FINITE- AND LARGE-SAMPLE INFERENCE FOR MODEL AND COEFFICIENTS IN HIGH-DIMENSIONAL LINEAR REGRESSION WITH REPRO SAMPLES

BY PENG WANG, MIN-GE XIE AND LINJUN ZHANG

Abstract In this paper, we present a new and effective simulation-based approach to conduct both finite- and large-sample inference for high-dimensional linear regression models. This approach is developed under the so-called repro samples framework, in which we conduct statistical inference by creating and studying the behavior of artificial samples that are obtained by mimicking the sampling mechanism of the data. We obtain confidence sets for (a) the true model corresponding to the nonzero coefficients, (b) a single or any collection of regression coefficients, and (c) both the model and regression coefficients jointly. We also extend our approaches to drawing inferences on functions of the regression coefficients. The proposed approach fills in two major gaps in the high-dimensional regression literature: (1) lack of effective approaches to address model selection uncertainty and provide valid inference for the underlying true model; (2) lack of effective inference approaches that guarantee finite-sample performances. We provide both finite-sample and asymptotic results to theoretically guarantee the performances of the proposed methods. In addition, our numerical results demonstrate that the proposed methods are valid and achieve better coverage with smaller confidence sets than the existing state-of-art approaches, such as debiasing and bootstrap approaches.

MSC 2010 subject classifications: Primary 00X00, 00X00; secondary 00X00
Keywords and phrases: high-dimensional inference, model selection inference

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1. Introduction  High-dimensional linear regression plays an important role in modern statistics, with applications ranging from signal processing [55] to econometrics [4, 38] to bioinformatics [54, 33]. There have been a large amount of literature on this topic in the past three decades, in the early part of which researchers focused more on estimation/detection problems such as coefficients estimation [12, 49, 15] and support recovery [62, 68]. More recently and starting with the pioneer work of [59, 45, 37] on the debiased LASSO, the more difficult task of inference comes to the central stage. Some recent works on inference include confidence interval construction [59, 45, 37], multiple testing of regression coefficients [40], and post-selection inference [48, 50, 39].

Despite many works on statistical inference for the high-dimensional linear model, several important open problems remain. First, most existing works focus on inference for regression coefficients, while inference for the true model (including uncertainty quantification for model selection) in a high dimensional regression model is mostly absent. This is partly due to the challenges arising from the discrete nature of the coefficients support, for which the conventional inference tools built for continuous parameters, such as the central limit theorem and bootstrap theorems, no longer apply. Furthermore, all the results in the literature on high-dimensional inference are asymptotic, relying on the assumption that the sample size goes to infinity, and there are no theories concerning the performance of these procedures under the finite-sample setting. However, the performances of these asymptotic procedures are often empirically unsatisfactory, especially in the high-dimensional setting with limited sample size. Therefore a procedure with guaranteed finite-sample performance is desirable. Finally, the post-selection inference framework attempts to sidestep the problem of model uncertainty by only making conditional inferences for regression coefficients of the predictors selected by a model selection procedure. In other words, if some predictor variables are significant but not selected, no inference will be available and one will miss some important signals.

To solve the above problems, we develop a repro samples method that quantifies both the uncertainty in model selection and that in estimation of regression coefficients (or their functions). Specifically, we provide a comprehensive inferential approach with which we can construct confidence sets for (a) the true model, (b) a single or any collection of regression coefficients, and (c) both the model and regression coefficients jointly. Moreover, the proposed repro samples approaches enjoy finite-sample performance guarantees without requiring a large sample size for all of (a)-(c), when used to make inference for the model, regression coefficients or both simultaneously. Although our work focuses primarily on finite-sample performances, we also provide several related large-sample results.

Consider the high-dimensional linear regression problem in which we observe an $n \times 1$ response vector $\mathbf{y}_{obs}$ with an $n \times p$ design matrix $\mathbf{X}$. Here, the dimension $p$ can be much larger than the sample size $n$. Suppose that the observed $\mathbf{y}_{obs}$ relates only to a subset of independent variables indexed by $\tau_0$ with

$$\mathbf{y}_{obs} = \mathbf{X}\beta_{0\text{full}} + \epsilon_{\text{rel}} = \mathbf{X}_{\tau_0}\beta_0 + \epsilon_{\text{rel}},$$

where $\epsilon_{\text{rel}} \sim \mathcal{N}(0, \sigma_0^2\mathbf{I}_n)$ is the realization of the error term associated with the observed data $\mathbf{y}_{obs}$, $\mathbf{I}_n$ is a $n \times n$ identity matrix, $(\tau_0, \beta_0, \sigma_0^2)$ are unknown model parameters, $\mathbf{X} = (\mathbf{X}_{\tau_0}, \mathbf{X}_{\tau_0}^C)$, $\beta_0^{\text{full}} = (\beta_0^T, \mathbf{0}^T_{\tau_0}^C)^T$ and $\tau_0^C = \{1, \ldots, p\} \backslash \tau_0$. We can re-express the above model as

$$(1) \quad \mathbf{y}_{obs} = \mathbf{X}\beta_{0\text{full}} + \sigma_0\mathbf{u}^{rel} = \mathbf{X}_{\tau_0}\beta_0 + \sigma_0\mathbf{u}^{rel},$$

where $\mathbf{u}^{rel}$ is the realization of the standardized error term $\mathbf{u} \sim \mathcal{N}(0, \mathbf{I}_n)$ and, compared with $\epsilon_{\text{rel}}$, it is free of the unknown $\sigma_0$. Corresponding to model (1) for the observed $\mathbf{y}_{obs}$ and under
the frequentist inference framework, there is a random sample (or population) version of data generation model

\[ Y = X \beta_0^{full} + \sigma_0 U = X_{\tau_0} \beta_0 + \sigma_0 U, \quad U \sim N(0, I_n), \]

of which model (1) is a realization.

Inference for the true model \( \tau_0 \) is almost entirely absent in high-dimensional settings, in contrast to the fact that the problem of estimating \( \tau_0 \), or model selection, has been well studied since the early research of high-dimensional statistics. Although there exist works on model confidence sets that tackle the discrete model space \([32, 28]\), the works are all in low-dimensional settings and require that the model space is small, which apparently does not hold in the high-dimensional regime. Moreover, the works of \([32, 28]\) involve sequential testing procedures against a pre-specified finite-dimensional full model, which can not be well-defined in the high-dimensional settings. Constructing model confidence sets for high-dimensional models remains a difficult open problem.

In comparison to the inference for \( \tau_0 \), there are considerably more works on conducting inference for the (continuous) regression coefficients, either for single (scalar) coefficient or for a subset or the entire \( \beta_0^{full} \) [e.g., 59, 37, 60, 23, among others]. However, all the existing approaches are justified by only large-sample theories. Specifically, the existing approaches need to rely on either higher-order estimation and its asymptotic properties, or certain model selection procedure and its asymptotic consistency. Note that accurate estimation of higher-order parameters such as variance-covariance matrix or its inverse is a notoriously challenging problem itself. The errors from the estimations often impact the inference of the coefficients. In addition, model selection consistency usually requires strong conditions, see, e.g., [62, 6]. Also, importantly, these methods rely on asymptotic properties and do not have any guaranteed finite-sample performance. In fact, we have frequently observed in our empirical studies that the finite-sample performance of these large-sample approaches are unsatisfactory, especially when the dimension \( p \) is large.

This paper proposes a repro samples approach, which allows us to make inferences for the true model \( \tau_0 \), the regression coefficients, and both simultaneously. Unlike the conventional Wald-test type of methods, the proposed approach directly provides us with the desired confidence sets without having to estimate \((\tau_0, \beta_0)\) or any other model parameters. The essential idea is to generate “synthetic (fake) residuals” by sampling from the residual distribution and find candidate models under which the synthetic residuals can generate an artificial \( y \) that resembles the observed \( y_{obs} \). After that, we construct both the confidence sets for \( \tau_0 \) and those for any subset or function of \( \beta_0 \), by checking each candidate model and see whether it is likely to reproduce \( y_{obs} \). The checking criterion is facilitated by a so-called nuclear mapping function. The nuclear mapping functions we construct are also able to handle the nuisance parameters since their distributions or conditional distributions are free of the nuisance parameters.

Compared to existing approaches such as bootstrap and other related large-sample approaches, the proposed approach has several advantages: first, the confidence sets have guaranteed finite-sample validity, and the corresponding large-sample supporting theories are also available; second, numerical studies suggest that the proposed approach efficiently constructs tight confidence sets, both for the true model \( \tau_0 \) and for subsets of \( \beta_0^{full} \), and improved performance over the state-of-art debiased method \([37, 59]\) on the inference of a single coefficient is also documented; third, our finite-sample theoretical results require weaker conditions than existing literature. Neither any conditions on the separation or strength of signals, such as the \( \beta \)-min condition \([62, 41]\), nor conditions on the design matrix, such as the restricted eigenvalue condition \([6, 59]\), are necessary to achieve the desired coverage rate, although weaker signals would typically require a higher computational cost. Overall, we provide an
all-inclusive method that subsumes existing inference approaches by two means: we consider a broader set of marginal and joint inference problems to account for uncertainties of both the model and regression coefficients; we provide supporting theories to guarantee both finite- and large-sample performances.

1.1. Contributions
To summarize, this paper has the following five major contributions.

1. We propose the repro samples framework to effectively construct model confidence set and quantify model selection uncertainty for the high-dimensional linear regression model. To the best of our knowledge, this is the only existing approach that is computationally efficient and that achieves the goal of constructing a performance-guaranteed model confidence set without splitting the data or a prior assumed candidate model set.

2. We develop a novel inference procedure for regression coefficients. Contrary to other existing methods, our approach does not rely on covariance matrix estimation or a consistent model selection procedure.

3. Theoretically, we show that the proposed inference procedures for both the model and the regression coefficients can achieve finite-sample coverage, while most literature on high-dimensional models focuses only on asymptotic properties. To our knowledge, the proposed method is the first approach that guarantees coverage for finite samples. Additionally, our theory suggests a complementary effect between computational power and sample size: one can achieve valid coverage as long as either is sufficiently large.

4. We do not need to impose the standard conditions that high-dimensional literature typically require to obtain a consistent estimation, such as the restricted isometry property or restricted eigenvalue conditions. Neither do we need to require signal strength conditions, which is usually necessary for consistent model selection.

5. Finally, through extensive numerical simulations, we show that our proposed method can produce smaller confidence sets than those of the state-of-art debiased LASSO estimators [59, 37]. Also, because we have finite-sample validity guarantee, our proposed method can achieve the desired coverage in the small sample size region, while other methods can not.

1.2. Connections with other simulation-based procedures
The repro samples framework is connected to other modern simulation-based procedures. As a technique to reproduce synthetic (“fake”) sample, it is in principle akin to the bootstrap [24, 13]. The difference is that bootstrap generates synthetic data from empirical distribution of estimated residuals that are based on model selection and regression coefficients estimation, while repro samples does so from the residual distribution without any parameter estimations preceding the repro samples procedure. More importantly, the bootstrap approach relies on large-sample central limit theorem (or large deviation theorem) to justify its validity, while the repro samples method can directly provide finite-sample inference without invoking any large-sample theory. Besides connections with the bootstrap, the repro samples method also inherits the “matching scheme” of the approximate Bayesian computation (ABC) approach [3], the inferential models [42] and the generalized fiducial inference [31]. Nevertheless, unlike these Bayesian or fiducial approaches, the proposed framework is a frequentist approach, and we do not require either a prior, or a summary (sufficient) statistics, or an approximate match within a pre-specified (ad-hoc) tolerance level. Finally, our framework is remotely related to the knock-off approach [2, 11] where artificial data are used to control the false discovery rate. See further discussions and comparisons in [57].
1.3. Related work There have been much efforts in recent years to develop inference procedures for regression coefficients of $\beta_0^{full}$ or functions of $\beta_0^{full}$ in high-dimensional linear regression models. On the inference of a single parameter among $\beta_0^{full}$, [61, 51, 37] propose the debiased LASSO estimator and develop its asymptotic distribution. Moreover, [13, 20, 21] modified the bootstrap procedure to consistently estimate the asymptotic distribution of lasso or adaptive lasso estimators for regression coefficients. Another class of methods utilize Neyman-Orthogonal estimating equations with an accurate estimation of the nuisance parameters [5, 16, 17, 19]. On simultaneous inference for a subset or all of $\beta_0^{full}$, [66, 44, 52] develop high-dimensional versions of chi-square tests, and [60, 23, 18] combine bootstrap with the debiased approach to construct simultaneous confidence sets. Moreover, [10, 9, 45, 63, 65] investigate constructing confidence regions (sets) for $\beta_0^{full}$. Also see [22] for a review on high-dimensional statistical inference. The current paper provides solutions to the same inference problems, plus inference problems on model selection. It also provides previously unavailable finite-sample results.

A recent work by the authors [57] provided a repro samples framework for statistical inference under a general setup in which the number of parameters $p$ is less than the number of observations $n$. The current paper focuses on the high-dimensional $p \gg n$ case that was not discussed in [57]. New procedures and theoretical results with conditions tailored to high-dimensional models that guarantee the performance of the proposed method in both finite and large-sample cases are developed.

1.4. Notation and identifiability condition In this paper, for any $k \in \mathbb{N}^+$, we use $[k]$ to denote the set $\{1, 2, \cdots, k\}$. For a vector $v$, let $v_i$ be the $i$-th coordinate of $v$. For a set $S$, we use $|S|$ to denote the cardinality of $S$. For two positive sequences $\{a_k\}$ and $\{b_k\}$, we write $a_k = O(b_k)$ (or $a_n \lesssim b_n$), and $a_k = o(b_k)$, if $\lim_{k \rightarrow \infty} (a_k/b_k) < \infty$ and $\lim_{k \rightarrow \infty} (a_k/b_k) = 0$, respectively. We also use $\mathbb{P}$ for probability and $\mathbb{E}$ for expectation in general. Sometimes, to stress the source of randomness, we add a subscription and use $\mathbb{P}_Q$ and $\mathbb{E}_Q$ to indicate the probability and expectation are taken over the random variable $Q$. We use $\overline{\mathbb{P}}$ and $\overline{\mathbb{E}}$ for empirical probability and expectation. For a $p$-dimensional vector $\beta$ and an indices set $\tau \subset \{1, \ldots, p\}$, we use $\beta_\tau$ to denote the sub-vector of $\beta$, containing all the entries of $\beta$ that are associated with the indices in $\tau$. The model space $\mathcal{M} = 2^{\{1,\ldots,p\}}$ is of size $2^p$ and it is the collection of all possible $\tau$ models. For a matrix $M \in \mathbb{R}^{n \times n}$, we use $\text{span}(M)$ to denote the vector space spanned by the columns of $M$: $\text{span}(M) = \{Mv : v \in \mathbb{R}^p\}$. We also call $M(M^\top M)^{-1}M^\top$ the projection matrix of $M$.

For $\tau_0$ defined in (1), there might be another model $\tilde{\tau}_0$ and corresponding coefficients $\beta_{\tilde{\tau}_0}$ such that $X_{\tau_0} \beta_0 = X_{\tilde{\tau}_0} \beta_{\tilde{\tau}_0}$. Then it is impossible to tell apart $\tau_0$ and $\tilde{\tau}_0$ even when knowing both $y_{\text{obs}}$ and the realized noise $u^{rel}$, since $y_{\text{obs}} = X_{\tau_0} \beta_0 + \sigma_0 u^{rel} = X_{\tilde{\tau}_0} \beta_{\tilde{\tau}_0} + \sigma_0 u^{rel}$. We refer this as an identifiability issue. To address this issue and uniquely define $\tau_0$, we follow the convectional practice in the high-dimensional regression literature [6] to re-define $\tau_0$ as the smallest model among the set $\{\tau \in \mathcal{M} : X_{\tau} \beta_\tau = X_{\tau_0} \beta_0, \text{ for some } \beta_\tau\}$:

$$\tau_0' = \arg\min_{\tau \in \mathcal{M}} |\tau|.$$  

Throughout the paper, we assume that the true model $\tau_0'$ defined in (3) is unique, which we refer as the identifiability condition. For notational simplicity, we will still refer $\tau_0'$ as $\tau_0$ and $\beta_{\tau_0'}$ as $\beta_0$ in the remaining of the paper.
Under the identifiability condition, we follow [47] and define the degree of separation between model \( \tau_0 \) and other models of equal or smaller model sizes as
\[
C_{\min} = \min_{\{\tau: \tau \neq \tau_0, |\tau| \leq |\tau_0|\}} \frac{1}{n \max(|\tau_0 \setminus \tau|, 1)} \|X_0 \beta_0 - X_0 \beta_\tau\|_2^2.
\]
By the identifiability condition, \( C_{\min} > 0 \). We remark that the notion \( C_{\min} \) is related to \( \beta_{\min} \) of the \( \beta \)-min condition in the literature. However, unlike existing literature, we do not impose any assumption on \( C_{\min} \) other than \( C_{\min} > 0 \). We only use it as a measure of separation.

Finally, we refer in this paper a simulated copy of artificial \( u^* \sim U \) as a repro copy of the realized \( u^{rel} \) and, for a potential set of values \( (\tau_0, \beta_0, \sigma^2) \), the artificial data \( y^* = X_\tau \beta_\tau + \sigma u^* \) as a repro sample of \( y^{obs} \). The key of our development is to study and relate this \( u^* \) with \( u^{rel} \) and \( y^* \) with \( y^{obs} \). We generally refer our method, developed by using the copies of \( (u^*, y^*) \), as a repro samples method. We will provide more details in each of the sections.

1.5. Organization The paper is organized as follows. Section 2 provides a repro samples framework for the inference of model selection in high-dimensional linear models, and provides both finite-sample and large-sample guarantees. Section 3 studies the inference of regression coefficients, including \( \beta_0^{full} \) and any linear transformation of \( \beta_0^{full} \), and further extends to the inference of any function of \( \beta_0^{full} \). A joint inference of model and coefficients \( (\tau_0, \beta_0) \) is also provided. Section 4 provides numerical illustrations of our proposed method, and compare the coverage and the size of the constructed confidence sets with the state-of-art debiased LASSO methods. In Section 5, we present technical proofs of our main results. Section 6 concludes the paper with a discussion of our results and future research directions. The proofs of other results and technical lemmas are deferred to the Appendix.

2. Inference for the true model \( \tau_0 \) In this section, we construct a model confidence set for high-dimensional linear regression models using a repro samples method. Since the model space is discrete and of a large size \( 2^p \), to reduce the search space and improve computational efficiency, we first introduce a notion of candidate models and develop a data-driven repro samples method to search for the candidate models in Section 2.1. In Section 2.2, we will then develop an inference procedure for the true model \( \tau_0 \) with provable guarantees. We will also utilize the data-driven candidate set in Section 3 when we conduct inference for subsets of regression coefficients, inference for functions of regression coefficients, as well as joint inference for model and regression coefficients.

2.1. Searching for candidate models To introduce the insight and intuition of our proposed procedure for the search of candidate models, we first investigate how we can recover the true model in an ideal (but unrealistic) case where we would have known the unobserved realization of the error terms \( u^{rel} \). In particular, Lemma 1 below suggests that \( \tau_0 \) defined in (3) can be expressed in terms of the given realization \( (y^{obs}, u^{rel}) \) through an optimization statement. We provide the proof of the following lemma in the Appendix.

**Lemma 1.** Let \( H_\tau \) be the projection matrix of \( X_\tau \) and \( H_{\tau,u^{rel}} \) be the projection matrix of \( (X_\tau, u^{rel}) \). Let \( \gamma_{(u^{rel}, \tau_0)}^2 = 1 - \min_{(\tau: |\tau| < |\tau_0|)} \frac{||I-H_{\tau,u^{rel}}X_0 \beta_0||^2}{||I-H_\tau X_0 \beta_0||^2} < 1 \). Then, given \( u^{rel} \), \( \tau_0 \) defined in (3) satisfies
\[
(4) \quad \tau_0 = \arg\min_{\tau} \left\{ \min_{\beta, \sigma} \left\{ \frac{||y^{obs} - X_\tau \beta_\tau - \sigma u^{rel}||_2^2 + \lambda |\tau|}{2} \right\} \right\},
\]
and moreover,
\[
(\tau_0, \beta_0, \sigma_0) = \arg\min_{\tau, \beta, \sigma} \left\{ \frac{||y^{obs} - X_\tau \beta_\tau - \sigma u^{rel}||_2^2 + \lambda |\tau|}{2} \right\},
\]
for any $0 < \lambda < n[1 - \gamma^2_{(u, \tau_0)}]C_{\min}$.

In practice, however, we do not know the underlying realization $u^{rel}$ and we can not directly apply Lemma 1. Nonetheless, the equation (4) provides us clues how to construct a set of candidate models for $\tau_0$. More specifically, we generate a large number of, say $d$, copies of Monte Carlo $u^*_1, \ldots, u^*_d \sim U$. Then instead of solving (4) with the realized $u^{rel}$, we compute

$$
\hat{\tau}_b = \arg\min_{\tau} \left\{ \min_{\beta, \sigma} \left\{ \|y_{obs} - X_{\tau} \beta_{\tau} - \sigma u^*_b \|^2 + \lambda |\tau| \right\} \right\},
$$

for each $u^*_b, b = 1, \ldots, d$. After that, we collect all $\hat{\tau}_b$'s to form a candidate set for $\tau_0$:

$$
S^{(d)} = \{ \hat{\tau}_b : b = 1, \ldots, d \}.
$$

Although we require $d$ to be a large number, the candidate set $S^{(d)}$ is often of reasonable size that is much smaller than $d$, since the mapping function from $u^*_b \in \mathbb{R}^n$ to $\hat{\tau}_b \in \mathcal{M} = 2^{\{1, \ldots, p\}}$ in (5) is a many-to-one mapping and many of the $d$ copies of $\hat{\tau}_b$'s obtained by (5) are identical.

The only difference between (5) and (4) is that we replace $u^{rel}$ with $u^*_b$. One could imagine that if some $u^*_b$ is in a neighbourhood of $u^{rel}$, then for such $u^*_b$'s, the event $\{ \hat{\tau}_b = \tau_0 \}$ is very likely to hold by Lemma 1. The size of such neighbourhood depends on the separation metric $C_{\min}$ and the sample size, yet its probability measure is always positive under the identifiability condition. As a result, as long as $d$, the number of Monte Carlo copies, is sufficiently large, eventually some $u^*_b$ will fall in this neighbourhood, leading to $\hat{\tau}_b = \tau_0$ and that the candidate set $S^{(d)}$ contains the true model $\tau_0$.

Formally, we summarize the above discussions in Theorems 1-2 below, in which we prove that $\mathbb{P}_{(u^*, Y)}(\tau_0 \notin S^{(d)}) \to 0$, in each of the following two cases: 1) the sample size $n$ is finite and $d \to \infty$; or 2) $d$ is finite and $n \to \infty$, respectively. Here, the probability $\mathbb{P}_{(u^*, Y)}(\cdot)$ refers to the joint distribution of $U$ and $U^d = (U^*_1, \ldots, U^*_d)$, where $U^*_b \sim U$ is a Monte Carlo copy of $U$, $b = 1, \ldots, d$. We provide the poofs of the two theorems in Section 5.

**Theorem 1.** Suppose $n - |\tau_0| > 4$. For any $\delta > 0$, there exists a constant $\gamma_0 > 0$ such that when $\lambda \in \left[ n\gamma_0^{1/2} \left\{ 2 + 2(|\tau_0| + 1)^{\log(p/2)} \right\}, n\gamma_0^{1/4}C_{\min}^{1/6} \right]$, the finite-sample probability bound that the true model is not included in the model candidates set $S^{(d)}$, obtained by (6) with the objective function (5), is as follows,

$$
\mathbb{P}_{(u^*, Y)}(\tau_0 \notin S^{(d)}) \leq \left( 1 - \frac{\delta n^{-1}}{n - 1} \right)^d + \delta.
$$

Therefore as $d \to \infty$, $\mathbb{P}_{(u^*, Y)}(\tau_0 \notin S^{(d)}) \to 0$, where $\delta > 0$ is arbitrarily small.

**Theorem 2.** Suppose $\frac{\lambda}{\sigma^2} \in \left[ 6\sigma_0^2 \left\{ (|\tau_0| + 1)^{\log(p/2)} \right\} + t, 0.05C_{\min} \right]$ for a positive constant $t > 0$. Then the finite-sample probability bound that the true model is not included in the confidence set $S^{(d)}$, obtained by (6) with the objective function (5) for any finite $d$ is as follows,

$$
\mathbb{P}_{(u^*, Y)}(\tau_0 \notin S^{(d)}) \leq 6 \exp \left\{ -\frac{n}{18\sigma_0^2} \{ 0.3C_{\min} - 36 \frac{\log(p + 1)}{n} \sigma_0^2 \} \right\} + 3 \exp \left\{ -\frac{nt}{3\sigma_0^2} \right\} + \exp \left\{ -nd \left( 0.23 - \frac{|\tau_0| \log(p) + 2}{n} \right) \right\},
$$

(8)
Therefore \( \mathbb{P}(\tau \notin S^{(d)}) \rightarrow 0 \) for any \( d \) as \( n \rightarrow \infty \), if \( \frac{\|\tau\| \log(p)}{n} < 0.23 \) and \( C_{\min} > 120 \left( \frac{|\tau|+2}{2+1} \right)^2 \sigma_0^2 / n \) when \( n \) is large enough.

The two theorems above suggest two complementary driving forces of the coverage validity: the sample size and the computation time. In cases where the sample is limited, Theorem 1 implies that we will have valid coverage as long as the computation time (linearly scaled with \( d \)) goes to infinity; in cases where the computational resources are limited, Theorem 2 then indicates collecting sufficient samples will result in valid coverage guarantee.

To put it succinctly, we summarize the aforementioned procedure in Algorithm 1 below.

**Algorithm 1** Search of Candidate Models

Input: Design matrix \( X \), response vector \( y_{\text{obs}} \), the number of Monte Carlo copies \( d \).

Output: Candidate Models \( S^{(d)} \).

Step 1: Simulate a large number \( d \) copies of \( u^* \sim U \sim N(0, I_n) \). Denote the \( d \) copies by \( u^*_b \), \( b = 1, \ldots, d \), respectively.

Step 2: Compute \( \hat{\tau}_{b,\lambda} = \arg\min_{\lambda} \max_{\beta_b, \sigma_b} \left[ \|\beta\|_1 + \|y_{\text{obs}} - X_\tau \beta + \sigma u^*_b\|^2 \right] \) for \( b = 1, \ldots, d \) and a grid values of \( \lambda \). For each \( b \), use certain selection criteria to pick a subset of all values of \( \lambda \), denoted as \( \Lambda_b \).

Step 3: Construct \( S^{(d)} = \{ \hat{\tau}_{b, \lambda} : \lambda \in \Lambda_b, b = 1, \ldots, d \} \).

**Remark 1** (Practical implementation of Algorithm 1). There are two practical issues to be addressed when we implement Algorithm 1. First, it is a common practice that we use some criteria to determine the value of the tuning parameter \( \lambda \). In this paper, we use the extended BIC [14] to determine \( \lambda \), due to its good empirical performance and asymptotic model selection consistency in high-dimensional settings. The second practical component is that solving an optimization problem with a \( L_1 \) penalty \( \lambda \| \tau \|_1 \) is often computationally difficult for high-dimensional data, and researchers typically use a surrogate to replace the \( L_1 \) penalty. In this paper, we adopt the adaptive LASSO [67] as a surrogate for the \( L_1 \) penalty in (5) because of its simplicity and convexity. One may also use other surrogates like the truncated LASSO penalty [46], smoothly clipped absolute deviation penalty [25], or the minimax concave penalty [58], among others. These surrogates may enjoy different computational and theoretical properties. However, since the implementation of penalty functions is not the focus of this paper, we will not dive into the topic any further.

2.2. Construction of Model Confidence Sets In this subsection, we construct the confidence sets for model \( \tau_0 \) by developing a repro samples method that is tailored to our problem.

For the ease of presenting the general idea of a repro samples method, let us first assume that we are interested in making a joint inference about \( \theta_0 = (\tau_0, \beta_0^T, \sigma_0)^T \) and describe how a repro samples method works in this case. The idea is that for any potential candidate value \( \theta = (\tau, \beta_0^T, \sigma)^T \), we can create an artificial repro sample data \( y^* = X_\tau \beta + \sigma u^* \), where \( u^* \sim N(0, I_n) \). If \( u^* \) is close to \( u^{\text{rel}} \) and \( \theta \) is equal or close to \( \theta_0 \), then we expect \( y^* \) and \( y_{\text{obs}} \) would be equal or close. Inversely, for a potential value \( \theta \), if we can find a \( u^* \) likely matching \( u^{\text{rel}} \) such that \( y^* \) matches \( y_{\text{obs}} \) (i.e., \( y_{\text{obs}} = y^* \)), then we keep this \( \theta \) as a potential estimate of \( \theta_0 \). Mathematically, we define a level-\( \alpha \) confidence set for \( \theta_0 \) as

\[
\Gamma_\alpha(y_{\text{obs}}) = \{ \theta : \exists u^* \text{ s.t. } y_{\text{obs}} = G(\theta, u^*), T(u^*, \theta) \in B_\alpha(0) \}. \tag{9}
\]

Here, the function \( T(\cdot, \cdot) \) is referred to as a nuclear mapping function and the set \( B_\alpha(0) \) is a fixed level-\( \alpha \) Borel set in \( \mathbb{R}^d \) such that

\[
\mathbb{P}_U(T(U, \theta) \in B_\alpha(0)) \geq \alpha. \tag{10}
\]
The interpretation of (9) is: for a potential value $\theta$, if there exists a $u^*$ satisfying $T(u^*, \theta) \in B_\alpha(\theta)$ such that the artificial data $y^* = X_\tau \beta_\tau + \sigma u^*$ matches with $y_{\text{obs}}$ (i.e., $y^* = y_{\text{obs}}$), then we keep this $\theta$ in the set. The repro samples method uses $P_U(T(U, \theta) \in B_\alpha(\theta))$, for a given $\theta$, as a way to quantify the uncertainty of $U$ thus also the uncertainty of $Y$. Also, for any nuclear mapping function $T(U, \theta)$, as long as we have a set $B_\alpha(\theta)$ such that (10) holds, we can show that the set $\Gamma_\alpha(\theta_{\text{obs}})$ in (9) is a level-$\alpha$ confidence set [57]. Here, the role of $T(U, \theta)$ under the repro samples framework is similar to that of a test statistic under the classical (Neyman-Pearson) hypothesis testing framework. Besides, a good choice for $T(U, \theta)$ is problem specific.

Now we extend the general method to make inference for only the unknown true model $\tau_0$. First, in order to define the nuclear mapping $T(u, \theta)$ for the inference for $\tau_0$, we write $y_\theta = X_\tau \beta_\tau + \sigma u$, for a $u \sim U$. This $y_\theta$ is a copy of artificial repro sample data generated from a given set of parameters $\theta = (\tau, \beta_\tau, \sigma)^\top$. The corresponding random version is

$$Y_\theta = X_\tau \beta_\tau + \sigma U.$$  \hfill (11)

Then based on the artificial repro data $(X, y_\theta)$, one can obtain an estimate of $\tau$, denoted by $\hat{\tau}(y_\theta)$. In this paper, we use

$$\hat{\tau}(y_\theta) = \arg \min_{\tau \in \mathbb{R}} \|y_\theta - X_\tau \beta_\tau\|^2 \text{ s.t. } |\hat{\tau}| \leq |\tau|.$$  

We define the nuclear mapping function for the inference of the true model $\tau_0$ as $T(u, \theta) = \hat{\tau}(y_\theta) = \hat{T}(y_\theta, \tau)$. In principle, we can choose to use another estimator of reasonable performance too.

Handling nuisance parameters is a ubiquitously challenging issue in statistical inference. Here, if we follow the general repro samples method, we need to find a Borel set $B_\alpha(\theta)$ that satisfies (10), i.e., $P_U(T(U, \theta) \in B_\alpha(\theta)) = P_U(\hat{T}(Y_\theta, \tau) \in B_\alpha(\theta)) \geq \alpha$, for the nuclear mapping $\hat{T}(y_\theta, \tau)$ defined above. However, the distribution of $\hat{T}(y_\theta, \tau)$ involves the entire parameter $\theta = (\tau, \beta_\tau^\top, \sigma)^\top$, including the nuisance parameters $\beta_\tau$ and $\sigma^2$. The task of directly obtaining $B_\alpha(\theta)$ is computationally challenging, if not infeasible. To overcome the impact of the nuisance parameters, we introduce below an effective conditional repro samples method to handle the nuisance parameters and construct a confidence set for $\tau_0$ with provable guarantees.

The idea of conditional repro samples method is to first find a quantity $W(U, \theta)$, such that the conditional distribution of the nuclear statistic $T(U, \theta)$ given $W(U, \theta) = w$ is free of the nuisance parameters $(\beta, \sigma)$. Assume we have such $W(U, \theta)$; we will discuss how to obtain $W(U, \theta)$ for our purpose later in the section. Then, based on the conditional distribution of $T(U, \theta)|W(U, \theta)$, we construct a Borel set $B_\alpha(\tau, w)$ that depends on $w$, the value of the random quantity $W(U, \theta)$, but not on $\beta, \sigma$, such that

$$P_U|W(T(U, \theta) \in B_\alpha(\tau, w)|W(U, \theta) = w) = P_U(\hat{T}(Y_\theta, \tau) \in B_\alpha(\tau, w)|W(U, \theta) = w) \geq \alpha.$$  \hfill (12)

Accordingly, the marginal probability $P_U(T(U, \theta) \in B_\alpha(\tau, W(U, \theta)) \geq \alpha$.

Now, instead of directly following (9), we construct a subset in the model space $M$:

$$\Gamma_\alpha(y_{\text{obs}}) = \{\tau \in \mathcal{M} : \exists u^* \text{ and } (\beta_\tau, \sigma) \text{ s.t. } y_{\text{obs}} = X_\tau \beta_\tau + \sigma u^*,$$

$$T(u^*, \theta) \in B_\alpha(\tau, W(u^*, \theta))\}.$$  \hfill (13)

The following theorem suggests that the newly constructed set $\Gamma_\alpha^*(y_{\text{obs}})$ is a level-$\alpha$ confidence set for the true model $\tau_0$, whose detailed proof is provided in Section 5.
Theorem 3. Suppose the conditional distribution of \( T(U, \theta) \) given \( W(U, \theta) = w \) is free of \((\beta_r, \sigma)\) and the Borel set \( B_\alpha(\tau, w) \) satisfies (12), then

\[
\mathbb{P}(\tau_0 \in \Gamma^\tau_\alpha(Y)) \geq \alpha,
\]

where the confidence set \( \Gamma^\tau_\alpha(Y) \) is defined following from (13).

The remaining task is to find the random quantity \( \mathbf{W}(U, \theta) \) and the Borel set \( B_\alpha(\tau, w) \) such that the conditional distribution of \( T(U, \theta) \) given \( W(U, \theta) = w \) is free of the nuisance parameters \((\beta, \sigma)\) and the inequality (12) holds. Note that we can rewrite (11) as \( Y_\theta = H_r Y_\theta + (I - H_r) Y_\theta + \sigma (I - H_r) U \), where \( H_r = X_r (X_r^\top X_r)^{-1} X_r^\top \) is the projection matrix of \( X_r \). Write \( A_\theta(U) = H_r Y_\theta = A_\theta(Y_\theta) \) and \( b_\theta(U) = \| (I - H_r) Y_\theta \| = \tilde{b}_\theta(Y_\theta) \). It follows that

\[
Y_\theta = A_\theta(U) + b_\theta(U) \frac{(I - H_r) U}{\|(I - H_r) U\|} = \tilde{A}_\theta(Y_\theta) + \tilde{b}_\theta(Y_\theta) \frac{(I - H_r) U}{\|(I - H_r) U\|}.
\]

In this equation, the “randomness” of \( U \) (and also \( Y_\theta \)) are split into three pieces, \( A_\theta(U), \tilde{b}_\theta(U) \) and \((I - H_r) U / \|(I - H_r) U\| \). Under model equation (11), \((A_\theta(U), b_\theta(U)) = \left( \tilde{A}_\theta(Y_\theta), \tilde{b}_\theta(Y_\theta) \right)\) is a sufficient statistic and the last piece \((I - H_r) U / \|(I - H_r) U\|\) is an ancillary statistic that is free of the nuisance parameters \((\beta_r, \sigma^2)\). Based on this partition, we define for our purpose \( \mathbf{W}(U, \theta) = (A_\theta(U), b_\theta(U)) = \left( \tilde{A}_\theta(Y_\theta), \tilde{b}_\theta(Y_\theta) \right) = \mathbf{w}(Y_\theta, \theta) \). It follows immediately that the conditional distribution of \( Y_\theta \mid \mathbf{W}(U, \theta) = w \) is free of \((\beta_r, \sigma^2)\). So is the conditional probability mass function of \( \tilde{T}(Y_\theta, \tau) \mid \mathbf{W}(U, \theta) = w \),

\[
p_{(w, \tau)}(\tau') = \mathbb{P}_{U \mid \mathbf{W}} \left\{ \tilde{T}(Y_\theta, \tau) = \tau' \mid \mathbf{W}(U, \theta) = w \right\},
\]

for any \( \tau' \in \mathcal{T} \). Note that, when given \((w, \tau)\), we can use the model equation (11) to generate many copies of \( Y_\theta \) by repeated draws from \( U \). Therefore we can obtain the conditional probability mass function in (14) through a Monte-Carlo method.

We define the Borel set \( B_\alpha(\tau, w) \) as

\[
B_\alpha(\tau, w) = \left\{ \tau^* \in \mathcal{M} : \sum_{\{\tau' : p_{(w, \tau)}(\tau') \leq p_{(w, \tau)}(\tau^*)\}} p_{(w, \tau)}(\tau') \geq 1 - \alpha \right\}.
\]

In Section 5, we provide a proof that the conditional probability

\[
\mathbb{P}_{Y_\theta \mid \mathbf{w}} \left\{ \tilde{T}(Y_\theta, \tau) \in B_\alpha(\tau, w) \mid \mathbf{W}(Y_\theta, \tau) = w \right\} \geq \alpha.
\]

It follows that, marginally, \( \mathbb{P}_{Y_\theta} \left\{ \tilde{T}(Y_\theta, \tau) \in B_\alpha(\tau, \mathbf{W}(Y_\theta, \tau)) \right\} \geq \alpha \). By (13) and using the candidate set \( S^{(d)} \), we define

\[
\Gamma^\tau_\alpha(Y_{obs}) = \Gamma^\tau_\alpha(Y_{obs}) \bigcap S^{(d)} = \left\{ \tau \in S^{(d)} : \tilde{T}(Y_{obs}, \tau) \in B_\alpha(\tau, \mathbf{W}(Y_{obs}, \tau)) \right\}.
\]

To obtain the confidence set, we use a Monte-Carlo algorithm to compute the conditional probability in (14). We summarize the procedure of constructing the above model confidence set in Algorithm 2, with the size of the Monte-Carlo simulations \( J \).
Algorithm 2 Confidence set construction for $\tau_0$

Input: Design matrix $X$, response vector $y_{obs}$, candidate set $S^{(d)}$, simulation size $J$

Output: Confidence set of $\tau_0$ for $\tau_0 \in S^{(d)}$ and $j \in 1, \ldots, J$

for $\tau_0 \in S^{(d)}$ do

Step 1: Calculate $w_{obs} = (a_{obs}, b_{obs}) = (H_{x}, y_{obs}, \|I - H_{x}\| y_{obs})$.

Step 2: Generate $u_j^* \sim \mathcal{N}(0, I_p)$, and compute

\[
y_j^* = a_{obs} + b_{obs} \frac{(I - H_{x})u_j^*}{\|I - H_{x}\| u_j^*}.
\]

In addition, obtain the estimated model $\hat{\tau}_j = \hat{\tau}(y_j^*)$ by

\[
\hat{\tau}(y_j^*) = \arg\min_{\tau \in T, \beta \in R^{(d)}} \|y_j^* - X_j \beta\|^2 \text{ s.t. } |\hat{\tau}| \leq |\tau_0|.
\]

end for

Step 3: Estimate $p(w_{obs}, \tau_0)(\tau)$ for all $\tau \in T$ by

\[
\hat{p}(w_{obs}, \tau_0)(\tau) = \frac{1}{J} \sum_{j=1}^{J} 1{\hat{\tau}_j = \tau},
\]

where $1(.)$ is the indicator function.

Step 3: Calculate

\[
\hat{T}(y_{obs}, \tau_0) = \arg\min_{\tau \in T, \beta \in R^{(d)}} \|y_{obs} - X \beta\|^2 \text{ s.t. } |\hat{T}| \leq |\tau_0|,
\]

Step 4: We then compute the estimated tail probability of $\hat{T}(y_{obs}, \tau_0)$ as

\[
\hat{F}(w_{obs}, \tau_0) \left\{ \hat{T}(y_{obs}, \tau_0) \right\} = \sum_{\{\tau \in \mathbb{P}(w_{obs}, \tau_0)(\tau) \leq p(w_{obs}, \tau_0)(\tau(y_{obs}))\}} \hat{p}(w_{obs}, \tau_0)(\tau).
\]

Step 5: We therefore obtain the level-$\alpha$ confidence set for $\tau_0$

\[
\hat{F}_\alpha^{(d)}(y_{obs}) = \left\{ \tau_0 \in S^{(d)} : \hat{F}(w_{obs}, \tau_0) \left\{ \hat{T}(y_{obs}, \tau_0) \right\} \geq 1 - \alpha \right\}.
\]

Theorem 4 below states that $\hat{F}_\alpha^{(d)}(y_{obs})$ in (17) is a level-$\alpha$ confidence set for $\tau_0$ with a guaranteed finite-sample coverage rate, if we can repeatedly generate a large number $(d)$ of Monte Carlo samples to construct the candidate set $S^{(d)}$. Theorem 5 states that even when the number of Monte Carlo copies $d$ is limited, $\hat{F}_\alpha^{(d)}(y_{obs})$ is still a level-$\alpha$ confidence set for $\tau_0$ if we have a large sample size $n$. Proofs of the theorems are in Section 5.

**THEOREM 4.** Under the conditions in Theorem 1, for any finite $n$ and $p$, and arbitrarily small $\delta > 0$, the coverage probability of model confidence set $\hat{F}_\alpha^{(d)}(y_{obs})$ constructed above is $P_{\{U^{(d)} \ Y\}} \left\{ \tau_0 \in \hat{F}_\alpha^{(d)}(Y) \right\} \geq \alpha - \delta - o(e^{-c_1 d})$ as $d \to \infty$ for some $c_1 > 0$. Further $\mathbb{P}_{Y|U^{(d)}} \left\{ \tau_0 \in \hat{F}_\alpha^{(d)}(Y) \right\} \geq \alpha - \delta - o_p(e^{-c_2 d})$.

**THEOREM 5.** Under the conditions in Theorem 2, for any finite $d$, the coverage probability of model confidence set $\hat{F}_\alpha^{(d)}(y_{obs})$ constructed above is $P_{\{U^{(d)} \ Y\}} \left\{ \tau_0 \in \hat{F}_\alpha^{(d)}(Y) \right\} \geq \alpha - o(e^{-c_2 n})$ as $n \to \infty$ for some $c_2 > 0$. Further $\mathbb{P}_{Y|U^{(d)}} \left\{ \tau_0 \in \hat{F}_\alpha^{(d)}(Y) \right\} \geq \alpha - o_p(e^{-c_2 n})$.

3. Inference for regression coefficients accounting for model selection uncertainty

We first propose a confidence set for any subset of $\beta_0^{(full)} = (\beta_{0,1}, \ldots, \beta_{0,p})^T$ while accounting for model selection uncertainty in Section 3.1. The work can be extended to make inference for any linear transformation of $\beta_0^{(full)}$. We then discuss two interesting special cases of practical importance in Section 3.2: (a) joint inference for all regression coefficients $\beta_0^{(full)}$;
and (b) inference for single regression coefficient $\beta_{0,i}, i = 1, \ldots, p$. Note that, most existing methods focus only on one of the two special cases, and there are few effective approaches on making inference for any subset or linear transformation of $\beta_{0}^{full}$ in the literature. Moreover, our work guarantees both the finite-sample and the large-sample coverage, while the existing methods provide only asymptotic inferences. In addition, our confidence set is a union of multiple smaller sets. In contrast, confidence sets produced by existing methods are single intervals or ellipsoid sets; see Section 3.2 for further comparisons.

3.1. Inference for a subset of regression coefficients. Let $\beta_{0,\Lambda}, \Lambda \subset \{1, \ldots, p\}$ be the collection of $\beta_{0,i}$’s that are of interests, leaving the remaining parameters $\beta_{0,i}, i \notin \Lambda, \sigma_0$ and $\tau_0$ as nuisance parameters. The subset $\Lambda$ is given based on one’s problem of interests, and it may overlap or separate from $\tau_0$. Here our strategy is to first remove the influence of $\beta_{0,i}, i \notin \Lambda$ and $\sigma_0$ by defining a nuclear mapping function that only involves $\eta_\Lambda = (\beta_\Lambda, \tau)$, where $\tau$ is a potential value of $\tau_0$. The role of the nuclear mapping is similar to test statistics in the classical hypothesis testing framework, but in general, the definition of the nuclear mapping is broader and more flexible than the definition of test statistics. See [57] for a detailed discussion. We then utilize the work in the previous section to handle the impact of $\tau$, leading to an inference statement focusing on $\beta_\Lambda$.

For a given $\eta_\Lambda = (\beta_\Lambda, \tau)$, we define the nuclear mapping as follows

$$\begin{align*}
T(u, \eta_\Lambda) = \begin{cases}
\frac{u^T \Omega_\Lambda u}{u^T (I - H_{r\backslash\Lambda}) u / (n - |\tau|)} & \text{if } \Lambda \cap \tau \neq \emptyset \text{ and } \beta_i = 0 \text{ for any } i \in \Lambda \setminus \tau \\
\infty & \text{if } \beta_i \neq 0 \text{ for any } i \in \Lambda \setminus \tau \\
0 & \text{if } \Lambda \cap \tau = \emptyset \text{ and } \beta_i = 0 \text{ for any } i \in \Lambda 
\end{cases},
\end{align*}$$

where $O_{r,\Lambda}$ is the projection matrix of $(I - H_{r\backslash\Lambda})X_{\Lambda \cap r}$, and $H_{r\backslash\Lambda}$ is the projection matrix of $X_{r\backslash\Lambda}$. We can rewrite the above nuclear mapping as a function of $y_\theta = X_r \beta_r + \sigma u$:

$$\begin{align*}
\hat{T}(y_\theta, \eta_\Lambda) = \begin{cases}
(y_\theta - X_\beta \beta_\Lambda)^T O_{r,\Lambda} (y_\theta - X_\beta \beta_\Lambda) & \text{if } \Lambda \cap \tau \neq \emptyset \text{ and } \beta_i = 0 \text{ for any } i \in \Lambda \setminus \tau \\
\infty & \text{if } \beta_i \neq 0 \text{ for any } i \in \Lambda \setminus \tau \\
0 & \text{if } \Lambda \cap \tau = \emptyset \text{ and } \beta_i = 0 \text{ for any } i \in \Lambda 
\end{cases}.
\end{align*}$$

Since when $\Lambda \cap \tau \neq \emptyset$ and $\beta_i = 0$ for any $i \in \Lambda \setminus \tau$, the distribution of the nuclear mapping defined above is $T(U, \eta_\Lambda) \sim \tilde{T}(Y_\theta, \eta_\Lambda)$, we let the Borel set be $B_{\eta_\Lambda}(\alpha) = [0, F_{r|\Lambda \cap r, n-|\tau|\Lambda}(\alpha)]$, such that $\mathbb{P}(\hat{T}(Y_\theta, \eta_\Lambda) \in B_{\eta_\Lambda}(\alpha)) \geq \alpha$. We can show that a valid level-$\alpha$ repro samples confidence set for $\eta_{0,\Lambda} = (\beta_{0,\Lambda}, \tau_0)$ is

$$\Gamma^r_{\alpha}(y_{obs}) = \left\{ \eta_\Lambda : \hat{T}(y_{obs}, \eta_\Lambda) \in B_{\alpha}(\eta_\Lambda) \right\}. $$

Now with both $\beta_{0,i}, i \notin \Lambda$ and $\sigma_0$ out of the picture, we need to deal with the only remaining nuisance parameter $\tau$. To handle the impact of $\tau$, we utilize the model candidate set $S^{(d)}$ constructed in Section 2.1 and take a union approach. That is, for certain $\beta_\Lambda$, if $(\beta_\Lambda, \tau)$ is defined above for any $\tau$ in the candidate set $S^{(d)}$, we then retain the $\beta_\Lambda$ in the confidence set for $\beta_{0,\Lambda}$. Specifically,

$$\Gamma^r_{\alpha}(y_{obs}) = \left\{ \beta_\Lambda : \hat{T}(y_{obs}, \eta_\Lambda) \in B_{\alpha}(\eta_\Lambda), \eta_\Lambda = (\beta_\Lambda, \tau) \text{ for some } \tau \in S^{(d)} \right\}$$

$$= \bigcup_{\tau \in S^{(d)}} \left\{ \beta_\Lambda : \hat{T}(y_{obs}, \eta_\Lambda) \in B_{\alpha}(\eta_\Lambda), \eta_\Lambda = (\beta_\Lambda, \tau) \right\}. $$

An illustration of such a confidence set is provided in Section 3.2 for the special cases that $\Lambda = \{1, \ldots, p\}$; see Figure 1.
We observe that inside the union in (22), each set is a confidence set based on certain model \( \tau \) in the candidate set \( S^{(d)} \). Although we do not know the true underlying model \( \tau_0 \), with Algorithm 1, we are able to construct a candidate set of reasonable size that would include \( \tau_0 \) with high probability. This enables us to guarantee the coverage rate, both in finite samples and asymptotically, as indicated in the following theorems. We provide detailed proofs of the two theorems in the Section 5.

**Theorem 6.** Under the conditions in Theorem 1, for any finite \( n \) and \( p \) and an arbitrarily small \( \delta > 0 \), the coverage probability of the confidence interval \( \Gamma_{\alpha}^{d_1} (Y) \) defined in (22) is \( P_{(\xi_t, Y)} \{ \beta_0, \Lambda \in \Gamma_{\alpha}^{d_1} (Y) \} \geq \alpha - \delta - o(e^{-c_1d}) \) for some \( c_1 > 0 \). Further \( P_{Y, \xi_t} \{ \beta_0, \Lambda \in \Gamma_{\alpha}^{d_1} (Y) \} \geq \alpha - \delta - o_p(e^{-c_1d}) \).

**Theorem 7.** Under the conditions in Theorem 2, for any finite \( d \), the coverage probability of \( \Gamma_{\alpha}^{d_1} (Y) \) defined in (22) is \( P_{(\xi_t, Y)} \{ \beta_0, \Lambda \in \Gamma_{\alpha}^{d_1} (Y) \} \geq \alpha - o(e^{-c_2n}) \) for some \( c_2 > 0 \). Further \( P_{Y, \xi_t} \{ \beta_0, \Lambda \in \Gamma_{\alpha}^{d_1} (Y) \} \geq \alpha - o_p(e^{-c_2n}) \).

**Remark 2** (Extension to make inference for any linear transformation of \( \beta_0^{full} \)). Let \( L \beta_0^{full} \) be a linear transformation of \( \beta_0^{full} \), where \( L \) is a \( l \times p \) transformation matrix. We then let \( \tilde{L} = \begin{bmatrix} \frac{L}{\text{I}_{(p-l) \times (p-l)}} \end{bmatrix} \), \( \tilde{\beta}_0^{full} = \tilde{L} \beta_0^{full} \), and \( \bar{X} = XL^{-1} \). The inference of \( L \beta_0^{full} \) based on the data \( (Y_{obs}, X) \) is now equivalently transformed to the inference of a subset of \( \tilde{\beta}_0^{full} \) based on the transformed data \( (Y_{obs}, \bar{X}) \). Therefore we are able to construct the confidence set for \( L \beta_0^{full} \) by applying (22) on \( (Y_{obs}, \bar{X}) \). Note that one should also derive the candidate set \( S^{(d)} \) from the transformed data \( (Y_{obs}, \bar{X}) \) using Algorithm 1.

3.2. Two special examples of interest  As stated in [59, 37], we are often interested in marginal inference for a single regression coefficient \( \beta_{0,i} \) in practice. Another interesting inference problem that has been studied in the literature is to jointly infer all regression coefficients \( \beta_0^{full} \) [60, 23]. In this subsection, we consider these interesting special cases and provide a new solution using the repro samples method.

**Inference for a single regression coefficient.** To obtain the repro samples confidence set for \( \beta_{0,i} \), we simplify the nuclear mapping function defined in (19) and (20) by making \( \Lambda = \{ i \} \). For a given \( \eta_i = (\beta_i, \tau) \), it is

\[
T(u, \eta_i) = \begin{cases} \frac{u^\top O_{\tau,i} u}{(1 - H_{\tau,i})u^\top (n - |\tau|)} & \text{if } i \in \tau \\ \infty & \text{if } i \notin \tau \text{ and } \beta_i \neq 0 \\ 0 & \text{if } i \notin \tau \text{ and } \beta_i = 0 \end{cases}
\]

\[
= \begin{cases} \frac{(y_\theta - X_i \beta_i)^\top O_{\tau,i} (y_\theta - X_i \beta_i)}{(y_\theta - X_i \beta_i)^\top (1 - H_{\tau,i})(y_\theta - X_i \beta_i)/(n - |\tau|)} & \text{if } i \in \tau \\ \infty & \text{if } i \notin \tau \text{ and } \beta_i \neq 0 \Rightarrow \tilde{T}(y_\theta, \eta_i), \\ 0 & \text{if } i \notin \tau \text{ and } \beta_i = 0 \end{cases}
\]

where \( O_{\tau,i} \) is the projection matrix of \( (I - H_{\tau,i})X_i \), and \( \tau_{-i} = \tau \setminus \{ i \} \). Note that for \( i \in \tau \), the nuclear statistics \( \tilde{T}(y_\theta, \eta_i) \) is equivalent to the square of t-statistics for testing \( H_0 : \beta_{0,i} = \beta_i \), obtained by fitting a linear regression of \( y_\theta \) on \( X_\tau \).
Then following from (22), we obtain the confidence set for $\beta_{0,i}$

$$
\Gamma_\alpha^{\beta}(y_{obs}) = \left\{ \beta_i : \hat{T}(y_{obs}, \eta_i) \in B_\alpha(\eta_i), \eta_i = (\beta_i, \tau) \text{ for some } \tau \in S^{(d)} \right\}
$$

(23)

$$
= \bigcup_{\tau \in S^{(d)}} \left\{ \beta_i : \hat{T}(y_{obs}, (\beta_i, \tau)) \leq F_{1,n-|\tau|}(\alpha) \right\},
$$

where we let $B_\alpha(\eta_i) = B_\alpha(\tau) = [0, F_{1,n-|\tau|}(\alpha)]$. Following Theorems 6 and 7, the set $\Gamma_\alpha^{\beta}(y_{obs})$ is a level-$\alpha$ confidence set for $\beta_{0,i}$.

**Remark 3 (Comparison with the debiased method).** We discuss the difference between our method and the debiased LASSO. First of all, our method offers the finite-sample coverage guarantee, while the debiased LASSO method can only produce the asymptotic coverage rate. More specifically, the debiased LASSO method needs the sample size $n \to \infty$ to make sure the bias, which comes from the regularized estimation and is of order $O(\sqrt{\log p/n})$, goes to 0. In contrast, our method bypasses the estimation step and constructs the confidence sets directly via the repro sampling framework, and is therefore unbiased in nature. Second, the debiased LASSO method [37] is designed to make inference for an individual regression coefficient. The idea of the debiased LASSO method was later generalized to make inference of functions of the regression coefficients, such as co-heritability[30] and group inference statistics [29]. However, such a generalization relies on specific forms of the functions and does not allow arbitrary functions. Our method, however, as we will show in Remark 5, can be used to construct the confidence sets for arbitrary functions. Third, we will show in Section 4.2 that, when the sample size is small, the debiased LASSO method may have either coverage issues or overly large intervals for large regression coefficients. Our method on the other hand can guarantee the coverage for both large and zero regression coefficients in this small sample setting with preferable interval lengths. We refer the readers to Section 4.2 for details.

**Joint inference for all regression coefficients.** Let $\Lambda = \{1, \ldots, p\}$ and we make a joint inference all regression coefficients $\beta_{0}^{full}$ here. Note that $\tau \subset \Lambda$, so $\tau \setminus \Lambda = \emptyset$. Following from (19) and (20), the nuclear mapping function for $\eta = (\beta, \tau) = ((\beta_\tau, 0_{|\tau|}), \tau)$ is

$$
T(u, \eta) = \frac{u^\top H_\tau u / |\tau|}{u^\top (I - H_\tau) u / (n - |\tau|)}
$$

(24)

$$
= \frac{(y_\theta - X_\tau \beta_\tau)^\top H_\tau (y_\theta - X_\tau \beta_\tau) / |\tau|}{(y_\theta - X_\tau \beta_\tau)^\top (I - H_\tau) (y_\theta - X_\tau \beta_\tau) / (n - |\tau|)}:= \hat{T}(y_\theta, \eta).
$$

We then let the Borel set be $B_\alpha(\eta) = B_\alpha(\tau) = [0, F_{|\tau|,n-|\tau|}(\alpha)]$, and construct the joint confidence set for $\beta_{0}^{full}$ following from (22).

$$
\Gamma_\alpha^{\beta}(y_{obs}) = \left\{ \beta : \hat{T}(y_{obs}, \eta) \leq F_{|\tau|,n-|\tau|}(\alpha), \beta = (\beta_\tau, 0_{|\tau|}), \eta = (\beta, \tau) \text{ for some } \tau \in S^{(d)} \right\}
$$

(25)

$$
= \bigcup_{\tau \in S^{(d)}} \left\{ \beta : \hat{T}(y_{obs}, \eta) \leq F_{|\tau|,n-|\tau|}(\alpha), \beta = (\beta_\tau, 0_{|\tau|}), \eta = (\beta, \tau) \right\}.
$$

Again, following Theorems 6 and 7, the set $\Gamma_\alpha^{\beta}(y_{obs})$ is a level-$\alpha$ confidence set for the entire vector $\beta_{0}^{full}$.
Remark 4 (Visualization of the confidence set $\Gamma^{\beta}(y_{\text{obs}})$ in (25)). We now use a 3-dimensional graph to present a visualization of the joint confidence set $\Gamma^{\beta}(y_{\text{obs}})$ for $\beta_0^{\text{full}}$. To do so, we consider a particular example of $p = 8$ with the true model $\tau_0 = \{1, 2\}$, for which our candidate set contains only three models $S^{(d)} = \{\{1, 2, 3\}, \{1, 2\}, \{1, 3\}\}$, each having three or less covariates. Unlike the confidence set obtained in [60, 23], which, in this example, would typically be a 8-dimensional shallow disc, our confidence set $\Gamma^{\beta}(y_{\text{obs}})$ is a union of three sets, one 3-dimensional ellipsoid and two 2-dimensional ellipsoids, corresponding to models $\{1, 2, 3\}$, $\{1, 2\}$ and $\{1, 3\}$, respectively. Plotted in Figure 1 are two components: (a) a confidence curve [56] plot of model $\tau_0$ plotted on the candidate model space $S^{(d)}$; and (b) the corresponding confidence regions of the coefficients in the three candidate models. The $y$-axis of plot (a) is the associated confidence level of each model computed via the conditional the corresponding function value of the joint confidence set in (25). To put it more clearly, for each $\tau$, $\tau \in S^{(d)}$, the associated confidence level of each model computed via the conditional probability in (14), therefore the plot demonstrates the uncertainty of the models. The figure on the right shows the level-95% confidence sets of $\beta$ (the two blue ones) for each of the three models in the candidate set $S^{(d)}$. It demonstrates that our algorithm produces a union of three sets of different dimensions in this example.

Figure 1: Plot for Displaying the Joint Confidence Sets

Figure 2: (a) Confidence curve [56] plot on $S^{(d)}$; (b) confidence sets of $\beta_\tau$ (one 3-dimensional ellipsoid and two 2-dimensional ellipsoids) of the three $\tau$ models in candidate set $S^{(d)} = \{\{1, 2, 3\}, \{1, 2\}, \{1, 3\}\}$. In (a), the red line instantiate the case where we aim to construct a level-0.95 ($\alpha = 0.95$) model confidence set. In this case, our 95% model confidence set for the true $\tau_0$ contains two models; i.e., $\Gamma^{\beta}(y_{\text{obs}}) = \{\{1, 2, 3\}, \{1, 2\}\}$. In (b), a 95% joint confidence set for $\beta_0^{\text{full}}$ is the union of these three confidence sets, one 3-dimensional on the $(\beta_1, \beta_2, \beta_3)$ space and two 2-dimensional ellipsoids on the $(\beta_1, \beta_2)$ and $(\beta_1, \beta_3)$ space, respectively (in each of the cases the remaining $\beta_j$’s are 0).

Remark 5 (Extension to make inference for any function of $\beta_0^{\text{full}}$). We can extend the joint confidence set in (25) to obtain a repro samples confidence set for any function of $\beta_0^{\text{full}}$, say $h(\beta_0^{\text{full}})$. To put it more clearly, for each $(\tau, \beta_\tau)$ in the confidence set (25), we collect the corresponding function value $h(\beta_\tau^{\text{full}})$, where $\beta_\tau^{\text{full}} = (\beta_\tau, 0_{\text{occ}})$ to form the confidence set for $h(\beta_0^{\text{full}})$, i.e. $\Gamma^h(y_{\text{obs}}) = \{h((\beta_\tau, 0_{\text{occ}})) : \tilde{T}(y_{\text{obs}}, \eta) \leq F_{\|\tau\|, n-|\tau|}(\alpha), \eta = (\tau, \beta_\tau) \text{ for } \tau \in S^{(d)}\}$.

3.3. Joint inference for model and regression coefficients Besides constructing confidence sets for the true model $\tau_0$ and certain regression coefficients $\beta_{\Lambda,0}$ respectively, we
are also able to construct joint confidence set for the model and coefficients \( \eta_0 = (\tau_0, \beta_0) \).
Specifically, let \( \eta_r = (\tau, \beta_r) \), we then follow (24) to define the nuclear mapping as

\[
T(u, \eta_r) = \frac{u^\top H_r u}{\|u\| (1 - H_r) u / (n - |\tau|)}
\]

\[
= \frac{(y_\theta - X_\tau \beta)^\top H_r (y_\theta - X_\tau \beta_r) / |\tau|}{(y_\theta - X_\tau \beta)^\top (1 - H_r) (y_\theta - X_\tau \beta_r) / (n - |\tau|)} = \tilde{T}(y_\theta, \eta_r).
\]

Then it follows immediately that \( \mathbb{P}_U \left\{ \tilde{T}(Y_\theta, \eta_r) \in B_{\eta_r}(\alpha) \right\} = \alpha \) if we let \( B_{\eta_r}(\alpha) = \left[ 0, F_{\tau,|\tau|,n-|\tau|}(\alpha) \right] \).

If we use the above nuclear mapping and follow a similar approach to (21) to construct the joint confidence set for \( \eta_0 = (\tau_0, \beta_0) \), the resulting confidence set is not tight for the true model \( \tau_0 \) since it includes all models in the model candidate set. To make the joint confidence set informative about \( \tau_0 \), we can limit \( \tau \) in a level-\( \alpha_1 \) model confidence set \( \Gamma_{\alpha_1}(y_{\text{obs}}) \) obtained in Section 2 using (17). Here, \( \alpha_1 \in (\frac{1}{2}, 1) \) and close to 1. Similarly, take another \( \alpha_2 \in (\frac{1}{2}, 1) \), and let \( \alpha = \alpha_1 + \alpha_2 - 1 \). Then we use a modified version of (25) to construct the confidence set for \( \eta_0 = (\tau_0, \beta_0) \):

\[
\Gamma_{\alpha}(y_{\text{obs}}) = \bigcup_{\tau \in \Gamma_{\alpha_1}(y_{\text{obs}})} \{ \eta_r : \tilde{T}(y_{\text{obs}}, \eta_r) \in B_{\alpha_2}(\eta_r) \}.
\]

The following Theorem (8) and (9), the proofs of which we provide in Section 5, guarantees that \( \Gamma_{\alpha}(y_{\text{obs}}) \) is a level-\( \alpha \) joint confidence set for \( \eta_0 \). If, for instance, we take \( \alpha_1 = \alpha_2 = 0.975 \), then \( \alpha = \alpha_1 + \alpha_2 - 1 = 0.95 \) and the above \( \Gamma_{\alpha}(y_{\text{obs}}) \) has at least 95% guaranteed coverage. This scheme also applies to the confidence set (22) discussed in the previous subsection, including the two special cases of \( \beta_{\lambda,0} \).

**THEOREM 8.** Under the conditions in Theorem 1, for any finite sample size \( n \) and an arbitrarily small \( \delta > 0 \), the coverage probability of the confidence interval \( \Gamma_{\alpha}^\| (Y) \) defined in (26) is \( P_{(\eta, Y)} \{ (\tau_0, \beta_0) \in \Gamma_{\alpha}^\| (Y) \} \geq \alpha - \delta - o(e^{-cd}) \) for some \( c_1 > 0 \), provided that \( \alpha_1 + \alpha_2 - 1 = \alpha \). Further \( P_{(\eta, Y)} \{ (\tau_0, \beta_0) \in \Gamma_{\alpha}^\| (Y) \} \geq \alpha - \delta - o_p(e^{-c_2d}) \).

**THEOREM 9.** Under the conditions in Theorem 2, for any finite \( d \), the coverage probability of the confidence interval \( \Gamma_{\alpha}^\| (Y) \) defined in (26) is \( P_{Y} \{ (\tau_0, \beta_0) \in \Gamma_{\alpha}^\| (Y) \} \geq \alpha - o(e^{-c_2n}) \) for some \( c_2 > 0 \), provided that \( \alpha_1 + \alpha_2 - 1 = \alpha \). Further \( P_{Y} \{ (\tau_0, \beta_0) \in \Gamma_{\alpha}^\| (Y) \} \geq \alpha - o_p(e^{-c_2n}) \).

4. Simulation studies In this section, we provide a set of comprehensive simulation studies to evaluate the numerical performance of the proposed repro samples methods. Section 4.1 focuses on making inference for the unknown underlying true model discussed in Section 2, and Section 4.2 addresses the two inference problems for regression coefficients discussed in Section 3.2.

4.1. Model candidates and inference for the true model \( \tau_0 \) In this subsection, we study the performance of the data-driven model candidate set \( S_{(d)} \) in (6), produced by Algorithm 1 and the repro samples model confidence set in (17), constructed by Algorithm 2. We carry out our numerical studies on synthetic data from the following three models:

\begin{itemize}
\item[(M1)] (Extremely High Dimension) Let \( \beta_0^{full} = (3, 2, 1.5, 0, \ldots, 0) \). For \( j_1, j_2 \in [p] \), the correlation between \( x_{j_1} \) and \( x_{j_2} \) is set to \( 0.5^{\min(|j_1 - j_2|)} \). We set \( n = 50, p = 1000 \) and \( \sigma = 1 \).
\end{itemize}
(M2) (Decaying Signal) Let $\beta_0^{full} = (2, 1.5, 1, 0.8, 0.6, 0, \ldots, 0)$. For $j_1, j_2 \in [p]$, the correlation between $x_{j_1}$ and $x_{j_2}$ is set to $0.1|j_1 - j_2|$. We let $n = 80$, $p = 150$ and $\sigma = 1$.

(M3) (High Dimension and Decaying Signal) Let $\beta_0^{full} = (3, 2, 1.5, 1, 0.8, 0.6, 0, \ldots, 0)$. For $j_1, j_2 \in [p]$, the correlation between $x_{j_1}$ and $x_{j_2}$ is set to $0.1|j_1 - j_2|$. We let $n = 100$, $p = 500$, and $\sigma = 1$.

The first model (M1) represents an extremely high-dimensional setting with $p \gg n$. The second model (M2) represents a challenging case where the signals are decaying with the weakest signal being just 0.5. We set Model (M3) by increasing the dimension of Model (M2) to investigate the performance of the proposed approach when both high-dimensional design matrix and weak signals are present in the data. We also add a strong signal of $\beta_{1,0} = 3$ to expand the range of signal strengths. To evaluate the frequentist performance of the proposed methods, we replicate the simulation for 200 times for each model.

When applying Algorithm 1 to obtain the model candidate set, we use the following extended BIC to choose the values of the tuning parameter $\lambda$ in (5).

$$
EBIC_{b, \zeta}(\lambda) = n \log \left( \frac{\| y_{obs} - X_{\hat{\theta}_{b,\lambda}} \hat{\beta}_{\hat{\theta}_{b,\lambda}} \|^2}{n} + |\hat{\theta}_{b,\lambda}| \log(n) + 2\zeta \log \left( \frac{p}{|\hat{\theta}_{b,\lambda}|} \right) \right).
$$

Here, $\hat{\theta}_{b,\lambda}$ is the solution to (5) with the tuning parameter $\lambda$, $\hat{\beta}_{\hat{\theta}_{b,\lambda}}$ is an estimation of $\beta_{\hat{\theta}_{b,\lambda}}$ and $0 \leq \zeta \leq 1$ can range between 0 and 1. To increase the efficiency of candidate models search, we pick multiple models for each $u^*_g$. Specifically, we pick all $\lambda$’s between $\lambda^0_0$ and $\lambda^1_b$ i.e. $\Lambda_b = [\lambda^0_0, \lambda^1_b]$, where $\lambda^0_0 = \arg\min_{\lambda} EBIC_{b, \zeta}(\lambda)$. This is equivalent to using all $0 \leq \zeta \leq 1$, because $\lambda^0_0$ is monotonically non-decreasing in $\zeta$, and [14] showed that the model selection consistency of extended BIC holds for some $0 \leq \zeta \leq 1$. When applying Algorithm 2 to obtain the model confidence set, we calculate the $\hat{\tau}(y^g_j)$ in (18) by obtaining the largest estimated model that is not larger than $|\tau_b|$ in the adaptive LASSO solution path. Also, in our analysis, we set the number of repro samples for the candidate set in Algorithm 1 to be $d = 1,000$ for model (M1). For Models (M2)-(M3) with weak signals, identifying the true model is a known challenging problem. In this case, we set the number of repro samples to be a large $d = 10,000$ for (M2) and $d = 100,000$ for (M3). Regarding the number of repro samples in Algorithm 2 for calculating the distribution of the nuclear statistics, we set $J = 200$ for all three models.

We compare the proposed repro samples approach with the residual bootstrap approach in the current literature (e.g., [13]). The numbers of bootstrap samples are 1,000, 10,000, and 100,000 for (M1), (M2) and (M3) respectively, the same as $d$, the numbers of repro samples for searching for the candidate models in our method. In each setting, the collection of all models obtained using the bootstrap samples form a bootstrap model candidate set. Here, in our study of the bootstrap method, we use three different tuning criteria, AIC, BIC and cross-validation (CV), to select models. The bootstrap model “confidence” sets are obtained by removing the least frequent model estimations from the bootstrap candidate model set, with the total (cumulative) frequency of the removed models not larger than 5%. We note that the bootstrap method here is an ad hoc method commonly used in current practice. Due to the discreteness of the model space and estimated models, there is no theoretical support to the “confidence” claim that such a bootstrap method can get a valid level-95% model confidence set for the true model $\tau_0$.

Table 1 compares the performance of the model candidate sets produced by the proposed repro samples approach and the typical residual bootstrap approaches with different tuning criteria. We report the average cardinality of the model candidate sets (Cardinality) and the percentage of simulation cases where the true model $\tau_0$ is included in the model candidate
| Method              | Cardinality of $S_{0.05}^{(d)}$ | Inclusion of $\Gamma_{0.05}$. |
|--------------------|---------------------------------|-------------------------------|
| Model M1: $n = 50, p = 1000$ |                                 |                               |
| Repro samples      | 2.605 (0.191)                   | 1.000 (0.000)                 |
| Bootstrap AIC      | 215.425 (10.855)                | 1.000 (0.000)                 |
| Bootstrap BIC      | 146.100 (7.423)                 | 1.000 (0.000)                 |
| Bootstrap CV       | 259.535 (11.891)                | 1.000 (0.000)                 |
| Model M2: $n = 80, p = 150$ |                                 |                               |
| Repro samples      | 29.455 (3.080)                  | 0.980 (0.010)                 |
| Bootstrap AIC      | 4350.850 (134.000)              | 1.000 (0.000)                 |
| Bootstrap BIC      | 2303.190 (75.708)               | 1.000 (0.000)                 |
| Bootstrap CV       | 5033.700 (134.233)              | 1.000 (0.000)                 |
| Model M3: $n = 100, p = 500$ |                                 |                               |
| Repro samples      | 4.710 (0.558)                   | 0.995 (0.005)                 |
| Bootstrap AIC      | 5088.030 (456.021)              | 1.000 (0.000)                 |
| Bootstrap BIC      | 2944.325 (245.670)              | 1.000 (0.000)                 |
| Bootstrap CV       | 6458.345 (570.104)              | 1.000 (0.000)                 |

Table 1: Comparison of Performance of the Model Confidence Sets

Table 2 reports the average cardinality of the confidence sets obtained using Algorithm 2 and their coverage of the true model $\tau_0$ out of the 200 repetitions. From Table 2, we can see that, for Model (M1), the model confidence set based on the repro samples approach only contains two models on average, while the sets by the bootstrap methods have sizes between 110 to 210. The coverage of the proposed approach is 100%, because the discrete nature of the model confidence sets could often preclude an exact confidence level of 95%. For example, if a candidate set only contains two models, excluding one of them could drop the confidence level well below 95%. For Models (M2) and (M3), the model confidence sets...
generated by the bootstrap are impractically large, containing between 1400-5000 models on average. Even with those many models, the bootstrap confidence set with AIC and BIC slightly undercovers the true model \( \tau_0 \) for (M3). On the contrary, for (M2) and (M3), the proposed approach manages to give a confidence set of around just 12 and 4 models on average respectively with a good coverage above 95\% under the decaying signal setting, where the minimum coefficient is only 0.6.

The above results demonstrate that the proposed repro samples method constructs valid and efficient model confidence sets for the true model \( \tau_0 \), even under the challenging settings of (M1) - (M3). On the contrary, the bootstrap method exaggerates the uncertainty of model selection by producing extremely large number of models in its “confidence” sets, rendering the results that are not very useful in practice.

### 4.2. Inference for regression coefficients accounting for model selection uncertainty

In this subsection, we evaluate the performance of the proposed repro samples confidence set for single regression coefficients in (23) and compare it with the existing “state-of-art” debiased methods. We also evaluate the performance of the joint confidence set for \( \beta_{1}^{\text{full}} \) in (25).

#### Table 3

| Model | \( \beta_{0,i} \) | \( \beta_{0,i} \neq 0 \) | \( \beta_{0,i} = 0 \) | \( \beta_{0,i} \neq 0 \) | \( \beta_{0,i} = 0 \) |
|-------|------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| M1    | 0.970(0.012)     | 0.310(0.033)          | 0.320(0.033)          | 0.970(0.012)          | 0.310(0.033)          |
|       | 0.960(0.014)     | 0.440(0.035)          | 0.320(0.033)          | 0.960(0.014)          | 0.440(0.035)          |
|       | 0.925(0.019)     | 0.517(0.033)          | 0.320(0.033)          | 0.925(0.019)          | 0.517(0.033)          |
| M2    | 0.990(0.007)     | 0.960(0.014)          | 0.960(0.014)          | 0.990(0.007)          | 0.960(0.014)          |
|       | 0.965(0.013)     | 0.915(0.020)          | 0.965(0.013)          | 0.965(0.013)          | 0.915(0.020)          |
|       | 0.955(0.016)     | 0.905(0.015)          | 0.955(0.016)          | 0.955(0.016)          | 0.905(0.015)          |
| M3    | 0.980(0.010)     | 0.870(0.024)          | 0.870(0.024)          | 0.980(0.010)          | 0.870(0.024)          |
|       | 0.950(0.015)     | 0.870(0.024)          | 0.870(0.024)          | 0.950(0.015)          | 0.870(0.024)          |
|       | 0.965(0.013)     | 0.865(0.024)          | 0.865(0.024)          | 0.965(0.013)          | 0.865(0.024)          |
|       | 0.950(0.014)     | 0.850(0.025)          | 0.850(0.025)          | 0.950(0.014)          | 0.850(0.025)          |

#### Table 4

| Model | \( \beta_{0,i} \) | \( \beta_{0,i} \neq 0 \) | \( \beta_{0,i} = 0 \) | \( \beta_{0,i} \neq 0 \) | \( \beta_{0,i} = 0 \) |
|-------|------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| M1    | 0.970(0.012)     | 0.310(0.033)          | 0.320(0.033)          | 0.970(0.012)          | 0.310(0.033)          |
|       | 0.960(0.014)     | 0.440(0.035)          | 0.320(0.033)          | 0.960(0.014)          | 0.440(0.035)          |
|       | 0.925(0.019)     | 0.517(0.033)          | 0.320(0.033)          | 0.925(0.019)          | 0.517(0.033)          |
| M2    | 0.990(0.007)     | 0.960(0.014)          | 0.960(0.014)          | 0.990(0.007)          | 0.960(0.014)          |
|       | 0.965(0.013)     | 0.915(0.020)          | 0.965(0.013)          | 0.965(0.013)          | 0.915(0.020)          |
|       | 0.955(0.016)     | 0.905(0.015)          | 0.955(0.016)          | 0.955(0.016)          | 0.905(0.015)          |
| M3    | 0.980(0.010)     | 0.870(0.024)          | 0.870(0.024)          | 0.980(0.010)          | 0.870(0.024)          |
|       | 0.950(0.015)     | 0.870(0.024)          | 0.870(0.024)          | 0.950(0.015)          | 0.870(0.024)          |
|       | 0.965(0.013)     | 0.865(0.024)          | 0.865(0.024)          | 0.965(0.013)          | 0.865(0.024)          |
|       | 0.950(0.014)     | 0.850(0.025)          | 0.850(0.025)          | 0.950(0.014)          | 0.850(0.025)          |

In Table 3, we compare the performance of the repro samples approach in terms of the constructed confidence sets for single regression coefficients with two stat-of-the-art debiased/de-sparsify approaches, one in [37] (debiased LASSO (JM), using the R codes provided by the authors at the website [36]) and the other in [59] (debiased LASSO (ZZ), using
the R codes provided by the authors). We notice that although the debiased LASSO (JM) could achieve the desired coverage rate on average, it significantly undercovers the non-zero coefficients (signals) for all models (M1-M3), especially for (M1) where the correlations among covariates are large. This phenomenon has been identified in [59, 37]. Although the LASSO estimator has a vanishing convergence rate for large sample size, when the sample size is limited, the large absolute correlations will result in a greater value in the estimation error $|\hat{\beta}_i - \beta_{0,i}|$ for nonzero $\beta_{0,i}$'s. This increases bias and makes the debiased methods undercover the signals. [59] provided an enhanced method, denoted by debiased LASSO (ZZ) in Table 3, to overcome this issue by including a few highly correlated independent variables when debiasing and enforcing small correlations between the score vector and covariates, making the confidence intervals larger. The enhanced debiased LASSO (ZZ) method indeed improved the coverage rates in the three simulation settings, however, they are achieved at the expenses of interval widths. On the other hand, the proposed repro samples approach successfully achieves the desired coverage for all the signals of all three models with confidence sets at least 40% shorter than those produced by debiased LASSO (ZZ). Moreover, compared to both of the debiased approaches, the repro samples confidence sets for the coefficients whose true values are zero appear to be much narrower, making the overall average width of the proposed confidence sets much smaller. In addition, the computing code of the enhanced debiased LASSO (ZZ) approach needs to pre-select the number of highly correlated predictors when calculating the score vector, and the choice of the pre-selected number is ad hoc. Contrarily the repro samples approach is a data-dependent procedure that does not involve such an ad hoc decision. After all, it is evident that when it comes to constructing confidence sets for single coefficients, the repro samples approach could achieve better coverage with narrower intervals.

To further investigate the differences between the performance of the proposed approach and that of the debiased LASSO, we compare in Table 4 the coverage rates and widths of the confidence sets produced by all the three approaches for each of the nonzero regression coefficients. We observe that the repro samples approach and debiased LASSO (ZZ) both achieve the desired coverage regardless of the signal strengths. However, the confidence intervals produced by debiased LASSO (ZZ) are at least 70% wider than those produced by the repro samples approach. On the contrary, the debiased LASSO (JM) uniformly undercovers the truths for all signals in all three models except for two coefficients in Model (M2). As expected, the under-coverage issue of the debiased LASSO (JM) approach is more serious when $p/n$ is larger, since the second order approximation is more difficult. For Model (M1) with $n = 50, p = 1000$, the coverage rate of the debiased LASSO is only around 30%-45%, and for Model (M3) with $n = 100, p = 500$ the coverage rate is around 85%-89%. When $p/n$ is relatively smaller as in Model (M2) with $n = 80, p = 150$, the coverage of debiased LASSO (JM) improves to over 91% although the under coverage issue still lingers. In terms of the width of the confidence sets, for Model (M1) with $n = 100, p = 500$, the widths of the repro samples confidence sets are less than half of those from the debiased LASSO (ZZ) and comparable to the debiased LASSO (JM), even though the coverage of the repro samples confidence sets are 10% higher in general. For the other two models, the repro samples confidence sets are also at least 40% shorter than the debiased LASSO (ZZ) confidence intervals for the signals, providing a more accurate assessment of the uncertainties of the estimation of these regression parameters. To sum up, the repro samples approach is able to cover all the signals with desired coverage rate and correctly quantify the uncertainty of parameter estimation regardless of the dimension of the design matrix and signal strength.

Besides getting the model confidence set and the confidence set for single coefficients, our repro samples method also provides a joint inference for $\beta_0^{full}$. To evaluate the performance of the joint confidence set for $\beta_0^{full}$ in (25), we apply (25) on the 200 simulated data sets for
models (M1)-(M3), and summarize the results in Table 5. Evidently, the proposed confidence set can achieve the desired coverage rate, since it covers the truth \( \beta_0^{full} \) 94%, 94.5% and 95% of the times for models (M1), (M2) and (M3), respectively. Moreover, the proposed confidence set, as opposed to those in [60, 23], has a sparse structure in the sense that the vast majority of dimensions of the joint confidence set corresponding to the zero regression coefficients are shrunk to [0,0], as illustrated by Table 5. This is because if variable \( X_i \) is not in any of the models in the model candidate set \( S^{(d)} \), then any value of \( \beta \) with nonzero \( \beta_i \) will be excluded from the confidence set, following from the union in (25). Such sparse confidence sets give researchers two advantages in practice: (1) the size/volume of the confidence set is substantially smaller, and therefore it is more informative; (2) it offers a new tool for confidently and efficiently screening variables. Here the proportions of the confidence set’s dimensions shrunk to [0,0] are above 98.5% for model (M1) and (M3) and 91.6% for model (M2), demonstrating that the number of variables left after screening is much smaller than \( n - 1 \), which is suggested for the sure independence screening approach [26, 27].

### Table 5

| Model | Coverage Rate | Proportions of Dimensions Shrunk to [0,0] |
|-------|---------------|------------------------------------------|
| M1: \( n = 50, p = 1,000 \) | 0.940 (0.016) | 0.997 (0.000) |
| M2: \( n = 80, p = 150 \) | 0.945 (0.016) | 0.916 (0.002) |
| M3: \( n = 100, p = 500 \) | 0.950 (0.015) | 0.986 (0.001) |

5. Technical proofs  In this section, we prove our main results Theorems 1-7. We would like to point out that Theorems 1 and 2 in Section 2.1 are particularly challenging. In both cases, we have to control the behavior of the repro samples \( U^* \) not only in relation to the error term \( U \), but also in relation to \( (I - H_T)X_{\tau_0}\beta_0 \) for any \( |\tau| \leq |\tau_0| \), within the proximity of which \( U^* \) could possibly lead to \( \tau \) instead of \( \tau_0 \). We also would like to note that there have not been any finite-sample theories like Theorem 1 in the literature.

In the following, we first prove Theorems 1 and 2, that is, when either the number of repro simulations \( d \) or the sample size \( n \) is large enough, our candidate model sets \( S^{(d)} \) will contain the true model \( \tau_0 \) with high probability.

5.1. Proof of Theorem 1  First we define a similarity measure between two vectors \( v_1, v_2 \) as the square of cosine of the angles between \( v_1 \) and \( v_2 \), i.e.

\[
\rho(v_1, v_2) = \frac{\|H_{v_1}v_2\|^2}{\|v_2\|^2} = \frac{(v_1^Tv_2)^2}{\|v_1\|^2\|v_2\|^2}.
\]

We therefore use \( \rho(u^*, u^{rel}) \) to measure the similarity between a single repro sample \( u^* \) and the realization \( u^{rel} \). Apparently, the closer \( \rho(u, u^{rel}) \) is to 1, the smaller the angle between \( u \) and \( u^{rel} \). Hence we use \( \rho(u, u^{rel}) \) to measure the similarity between \( u \) and \( u^{rel} \).

We then present a technical lemma that derives the probability bound of obtaining the true model \( \tau_0 \) when the repro sample \( u^* \) falls within close proximity of \( u^{rel} \) in that \( \rho(u^*, u^{rel}) > 1 - \gamma_2^2 \) for a small \( \gamma_2 > 0 \). We provide the proof of Lemma 2 in the appendix.

**Lemma 2.** Suppose \( n - |\tau_0| > 4 \). Let \( U^* \) be a random repro sample of \( U \), such that \( U^*, U \sim N(0, I_0) \), and

\[
\hat{\tau}_{U^*} = \arg\min_{\tau} \left\{ \min_{\beta, \sigma} \|Y - X_{\tau}\beta - \sigma U^*\|^2 + \lambda|\tau| \right\}.
\]
Then for any $0 < \gamma_2^{1/4} < \min \left\{ \frac{C_{\min}}{|\tau_0|^2}, \frac{24}{2^2(2|\tau_0|+1)\log(p/2)/n}, 0.35 \right\}$ such that $C_{\min} > 52\sqrt{2} \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2$ and $\lambda \in \left[ n\gamma_2^{1/2} \left\{ 2 + 2(|\tau_0| + 1)\log(p/2)/n \right\} , n\gamma_2^{1/4} C_{\min} 6 \right]$, 

$$
\mathbb{P}(U, U^*) \left\{ \hat{r}_U \neq \tau_0, \rho(U^*, U) > 1 - \gamma_2^2 \right\} 
\leq 3 \exp \left\{ - \frac{n}{26\sigma_0^2} \left[ \frac{C_{\min}}{\sqrt{\gamma_2}} - 52 \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2 \right] \right\} + 3 \exp \left\{ - \frac{n}{4\gamma_2^{1/4} \sigma_0^2} \right\} 
+ 4(64\gamma_2) \frac{n^{-|\tau_0|-1}}{6} p|\tau_0| + 2\gamma_2^{n^{-|\tau_0|-1}} (\sqrt{n}p)|\tau_0|.
$$

Unlike existing literature in the high-dimensional regime, the results in Lemma 2 do not require any conditions on $C_{\min}$, nor do they even depend on any conditions necessary for achieving consistent regression parameter estimation. This is because the probability bound on the right-hand side of Eq. (27) depends on $C_{\min}$ only through $C_{\min}/\sqrt{\gamma_2}$. When the quantity $C_{\min}/\sqrt{\gamma_2}$ becomes larger, the probability bound becomes smaller. Therefore no matter how small $C_{\min}$ is, as long as $C_{\min} > 0$, the quantity $C_{\min}/\sqrt{\gamma_2}$ can be arbitrarily large when $\gamma_2$ approaches 0. Consequently, however small the separation between the true model $\tau_0$ and the alternative models is, we can always recover $\tau_0$ with high probability with a repro sample $U^*$ that is close to $U$.

By the finite-sample probability bound obtained in the above lemma, when $\gamma_2$ goes to 0, that is, $U^*$ proximate $U$ more closely, the probability of $\hat{r}_U \neq \tau_0$ goes to 0 for any finite $n$ and $p$. This indicates that we do not need $U^*$ to hit $U$ exactly, rather we would only need $U^*$ to be in a neighborhood of $U$ in order to recover $\tau_0$ with high probability. Additionally we observe that as the sample size $n$ goes larger, the probability bounds in Lemma 2 decay exponentially. Therefore, for larger sample, the estimation $\hat{r}_{U^*} = \tau_0$ with large probability even for a large $\gamma_2$. As a result, the neighbourhood of $U^{rel}$, within which $U$ yields $\hat{r}_{U^*} = \tau_0$ with high probability, will expand as the sample size $n$ grows larger.

As Lemma 2 shows the probability of a single sample $U$ being close to $U^*$, in the following Lemma 3, we develop the probability bound for at least one of the $d$ independent samples of $U$ being close to $U^*$. This probability bound then implies a finite-sample probability bound of $\tau_0$ not included in the candidate set $S^{(d)}$ constructed by Algorithm 1. The proof of Lemma 3 is deferred to the appendix.

**Lemma 3.** Suppose $n - |\tau_0| > 4$. Then for any $0 < \gamma_2^{1/4} < \min \left\{ \frac{C_{\min}}{|\tau_0|^2}, \frac{C_{\min}}{2\{2^2(2|\tau_0|+1)\log(p/2)/n\}}, 0.35 \right\}$, such that $C_{\min} > 52\sqrt{2} \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2$, and $\lambda \in \left[ n\gamma_2^{1/2} \left\{ 2 + 2(|\tau_0| + 1)\log(p/2)/n \right\} , n\gamma_2^{1/4} C_{\min} 6 \right]$, the finite-sample probability bound that the true model is not covered by the model candidates set $S^{(d)}$, obtained by Algorithm 1 with the objective function (5), is as follows,

$$
\mathbb{P}(\mu, \chi) (\tau_0 \notin S^{(d)}) \leq 3 \exp \left\{ - \frac{n}{26\sigma_0^2} \left[ \frac{C_{\min}}{\sqrt{\gamma_2}} - 52 \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2 \right] \right\} 
+ 3 \exp \left\{ - \frac{n}{4\gamma_2^{1/4} \sigma_0^2} \right\} 
+ 4(64\gamma_2) \frac{n^{-|\tau_0|-1}}{6} p|\tau_0| + 2\gamma_2^{n^{-|\tau_0|-1}} (\sqrt{n}p)|\tau_0| + \left( 1 - \frac{\gamma_2^{n-1}}{n-1} \right)^d.
$$
We are now to present the proof of Theorem 1

**Proof of Theorem 1**: The first four terms of (28) go to 0 as $\gamma_2$ goes to 0. Therefore for any $\delta > 0$, there exists a $\gamma_0 > 0$, such that when $\gamma_2 = \gamma_0$, sum of the first four terms of (28) is smaller than $\delta$, which implies the probability bound in (7). \hfill $\blacksquare$

5.2. Proof of Theorem 2

Similar to the last section, we first introduce a key lemma.

**Lemma 4.** For any finite $n$ and $p$, if
\[
\frac{\lambda}{n} \in \left[ \frac{3\sigma_0^2(|\tau_0|) + 1}{3} \left( \log(p - |\tau_0|) + \log(|\tau_0|) + \frac{2}{3} \right) + t, \frac{(1 - \gamma_1^2)C_{\min}}{6} \right],
\]
a finite-sample probability bound that the true model is not covered by the model candidates set $S^{(d)}$, obtained by Algorithm 1 with the objective function (5), is as follows,
\[
P_{(\hat{U}, Y)}(\tau_0 \notin S^{(d)}) \leq L(\gamma_1) + 3 \exp \left( \frac{nt}{3\sigma_0^2} \right) + \left[ 2\arccos(\gamma_1) \right]^{\min + |\tau_0| - |\beta_0|} d,
\]
where
\[
L(\gamma_1) = 6 \exp \left[ -\frac{n}{18\sigma_0^2} \left\{ (1 - \gamma_1^2)C_{\min} - 36\frac{\log p}{n}\sigma_0^2 \right\} \right],
\]
and $\cos(0.3\pi) < \gamma_1 < 1$ is any real number.

Lemma 4 aims to offer insights on the asymptotic property of the candidate set $S^{(d)}$, therefore, it gives a different probability bound than Lemma 3. The interpretation is that for any fixed $d$, the probability of $\tau_0 \notin S^{(d)}$ is $O(e^{-n})$ under the conditions in Theorem 2. This provides us the insight that for large samples, we actually do not need an extremely large number of repro samples in order to recover the true model in the candidate set $S^{(d)}$.

To explain the intuition behind the probability bound in Lemma 4, we denote the angle between the repro sample $U^*$ and $(I - H_r)X_{\tau_0}\beta_0$ as $\gamma_1^r$. If $\gamma_1^r \geq \gamma_1$ for all $|\tau| \leq |\tau_0|$, then the probability of $\hat{\tau}_U, \neq \tau_0$ is bounded by the first two terms of (29). The reason that we want to bound $U^*$ away from $(I - H_r)X_{\tau_0}\beta_0$ is that when $U^* \approx (I - H_r)X_{\tau_0}\beta_0$, $X_r$ will explain $Y - U^*$ as well as $X_{\tau_0}$, possibly leading to $\hat{\tau}_U = \tau \neq \tau_0$. The last term of (29) is derived from the probability bound that $\gamma_1^r \leq \gamma_1$ for some $|\tau| \leq |\tau_0|$ for all the $d$ copies of repro samples $U^*$. Therefore, all the three terms together give a probability bound for $\tau_0 \notin S^{(d)}$.

We now present the proof of Theorem 2.

**Proof of Theorem 2.** By Lemma 4, we obtain (8) by making $\gamma_1^2 = 0.7$. The lower bound for $\frac{1}{\alpha}$ is simplified by applying the inequality $\log(|\tau_0|) + \log(p - |\tau_0|) \leq 2\log(p/2)$. \hfill $\blacksquare$

We then proceed to the proof of Theorem 3-5, showing the validity of the constructed confidence set.

5.3. Proof of Theorems 3-5

**Proof of Theorem 3.** The proof of Theorem 3 is a direct consequence of our repro samples idea.
\[
P(\tau_0 \in \Gamma_\alpha(Y)) \geq P(T(U, \theta) \in B_\alpha(\tau, W(U, \theta)) = E\{P(T(U, \theta) \in B_\alpha(\tau, W(U, \theta)|W(U, \theta)) \} \geq \alpha
\]
\hfill $\blacksquare$
Proof of Theorem 4. First, for a given $\tau$, the distribution of $(I - H_\tau)U \mid (I - H_\tau)Y_\theta \mid (I - H_\tau)Y_\theta$ is free of $(\beta_\tau, \sigma)$. Therefore $(I - H_\tau)Y_\theta \mid (I - H_\tau)Y_\theta$ is ancillary for $(\beta_\tau, \sigma)$. Because $\widetilde{W}(Y_\theta, \tau)$ is minimal sufficient for $(\beta_\tau, \sigma)$, then by Basu’s theorem $\widetilde{W}(Y_\theta, \tau)$ is independent of $(I - H_\tau)U \mid (I - H_\tau)U$. Apparently, $A_\theta(U) = \tilde{A}_{\tau}(Y_\theta)$ and $b_\theta(U) = \tilde{b}_{\tau}(Y_\theta)$ are independent. It then follows that $A_{\tau}(Y_\theta)$, $\tilde{b}_{\tau}(Y_\theta)$ and $(I - H_\tau)U \mid (I - H_\tau)U$ are mutually independent. As a result, we conclude that the conditional distribution

$$\{Y_\theta \mid \widetilde{W}(Y_\theta, \tau) = (a_{obs}, b_{obs})\} \sim \left\{a_{obs} + b_{obs} \frac{(I - H_\tau)U}{\|I - H_\tau\|} \right\} \sim Y^*,$$

where $Y^* = \{a_{obs} + b_{obs} \frac{(I - H_\tau)U^*}{\|I - H_\tau\|}\}$ and $U^* \sim U$, is free of $(\beta_\tau, \sigma)$ for any $a_{obs}, b_{obs}$. Then the conditional probability in (14) is free of $(\beta_\tau, \sigma)$, hence the Borel set $B_\alpha(\tau, w)$ defined (15) is also free of $(\beta_\tau, \sigma)$. Moreover, it follows from (15) that

$$P_{Y_\theta|W} \left\{T(Y_\theta, \tau) \in B_\alpha(\tau, w) \mid \widetilde{W}(Y_\theta, \tau) = w \right\}$$

which proves (16). Then following from (16), (17) and Theorem 3,

$$P_{(U_\delta, Y)} \left\{\tau_0 \not\in \tilde{\Gamma}_\alpha(Y) \right\} \leq P_{(U_\delta, Y)} \left\{\tau_0 \not\in \tilde{\Gamma}_\alpha(Y) \right\} + P_{(U_\delta, Y)} \left\{0 \leq \tilde{\Gamma}_\alpha(Y) \right\}$$

$$\leq 1 - \alpha + P_{(U_\delta, Y)} \left\{\tau_0 \not\in S(D) \right\}.$$

Then it follows from Theorem 1 that $P_{(U_\delta, Y)} \left\{\tau_0 \not\in S(D) \right\} = o(e^{-c_1 d})$ for some $c_1 < -\log \left(1 - \frac{n^{\gamma - 1}}{n} \right)$. Therefore $P_{(U_\delta, Y)} \left\{\tau_0 \not\in \tilde{\Gamma}_\alpha(Y) \right\} \leq 1 - \alpha + o(e^{-c_1 d})$. Further let $c_\delta = -\log \left(1 - \frac{n^{\gamma - 1}}{n} \right)$, then by Markov Inequality and Theorem 1

$$P_{(U_\delta)} \left[ P_{Y_\theta|U_\delta} \left\{\tau_0 \not\in S(D) \right\} - \delta \geq e^{-c_1 d} \right] \leq \frac{E_{U_\delta} \left[ P_{Y_\theta|U_\delta} \left\{\tau_0 \not\in S(D) \right\} - \delta \right]}{e^{-c_1 d}}$$

$$\leq \frac{P_{(U_\delta, Y)} \left\{\tau_0 \not\in S(D) \right\} - \delta}{e^{-c_1 d}} = e^{-(c_\delta - c_1)d} \to 0,$$

as $d \to \infty$. The last part of Theorem 4 then follows immediately.

Proof of Theorem 5. Under the conditions in Theorem 2, we make the constant $c_2 > 0$ and

$$c_2 < c_a = \min \left\{ \frac{1}{18 \sigma_0^2} \left( 0.3 C_{min} - 36 \log(p + 1) \right) - \sigma_0^2, \frac{t}{3 \sigma_0^2} d (0.23 - \frac{|\tau_0| \log(p + 2)}{n}) \right\}.$$

Then Theorem 5 follows from (30), Theorem 2 and the following

$$P_{(U_\delta, Y)} \left[ P_{Y_\theta|U_\delta} \left\{\tau_0 \not\in S(D) \right\} \right] \geq C_n e^{-(c_2 n)} \leq \frac{E_{U_\delta} \left[ P_{Y_\theta|U_\delta} \left\{\tau_0 \not\in S(D) \right\} \right]}{e^{-(c_2 n)}}$$

$$= \frac{P_{(U_\delta, Y)} \left\{\tau_0 \not\in S(D) \right\}}{e^{-(c_2 n)}} = e^{-(c_n - c_2)n} \to 0,$$

as $d \to \infty$. The last part of Theorem 4 then follows immediately.
as $n \to \infty$. 

Next, we present the proofs of Theorems 6 and 7, showing the validity of the inference for any subset of regression coefficients, both in finite samples and asymptotically.

5.4. Proofs of Theorems 6 and 7

**Proof of Theorem 6.** We first write

\[
P_Y\{\beta_{0,\Lambda} \not\in \Gamma_{\alpha}^{\beta}(Y)\} = P_Y\{\beta_{0,\Lambda} \not\in \Gamma_{\alpha}^{\beta}(Y), \tau_0 \in S^{(d)}\} + P_Y\{\beta_{0,\Lambda} \not\in \Gamma_{\alpha}^{\beta}(Y), \tau_0 \not\in S^{(d)}\}.
\]

Then let $\eta_{0,\Lambda} = (\tau_0, \beta_{0,\Lambda})$, 

\[
P_Y\{\beta_{0,\Lambda} \not\in \Gamma_{\alpha}^{\beta}(Y), \tau_0 \in S^{(d)}\} \leq P_U\{\tilde{T}(Y, \eta_{0,\Lambda}) \in B_{\eta_{0,\Lambda}}(\alpha)\} = 1 - \alpha.
\]

Therefore, from the above and Theorem 1, 

\[
P_Y\{\beta_{0,\Lambda} \not\in \Gamma_{\alpha}^{\beta}(Y), \tau_0 \not\in S^{(d)}\} \leq P \{\tau_0 \not\in S^{(d)}\} = \delta + o(e^{-c_1d}),
\]

for some $c_1 < -\log \left(1 - \frac{n^{-1}}{n-1}\right)$. Theorem 6 then follows immediately from the above and (31). 

**Proof of Theorem 7.** Define the constant $c_2$ as in (32). It follows from Theorem 2 that 

\[
P_Y\{\beta_{0,\Lambda} \not\in \Gamma_{\alpha}^{\beta}(Y), \tau_0 \not\in S^{(d)}\} \leq P \{\tau_0 \not\in S^{(d)}\} = o(e^{-c_2n}).
\]

Hence Theorem 7 follows from (33), (34), (35) and the above. 

5.5. Proofs of Theorems 8 and 9

**Proof of Theorems 8 and 9.** Since  

\[
\{\tilde{T}(y_{obs}, \eta_\tau) \in B_{\alpha_2}(\eta_\tau), \tau \in \Gamma_{\alpha_1}(y_{obs})\} = \{\tilde{T}(y_{obs}, \eta_\tau) \not\in B_{\alpha_2}(\eta_\tau) \} \cup \{\tau \not\in \Gamma_{\alpha_1}(y_{obs})\},
\]

we have $P(\eta_0 \not\in \Gamma_{\alpha_1}(Y)) \leq P(\tilde{T}(Y, \eta_0) \not\in B_{\alpha_2}(\eta_0)) + P(\tau_0 \not\in \Gamma_{\alpha_1}(Y))$. Then, Theorem 8 follows from the above inequality and Theorem 4 and Theorem 9 follows from the above inequality and Theorem 5. 

6. Discussion

In this article, we develop a repro samples method to solve the inferential problems concerning high-dimensional linear regression models. We propose novel statistical methods and algorithms, with supporting theories, to construct performance-guaranteed confidence sets for the unknown underlying true model, as well as for a single or a subset of regression coefficients. Our work provides a solution to a challenging open problem in the high-dimensional statistics literature: how to infer the true model and quantify model selection uncertainty. Besides, the proposed confidence sets theoretically guarantee the coverage rate in both finite- and large-samples, as opposed to existing literature that usually relies on asymptotic results requiring the sample size to go to infinity. In addition, numerical studies demonstrate that the proposed methods are valid and efficient, and they outperform the existing methods.

The paper contains three technical innovations.

1. We develop a data-driven approach to obtain a efficient model candidate set, which is able to cover the true model with high probability by including just a reasonable number of model candidates. Using this model candidate set effectively addresses the computational
issue since it avoids searching the entire model space. The approach is based on the matching attempt of repro samples with the observed data, leading to the many-to-one mapping function in (5). Specifically, this many-to-one mapping tells us that there always exists a neighbourhood of \( U \), within which a repro copy \( U^* \) can help recover the true model with a high probability. With this insight, we propose a formal procedure and provide supporting theories and numerical evidence, both of which also help to outline trade-offs among sample size, the signal strength, and the performance of the model candidate set.

2. When making inference for the unknown model, we develop a conditional repro samples approach to remove the impact of the nuisance parameters \((\beta, \sigma^2)\). This conditional approach works in general for inference problems beyond the scope of this paper. In particular, let \( \theta_0 = (\nu_0, \xi_0) \), where \( \nu_0 \) and \( \xi_0 \) are interested and nuisance parameters, respectively. If we have a nuclear mapping \( T(U, \theta) \) and a quantity \( W(U, \theta) \), such that the conditional distribution of \( T(U, \theta) \) given \( W(U, \theta) = w \) is free of \( \xi \), then there exists a Borel set \( B_\alpha(\nu, w) \) free of the nuisance \( \xi \) such that \( P(T(U, \theta) \in B_\alpha(\nu, w)|W(U, \theta) = w) \geq \alpha \).

3. We propose confidence sets both for a single and for any subset of regression coefficients. In contrast, existing literature only focus on one aspect of these inference problems. This is because unlike existing approaches, we take a union of intervals or multi-dimensional ellipsoids based on each model in the model candidate set. Thereby, our approach takes into account the uncertainty in model estimation. Not only does it provides the desired coverage, it also produces confidence sets that are sparse and generally smaller than the existing methods, including the debiased approach.

Finally, there are several potential directions for extensions of the work. First, in this paper, we considered the model (2) with the Gaussian error \( U \sim N(0, 1) \). It is possible to extend it to other given distributions or a generalized linear model setting. In these extensions, the conditional approach to handle nuisance regression parameters may not directly apply, but we may use asymptotic arguments to justify their validity and coverage statements. Moreover, another research direction is how to handle weak signals. Even though we do not need any condition on the signal strength, the proposed approaches may demand a large computational cost when weak signals are present. Therefore a natural question is, under limited computational resources, how to adjust the proposed approaches for weak signals. Additionally, the identifiability condition or \( C_{\min} > 0 \) ensures that there is no perfect co-linearity between the true model and an alternative model of equal size. When there is, then multiple equivalent “true” models may exist. The proposed approach is still valid to cover one of these “true” models. Further research, however, is still needed if we would like to have a confident set to cover all of these equivalent “true” models. These topics are outside the scope of the current paper and will be reported in other articles.

7. Acknowledgements The authors wish to thank Professors Cun-Hui Zhang and Zijian Guo for their insightful knowledge and in-depth discussions on the topic of high dimensional regressions, which helped improve the quality of this article. The authors also wish to thank Professor Cun-Hui Zhang for sharing the R code that was used in their seminal paper proposing the debiased method [59].
APPENDIX A: AN ALTERNATIVE FORMULATION IN SECTION 2

In Section 2, we obtain the candidate set by solving the objective function (5). In addition to (5), there is also an almost equivalent form that imposes a constraint on \(|\tau| = \|\beta_r\|_0\) other than adding a regularization term, i.e.

\[
\min \|y_{\text{obs}} - X_r\beta_r - \sigma U^*_b\|_2^2, \quad \text{s.t. } |\tau| \leq k,
\]

where \(k\) is a constraint on the model size, playing a similar role as the \(\lambda\) in (5). One can opt to use (36) in Step 2 of Algorithm 1. Similarly, we can obtain the following results, where Theorem 10, Lemma 5, Lemma 6 and Theorem 11 are counterparts of Theorem 1, Lemma 2, Lemma 3 and Theorem 2 respectively. We provide the proofs of the following theorems and lemmas in Appendix B.

**Theorem 10.** For any \(\delta > 0\), there exists a constant \(\gamma_\delta\) such that under the constraint \(|\tau| \leq |\tau_0|\), the finite-sample probability bound that the true model is not covered by the model candidates set \(S^{(d)}\), obtained by Algorithm 1 with the objective function (36), is as follows,

\[
\mathbb{P}_{(U^*, Y)}(\tau_0 \notin S^{(d)}) \leq \left\{ 1 - \frac{(\gamma_\delta)^{n-1}}{n-1} \right\} + \delta.
\]

Therefore as \(d \to \infty\), \(\mathbb{P}_{(U^*, Y)}(\tau_0 \notin S^{(d)}) \to 0\).

**Lemma 5.** Suppose \(n - |\tau_0| > 4\). Under the constraint \(|\tau| \leq |\tau_0|\), let \(U^*\) be a random repro sample of \(U\), such that \(U^*, U \sim N(0, I_n)\), and

\[
\hat{\tau}_{U^*} = \arg \min_{\{\tau: |\tau| \leq |\tau_0|\}} \left\{ \min_{\beta, \sigma} \|Y - X_r\beta_r - \sigma U^*\|_2^2 \right\}.
\]

Then for any \(0 < \gamma_2 < 1/64\) such that \(C_{\min} > 24\sqrt{\gamma_2} \left( \log(p/2) \frac{n}{n} + \gamma_2 \right) \sigma_0^2\),

\[
\mathbb{P}_{(U, U^*)}\{ \hat{\tau}_{U^*} \neq \tau_0, \rho(U^*, U) > 1 - \gamma_2 \} \leq 3 \exp \left\{ - \frac{n}{12\sigma_0^2} \left[ C_{\min} \sqrt{\gamma_2} - 24 \left( \log(p/2) \frac{n}{n} + \gamma_2 \right) \sigma_0^2 \right] \right\} + 4(64\gamma_2)^{n-|\tau_0|-1}p^{||\tau_0||} + 2\gamma_2^{n-|\tau_0|-1}(\sqrt{n}p)^{|\tau_0|}.
\]

**Lemma 6.** Suppose \(n - |\tau_0| > 4\). Then for any \(0 < \gamma_2 < 1/64\) such that \(C_{\min} > 24\sqrt{\gamma_2} \left( \log(p/2) \frac{n}{n} + \gamma_2 \right) \sigma_0^2\), the finite-sample probability bound that the true model is not covered by the model candidates set \(S^{(d)}\), obtained by Algorithm 1 with the objective function (36), is as follows,

\[
\mathbb{P}_{(U^*, Y)}(\tau_0 \notin S^{(d)}) \leq 3 \exp \left\{ - \frac{n}{12\sigma_0^2} \left[ C_{\min} \sqrt{\gamma_2} - 24 \left( \log(p/2) \frac{n}{n} + \gamma_2 \right) \sigma_0^2 \right] \right\} + 4(64\gamma_2)^{n-|\tau_0|-1}p^{||\tau_0||} + 2\gamma_2^{n-|\tau_0|-1}(\sqrt{n}p)^{|\tau_0|} + \left( 1 - \frac{\gamma_2}{n-1} \right)^d.
\]

**Theorem 11.** Under the constraint \(|\tau| \leq |\tau_0|\), the probability bound that the true model is not covered by the model candidates set \(S^{(d)}\), obtained by Algorithm 1 with the objective
function (36) for any finite $d$ is as follows,

$$\mathbb{P}_{(U^N, Y)}(\tau_0 \not\in S(d)) \leq 6 \exp \left[ - \frac{n}{18\sigma_0^2} \left\{ 0.3C_{\min} - 36 \frac{\log(p)}{n} - \sigma_0^2 \right\} \right]$$

(38)

$$+ \exp \left\{ -\eta d \left( 0.23 - \frac{|\tau_0| \log(p) + 2}{n} \right) \right\}.$$  

Therefore $\mathbb{P}_{(U^N, Y)}(\tau_0 \not\in S(d)) \to 0$ for any $d$ as $n \to \infty$, if $\frac{|\tau_0| \log(p)}{n} < 0.23$ and $C_{\min} > 120 \frac{\log(p+1)}{n} \sigma_0^2$ when $n$ is large enough.

APPENDIX B: TECHNICAL PROOFS

B.1. Proof of Lemma 1

PROOF OF LEMMA 1. By the definition (3), there exist a $\beta_0$ and a $\sigma_0$ such that $X_{\tau_0} \beta_0 = y_{obs} - \sigma_0 u^{rel}$. Since

$$0 \leq \min_{\tau, \beta, \sigma} \| y_{obs} - X_{\tau} \beta - \sigma u^{rel} \|^2 \leq \| y_{obs} - X_{\tau_0} \beta_0 - \sigma_0 u^{rel} \|^2 = 0,$$

it follows that

$$\min_{\tau, \beta, \sigma} \| y_{obs} - X_{\tau} \beta - \sigma u^{rel} \|^2 = 0.$$

Now, let

$$\tilde{\tau}, \beta_{\tilde{\tau}}, \sigma_{\tilde{\tau}} = \arg \min_{\tau, \beta, \sigma} \{ \lambda |\tau| + \| y_{obs} - X_{\tau} \beta - \sigma u^{rel} \|^2 \}.$$  

(39)

We show below that $\| y_{obs} - X_{\tilde{\tau}} \beta_{\tilde{\tau}} - \sigma_{\tilde{\tau}} u^{rel} \|^2 = 0$ using the “proof by contradiction” method.

First, we show that, if $\| y_{obs} - X_{\tilde{\tau}} \beta_{\tilde{\tau}} - \sigma_{\tilde{\tau}} u^{rel} \|^2 \neq 0$, then size of $\tilde{\tau}$ must be smaller than $\tau_0$, i.e. $|\tilde{\tau}| < |\tau_0|$. This is because otherwise if $|\tilde{\tau}| \geq |\tau_0|$, then $\lambda |\tilde{\tau}| + \| y_{obs} - X_{\tau_0} \beta_0 - \sigma_0 u^{rel} \|^2 > \lambda |\tau_0| = \lambda |\tau_0| + \| y_{obs} - X_{\tau_0} \beta_0 - \sigma_0 u^{rel} \|^2$, which contradicts with (39).

Now, with the triplet $(\tilde{\tau}, \beta_{\tilde{\tau}}, \sigma_{\tilde{\tau}})$ defined in (39) and $|\tilde{\tau}| < |\tau_0| < n$, we have for the given $\tilde{\tau}$,

$$\| y_{obs} - X_{\tilde{\tau}} \beta_{\tilde{\tau}} - \sigma_{\tilde{\tau}} u^{rel} \|^2 \geq \| (I - H_{\tilde{\tau}, u^{rel}}) Y_{obs} \|,$$

where $H_{\tilde{\tau}, u^{rel}} = X_{\tilde{\tau}, u^{rel}} (X_{\tilde{\tau}, u^{rel}}^T X_{\tilde{\tau}, u^{rel}})^{-1} X_{\tilde{\tau}, u^{rel}}^T$ with $X_{\tilde{\tau}, u^{rel}} = (X_{\tilde{\tau}}, u^{rel})$ is the projection matrix to the space expanded by $X_{\tilde{\tau}}$ and $u^{rel}$. It follows that

$$\| y_{obs} - X_{\tilde{\tau}} \beta_{\tilde{\tau}} - \sigma_{\tilde{\tau}} u^{rel} \|^2 \geq \| (I - H_{\tilde{\tau}, u^{rel}}) Y_{obs} \| = \| (I - H_{\tilde{\tau}, u^{rel}}) X_0 \beta_0 \|,$$

where the equality holds because $u^{rel}$ is orthogonal to $(I - H_{\tilde{\tau}, u^{rel}})$.

By (40), the definitions of $\gamma_{(u^{rel}, \tau_0)}^2$ and $C_{\min}$, and under the condition that $0 < \lambda \leq n \left\{ 1 - \gamma_{(u^{rel}, \tau_0)}^2 \right\} C_{\min},$

$$\| y_{obs} - X_{\tilde{\tau}} \beta_{\tilde{\tau}} - \sigma_{\tilde{\tau}} u^{rel} \|^2 + \lambda |\tilde{\tau}| \geq \| (I - H_{\tilde{\tau}, u^{rel}}) X_0 \beta_0 \|^2 + \lambda |\tilde{\tau}|$$

$$\geq \left\{ 1 - \gamma_{(u^{rel}, \tau_0)}^2 \right\} \| (I - H_{\tilde{\tau}}) X_0 \beta_0 \|^2 + \lambda |\tilde{\tau}|$$

$$\geq \left\{ 1 - \gamma_{(u^{rel}, \tau_0)}^2 \right\} n |\tau_0| \setminus \tilde{\tau} \{ C_{\min} + \lambda |\tau_0| - \lambda |\tau_0| \setminus \tilde{\tau} \}$$

$$\geq \lambda |\tau_0| = \lambda |\tau_0| + \| y_{obs} - X_{\tau_0} \beta_0 - \sigma_0 u^{rel} \|^2,$$

which contradicts with (39). Thus, $\| y_{obs} - X_{\tilde{\tau}} \beta_{\tilde{\tau}} - \sigma_{\tilde{\tau}} u^{rel} \|^2 \neq 0$ does not hold and we only have $\| y_{obs} - X_{\tilde{\tau}} \beta_{\tilde{\tau}} - \sigma_{\tilde{\tau}} u^{rel} \|^2 = 0$. Because $u^{rel} \not\in \text{span}(X_0, X_{\tau_0})$ for any $\tau$ with $|\tau| \leq |\tau_0|$, by definition (3), we have $\tilde{\tau} = \tau_0$ and thus the conclusion of the lemma follows.
B.2. Proof of Lemma 2 and Lemma 5  

Before we proceed to the proofs of Lemma 2 and Lemma 5, we first provide a few technical lemmas that can facilitate the proofs.

**Lemma 7.** For any \( \tau \) and \( u^* \),

\[
I - H_{\tau, u^*} = I - H_{\tau} - O_{\tau^+, u^*},
\]

where \( H_{\tau, u^*} = (X_{\tau} u^*) \left( \begin{array}{c} X_{\tau}^T X_{\tau} X_{\tau}^T u^* \\ (u^*)^T X_{\tau} (u^*)^T u^* \end{array} \right)^{-1} \left( \begin{array}{c} X_{\tau}^T u^* \\ (u^*)^T \end{array} \right) \) is the projection matrix on the space spanned by \( (X_{\tau} u^*) \) and \( O_{\tau^+, u^*} = \frac{(I - H_{\tau}) u^* (u^*)^T (I - H_{\tau})}{(u^*)^T (I - H_{\tau}) u^*} \) is the projection matrix on the space spanned by \( (I - H_{\tau}) u^* \).

**Proof.** By a direct calculation, we have

\[
I - H_{\tau, u^*} = I - (X_{\tau} u^*) \left( \begin{array}{c} X_{\tau}^T X_{\tau} X_{\tau}^T u^* \\ (u^*)^T X_{\tau} (u^*)^T u^* \end{array} \right)^{-1} \left( \begin{array}{c} X_{\tau}^T u^* \\ (u^*)^T \end{array} \right) - \frac{(X_{\tau}^T X_{\tau})^{-1} X_{\tau}^T u^*}{(u^*)^T (I - H_{\tau}) u^*} \frac{1}{(u^*)^T (I - H_{\tau}) u^*} \left( \begin{array}{c} X_{\tau}^T u^* \\ (u^*)^T \end{array} \right) = I - (X_{\tau} u^*) \left( \begin{array}{c} X_{\tau}^T X_{\tau} X_{\tau}^T u^* \\ (u^*)^T X_{\tau} (u^*)^T u^* \end{array} \right)^{-1} \left( \begin{array}{c} X_{\tau}^T u^* \\ (u^*)^T \end{array} \right) + \frac{X_{\tau}^T X_{\tau} X_{\tau}^T u^*}{(u^*)^T (I - H_{\tau}) u^*} - \frac{u^* (u^*)^T}{(u^*)^T (I - H_{\tau}) u^*} \frac{(I - H_{\tau})}{(u^*)^T (I - H_{\tau}) u^*} \]

Let \( \rho(v_1, v_2) = \cos^2(\theta) \) be the square of the cosine of the angle between any two \( n \times 1 \) vectors \( v_1 \) and \( v_2 \). Further, for any given \( \tau \), let \( \rho_{\tau^+} (v_1, v_2) = \rho \{ (I - H_\tau) v_1, (I - H_\tau) v_2 \} \) be the cosine of the angle between \( (I - H_\tau) v_1 \) and \( (I - H_\tau) v_2 \).

**Lemma 8.** Suppose \( |\tau| < n \). For any \( -1 \leq \gamma_1, \gamma_2 \leq 1 \), if \( U^* \sim U \sim N(0, I) \),

\[
P_{U^*} \{ \rho_{\tau^+} (U^*, X_0 \beta_0) < \gamma_1 \} = P_{U} \{ \rho_{\tau^+} (U, X_0 \beta_0) < \gamma_2^2 \} > 1 - 2 \{ \arccos(\gamma_1) \}^{n-|\tau|-1},
\]

and

\[
P_{(U^*, U)} \{ \rho(U^*, U) > 1 - \gamma_2^2 \} > \frac{\gamma_2^{n-1}}{n}.
\]

Further more \( \rho_{\tau^+} (U^*, X_0 \beta_0) \) and \( \rho(U^*, U) \) are independent.

**Proof.** Let \( (I - H_\tau) = \sum_{i=1}^{n-|\tau|} D_i D_i^\top \) be the eigen decomposition of \( (I - H_\tau) \). Denote by \( Z_i = D_i \) and \( w_i = D_i X_0 \beta_0 \), for \( i = 1, \ldots, n - |\tau| \). It follows that \( Z_1, \ldots, Z_{n-|\tau|} \) are independent.
i.i.d $N(0, 1)$ and
\[
\mathbb{P}_{U^*} \{ \rho_{\tau^+}(U^*, X_0^{\beta_0}) < \gamma^n_2 \} = \mathbb{P}_{U} \{ \rho_{\tau^+}(U, X_0^{\beta_0}) < \gamma^n_2 \}
\]
\[
= \mathbb{P}_{U} \left\{ \sum_{i=1}^{n-|\tau|} w_i Z_i \right\} \sqrt{\sum_{i=1}^{n-|\tau|} w_i^2 / \sum_{i=1}^{n-|\tau|} Z_i^2} < \gamma^n_1 \}
\]
\[
= \mathbb{P}_{U} \{ \cos(\varphi) < \gamma^n_1 \},
\]
where $\varphi = \varphi(U)$ (or $\pi - \varphi$) is the angle between $(Z_1, \ldots, Z_{n-|\tau|})$ and $(w_1, \ldots, w_{n-|\tau|})$ for $0 \leq \varphi \leq \pi$.

We transform the co-ordinates of $Z_1, \ldots, Z_{n-|\tau|}$ into sphere co-ordinates, with $\varphi$ as the first angle coordinate. It follows from the Jacobian of the spherical transformation the density function of $\varphi$

\[
f(\varphi) = \sin^{n-|\tau|-2}(\varphi)/c, \quad 0 \leq \varphi \leq \pi,
\]
where $c = \int_0^\pi \sin^{n-|\tau|-2}(\varphi) d\varphi = 2 \int_0^{\pi/2} \sin^{n-|\tau|-2}(\varphi) d\varphi$ is is the normalizing constant.

Note that, for $0 < \varphi < \pi/2$, we have

\[
\frac{2}{\pi} \varphi < \sin(\varphi) < \min\{\varphi, 1\} = \varphi 1_{(0 < \varphi < 1)} + 1_{(1 \leq \varphi < \pi/2)},
\]
where $1_{(\cdot)}$ is an indicator function. It follows that

\[
\frac{\pi}{2(n - |\tau| - 1)} < c < \frac{1}{n - |\tau| - 1} + \left(\frac{\pi}{2} - 1\right) < 2.
\]

Therefore, we have

\[
\mathbb{P}_{U} \{ \cos(\varphi) < \gamma^n_1 \} = \frac{2}{c} \int_{\arccos(\gamma^n_1)}^{\pi/2} \sin^{n-|\tau|-2}(s) ds = 1 - \frac{2}{c} \int_0^{\arccos(\gamma^n_1)} \sin^{n-|\tau|-2}(s) ds
\]
\[
> 1 - \frac{2(n - |\tau| - 1) \int_{\arccos(\gamma^n_1)}^{\pi/2} \sin^{n-|\tau|-2}(s) ds}{\pi} = 1 - 2\{\arccos(\gamma^n_1)\}^{n-|\tau|-1}.
\]

Next conditioning on $U^* = u^*$, with similar procedure as above but replacing $n - |\tau|$ with $n$, we can show that

\[
\mathbb{P}_{U} \{ \| (u^*)^T U \| / (\| u^* \| \| U \| ) > \sqrt{1 - \gamma^n_2} \left\| u^* \right\| \} = \mathbb{P}_{U} \{ \cos(\psi) > \sqrt{1 - \gamma^n_2} \left\| u^* \right\| \}
\]
\[
(41) \quad = \frac{2}{c_1} \int_0^{\arcsin \gamma_2} \sin^{n-2}(s) ds
\]
\[
> \frac{2}{c_1} \int_0^{\arcsin \gamma_2} \left( \frac{s \gamma_2}{\arcsin \gamma_2} \right)^{n-2} ds > \frac{\gamma_2^{n-2} \arcsin \gamma_2}{n - 1},
\]
where $\psi = \psi(u^*, u)$ (or $\pi - \psi$) is the angle between $u$ and $u^*$ and the normalizing constant $c_1 = \int_0^\pi \sin^{n-2}(\psi) d\psi = 2 \int_0^{\pi/2} \sin^{n-2}(\psi) d\psi$. The same derivation works when the conditional is on $U = u$:

\[
\mathbb{P}_{U^*} \{ \| U^*^T u \| / (\| U^* \| \| u \| ) > \sqrt{1 - \gamma^n_2} \left\| u \right\| \} = \mathbb{P}_{U} \{ \cos(\psi) > \sqrt{1 - \gamma^n_2} \left\| u \right\| \}
\]
\[
(42) \quad = \frac{2}{c_1} \int_0^{\arcsin \gamma_2} \sin^{n-2}(s) ds > \frac{\gamma_2^{n-2} \arcsin \gamma_2}{n - 1},
\]
Because (41) and (42) do not involve \( u^* \) or \( u \), we have
\[
\mathbb{P}(u^*, u) \{ \rho(u^*, u) > 1 - \gamma_2^2 \} = \mathbb{P}_\epsilon \left\{ \rho(u^*, u) > 1 - \gamma_2^2 \right\} \]
\[
= \mathbb{P}_U \left\{ \rho(u^*, u) > 1 - \gamma_2^2 \right\} > \frac{\gamma_2^{n-2} \arcsin \gamma_2}{n-1}.
\]
The above statement also suggests that \( \rho(u^*, u) \) and \( u^* \) are independent, therefore
\[
\rho(u^*, u) \text{ and } \rho_{\tau^*}(u^*, X_0\beta_0) \text{ are independent.}
\]

**Lemma 9.** Let
\[
E(\gamma_1, \gamma_2) = \left\{ \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^*}(u^*, X_0\beta_0) < \gamma_2^2, \rho(u^*, u) > 1 - \gamma_2^2 \right\},
\]
for any \( 0 < \gamma_1, \gamma_2 < 1 \) and \( \rho(u, \tau) = \frac{\|H_r u\|^2}{\|u\|^2} \). Then
\[
\left\{ \rho(u^*, u) > 1 - \gamma_2^2, \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^*}(u^*, X_0\beta_0) < \gamma_2^2, \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho(u, \tau) < 1 - \gamma_2 \right\}
\]
\[
\subseteq E(\gamma_1, \gamma_2),
\]
where \( \gamma_1 = (1 - \sqrt{2} - \gamma_2^2) \).

**Proof of Lemma 9.** Denote by \( g_r(U) = \frac{\|I-H_r\|}{\|U\|} \) and \( g_r(U^*) = \frac{\|I-H_r\|}{\|U^*\|} \). For each \( U^* \), given \( \{ U \in \cap_{\{\tau; |\tau| \leq |\tau_0|\}} A(\gamma_1^2, \tau) \} \), we have
\[
\frac{1}{\|I-H_r\|U^*\|(U^*)^\top(I-H_r)X_0\beta_0}
\]
\[
= \frac{1}{\|U\|} U^\top(I-H_r)X_0\beta_0 + (\frac{(U^*)^\top/\|U^*\|-U^\top/\|U\|}{\|I-H_r\|})(I-H_r)X_0\beta_0
\]
\[
+ \left( \frac{1}{\|I-H_r\|U^*\|} - \frac{1}{\|U^*\|} \right) (U^*)^\top(I-H_r)X_0\beta_0
\]
\[
\leq \frac{\|I-H_r\|U}{\|U\|} + \frac{1}{\|I-H_r\|U\|} U^\top(I-H_r)X_0\beta_0 + \frac{\|U^*\|}{\|U^*\|} U^\top(I-H_r)X_0\beta_0
\]
\[
+ \frac{\|U^*\|}{\|U^*\|} (U^*)^\top(I-H_r)X_0\beta_0
\]
\[
\leq g_r(U) \gamma_1 \|I-H_r\|X_0\beta_0 + \sqrt{2 - 2 \frac{(U^*)^\top U}{\|U^*\|^2}\|I-H_r\|X_0\beta_0}
\]
\[
+ (1 - g_r(U)) \frac{1}{\|I-H_r\|U^*\|} (U^*)^\top(I-H_r)X_0\beta_0
\]
\[
\leq g_r(U) \gamma_1 \|I-H_r\|X_0\beta_0 + \sqrt{2 - 2 \sqrt{1 - \gamma_2^2}} \|I-H_r\|X_0\beta_0
\]
\[
+ (1 - g_r(U)) \frac{1}{\|I-H_r\|U^*\|} (U^*)^\top(I-H_r)X_0\beta_0.
It then follows that
\[
\frac{1}{\| (I - H_r) U \|^2} (U^*)^\top (I - H_r) X_0 \beta_0 \\
\leq \frac{g_T(U)}{g_T(U^*)} \gamma_1 \| (I - H_r) X_0 \beta_0 \| + \frac{1}{g_T(U^*)} \sqrt{2 - 2 \sqrt{1 - \gamma_2^2}} \| (I - H_r) X_0 \beta_0 \|
\]

Further because \( \| (I - H_T) U^* \| \leq \| (I - H_T U) U^* \| \), if \((U^*, U) \in B(\gamma_2)\) we have
\[
g_T(U^*) \leq \frac{\| (I - P_U) U^* \| + \| (P_U - H_T P_U) U^* \|}{\| U^* \|} \\
\leq \gamma_2 + \frac{\| (I - H_T) P_U U^* \|}{\| P_U U^* \|} = \gamma_2 + g_T(U).
\]

Similarly, we can show that \( g_T(U) \leq g_T(U^*) + \gamma_2 \). Then
\[
\frac{g_T(U^*)}{g_T(U)} \geq 1 - \frac{\gamma_2}{g_T(U)}.
\]

It then follows that a sufficient condition for \( \| (I - H_T) U \|^2 (U^*)^\top (I - H_r) X_0 \beta_0 \leq \gamma_1 \) is
\[
\gamma_1 \leq \left( 1 - \frac{\gamma_2}{g_T(U)} \right) \gamma_1 - \sqrt{2 - 2 \sqrt{1 - \gamma_2^2}} \leq \frac{g_T(U^*)}{g_T(U)} \gamma_1 - \sqrt{2 - 2 \sqrt{1 - \gamma_2^2}}
\]

Because it follows from \( \rho(U, \tau) < 1 - \gamma_2 \) that \( g_T(U) = \sqrt{1 - \rho^2(U, \tau)} > \sqrt{\gamma_2}, \) the above holds for \( \gamma_1 = (1 - \sqrt{\gamma_2}) \gamma_1 - \sqrt{2 - 2 \sqrt{1 - \gamma_2^2}}. \) Therefore
\[
\{ \rho(U^*, U) > 1 - \gamma_2^2 \} \cap \left\{ \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_T(U^*, X_0 \beta_0) < \gamma_1^2, \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho(U, \tau) < 1 - \gamma_2 \right\} \\
\subset E(\gamma_1, \gamma_2).
\]

**Lemma 10.** Suppose \( n - |\tau_0| > 4 \). For any \( 0 < \tilde{\gamma}_1, \gamma_2 < 1 \),
\[
\mathbb{P} \left( U \notin \left\{ \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_T(U^*, X_0 \beta_0) < \gamma_1^2, \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho(U, \tau) < 1 - \gamma_2 \right\} \right) \\
\leq \mathbb{P} \left( \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_T(U, X_0 \beta_0) \geq \gamma_1^2 \right) + \mathbb{P} \left( \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho(U, \tau) \geq 1 - \gamma_2 \right) \\
\leq 4(\arccos \tilde{\gamma}_1)^{n - |\tau_0| - 1} |\tau|^{\rho} + 2 \gamma_2 \frac{n - |\tau_0| - 1}{2} (\sqrt{n})^{-1}.
\]

**Proof of Lemma 10.** Let \( g_T^2(u) = \| (I - H_r) u \|^2 = \frac{\| (I - H_r) u \|^2}{\| (I - H_r) u \|^2 + \| H_r u \|^2} \), then if \( n - |\tau| > 4 \) and \( \gamma_2 < 0.6 \),
\[
\mathbb{P}_U(\rho(U, \tau) \geq 1 - \gamma_2) = \mathbb{P}_U(g_T(U) > \sqrt{\gamma_2}) = \mathbb{P}_U \left( \frac{\| (I - H_T) U \|^2}{\| H_T U \|^2} > \frac{\gamma_2}{1 - \gamma_2} \right) \\
= 1 - F_{n - |\tau|, |\tau|} \left( \frac{\gamma_2/(n - |\tau|)}{(1 - \gamma_2)/|\tau|} \right) \geq 1 - \left( \frac{n - |\tau|}{2} \right)^{|\tau|} 2^{\frac{n - |\tau| - 1}{2}}.
\]
The last inequality holds because when \( n - |\tau| > 4 \) and \( \gamma_2 < 0.6 \),

\[
F_{n - |\tau|, |\tau|} \left( \frac{\gamma_2 / (n - |\tau|)}{(1 - \gamma_2) / |\tau|} \right) = \frac{\int_0^\gamma_2 t^{n - |\tau| - 1} (1 - t)^{\frac{|\tau|}{2} - 1} dt}{B \left( \frac{n - |\tau|}{2}, \frac{|\tau|}{2} \right)} \leq \frac{\gamma_2^{n - |\tau| - 1}}{B \left( \frac{n - |\tau|}{2}, \frac{|\tau|}{2} \right)},
\]

where \( B \left( \frac{n - |\tau|}{2}, \frac{|\tau|}{2} \right) \) is the beta function and

\[
B \left( \frac{n - |\tau|}{2}, \frac{|\tau|}{2} \right) \geq \left( \frac{n - |\tau|}{2} \right)^{-\frac{|\tau|}{2}}.
\]

Therefore it follows from the above, Lemma 8 and Lemma 9 that

\[
\Pr \left( U \notin \left\{ \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau \perp \tau_0} (U, X_0 \beta_0) < \tilde{\gamma}_1^2, \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho(U, \tau) < 1 - \gamma_2 \right\} \right) \leq \Pr \left( \max_{|\tau| \leq |\tau_0|} \rho_{\tau \perp \tau_0} (U, X_0 \beta_0) \geq \tilde{\gamma}_1^2 \right) + \Pr \left( \max_{|\tau| \leq |\tau_0|} \rho(U, \tau) \geq 1 - \gamma_2 \right) \\
\leq \sum_{|\tau| = 1}^{|\tau_0|} \left( \frac{p}{|\tau|} \right) \left\{ 2(\arccos \tilde{\gamma}_1)^{n - |\tau| - 1} + \left( \frac{n - |\tau|}{2} \right)^{\frac{|\tau|}{2}} \frac{n - |\tau| - 1}{\gamma_2^{n - |\tau| - 1}} \right\} \\
\leq \sum_{|\tau| = 1}^{|\tau_0|} p|\tau| \left\{ 2(\arccos \tilde{\gamma}_1)^{n - |\tau| - 1} + \left( \frac{n - |\tau|}{2} \right)^{\frac{|\tau|}{2}} \frac{n - |\tau| - 1}{\gamma_2^{n - |\tau| - 1}} \right\} \\
\leq 2(\arccos \tilde{\gamma}_1)^{n - |\tau_0| - 1} p|^\tau_0| \sum_{k=0}^{n - |\tau_0| - 1} \left( \frac{\arccos \tilde{\gamma}_1}{p} \right)^k + \gamma_2^{n - |\tau_0| - 1} \left( \sqrt{np} \right)^{|\tau_0|} \sum_{k=0}^{n - |\tau_0| - 1} \left( \frac{\gamma_2}{np} \right)^{k/2} \\
\leq 4(\arccos \tilde{\gamma}_1)^{n - |\tau_0| - 1} p|^\tau_0| + 2\gamma_2^{n - |\tau_0| - 1} \left( \sqrt{np} \right)^{|\tau_0|}.
\]

\[\square\]

**Proof of Lemma 5.** For a fixed \( \tau \), let

\[
D(\tau, u^*) = \min_{\beta_\tau, \sigma} \| Y - X_\tau \beta_\tau - \sigma u^* \|_2^2 = \| (I - H_{\tau, u^*}) Y \|_2^2,
\]

where \( Y = X_0 \beta_0 + \sigma_0 U \) is a random sample from the true model (2) with the error term \( U \sim N(0, I_n) \), and \( H_{\tau, u^*} \) is the projection matrix for \( (X_\tau, u^*) \).

Define

\[
\hat{\tau}_{u^*} = \arg \min_{\{\tau \} : |\tau| \leq |\tau_0|} D(\tau, u^*).
\]

By (36) with constraint \( |\tau| = \| \beta_\tau \|_0 \leq |\tau_0| \), if there exists a \( \tau \) with \( |\tau| \leq |\tau_0| \), such that \( \{ D(\tau, u^*) - D(\tau_0, u^*) < 0 \} \), then \( \{ \hat{\tau}_{u^*} \neq \tau_0 \} \). On the other hand, if \( \{ \hat{\tau}_{u^*} \neq \tau_0 \} \), then \( D(\hat{\tau}_{u^*}, u^*) - D(\tau_0, u^*) \leq 0 \). Thus, \( \{ \hat{\tau}_{u^*} \neq \tau_0 \} \) \( \{ D(\tau, u^*) - D(\tau_0, u^*) < 0 \} \) \( \{ \hat{\tau}_{u^*} \neq \tau_0 \} \).

For each \( Y \),

\[
D(\tau, u^*) - D(\tau_0, u^*) = \| (I - H_{\tau, u^*}) Y \|_2^2 - \| (I - H_{\tau_0, u^*}) Y \|_2^2 \\
= \| (I - H_{\tau, u^*})(X_0 \beta_0 + \sigma_0 U) \|_2^2 - \sigma_0^2 \| (I - H_{\tau_0, u^*}) U \|_2^2 \\
= \| (I - H_{\tau_0, u^*}) X_0 \beta_0 \|_2^2 + 2\sigma_0 U^T (I - H_{\tau, u^*}) X_0 \beta_0 - \sigma_0^2 U^T (H_{\tau, u^*} - H_{\tau_0, u^*}) U.
\]
Now, define an event set

\[(44) \quad E(\gamma_1, \gamma_2) = \left\{ (u^*, u) : \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^+}(u^*, X_0\beta_0) < \gamma_1^2, \rho(u^*, u) > 1 - \gamma_2^2 \right\}, \]

we have, for any \( \delta \in (0, 1), \)

\[
P_{(U^*, U)} \{ D(\tau, U^*) - D(\tau_0, U^*) < 0, (U^*, U) \in E(\gamma_1, \gamma_2) \}
\leq P_{(U^*, U)} \left\{ (1 - \gamma_1^2) \| (I - H_\tau) X_0\beta_0 \|^2 - \sigma_0^2 U^T (H_\tau U^* - H_{\tau_0} U^*) U \right.
\]

\[
+ 2\sigma_0 U^T (I - H_\tau U^*) X_0\beta_0 < 0, (U^*, U) \in E(\gamma_1, \gamma_2) \}
\leq P_{(U^*, U)} \left\{ (1 - \gamma_1^2) (1 - \delta) \| (I - H_\tau) X_0\beta_0 \|^2 \right.
\]

\[
- \sigma_0^2 U^T (H_\tau U^* - H_{\tau_0} U^*) U < 0, (U^*, U) \in E(\gamma_1, \gamma_2) \}
\leq P_{(U^*, U)} \left\{ (1 - \gamma_1^2) \delta \| (I - H_\tau) X_0\beta_0 \|^2 \right.
\]

\[
+ 2\sigma_0 U^T (I - H_\tau U^*) X_0\beta_0 < 0, (U^*, U) \in E(\gamma_1, \gamma_2) \}
= (I_1) + (I_2).

To derive an upper bound for \((I_1), \) we note that, by Lemma 7, for any \((U^*, U)\) that satisfies

\[
\rho(U^*, U) > 1 - \gamma_2^2,
\]

\[
U^T (H_\tau U^* - H_{\tau_0} U^*) U = U^T (I - H_\tau U^*) U - U^T (I - H_{\tau_0} U^*) U \leq U^T (I - H_{\tau_0} U^*) U
\]

\[
= \| (I - H_{\tau_0} - O_{\tau_0^+ U^*}) U \|^2 = \| (I - H_{\tau_0}) (I - O_{\tau_0^+ U^*}) U \|^2
\leq \| (I - H_{\tau_0}) (I - H_U U^*) U \|^2 \leq \| (I - H_U U^*) U \|^2 \leq \| U \|^2,
\]

where \(O_{\tau_0^+ U^*}\) is the projection matrix of \((I - H_{\tau_0}) U^*\) and the first inequality follows from the definition of projection. It follows from the definition of \(C_{\min}\) that,

\[
(I_1) < P_{(U^*, U)} \left\{ \| U \|^2 > \frac{(1 - \gamma_1^2) (1 - \delta)}{\gamma_2^2} \| (I - H_\tau) X_0\beta_0 \|^2 \right\}, (U^*, U) \in E(\gamma_1, \gamma_2) \}
\]

\[
< P_{(U^*, U)} \left\{ \| U \|^2 > \frac{(1 - \gamma_1^2) (1 - \delta)}{\gamma_2^2} \| (I - H_\tau) X_0\beta_0 \|^2 \right\}
\leq P_{\chi^2_n} \left\{ \frac{(1 - \gamma_1^2) (1 - \delta) n \| \tau_0 \| \tau |C_{\min}|}{\gamma_2^2 \sigma_0^2} \right\}
\leq \exp \left\{ -\frac{n}{2} \log(1 - 2t_1) - t_1 \frac{(1 - \gamma_1^2) (1 - \delta) n \| \tau_0 \| \tau |C_{\min}|}{\gamma_2^2 \sigma_0^2} \right\},
\]

for any \(0 < t_1 < 1/2,\) where \(\chi^2_n\) is a random variable that follows \(\chi^2\) distribution. The last inequality is derived from Markov inequality and moment generating function of chi-square distribution.

For \((I_2),\) we note that, for any \((U^*, U)\) such that \(\rho(U^*, U) > 1 - \gamma_2^2, \| (I - H_\tau - O_{\tau_0^+ U^*}) U \|^2 = \| (I - H_\tau)(I - O_{\tau_0^+ U^*}) U \|^2 \leq \| (I - H_\tau)(I - H_U U^*) U \|^2 \leq \| (I - H_U U^*) U \|^2 \leq \gamma_2^2 \| U \|^2.\)
Therefore, 
\[
(I_2) \leq \mathbb{P}(U^* U) \left\{ \frac{(1 - \gamma_1^2)\delta}{\sigma_0^2} \| (I - H_r) X_0 \beta_0 \| < 2\sigma_0 \| U^* (I - H_r) X_0 \beta_0 \|, (U^*, U) \in \mathcal{E}(\gamma_1, \gamma_2) \right\}
\]
\[
\leq \mathbb{P}(U^* U) \left\{ \frac{(1 - \gamma_1^2)\delta}{\sigma_0^2} \| (I - H_r) X_0 \beta_0 \| < 2\sigma_0 |\gamma_2| \| (I - H_r) X_0 \beta_0 \|, (U^*, U) \in \mathcal{E}(\gamma_1, \gamma_2) \right\}
\]
\[
= \mathbb{P}(U^* U) \left\{ \frac{n}{\sqrt{(1 - \gamma_1^2)\delta^2}} \frac{n |\tau| C_{\text{min}}}{\sigma_0^2} \right\}
\]
\[
\leq \exp \left\{ -\frac{n}{2} \log(1 - 2t_2) - t_2 \frac{(1 - \gamma_1^2)\delta^2}{\sigma_0^2} \right\},
\]
for any \(0 < t_2 < 1/2\).

Now, by making of \((1 - \gamma_1^2)(1 - \delta) = (1 - \gamma_1^2)\delta^2/4\), we obtain \(\delta = \frac{2}{1 - \gamma_1^2}(\sqrt{2 - \gamma_1^2} - 1)\). Further we make \(t_1 = t_2 = \frac{\gamma_2}{2\varrho_1^2}\), so we have \(-\frac{n}{2} \log(1 - 2t_1) = -\frac{n}{2} \log(1 - 2t_2) = -\frac{n}{2} \log(1 - \frac{\gamma_2}{2\varrho_1^2}) \leq 2n\gamma_2\). Then, intersect with the event \(\{(U^*, U) \in \mathcal{E}(\gamma_1, \gamma_2)\}\), we have
\[
\mathbb{P}(U^* U) \{ \tilde{\tau} U \neq \tau_0, (U^*, U) \in \mathcal{E}(\gamma_1, \gamma_2) \}
\]
\[
< \sum_{i=1}^{\lfloor |\tau_0| \rfloor} \sum_{j=0}^i \frac{p - |\tau_0|}{j} \frac{|\tau_0|}{i} \exp \left\{ -\left( \sqrt{2 - \gamma_1^2} - 1 \right)^2 \frac{n i C_{\text{min}}}{2.04 \gamma_2 \sigma_0^2} + 2n\gamma_2 \right\}
\]
\[
< \sum_{i=1}^{\lfloor |\tau_0| \rfloor} \sum_{j=0}^i \frac{p - |\tau_0|}{j} \frac{|\tau_0|}{i} \exp \left\{ -\frac{i C_{\text{min}}}{12 \sigma_0^2} \left( \frac{1 - \gamma_1^2}{\gamma_2} \right)^2 + 2n\gamma_2 \right\}.
\]
The last inequality holds since \((\sqrt{2 - \gamma_1^2} - 1)^2 \geq 1.02 (1 - \gamma_1^2)^2/6\) for \(\gamma_1^2 \in (0, 1)\). Since \(\binom{a}{b} \leq a^b \text{ and } \log(p - |\tau_0|) + \log(|\tau_0|) \leq \log(p/4) = 2\log(p/2)\), it follows
\[
\mathbb{P}(U^* U) \{ \tilde{\tau} U \neq \tau_0, (U^*, U) \in \mathcal{E}(\gamma_1, \gamma_2) \}
\]
\[
< \sum_{i=1}^{\lfloor |\tau_0| \rfloor} \frac{p - |\tau_0|}{i} \exp \left\{ -\frac{i C_{\text{min}}}{12 \sigma_0^2} \left( \frac{1 - \gamma_1^2}{\gamma_2} \right)^2 + 2n\gamma_2 \right\}
\]
\[
< 2 \sum_{i=1}^{\lfloor |\tau_0| \rfloor} \exp \left\{ -\frac{i C_{\text{min}}}{12 \sigma_0^2} \left( \frac{1 - \gamma_1^2}{\gamma_2} \right)^2 + 2\log(p/2) \right\}
\]
\[
< \exp \left\{ -\frac{i C_{\text{min}}}{12 \sigma_0^2} \left( \frac{1 - \gamma_1^2}{\gamma_2} \right)^2 + 2\log(p/2) \right\}.
\]
(45) \[ < 3 \exp \left\{ \frac{n}{12 \sigma_0^2} \left[ \frac{(1 - \gamma_1^2)^2}{\gamma_2} C_{\min} - 24 \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2 \right] \right\} = L_0(\gamma_1, \gamma_2), \]

since \( \frac{(1 - \gamma_1^2)^2}{\gamma_2} C_{\min} - 24 \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2 > 0. \) The last inequality holds because

\[ \mathbb{P}(U^*, U) \{ \hat{\tau} U^* \neq \tau_0, (U^*, U) \in E(\gamma_1, \gamma_2) \} \]
\[ \leq [2 + \mathbb{P}(U^*, U) \{ \hat{\tau} U^* \neq \tau_0, (U^*, U) \in E(\gamma_1, \gamma_2) \}] \]
\[ \leq \exp \left\{ -n \left[ \frac{C_{\min} (1 - \gamma_1^2)^2}{\gamma_2} \frac{2 \log(p/2)}{n} - 2 \gamma_2 \right] \right\} \]
\[ \leq 3 \exp \left\{ -n \left[ \frac{C_{\min} (1 - \gamma_1^2)^2}{\gamma_2} \frac{2 \log(p/2)}{n} - 2 \gamma_2 \right] \right\}. \]

It then follows from Lemma 9 and Lemma 10 that

\[ \mathbb{P}(U^*, U) (\hat{\tau} U^* \neq \tau_0, \rho(U^*, U) > 1 - \gamma_2) \]
\[ \leq \mathbb{P}(U^*, U) \{ \hat{\tau} U^* \neq \tau_0, (U^*, U) \in E(\gamma_1, \gamma_2) \} + \mathbb{P} \left( \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho(\tau, U, \tau_0 \beta_0) \geq \tilde{\gamma}_1 \right) \]
\[ + \mathbb{P} \left( \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho(U, \tau) \geq 1 - \gamma_2 \right) \]
\[ \leq 3 \exp \left\{ -n \left[ \frac{C_{\min} (1 - \gamma_1^2)^2}{\gamma_2} \frac{2 \log(p/2)}{n} - 2 \gamma_2 \right] \right\} \]
\[ + 4(\arccos(1 - \gamma_1) - |\tau_0| - 1) \frac{(\sqrt{n})^{|\tau_0|}}{n} \]
\[ + 2 \gamma_2 n^{-|\tau_0| - 1} \frac{1}{(\sqrt{n})^{|\tau_0|}}. \]

We then make \( \gamma_1 = \sqrt{1 - \gamma_2^{1/4}} \), from which we have \( \tilde{\gamma}_1 = (1 - \sqrt{\gamma_2}) \sqrt{1 - \gamma_2^{1/4}} - \sqrt{2 - 2\sqrt{1 - \gamma_2^2}} \geq 1 - 1.6 \gamma_2^{1/3} > 0 \) for \( \gamma_2 \in [0, 0.24] \). Therefore \( \arccos(1 - 1.6 \gamma_2^{1/3}) \leq 2 \gamma_2^{1/6} < 1. \) Hence the above probability bound reduces to

\[ \mathbb{P}(U^*, U) (\hat{\tau} U^* \neq \tau_0, \rho(U^*, U) > 1 - \gamma_2) \]
\[ \leq 3 \exp \left\{ -n \left[ \frac{C_{\min} (1 - \gamma_1^2)^2}{\gamma_2} \frac{2 \log(p/2)}{n} - 2 \gamma_2 \right] \right\} \]
\[ + 4(64 \gamma_2) n^{-|\tau_0| - 1} \frac{1}{(\sqrt{n})^{|\tau_0|}} \]
\[ + 2 \gamma_2 n^{-|\tau_0| - 1} \frac{1}{(\sqrt{n})^{|\tau_0|}}. \]

\[ \square \]

**Proof of Lemma 2.** By Lemma 7, we let \( D(\tau, u^*) = \frac{1}{2} ||(I - H_{\tau, u^*})Y||^2 + \lambda |\tau| = \frac{1}{2} ||(I - H_{\tau}) Y||^2 + \lambda |\tau| \) for any \( \tau \neq \tau_0 \), then

\[ D(\tau, u^*) - D(\tau_0, u^*) \]
\[ = ||(I - H_{\tau}) - (I - H_{\tau_0})||Y||^2 - ||(I - H_{\tau_0}) - (I - H_{\tau})||Y||^2 + \lambda(|\tau| - |\tau_0|) \]
\[ = ||(I - H_{\tau}) - (I - H_{\tau_0})||X_0 \beta_0||Y||^2 - U^T (H_{\tau} - H_{\tau_0}) U \]
\[ + 2U^T (I - H_{\tau}) X_0 \beta_0 + 2\lambda(|\tau| - |\tau_0|). \]
Let $E(\gamma_1, \gamma_2)$ be the event defined in (44), then
\[
\mathbb{P}_{(U^*, U)} \{D(\tau, U^*) - D(\tau_0, U^*) < 0, (U^*, U) \in E(\gamma_1, \gamma_2)\}
\]
\[
\leq \mathbb{P}_{(U^*, U)} \{(1 - \gamma_1^2)\|I - H_{\tau}\|X_0\beta_0\| - \sigma^2_0 U^T(H_{\tau} + O_{\tau^+} - H_{\tau_0} - O_{\tau_0^+})U + 2\sigma_0 U^T(I - H_{\tau} - O_{\tau^+})X_0\beta_0 + 2\lambda(\|\tau| - |\tau_0|) < 0, (U^*, U) \in E(\gamma_1, \gamma_2)\}
\]
\[
\leq \mathbb{P}_{(U^*, U)} \{(1 - \gamma_1^2)\|I - H_{\tau}\|X_0\beta_0\|^2 - \sigma^2_0 U^T(H_{\tau} + O_{\tau^+} - H_{\tau_0} - O_{\tau_0^+})U + \lambda(\|\tau| - |\tau_0|)\}
\]
\[
+ \mathbb{P}_{(U^*, U)} \{(1 - \gamma_1^2)\|I - H_{\tau}\|X_0\beta_0\|^2
\]
\[
+ 2\sigma_0 U^T(I - H_{\tau} - O_{\tau^+})X_0\beta_0 + \lambda(\|\tau| - |\tau_0|) < 0\}
\]
\[
= (I_1) + (I_2),
\]
for any $\delta \in (0, 1)$.

To derive an upper bound for $I_1$, we have
\[
\|(I - H_{\tau} - O_{\tau^+})U\|^2 = \|(I - H_{\tau})(I - O_{\tau^+})U\|^2
\]
\[
\leq \|(I - H_{\tau})(I - O_{\tau^+})U\|^2 \leq \|(I - O_{\tau^+})U\|^2 \leq \gamma_2^2\|U\|^2.
\]
First,
\[
U^T(I - H_{\tau} - O_{\tau^+})X_0\beta_0 = U^T(I - H_{\tau} - O_{\tau^+})(I - H_{\tau})X_0\beta_0
\]
\[
\leq \|U^T(I - H_{\tau} - O_{\tau^+})\|\|(I - H_{\tau})X_0\beta_0\|.
\]
Then
\[
U^T(H_{\tau} + O_{\tau^+} - H_{\tau_0} - O_{\tau_0^+})U \leq 2\gamma_2\|U\|^2.
\]
Because
\[
\|U^T(I - H_{\tau} - O_{\tau^+})\|^2 \leq \gamma_2^2\|U\|^2,
\]
it then follows if $|\tau| \leq |\tau_0|$ and $\frac{\lambda}{n} < \frac{1}{2} \min \{\frac{(1 - \gamma_1^2)C_{\min}}{|\tau_0|}, \frac{\sqrt{(1 - \gamma_1^2)C_{\min}}}{|\tau_0|}\}$,
\[
(I_1) \leq \mathbb{P}_{(U^*, U)} \left\{ \|U\|^2 > \frac{(1 - \gamma_1^2)(1 - \delta)\|I - H_{\tau}\|X_0\beta_0\|^2 + \lambda(\|\tau| - |\tau_0|)}{\gamma_2^2\sigma_0^2} \right\}
\]
\[
\leq \mathbb{P} \left\{ \lambda_n^2 > \frac{(1 - \gamma_1^2)(1 - \delta - 1/6) nC_{\min}}{\gamma_2^2} \right\}
\]
\[
\leq \exp \left\{ -\frac{n}{2} \log(1 - 2t_1) - t_1 \frac{(1 - \gamma_1^2)(1 - \delta - 1/6) nC_{\min}}{\gamma_2^2} \right\},
\]
for any $0 < t_1 < 1/2$. Otherwise when $|\tau| > |\tau_0|$, we would have
\[
(I_1) \leq \exp \left\{ -\frac{n}{2} \log(1 - 2t_1) - t_1 \frac{\lambda(\|\tau| - |\tau_0|)}{\gamma_2^2\sigma_0^2} \right\}.
\]
The above inequalities are derived from Markov inequality and moment generating function of chi-square distribution. For $(I_2)$, if $\frac{\lambda}{n} < \frac{1}{6} \min \{\frac{(1 - \gamma_1^2)C_{\min}}{|\tau_0|}, \frac{\sqrt{(1 - \gamma_1^2)C_{\min}}}{|\tau_0|}\}$, by
Cauchy-Schwartz inequality when $|\tau| \leq |\tau_0|$ we have

\[(I_2)\]

\[
P_{(U^*, U)} \left\{ (1 - \gamma_1^2) \delta \|(I - H_\tau)X_0\beta_0\|^2 \leq 2\sigma_0 \|U^T (I - H_\tau - O_{\tau^\perp U^*})\| \|(I - H_\tau)X_0\beta_0\| - \lambda(|\tau| - |\tau_0|) \right\} \]

\[
= P_{(U^*, U)} \left\{ 2\sigma_0 \|U^T (I - H_\tau - O_{\tau^\perp U^*})\| > (1 - \gamma_1^2)(\delta - 1/6)\|(I - H_\tau)X_0\beta_0\| + \lambda(|\tau| - |\tau_0|) \right\} \]

\[
\leq P_{(U^*, U)} \left\{ \|U\|^2 > \frac{(1 - \gamma_1^2)^2(\delta - 1/6)^2 \|(I - H_\tau)X_0\beta_0\|^2}{4\gamma_2^2} \right\} \]

\[
\leq \mathbb{P} \left\{ \chi_n^2 > \frac{(1 - \gamma_1^2)^2(\delta - 1/6)^2 niC_{\min}}{4\gamma_2^2 \sigma_0^2} \right\} \]

\[
\leq \exp \left\{ -\frac{n}{2} \log(1 - 2t_2) - t_2 \frac{(1 - \gamma_1^2)^2(\delta - 1/6)^2 niC_{\min}}{4\gamma_2^2 \sigma_0^2} \right\} ,
\]

for any $0 < t_2 < 1/2$.

When $|\tau| > |\tau_0|$, from the fact that $(1 - \gamma_1^2)\delta \|(I - H_\tau)X_0\beta_0\|^2 + 2U^T (I - H_\tau - O_{\tau^\perp U^*})X_0\beta_0 \geq -\|U^T (I - H_\tau - O_{\tau^\perp U^*})\|/\gamma_2^2$, we have

\[(I_2) \leq P_{(U^*, U)} \left\{ \|U^T (I - H_\tau - O_{\tau^\perp U^*})\|^2 > (1 - \gamma_1^2)\delta \lambda(|\tau| - |\tau_0|) \right\} \]

\[
\leq P_{(U^*, U)} \left\{ \|U\|^2 / \sigma_0^2 > \frac{(1 - \gamma_1^2)\delta \lambda(|\tau| - |\tau_0|)}{\gamma_2^2 \sigma_0^2} \right\} \]

\[
\leq \exp \left\{ -\frac{n}{2} \log(1 - 2t_2) - t_2 \frac{(1 - \gamma_1^2)\delta \lambda(|\tau| - |\tau_0|)}{\gamma_2^2 \sigma_0^2} \right\} ,
\]

Now, by making of $(1 - \gamma_1^2)(1 - \delta - 1/6) = (1 - \gamma_1^2)^2(\delta - 1/6)^2/4$, we obtain $\delta = \frac{2}{1 - \gamma_1^2} \left( \frac{2}{3} - \frac{\gamma_2^2}{3} \right) - 1 + \frac{1}{6}$. Further we make $t_1 = t_2 = \frac{2\gamma_2}{3\sigma_0}$, so we have $-\frac{n}{2} \log(1 - 2t_1) = -\frac{n}{2} \log(1 - \frac{\gamma_2}{3\sigma_0}) \leq 2n\gamma_2$. Then, intersect with the event \{(U^*, U) \in E(\gamma_1, \gamma_2)\}, we have

\[
P_{(U^*, U)} \left\{ \hat{\tau}_{U^*} \neq \tau_0, (U^*, U) \in E(\gamma_1, \gamma_2) \right\} \]

\[
\leq 2 \sum_{i=1}^{\gamma_0} \sum_{j=0}^{i} \left( p - |\tau_0| \right) \left( |\tau_0| \right) \exp \left\{ -\left( \sqrt{\frac{5}{3} - \frac{\gamma_2^2}{3\gamma_1^2}} - 1 \right) \frac{niC_{\min}}{2.04\gamma_2^2 \sigma_0^2} + 2n\gamma_2 \right\} \]

\[
+ 2 \sum_{i=0}^{\gamma_0} \sum_{j=i+1}^{p} \left( p - |\tau_0| \right) \left( |\tau_0| \right) \exp \left\{ -\left( \sqrt{\frac{5}{3} - \frac{\gamma_2^2}{3\gamma_1^2}} - 1 \right) \frac{\lambda(j - i)}{1.02\gamma_2^2 \sigma_0^2} \right\} + 2\gamma_2 n \]

\[
\leq 2 \sum_{i=1}^{\gamma_0} \sum_{j=0}^{i} \left( p - |\tau_0| \right) \left( |\tau_0| \right) \exp \left\{ -\frac{niC_{\min} (1 - \gamma_1^2)^2}{26\sigma_0^2} + 2n\gamma_2 \right\} \]

\[
+ 2 \sum_{i=0}^{\gamma_0} \sum_{j=i+1}^{p} \left( p - |\tau_0| \right) \left( |\tau_0| \right) \exp \left\{ -\frac{(1 - \gamma_1^2)\lambda(j - i)}{4\gamma_2 \sigma_0^2} + 2\gamma_2 n \right\} .
\]
The last inequality holds since \((\sqrt{\frac{5}{3}} - \frac{2}{\sqrt{3}})^2 - 1)^2 \geq 1.02(1 - \gamma_1^2)^2/13\) for \(\gamma_1 \in (0, 1)\).

By similar calculation to that in (45), the first part of the above can be bounded by

\[
L_\rho(\gamma_1, \gamma_2) = 3 \exp \left\{ -\frac{n}{26\sigma_0^2} \left[ \frac{(1 - \gamma_1^2)^2}{\gamma_2} C_{\min} - \frac{\log(\rho/2)}{n} + \gamma_2 \right] \right\}.
\]

As for the second part,

\[
2 \sum_{i=0}^{\gamma_0} \sum_{j=i+1}^{p} \left( p - |\tau_0| \right) \left( |\tau_0| \right) \exp \left\{ -\frac{(1 - \gamma_1^2)\lambda(j - i)}{4\gamma_2\sigma_0^2} + 2\gamma_2 n \right\}
\]

\[
\leq 2 \sum_{i=0}^{\gamma_0} |\tau_0|^i \exp \left\{ \gamma_2 n + \frac{(1 - \gamma_1^2)\lambda i}{4\gamma_2\sigma_0^2} \right\} \sum_{j=i+1}^{p} \exp \left\{ -\frac{(1 - \gamma_1^2)\lambda}{4\gamma_2\sigma_0^2} \right\} \gamma_2 n + \log(p - |\tau_0|) + |\lambda_0| \log(p - |\tau_0|) \right\}
\]

\[
\leq 2 \exp \left\{ -\frac{(1 - \gamma_1^2)\lambda}{4\gamma_2\sigma_0^2} \right\} \gamma_2 n + \log(p - |\tau_0|) + |\lambda_0| \log(p - |\tau_0|) \right\}
\]

\[
\leq 3 \exp \left\{ -\frac{1 - \gamma_1^2}{4\gamma_2\sigma_0^2} \right\} n, \]

if \(\frac{\lambda(1)}{n} + t, \frac{1}{B} \min \left\{ (1 - \gamma_1^2)C_{\min}, (1 - \gamma_1^2)C_{\min} \right\} \), where

\[
\lambda_0(1) = \frac{4\gamma_2\sigma_0^2}{1 - \gamma_1^2} \left[ \gamma_2 n + (|\tau_0| + 1) \log(p - |\tau_0|) \right].
\]

It then follows from Lemma 9 and Lemma 10 that

\[
P_{(U^*, U)}(\hat{\tau}_U \neq \tau_0, \rho(U^*, U) > 1 - \gamma_2^2)
\]

\[
\leq P_{(U^*, U)}(\hat{\tau}_U \neq \tau_0, (U^*, U) \in E(\gamma_1, \gamma_2)) + P\left( \max_{\rho \neq \rho_0, |\tau| \leq |\tau_0|} \rho(\epsilon, X_0\beta_0) \geq \gamma_1^2 \right)
\]

\[
+ P\left( \max_{\rho \neq \rho_0, |\tau| \leq |\tau_0|} \rho(\epsilon, \tau) \geq 1 - \gamma_2 \right)
\]

\[
\leq L_\rho(\gamma_1, \gamma_2) + 3 \exp \left\{ -\frac{1 - \gamma_1^2}{4\gamma_2\sigma_0^2} \right\} n + 4(\arccos \gamma_1)n - |\tau_0| - 1p|\tau_0|
\]

\[
+ 2\gamma_2 \frac{n - |\tau_0| - 1}{\sqrt{np}}|\tau_0|.
\]

We then make \(\gamma_1 = \sqrt{1 - \gamma_2^2/4}\), from which we have \(\gamma_1 = (1 - \sqrt{\gamma_2})\sqrt{1 - \gamma_2^2/4} - \sqrt{2 - 2\sqrt{1 - \gamma_2^2}} \geq 1 - 1.6\gamma_2^{1/3} > 0\) for \(\gamma_2 \in [0, 0.24]\). Therefore \(\arccos \gamma_1 \leq \arccos(1 - 1.6\gamma_2^{1/3}) \leq 2\gamma_2^{1/6} < 1\). In addition, we make \(t = \sqrt{\gamma_2}\). Hence the above probability bound reduces to

\[
P_{(U^*, U)}(\hat{\tau}_U \neq \tau_0, \rho(U^*, U) > 1 - \gamma_2^2)
\]
\[ \leq 3 \exp \left\{ -\frac{n}{26\sigma_0^2} \left[ C_{\text{min}} - 52 \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2 \right] \right\} + 3 \exp \left( -\frac{n}{4\gamma_2^2 \sigma_0^2} nt \right) \\
+ 4(64\gamma_2) \frac{n-|\tau_0|-1}{n} p^{\rho_{\tau_0}} + 2\gamma_2 \frac{n-|\tau_0|-1}{n} (\sqrt{np})^{\rho_{\tau_0}} \\
\leq 3 \exp \left\{ -\frac{n}{26\sigma_0^2} \left[ C_{\text{min}} - 52 \left( \frac{\log(p/2)}{n} + \gamma_2 \right) \sigma_0^2 \right] \right\} + 3 \exp \left( -\frac{n}{4\gamma_2^2 \sigma_0^2} nt \right) \\
+ 4(64\gamma_2) \frac{n-|\tau_0|-1}{n} p^{\rho_{\tau_0}} + 2\gamma_2 \frac{n-|\tau_0|-1}{n} (\sqrt{np})^{\rho_{\tau_0}}, \]

where \( \gamma_2 < 1/64 \) since \( \gamma_2^{1/4} < 0.35 \).

Moreover it follows from the fact \( \log |\tau_0| + \log(p - |\tau_0|) \leq 2 \log(p/2) \) that when \( \gamma_2^{1/4} \leq \frac{C_{\text{min}}}{|\tau_0|^2} \wedge \frac{C_{\text{min}}}{24(2+2(|\tau_0|+1)\log(p/2)/n)} \) and \( t = \sqrt{\gamma_2} \),

\[
\frac{\lambda_0^{(1)}}{n} + t \leq 4\gamma_2^{1/2} \left\{ \gamma_2 + 1 + 2\gamma_2^{1/4} (|\tau_0| + 1) \left( \frac{\log(p/2)}{n} \right) \right\} \\
< 4\gamma_2^{1/2} \left\{ 2 + 2(|\tau_0| + 1) \frac{\log(p/2)}{n} \right\} \\
< \frac{1}{6} \gamma_2^{1/4} C_{\text{min}} \leq \frac{1}{6|\tau_0|} \sqrt{C_{\text{min}}}. \]

The result in Lemma 2 then follows immediately. \( \square \)

### B.3. Proof of Lemma 3 and Lemma 6

**Lemma 11.** Suppose \( U_1^*, \ldots, U_d^* \) are \( d \) i.i.d. copies of \( U^* \sim N(0, I) \), then

\[ \mathbb{P} \left( \bigcap_{b=1}^{d} \{ \rho(U_b^*, U) \leq 1 - \gamma_2^2 \} \right) \leq \left( 1 - \frac{\gamma_2^{n-1}}{n-1} \right)^d. \]

**Proof of Lemma 11.** By (42), \( \rho(U_b^*, U) \) and \( U \) are independent. It then follows from Lemma 8 and the fact arcsin(\( \gamma_2 \)) > \( \gamma_2 \) that

\[ \mathbb{P} \left( \bigcap_{b=1}^{d} \{ \rho(U_b^*, U) \leq 1 - \gamma_2^2 \} \right) \]

\[ = E \left\{ \mathbb{P} \left( \bigcap_{b=1}^{d} \{ \rho(U_b^*, U) \leq 1 - \gamma_2^2 \} \Big| U \right) \right\} \]

\[ = E \left\{ (1 - \mathbb{P}(\rho(U^*, U) > 1 - \gamma_2^2 | U))^{d} \right\} \]

\[ = (1 - \mathbb{E}(\rho(U^*, U) > 1 - \gamma_2^2))^{d} \]

\[ \leq \left( 1 - \frac{\gamma_2^{n-2} \arcsin(\gamma_2)}{n-1} \right)^d \leq \left( 1 - \frac{\gamma_2^{n-1}}{n-1} \right)^d. \]

\( \square \)
PROOF OF LEMMA 6. We can decompose the probability $\tau_0 \notin S^{(d)}$ into
\[ \mathbb{P}(\tau_0 \notin S^{(d)}) = \mathbb{P}\left(\tau_0 \notin S^{(d)}, \bigcup_{b=1}^{d} \{\rho(U_b^*, U) > 1 - \gamma_2^2\}\right) + \mathbb{P}\left(\tau_0 \notin S^{(d)}, \bigcap_{b=1}^{d} \{\rho(U_b^*, U) \leq 1 - \gamma_2^2\}\right) \]
\[ \leq \mathbb{P}(\tilde{\tau}U \neq \tau_0, \rho(U_b^*, U) > 1 - \gamma_2^2 \text{ for some } b) + \mathbb{P}\left(\bigcap_{b=1}^{d} \{\rho(U_b^*, U) \leq 1 - \gamma_2^2\}\right) \]
(47)
\[ \leq \mathbb{P}(\tilde{\tau}U \neq \tau_0, \rho(U_b^*, U) > 1 - \gamma_2^2) + \mathbb{P}\left(\bigcap_{b=1}^{d} \{\rho(U_b^*, U) \leq 1 - \gamma_2^2\}\right). \]

Then the probability bound in (37) follows immediately from Lemma 5 and Lemma 11. □

PROOF OF LEMMA 3. By (47), the probability bound in (28) follows immediately from Lemma 2 and Lemma 11. □

B.4. Proof of Theorem 11 and Lemma 4. In order to prove Theorem 11, we first present a technical lemma, which is a counterpart of Lemma 4. We will first prove Lemma 12, and follow the similar strategy to prove Lemma 4.

LEMMA 12. Under the constraint $|\tau| \leq |\tau_0|$, the finite-sample probability bound that the true model is not covered by the model candidate set $S^{(d)}$, obtained by Algorithm 1 with the objective function (36), is as follows,
\[ \mathbb{P}(\{\tau^*, \gamma\} (\tau_0 \notin S^{(d)}) \leq L(\gamma_1) + \left[2\{\arccos(\gamma_1)\} \right]^{d} \]
\[ \text{where} \]
\[ L(\gamma_1) = 6 \exp\left[-\frac{n}{18\sigma_0^2} \left\{ (1 - \gamma_1^2) C_{\min} - 36 \frac{\log p}{n} \frac{\log p}{\sigma_0^2} \right\} \right], \]
and $\cos(0.3\pi) < \gamma_1 < 1$ is any real number.

PROOF OF LEMMA 12. By (43), for any $\delta \in (0, 1)$ an any $u^*$ such that
\[ \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^*}(u^*, X_0\beta_0) < \gamma_1^2, \]
we have
\[ \mathbb{P}(D(\tau, u^*) - D(\tau_0, u^*) < 0) \]
\[ \leq \mathbb{P}(\{1 - \gamma_1^2\}(I - H_{\tau})X_0\beta_0\|^2 - \sigma_0^2 U^T(H_{\tau,u^*} - H_{\tau_0,u^*})U \]
\[ + 2\sigma_0 U^T(I - H_{\tau,u^*})X_0\beta_0 < 0\}
\[ \leq \mathbb{P}(\{1 - \gamma_1^2\}(1 - \delta)(I - H_{\tau})X_0\beta_0\|^2 - \sigma_0^2 U^T(H_{\tau,u^*} - H_{\tau_0,u^*})U < 0\}
\[ + \mathbb{P}(\{1 - \gamma_1^2\}\delta(I - H_{\tau})X_0\beta_0\|^2 + 2\sigma_0 U^T(I - H_{\tau,u^*})X_0\beta_0 < 0\}
\[ = (I_1) + (I_2). \]
By Lemma 4 of [47], we bound the log of the moment generating function $M(t)$ of 
$U^T(H_{r,u^*} - H_{r_0,u^*})U$

$$\log\{M(t)\} = \sum_{r=1}^{\infty} 2^{r-1} t^r \text{tr}\{(H_{r,u^*} - H_{r_0,u^*})^r\}$$

(49)

$$\leq t(|\tau| - |\tau_0|) + \frac{t^2}{1 - 2t} \text{tr}\{(H_{r,u^*} - H_{r_0,u^*})^2\} \leq 2t|\tau| - |\tau_0| \leq 2t|\tau_0| - \tau,$$

for any $0 < t < 1/2$. Therefore by Markov Inequality

$$(I_1) \leq \exp\left\{2t_1|\tau| - |\tau_0| - \frac{t_1(1 - \delta)(1 - \gamma_1^2)n|\tau_0|}{\sigma_0^2}\right\},$$

for any $0 < t_1 < 1/2$. Further because $2\sigma_0 U^T(I - H_{r,u^*})X_0\beta_0$ follows $N(0, \sigma_0^2(I - H_{r,u^*})X_0\beta_0)^2$, then by Markov inequality and moment generating function of the normal distribution, we have

$$(I_2) \leq \exp\left\{\frac{(2t_2^2 - \delta t_2)(1 - \gamma_1^2)n|\tau_0|}{\sigma_0^2} \tau|C_{\min}\right\}$$

for any $0 < t_2 < 1/2$. It then follows that

$$\mathbb{P}_U(\hat{\tau}_{u^*} \neq \tau_0) \leq \sum_{i=0}^{\tau_0} \sum_{j=0}^{i} \binom{|\tau_0|}{i} \binom{p - |\tau_0|}{j} \left[\exp\left\{2t_1j - \frac{t_1(1 - \delta)(1 - \gamma_1^2)n|\tau_0|}{\sigma_0^2}\right\} + \exp\left\{\frac{(2t_2^2 - \delta t_2)(1 - \gamma_1^2)n|\tau_0|}{\sigma_0^2}\right\}\right].$$

We can make $t_1 = t_2 = 1/3$, $\delta = 5/6$, therefore $t_1(1 - \delta) = -(2t_2^2 - \delta t_2) = 1/18$. Then by the fact that $\left(\frac{a}{b}\right) \leq a^b$, the probability bound above can be simplified as

$$\mathbb{P}_U(\hat{\tau}_{u^*} \neq \tau_0) \leq \sum_{i=0}^{\tau_0} \sum_{j=0}^{i} (p - |\tau_0|)^j |\tau_0|^i \exp\left\{-\frac{(1 - \gamma_1^2)nC_{\min}}{18\sigma_0^2} i + \frac{2}{3} j\right\}$$

$$= 2 \sum_{i=0}^{\tau_0} \exp\left[-i \left\{\frac{(1 - \gamma_1^2)nC_{\min}}{18\sigma_0^2} - \log|\tau_0|\right\}\right] \sum_{j=0}^{i} \exp\left[j \left\{\frac{2}{3} + \log(p - |\tau_0|)\right\}\right].$$

Then we have

$$\sum_{j=0}^{i} \exp\left[j \left\{\frac{2}{3} + \log(p - |\tau_0|)\right\}\right] \leq \exp\left[i \left\{\frac{2}{3} + \log(p - |\tau_0|)\right\}\right] - 1 \leq \frac{\exp\left[i \left\{\frac{2}{3} + \log(p - |\tau_0|)\right\}\right]}{1 - e^{-2/3}}.$$

It then follows from $\log(p - |\tau_0|) + \log(|\tau_0|) \leq 2\log p - 1$ that

$$\mathbb{P}_U(\hat{\tau}_{u^*} \neq \tau_0) \leq \frac{2}{1 - e^{-2/3}} \sum_{i=1}^{\tau_0} \exp\left[-i \left\{\frac{(1 - \gamma_1^2)nC_{\min}}{18\sigma_0^2} - 2\log p\right\}\right].$$
we have the probability bound
\[ P(U (\tau_\ast \neq \tau_0)) \leq \frac{2}{1 - e^{-2/3}} + \frac{3 - e^{-2/3}}{1 - e^{-2/3}} \exp \left[ -\frac{n}{18\sigma_0^2} \left( 1 - \gamma_1^2 \right) C_{\min} - 36 \frac{\log p}{n} \sigma_0^2 \right] \]

It then follows that for any
\[ u^* \in \left\{ \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (u^*, X_0|\beta_0) < \gamma_1^2 \right\}, \]
we have the probability bound
\[ P(U (\tilde{\tau}_u \neq \tau_0)) \leq \frac{2}{1 - e^{-2/3}} + \frac{3 - e^{-2/3}}{1 - e^{-2/3}} \exp \left[ -\frac{n}{18\sigma_0^2} \left( 1 - \gamma_1^2 \right) C_{\min} - 36 \frac{\log p}{n} \sigma_0^2 \right] \]

By Lemma 8
\[ P(U^\ast (\max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^*, X_0|\beta_0) \geq \gamma_1^2)) \leq \sum_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} P(U^\ast (\rho_\tau (U^*, X_0|\beta_0) \geq \gamma_1^2)) \]
\[ \leq \sum_{\{\tau: |\tau| \leq |\tau_0|\}} 2 |\arccos(\gamma_1)| n^{-|\tau| - 1} = \sum_{k=1}^{|\tau_0|} \binom{p}{k} 2 |\arccos(\gamma_1)| n^{-k-1} \]

Then let \( i_{\min} = \arg \min_{1 \leq i \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_i, X_0|\beta_0), \) we have
\[ P(\mathcal{U}^\ast, Y) \left( 0 \notin S(d) \right) \leq P(\mathcal{U}^\ast, Y) \left( 0 \notin S(d), \min_{1 \leq i \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_i, X_0|\beta_0) < \gamma_1^2 \right) \]
\[ + P(\mathcal{U}^\ast, Y) \left( 0 \notin S(d), \min_{1 \leq i \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_i, X_0|\beta_0) \geq \gamma_1^2 \right) \]
\[ \leq P(\mathcal{U}^\ast, Y) \left( 0 \notin S(d), \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_{i_{\min}}, X_0|\beta_0) < \gamma_1^2 \right) \]
\[ + P(\mathcal{U}^\ast, Y) \left( \max_{1 \leq i \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_i, X_0|\beta_0) \geq \gamma_1^2 \right) \]
\[ \leq P(\mathcal{U}^\ast, Y) \left( 0 \notin S(d), \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_{i_{\min}}, X_0|\beta_0) < \gamma_1^2 \right) \]
\[ \times P(\mathcal{U}^\ast) \left( \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_{i_{\min}}, X_0|\beta_0) < \gamma_1^2 \right) \]
\[ + P(\mathcal{U}^\ast, Y) \left( \min_{1 \leq i \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_\tau (U^\ast_i, X_0|\beta_0) \geq \gamma_1^2 \right) \]
\[
\leq \max \left\{ P_U(\hat{\tau}_{u^*} \neq \tau_0) : \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^+}(u^*, X_{0\beta_0}) < \gamma_1^2 \right\} \\
+ \prod_{i=1}^d \mathbb{P}_{U_{i^*}} \left\{ \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^+}(U_{i^*}, X_{0\beta_0}) \geq \gamma_1^2 \right\} \\
\leq L(\gamma_1) + \left[ 2(\arccos(\gamma_1))^{n-|\tau_0|-1}p_{|\tau_0|} \right]^d.
\]

\[\square\]

**Proof of Lemma 4.** By Lemma 7, we let \( D(\tau, u^* ) = \frac{1}{2} \| (I - H_{\tau, u^*}) Y \|^2 + \lambda |\tau| = \frac{1}{2} \| (I - H_{\tau} - O_{\tau^0, u}) y \|^2 + \lambda |\tau| \) for any \( \tau \neq \tau_0 \). Then By (46), for any \( \delta \in (0, 1) \) an any \( u^* \) such that

\[
\max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^+}(u^*, X_{0\beta_0}) < \gamma_1^2,
\]

we have

\[
\mathbb{P}_U \{ D(\tau, u^*) - D(\tau_0, u^*) < 0 \} \\
\leq \mathbb{P}_U \{ (1 - \gamma_1^2)(I - H_{\tau}) X_{0\beta_0} \|^2 - \sigma_0^2 U^T (H_{\tau} + O_{\tau^+ u^*} - H_{\tau_0} - O_{\tau^0 u}) U \\
+ 2\sigma_0 U^T (I - H_{\tau} - O_{\tau^0 u}) X_{0\beta_0} + 2\lambda(|\tau| - |\tau_0|) < 0 \} \\
\leq \mathbb{P}_U \{ (1 - \gamma_1^2)(1 - \delta)(I - H_{\tau}) X_{0\beta_0} \|^2 - \sigma_0^2 U^T (H_{\tau} + O_{\tau^+ u^*} - H_{\tau_0} - O_{\tau^0 u}) U \\
+ \lambda(|\tau| - |\tau_0|) < 0 \} \\
+ \mathbb{P}_U \{ (1 - \gamma_1^2)\delta (I - H_{\tau}) X_{0\beta_0} \|^2 + 2\sigma_0 U^T (I - H_{\tau} - O_{\tau^+ u^*}) X_{0\beta_0} \\
+ \lambda(|\tau| - |\tau_0|) < 0 \} = (I_1) + (I_2). \]

Then it follows from (49) and Markov Inequality

\[
(I_1) \leq \exp \left\{ 2t_1 |\tau \setminus \tau_0| - t_1(1 - \delta)(1 - \gamma_1^2)n|\tau_0 \setminus \tau| C_{\min} + t_1 \lambda(|\tau| - |\tau_0|) \right\}.
\]

for any \( 0 < t_1 < 1/2 \). Further because \( 2\sigma_0 U^T (I - H_{\tau, u^*}) X_{0\beta_0} \) follows \( N(0, \sigma_0^2 \| (I - H_{\tau, u^*}) X_{0\beta_0} \|^2) \), then by Markov inequality and moment generating function of the normal distribution, we have

\[
(I_2) \leq \exp \left\{ \frac{(2t_2 - \delta t_2)(1 - \gamma_1^2)n|\tau_0 \setminus \tau| C_{\min} + t_2 \lambda(|\tau| - |\tau_0|)}{\sigma_0^2} \right\}.
\]

for any \( 0 < t_2 < 1/2 \). It then follows that

\[
\mathbb{P}_U(\hat{\tau}_{u^*} \neq \tau_0) \\
\leq \sum_{i=1}^{|\tau_0|} \sum_{j=0}^i \binom{|\tau_0|}{i} \binom{p - |\tau_0|}{j} \left[ \exp \left\{ \frac{(2t_1^2 - \delta t_1)(1 - \gamma_1^2)n_i C_{\min} + t_1 \lambda(i - j)}{\sigma_0^2} \right\} \right] \\
+ \exp \left\{ \frac{-t_1(1 - \delta)t_2(1 - \gamma_1^2)n_i C_{\min} + t_2 \lambda(i - j) + 2t_2 j}{\sigma_0^2} \right\} \\
+ \sum_{i=0}^{|\tau_0|} \sum_{j=i+1}^p \binom{|\tau_0|}{i} \binom{p - |\tau_0|}{j} \left[ \exp \left\{ \frac{t_1 \lambda(i - j)}{\sigma_0^2} \right\} + \exp \left\{ \frac{t_2 \lambda(i - j) + 2t_2 j}{\sigma_0^2} \right\} \right].
\]
We can make $\delta = 1/2$, $t_1 = t_2 = 1/3$, then by (50), if

$$\lambda \leq \frac{3\sigma_0^2(|\tau_0|)}{n} \left\{ \log(p - |\tau_0|) + \log(|\tau_0|) + \frac{2}{3} \right\} + 6 \left( 1 - \frac{\gamma_1^2}{3} \right) C_{\min},$$

we have

$$\mathbb{P}(\hat{u} \neq \tau_0) \leq 2 \sum_{i=1}^{\tau_0} \sum_{j=0}^i (p - |\tau_0|)^j |\tau_0|^i \exp \left\{ -\frac{(1 - \gamma_1^2) \tau_0 C_{\min} \lambda(i - j) + 2}{18\sigma_0^2} + \frac{\lambda(i - j) + 2}{3} \right\}$$

$$+ 2 \sum_{i=0}^{\tau_0} \sum_{j=0}^i (p - |\tau_0|)^j |\tau_0|^i \exp \left\{ -\frac{\lambda(i - j) + 2}{3\sigma_0^2} + \frac{2}{3} \right\}$$

$$\leq L(\gamma_1) + 2 \sum_{i=0}^{\tau_0} \exp \left\{ -\frac{\lambda(i - j) + 2}{3\sigma_0^2} + \frac{2}{3} \right\}$$

Then let $i_{\min} = \arg \min_{1 \leq i \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau}^\perp(U^*_i, X_0^0)$, by (51) we have

$$\mathbb{P}(\hat{u} \notin S^{(d)}) \leq \mathbb{P}(\hat{u} \notin S^{(d)}) \left\{ \tau_0 \notin S^{(d)}, \min_{1 \leq r \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^\perp}(U^*_r, X_0^0) < \gamma_1^2 \right\}$$

$$+ \mathbb{P}(\hat{u} \notin S^{(d)}) \left\{ \tau_0 \notin S^{(d)}, \min_{1 \leq r \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^\perp}(U^*_r, X_0^0) \geq \gamma_1^2 \right\}$$

$$\leq \mathbb{P}(\hat{u} \notin S^{(d)}) \left\{ \hat{u} \neq \tau_0, \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^\perp}(U^*_{\min}, X_0^0) < \gamma_1^2 \right\}$$

$$+ \mathbb{P}(\hat{u} \notin S^{(d)}) \left\{ \min_{1 \leq r \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^\perp}(U^*_r, X_0^0) \geq \gamma_1^2 \right\}$$

$$\leq \mathbb{P}(\hat{u} \notin S^{(d)}) \left\{ \hat{u} \neq \tau_0, \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^\perp}(U^*_{\min}, X_0^0) < \gamma_1^2 \right\}$$

$$+ \mathbb{P}(\hat{u} \notin S^{(d)}) \left\{ \min_{1 \leq r \leq d} \max_{\tau \neq \tau_0, |\tau| \leq |\tau_0|} \rho_{\tau^\perp}(U^*_r, X_0^0) \geq \gamma_1^2 \right\}$$

$$\leq \max \left\{ \mathbb{P}(\hat{u} \neq \tau_0) : \max_{1 \leq r \leq d} \rho_{\tau^\perp}(u, X_0^0) < \gamma_1^2 \right\}$$

$$+ \prod_{i=1}^d \mathbb{P}(u_i \neq \tau_0) \left\{ \max_{1 \leq r \leq d} \rho_{\tau^\perp}(U^*_r, X_0^0) \geq \gamma_1^2 \right\}$$
\[ L(\gamma_1) + 3\exp\left(-\frac{nt}{3\sigma^2_0}\right) + \left[2\{\arccos(\gamma_1)\}^n - |\tau_0| - 1\right]^{\frac{d}{\tau_0}}. \]

\[ \square \]

**Proof of Theorem 11.** By Lemma 12, we make $\gamma_1^2 = 0.7$, then the probability bound (38) follows from (48).

\[ \square \]

**REFERENCES**

[1] ATHEY, S., IMBENS, G. W. and WAGER (2018). Approximate Residual Balancing: De-Biased Inference of Average Treatment Effects in High Dimensions. arXiv:1604.07125 [econ, math, stat].

[2] BARBER, R. F. and CANDÉS, E. J. (2015). Controlling the False Discovery Rate via Knockoffs. The Annals of Statistics 43 2055–2085.

[3] BEAUMONT, M. A., ZHANG, W. and BALDING, D. J. (2002). Approximate Bayesian Computation in Population Genetics. Genetics 162 2025–2035.

[4] BELLONI, A., CHERNELZHUKOV, V., CHERNOZHUKOV, D., HANSEN, C. and KATO, K. (2018). High-dimensional econometrics and regularized GMM. arXiv preprint arXiv:1806.01888.

[5] BELLONI, A., CHERNELZHUKOV, V., FERNÁNDEZ-VAL, I. and HANSEN, C. (2017). Program Evaluation and Causal Inference with High-Dimensional Data. Econometrica 85 233–298.

[6] BÜHLMANN, P. and VAN DE GEEER, S. (2011). Statistics for High-dimensional Data: Methods, Theory and Applications. Springer Science & Business Media.

[7] CAI, T., CAI, T. and GUO, Z. (2019). Individualized Treatment Selection: An Optimal Hypothesis Testing Approach In High-dimensional Models. arXiv:1904.12891 [math, stat].

[8] CAI, T. and GUO, Z. (2020). Semisupervised Inference for Explained Variance in High Dimensional Linear Regression and Its Applications. Journal of the Royal Statistical Society: Series B (Statistical Methodology).

[9] CAI, T. T. and GUO, Z. (2017). Confidence Intervals for High-Dimensional Linear Regression: Minimax Rates and Adaptivity. The Annals of statistics 45 615–646.

[10] CAI, T. T. and GUO, Z. (2018). Accuracy Assessment for High-Dimensional Linear Regression. The Annals of Statistics 46 1807–1836.

[11] CANDÉS, E., FAN, Y., JANSON, L. and LV, J. (2018). Panning for Gold: ‘Model-X’ Knockoffs for High Dimensional Controlled Variable Selection. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 80 551–577.

[12] CANDÉS, E. and TAO, T. (2007). The Dantzig selector: Statistical estimation when p is much larger than n. The annals of Statistics 35 2313–2351.

[13] CHATTERJEE, A. and LAHIRI, S. N. (2011). Bootstrapping Lasso Estimators. Journal of the American Statistical Association 106 608–625.

[14] CHEN, J. and CHEN, Z. (2008). Extended Bayesian Information Criteria for Model Selection with Large Model Spaces. Biometrika 95 759–771.

[15] CHEN, S. S., DONOHO, D. L. and SAUNDERS, M. A. (2001). Atomic decomposition by basis pursuit. SIAM review 43 129–159.

[16] CHERNELZHUKOV, V., CHERNOZHUKOV, D., DEMIRER, M., DUFOLO, E., HANSEN, C. and NEWEY, W. (2017). Double/Debiased/Neyman Machine Learning of Treatment Effects. American Economic Review 107 261–65.

[17] CHERNELZHUKOV, V., CHERNOZHUKOV, D., DEMIRER, M., DUFOLO, E., HANSEN, C., NEWEY, W. and ROBINS, J. (2018). Double/Debiased Machine Learning for Treatment and Structural Parameters. Oxford University Press Oxford, UK.

[18] CHERNELZHUKOV, V., CHERNOZHUKOV, D. and KATO, K. (2017). Central Limit Theorems and Bootstrap in High Dimensions. The Annals of Probability 45 2309–2352.

[19] CHERNELZHUKOV, V., HANSEN, C. and SPINDLER, M. (2015). Post-Selection and Post-Regularization Inference in Linear Models with Many Controls and Instruments. American Economic Review 105 486–90.

[20] Das, D., Gregory, K. and Lahiri, S. N. (2019). Perturbation Bootstrap in Adaptive Lasso. The Annals of Statistics 47 2080–2116.

[21] Das, D. and Lahiri, S. N. (2019). Distributional Consistency of the Lasso by Perturbation Bootstrap. Biometrika 106 957–964.

[22] DEZEURE, R., BÜHLMANN, P., MEIER, L. and MEINSHAUSEN, N. (2015). High-Dimensional Inference: Confidence Intervals, SpSp-Values and R-Software Hdi. Statistical Science 30 533–558.
[23] DEZEURE, R., BÜHLMANN, P. and ZHANG, C.-H. (2017). High-Dimensional Simultaneous Inference with the Bootstrap. *Test* **26** 685–719.
[24] EFRON, B. (1992). Bootstrap Methods: Another Look at the Jackknife. In *Breakthroughs in Statistics* 569–593, Springer.
[25] FAN, J. and LI, R. (2001). Variable Selection via Nonconcave Penalized Likelihood and Its Oracle Properties. *Journal of the American Statistical Association* **96** 1348–1360.
[26] FAN, J. and LV, J. (2008). Sure Independence Screening for Ultrahigh Dimensional Feature Space. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **70** 849–911.
[27] FAN, J. and LV, J. (2018). Sure independence screening. *Wiley StatsRef: Statistics Reference Online*.
[28] FERRARI, D. and YANG, Y. (2015). Confidence Sets for Model Selection by F-testing. *Statistica Sinica* 1637–1658.
[29] GUO, Z., RENAX, C., BÜHLMANN, P. and CAI, T. T. (2020). Group Inference in High Dimensions with Applications to Hierarchical Testing. *arXiv:1909.01503 [stat]*.
[30] GUO, Z., WANG, W., CAI, T. T. and LI, H. (2019). Optimal Estimation of Genetic Relatedness in High-Dimensional Linear Models. *Journal of the American Statistical Association* **114** 358–369.
[31] HANNING, J., IYER, H., LÁI, R. C. S. and LEE, T. C. M. (2016). Generalized Fiducial Inference: A Review and New Results. *Journal of the American Statistical Association* **111** 1346–1361.
[32] HANSEN, P. R., LUNDE, A. and NASON, J. M. (2011). The Model Confidence Set. *Econometrica* **79** 453–497.
[33] HILAFU, H. and SAFO, S. E. (2022). Sparse sliced inverse regression for high dimensional data analysis. *BMC bioinformatics* **23** 1–19.
[34] JANSON, L., BARBER, R. F. and CANDÉS, E. (2016). EigenPrism: Inference for High-Dimensional Signal-to-Noise Ratios. *arXiv:1505.02097 [stat]*.
[35] JAVANMARD, A. and LEE, J. D. (2019). A Flexible Framework for Hypothesis Testing in High-dimensions. *arXiv:1704.07971 [cs, math, stat]*.
[36] JAVANMARD, A. and MONTANARI, A. Confidence Intervals and Hypothesis Testing for High-Dimensional Regression. *https://web.stanford.edu/~montanar/sslasso/code.html*.
[37] JAVANMARD, A. and MONTANARI, A. (2014). Confidence Intervals and Hypothesis Testing for High-Dimensional Regression. *The Journal of Machine Learning Research* **15** 2869–2909.
[38] KOROBLIS, D. (2021). High-dimensional macroeconomic forecasting using message passing algorithms. *Journal of Business & Economic Statistics* **39** 493–504.
[39] LEINER, J., DUAN, B., WASSERMAN, L. and RAMDAS, A. (2021). Data fission: splitting a single data point. *arXiv preprint arXiv:2112.11079*.
[40] LIU, W. (2013). Gaussian graphical model estimation with false discovery rate control. *The Annals of Statistics* **41** 2948–2978.
[41] LV, S., YOU, M., LIN, H., LIAN, H. and HUANG, J. (2018). On the Sign Consistency of the Lasso for the High-dimensional Cox Model. *Journal of Multivariate Analysis* **167** 79–96.
[42] MARTIN, R. and LIU, C. (2015). *Inferential Models: Reasoning with Uncertainty*. Chapman & Hall/CRC.
[43] MEINSHAUSEN, N., MEIER, L. and BÜHLMANN, P. (2009). P-Values for High-Dimensional Regression. *Journal of the American Statistical Association* **104** 1671–1681.
[44] MITRA, R. and ZHANG, C.-H. (2016). The Benefit of Group Sparsity in Group Inference with De-Biased Scaled Group Lasso. *Electronic Journal of Statistics* **10** 1829–1873.
[45] NICKL, R. and VAN DE GEER, S. (2013). Confidence Sets in Sparse Regression. *The Annals of Statistics* **41** 2858–2876.
[46] SHEN, X., PAN, W. and ZHU, Y. (2012). Likelihood-Based Selection and Sharp Parameter Estimation. *Journal of the American Statistical Association* **107** 223–232.
[47] SHEN, X., PAN, W., ZHU, Y. and ZHOU, H. (2013). On Constrained and Regularized High-Dimensional Regression. *Annals of the Institute of Statistical Mathematics* **65** 807–832.
[48] TAYLOR, J. and TIBSHIRANI, R. J. (2015). Statistical learning and selective inference. *Proceedings of the National Academy of Sciences* **112** 7629–7634.
[49] TIBSHIRANI, R. (1996). Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society: Series B (Methodological)* **58** 267–288.
[50] TIBSHIRANI, R. J., TAYLOR, J., LOCKHART, R. and TIBSHIRANI, R. (2016). Exact post-selection inference for sequential regression procedures. *Journal of the American Statistical Association* **111** 600–620.
[51] VAN DE GEER, S., BÜHLMANN, P., RITOV, Y. and DEZEURE, R. (2014). On Asymptotically Optimal Confidence Regions and Tests for High-Dimensional Models. *The Annals of Statistics* **42** 1166–1202.
[52] VAN DE GEER, S. and STUCKY, B. (2016). χ 2-Confidence Sets in High-Dimensional Regression. In *Statistical Analysis for High-Dimensional Data* 279–306, Springer.
[53] Verzelen, N. and Gassiat, E. (2018). Adaptive Estimation of High-Dimensional Signal-to-Noise Ratios. *Bernoulli* **24** 3683–3710.

[54] Wang, H., Lengerich, B. J., Aragam, B. and Xing, E. P. (2019). Precision Lasso: accounting for correlations and linear dependencies in high-dimensional genomic data. *Bioinformatics* **35** 1181–1187.

[55] Wang, X., Benesty, J., Chen, J. and Cohen, I. (2020). Beamforming with small-spacing microphone arrays using constrained/generalized LASSO. *IEEE Signal Processing Letters* **27** 356–360.

[56] Xie, M.-G. and Singh, K. (2013). Confidence Distribution, the Frequentist Distribution Estimator of a Parameter: A Review. *International Statistical Review* **81** 3–39.

[57] Xie, M.-G. and Wang, P. (2022). Repro Samples Method for Finite- and Large-Sample Inferences. *arXiv e-prints arXiv.2206.06421*.

[58] Zhang, C.-H. (2010). Nearly Unbiased Variable Selection under Minimax Concave Penalty. *The Annals of statistics* **38** 894–942.

[59] Zhang, C.-H. and Zhang, S. S. (2014). Confidence Intervals for Low Dimensional Parameters in High Dimensional Linear Models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **76** 217–242.

[60] Zhang, X. and Cheng, G. (2017). Simultaneous Inference for High-Dimensional Linear Models. *Journal of the American Statistical Association* **112** 757–768.

[61] Zhang, Y., d’Aspremont, A. and Ghoul, L. E. (2012). Sparse PCA: Convex Relaxations, Algorithms and Applications. In *Handbook on Semidefinite, Conic and Polynomial Optimization*, (M. F. Anjos and J. B. Lasserre, eds.). *International Series in Operations Research & Management Science* **166** 915–940. Springer US.

[62] Zhao, P. and Yu, B. (2006). On model selection consistency of Lasso. *The Journal of Machine Learning Research* **7** 2541–2563.

[63] Zhou, K., Li, K.-C. and Zhou, Q. (2019). Honest Confidence Sets for High-Dimensional Regression by Projection and Shrinkage. *arXiv preprint arXiv:1902.00355*.

[64] Zhu, Y. and Bradic, J. (2017). A Projection Pursuit Framework for Testing General High-Dimensional Hypothesis. *arXiv:1705.01024 [math, stat]*.

[65] Zhu, Y. and Bradic, J. (2018). Linear Hypothesis Testing in Dense High-Dimensional Linear Models. *Journal of the American Statistical Association* **113** 1583–1600.

[66] Zhu, Y., Shen, X. and Pan, W. (2020). On High-Dimensional Constrained Maximum Likelihood Inference. *Journal of the American Statistical Association* **115** 217–230.

[67] Zou, H. (2006). The Adaptive Lasso and Its Oracle Properties. *Journal of the American Statistical Association* **101** 1418–1429.

[68] Zou, H. and Hastie, T. (2005). Regularization and variable selection via the elastic net. *Journal of the royal statistical society: series B (statistical methodology)* **67** 301–320.