Optimal Semi-supervised Estimation and Inference for High-dimensional Linear Regression

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Abstract

There are many scenarios such as the electronic health records where the outcome is much more difficult to collect than the covariates. The data with the observed outcomes are called labeled, and those without the outcomes are referred to as unlabeled. In this paper, we consider the linear regression problem with such a data structure under the high dimensionality. Clearly, any supervised estimators can only use the labeled data. Our goal is to investigate when and how the unlabeled data can be exploited to improve the estimation and inference of the regression parameters in linear models, especially in light of the fact that such linear models may be misspecified in data analysis. In particular, we address the following two important questions. (1) Can we use the labeled data as well as the unlabeled data to construct a semi-supervised estimator such that its convergence rate is faster than the supervised estimators (e.g., lasso and Dantzig selector)? (2) Can we construct confidence intervals or hypothesis tests that are guaranteed to be more efficient or powerful than the supervised estimators? To address the first question, we establish the minimax lower bound for parameter estimation in the semi-supervised setting. We show that the upper bound from the supervised estimators that only use the labeled data cannot attain this lower bound; thus there is a gap between the two bounds. We close this gap by proposing a new semi-supervised estimator which attains the lower bound and therefore improves the rate of the supervised estimators under mild conditions. To address the second question, based on our proposed semi-supervised estimator, we propose two additional estimators for semi-supervised inference, the efficient estimator and the safe estimator. The former is fully efficient if the unknown conditional mean function is estimated consistently, but may not be more efficient than the supervised approach otherwise. The latter usually does not aim to provide fully efficient inference, but is guaranteed to be no worse than the supervised approach, no matter whether the linear model is correctly specified or the conditional mean function is consistently estimated. Thus, it provides a safe use of the unlabeled data for inference. Thorough numerical simulations and real data analysis are provided to back up our theoretical results.

Keyword: Semi-supervised learning, Minimax optimality, High-dimensional inference, Sparsity, Model misspecification

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1 Introduction

Thanks to the development of modern technology, big datasets are routinely collected in many areas including health care, business, epidemiology and social science. Not surprisingly, the availability of large datasets increases the chance of complications and heterogeneity. For example, the response variable(s) may be missing due to various reasons. In Electronic Health Records (EHR) based association studies, one major challenge is the lack of gold-standard health outcomes or phenotypes. The validated phenotypes are often obtained by manual chart reviews, which are often prohibitively expensive. In reality, only a very small subset of patients can be annotated by experts. For the rest of the patients, we only observe their covariate information, which is often high-dimensional.

Developing efficient statistical methods to analyze such data is a timely and important problem. We consider the following so-called semi-supervised setting. Let \( Y \) denote the outcome variable and \( X \) denote the \( p \)-dimensional covariates. In addition to \( n \) i.i.d. samples \( (Y_1, X_1), \ldots, (Y_n, X_n) \sim (Y, X) \), we also observe \( N \) i.i.d. data consisting of only covariates, \( X_{n+1}, \ldots, X_{N+n} \sim X \). Following the convention, the former is referred to as labeled data and the latter is called unlabeled data. For notation simplicity, we denote by \( Y = (Y_1, \ldots, Y_n)^T \in \mathbb{R}^n \), \( X = (X_1, \ldots, X_n)^T \in \mathbb{R}^{n \times p} \) the outcomes and covariates from the labeled data, respectively, and \( \bar{X} = (X_1, \ldots, X_{N+n})^T \in \mathbb{R}^{(N+n) \times p} \) the covariates from the labeled data as well as the unlabeled data. In this work, we focus on high-dimensional problems; namely, \( p \) can be much larger than \( n \). The size of the unlabeled data \( N \) is allowed but not required to be larger than \( n \).

We consider the so-called assumption lean regression framework (Buja et al., 2019; Berk et al., 2019),

\[
Y = f(X) + \epsilon, \tag{1.1}
\]

where \( f(X) = E(Y|X) \) is the unknown conditional mean function, \( \epsilon \) is the random error independent of \( X \in \mathbb{R}^p \) with \( E(\epsilon) = 0 \), \( E(\epsilon^2) = \sigma^2 \), and \( \sigma^2 \) is an unknown parameter. We assume that \( X \) and \( Y \) are centered with \( E(X) = 0 \) and \( E(f(X)) = 0 \). On the one hand, we would like to put as fewer model assumptions on \( f(X) \) as possible to make the model more flexible. On the other hand, for the purpose of interpretability, we often fit simple parametric models such as linear regression to explain the association between \( Y \) and \( X \) in many practical data analysis. To meet both ends, we focus on the linear regression as a working model where the true data generating process follows (1.1). Since

\[
\mathbb{E}[(Y - X^T \theta)^2] = \mathbb{E}[(f(X) - X^T \theta)^2] + \sigma^2,
\]

the regression coefficients in a linear model correspond to the \( L_2(\mathbb{P}) \) projection of \( f(X) \) onto the linear space spanned by \( X \), i.e.,

\[
\theta^* = \arg \min_{\theta \in \mathbb{R}^p} \mathbb{E}[(f(X) - X^T \theta)^2] \in \mathbb{R}^p
\]

which describes the linear dependence between \( Y \) and \( X \). We note that since \( E(X) = 0 \) and \( E(f(X)) = 0 \), the intercept parameter in the working linear regression is 0. Thus, we do not include the intercept parameter in the definition of \( \theta^* \). Our goal is to estimate the high-dimensional parameter \( \theta^* \) and further construct confidence intervals or hypothesis tests for some linear functional of \( \theta^* \), i.e., \( v^T \theta^* \) for some given \( v \in \mathbb{R}^p \).

In the supervised setting with \( n \) labeled observations, a number of penalized estimators have been proposed to estimate \( \theta^* \), such as lasso (Tibshirani, 1996) and Dantzig selector (Candes and...
For statistical inference, there has been some recent research on debiased lasso estimators for hypothesis tests and confidence intervals, for example, Zhang and Zhang (2014); Van de Geer et al. (2014); Javanmard and Montanari (2014); Cai and Guo (2017); Ning and Liu (2017); Neykov et al. (2018), a list that is far from exhaustive. While significant progress has been made towards understanding the estimation and inference in the fully supervised setting, there is very limited research in the semi-supervised setting. It is important to observe that under (1.1), since the linear regression is the working model, the covariate $X$ is no longer the ancillary statistic for the regression parameter $\theta^*$. Therefore, the information of $X$ in the unlabeled data may improve the estimation and inference of $\theta^*$. In particular, we answer two critical questions the presence of the unlabeled data poses.

Q1: Can we use the labeled data as well as the unlabeled data to construct a semi-supervised estimator for $\theta^*$ such that its convergence rate is faster than the supervised estimators (e.g., lasso and Dantzig selector)?

In the literature, Bellec et al. (2018) proposed a modified lasso estimator of $\theta^*$ in the semi-supervised setting and showed that the excess risk of their estimator in prediction has the same rate of convergence as the standard lasso estimator. Their results neither confirm nor deny the existence of estimators with improved statistical rate when unlabeled data are available. To the best of our knowledge, this question remains an open problem.

In Theorem 1, we establish the minimax lower bound for the estimation of $\theta^*$ in the semi-supervised setting. Based on the lower bound, when $N$ is sufficiently large, the error term due to the model misspecification or equivalently the nonlinearity of $f(X)$ becomes ignorable. This reveals one potential benefit from using the unlabeled data in that the estimation of $\theta^*$ can be more robust to the model misspecification. Moreover, we show that the fully supervised estimators (e.g., lasso and Dantzig selector) do not attain this lower bound. To demonstrate how to achieve this lower bound, in Section 2.2 we propose an estimator $\hat{\theta}_D$ under the assumption that the unknown conditional mean function $f(X)$ can be consistently estimated. We show in Theorem 2 that the proposed estimator $\hat{\theta}_D$ attains the minimax lower bound (up to the log $s$ factor). For this reason, we refer $\hat{\theta}_D$ as the optimal semi-supervised estimator. As a byproduct of this theorem, our estimator $\hat{\theta}_D$ has a faster convergence rate than the supervised estimators.

Q2: Does there exist an estimator of the linear functional of $\theta^*$ that is asymptotically normal and is guaranteed to be more efficient than the supervised estimator (e.g., debiased lasso)?

In the literature, several methods have been proposed to address this question in low-dimensional setting with $p$ fixed. Azriel et al. (2016) proposed an adjusted linear regression approach and Chakrabortty and Cai (2018) proposed an efficient and adaptive semi-supervised estimator (EASE) based on non-parametric imputation. Both methods produce more efficient estimators for each component of $\theta^*$ than the least square estimator (LSE) using only labeled data. However, they do not guarantee the efficiency improvement if the parameter of interest is the linear combination of $\theta^*$ (e.g., $\theta_1^* + \theta_2^*$). Therefore, none of the existing methods provides a satisfactory answer to this question, even when $p$ is fixed.
Following our answer to Q1, while the estimator \( \hat{\theta}_D \) is rate optimal, the limiting distribution of \( \hat{\theta}_D \) is intractable due to the regularization. To construct confidence intervals and hypothesis tests, we further propose two estimators based on the existing debiased lasso approach (Zhang and Zhang, 2014; Van de Geer et al., 2014; Javanmard and Montanari, 2014; Cai and Guo, 2017; Ning and Liu, 2017; Neykov et al., 2018). In particular, using \( \hat{\theta}_D \) as an initial estimator, we construct a one-step estimator \( \hat{\theta}^{d} \). In Theorem 3, we show that the estimator \( v^T \hat{\theta}^d \) is asymptotically normal and attains the semi-parametric efficiency bound when \( n \ll N \). For this reason, we call \( \hat{\theta}^d \) efficient semi-supervised estimator. However, this estimator depends on the consistency of the estimate of \( f(X) \).

If \( f(X) \) cannot be consistently estimated, the estimator \( v^T \hat{\theta}^d \) is not guaranteed to be more efficient than the supervised debiased lasso estimators (Van de Geer et al., 2014). To address the question Q2, we further propose a safe semi-supervised estimator which does not require the estimate of \( f(X) \). The main idea is to construct a set of unbiased estimating functions and decorrelate the score function to reduce the variability. In Theorem 5, we show that the corresponding estimator \( v^T \hat{\theta}_S^{d,\psi} \) is asymptotically normal, where \( \psi \) is a tuning parameter. When the linear model is misspecified and \( \lim_{n \to \infty} \frac{n}{n+N} = \rho \) for some \( 0 \leq \rho < 1 \), the estimator \( v^T \hat{\theta}_S^{d,\psi} \) with \( 0 < \psi < 2 \) is strictly more efficient than the debiased lasso, leading to more powerful hypothesis tests and shorter confidence intervals. We attain the maximum variance reduction by choosing \( \psi = 1 \). In addition, if either the linear model is correctly specified \( f(X) = X^T \theta^* \) or the size of the unlabeled data is small \( \lim_{n \to \infty} \frac{n}{n+N} = 1 \) (i.e., \( N \ll n \)), the estimator \( v^T \hat{\theta}_S^{d,\psi} \) is asymptotically equivalent to the debiased lasso estimator. In summary, the estimator \( v^T \hat{\theta}_S^{d,\psi} \) provides a safe use of the unlabeled data, since it is always no worse than the supervised estimators, no matter whether the linear model is correctly specified or the conditional mean function is consistently estimated.

1.1 Other related work

In computer science, a large number of classification algorithms have been developed under semi-supervised setting, which mainly focus on the data with discrete labels; see Zhu (2005); Chapelle et al. (2009) for some surveys. Common assumptions such as manifold assumption and cluster assumption were made in the literature in order to obtain fast rate of convergence in classification (Rigollet, 2006). In non-parametric regression problem, Wasserman and Lafferty (2008) showed that unlabeled data do not always help to improve the rate of the mean squared error, but with semi-supervised smoothness assumption the estimator with faster rate was developed.

Recently, there are progress considering how to safely make use of the unlabeled data to achieve an estimator with smaller asymptotic variance for inference. Zhang et al. (2019) proposed a general semi-supervised inference framework to improve the estimation of the population mean \( \mathbb{E}(Y) \) without specific distributional assumptions relating \( Y \) and \( X \). They allowed the dimension of \( X \) to grow but no faster than \( n^{1/2} \). Therefore, the results cannot be used in high-dimensional setting. With high-dimensional data, Zhang and Bradic (2019) proposed semi-supervised estimators of population mean and variance and established their asymptotic distributions. By fitting a working linear regression, one can rewrite \( \mathbb{E}(Y) \) as a linear combination of \( \theta^* \), \( \mathbb{E}(Y) = \mathbb{E}(X^T \theta^*) \). The way they utilized the unlabeled data is to estimate \( \mathbb{E}(X) \) by \( \sum_{i=n+1}^{n+N} X_i/N \). It is of interest to note that, they required \( \lim_{n \to \infty} \frac{n}{n+N} < 1/2 \) to guarantee the safe inference on \( \mathbb{E}(Y) \) (i.e., more efficient than the
sample mean of $Y$ in the labeled data). In comparison, our proposed safe semi-supervised inference requires a weaker condition $\lim_{n \to \infty} \frac{n}{n+N} < 1$. In high dimensional regime, Cai and Guo (2020) considered how to estimate the explained variance $\theta^T \Sigma \theta^*$ in the semi-supervised setting. Their estimator achieved the optimal rate of convergence and was asymptotically normal. However, their results were established under the assumption that the working linear model is correctly specified, which differed from our assumption lean framework.

1.2 Organization of the Paper

The rest of this paper is organized as follows. In Section 2, we first give the minimax lower bound for semi-supervised estimation, then introduce the proposed estimator and its corresponding upper bound. In Section 3 we devote ourselves into semi-supervised inference, where we propose an efficient procedure provided that the conditional mean function is consistently estimated, and a safe procedure which is guaranteed to be no worse than the one using only the labeled data. Numerical experiments and a real data application are in Sections 4 and 5, respectively. The paper is concluded with a discussion section. All the technical proofs are contained in the appendix.

1.3 Notations

The following notation is adopted throughout this paper. For $v = (v^{(1)}, \ldots, v^{(p)})^T \in \mathbb{R}^p$, and $1 \leq q \leq \infty$, we define $\|v\|_q = (\sum_{i=1}^{p} |v^{(i)}|^q)^{1/q}$, $\|v\|_0 = |\text{supp}(v)|$, where $\text{supp}(v) = \{i : v^{(i)} \neq 0\}$ and $|A|$ is the cardinality of a set $A$. Denote $\|v\|_{\infty} = \max_{1 \leq i \leq p} |v^{(i)}|$ and $v^\otimes 2 = vv^T$. For a matrix $M = [M_{ij}]$, $M_i$ and $M_j$ denote the $i$-th row and $j$-th column respectively. Define $\|M\|_{\max} = \max_{ij} |M_{ij}|$, $\|M\|_1 = \max_i \sum_j |M_{ij}|$, $\|M\|_\infty = \max_j \sum_i |M_{ij}|$. If the matrix $M$ is symmetric, then $\lambda_{\min}(M)$ and $\lambda_{\max}(M)$ are the minimal and maximal eigenvalues of $M$. We denote $I_p$ by the $p \times p$ identity matrix. For $S \subseteq \{1, \ldots, p\}$, let $v_S = \{v^{(k)} : k \in S\}$ and $S^c$ be the complement of $S$. For matrix $X \in \mathbb{R}^{n \times p}$ and index set $D \subseteq \{1, \ldots, n\}$, $X_D = \{X_i : i \in D\}^T \in \mathbb{R}^{|D| \times p}$. For a function $f$, let $\|f\|_2^2 = \mathbb{E}[f(X)^2]$ denote the $L_2(\mathbb{P})$ norm of $f$.

For two positive sequences $a_n$ and $b_n$, we write $a_n \asymp b_n$ if $C \leq a_n/b_n \leq C'$ for some $C, C' > 0$. Similarly, we use $a \lesssim b$ to denote $a \leq Cb$ for some constant $C > 0$. Given $a, b \in \mathbb{R}$, let $a \vee b$ and $a \wedge b$ denote the maximum and minimum of $a$ and $b$. For notational simplicity, we use $C, C', C''$ to denote generic constants, whose values can change from line to line. To characterize the tail behavior of random variables, we introduce the following definition.

**Definition 1** (Sub-Gaussian variable and vector). A random variable $X$ is called sub-Gaussian if there exists some positive constant $K_2$ such that $\mathbb{P}(|X| > t) \leq \exp(1 - t^2/K_2^2)$ for all $t \geq 0$. The sub-Gaussian norm of $X$ is defined as $\|X\|_{\psi_2} = \sup_{p \geq 1} p^{-1/2}(\mathbb{E}|X|^p)^{1/p}$. A vector $X \in \mathbb{R}^p$ is a sub-Gaussian vector if the one-dimensional marginals $v^T X$ are sub-Gaussian for all $v \in \mathbb{R}^p$, and its sub-Gaussian norm is defined as $\|X\|_{\psi_2} = \sup_{\|v\|_2 = 1} \|v^T X\|_{\psi_2}$.
2 Optimal Rate in Semi-supervised Estimation

In Section 2.1, we present the minimax lower bound for the estimation of $\theta^*$ in the semi-supervised setting. A key message from the lower bound is that the benefit of using the unlabeled data is to mitigate the error due to model misspecification. In Section 2.2, we propose a new estimator that nearly attains the lower bound. Throughout the paper, we consider the random design.

2.1 Minimax lower bound for semi-supervised estimation

Recall that in the semi-supervised setting we observe $n$ i.i.d. labeled data $(Y_1, X_1), ..., (Y_n, X_n)$ and additional $N$ unlabeled data $X_{n+1}, ..., X_{N+n} \sim X$. Let $P_{X,Y}$ and $P_X$ denote the joint distribution of $(X, Y)$ and the marginal distribution of $X$, respectively. To establish the minimax lower bound, we consider the following class of distributions

$$\mathcal{P}_{\Phi, \sigma} = \{P_{X,Y} \mid Y = f(X) + \epsilon, \|\theta^*\|_0 \leq s, \text{ and } \text{Var}(\epsilon) = \sigma^2, \mathbb{E}(f(X) - X^T \theta^*)^2 \leq \Phi^2, P_X \in \mathcal{P}_X\},$$

where $f(X) = \mathbb{E}(Y | X)$, $\theta^* = \arg\min_{\theta \in \mathbb{R}} \mathbb{E}[(f(X) - X^T \theta)^2]$ depends on the distribution $P_{X,Y}$ implicitly, and $\mathcal{P}_X = \{P_X | \mathbb{E}[X] = 0, \text{Var}(X_j) = 1 \text{ and } \lambda_{\min}(\text{Cov}(X)) \geq C_{\text{min}} > 0\}$ with some constant $C_{\text{min}}$. For notational simplicity, we write $\mathbb{E}(\cdot)$ for $\mathbb{E}_{P_{X,Y}}(\cdot)$. We note that, $\mathcal{P}_{\Phi, \sigma}$ is indexed by two non-negative parameters $\Phi^2$ and $\sigma^2$, where the former controls the magnitude of model misspecification $f(X) - X^T \theta^*$ or equivalently the nonlinearity of $f(X)$ in the second moment and the latter is the variance of $\epsilon$. In particular, we allow $\Phi^2$ to grow with $n$ in our framework.

The following theorem offers the lower bound for the convergence rate of any estimator of $\theta^*$ over the class of distributions $\mathcal{P}_{\Phi, \sigma}$.

**Theorem 1.** If $s \log(p/s) \leq Cn, (s - 1)c_1 \log(p/s) \leq 8(n + N)$ for some absolute constants $C, c_1$ and $2 \leq s \leq (n - 1)/4$, we have that for any $1 \leq q \leq \infty$,

$$\inf_{\hat{\theta}} \sup_{P_{X,Y} \in \mathcal{P}_{\Phi, \sigma}} \mathbb{P}_{P_{X,Y}} [||\hat{\theta} - \theta^*||_q \geq c_1 s^{1/q} \left(\Phi \sqrt{\frac{\log(p/s)}{n + N}} + \sigma \sqrt{\frac{\log(p/s)}{n}}\right)] > c_2,$$

where $\inf_{\hat{\theta}}$ denotes the infimum over all estimators of $\theta^*$, $c_1$ and $c_2$ are some positive constants and we simply denote $s^{1/\infty} = 1$.

**Remark 1.** (1) The lower bound (2.1) consists of two components. Up to some absolute constants, the first term $s^{1/q} \Phi \sqrt{\log(p/s)/(n + N)}$ corresponds to the error due to potential model misspecification and the second term $s^{1/q} \sigma \sqrt{\log(p/s)/n}$ comes from the uncertainty inherited from the randomness of the error $\epsilon$, which always exists even if the regression function is linear $f(X) = X^T \theta^*$. In this case, we have $\Phi = 0$ and the lower bound agrees with the existing result for sparse linear regression (Verzelen, 2012; Bellec et al., 2018).

(2) The sample size of the unlabeled data $N$ plays an important role in the lower bound (2.1). We first consider the case $\Phi \sigma \sqrt{\frac{n}{n+N}} \to \infty$, which may happen if $\Phi \to \infty$. In Appendix B.1, we construct examples in which we have $\Phi \asymp s^{1/2}$ so that $\Phi$ tends to infinity as the sparsity grows. In this case, the dominating term in the lower bound is $s^{1/q} \Phi \sqrt{\log(p/s)/(n + N)}$, which can be
Figure 1: Plot of the lower bound with $q = 1$ in Theorem 1 (the solid curve) and the upper bound from Dantzig in (2.3) (the dashed line) against the value of $(N + n)/n$. In the plot, we fix $n$ and vary the value of $N$. The region between these two lines corresponds to the gap between the lower bound and the upper bound for the supervised estimator.

reduced as $N$ increases. If $N$ is sufficiently large such that $\frac{\Phi}{\sigma} \sqrt{\frac{n}{n+N}} \rightarrow c < \infty$, the lower bound attains its minimum $s^{1/q}\sigma \sqrt{\frac{\log(p/s)}{n}}$, which can be viewed as the irreducible error in the semi-supervised setting since a further increase of $N$ would no longer decrease the lower bound. As an illustration, we plot the lower bound in Figure 1.

(3) In the following, we compare the lower bound with the upper bound from the following supervised Dantzig selector, which only uses the labeled data,

$$\hat{\theta}_L = \arg \min_{\| \theta \|_1} \text{ s.t. } \left\| \frac{1}{n} \sum_{i=1}^{n} (Y_i - X_i^T \theta)X_i \right\|_{\infty} \leq \lambda_L, \quad (2.2)$$

where $\lambda_L$ is a tuning parameter. Under the same assumption lean framework, we show in Lemma 11 that the upper bound for $\| \hat{\theta}_L - \theta^* \|_1$ is

$$s(\Phi + \sigma) \sqrt{\frac{\log p}{n}}, \quad (2.3)$$

which differs from the lower bound in (2.1) with $q = 1$ (ignoring the log $s$ factor); see Figure 1. Moreover, under the condition $N \gg n$, it can be easily shown that the lower bound in (2.1) is strictly smaller in order than the upper bound of $\hat{\theta}_L$ if and only if $\Phi/\sigma \rightarrow \infty$. In this case, the fully supervised estimator does not attain the lower bound and thus is sub-optimal in the minimax sense; see Figure 1.
2.2 Optimal semi-supervised estimator

**Motivation.** To motivate our estimator, we first briefly explain how the convergence rate of \( \hat{\theta}_L \) in (2.2) is derived. Following the standard argument in Bickel et al. (2009), the Dantizig selector satisfies \( \| \hat{\theta}_L - \theta^* \|_1 = O_p(s \lambda_L) \), where the tuning parameter \( \lambda_L \gtrsim \frac{1}{n} \sum_{i=1}^{n} X_i (Y_i - X_i^T \theta^*) \|_\infty \). In the proof of Lemma 11, we further show that \( \frac{1}{n} \sum_{i=1}^{n} X_i (Y_i - X_i^T \theta^*) \|_\infty \lesssim \sqrt{\frac{\log p}{n} \{ \mathbb{E} (Y_i - X_i^T \theta^*)^2 \}^{1/2}} \) with high probability. The desired bound (2.3) is obtained by noting that
\[
\mathbb{E} (Y_i - X_i^T \theta^*)^2 = \mathbb{E} (Y_i - f(X_i))^2 + \mathbb{E} (f(X_i) - X_i^T \theta^*)^2 \leq \sigma^2 + \Phi^2, \tag{2.4}
\]
as \( \mathbb{E} (\epsilon | X) = 0 \), where \( \mathbb{E} (\epsilon^2) = \sigma^2 \) and \( \mathbb{E} (f(X) - X^T \theta^*)^2 \leq \Phi^2 \). In view of (2.3) and Remark 1 (3), we see that the slow rate of \( \hat{\theta}_L \) is driven by the \( \mathbb{E} (f(X) - X^T \theta^*)^2 \) term in (2.4).

**Key Step.** To reduce the effect of \( \Phi^2 \) in the upper bound, our key idea is to decompose the score function
\[
\frac{1}{n} \sum_{i=1}^{n} X_i (Y_i - X_i^T \theta^*) = \frac{1}{n} \sum_{i=1}^{n} X_i (Y_i - f(X_i)) + \frac{1}{n} \sum_{i=1}^{n} X_i (f(X_i) - X_i^T \theta^*),
\]
and replace the last term with \( \frac{1}{n+N} \sum_{i=1}^{n+N} X_i (f(X_i) - X_i^T \theta^*) \), the sample average over both labeled and unlabeled data. This leads to the following modified score function
\[
\frac{1}{n} \sum_{i=1}^{n} X_i (Y_i - f(X_i)) + \frac{1}{n+N} \sum_{i=1}^{n+N} X_i (f(X_i) - X_i^T \theta^*) = \xi - \hat{\Sigma}_{n+N} \theta^*, \tag{2.5}
\]
where \( \hat{\Sigma}_{n+N} = \frac{1}{n+N} \sum_{i=1}^{n+N} X_i^2 \) and
\[
\xi = \frac{1}{n} \sum_{i=1}^{n} X_i Y_i - \frac{1}{n} \sum_{i=1}^{n} X_i f(X_i) + \frac{1}{n+N} \sum_{i=1}^{n+N} X_i f(X_i). \tag{2.6}
\]

**Computation of \( \bar{\xi} \).** To compute \( \bar{\xi} \), we need to find an estimator for \( f(\cdot) \), the unknown conditional mean function. For model flexibility, we can use semiparametric/nonparametric techniques to estimate \( f(\cdot) \) and will discuss some examples of \( \hat{f}(\cdot) \) later, such as in Remark 2. A serious challenge may arise from deriving the theoretical property of our proposed optimal semi-supervised estimator if we use all data to obtain \( \hat{f}(\cdot) \) due to the dependence between the estimator \( \hat{f}(\cdot) \) and the data \( (X_i, Y_i) \) in the sample average from \( \bar{\xi} \). To bypass this challenge, we adopt the popular cross-fitting technique that was devised for semiparametric estimation problems (Bickel, 1982; Schick, 1986) as well as for high-dimensional data (Robins et al., 2017; Chernozhukov et al., 2018). For notational simplicity, we denote by \( D^* \) the labeled data and \( D \) the full dataset with both labeled and unlabeled data. Without loss of generality, we split the labeled data \( D^* \) into two folds \( D_1^* \) and \( D_2^* \) with size \( n_1 = n_2 = n/2 \). Similarly, we split the unlabeled data into two folds \( U_1 \) and \( U_2 \) with size \( N_1 = N_2 = N/2 \). Merging with \( D_1^* \) and \( D_2^* \) respectively, we obtain two independent data sets \( D_1 = D_1^* \cup U_1 \) and \( D_2 = D_2^* \cup U_2 \). Next, for \( j = 1, 2 \), we train the estimator \( \hat{f}^{-j} \) using the data \( D^* \setminus D_j^* \) and then construct
\[
\bar{\xi}_j = \frac{1}{n_j} \sum_{i \in D_j^*} X_i Y_i - \frac{1}{n_j} \sum_{i \in D_j^*} X_i \hat{f}^{-j}(X_i) + \frac{1}{n_j + N_j} \sum_{i \in D_j} X_i \hat{f}^{-j}(X_i). \tag{2.7}
\]
In view of the modified score function (2.5), replacing $\bar{\xi}$ with $\hat{\xi} = (\hat{\xi}_1 + \hat{\xi}_2)/2$, we propose the following estimator

$$
\hat{\theta}_D = \arg\min \|\theta\|_1, \quad \text{s.t.} \quad \|\hat{\Sigma}_{n+N}\theta - \hat{\xi}\|_{\infty} \leq \lambda_D.
$$

(2.8)

### 2.3 Upper bound of the proposed estimator

Now we develop the theoretical property of the proposed estimator $\hat{\theta}_D$.

**Assumption 1.** We make the following assumptions:

(A1) $\Sigma^{-1/2}X$ is a zero mean sub-gaussian vector with bounded sub-gaussian norm and $\text{Cov}(X) = \Sigma$ has smallest eigenvalue $\Lambda_{\min}(\Sigma) \geq C_{\min} > 0$ for some positive constant $C_{\min}$. Moreover, $\max_{1 \leq j \leq p} \Sigma_{jj} = O(1)$.

(A2) $\max_{1 \leq i \leq n+N} \|X_i\|_{\infty} \leq K_1$ where we allow $K_1$ to diverge with $(n,N,p)$.

(A3) $E(\epsilon^2) = \sigma^2$ and $E[(f(X) - X^T\theta^*)^2] \leq \Phi^2$.

(A4) $\theta^*$ is $s$-sparse with $\|\theta^*\|_0 = s$, and $s \log p / (n+N) = O(1)$.

Assumption (A1) is a standard technical condition for $X$ in order to verify the restricted eigenvalue (RE) condition (Bickel et al., 2009). Assumption (A2) imposes the boundedness of the covariates, which simplifies the analysis when the linear model is misspecified (Bühlmann and Van de Geer, 2015). In particular, when $X_i$ is uniformly bounded, $K_1$ becomes a constant. If each component of $X_i$ is Gaussian or sub-Gaussian, Assumption (A2) still holds with high probability with $K_1 = \sqrt{\log[p(n+N)]}$. Assumption (A3) only requires the existence of the second moment of $\epsilon$ and $f(X) - X^T\theta^*$. We note that, unlike most of the work in high-dimensional statistics including Bickel et al. (2009), we do not assume the residual $Y - X^T\theta^*$ is sub-Gaussian. This is because the misspecified model $Y - X^T\theta^* = \epsilon + (f(X) - X^T\theta^*)$ contains the nonlinearity term $f(X) - X^T\theta^*$ which can be large. While we only assume the moment condition in Assumption (A3), the boundedness in Assumption (A2) enables us to apply the Nemirovski moment inequality (Lemma 8) to control the deviation of the sample estimates from their population. Assumption (A4) is the sparsity condition. In particular, Bühlmann and Van de Geer (2015) provided some sufficient conditions on $f(X)$ and the distribution of $X$ under which $\theta^*$ is sparse in the misspecified model. We further require $s \log p / (n+N) = O(1)$ to verify the RE condition under the random design; see Lemma 9.

Given Assumption 1, the following theorem shows that the proposed estimator $\hat{\theta}_D$ in (2.8) achieves the near optimal rate for estimating $\theta^*$. For the purpose of inference, we only present the asymptotic results, where $n,p \to \infty$ and $N$ can be either fixed or tends to infinity as well.

**Theorem 2.** Suppose Assumption 1 holds and the estimator $\hat{f}^{-j}(X)$ satisfies

$$
\|\hat{f}^{-j} - f\|_2 = O_p(b_n),
$$

...
for \( j = 1, 2 \), where \( b_n \) is a deterministic sequence. With tuning parameter \( \lambda_D \propto K_1(\Phi \sqrt{\frac{\log p}{n+N}} + \sigma \sqrt{\frac{\log p}{n}} + b_n \sqrt{\frac{\log p}{n}}) \), the estimator \( \hat{\theta}_D \) in (2.8) achieves the following error bounds

\[
\|\hat{\theta}_D - \theta^*\|_1 = O_p\left( K_1 s \left\{ \Phi \sqrt{\frac{\log p}{n+N}} + (\sigma + b_n) \sqrt{\frac{\log p}{n}} \right\} \right),
\]

\[
\|\hat{\theta}_D - \theta^*\|_2 = O_p\left( K_1 s^{1/2} \left\{ \Phi \sqrt{\frac{\log p}{n+N}} + (\sigma + b_n) \sqrt{\frac{\log p}{n}} \right\} \right).
\]

Moreover, if \( b_n/\sigma = o(1) \) and \( K_1 = O(1) \), we obtain

\[
\|\hat{\theta}_D - \theta^*\|_1 = O_p\left( s \left\{ \Phi \sqrt{\frac{\log p}{n+N}} + \sigma \sqrt{\frac{\log p}{n}} \right\} \right),
\]

\[
\|\hat{\theta}_D - \theta^*\|_2 = O_p\left( s^{1/2} \left\{ \Phi \sqrt{\frac{\log p}{n+N}} + \sigma \sqrt{\frac{\log p}{n}} \right\} \right),
\]

which match the minimax lower bound with \( q = 1, 2 \) in Theorem 1 up to a \( \log s \) factor.

**Remark 2.** Assume that \( \sigma^2 \) is bounded away from 0 by a constant. In order to attain the near minimax optimal rate, we only need a very mild condition on \( \hat{f}^j \), that is \( \hat{f}^j \) is consistent in the \( L_2(\mathbb{P}) \) norm. If the knowledge of \( f(X) \) is available to some extent, we can leverage this information to construct estimators of \( f(X) \). For example, if \( f(X_i) \) can be well approximated by sparse additive models \( f(X_i) = \sum_{k \in S} f_k(X_{ik}) \) for some set \( S \subseteq \{1, \ldots, p\} \) with small cardinality, then we can directly apply the existing estimators in the literature, see Lin and Zhang (2006); Meier et al. (2009); Huang et al. (2010); Raskutti et al. (2012) among many others. In particular, Corollary 2 in Huang et al. (2010) implies that their adaptive group lasso estimator \( \hat{f} \) satisfies \( \|\hat{f} - f\|_2 = O_p(n^{-d/(2d+1)}) \), where \( d \) is the smoothness of the function \( f_k(\cdot) \). This meets the condition \( b_n = o(1) \).

**Remark 3.** In a recent work, Bellec et al. (2018) proposed a modified lasso estimator for prediction in the semi-supervised setting, which can be reformatted as the following Dantzig selector

\[
\hat{\theta}_U = \arg\min \|\theta\|_1, \quad \text{s.t.} \quad \|\hat{\Sigma}_{n+N}\theta - \frac{1}{n} \sum_{i=1}^n X_i Y_i\|_\infty \leq \lambda_U,
\]

where \( \hat{\Sigma}_{n+N} = \frac{1}{n+N} \sum_{i=1}^{n+N} X_i^\otimes 2 \). They showed that if a large number of unlabeled data are used to compute \( \hat{\Sigma}_{n+N} \), it becomes more plausible to assume that the compatibility (or RE) constant is bounded away from zero. Moreover, they proved that the error bound for the excess risk in prediction remains \( O_p(s \log p/n) \) under certain conditions, including \( |Y| \leq C \) for some constant \( C > 0 \) which indeed implies \( \Phi \) and \( \sigma = O(1) \) by their proof of Theorem 7. To make a fair comparison of \( \hat{\theta}_U \) with our estimator \( \hat{\theta}_D \), we show that under the same conditions in our Theorem 2,

\[
\|\hat{\theta}_U - \theta^*\|_1 = O_p\left( s(\Phi + \sigma + (\theta^* \hat{\Sigma} \theta^*)^{1/2}) \sqrt{\frac{\log p}{n}} \right).
\]

The proof is deferred to Appendix B.2. It is seen that \( \hat{\theta}_U \) has a slower rate than our estimator \( \hat{\theta}_D \) if \( \Phi/\sigma \to \infty \) or \( \theta^* \hat{\Sigma} \theta^*/\sigma^2 \to \infty \). Perhaps, a more surprising fact is that the convergence rate of
\[ \hat{\theta}_U \] can be even slower than the fully supervised estimator \( \hat{\theta}_L \) in (2.3) if \( \theta^* \Sigma \theta^*/(\sigma^2 + \Phi^2) \to \infty. \) Indeed, our simulation studies confirm that the estimator \( \hat{\theta}_U \) often produces larger estimation error than the lasso/Dantzig selector that only use the labeled data.

Finally, we note that the estimator \( \hat{\theta}_U \) can be considered as an extreme case of our estimator \( \hat{\theta}_D \) that does not account for the estimated conditional mean function in (2.7) (i.e., set \( \hat{f}^{-j} = 0 \) in \( \hat{\xi}_j \)). This remark shows that, if \( f(\cdot) \) is poorly estimated, it may not be beneficial to estimate \( \Sigma \) by \( \hat{\Sigma}_{n+N} \) as in (2.9), a common procedure to incorporate the information from unlabeled data.

### 3 Semi-supervised Inference

In this section, we address the inference problem for a linear combination of \( \theta^* \) under the semi-supervised setting. In Section 3.1, we consider the case where there exists a proper estimator of the unknown conditional mean function \( f(X) \). An efficient semi-supervised inference procedure is proposed. We further extend our method in Section 3.2 to a more general case where we do not require the estimation of \( f(X) \). We propose a safe semi-supervised inference approach that guarantees the efficiency improvement over the supervised debiased estimators.

#### 3.1 Efficient semi-supervised inference

Motivated by the formulation of the regularized estimator \( \hat{\theta}_D \) in (2.8), we can view \( h(\tilde{X}, Y; \theta) = \tilde{\Sigma}_{n+N} \theta - \tilde{\xi} \) as an estimating function for \( \theta \). Borrowing the idea from the classical one-step estimator and the debiased lasso, we construct the following estimator,

\[
\hat{\theta}^d = \hat{\theta}_D - \hat{\Omega} h(\tilde{X}, Y; \hat{\theta}_D) = \hat{\theta}_D + \hat{\Omega} (\tilde{\xi} - \tilde{\Sigma}_{n+N} \hat{\theta}_D),
\]  

(3.1)

where \( \hat{\Omega} \) is an estimator of the precision matrix \( \Omega = \Sigma^{-1} \). To be specific, we consider the following node-wise lasso estimator (Meinshausen and Bühlmann, 2006) based on both labeled and unlabeled data \( \tilde{X} \). For \( k \in [p] \), we define the vector \( \hat{\gamma}_k = \{\hat{\gamma}_{k,j} : j \in [p] \text{ and } j \neq k\} \) as

\[
\hat{\gamma}_k = \arg\min_{\gamma \in \mathbb{R}^p} \left\{ \frac{1}{n+N}\|\tilde{X}_k - \tilde{X}_{-k}\gamma\|^2_2 + 2\lambda_k\|\gamma\|_1 \right\}.
\]  

(3.2)

Denote by

\[
\hat{C} = \begin{bmatrix}
1 & -\hat{\gamma}_{1,2} & \cdots & -\hat{\gamma}_{1,p} \\
-\hat{\gamma}_{2,1} & 1 & \cdots & -\hat{\gamma}_{2,p} \\
\vdots & \vdots & \ddots & \vdots \\
-\hat{\gamma}_{p,1} & -\hat{\gamma}_{p,2} & \cdots & 1
\end{bmatrix}
\]

and let

\[
\hat{T}^2 = \text{diag}(\hat{\tau}_1^2, \ldots, \hat{\tau}_p^2), \text{ where } \hat{\tau}_k^2 = \frac{1}{n+N}(\tilde{X}_k - \tilde{X}_{-k}\hat{\gamma}_k)^T \tilde{X}_k.
\]  

(3.3)

The node-wise lasso estimator is defined as

\[
\hat{\Omega} = \hat{T}^{-2}\hat{C}.
\]  

(3.4)
Assumption 2. Denote $\Omega = \Sigma^{-1}$. Assume $\max_{1 \leq i \leq n+N} \|\Omega X_i\|_\infty \leq K_2$, and $\max_{1 \leq k \leq p} \|\Omega_k\|_0 \leq s_\Omega$ satisfies $K^2 s_\Omega \sqrt{n} \log p/(n+N) = o(1)$, where $K = K_1 \lor K_2$ with $K_1$ defined in Assumption 1.

Assumption 2 and (A2) in Assumption 1 together imply the strong boundedness condition for some $b$.

Assumption 2. Denote $\Omega$ and $\hat{\Omega}$ in the matrix $L_\infty$ norm. While it is possible to relax the sparsity assumption $\max_{1 \leq k \leq p} \|\Omega_k\|_0 \leq s_\Omega$ (Javanmard and Montanari, 2014), we make this assumption in order to show the proposed estimator is regular and asymptotically linear, which facilitates the comparison with other competing estimators in terms of asymptotic efficiency. Finally, we note that Assumptions 1 and 2 do not impose or imply any upper bound on $\Lambda_{\max}(\Sigma)$. For example, we allow $\Sigma$ to be an equicorrelation matrix, whose largest eigenvalue is proportional to the dimension $p$. Given these assumptions, the following theorem shows that $v^T \hat{\theta}^d$ is asymptotically normal for a linear functional $v^T \theta^*$. 

Theorem 3. Suppose Assumptions 1 and 2 hold. By choosing $\lambda_D \asymp K_1(\Phi \sqrt{\log p/n} + \sqrt{\sigma \log p/n} + b_n \sqrt{\log p/n})$ and $\lambda_k \asymp K_2 \sqrt{\log p/n}$ uniformly over $k$, we obtain that for any $v \neq 0 \in \mathbb{R}^p$,

$$v^T(\hat{\theta}^d - \theta^*) = \frac{1}{n} \sum_{i=1}^{n} v^T W_i(Y_i - f(X_i)) + \frac{1}{n+1} \sum_{i=1}^{n+N} v^T W_i(f(X_i) - X_i^T \theta^*) + O_p(\delta_n), \quad (3.5)$$

where $W_i = \Omega X_i$ and $\delta_n = \|v\|_1(\hat{R}_1 + R_2)$ with

$$R_1 = K_1 K(s \lor s_\Omega) \left( \Phi \log p/n + (\sigma + b_n) \log p/n \sqrt{n/(n+N)} \right), \quad R_2 = K_2 b_n \sqrt{\log p/n}$$

and $b_n$ is defined in Theorem 2. In addition, if

$$\frac{n^{1/2} \delta_n}{(v^T (\sigma^2 \Omega + \frac{n}{n+N} \Gamma) v)^{1/2}} = o(1) \quad (3.6)$$

with $\Gamma = \mathbb{E}(W_i^{\otimes 2}(f(X_i) - X_i^T \theta^*))$, $\epsilon$ and $\eta(X) = f(X) - X^T \theta^*$ satisfy

$$\|v\|_1^{2+\delta} K_2^2 + \frac{\mathbb{E}(|\epsilon|^{2+\delta})}{n^{\delta/2} (\sigma^2 \Omega v)^{1+\delta/2}} + \frac{\mathbb{E}|\eta(X)|^{2+\delta}}{(n+1)\delta/2 (v^T \Gamma v)^{1+\delta/2}} = o(1), \quad (3.7)$$

for some $\delta > 0$, then

$$\frac{n^{1/2} v^T(\hat{\theta}^d - \theta^*)}{(v^T (\sigma^2 \Omega + \frac{n}{n+N} \Gamma) v)^{1/2}} \overset{d}{\rightarrow} \mathcal{N}(0, 1). \quad (3.8)$$

The asymptotic expansion of $v^T(\hat{\theta}^d - \theta^*)$ is presented in (3.5), where the remainder term $\delta_n$ consists of two components $R_1$ and $R_2$, which come from the cross product of the estimation errors of $\hat{\Omega}$ and $\hat{\theta}_D$ in Theorem 2 and the plug-in error of $\hat{f}^{-1}$ in $\xi$, respectively. To establish the asymptotic normality of $v^T(\hat{\theta}^d - \theta^*)$, we further need to assume that $\delta_n$ is sufficiently small and the Lyapunov condition holds so that one can apply the central limit theorem to the leading terms in (3.5). These
two conditions are rigorously formulated in (3.6) and (3.7). To further simplify (3.6) and (3.7), assume that \( \sigma^2 v^T \Omega v \geq C\|v\|^2_2 \) and \( v^T \Gamma v \geq C\|v\|^2_2 \) for some constant \( C \), \( \mathbb{E}[|\epsilon|^{2+\delta}] \), \( \mathbb{E}[\eta(X)]^{2+\delta} \), \( K \) are all \( O(1) \) and \( b_n = o(1) \). Under these mild conditions, (3.6) and (3.7) are implied by

\[
\frac{\|v\|_1}{\|v\|_2} \left[ \frac{(s \vee s_0) \log p}{\sqrt{n + N}} + b_n \sqrt{\log p + n^{-\frac{\delta}{2(2+\delta)}}} \right] = o(1).
\]  

(3.9)

**Remark 4.** (1) The bound (3.9) requires the ratio \( \|v\|_1/\|v\|_2 \) cannot be too large which excludes the case that \( v \) has many large entries (e.g., \( v = (1,1,...,1)^T \)). This observation agrees with the theoretical results in Cai and Guo (2017), as the debiased estimator does not yield optimal confidence intervals for \( v^T \theta^* \) when \( v \) is a dense vector. To see some concrete examples that our results are applicable, we first note that if \( v = e_j \) the jth basis vector in \( \mathbb{R}^p \), then \( v^T \hat{\theta}^d = \hat{\theta}^d_j \) reduces to the estimate of \( \theta_j \). Our condition (3.9) becomes \( (s \vee s_0) \log p = o(\sqrt{n + N}) \) and \( b_n = o(1/\sqrt{\log p}) \). The former is a standard condition for debiased inference adapted to the semi-supervised setting and the latter is slightly stronger than the consistency of \( \hat{f}^{-j} \) required in Theorem 2; see Remark 2 for details. The same comments are applicable if the parameter of interest \( v^T \theta^* \) is a linear combination of \( \theta^* \) with \( \|v\|_2 \) fixed.

Indeed, the set of vector \( v \) in \( \mathbb{R}^p \) satisfying (3.9) forms a cone \( \left\{ \frac{\|v\|_1}{\|v\|_2} \leq t_n \left[ \frac{(s \vee s_0) \log p}{\sqrt{n + N}} + b_n \sqrt{\log p + n^{-\frac{\delta}{2(2+\delta)}}} \right]^{-1} \right\} \) for some \( t_n = o(1) \). Compared to Cai and Guo (2017) who proposed the debiased estimator for \( v^T \theta^* \) with sparse \( v \), the cone condition (3.9) may still hold if \( v \) is approximately sparse with many small but nonzero entries. Our results are still applicable in this case.

(2) Assuming \( \|v\|_1/\|v\|_2 \) is a constant and \( N \gg n \), we can see from (3.9) that in the semi-supervised setting we need \( (s \vee s_0) \log p = o(\sqrt{N}) \), which is much weaker than the similar condition \( (s \vee s_0) \log p = o(\sqrt{n}) \) for the supervised estimators (up to some logarithmic factors). Thus, with a large amount of unlabeled data, our inference results may still hold for models with large \( s \).

**Remark 5.** (Efficiency improvement and semi-parametric efficiency bound). We first note that, when the linear model is correctly specified i.e. \( f(X) = X^T \theta^* \), we have \( \Gamma = 0 \) and the asymptotic variance of \( v^T \hat{\theta}^d \) reduces to \( \sigma^2 v^T \Omega v \), which agrees with the asymptotic variance of the debiased estimator in fully supervised setting and also matches the semi-parametric efficiency bound. In this case, the information of \( X \) contained in the unlabeled data is ancillary and does not contribute to the inference on \( \theta \); see also Azriel et al. (2016); Chakrabortty and Cai (2018).

In the following, we assume \( \Gamma \) is strictly positive definite. Recall that our asymptotic analysis requires \( n, p \to \infty \) and allows \( N \) to be either fixed or grow with \( n \). In the following, we discuss the asymptotic variance of \( v^T \hat{\theta}^d \) in (3.9) according to the magnitude of \( N \).

(1) \( \lim_{n \to \infty} \frac{n}{\sqrt{n + N}} = 1 \). Denote \( \mathbf{K} = \mathbb{E}[X^2(Y - X^T \theta^*)^2] \). It is seen that \( \mathbf{K} = \sigma^2 \mathbf{\Sigma} + \mathbf{\Sigma} \Gamma \mathbf{\Sigma} \). In this case, the asymptotic variance of \( v^T \hat{\theta}^d \) reduces to \( v^T (\sigma^2 \Omega + \Gamma) v = v^T \Omega \mathbf{K} \Omega v \), which is the asymptotic variance of the debiased estimator in the fully supervised setting; see Bühlmann and Van de Geer (2015); Ning and Liu (2017). As expected, when \( N \ll n \), the amount of unlabeled data is not sufficiently large to improve the asymptotic efficiency of the estimator.

(2) \( \lim_{n \to \infty} \frac{n}{\sqrt{n + N}} = \rho \) for some \( 0 < \rho < 1 \). In this case, the asymptotic variance \( v^T (\sigma^2 \Omega + \rho \Gamma) v \) is strictly smaller than \( v^T \hat{\theta}^d \). Thus, the unlabeled data can be used to improve the asymptotic efficiency for inference.
(3) \( \lim_{n \to \infty} \frac{n}{n+N} = 0 \). In the case, the asymptotic variance becomes \( \sigma^2 v^T \Omega v \). Indeed, if the distribution of \( X \) is known, the semi-parametric efficiency bound for estimating \( v^T \theta^* \) is exactly \( \sigma^2 v^T \Omega v \) as well; see Chakrabortty and Cai (2018) and the reference therein. Thus, when \( N \gg n \), our estimator attains the semi-parametric efficiency bound.

In the following, we consider how to estimate the asymptotic variance of \( v^T \hat{\theta}^d \). To estimate \( \sigma^2 \), we apply the cross-fitting technique. Specifically, for \( j = 1, 2 \), define

\[
\hat{\sigma}_j^2 = \frac{1}{n_j} \sum_{i \in D_j^c} (Y_i - \hat{f}^{-j}(X_i))^2.
\]

We estimate \( \sigma^2 \) by \( \hat{\sigma}^2 = (\hat{\sigma}_1^2 + \hat{\sigma}_2^2)/2 \). Similarly, define

\[
\hat{\Gamma}_j = \frac{1}{n_j + N_j} \sum_{i \in D_j} (\hat{\eta}_i^{-j})^2 \hat{\Omega} X_i X_i^T \hat{\Omega},
\]

where \( \hat{\eta}_i^{-j} = \hat{f}^{-j}(X_i) - \hat{\theta}^d_j X_i \) and \( \hat{\Omega} \) is defined in (3.4). We then estimate \( \Gamma \) by \( \hat{\Gamma} = (\hat{\Gamma}_1 + \hat{\Gamma}_2)/2 \).

The following Proposition shows that the asymptotic variance of \( v^T \hat{\theta}^d \) can be consistently estimated by the plug-in estimator \( v^T (\hat{\sigma}^2 \hat{\Omega} + \frac{n}{n+N} \hat{\Gamma}) v \).

**Proposition 4.** Suppose the conditions in Theorems 2 and 3 hold. To simplify the presentation, we further assume \( \mathbb{E}(\xi^4) = O(1), \mathbb{E}(\eta^4(X)) = O(1) \) and \( K \sqrt{\frac{2 \log p}{n+N}} = o(1) \). Then

\[
\left| v^T (\hat{\sigma}^2 \hat{\Omega} + \frac{n}{n+N} \hat{\Gamma}) v - v^T (\sigma^2 \Omega + \frac{n}{n+N} \Gamma) v \right| = O_P \left( \frac{\|v\|_2^2 (\frac{1}{\sqrt{n}} + b_n^2) + \text{Rem}_N}{\sqrt{n+N}} \right),
\]

where

\[
\text{Rem}_N = \frac{n}{n+N} K^2 \|v\|^2 b_n + K^3 \|v\|^2 \left( s \lor s_\Omega \right) \sqrt{\frac{\log p}{n+N}}.
\]

Under the additional assumptions \( \sigma^2 v^T \Omega v \geq C \|v\|_2^2 \) and \( \text{Rem}_N/\|v\|_2^2 = o(1) \), we have

\[
\frac{n^{1/2} v^T (\hat{\theta}^d - \theta^*)}{(v^T (\hat{\sigma}^2 \hat{\Omega} + \frac{n}{n+N} \hat{\Gamma}) v)^{1/2}} \xrightarrow{d} \mathcal{N}(0,1).
\]

To better understand the convergence rate of the estimated asymptotic variance, we decompose the error in (3.10) into two terms, \( \|v\|_2^2 (\frac{1}{\sqrt{n}} + b_n^2) \) and \( \text{Rem}_N \). The former is due to the estimation error of \( \hat{\sigma}^2 \) and the latter comes from the error of \( \hat{\Gamma} \) and \( \hat{\Omega} \). It is of interest to note that, if \( N \gg n \), the error term \( \text{Rem}_N \) may vanish to 0 fast enough, so that the convergence rate of the estimated asymptotic variance in (3.10) is dominated by \( \|v\|_2^2 (\frac{1}{\sqrt{n}} + b_n^2) \). In addition, for many practical estimators \( \hat{f}^{-j} \), such as the group lasso estimator for sparse additive models in Remark 2, its convergence rate in \( L_2(\mathbb{P}) \) norm is no slower than \( n^{-1/4} \), that is \( b_n = o(n^{-1/4}) \). In this case, the rate in (3.10) further reduces to \( \|v\|_2^2 / \sqrt{n} \), which is the best possible rate for estimating the variance even if \( \Omega, \Gamma \) and \( f(X) \) are known. Thus, the unlabeled data lead to a more accurate estimate of the asymptotic variance.

Finally, from (3.12) we can construct the \( (1 - \alpha) \) confidence interval for \( v^T \theta^* \) as \( [v^T \hat{\theta}^d - z_{1-\alpha/2} n^{-1/2} s_d, v^T \hat{\theta}^d + z_{1-\alpha/2} n^{-1/2} s_d] \), where \( z_{1-\alpha/2} \) is the \( 1 - \alpha/2 \) quantile of a standard normal distribution and \( s_d = (v^T (\hat{\sigma}^2 \hat{\Omega} + \frac{n}{n+N} \hat{\Gamma}) v)^{1/2} \). Similarly, if one is interested in testing the hypothesis \( H_0 : v^T \theta^* = 0 \), we can construct the test statistic \( n^{1/2} v^T \hat{\theta}^d / (v^T (\hat{\sigma}^2 \hat{\Omega} + \frac{n}{n+N} \hat{\Gamma}) v)^{1/2} \) based on (3.12).
3.2 Safe semi-supervised inference

To construct the estimator $\hat{\theta}^d$ in the previous section, one assumption we make is that the conditional mean function $f(X)$ is consistently estimated with the desired rate. If this assumption fails, there is no guarantee that the estimator $\hat{\theta}^d$ attains the semi-parametric efficiency bound or outperforms the supervised estimator. To tackle this problem, in this section we propose a new safe semi-supervised inference approach, which does not rely on the estimation of the conditional mean function $f(X)$ but guarantees the efficiency improvement.

Given any $p$-dimensional function $m(X) : \mathbb{R}^p \rightarrow \mathbb{R}$, we first construct a set of unbiased estimating functions $Xm(X) - \mu$, where $\mu = \mathbb{E}[Xm(X)]$. While these functions do not directly involve the unknown parameter $\theta^*$, they play an important role in the safe semi-supervised inference approach. Using $Xm(X) - \mu$ as covariates, we postulate a $p$-variate working regression model with response variables $X(Y - X^T\theta^*)$, i.e.

$$X(Y - X^T\theta^*) = B^T(Xm(X) - \mu) + E,$$  \hspace{1cm} (3.13)

where $E \in \mathbb{R}^p$ is the error vector and the coefficient matrix $B \in \mathbb{R}^{p \times p}$ is

$$B = \{\mathbb{E}[(Xm(X) - \mu)^{\otimes 2}]\}^{-1}\mathbb{E}[(Xm(X)(Y - X^T\theta^*))].$$

Since (3.13) is only a working model, the error $E$ and covariates $Xm(X) - \mu$ are not necessarily independent. Recall that the response variable $X(Y - X^T\theta^*)$ corresponds to the score function of $\theta^*$ in the linear regression model, and can be rewritten as $X(\epsilon + \eta(X))$, where $\epsilon = Y - f(X)$ and $\eta(X) = f(X) - X^T\theta^*$ is the nonlinear effect. Since $\epsilon$ and $Xm(X) - \mu$ are independent, the goal of model (3.13) is to explain the nonlinear effect $X\eta(X)$ by the covariates $Xm(X) - \mu$. Indeed, we show in Remark 7 that the optimal choice of $m(X)$ is $m(X) = f(X) - X^T\theta^* = \eta(X)$ and in this case the nonlinear effect $X\eta(X)$ can be perfectly explained by $Xm(X) - \mu$.

Given $Xm(X) - \mu$ and the coefficient matrix $B$, we define a class of unbiased estimating functions for $\theta^*$ as $h_\psi(X,Y;\theta) = \bar{\xi}_\psi - XX^T\theta = X(Y - X^T\theta) - \psi B^T(Xm(X) - \mu)$, where

$$\bar{\xi}_\psi = XY - \psi B^T(Xm(X) - \mu),$$  \hspace{1cm} (3.14)

with $\psi \in \mathbb{R}$ being a tuning parameter that balances two unbiased functions $Xm(X) - \mu$ and $X(Y - X^T\theta^*)$. In particular, we have $\mathbb{E}(h_\psi(X,Y;\theta^*)) = 0$ for any $\psi$. Indeed, we show in Remark 6 that the optimal choice of $\psi$ is $\psi = 1$, which implies $h_\psi(X,Y;\theta^*) = E$ in view of (3.13). Thus, from a geometric perspective, $h_\psi(X,Y;\theta)$ is the residual by projecting the score function $X(Y - X^T\theta)$ onto the set of unbiased estimating functions $Xm(X) - \mu$ in the $L_2(\mathbb{P})$ norm. Following the insight from the above geometric interpretation, we now propose the safe semi-supervised inference approach.

To formulate the inference procedure, we first consider how to estimate the coefficient matrix $B$. In view of (3.13) and the followup discussion, to estimate $B$, we can either pre-specify a nonlinear function $m(X)$ or perhaps use a more flexible approach to estimate $m(X)$ from the data. To see this, we can define $m(X) = \arg\min_{g \in \mathcal{G}} \mathbb{E}[(Y - g(X))^2]$, where $\mathcal{G}$ is a pre-specified class of functions of $X$. For example, $\mathcal{G} = \{\sum_{j=1}^p \alpha_j X_j + \sum_{1 \leq k < l \leq p} \beta_{kl} X_k X_l : \alpha_j, \beta_{kl} \in \mathbb{R}\}$ corresponds to the class
of functions with main effects and the second-order interactions. By fitting a penalized interaction model as in Zhao et al. (2016), we can construct an estimator \( \hat{m}(X) \). In the rest of the paper, we assume an estimator \( \hat{m}(X) \) of \( m(X) \) is available. The detailed technical conditions on \( \hat{m}(X) \) are shown in Assumption 3 and Theorem 5. Similar to Section 2.2, we apply a cross-fitting approach to estimate \( B \). Recall that we use \( D_j^* \) to denote the \( j \)th fold of labeled data and \( D_j \) to denote the \( j \)th fold of labeled and unlabeled data. Given the estimator \( \hat{m}^{-j}(\cdot) \) obtained from the labeled data \( D^* \setminus D_j^* \) for \( j = 1, 2 \), we can estimate the \( k \)th column of \( B \) by

\[
\hat{B}^j_k = \arg \min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i \in D_j^*} \left\{ X_{ik}(Y_i - X_i^T \hat{\theta}_L) - \beta^T (X_i \hat{m}^{-j}(X_i) - \hat{\mu}^j) \right\}^2 + \lambda_k \|\beta\|_1,
\]

where \( \hat{\theta}_L \) is the Dantzig estimator in (2.2), \( \hat{\mu}^j = \frac{1}{n_j} \sum_{i \in D_j^*} \hat{m}^{-j}(X_i) X_i \) and \( \lambda_k \) is a tuning parameter. We note that it is possible to estimate \( \mu = \mathbb{E}[m(X)] \) by using both labeled and unlabeled data \( D_j \). However, the rate of the estimator \( \hat{B}^j_k \) remains the same. The final estimator of \( B_k \) is \( \hat{B}_k = (\hat{B}_k^1 + \hat{B}_k^2)/2 \), and this leads to \( \hat{B} = (\hat{B}_1, ..., \hat{B}_p) \).

Motivated by the form of \( \xi_\psi \) in (3.14), we construct the following estimate of \( \xi = \mathbb{E}(XY) \),

\[
\hat{\xi}_{S,\psi} = \frac{\sum_{i=1}^n X_i Y_i}{n} - \frac{\psi}{2} \hat{B}^2 \sum_{j=1}^2 \left( \sum_{i \in D_j^*} \frac{X_i \hat{m}^{-j}(X_i)}{n_j} - \frac{\sum_{i \in D_j} X_i \hat{m}^{-j}(X_i)}{n_j + N_j} \right),
\]

where we apply the cross-fitting technique again, and \( n_j = |D_j^*| \) and \( n_j + N_j = |D_j| \). We note that different from the estimator \( \hat{\mu}^j \) used in \( \hat{B}^j_k \), we estimate \( \mu \) by \( \frac{1}{n_j + N_j} \sum_{i \in D_j} X_i \hat{m}^{-j}(X_i) \) in (3.16), which incorporates the information from the unlabeled data.

Similar to the estimator \( \hat{\theta}^d \) in (3.1), we propose the following safe semi-supervised estimator

\[
\hat{\theta}^d_{S,\psi} = \hat{\theta}_L + \hat{\Omega}(\hat{\xi}_{S,\psi} - \hat{\Sigma}_n \hat{\theta}),
\]

where \( \hat{\theta}_L \) is the supervised Dantzig estimator in (2.2), \( \hat{\xi}_{S,\psi} \) is defined in (3.16), \( \hat{\Sigma}_n = \frac{1}{n} \sum_{i=1}^n X_i^{\otimes 2} \) and \( \hat{\Omega} \) is the node-wise lasso estimator in (3.4). It is worthwhile to note that we estimate \( \Sigma \) by \( \hat{\Sigma}_n \) in (3.17), whereas we use \( \hat{\Sigma}_{n+N} = \frac{1}{n+N} \sum_{i=1}^{n+N} X_i^{\otimes 2} \) in the estimator \( \hat{\theta}^d \). Indeed, this is a critical difference as replacing \( \hat{\Sigma}_n \) with \( \hat{\Sigma}_{n+N} \) in (3.17) corresponds to an estimating function different from \( h_\psi(X, Y; \theta) \) and therefore no longer leads to a more efficient estimator.

**Assumption 3.** To show the theoretical properties of \( \hat{\theta}^d_{S,\psi} \), we make the following assumptions:

**(E1)** The smallest eigenvalue of \( \mathbb{E}[(Xm(X) - \mu)^{\otimes 2}] \) is lower bounded by a positive constant. Assume that the second moment of the residual \( E_j \) in (3.13) is less than \( C \), and \( |m(X_i)| \leq C \) for some constant \( C \). The estimator \( \hat{m}^{-j}(\cdot) \) satisfies \( \|\hat{m}^{-j} - m\|_2 = O_p(c_n) \) for a deterministic sequence \( c_n \). We require \( s_B K_2(c_n + \sqrt{\frac{\log p}{n}}) = o(1) \) and \( \sqrt{s_{\log p}/n} = O(1) \).

**(E2)** The columns of the matrix \( B \) are sparse with \( \max_{1 \leq k \leq p} \|B_k\|_0 = s_B \) and \( \max_{1 \leq k \leq p} \|B_k\|_1 \leq L_B \) for some \( L_B \) that may grow with \( n \).

**(E3)** \( \|\Omega\|_\infty \leq L_\Omega \) and \( (K_1 L_\Omega)^2 s_\Omega \sqrt{\log p/(n + N)} = o(1) \), where \( s_\Omega \) is the maximum rowwise sparsity of \( \Omega \) defined in Assumption 2.
\((E4)\) \(\mathbb{E}|\epsilon|^{2+\delta} = O(1)\) and \(\mathbb{E}|\eta|^{2+\delta} = O(1)\), where \(\epsilon = Y - f(X)\) and \(\eta = f(X) - X^T\theta^*\).

Assumption (E1) guarantees that the RE condition holds for the estimation of \(B_k\) in \((3.15)\). Assumption (E2) is the sparsity assumption of \(B_k\). For example, in the ideal case we can choose \(m(X) = f(X) - X^T\theta^*\) and then \(B = I_p\) is sparse. We note that there are other practical settings that the sparsity assumption of \(B_k\) is reasonable (e.g., \(X\) is blockwise independent). We defer the detailed discussion to Appendix B.3. In Assumption (E2), we further require that the matrix \(L_\infty\) norm of \(B\) is bounded by \(L_B\), which is used to establish the rate of \(\hat{B}\). Assumption (E3) is similar to Assumption 2. In particular, to control the remainder term in the asymptotic expansion of \(\hat{\theta}^d_{S,\psi}\), we need \(\|\Omega\|_\infty \leq L_\Omega\). Together with the boundedness assumption \(\|X_i\|_\infty \leq K_1\) in Assumption 1, it implies \(\|\Omega X_i\|_\infty \leq \|\Omega\|_\infty \|X_i\|_\infty \leq K_1 L_\Omega\). Replacing \(K\) in Assumption 2 with \(K_1 L_\Omega\), (E3) is equivalent to Assumption 2. Assumption (E4) assumes that \(\epsilon\) and \(\eta\) has bounded \((2 + \delta)\) moment, which is used to simplify the Lyapunov condition.

Denote
\[
\Gamma_{\psi} = \mathbb{E}(T_{i_1}^{(2)}) - \frac{N(2\psi - \psi^2)}{n + N} \mathbb{E}(T_{i_2}^T T_{i_1}^{(2)}) \mathbb{E}(T_{i_2}^T) - \mathbb{E}(T_{i_2} T_{i_1}^{(2)}),
\]
where \(T_{i_1} = X_i(Y_i - X_i^T \theta^*)\) and \(T_{i_2} = X_i m(X_i) - \mu\).

**Theorem 5.** Suppose Assumptions 1 and 3 hold. We choose \(\lambda_{1} \propto K_1 \sqrt{\frac{1}{\log p}} + \lambda_{2} \propto \lambda_{opt} \) in \((2.2)\), \(\lambda_k \propto K \sqrt{\frac{1}{n + N}}\) in \((3.2)\) and \(\tilde{\lambda}_k = \tilde{\lambda}_{opt} \) in \((3.15)\), where \(\tilde{\lambda}_{opt}\) is defined in Proposition 12. Then for any \(v \neq 0 \in \mathbb{R}^p\),
\[
v^T(\hat{\theta}^d_{S,\psi} - \theta^*) = v^T \Omega \left( \frac{X^T(Y - X \theta^*)}{n} - \psi B^T \left( \frac{\sum_{i=1}^n X_i m(X_i)}{n + N} \right) \right) + O_p(\tilde{\delta}_n),
\]
where
\[
\tilde{\delta}_n = \|v\|_1 L_\Omega K_2 \sqrt{\frac{\log p}{n}} \sqrt{\frac{\log p}{n + N} + s_B \sqrt{\log p} + c_n} + K_1 (s + s_B) \sqrt{\frac{\log p}{n}}
\]
with \(c_n\) defined in Assumption 3 (E1). In addition, if \(v^T \Omega_{\psi}^T V \geq C \|v\|_2^2\) for some constant \(C\), then
\[
\frac{n^{1/2} v^T(\hat{\theta}^d_{S,\psi} - \theta^*)}{(v^T \Omega_{\psi}^T V v)^{1/2}} \xrightarrow{d} N(0, 1).
\]

In a similar spirit to Theorem 3, the remainder term \(\tilde{\delta}_n\) in the asymptotic expansion of \(v^T(\hat{\theta}^d_{S,\psi} - \theta^*)\) characterizes the effect of the plug-in estimators \(\hat{\Omega}, \hat{B}\) and \(\hat{\theta}_L\) and \((3.19)\) is the Lyapunov condition under Assumption (E4). To further simplify the conditions in Theorem 5, we assume
\[ \|v\|_1/\|v\|_2, K_1, L_\Omega, L_B \text{ are all of order } O(1). \]

As a result, (3.19) always holds and the condition \( \delta_n/\|v\|_2 = o(n^{-1/2}) \) is implied by

\[
s_\Omega \frac{\log p}{\sqrt{n + N}} + (s \vee s_B) \frac{\log p}{\sqrt{n}} + s_B^{1/2} c_n \sqrt{\log p} = o(1). \tag{3.21}
\]

Compared to (3.9) for Theorem 3, we need a slightly stronger condition \( s(\log p/\sqrt{m}) = o(1) \) in (3.21). This is because \( \hat{\theta}_L \) is not only used as an initial estimator when constructing the one-step estimator \( \hat{\theta}_{S,\psi}^d \) but also used as a plug-in estimator to estimate \( B \) in (3.15). The error of \( \hat{\theta}_L \) accumulates in the asymptotic expansion of \( v^T(\hat{\theta}_{S,\psi}^d - \theta^*) \), leading to the slow order \( s(\log p/\sqrt{m}) \) in (3.21). In terms of the rate of \( \hat{m}^{-j} \) in the \( L_2(\mathbb{P}) \) norm, (3.21) requires \( c_n = o((s_B \log p)^{-1/2}) \), which is also slightly stronger than the condition for \( \hat{f}^{-j} \) in (3.9).

**Remark 6 (Efficiency improvement and optimality).** Similar to Remark 5, we first note that when the linear model is correctly specified i.e. \( f(X) = X^T \theta^* \), we have \( \mathbb{E}(T_2 T_1^T) = 0 \) and \( \Gamma_\psi = \sigma^2 \Sigma \). Thus, the asymptotic variance of \( v^T \hat{\theta}_{S,\psi}^d \) reduces to \( \sigma^2 v^T \Omega v \), which agrees with the asymptotic variance of the supervised debiased estimator.

In the following, we assume \( \mathbb{E}(T_2 T_1^T) = \mathbb{E}(X \otimes^2 m(X)) \) is of full rank. Since \( \mathbb{E}(T_2^{\otimes 2}) \) is strictly positive definite by Assumption (E1), it implies that \( \mathbb{E}(T_2 T_1^T) \mathbb{E}(T_2^{\otimes 2})^{-1} \mathbb{E}(T_2 T_1^T) \) is strictly positive definite. Similar to Remark 5, we consider the following two cases.

1. \( \lim_{n \to \infty} \frac{n}{n + N} = 1 \). Recall that the asymptotic variance of the supervised debiased estimator is \( v^T \Omega K \Omega v \), where \( K = \mathbb{E}(T_1^{\otimes 2}) \) with \( T_{11} = X_i (Y_i - X_i^T \theta^*) \). In this case, the asymptotic variance of \( v^T \hat{\theta}_{S,\psi}^d \) is identical to \( v^T \Omega K \Omega v \). There is no efficiency improvement when \( n \gg N \).

2. \( \lim_{n \to \infty} \frac{n}{n + N} = \rho \) for some \( 0 \leq \rho < 1 \). In this case, the asymptotic variance \( v^T \Omega \Gamma_\psi \Omega v \) is strictly smaller than \( v^T \Omega K \Omega v \) provided \( 2\rho - \rho^2 > 0 \), i.e. \( 0 < \rho < 2 \). Thus, we conclude that our estimator \( v^T \hat{\theta}_{S,\psi}^d \) with \( 0 < \rho < 2 \) is more efficient than the supervised estimator. In view of the form of \( \Gamma_\psi \), the variance reduction becomes more evident as \( \rho \) goes to 0 (i.e., \( N \) increases).

Another interesting fact is that the asymptotic variance \( v^T \Omega \Gamma_\psi \Omega v \) is minimized when taking \( \psi = 1 \). Thus, the estimator \( v^T \hat{\theta}_{S,\psi=1}^d \) is optimal within the following class of estimators \( \{v^T \hat{\theta}_{S,\psi}^d : \psi \in \mathbb{R}\} \) in terms of asymptotic efficiency.

**Remark 7 (Comparison with the estimator \( \hat{\theta}_d \)).** To see the connection of the two estimators \( \hat{\theta}_d \) and \( \hat{\theta}_{S,\psi}^d \) in (3.1) and (3.17), consider the ideal case with \( m(X) = f(X) - X^T \theta^* \). From (3.18), we can show that with \( \psi = 1 \)

\[
\Gamma_\psi = \sigma^2 \Sigma + \mathbb{E}(X \otimes^2 \eta^2) - \frac{N}{n + N} \mathbb{E}(X \otimes^2 \eta^2) = \sigma^2 \Sigma + \frac{n}{n + N} \mathbb{E}(X \otimes^2 \eta^2)
\]

where \( \eta = f(X) - X^T \theta^* \). The asymptotic variances of \( v^T \hat{\theta}_d \) and \( v^T \hat{\theta}_{S,\psi}^d \) are identical, since \( v^T \Omega \Gamma_\psi \Omega v = v^T (\sigma^2 \Omega + \frac{n}{n + N} \Gamma) v \), where \( \Gamma = \Omega \mathbb{E}(X \otimes^2 \eta^2) \Omega \). Thus, in the ideal case when \( f(X) \) is known, using \( \hat{\theta}_{S,\psi}^d \) with \( m(X) = f(X) - X^T \theta^* \) would not suffer efficiency loss compared to \( \hat{\theta}_d \) and
both estimators improve the efficiency of the debiased estimator (and attains the semi-parametric efficiency bound under certain conditions); see Remark 5 and 6. However, if there is no sufficient information for us to estimate \( f(X) \) consistently, the estimator \( \mathbf{v}^T \hat{\mathbf{d}} \) may not improve the efficiency of the debiased estimator, whereas \( \mathbf{v}^T \hat{\mathbf{d}}_{S,\psi} \) does not rely on the estimation of \( f(X) \) and guarantees the efficiency improvement for any \( m(X) \) that satisfies the conditions in Theorem 5. We note that the amount of efficiency improvement of \( \mathbf{v}^T \hat{\mathbf{d}}_{S,\psi} \) depends on the choice of \( m(X) \). Unless we choose \( m(X) = f(X) - X^T \theta^* \), the estimator \( \mathbf{v}^T \hat{\mathbf{d}}_{S,\psi} \) in general would not attain the semi-parametric efficiency bound.

From Remarks 6 and 7, we can see that the estimator \( \mathbf{v}^T \hat{\mathbf{d}}_{S,\psi} \) provides a safe use of the unlabeled data, since it is no worse than the supervised approach, no matter whether the linear model is correctly specified or the conditional mean function is consistently estimated.

As mentioned in the introduction, when the dimension \( p \) is fixed, Azrieli et al. (2016) and Chakrabortty and Cai (2018) investigated how to incorporate the unlabeled data to improve the estimation efficiency for \( \theta_j^* \). In addition to the technical challenges arise from the high dimensionality, the way we construct our estimator \( \hat{\theta}_{S,\psi}^d \) is different from theirs. Unlike \( \hat{\theta}_{S,\psi}^d \), their estimators can not guarantee the efficiency improvement if the parameter of interest is the linear combination of \( \theta^* \) (e.g., \( \theta_1^* + \theta_2^* \)). We refer to Appendix B.4 for more detailed discussions.

Finally, we consider how to estimate the asymptotic variance of \( \mathbf{v}^T \hat{\mathbf{d}}_{S} \). Recall that \( \hat{\Omega} \) is an estimator of \( \Omega \) defined in (3.4). To estimate \( \Gamma_{\psi} \) in (3.18), we note that \( \hat{\mathbf{B}}^T \) is an estimate of \( \mathbb{E}(\mathbf{T}_{i1}^2)^T \{\mathbb{E}(\mathbf{T}_{i2}^2)\}^{-1} \). We can further estimate \( \hat{\mathbf{M}}_1 = \mathbb{E}(\mathbf{T}_{i1}^2) \) and \( \hat{\mathbf{M}}_2 = \mathbb{E}(\mathbf{T}_{i2}^2) \) by

\[
\hat{\mathbf{M}}_1 = \frac{1}{n} \sum_{i=1}^{n} (Y_i - X_i^T \hat{\mathbf{d}}_L)^2 X_i^2
\]

and \( \hat{\mathbf{M}}_2 = (\hat{\mathbf{M}}_1^T + \hat{\mathbf{M}}_2^T)/2 \), where

\[
\hat{\mathbf{M}}_2^i = \frac{1}{n_j} \sum_{i \in D_j^*} (Y_i - X_i^T \hat{\mathbf{d}}_L) \hat{m}^{-j}(X_i) X_i^2.
\]

Given these estimates, an estimator of \( \Gamma_{\psi} \) is defined as

\[
\hat{\Gamma}_{\psi} = \hat{\mathbf{M}}_1 - \frac{N(2\psi - \psi^2)}{n + N} \hat{\mathbf{B}}^T \hat{\mathbf{M}}_2.
\]

**Proposition 6.** Suppose the conditions in Theorem 5 hold, and assume \( \mathbb{E}(\epsilon^4) = O(1), \mathbb{E}(\eta^4) = O(1) \) and \( Rem = o(1) \), where

\[
Rem = K_1(p + \frac{1}{2} L_B)\left(\frac{\log p}{n} + c_n\right) + K_2 \sqrt{\frac{s B}{n}} L_B + K_1 L_B \sqrt{\frac{s \log p}{n}}. \tag{3.22}
\]

Under these assumptions, we can show that

\[
\mathbf{v}^T \hat{\Omega} \hat{\Gamma}_{\psi} \hat{\Omega} \mathbf{v} - \mathbf{v}^T \Omega \Gamma_{\psi} \Omega \mathbf{v} = O_p \left( \|\mathbf{v}\|^2 (R_1 + R_2 + R_3) \right), \tag{3.23}
\]
apply the group lasso with spline basis to estimate a sparse additive regression function \( \hat{\theta} \). For the proposed methods. To compute our optimal semi-supervised estimator \( \hat{\theta} \) from 1 to 8. We repeat the simulation 100 times.

\( n \), where \( n \) and \( s \)

\[ R_1 = K_1 L_{\Omega}^2 s_\Omega \sqrt{\frac{\log p}{n + N}} \| \Gamma_\psi \|_{\max}, \quad R_2 = K_1^3 L_{\Omega}^2 \sqrt{\frac{s \log p}{n}}, \quad R_3 = \frac{NK_1^2 L_{\Omega}^2}{n + N} Rem, \]

with \( Rem \) defined in (3.22). Thus, if \( \| \nu \|^2_1 (R_1 + R_2 + R_3) / \| \nu \|^2_2 = o(1) \), we have

\[ \frac{n^{1/2} \nu^T (\hat{\theta}_{S,\psi}^d - \theta^*)}{(v^T \Omega_\psi \Omega v)^{1/2}} \xrightarrow{d} N(0, 1). \] (3.24)

We note that the three terms \( R_1, R_2 \) and \( R_3 \) in the convergence rate (3.23) are inherited from the estimation errors of \( \hat{\Omega}, \hat{\theta}_L \) and \( \hat{B} \), respectively. To further simplify the conditions in Proposition 6, let us consider the case that \( \| \nu \|^1_1 / \| \nu \|^2_2, K_1, L_\Omega, L_B \) and \( \| \Gamma_\psi \|_{\max} \) are all of order \( O(1) \). In this case, the asymptotic normality in (3.24) is valid provided \( (s \vee s_B) \sqrt{\frac{\log p}{n}} = o(1) \), \( s_\Omega \sqrt{\frac{\log p}{n + N}} = o(1) \) and \( s_B c_n = o(1) \).

## 4 Simulation Studies

### 4.1 Data generating models and practical implementation

We first generate a \( p \)-dimensional multivariate normal random vector \( U \sim N(0, \Sigma) \) with \( \Sigma_{jk} = 0.3^{j-k} \). We set the covariate \( X = (X_1, ..., X_p) \) to be \( X_1 = |U_1| \) and \( X_j = U_j \) for \( 1 < j \leq p \). The reason we take \( X_1 = |U_1| \) is that this transformation implies \( \mathbb{E}(X_i X_j) = 0 \) for \( j \neq 1 \) but the parameter \( \theta_1^* \) for centered \( X_1 \) is nonzero. We consider the following two data generating models for \( Y \). For model 1, we consider an additive model

\[ Y = 0.5X_1^2 + 0.8X_3^3 - (X_4 - 2)^2 + 2(X_5 + 1)^2 + 2X_6 + \epsilon, \]

where \( \epsilon \sim N(0, 1) \). To calculate the corresponding regression parameter \( \theta^* \) under the working linear model, we first center \( Y \) and \( X_1 \) so that their means are 0. By Proposition 4 in Bùhlmann and Van de Geer (2015), we know that the support of \( \theta^* \) is \( S = \{1, 3, 4, 5, 6\} \) and \( \theta_j^* \) for any \( j \in S \) is given by the \( L_2(\mathbb{P}) \) projection in the sub-model only with the variable \( X_j \) (e.g., \( \theta_3^* = \arg\min \mathbb{E}(0.8X_3^3 - \theta_3 X_3)^2 \)). After some calculation, we obtain \( \theta^* = (1.1, 0, 2.4, 4, 4, 2, 0, ..., 0) \), which is sparse.

For model 2, we have

\[ Y = 0.6(X_1 + X_2)^2 + 0.4X_3^3 - X_5 + 2X_6 + \epsilon, \]

where \( \epsilon \sim N(0, 1) \). The model is non-additive since it includes an interaction term between \( X_1 \) and \( X_2 \). We can show that the corresponding regression parameter \( \theta^* \) is \( (1.48, 1.04, 0, 1.2, -1, 2, 0, ..., 0) \).

Under each data generating model, we consider several combinations of \( (n, p) \) and vary the ratio \( N/n \) from 1 to 8. We repeat the simulation 100 times.

Before we proceed to illustrate the results, we discuss several practical implementation issues for the proposed methods. To compute our optimal semi-supervised estimator \( \hat{\theta}_D \) in (2.8), we apply the group lasso with spline basis to estimate a sparse additive regression function \( \hat{f} \) (Huang
et al., 2010). To be specific, we use the cubic spline basis with degree of freedom \( df = 5 \). To select the penalty parameter in group lasso and make computation easier, the BIC criterion is used; see Section 4 in Huang et al. (2010) for the definition. After we derive the estimator \( \hat{f} \) and subsequently \( \hat{\xi} \), we modify the source code in the flare package to compute the Dantzig type estimator \( \hat{\theta}_D \), where the tuning parameter \( \lambda_D \) is selected by 5 fold cross-validation. Given the estimator \( \hat{\theta}_D \), we can compute the one-step estimator \( \hat{\theta}^d \) in (3.1) for inference, where \( \hat{\Omega} \) is obtained by the node-wise lasso using the glmnet package with tuning parameter selected by 5 fold cross-validation.

To implement the safe semi-supervised method, we choose \( \hat{m}(\cdot) = \hat{f}(\cdot) \) the estimated sparse additive function obtained previously. We estimate each column of the coefficient matrix \( B \) by (3.15) using lasso with tuning parameters selected by cross-validation. Given the estimator \( \hat{\theta}^d \), we can compute the one-step estimator \( \hat{\theta}^d \) in (3.1) for inference, where \( \hat{\Omega} \) is obtained by the node-wise lasso using the glmnet package with tuning parameter selected by 5 fold cross-validation.

4.2 Numerical results

We first compare the estimation error of several sparse estimators \( \hat{\theta}_D \) in (2.8) (O-SSL), \( \hat{\theta}_S \) in (4.1) (S-SSL), \( \hat{\theta}_L \) in (2.2) (Dantzig) and \( \hat{\theta}_U \) in (2.9) (U-Dantzig). The \( L_2 \) and \( L_1 \) estimation error under Model 1 with \( p = 200 \) and \( n = 100 \) is shown in Figure 2. Since the true data generating model is additive, O-SSL has the smallest error among the four estimators, which agrees with our results in Theorem 2. While S-SSL is sub-optimal, it still outperforms Dantzig and U-Dantzig by a large margin. One interesting observation is that U-Dantzig performs much worse than the fully supervised estimator Dantzig. Thus, using the sample covariance \( \hat{\Sigma}_{n+N} \) from both labeled and unlabeled data in the Dantzig selector may not provide any empirical improvement; see Remark 3 for the theoretical justification. In addition, as the size of unlabeled data \( N \) increases, the improvement of our estimators O-SSL and S-SSL is more overwhelming, whereas the performance of U-Dantzig tends to deteriorate. The simulation results with \( p = 500 \) and \( n = 200 \) demonstrate the same patterns and are deferred to Appendix C.

The \( L_1 \) and \( L_2 \) estimation error under Model 2 with \( p = 500 \) and \( n = 200 \) is shown in Figure 3. Since Model 2 includes an interaction term between \( X_1 \) and \( X_2 \), the sparse additive model is inconsistent for the true regression function. Thus our O-SSL estimator is no longer optimal. This is validated from the first panel of Figure 3, where the \( L_2 \) estimation error of O-SSL is slightly larger than Dantzig. In contrast, our S-SSL estimator leads to the smallest estimation error and provides a safe use of unlabeled data even if the imposed conditional mean model is incorrect.

To compare the inference results, we also consider two versions of debiased lasso estimators,

\[
\hat{\theta}^d_1 = \hat{\theta}_{lasso} + \hat{\Omega} \left( \frac{1}{n} \sum_{i=1}^{n} X_i Y_i - \hat{\Sigma}_n \hat{\theta}_{lasso} \right), \quad \hat{\theta}^d_2 = \hat{\theta}_{lasso} + \hat{\Omega} \left( \frac{1}{n} \sum_{i=1}^{n} X_i Y_i - \hat{\Sigma}_n \hat{\theta}_{lasso} \right),
\]
Figure 2: The $L_2$ and $L_1$ estimation error under Model 1 with $p = 200$ and $n = 100$. The length of the vertical bar represents the magnitude of the sample standard deviations.

Figure 3: The $L_2$ and $L_1$ estimation error under Model 2 with $p = 500$ and $n = 200$. The length of the vertical bar represents the magnitude of the sample standard deviations.
Figure 4: The length and empirical coverage rate (shown in the number) of 95% CIs under Model 1 with $p = 200$ and $n = 100$. The top left panel is drawn by averaging over all the covariates not in the support set. The rest are for the coefficients of $X_1$, $X_5$ and $X_6$ in the support set.

where $\hat{\theta}_{lasso}$ and $\bar{\Omega}$ are the standard lasso and node-wise lasso estimator applied to the labeled data. The only difference between $\hat{\theta}_d^1$ and $\hat{\theta}_d^2$ is the way of estimating the precision matrix $\Omega$. The two estimators $\hat{\theta}_d^1$, $\hat{\theta}_d^2$ and the associated confidence intervals can be computed using the hdi package with Robust option.

In Figure 4, we compare the performance of 95% confidence intervals (CIs) associated with $\hat{\theta}_d^l$ in (3.1) (O-SSL), $\hat{\theta}_{S,\psi=1}^d$ in (3.17) (S-SSL), $\hat{\theta}_1^d$ (D-Lasso1) and $\hat{\theta}_2^d$ in (4.2) (D-Lasso2) under Model 1 with $p = 200$, $n = 100$. For simplicity, we still call our estimators as O-SSL and S-SSL. Recall that under Model 1, the support set is $S = \{1, 3, 4, 5, 6\}$. The top left panel contains the length and empirical coverage rate (shown in the number) of 95% CIs averaged over all the covariates not in the support set (denoted by $X_0$). Similarly, the rest of panels compare the CIs for the coefficients of three covariates $X_1$, $X_5$ and $X_6$ in the support set. It is seen that the coverage rates of all the methods are very close to the desired level 0.95. Our O-SSL method as guaranteed in Theorem 3, produces the shortest CIs among all four methods. The CIs from the S-SSL method are always shorter than those from D-Lasso1 and D-Lasso2, which agrees with Theorem 5. As expected, the CIs from both O-SSL and S-SSL become shorter as the size of unlabeled data $N$ increases. Finally, we note that the length of CIs from D-Lasso1 and D-Lasso2 is very similar, which shows that the way of estimating $\Omega$ has little effect on debiased lasso estimators. The former is slightly shorter for the covariates not in the support set ($X_0$) but longer for $X_1$, $X_5$ and $X_6$. Additional simulation results with $p = 500$, $n = 200$ are deferred to Appendix C.
Figure 5: The length and empirical coverage rate (shown in the number) of 95% CIs under Model 2 with \( p = 500 \) and \( n = 200 \). The top left panel is drawn by averaging over all the covariates not in the support set. The rest are for the coefficients of \( X_1, X_2 \) and \( X_6 \) in the support set.

We illustrate the inference results under Model 2 with \( p = 500, n = 200 \) in Figure 5. Although the CI from O-SSL is still shorter than D-Lasso1, it is no longer valid for the inference, as we can see a relatively low coverage rate for \( X_1 \). This results from a poor estimation of conditional mean as the true model is no longer additive. However, S-SSL is still reliable in this scenario and shows a plausible improvement in efficiency, which becomes more significant as \( N \) increases. Additional simulation results are deferred to Appendix C.

In summary, O-SSL outperforms the other methods when the conditional mean function is estimated consistently. However, in practice, estimation of the conditional mean function can be difficult especially with high-dimensional covariates. In this case, we recommend S-SSL as it provides a safe use of unlabeled data even if the imposed conditional mean model is incorrect.

5 Real Data Application

In this section, we apply our proposed method to a real data example, where the data set is from the Medical Information Mart for Intensive Care III (MIMIC-III) database (Johnson et al., 2016). MIMIC-III is an openly available electronic health records system developed by the MIT Lab for Computational Physiology. It comprises deidentified health-related data associated with intensive care unit patients with rich information including demographics, vital signs, laboratory test, medications, and so on. Our initial motivation for this data analysis is the association study for
the albumin level in the blood sample, a very indicative biomarker correlated with the phenotypes of different types of diseases (Phillips et al., 1989). We focus on a subset with around 4800 patients of the whole database that the albumin level is available.

Some data cleaning strategy is inevitable for handling electronic health records database. In our situation, around 54% covariates contain missing values. Among these covariates with missing values, the missingness proportions are 9.4% on average and the range is from 0.2% to 30.8%. For those missing values, we simply impute them using the mean of observed samples, the so-called mean imputation. For many clinical markers with continuous scale, the database collects the minimum, the maximum, as well as the mean, values across a certain period of time. To alleviate the potential collinearity among these variables but also to maintain as much information as possible, we decide to only include the maximum and the mean values in our analysis. Additionally, we convert the categorical variables, such as gender and marital status, to dummy variables. The number of features after data pre-processing is $p = 160$. We randomly sample 900 observations out of 4811 patients and divide them into $n = 100$ labeled data and $N = 800$ unlabeled data, where the value of the outcome variable albumin is removed for the 800 unlabeled data. We also vary the size of the labeled and unlabeled data in this analysis.

Firstly, same as the simulations, we apply the hdi package to compute the debiased lasso estimator D-Lasso1 with robust option using the labeled data. Due to multiple testing, the p-value for each covariate is corrected using the default holm approach. The three variables iron binding capacity, calcium, and alkaline phosphatase are significant with corrected p-values smaller than 0.05. We also applied the method D-Lasso2. Its result is quite similar therefore omitted.

Next we apply our O-SSL and S-SSL methods. The O-SSL estimator is implemented in the same way as the simulation studies. In the S-SSL method implementation, we consider the working model $\hat{\theta}^0$ as the linear model with lasso where the explanatory variables also include the squared terms and interaction terms of the three identified variables iron binding capacity, calcium, and alkaline phosphatase. It shows that, in this working model, the coefficients of the interaction terms between iron binding capacity and calcium, and between iron binding capacity and alkaline phosphatase are nonzero; therefore, this working model indeed exhibits some non-linearity between the outcome and the covariate variables. In either O-SSL or S-SSL, the p-values are corrected using the same holm method.

The results are summarized in Table 1. All the three methods D-Lasso1, O-SSL and S-SSL identify the three variables iron binding capacity, calcium, and alkaline phosphatase as significant at the FWER 5% level, with the average confidence interval length 0.11, 0.08, and 0.09, respectively. Besides, the O-SSL method selects nine additional variables, and the S-SSL method provides a more parsimonious model with three additional variables. The variables hemoglobin and lymphocytes are selected by both of the two methods. The S-SSL method selects the variable white blood cells as well. In the medical literature, there are various evidence documenting the associations between the albumin level in the blood sample with our selected biomarkers here, such as with the hemoglobin level (Fukui et al., 2008), with the lymphocytes level (Alagappan et al., 2018), and with the count of the white blood cells (Cavalot et al., 2002). More interestingly,
researchers recently started to use the so-called HALP score, a combination of hemoglobin, albumin, lymphocyte, and platelet levels in the blood sample (Chen et al., 2015), as a prognostic factor for various disease types (Peng et al., 2018; Guo et al., 2019; Shen et al., 2019; Tojek et al., 2019). Our statistical results are consistent with the medical literature.

Table 1 also shows that, while the successful implementation of the O-SSL method needs the correct specification of the conditional mean model, both O-SSL and S-SSL achieve more efficiency gains compared to the D-Lasso1 method, in the sense that they have shorter confidence intervals and would be more powerful for conducting hypothesis tests.

6 Discussion

In this paper, we first establish the minimax lower bound for the estimation of $\theta^*$ in the semi-supervised setting. We show that the simple supervised estimator cannot attain this lower bound and thus there is a gap between the two. We close this gap by proposing a new semi-supervised estimator $\hat{\theta}_D$ which attains the lower bound. To construct confidence intervals and hypothesis tests, we further propose two semi-supervised estimators $\mathbf{v}^T \hat{\theta}_d$ and $\mathbf{v}^T \hat{\theta}_{d,\psi}$ for $\mathbf{v}^T \theta^*$. The former is fully efficient if $f(X)$ is estimated consistently, but may not be more efficient than the supervised approach otherwise. The latter does not aim to provide fully efficient inference, but is guaranteed to be no worse than the supervised approach, no matter whether $f(X) = X^T \theta^*$ or $f(X)$ is estimated consistently. Thus, it provides a safe use of the unlabeled data for inference.

There are several future directions that warrant further investigation. First, in many biomedical studies, the outcome variable of interest is often binary or discrete. It is of both practical and theoretical importance to generalize the method and theory to models that can deal with discrete data, such as generalized linear models. Second, in some applications, the labeled and unlabeled data are collected under different conditions or from different populations. In this case, it is more appropriate to assume that the marginal distribution of $X$ in the unlabeled data differs from that in the labeled data (Kawakita and Kanamori, 2013). With different marginal distributions of $X$, it is unclear whether and how the unlabeled data can be used to improve the estimation and inference. We plan to study this problem in the future.

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|                                | D-Lasso1 | S-SSL          | O-SSL          |
|--------------------------------|----------|----------------|----------------|
|                                | Est.     | len/2          | pval           | CI             | Est.     | len/2          | pval           | CI             | Est.     | len/2          | pval           | CI             |
| iron binding capacity_mean     | 0.153    | 0.055          | <E-05          | (0.1,0.21)     | 0.142    | 0.050          | <E-05          | (0.09,0.19)    | 0.165    | 0.038          | <E-14          | (0.13,0.2)     |
| calcium_mean                   | 0.144    | 0.056          | <E-04          | (0.1,0.21)     | 0.138    | 0.043          | <E-07          | (0.1,0.18)     | 0.148    | 0.038          | <E-11          | (0.11,0.19)    |
| alkaline phosphatase_mean      | -0.128   | 0.059          | 0.003          | (-0.2,-0.07)   | -0.119   | 0.047          | <E-03          | (-0.17,-0.07)  | -0.115   | 0.040          | <E-05          | (-0.16,-0.07)  |
| hemoglobin_mean                | 0.101    | 0.058          | 0.093          | (0.04,0.16)    | 0.096    | 0.047          | 0.008          | (0.05,0.14)    | 0.107    | 0.039          | <E-04          | (0.07,0.15)    |
| lymphocytes_mean               | 0.097    | 0.055          | 0.088          | (0.0,0.16)     | 0.081    | 0.038          | 0.005          | (0.04,0.12)    | 0.077    | 0.038          | 0.014          | (0.04,0.11)    |
| white blood cells_mean         | -0.074   | 0.058          | 1              | (-0.14,-0.02)  | -0.078   | 0.043          | 0.049          | (-0.12,-0.04)  | -0.061   | 0.040          | 0.364          | (-0.1,-0.02)   |
| resprate_max                   | -0.033   | 0.059          | 1              | (-0.09,0.03)   | -0.048   | 0.043          | 1              | (-0.09,0)      | -0.076   | 0.039          | 0.019          | (-0.11,-0.04)  |
| resprate_mean                  | -0.033   | 0.059          | 1              | (-0.09,0.03)   | -0.039   | 0.046          | 1              | (-0.09,0.01)   | -0.076   | 0.039          | 0.019          | (-0.11,-0.04)  |
| hr_max                         | -0.083   | 0.056          | 0.55           | (-0.13,-0.02)  | -0.061   | 0.050          | 1              | (-0.11,-0.01)  | -0.07    | 0.038          | 0.045          | (-0.11,-0.03)  |
| temp_max                       | -0.067   | 0.051          | 1              | (-0.12,-0.02)  | -0.052   | 0.038          | 1              | (-0.11,-0.01)  | -0.076   | 0.038          | 0.017          | (-0.11,-0.03)  |
| transferrin_mean               | 0.070    | 0.055          | 1              | (0.01,0.12)    | 0.049    | 0.050          | 1              | (0.0,0.1)      | 0.072    | 0.038          | 0.031          | (0.03,0.11)    |
| anion gap_mean                 | 0.094    | 0.058          | 0.21           | (0.03,0.15)    | 0.078    | 0.045          | 0.102          | (0.03,0.12)    | 0.075    | 0.039          | 0.027          | (0.04,0.11)    |
| hematocrit_mean                | 0.102    | 0.058          | 0.08           | (-0.03,0.2)    | 0.076    | 0.042          | 0.059          | (0.03,0.12)    | 0.073    | 0.039          | 0.037          | (0.03,0.11)    |

Table 1: The point estimates, confidence intervals (and the length) and corrected p-values from the D-Lasso1, S-SSL and O-SSL methods when $n = 100$, $N = 800$. 
A Proofs

A.1 Preliminary Lemmas

We start with several basic lemmas that we will apply in our proofs.

**Lemma 7** (Lemma B.1 in Chernozhukov et al. (2018)). Let \( \{X_n, Y_n\} \) be sequences of random variables. If for any \( c > 0, \mathbb{P}(|X_n| > cY_n) = o_p(1) \). Then \( X_n = o_p(1) \).

**Lemma 8** (Nemirovski moment inequality, Lemma 14.24 in Bhlmann and Van de Geer (2011)). For \( m \geq 1 \) and \( p > e^{m-1} \), we have

\[
\mathbb{E}
\left[
\max_{1 \leq k \leq p} \left| \sum_{i=1}^{n} (\gamma_k(Z_i) - \mathbb{E}[\gamma_k(Z_i)]) \right|^m
\right]
\leq (8 \log 2p)^m \mathbb{E}
\left[
\left( \max_{1 \leq k \leq p} \sum_{i=1}^{n} \gamma_k^2(Z_i) \right)^{m/2}
\right]
\tag{A.1}
\]

**Lemma 9** (Theorem 3.1 in Rudelson and Zhou (2012)). Assume that \( X \in \mathbb{R}^{n \times p} \) has zero mean and covariance \( \Sigma \). Furthermore, assume that the rows of \( X \Sigma^{-1/2} \in \mathbb{R}^{n \times p} \) are independent sub-gaussian random vector with a bounded sub-gaussian constant and \( \Lambda_{\min}(\Sigma) > C_{\min} > 0, \max_{1 \leq j \leq p} \Sigma_{jj} = O(1) \). Set \( 0 < \delta < 1, 0 < s_0 < p, \) and \( L > 0 \). Define the following event,

\[
B_\delta(n, s_0, L) = \{ X \in \mathbb{R}^{n \times p} : (1 - \delta) \sqrt{C_{\min}} \leq \frac{\|Xv\|_2}{\sqrt{n}\|v\|_2}, \forall v \in C(s_0, L) \text{ s.t. } v \neq 0 \}.
\tag{A.2}
\]

and \( C(s_0, L) = \{ \theta \in \mathbb{R}^p : \exists S \subseteq \{1, \ldots, p\}, |S| = s_0, \|\theta_{S^c}\|_1 \leq L\|\theta_S\|_1 \} \). Then, there exists a constant \( c_1 = c(L, \delta) \) such that, for sample size \( n \geq c_1 s_0 \log(p/s_0) \), we have

\[
\mathbb{P}(B_\delta(n, s_0, L)) \geq 1 - e^{-\delta^2 n}.
\tag{A.3}
\]

A.2 Proof of Theorem 1

The lower bound consists of two parts. By taking \( f(X) = X^T \theta^\star \), that is the linear model is correctly specified, the proof in Proposition 6.4 of Verzelen (2012) with conditions \( s \log(p/s) \leq C' n \) and \( 2 \leq s \leq (n - 1)/4 \) directly implies

\[
\inf_{\hat{\theta}} \sup_{P_{X,Y} \in \mathcal{P}_{\theta,\sigma}} \mathbb{P}_{P_{X,Y}} \left[ \|\hat{\theta} - \theta^\star\|_q \geq c_1 s^{1/q} \sqrt{\frac{\log(p/s)}{n}} \right] > c_2.
\]

To establish the lower bound \( s^{1/q} \Phi \sqrt{\log(p/s)/(n + N)} \), we first construct a set of hypotheses and then apply Theorem 2.7 in Tsybakov (2008). Define the set \( \mathcal{M} = \{ x \in \{0, 1\}^{p-1} : \|x\|_0 = s \} \). It follows from the Varshamov-Gilbert bound (e.g., Lemma 2.9 in Tsybakov (2008)) and Lemma A.3 in Rigollet and Tsybakov (2011) that there exists a subset \( \mathcal{M}' \) of \( \mathcal{M} \) such that for any \( x, x' \) in \( \mathcal{M}' \) with \( x \neq x' \), we have

\[
\rho_H(x, x') > \frac{s}{16}, \quad \text{and} \quad \log |\mathcal{M}'| \geq c_1' s \log \left( \frac{P}{s} \right),
\tag{A.4}
\]

where \( \rho_H \) denotes the Hamming distance and \( c_1' > 0 \) is an absolute constant. Denote the element of the finite set \( \mathcal{M}' \) by \( w^j \) and the index set for the nonzero entries by \( [j] \). For each \( w^j \in \mathbb{R}^{p-1} \), we
add a zero as the first entry to obtain a \( p \)-dimensional vector \((0, w^j)\), and for notational simplicity, we still call it \( w^j \).

Next, we construct a finite set of hypotheses by perturbing the distribution of \( X \). Denote \( N = (N_1, \ldots, N_p) \sim \mathcal{N}(0, I_p) \). Let us consider the following hypotheses

\[
H_0 : X = (X_1, \ldots, X_p) \text{ with } X_\ell = N_\ell,
\]

\[
H_j : X = (X_1, \ldots, X_p) \text{ with } X_\ell = \begin{cases} \rho(N_1^2 - 1) + \sqrt{1 - 2\rho^2} N_\ell, & \text{if } w^j_\ell = 1, \\ N_\ell, & \text{if } w^j_\ell = 0, \end{cases}
\]

for \( j = 1, \ldots, |M'| \), where \( \rho > 0 \) is a quantity to be chosen later. Let \( \mathbb{E}_j \) denote the expectation under \( H_j \). Clearly, \( \mathbb{E}_j(X_\ell) = 0 \). After some simple calculation, we can verify that for \( j = 1, \ldots, |M'| \),

\[
\mathbb{E}_j[X_\ell X_m] = \begin{cases} 2\rho^2 & \text{if } w^j_\ell \text{ and } w^j_m \neq 0 \text{ and } \ell \neq m, \\ 1 & \text{if } \ell = m, \\ 0 & \text{otherwise}. \end{cases} \tag{A.5}
\]

Denote by \( M = \mathbb{E}_j(XX^T) \) the covariance matrix of \( X \) under \( H_j \). From (A.5), there exists a permutation matrix \( P \) such that \( M = PBP^T \), where \( B = \text{diag}(A, I_{p-s}) \) and \( A \) is a \( s \)-dimensional equicorrelation matrix with the off-diagonal entry \( 2\rho^2 \) and the diagonal entry \( 1 \). Assume that the \((\lambda, v)\) are the eigenvalue and corresponding eigenvector of \( B \). Following the definition of eigenvalues, \( (\lambda, P^Tv) \) are the eigenvalue and eigenvector of \( M \). As a result, \( \lambda_{\min}(M) = \lambda_{\min}(B) = \lambda_{\min}(A) = 1 - 2\rho^2 \), where the last two equalities follow from the property of the block diagonal matrix and equicorrelation matrix. With the choice of \( \rho \) as specified in (A.10), we can derive that \( \lambda_{\min}(M) > 1/2 \) and therefore \( M \) is positive definite.

We further choose \( f(X) = \frac{\Phi}{\sqrt{3}} X_1^2 \). Our next step is to verify that the corresponding estimand \( \theta^j = (\mathbb{E}_j(XX^T))^{-1}\mathbb{E}_j(Xf(X)) \) is \( s \)-sparse. To this end, we first note that \( \mathbb{E}_j[Xf(X)] = \frac{2}{\sqrt{3}} \Phi \rho w^j \). To calculate \( M^{-1} \), we first rewrite the equicorrelation matrix \( A \) as \( A = (1 - 2\rho^2)I_s + 2\rho^2 1_s 1_s^T \), where \( 1_s \) is a \( s \)-dimensional vector of 1. The Woodbury formula implies

\[
A^{-1} = \frac{1}{1 - 2\rho^2} I_s - \frac{2\rho^2}{(1 - 2\rho^2)(1 + 2(s - 1)\rho^2)} 1_s 1_s^T.
\]

Thus, we obtain \( M^{-1} = PB^{-1}P^T \) with \( B^{-1} = \text{diag}(A^{-1}, I_{p-s}) \). Let \( e_\ell \) denote the canonical basis in \( \mathbb{R}^p \) with the \( t \)th entry being 1 and the rest being 0. Note that the permutation matrix \( P \) can be written as \( P = (e_{j_1}, \ldots, e_{j_s}, e_{j_{s+1}}, \ldots, e_{j_p}) \), where the indexes \( j_1, \ldots, j_s \) belong to \([j]\) and \( j_{s+1}, \ldots, j_p \) are not in \([j]\). Combining the above argument, the estimand \( \theta^j \) under hypothesis \( H_j \) is given by

\[
\theta^j = \frac{2\Phi \rho}{\sqrt{3}} PB^{-1}P^T w^j = \frac{2\Phi \rho}{\sqrt{3}} PB^{-1} \begin{pmatrix} 1_s \\ 0_{p-s} \end{pmatrix} = \frac{2\Phi \rho}{\sqrt{3}} P \begin{pmatrix} A^{-1}1_s \\ 0_{p-s} \end{pmatrix}
\]

\[
= \frac{2\Phi \rho}{\sqrt{3}(1 + 2(s - 1)\rho^2)} w^j, \tag{A.6}
\]

from which we know \( \theta^j \) is \( s \)-sparse. It is easily seen that under \( H_0 \) the corresponding estimand is \( \theta^0 = 0 \).
In the sequel, we will verify $\mathbb{E}_j(f(X) - X^T \theta^j)^2 \leq \Phi^2$ holds. Recall that $N = (N_1, ..., N_p) \sim N(0, I_p)$. By (A.6), we have

$$
\mathbb{E}_j(f(X) - X^T \theta^j)^2 = \mathbb{E} \left[ \left( \frac{\Phi}{\sqrt{3}} N_1^2 - \frac{2s\Phi^2}{\sqrt{3}(1 + 2(s-1)\rho^2)(N_1^2 - 1) - \frac{2\Phi\rho(1 - 2\rho^2)}{\sqrt{3}(1 + 2(s-1)\rho^2)} \sum_{k \in [j]} N_k)^2} \right) \right]
$$

$$
= \frac{\Phi^2}{3} \left( 3 - \frac{4s\rho^2}{1 + 2(s-1)\rho^2} \right) \leq \Phi^2.
$$

Obviously, under $H_0$ we have $\mathbb{E}_0(f(X) - X^T \theta^0)^2 = \Phi^2$. Therefore, we have shown that the distribution of $(X, Y)$ under the hypotheses $H_j$ for $j = 0, ..., |\mathcal{M}'|$ belongs to the class of distributions $\mathcal{P}_{\Phi, \sigma}$.

To apply Theorem 2.7 in Tsybakov (2008), we need to (1) lower bound $\|\theta^j - \theta^{j'}\|_q$ for $0 \leq j < j' \leq |\mathcal{M}'|$ and (2) upper bound the Kullback-Leibler divergence between the probability measure of the data denoted by $\mathcal{P}_j$ and $\mathcal{P}_0$ under $H_j$ and $H_0$. For (1), we have from (A.6) that for $1 \leq j < j' \leq |\mathcal{M}'|$

$$
\|\theta^j - \theta^{j'}\|_q = \frac{2\Phi\rho}{\sqrt{3} + 2\sqrt{3}(s-1)\rho^2} \rho_{1/4}(w^j, w^{j'}) \geq \frac{2s^{1/q}\Phi\rho}{16^{1/4}\Phi\rho},
$$

where the last step follows from (A.4). Since $\theta^0 = 0$, for $j = 0$ and $j' \geq 1$ we have

$$
\|\theta^j - \theta^{j'}\|_q = \frac{2s^{1/q}\Phi\rho}{\sqrt{3}(1 + 2(s-1)\rho^2)}.
$$

To quantify the Kullback-Leibler divergence, recall that the data in matrix form can be written as $(Y, \tilde{X})$, where $\tilde{X} = (X_1, ..., X_{n+N})^T$ and $Y = (Y_1, ..., Y_n)^T$. With a slight change of notation, we use $X_{il}$ to denote the $\ell$th component of $X_i$ for $1 \leq \ell \leq p$ and $1 \leq i \leq n + N$. Under $H_j$, the data distribution can be decomposed as

$$
p_j(Y, \tilde{X}) = p(Y|X)p_j(\tilde{X}) = p(Y|X) \prod_{i=1}^{n+N} p_j(X_i)
$$

$$
= p(Y|X) \prod_{i=1}^{n+N} p_j(X_{i,-\{j,1\}})p_j(X_{i,\{j\}}|X_{i1})p_j(X_{i1}),
$$

where we note that the p.d.f. $p(Y|X)$ remains the same across $j$ and $X_{i,-\{j,1\}}$ stands for the subvector of $X_i$ by excluding the indexes in $\{j,1\}$. From the above decomposition, the Kullback-Leibler divergence is given by

$$
\mathcal{K}(\mathcal{P}_j, \mathcal{P}_0) = \mathbb{E}_j \left[ \log \frac{p(Y|X)p_j(\tilde{X})}{p(Y|X)p_0(X)} \right] = (n + N)\mathbb{E}_j \left[ \log \frac{p_j(X_{i,\{j\}}|X_{i1})}{p_0(X_{i,\{j\}}|X_{i1})} \right].
$$

Furthermore, notice that

$$
p_j(X_{i,\{j\}}|X_{i1}) = \prod_{k \in [j]} p_j(X_{ik}|X_{i1}) = \prod_{k \in [j]} \left( \frac{1}{\sqrt{2\pi(1 - 2\rho^2)}} \exp \left\{ - \frac{(X_{ik} - \rho(X_{i1}^2 - 1))^2}{2(1 - 2\rho^2)} \right\} \right),
$$

30
\[ p_0(X_{i,j}|X_{11}) = \prod_{k \in [j]} p_0(X_{ik}|X_{11}) = \prod_{k \in [j]} \left( \frac{1}{\sqrt{2\pi}} \exp \left\{ - \frac{X_{ik}^2}{2} \right\} \right). \]

Hence, with some index \( k \in [j] \) we obtain

\[
\mathcal{K}(P_j, P_0) = \frac{(n+N)s}{2} \left( \mathbb{E}_j \left[ \frac{(X_{ik} - \rho(X_{1i}^2 - 1))^2}{(1 - 2\rho^2)} \right] - \log(1 - 2\rho^2) + \mathbb{E}_j[X_{ik}^2] \right) = \frac{(n+N)s}{2} \left( 1 - \log(1 - 2\rho^2) - \frac{1}{(1 - 2\rho^2)} \mathbb{E}_j[X_{ik}^2 + \rho^2((X_{1i})^2 - 1)^2 - 2\rho X_{ik}(X_{1i}^2 - 1)] \right) = \frac{(n+N)s}{2} \log \left( 1 + \frac{2\rho^2}{1 - 2\rho^2} \right) \leq \frac{s(n+N)\rho^2}{1 - 2\rho^2}. \tag{A.9} \]

We set

\[
\rho = \frac{1}{4\sqrt{2}} \sqrt{\frac{c'_1 \log(p/s)}{n + N}}, \tag{A.10} \]

where \( c'_1 \) is specified in (A.4). Given the condition \( \frac{(s-1)c'_1 \log(p/s)}{8(n+N)} \leq 1 \) and \( s \geq 2 \), we have \( 1 - 2\rho^2 \geq \frac{1}{2} \).

Then from (A.9) the Kullback-Leibler divergence can be bounded as follows

\[
\mathcal{K}(P_j, P_0) \leq \frac{s(n+N)\rho^2}{1 - 2\rho^2} \leq \frac{c'_1 s \log(p/s)}{16} \leq \frac{1}{16} \log |\mathcal{M}'|, \]

where the last inequality follows from (A.4). Finally, with the choice of \( \rho \) in (A.10), we obtain from (A.7) and (A.8) that

\[
\|\hat{\theta}' - \theta'\|_q \geq \frac{s^{1/q} \Phi}{3\sqrt{6}16^{1/q}} \sqrt{\frac{c'_1 \log(p/s)}{n + N}},
\]

where we use the inequality \( 1 + 2(s-1)\rho^2 \leq 3/2 \). We complete the proof by applying Theorem 2.7 in Tsybakov (2008).

### A.3 Proof of Theorem 2

**Proof.** We can rewrite that

\[
\hat{\xi}_j = \frac{1}{n_j} \sum_{i \in D_j^*} \left\{ X_i Y_i - (\hat{f}^{-j}(X_i) X_i - \sum_{k \in D_j} \frac{\hat{f}^{-j}(X_k) X_k}{n_j + N_j}) \right\} = \frac{1}{n_j} \sum_{i \in D_j^*} \left\{ X_i Y_i - (f(X_i) X_i - \sum_{k \in D_j} \frac{f(X_k) X_k}{n_j + N_j}) + (f(X_i) X_i - \sum_{k \in D_j} \frac{f(X_k) X_k}{n_j + N_j}) - (\hat{f}^{-j}(X_i) X_i - \sum_{k \in D_j} \frac{\hat{f}^{-j}(X_k) X_k}{n_j + N_j}) \right\}.
\]

Denote

\[
I_1 = \frac{1}{n_j} \sum_{i \in D_j^*} \left\{ f(X_i) X_i - \sum_{k \in D_j} \frac{f(X_k) X_k}{n_j + N_j} - (\hat{f}^{-j}(X_i) X_i - \sum_{k \in D_j} \frac{\hat{f}^{-j}(X_k) X_k}{n_j + N_j}) \right\}. \tag{A.11} \]
Next, we aim to show that $\|I_i\|_\infty = O_p(K_1 b_n \sqrt{\log p})$. To this end, we further decompose $I$ as

$$
\|I_i\|_\infty = \left\| \frac{1}{n_j} \sum_{i \in D_j} \{f(X_i)X_i - \hat{f}^{-j}(X_i)X_i\} - \frac{1}{n_j + N_j} \sum_{i \in D_j} \{f(X_i)X_i - \hat{f}^{-j}(X_i)X_i\} \right\|_\infty
$$

$$
\leq \left\| \frac{1}{n_j} \sum_{i \in D_j} \{(f(X_i) - \hat{f}^{-j}(X_i))X_i\} - \mathbb{E}_{D_j^{-j}}[(f(X) - \hat{f}^{-j}(X))X] \right\|_\infty
$$

$$
+ \left\| \frac{1}{n_j + N_j} \sum_{i \in D_j} \{(f(X_i) - \hat{f}^{-j}(X_i))X_i\} - \mathbb{E}_{D_j^{-j}}[(f(X) - \hat{f}^{-j}(X))X] \right\|_\infty,
$$

(A.12)

where $\mathbb{E}_{D_j^{-j}}$ denotes the conditional expectation given the data in $D_j^{-j} = D^* \setminus D_j$. Let us denote $g_k(X) = (f(X) - \hat{f}^{-j}(X))X_k$ and $\gamma_k(X) = g_k(X) - \mathbb{E}_{D_j^{-j}}[g_k(X)]$. From (A.12), it suffices to upper bound $\max_{1 \leq k \leq p} \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i)$ and $\max_{1 \leq k \leq p} \frac{1}{n_j + N_j} \sum_{i \in D_j} \gamma_k(X_i)$, respectively.

We know

$$
\mathbb{E}_{D_j^{-j}} \left[ \max_{1 \leq k \leq p} \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i) \right] \leq n_j K_1^2 \| \hat{f}^{-j} - f \|_2^2,
$$

(A.13)

which follows from $\|X\|_\infty \leq K_1$ in Assumption 1. Therefore, with the application of lemma 8 by choosing $m = 2$, we can show

$$
\mathbb{E}_{D_j^{-j}} \left[ \max_{1 \leq k \leq p} \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i) \right] \leq K_1^2 \frac{8 \log(2p)}{n_j} \| \hat{f}^{-j} - f \|_2^2.
$$

Furthermore, the Markov inequality implies for any $c > 0$

$$
P\left( \max_{1 \leq k \leq p} \left| \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i) \right| \geq c K_1 b_n \sqrt{\frac{\log 2p}{n_j} D_j^{-j}} \right)
$$

$$
\leq \frac{\mathbb{E}_{D_j^{-j}} \left[ \max_{1 \leq k \leq p} \left| \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i) \right|^2 \right]}{c^2 K_1^2 b_n^2} \frac{n_j}{\log(2p)} \wedge 1
$$

$$
\leq \frac{8 \| \hat{f}^{-j} - f \|_2^2}{c^2 b_n^2} \wedge 1.
$$

(A.14)

For any $\epsilon > 0$, let $c' = 2 \epsilon$ be a sufficiently large constant such that the event $\mathcal{E} = \{ \| \hat{f}^{-j} - f \|_2^2 \leq c' b_n^2 \}$ holds with probability at least $1 - \epsilon$. From (A.14), we know that

$$
P\left( \max_{1 \leq k \leq p} \left| \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i) \right| \geq c K_1 b_n \sqrt{\frac{\log 2p}{n_j} D_j^{-j}} \right)
$$

$$
= \mathbb{E} \left[ P\left( \max_{1 \leq k \leq p} \left| \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i) \right| \geq c K_1 b_n \sqrt{\frac{\log 2p}{n_j} D_j^{-j}} \right) \right]
$$

$$
\leq \mathbb{E} \left[ \frac{8 \| \hat{f}^{-j} - f \|_2^2}{c^2 b_n^2} \wedge 1 \right] I(\mathcal{E}) + \mathbb{E} \left[ \frac{8 \| \hat{f}^{-j} - f \|_2^2}{c^2 b_n^2} \wedge 1 \right] I(\mathcal{E}^c)
$$

$$
\leq \frac{8c'}{c^2} + \mathbb{P}(\mathcal{E}^c) \leq 2\epsilon.
$$
where the last step holds by taking \( c^2 = 8d'/\epsilon \) and the definition \( \mathbb{P}(\mathcal{E}^c) \leq \epsilon \). This implies

\[
\max_{1 \leq k \leq p} \left| \frac{1}{n_j} \sum_{i \in D_j} \gamma_k(X_i) \right| = O_p(K_1b_n \sqrt{\frac{\log p}{n_j}}).
\]

Following the same argument, the following probability bound holds

\[
\max_{1 \leq k \leq p} \left| \frac{1}{n_j + N_j} \sum_{i \in D_j} \gamma_k(X_i) \right| = O_p(K_1b_n \sqrt{\frac{\log p}{n_j + N_j}}).
\]

The rest of the proof follows the same line as in the proof of Theorem 7.1 in Bickel et al. (2009).

Recall that we assume for \( j = \{1, 2\}, n_j = n/2 \) and \( N_j = N/2 \). We can show that

\[
\left\| \sum_{i=1}^{n+|N|} X_iX_i^T \theta^* \right\|_\infty = \left\| \sum_{i=1}^{n+|N|} X_i(X_i^T \theta^* - \hat{\theta}_1 + \hat{\theta}_2) \right\|_\infty + O_p(K_1b_n \sqrt{\frac{\log p}{n}})
\]

\[
\leq \left\| \sum_{i=1}^{n+|N|} X_i(X_i^T \theta^* - f(X_i)) \right\|_\infty + \left\| \sum_{i=1}^{n+|N|} X_i^T(Y_i - f(X_i)) \right\|_\infty + O_p(K_1b_n \sqrt{\frac{\log p}{n}})
\]

\[
= O_p(K_1 \Phi \sqrt{\frac{\log p}{n+N}}) + O_p(K_1 \sigma \sqrt{\frac{\log p}{n}}) + O_p(K_1b_n \sqrt{\frac{\log p}{n}}).
\]

where the last probability bound holds by the same argument in the proof of example 14.3 in Bhlmann and Van de Geer (2011).

Then, if we set \( \lambda_D = C'K_1(\Phi \sqrt{\frac{\log p}{n+N}} + \sigma \sqrt{\frac{\log p}{n}} + b_n \sqrt{\frac{\log p}{n}}) \) for sufficiently large \( C' \), (A.15) implies

\[
\lambda_D \geq \left\| \sum_{i=1}^{n+|N|} X_iX_i^T \theta^* - \hat{\theta}_1 + \hat{\theta}_2 \right\|_\infty
\]

holds with probability tending to 1. Let \( \delta = \hat{\theta}_D - \theta^* \). By the construction of Dantzig estimator, when (A.16) holds, we have \( ||\delta_T||_1 \leq ||\delta_T||_1 \) where \( T \) denotes the support of \( \theta^* \) and

\[
\frac{1}{n+N} ||\tilde{X}^T \tilde{X} \delta||_\infty \leq \frac{1}{n+N} ||\tilde{X}^T \tilde{X} \hat{\theta}_D||_\infty - \frac{\xi_1 + \xi_2}{2} + \frac{1}{n+N} ||\tilde{X}^T \tilde{X} \theta^*||_\infty - \frac{\xi_1 + \xi_2}{2} \leq 2\lambda_D.
\]

Therefore,

\[
\frac{1}{n+N} ||\tilde{X} \delta||_2^2 = \frac{1}{n+N} \delta^T \tilde{X}^T \tilde{X} \delta
\]

\[
\leq \frac{1}{n+N} ||\delta^T \tilde{X}^T \tilde{X}||_\infty ||\delta||_1
\]

\[
\leq 2\lambda_D \times 2||\delta_T||_1 \leq 4\lambda_D \sqrt{s} ||\delta_T||_2.
\]

With smallest eigenvalue condition (A1) and Lemma 9, we know on the event of \( \mathcal{B}_{c_1} (n+N,s,1) \),

\[
\frac{1}{n+N} ||\tilde{X} \delta||_2^2 \geq (1-c_1)^2 \gamma_{\min} ||\delta_T||_2^2.
\]

Therefore,

\[
||\delta_T||_2 \leq \frac{4\lambda_D \sqrt{s}}{(1-c_1)^2 \gamma_{\min}}.
\]

Above all, we know\( ||\delta||_1 \leq 2||\delta_T||_1 \leq 2\sqrt{s} ||\delta_T||_2 \leq \frac{8\lambda_D s}{(1-c_1)^2 \gamma_{\min}}. \) As a byproduct, we can show that\( ||\delta||_2 \leq \lambda_D \sqrt{s} \). This completes the proof.
A.4 Proof of Theorem 3

Proof. We will first derive some preliminary probability bounds that will be used later in the proof. With (A1)-(A5) in Assumptions (1) and (2), we can verify the assumptions (B1)-(B4) for strongly bounded case in Theorem 2.4 of Van de Geer et al. (2014) holds with \( K = K_1 \vee K_2 \). In particular, we have

\[
|X^{(-k)}^T \gamma_k| = |X^{(-k)}^T \Sigma_{-k,-k}^{-1} \Sigma_{-k,k}| = |X^{(-k)}^T \Omega_{-k,k}| \Omega_{kk}^{-1} \\
= |X^{(-k)}^T \Omega_{-k,k}|(\Sigma_{kk} - \Sigma_{k,-k} \Sigma_{-k,k}^{-1} \Sigma_{-k,k}) = O(K_2),
\]

uniformly over \( 1 \leq k \leq p \).

Under the the strongly bounded case with \( s_\Omega = o(\frac{n+N}{\log p}) \), and \( \max_k \Sigma_{kk} = O(1) \), we can apply Theorem 2.4 and Lemma 5.3 in Van de Geer et al. (2014) and claim that the nodewise lasso estimator satisfies

\[
||\hat{\Omega} - \Omega||_\infty = O_p(Ks_\Omega \sqrt{\frac{\log p}{n+N}}), \quad ||I_p - \hat{\Omega} \Sigma_{n+N}||_{\max} = O_p(K \sqrt{\frac{\log p}{n+N}}).
\]

The first probability bound in (A.17) is directly from Theorem 2.4 of Van de Geer et al. (2014). To see the second probability bound, with the formulation of \( \hat{\Omega} \) and notation from nodewise Lasso (3.3), we know for each row of \( \hat{\Omega} \),

\[
||\hat{\Sigma}_{n+N} \Omega_k^T - e_k||_\infty \leq \lambda_k/\tilde{\tau}_k^2,
\]

where \( e_k \) is the unit vector. Furthermore, invoking Lemma 5.3 in Van de Geer et al. (2014), we know when we choose a suitable tuning parameter \( \lambda_k = K_1 \sqrt{\frac{\log p}{n+N}} \) uniformly over \( k \), we have \( \max_k 1/\tilde{\tau}_k^2 = O_p(1) \). Hence, \( ||I_p - \hat{\Omega} \Sigma_{n+N}||_{\max} \leq \max_k (\lambda_k/\tilde{\tau}_k^2) = O_p(K_1 \sqrt{\frac{\log p}{n+N}}) \).

In addition, recalling from the derivation of (A.15) we have

\[
||\frac{X^T(Y - f_n)}{n} + \frac{X^T(\theta_{n+N} - \bar{\theta}_{n+N})}{n+N}||_\infty = O_p(K_1\sigma \sqrt{\frac{\log p}{n}} + K_1 \Phi \sqrt{\frac{\log p}{n+N}}),
\]

where \( f_n = (f(X_1), ..., f(X_n))^T \) and \( \theta_{n+N} \) is defined similarly.

Given the above preliminary results, we focus on deriving the limiting distribution of \( v^T(\hat{\theta}^d - \theta^*) \). Recall that we use the following notation \( \tilde{f}_{D_j} = \{\tilde{f}^{-j}(X_i) : i \in D_j\} \), \( \tilde{f}_{\hat{D}_j} = \{\tilde{f}^{-j}(X_i) : i \in \hat{D}_j\} \), and \( f_{D_j} \) and \( f_{\hat{D}_j} \) are defined similarly. We decompose the term \( v^T(\hat{\theta}^d - \theta^*) \) as

\[
v^T(\hat{\theta}^d - \theta^*) = v^T \left\{ (I_p - \hat{\Omega} \Sigma_{n+N}) (\hat{\theta}_D - \theta^*) + \hat{\Omega} \sum_{j=1}^{2} \left( \frac{X_{D_j}^T(Y_{D_j} - \tilde{f}_{D_j})}{2n_j} + \frac{X_{D_j}^T(\bar{f}_{D_j} - \bar{\theta}^*)}{2n_j + 2N_j} \right) \right\}
\]

\[
= v^T \left\{ (I_p - \hat{\Omega} \Sigma_{n+N}) (\hat{\theta}_D - \theta^*) + (\hat{\Omega} - \Omega) \left( \frac{X^T(Y - f_n)}{n} + \frac{X^T(\theta_{n+N} - \bar{\theta}_{n+N})}{n+N} \right) \right\}
\]

\[
+ \hat{\Omega} \left( \frac{X^T(Y - f_n)}{n} + \frac{X^T(\theta_{n+N} - \bar{\theta}_{n+N})}{n+N} \right) - \Omega \sum_{j=1}^{2} \left( \frac{X_{D_j}^T(\hat{f}_{D_j} - \tilde{f}_{D_j})}{2n_j} + \frac{X_{D_j}^T(\hat{f}_{D_j} - \tilde{f}_{D_j})}{2n_j + 2N_j} \right)
\]

\[
+ (\hat{\Omega} - \Omega) \sum_{j=1}^{2} \left( \frac{X_{D_j}^T(\hat{f}_{D_j} - \tilde{f}_{D_j})}{2n_j} + \frac{X_{D_j}^T(\hat{f}_{D_j} - \tilde{f}_{D_j})}{2n_j + 2N_j} \right).
\]
Therefore, with the preliminary results above in hand, we can show that

\[
\| (I_p - \tilde{\Theta} \tilde{\Sigma}_{n+N}) (\tilde{\theta}_D - \theta^*) \|_\infty \leq \| I_p - \tilde{\Theta} \tilde{\Sigma}_{n+N} \|_{\max} \| \tilde{\theta}_D - \theta^* \|_1
\]

\[
= O_p \left( K_1 K s_\Omega \left( \Phi \frac{\log p}{n + N} + \sigma \frac{\log p}{\sqrt{n(n + N)}} + b_n \frac{\log p}{\sqrt{n(n + N)}} \right) \right)
\]

from (A.17) and Theorem 2. Similarly,

\[
\| (\tilde{\Theta} - \Theta) \left( \frac{X^T(Y - f_n)}{n} + \frac{\tilde{X}^T(f_{n+N} - \tilde{X} \theta^*)}{n + N} \right) \|_\infty
\]

\[
\leq \| \tilde{\Theta} - \Theta \|_\infty \| \frac{X^T(Y - f_n)}{n} + \frac{\tilde{X}^T(f_{n+N} - \tilde{X} \theta^*)}{n + N} \|_\infty
\]

\[
= O_p \left( K_1 K s_\Omega \left( \Phi \frac{\log p}{n + N} + \sigma \frac{\log p}{\sqrt{n(n + N)}} \right) \right),
\]

from (A.18) and (A.17). Following the similar argument in the analysis of \( I_1 \) in (A.12) together with the assumption that \( \| W \|_\infty = \| \Omega X \|_\infty \leq K_2 \), we obtain

\[
\| \tilde{\Omega} \sum_{j=1}^{2} \left( \frac{X^T_D (\hat{\theta}_D^j - \hat{\theta}_D^j)}{2n_j} + \frac{\tilde{X}^T_D (f_{D_j} - \hat{\theta}_D^j)}{2n_j + 2N_j} \right) \|_\infty = O_p \left( K_2 b_n \sqrt{\frac{\log p}{n}} \right).
\]

Similarly, we have

\[
\| (\Omega - \tilde{\Omega}) \sum_{j=1}^{2} \left( \frac{X^T_D (\hat{\theta}_D^j - \hat{\theta}_D^j)}{2n_j} + \frac{\tilde{X}^T_D (f_{D_j} - \hat{\theta}_D^j)}{2n_j + 2N_j} \right) \|_\infty
\]

\[
\leq \| \Omega - \tilde{\Omega} \|_\infty \| \sum_{j=1}^{2} \left( \frac{X^T_D (\hat{\theta}_D^j - \hat{\theta}_D^j)}{2n_j} + \frac{\tilde{X}^T_D (f_{D_j} - \hat{\theta}_D^j)}{2n_j + 2N_j} \right) \|_\infty
\]

\[
= O_p \left( K_1 K b_n s_\Omega \frac{\log p}{\sqrt{n(n + N)}} \right).
\]

Collecting the above probability bounds and plugging into (A.19), we obtain

\[
v^T (\tilde{\theta}_D - \theta^*) = v^T \Omega \left( \frac{X^T(Y - f_n)}{n} + \frac{\tilde{X}^T(f_{n+N} - \tilde{X} \theta^*)}{n + N} \right) + O_p(\delta_n)
\]

\[
= \frac{1}{n} \sum_{i=1}^{n} v^T W_i (Y_i - f(X_i)) + \frac{1}{n + N} \sum_{i=1}^{n+N} v^T W_i (f(X_i) - X_i^T \theta^*) + O_p(\delta_n)
\]

\[
= \sum_{i=1}^{n+N} \xi_i + O_p(\delta_n).
\]  

(A.20)

where

\[
\xi_i = \begin{cases} 
\frac{1}{n} v^T W_i (Y_i - f(X_i)) + \frac{v^T}{n} (f(X_i) - X_i^T \theta^*) & \text{for } 1 \leq i \leq n, \\
\frac{1}{n+N} v^T W_i (f(X_i) - X_i^T \theta^*) & \text{for } n + 1 \leq i \leq n + N
\end{cases}
\]

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and
\[ \delta_n = \|v\|_1 \left[ K_1 K(s \vee s_0) \left( \Phi \frac{\log p}{p + N} + \sigma \frac{\log p}{\sqrt{n(n + N)}} + b_n \frac{\log p}{\sqrt{n(n + N)}} \right) + K_2 b_n \sqrt{\frac{\log p}{n}} \right]. \]

In the following, we will apply the Lindeberg-Feller Central Limit Theorem to (A.20). First, we note that \( \mathbb{E}W_i(Y_i - f(X_i)) = 0 \) and \( \mathbb{E}W_i(f(X_i) - X_i^T \theta^*) = 0 \). Denote \( \eta_i = f(X_i) - X_i^T \theta^* \). We have
\[
\sum_{i=1}^{n+N} \mathbb{E}(\xi_i^2) = \sum_{i=1}^{n} \frac{1}{n^2} \mathbb{E}\{v_i^T W_i(\epsilon_i + \frac{n}{n+N} \eta_i)\}^2 + \sum_{i=n+1}^{n+N} \frac{1}{(n+N)^2} \mathbb{E}(v_i^T W_i \eta_i)^2
\]
\[
= \frac{1}{n^2} v_i^T (\sigma^2 \Omega + \frac{n}{n+N} \Gamma) v := t_n^2,
\]
where \( \Gamma = \text{Cov}(W(f(X) - X^T \theta^*)) \). The Lyapunov condition holds as follows
\[
\sum_{i=1}^{n+N} \mathbb{E}\|\xi_i\|_{t_n^{2+\delta}}^2 \leq \frac{\|v\|_{t_n^{2+\delta}}^2 K_2^{2+\delta} (\sum_{i=1}^{n} \mathbb{E}(\epsilon_i + \frac{n}{n+N} \eta_i))^{2+\delta}/n^{2+\delta} + \sum_{i=n+1}^{n+N} \mathbb{E}\|\eta_i\|_{t_n^{2+\delta}}^2/(n+N)^{2+\delta})}{t_n^{2+\delta}}
\]
\[
\leq \|v\|_{t_n^{2+\delta}}^2 K_2^{2+\delta} \left( \mathbb{E}\|\epsilon_i\|_{t_n^{2+\delta}}^2 + \frac{\|\eta_i\|_{t_n^{2+\delta}}^2}{n^2} + \frac{\|\eta_i\|_{t_n^{2+\delta}}^2}{n^2} N/(n+N)^{2+\delta} \right) / n^{2+\delta}
\]
\[
\leq \frac{2^{1+\delta}\|v\|_{t_n^{2+\delta}}^2 K_2^{2+\delta} \mathbb{E}\|\xi_i\|_{t_n^{2+\delta}}^2}{n^{2+\delta}(\sigma^2 v_i^T \Omega v_i)^{1+\delta/2}} + \frac{\|v\|_{t_n^{2+\delta}}^2 K_2^{2+\delta} (\mathbb{E}\|\eta_i\|_{t_n^{2+\delta}}^2 + \mathbb{E}\|\eta_i\|_{t_n^{2+\delta}}^2 N/(n+N)^{2+\delta})}{(n+N)^{1+\delta/2}(v_i^T \Gamma v_i)^{1+\delta/2}} \rightarrow 0,
\]
where the first inequality follows from \( \|W\|_\infty = \|\Omega X\|_\infty \leq K_2 \) and the second one is due to the convexity of the function \( x^{2+\delta} \) for \( x > 0 \). Therefore, the Lindeberg-Feller Central Limit Theorem leads to
\[
\sum_{i=1}^{n+N} \xi_i/t_n \xrightarrow{d} \mathcal{N}(0, 1).
\]
From (A.20) we obtain
\[
\frac{v^T(\hat{\theta}^d - \theta^*)}{t_n} = \sum_{i=1}^{n+N} \xi_i/t_n + O_p(\delta_n/t_n) \xrightarrow{d} \mathcal{N}(0, 1),
\]
as \( \delta_n/t_n = o(1) \). This completes the proof.

\[ \square \]

A.5 Proof of Proposition 4

Lemma 10. Under the same conditions in Proposition 4, we have
\[
|\hat{\sigma}^2 - \sigma^2| = O_p(n^{-1/2} + b_n^2),
\]
and
\[
|v^T(\hat{\Gamma} - \Gamma)v| = O_p\left( K_2^2 \|v\|^2(b_n + K \sqrt{\frac{s \log p}{n} + \frac{K^2 s \log p}{n}} + K s \Omega \sqrt{\frac{\log p}{n+N}}) \right).
\]
Proof of Lemma 10. To show (A.21), it suffices to upper bound \( \hat{\sigma}_j^2 - \sigma^2 \), that is

\[
\hat{\sigma}_j^2 - \sigma^2 = \frac{1}{n_j} \sum_{i \in D_j^*} (Y_i - f(X_i) + f(X_i) - \hat{f}^{-j}(X_i))^2 - \sigma^2 \\
= \frac{1}{n_j} \sum_{i \in D_j^*} (\epsilon_i^2 - \sigma^2) + 2 \frac{2}{n_j} \sum_{i \in D_j^*} \epsilon_i(f(X_i) - \hat{f}^{-j}(X_i)) + \frac{1}{n_j} \sum_{i \in D_j^*} (f(X_i) - \hat{f}^{-j}(X_i))^2.
\tag{A.23}
\]

Chebyshev’s inequality together with the assumption \( \mathbb{E}(\epsilon^4) \leq C \) implies \( \frac{1}{n_j} \sum_{i \in D_j^*} (\epsilon_i^2 - \sigma^2) = O_p(n^{-1/2}) \). As in the derivation of (A.14) we have

\[
P \left( \frac{1}{n_j} \sum_{i \in D_j^*} \epsilon_i(f(X_i) - \hat{f}^{-j}(X_i)) > c\sigma_b/\sqrt{n_j} \right) \leq \frac{\| \hat{f}^{-j} - f \|^2}{c^2 \sigma_b^2} \wedge 1.
\]

As a result, we have

\[
\frac{1}{n_j} \sum_{i \in D_j^*} \epsilon_i(f(X_i) - \hat{f}^{-j}(X_i)) = O_p(1/n^{1/2}).
\]

Similarly, \( \frac{1}{n_j} \sum_{i \in D_j^*} (f(X_i) - \hat{f}^{-j}(X_i))^2 \lesssim \| \hat{f}^{-j} - f \|_2^2 = O_p(b_n^2) \). Plugging into (A.23), we have \( |\hat{\sigma}_j^2 - \sigma^2| = O_p(n^{-1/2} + b_n^2) \), which further implies (A.21).

To show (A.22), we decompose \( v^T(\hat{\Gamma}_j - \Gamma)v \) as follows

\[
v^T(\hat{\Gamma}_j - \Gamma)v = v^T\hat{\Omega} - \frac{1}{n_i + N_j} \sum_{i \in D_j} X_i X_i^T (\hat{\eta}_i^j - \eta_i^j) \hat{\Omega} v + v^T\hat{\Omega} \frac{1}{n_i + N_j} \sum_{i \in D_j} \{X_i X_i^T \hat{\eta}_i^2 - \mathbb{E}(X_i X_i^T \hat{\eta}_i^2)\} \hat{\Omega} v \\
+ v^T(\hat{\Omega} - \Omega) \mathbb{E}(X_i X_i^T \hat{\eta}_i^2) \hat{\Omega} v + v^T\Omega \mathbb{E}(X_i X_i^T \hat{\eta}_i^2)(\hat{\Omega} - \Omega)v \tag{A.24}
\]

Let us first consider \( T_1 \), which can be rewritten as

\[
T_1 = \frac{1}{n_i + N_j} \sum_{i \in D_j} (v^T\hat{\Omega} X_i)^2 [\hat{\eta}_i^j - \eta_i]^2 + \frac{1}{n_i + N_j} \sum_{i \in D_j} (v^T\hat{\Omega} X_i)^2 \eta_i [\hat{\eta}_i^j - \eta_i].
\]

We know that \( |v^T\hat{\Omega} X_i| \leq \|v\|_1 \|\hat{\Omega} X_i\|_\infty \leq \|v\|_1 (\|\hat{\Omega} X_i\|_\infty + \|\hat{\Omega} - \Omega\|_\infty \|X_i\|_\infty) \lesssim K \|v\|_1 \), since \( Ks\Omega(\log p/(n+N))^{1/2} = o(1) \). In addition, \( (\hat{\eta}_i^j - \eta_i)^2 \leq 2(\hat{f}^{-j}(X_i) - f(X_i))^2 + 2(\hat{X}_i^T(\theta_D - \theta^*))^2 \). Combining these results, Theorem 2 and \( b_n = o(1) \), we derive

\[
\left| \frac{1}{n_i + N_j} \sum_{i \in D_j} (v^T\hat{\Omega} X_i)^2 [\hat{\eta}_i^j - \eta_i]^2 \right| = O_p\left( K^2 \|v\|_1^2 (b_n^2 + \frac{K^2 s \log p}{n}) \right).
\]
and
\[
\left| \frac{1}{n_i + N_j} \sum_{i \in D_j} (v^T \hat{\Omega} X_i)^2 \eta_i^2 \hat{\eta}_i^j - \eta_i^j \right|
\leq \left| \frac{1}{n_i + N_j} \sum_{i \in D_j} (v^T \Theta X_i)^2 \eta_i^2 \right|^{1/2} \left| \frac{1}{n_i + N_j} \sum_{i \in D_j} (v^T \hat{\Omega} X_i)^2 \hat{\eta}_i^j - \eta_i^j \right|^{1/2}
= O_p \left( K^2 \|v\|_1^2 \left(n_i + K \sqrt{s \log \frac{p}{n}} \right) \right),
\]
where the first step holds by Cauchy–Schwarz inequality. This implies the following rate for $T_1$:
\[
|T_1| = O_p \left( K^2 \|v\|_1^2 \left(n_i + K \sqrt{s \log \frac{p}{n} + K^2 s \log \frac{p}{n}} \right) \right).
\]
For $T_2$, we can show that
\[
T_2 = v^T (\hat{\Omega} - \Omega) Z_n (\hat{\Omega} - \Omega) v + 2 v^T (\hat{\Omega} - \Omega) Z_n \Omega v + v^T \Omega Z_n \Omega v
\]
where $Z_n = \frac{1}{n_i + N_j} \sum_{i \in D_j} \{X_i X_i^T \eta_i^2 - \mathbb{E}(X_i X_i^T \eta_i^2)\}$. We can bound the three terms in the right hand side of the above equation separately. As an illustration, we have
\[
v^T (\hat{\Omega} - \Omega) Z_n (\hat{\Omega} - \Omega) v \leq \|v\|_1^2 \|\hat{\Omega} - \Omega\|_\infty^2 \|Z_n\|_{\text{max}} = O_p \left( \|v\|_1^2 K^2 s \log \frac{p}{n + N} K^2 \sqrt{\log p \frac{p}{n + N}} \right),
\]
where in the last step holds we plugin the rate of $\hat{\Omega}$ in (A.17) and apply Lemma 8 to upper bound $\|Z_n\|_{\text{max}}$ (as $X_i$ is uniformly bounded by $K_1 \leq K$ and $\mathbb{E}(\eta_i^2)$ is bounded as well). Using a similar argument, one can derive
\[
|v^T (\hat{\Omega} - \Omega) Z_n \Omega v| = \|v\|_1 \|\hat{\Omega} - \Omega\|_\infty \|Z_n \Omega v\|_\infty = O_p \left( \|v\|_1^2 K s \sqrt{\log p \frac{p}{n + N} K^2 \sqrt{\log p \frac{p}{n + N}}} \right),
\]
and
\[
v^T \Omega Z_n \Omega v = O_p \left( \|v\|_1^2 K^2 \sqrt{\log p \frac{p}{n + N}} \right).
\]
Under the additional assumption that $K s \Omega (\log p/(n + N))^{1/2} = o(1)$, we can simplify the rate of $T_2$ as
\[
|T_2| = O_p \left( \|v\|_1^2 K^2 \sqrt{\log p \frac{p}{n + N}} \right).
\]
Finally, let us consider $T_3$ and $T_4$. For $T_3$, we have
\[
T_3 = v^T (\hat{\Omega} - \Omega) \mathbb{E}(X_i X_i^T \eta_i^2 \Omega v) + v^T (\hat{\Omega} - \Omega) \mathbb{E}(X_i X_i^T \eta_i^2)(\hat{\Omega} - \Omega) v,
\]
where the first term is identical to $T_4$ and therefore it suffices to only consider the rate of $T_3$. Since $\mathbb{E}(X_i X_i^T \eta_i^2 \Omega v) \|\infty \leq \|v\|_1 K^2 \mathbb{E}(\eta_i^2) \| \leq \|v\|_1 K^2$ and $\mathbb{E}(X_i X_i^T \eta_i^2) \|_{\text{max}} \leq K^2$, we have
\[
|T_3| \lesssim \|v\|_1 K s \Omega \sqrt{\log p \frac{p}{n + N} \|v\|_1 K^2} = O_p \left( \|v\|_1^2 K^3 s \Omega \sqrt{\log p \frac{p}{n + N}} \right).
\]
Collecting the upper bounds for $T_1, \ldots, T_4$, from (A.24) we obtain the rate in (A.22).
Proof of Proposition 4. Note that $v^T \Omega v \leq \|v\|^2 \lambda_{\max}(\Omega) \lesssim \|v\|_2^2$ since $\lambda_{\max}(\Omega) = 1/\lambda_{\min}(\Sigma) \leq 1/C$. From Lemma 10, we can show that

\[
v^T \sigma^2 \Omega v - v^T \sigma^2 \Omega v = (\hat{\sigma}^2 - \sigma^2) v^T \Omega v + (\hat{\sigma}^2 - \sigma^2) v^T (\hat{\Omega} - \Omega) v + \sigma^2 v^T (\hat{\Omega} - \Omega) v
\]

\[
\lesssim \|v\|^2 (n^{-1/2} + b_n^2) + (n^{-1/2} + b_n^2) \|v\|_1 \|v\|_\infty K \sigma^2 \Omega \sqrt{\frac{\log p}{n + N}} + \|v\|_1 \|v\|_\infty K \sigma^2 \Omega \sqrt{\frac{\log p}{n + N}}
\]

\[
= O_p \left( \|v\|^2 (n^{-1/2} + b_n^2) + \|v\|_1 \|v\|_\infty K \sigma^2 \Omega \sqrt{\frac{\log p}{n + N}} \right).
\]

This implies

\[
\left| v^T (\hat{\sigma}^2 \Omega + \frac{n}{n + N} \hat{\Gamma}) v - v^T (\sigma^2 \Omega + \frac{n}{n + N} \Gamma) v \right|
\]

\[
= O_p \left( \|v\|^2 (n^{-1/2} + b_n^2) + \|v\|_1 \|v\|_\infty K \sigma^2 \Omega \sqrt{\frac{\log p}{n + N}} \right) + K^2 \|v\|^2 \left( \frac{nb_n}{n + N} + K \sqrt{\frac{n}{n + N}} \frac{s \log p}{n + N} + \frac{K^2 s \log p}{n + N} + K \sigma^2 \Omega \sqrt{\frac{\log p}{n + N}} \right) + \frac{n}{n + N} \frac{\log p}{n + N}.
\]

By applying the condition $K(s \log p/(n+N))^{1/2} = o(1)$ and $n/(n+N) \leq 1$, we can further simplify the above rate and derive (3.10). Note that $v^T (\sigma^2 \Omega + \frac{n}{n+N} \Gamma) v \geq C \|v\|_2^2$ which together with (3.10) leads to

\[
\left| v^T (\hat{\sigma}^2 \Omega + \frac{n}{n + N} \hat{\Gamma}) v - v^T (\sigma^2 \Omega + \frac{n}{n + N} \Gamma) v - 1 \right| = O_p (n^{-1/2} + b_n^2 + \text{Rem}_N/\|v\|_2^2).
\]

Finally, (3.12) holds by Theorem 3 and the Slutsky Theorem. This completes the proof. \qed

A.6 Proof of Theorem 5

We first state several propositions and lemmas which are used in the proof.

**Lemma 11.** Assume that Assumption 1 holds. Consider the Dantzig selector $\hat{\theta}_L$ in (2.2) with $\lambda_L \asymp K_1 \sqrt{(s^2 + \Phi^2) \log p / n}$. We have

\[
\|\hat{\theta}_L - \theta^*\|_1 = O_p(s \lambda_L), \quad \text{and} \quad \frac{1}{n} \sum_{i=1}^{n} [X_i^T (\hat{\theta}_L - \theta^*)]^2 = O_p(s \lambda_L^2).
\]

Moreover, we have

\[
\|\hat{\Sigma}_n (\hat{\theta}_L - \theta^*)\|_\infty = O_p(\lambda_L),
\]

where $\hat{\Sigma}_n = \frac{1}{n} \sum_{i=1}^{n} X_i \otimes X_i^T$.

**Proof.** The proof of the convergence rate of $\hat{\theta}_L$ in (A.25) is similar to Theorem 7.1 in Bickel et al. (2009). The key step is to derive

\[
\|\frac{1}{n} \sum_{i=1}^{n} X_i (Y_i - X_i^T \theta^*)\|_\infty \lesssim K_1 (s^2 + \Phi^2)^{1/2} \sqrt{\frac{\log p}{n}},
\]

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which is implied by Lemma 8 together with \( \mathbb{E}(Y_i - X_i^T \theta^*)^2 = \sigma^2 + \Phi^2 \) and \( \|X_i\|_\infty \leq K_1 \). The rest of the proof is omitted. To show the rate of \( \|\hat{\Sigma}_n(\hat{\theta}_L - \theta^*)\|_\infty \), we note that, with \( \lambda_L = CK_1 \sqrt{(\sigma^2 + \Phi^2) \log p \over n} \) for some sufficiently large \( C \), we have

\[
\|\hat{\Sigma}_n(\hat{\theta}_L - \theta^*)\|_\infty \leq \frac{1}{n} \sum_{i=1}^n X_i(Y_i - X_i^T \hat{\theta}_L)\|_\infty + \frac{1}{n} \sum_{i=1}^n X_i(Y_i - X_i^T \theta^*)\|_\infty \leq 2\lambda,
\]

where we invoke the KKT condition of \( \hat{\theta}_L \) in the last step.

\[ \square \]

**Proposition 12.** Under the same conditions in Theorem 5, for any \( \tilde{\lambda}_k = \tilde{\lambda} \geq CK_1(c_n + \sqrt{\log p/n}) \), we obtain that

\[
\|\hat{B}_k - B_k\|_1 \lesssim s_B \tilde{\lambda} + \tilde{\lambda}^{-1} \left[K_1 L_B(c_n + \sqrt{\log p / n}) + K_1^2 \sqrt{s(\sigma^2 + \Phi^2) \log p \over n}\right]^2.
\]

Define

\[
\tilde{\lambda}_{opt} = \arg \min_{\tilde{\lambda} \geq CK_1(c_n + \sqrt{\log p/n})} s_B \tilde{\lambda} + \tilde{\lambda}^{-1} \left[K_1 L_B(c_n + \sqrt{\log p / n}) + K_1^2 \sqrt{s(\sigma^2 + \Phi^2) \log p \over n}\right]^2.
\]

By choosing \( \tilde{\lambda}_k = \tilde{\lambda}_{opt} \), we obtain

\[
\|\hat{B}_k - B_k\|_1 \lesssim K_1(s_B + s_B^{1/2} L_B) \left(\sqrt{\log p / n} + c_n\right) + K_1^2 \sqrt{s s_B(\sigma^2 + \Phi^2) \log p \over n},
\]

which holds uniformly over \( 1 \leq k \leq p \).

\[ \square \]

**Proof.** The proof is deferred to Appendix A.8.

Now we are ready to prove Theorem 5. For notational simplicity, we use \( \hat{\theta}^d_S \) for \( \hat{\theta}^d_{S, \psi} \), \( \hat{\xi}_S \) for \( \hat{\xi}_{S, \psi} \) and \( \hat{\theta} \) for \( \hat{\theta}_L \). We can rewrite

\[
v^T(\hat{\theta}^d_S - \theta^*) = v^T(\hat{\theta} - \theta^* - \hat{\Omega} \hat{\Sigma}_n(\hat{\theta} - \theta^*) + \hat{\Omega}(\hat{\xi}_S - \hat{\Sigma}_n \theta^*))
\]

\[
= v^T \left\{ (I_p - \hat{\Omega} \hat{\Sigma}_n)(\hat{\theta} - \theta^*) + J \right\}
\]

\[
= v^T \left\{ (I_p - \Omega \hat{\Sigma}_n)(\hat{\theta} - \theta^*) + (\Omega - \hat{\Omega}) \hat{\Sigma}_n(\hat{\theta} - \theta^*) + J \right\} ,
\]

where

\[
J = \hat{\Omega} \left( \frac{X^T(Y - X \theta^*)}{n} - \frac{\psi}{2} \hat{B} \sum_{j=1}^2 \left( \frac{\sum_{i \in D_j^*} X_i \bar{m}^{-j}(X_i)}{n_j} - \frac{\sum_{i \in D_j} X_i \bar{m}^{-j}(X_i)}{n_j + N_j} \right) \right).
\]

We notice that \( \|\Omega X_i\|_\infty \leq \|\Omega\|_\infty \|X_i\|_\infty \leq L_\Omega K_1 \), applying Hoeffding inequality, \( \|I_p - \Omega \hat{\Sigma}_n\|_{\max} = O_p(K_1^2 L_\Omega \sqrt{\log p \over n}) \). Hence,

\[
\| (I_p - \Omega \hat{\Sigma}_n)(\hat{\theta} - \theta^*) \|_\infty \leq \| I_p - \Omega \hat{\Sigma}_n \|_{\max} \| \hat{\theta} - \theta^* \|_1 \lesssim K_1^3 L_\Omega (\sigma^2 + \Phi^2)^{1/2} s \log p \over n ,
\]

(A.27)
where we use the convergence rate of $\hat{\theta}$ in Lemma 11. Moreover, we know
\[
\|(\Omega - \hat{\Omega})\Sigma_n(\hat{\theta} - \theta^*)\|_\infty \leq \|\Omega - \hat{\Omega}\|_\infty \|\Sigma_n(\hat{\theta} - \theta^*)\|_\infty \lesssim K_1^2 L_\Omega s_\Omega \frac{(\sigma^2 + \Phi^2)^{1/2}\log p}{\sqrt{(n+N)n}},
\] (A.28)
followed by (A.17) (we replace $K$ with $K_1 L_\Omega$) and again Lemma 11. Now, we focus on the term $J$. We rewrite $J$ as
\[
J = \frac{X^T(Y - X\theta^*)}{n} - \psi B^T\left(\sum_{i=1}^n X_im(X_i) - \sum_{i=1}^{n+N} X_im(X_i)\right)
\]
\[
+ (\hat{\Omega} - \Omega)\frac{X^T(Y - X\theta^*)}{n} - \psi B^T\left(\sum_{i=1}^n X_im(X_i) - \sum_{i=1}^{n+N} X_im(X_i)\right)\]
\[
+ \frac{(\hat{\Omega} - \Omega)(\xi_S - \xi_0)}{J_2} + \frac{\Omega(\xi_S - \xi_0)}{J_3},
\]
where
\[
\xi_0 = \frac{X^TY}{n} - \psi B^T\left(\sum_{i=1}^n X_im(X_i) - \sum_{i=1}^{n+N} X_im(X_i)\right).
\]
In the following, we will show that the three terms $\|J_k\|_\infty$ for $k = 1, 2, 3$ are sufficiently small. We first recall that
\[
\left\| \frac{1}{n} \sum_{i=1}^n X_im(X_i) - \mu \right\|_\infty \lesssim K_1 \sqrt{\frac{\log p}{n}}, \quad \left\| \frac{1}{n} \sum_{i=1}^n X_i(Y_i - X_i^T\theta^*) \right\|_\infty \lesssim K_1 (\sigma^2 + \Phi^2)^{1/2} \sqrt{\frac{\log p}{n}},
\]
by Hoeffding inequality and Lemma 8. For $J_1$, it holds that
\[
\|J_1\|_\infty \leq \|\hat{\Omega} - \Omega\|_\infty \left\| \frac{X^TY}{n} - \psi \frac{n}{n} \left(\sum_{i=1}^n Xim(X_i) - \sum_{i=1}^{n+N} Xim(X_i)\right) \right\|_\infty
\]
\[
\leq \|\hat{\Omega} - \Omega\|_\infty \left[ \left\| \frac{1}{n} \sum_{i=1}^n X_i(Y_i - X_i^T\theta^*) \right\|_\infty + \|\psi\|L_B \left\| \frac{1}{n} \sum_{i=1}^n X_i m(X_i) - \mu \right\|_\infty \right.
\]
\[
+ \|\psi\|L_B \left\| \frac{1}{n} \sum_{i=1}^{n+N} X_i m(X_i) - \mu \right\|_\infty \]
\[
\lesssim K_1^2 L_\Omega ((\sigma^2 + \Phi^2)^{1/2} + L_B) s_\Omega \frac{\log p}{\sqrt{(n+N)n}}.
\] (A.29)
To upper bound the supnorm of $J_2$ and $J_3$, we need the following bounds. First, by Proposition 12, we have
\[
\left\| (\hat{B} - B)^T \left( \sum_{i=1}^n \frac{Xim(X_i)}{n} - \sum_{i=1}^{n+N} \frac{Xim(X_i)}{n+N} \right) \right\|_\infty
\]
\[
\leq \max_k \|\hat{B}_k - B_k\|_1 \left[ \left\| \frac{1}{n} \sum_{i=1}^n X_i m(X_i) - \mu \right\|_\infty + \left\| \frac{1}{n} \sum_{i=1}^{n+N} X_i m(X_i) - \mu \right\|_\infty \right]
\]
\[
\lesssim K_1^2 (s_B + s_B^{1/2} L_B) \left( \frac{\log p}{n} + c_n \sqrt{\frac{\log p}{n}} \right) + K_1 \sqrt{s_B (\sigma^2 + \Phi^2) \log p / n}.
\]
Furthermore, using a similar argument in the analysis of (A.12) in the proof of Theorem 2, we have

\[
\left\| \mathbf{B}^T \frac{1}{2} \sum_{j=1}^{2} \left( \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j} - \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j + N_j} \right) \right\|_{\infty} \\
\leq L_B \max_{j=1,2} \left\| \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j} - \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j + N_j} \right\|_{\infty} \\
\lesssim K_1 L_B c_n \sqrt{\frac{\log p}{n}}.
\]

Under the condition \( s_B K_1^2 (c_n + \sqrt{\frac{\log p}{n}}) = o(1) \), one can easily verify that max\( k \left\| \hat{B}_k - B_k \right\|_1 \lesssim L_B + K_1^2 \sqrt{\frac{s_B (\sigma^2 + \Phi^2) \log p}{n}} \), and therefore,

\[
\left\| (\hat{B} - B)^T \frac{1}{2} \sum_{j=1}^{2} \left( \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j} - \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j + N_j} \right) \right\|_{\infty} \\
\lesssim K_1 L_B c_n \sqrt{\frac{\log p}{n}} + c_n K_1^3 \sqrt{\frac{s_B (\sigma^2 + \Phi^2) \log p}{n}},
\]

which is of smaller order than the previous two terms. Given these bounds, we can decompose and bound \( \| \xi_0 - \hat{\xi}_S \|_{\infty} \) as

\[
\| \xi_0 - \hat{\xi}_S \|_{\infty} = \| \psi \| \times \left\| \frac{1}{2} \mathbf{B}^T \sum_{j=1}^{2} \left( \frac{\sum_{i \in D_j} X_i \hat{m}^{-j}(X_i)}{n_j} - \frac{\sum_{i \in D_j} X_i \hat{m}^{-j}(X_i)}{n_j + N_j} \right) \right\|_{\infty} \\
- \mathbf{B}^T \left( \frac{\sum_{i=1}^{n} X_i m(X_i)}{n} - \frac{\sum_{i=1}^{n+N} X_i m(X_i)}{n+N} \right) \right\|_{\infty} \\
\leq \left\| (\hat{B} - B)^T \left( \frac{\sum_{i=1}^{n} X_i m(X_i)}{n} - \frac{\sum_{k=1}^{n+N} X_i m(X_i)}{n+N} \right) \right\|_{\infty} \\
+ \left\| (\hat{B} - B)^T \frac{1}{2} \sum_{j=1}^{2} \left( \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j} - \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j + N_j} \right) \right\|_{\infty} \\
+ \left\| \mathbf{B}^T \frac{1}{2} \sum_{j=1}^{2} \left( \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j} - \frac{\sum_{i \in D_j} X_i (\hat{m}^{-j}(X_i) - m(X_i))}{n_j + N_j} \right) \right\|_{\infty} \\
\lesssim K_1^2 (s_B + s_B^{1/2} L_B) \left( \frac{\log p}{n} + c_n \sqrt{\frac{\log p}{n}} \right) + K_3 \frac{\sqrt{s_B (\sigma^2 + \Phi^2) \log p}}{n}.
\]

Thus, for \( J_2 \) and \( J_3 \) we have

\[
\| J_3 \| \lesssim L_1 \left[ K_2^2 (s_B + s_B^{1/2} L_B) \left( \frac{\log p}{n} + c_n \sqrt{\frac{\log p}{n}} \right) + K_3 \frac{\sqrt{s_B (\sigma^2 + \Phi^2) \log p}}{n} \right]. \tag{A.30}
\]

Since we have \( K_1 L_1 \sqrt{\frac{\log p}{n+N}} = o(1) \), \( \| J_2 \|_{\infty} \) is of smaller order than that of \( \| J_3 \|_{\infty} \). Thus, from (A.29) and (A.30), we have

\[
J = \Omega \left( \frac{\mathbf{X}^T (\mathbf{Y} - \mathbf{X} \theta^*)}{n} - \psi \mathbf{B}^T \left( \frac{\sum_{i=1}^{n} X_i m(X_i)}{n} - \frac{\sum_{i=1}^{n+N} X_i m(X_i)}{n+N} \right) \right) + \text{Rem}_n,
\]

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where
\[ \| Rem \|_\infty \lesssim L_\Omega K_1^2 \left[ \left( \left( \sigma^2 + \Phi^2 \right)^{1/2} + L_B \right) s_\Omega \frac{\log p}{\sqrt{(n+N)n}} \right. \]
\[ \left. + \left( s_B + s_B^{1/2} L_B \right) \left( \frac{\log p}{n} + c_n \sqrt{\frac{\log p}{n}} + K_1 \frac{\sqrt{ss_B \left( \sigma^2 + \Phi^2 \right) \log p}}{n} \right) \right]. \]

Finally, combining with (A.27) and (A.28), we obtain from (A.26) that
\[ v^T \left( \theta_S^d - \theta^* \right) = v^T \Omega \left( X^T \left( Y - X \theta^* \right) \right. \]
\[ \left. - \psi B^T \left( \sum_{i=1}^n X_i m(X_i) \right) + \sum_{i=1}^{n+N} X_i m(X_i) \right) + O_p(\tilde{\delta}), \]

where
\[ \tilde{\delta} = \|v\|_1 L_\Omega K_1^2 \left[ \left( \left( \sigma^2 + \Phi^2 \right)^{1/2} + L_B \right) s_\Omega \frac{\log p}{\sqrt{(n+N)n}} \right. \]
\[ \left. + \left( s_B + s_B^{1/2} L_B \right) \left( \frac{\log p}{n} + c_n \sqrt{\frac{\log p}{n}} + K_1 \frac{\sqrt{ss_B \left( \sigma^2 + \Phi^2 \right) \log p}}{n} \right) \right]. \]

To show the asymptotic normality of \( v^T \left( \theta_S^d - \theta^* \right) \), we denote
\[ \xi_i = \begin{cases} \frac{1}{n} v^T \Omega \left\{ T_{i1} - \frac{n_\psi}{n+N} B^T T_{i2} \right\} & \text{for } 1 \leq i \leq n, \\ \frac{\psi}{n+N} v^T \Omega B^T T_{i2} & \text{for } n+1 \leq i \leq n+N, \end{cases} \]
where \( T_{i1} = X_i (Y_i - X_i^T \theta^*) \) and \( T_{i2} = X_i m(X_i) - \mu \). One can rewrite (A.31) as
\[ v^T \left( \theta_S^d - \theta^* \right) = \sum_{i=1}^{n+N} \xi_i + O_p(\tilde{\delta}). \]

To apply the Lindeberg-Feller Central Limit Theorem, we first note that \( \mathbb{E}(\xi_i) = 0 \). Furthermore,
\[ \sum_{i=1}^{n+N} \mathbb{E}(\xi_i^2) = \frac{1}{n} v^T \Omega \left( \mathbb{E}(T_{i1}^{\otimes 2}) - \frac{2n_\psi}{n+N} B^T \mathbb{E}(T_{i2} T_{i1}^T) + \frac{N^2 \psi^2}{(n+N)^2} B^T \mathbb{E}(T_{i2}^{\otimes 2}) B \right) \Omega v \]
\[ + \frac{\psi^2 N}{(n+N)^2} v^T \Omega B^T \mathbb{E}(T_{i2}^{\otimes 2}) B \Omega v \]
\[ = \frac{1}{n} v^T \Omega \left( \mathbb{E}(T_{i1}^{\otimes 2}) - \frac{2n_\psi}{n+N} B^T \mathbb{E}(T_{i2} T_{i1}^T) + \frac{N \psi^2}{n+N} B^T \mathbb{E}(T_{i2}^{\otimes 2}) B \right) \Omega v. \]

Recall that \( B = \{ \mathbb{E}(T_{i2}^{\otimes 2}) \}^{-1} \mathbb{E}(T_{i2} T_{i1}^T) \). Thus, we have
\[ \sum_{i=1}^{n+N} \mathbb{E}(\xi_i^2) = \frac{1}{n} v^T \Omega \left( \mathbb{E}(T_{i1}^{\otimes 2}) - \frac{N(2\psi - \psi^2)}{n+N} \mathbb{E}(T_{i2} T_{i1}^T) \{ \mathbb{E}(T_{i2}^{\otimes 2}) \}^{-1} \mathbb{E}(T_{i2} T_{i1}^T) \right) \Omega v := t_n^2. \]

Note that \( \mathbb{E}\|T_{i1}\|_{\infty}^{2+\delta} \leq K_1^{2+\delta} \mathbb{E}\|\varepsilon_i\|_{\infty}^{2+\delta} \leq K_1^{2+\delta} \) and \( \mathbb{E}\|T_{i2}\|_{\infty}^{2+\delta} \leq K_1^{2+\delta} \). In addition, our assumption implies \( t_n^{2+\delta} \geq C\|v\|_{2}^{2+\delta}/n^{1+\delta/2} \). Finally, we can verify that the Lyapunov condition...
holds
\[
\sum_{i=1}^{n+N} \mathbb{E} [\xi_i]^{2+\delta} \leq \frac{\|v\|^{2+\delta} L_i^{2+\delta}}{n^{1+\delta}} [\frac{1}{n^{1+\delta}} \mathbb{E} \|T_i\| + \frac{N \psi}{n + N} B^T T_{i2} \|T_i\|^{2+\delta} + \frac{\psi^{2+\delta} N}{(n + N)^{2+\delta}} \mathbb{E} \|B^T T_{i2}\|^{2+\delta}]
\]
\[
\lesssim (\|v\| L \Omega K_i)^{2+\delta} \frac{1}{n^{\delta/2}} \left( 1 + \frac{L_i^{2+\delta} N}{n + N} \right) \to 0.
\]

Therefore, we obtain the desired result by applying the Lindeberg-Feller Central Limit Theorem and Slutsky Theorem. This completes the proof.

### A.7 Proof of Proposition 6

**Proof.** We first establish the rate of \( \hat{M}_1 \) and \( \hat{M}_2 \) in the elementwise supnorm. Define \( M_1 = \mathbb{E}((Y_i - X_i^T \theta^*)^2 X_i^{\otimes 2}) \). We note that
\[
\| \hat{M}_1 - M_1 \|_{\text{max}} \leq \left\| \frac{1}{n} \sum_{i=1}^{n} (Y_i - X_i^T \theta^*)^2 X_i^{\otimes 2} - M_1 \right\|_{\text{max}} + \left\| \frac{2}{n} \sum_{i=1}^{n} (Y_i - X_i^T \hat{\theta}_L - \theta^*)^2 X_i^{\otimes 2} \right\|_{\text{max}}
\]
\[
+ \left\| \frac{1}{n} \sum_{i=1}^{n} [X_i^T (\hat{\theta}_L - \theta^*)] X_i^{\otimes 2} \right\|_{\text{max}} \lesssim K_1^3 \sqrt{s \log p}.
\]

where we use the moment inequality in Lemma 8 and Lemma 11. Similarly, define \( M_2 = \mathbb{E}((T_{i2} T_{i1}^T) \). Since \( \hat{M}_2 \) is constructed by sample splitting, it suffices to derive the rate of \( \hat{M}_2 - M_2 \). Following the same type of argument, we can show that
\[
\| \hat{M}_2 - M_2 \|_{\text{max}} \leq \left\| \frac{1}{n} \sum_{i \in D_j^*} (Y_i - X_i^T \hat{\theta}_L) (\hat{m}^{-1}(X_i) - m(X_i)) X_i^{\otimes 2} \right\|_{\text{max}} + \left\| \frac{1}{n} \sum_{i \in D_j^*} X_i^T (\hat{\theta}_L - \theta^*) m(X_i) X_i^{\otimes 2} \right\|_{\text{max}}
\]
\[
+ \left\| \frac{1}{n} \sum_{i \in D_j^*} (Y_i - X_i^T \theta^*) m(X_i) X_i^{\otimes 2} - M_2 \right\|_{\text{max}} \lesssim K_1^2 c_n + K_1^3 \sqrt{s \log p}.
\]

Together with Proposition 12, we have
\[
\| \hat{B}^T \hat{M}_2 - B^T M_2 \|_{\text{max}} \leq \| \hat{B} - B \|_{\infty} \| \hat{M}_2 - M_2 \|_{\text{max}} + \| \hat{B} - B \|_{\infty} \| M_2 \|_{\text{max}} + \| B \|_{\infty} \| \hat{M}_2 - M_2 \|_{\text{max}}
\]
\[
\lesssim K_1^2 \text{Rem},
\]

where
\[
\text{Rem} = K_1 (s_B + s_B^{1/2} L_B) \sqrt{\frac{\log p}{n}} + c_n + K_2 \sqrt{s_B \log p} + K_1 L_B \sqrt{\frac{s \log p}{n}}.
\]

As a result,
\[
\| \hat{\Gamma}_\psi - \Gamma_\psi \|_{\text{max}} \lesssim K_1^3 \sqrt{\frac{s \log p}{n}} + \frac{NK_1^2}{n + N} \text{Rem}.
\]
One can easily show that \( \|\Gamma_\psi\|_{\text{max}} \lesssim K_1^2 + \frac{N}{n+N} LB K_1^2 \), which implies

\[
\|\hat{\Gamma}_\psi\|_{\text{max}} \leq \|\Gamma_\psi\|_{\text{max}} + \|\hat{\Gamma}_\psi - \Gamma_\psi\|_{\text{max}} \lesssim K_1^2 + \frac{N}{n+N} LB K_1^2
\]

under the assumption that \( \text{Rem} = o(1) \) and \( K_1 \sqrt{\frac{\log p}{n}} = o(1) \). Similarly, \( \|\hat{\Omega}\|_{\infty} \lesssim L_\Omega \) since \( \|\hat{\Omega} - \Omega\|_{\infty} = o(1) \). Finally, we can establish the rate of convergence of the estimated variance

\[
|v^T \hat{\Omega}_\psi \hat{\Omega} v - v^T \Omega \Gamma_\psi v|
\leq |v^T (\hat{\Omega} - \Omega) \hat{\Omega} v| + |v^T \Omega (\hat{\Omega} - \Omega) v| + |v^T (\hat{\Gamma}_\psi - \Gamma_\psi) \Omega v|
\lesssim \|v\|_2^2 (L_\Omega \|\hat{\Omega} - \Omega\|_{\text{max}} + L_\Omega^2 \|\hat{\Gamma}_\psi - \Gamma_\psi\|_{\text{max}})
\lesssim \|v\|_2^2 \left[ K_1^3 L_\Omega^2 \sqrt{\frac{\log p}{n+N}} \|\Gamma_\psi\|_{\text{max}} + K_1^3 L_\Omega^2 \sqrt{\frac{\log p}{n+N}} + \frac{N K_1^2 L_\Omega^2}{n+N} \text{Rem} \right],
\]

which proves (3.23). The proof of (3.24) is immediate by the Slutsky Theorem.

\[ \Box \]

### A.8 Proof of Proposition 12

**Proof.** To show Proposition 12, it suffices to show that the same rate of convergence holds for \( \hat{B}_j \).

For simplicity of presentation, we use the notation \( \hat{\theta}_L = \hat{\theta} \), \( \hat{B}_k = \hat{\beta} \), \( B_k = \beta \), \( \Delta = \beta - \hat{\beta} \) and \( \lambda = \hat{\lambda}, \hat{Z}_i = X_i \hat{m}^{-j}(X_i) - \hat{\mu}^j \) and \( Z_i = X_i m(X_i) - \mu \). We start from the inequality

\[
\frac{1}{n_j} \sum_{i \in D_j^*} \{X_{ik}(Y_i - X_i^T \hat{\theta}) - \hat{\beta}^T(X_i \hat{m}^{-j}(X_i) - \hat{\mu}^j)\}^2 + \lambda \|\hat{\beta}\|_1
\leq \frac{1}{n_j} \sum_{i \in D_j^*} \{X_{ik}(Y_i - X_i^T \hat{\theta}) - \beta^T(X_i \hat{m}^{-j}(X_i) - \mu^j)\}^2 + \lambda \|\beta\|_1.
\]

Following the standard argument in the analysis of Lasso (e.g., the proof of Theorem 7.1 in Bickel et al. (2009)), the above inequality reduces to

\[
\hat{\Delta}^T \hat{F} \hat{\Delta} \leq \lambda \|\beta\|_1 - \lambda \|\hat{\beta}\|_1 + \frac{2}{n_j} \sum_{i \in D_j^*} \{X_{ik}(Y_i - X_i^T \hat{\theta}) - \beta^T \hat{Z}_i\} \hat{Z}_i^T \hat{\Delta}
= \lambda \|\beta\|_1 - \lambda \|\hat{\beta}\|_1 + I_1 + I_2 + I_3 + I_4,
\]

where

\[
I_1 = \frac{2}{n_j} \sum_{i \in D_j^*} \{X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i\} Z_i^T \hat{\Delta},
\]

\[
I_2 = \frac{2}{n_j} \sum_{i \in D_j^*} \{X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i\} (\hat{Z}_i - Z_i)^T \hat{\Delta},
\]

\[
I_3 = -\frac{2}{n_j} \sum_{i \in D_j^*} X_{ik} X_i^T (\hat{\theta} - \theta^*) \hat{Z}_i^T \hat{\Delta}, \text{ and } I_4 = -\frac{2}{n_j} \sum_{i \in D_j^*} \beta^T (\hat{Z}_i - Z_i) \hat{Z}_i^T \hat{\Delta}.
\]
To bound $I_1$, we note that $\mathbb{E}\{X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i\} Z_i = 0$ by the definition of $\beta$. To invoke Lemma 8, we control the second moment as

$$\mathbb{E}\left[ \max_{1 \leq j \leq p} \{X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i\}^2 \right] \lesssim K_1^2 \mathbb{E}\left[ \{X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i\}^2 \right] \lesssim K_1^2,$$

where first step $|Z_{ij}| = |X_{ij} m(X_i) - \mu_j| \lesssim K_1$ holds as $|X_{ij}| \leq K_1$ and $|m(X_i)| \leq C$ and second step relies on the assumption that the second moment of $X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i$ is bounded. Therefore, applying Holder inequality and Lemma 8 with $m = 2$, we have

$$|I_1| \lesssim \left\| \frac{1}{n_j} \sum_{i \in D_j^*} \{X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i\} Z_i \right\|_\infty \|\hat{\Delta}\|_1 \lesssim K_1 \sqrt{\frac{\log p}{n}} \|\hat{\Delta}\|_1. \quad (A.33)$$

Similarly, we have $|I_2| \lesssim \left\| \frac{1}{n_j} \sum_{i \in D_j} E_{ik}(\hat{Z}_i - Z_i) \right\|_\infty \|\hat{\Delta}\|_1$, where $E_{ik} = X_{ik}(Y_i - X_i^T \theta^*) - \beta^T Z_i$. Furthermore, we notice that

$$\frac{1}{n_j} \sum_{i \in D_j^*} E_{ik}(\hat{Z}_i - Z_i) = \frac{1}{n_j} \sum_{i \in D_j^*} E_{ik} X_i(\hat{m}^{-j}(X_i) - m(X_i))$$

$$- \left( \frac{1}{n_j} \sum_{i \in D_j^*} E_{ik} \right) \frac{1}{n_j} \sum_{i \in D_j^*} [X_i \hat{m}^{-j}(X_i) - \mathbb{E}(X_i m(X_i))].$$

For the first term, we can apply Cauchy–Schwarz inequality to show that

$$\max_{1 \leq l \leq p} \left\| \frac{1}{n_j} \sum_{i \in D_j^*} E_{ik} X_{il}(\hat{m}^{-j}(X_i) - m(X_i)) \right\|$$

$$\leq \max_{1 \leq l \leq p} \left\| \frac{1}{n_j} \sum_{i \in D_j^*} E_{ik}^2 X_{il}^2 \right\|^{1/2} \left\| \frac{1}{n_j} \sum_{i \in D_j^*} (\hat{m}^{-j}(X_i) - m(X_i))^2 \right\|^{1/2} \lesssim K_1 c_n, \quad (A.34)$$

where in the last step we invoke Lemma 8 again to show $\max_{1 \leq l \leq p} \left\| \frac{1}{n_j} \sum_{i \in D_j^*} E_{ik}^2 X_{il}^2 - \mathbb{E}(E_{ik}^2 X_{il}^2) \right\| \lesssim K_1^2 \sqrt{\frac{\log p}{n}}$ and $\mathbb{E}(E_{ik}^2 X_{il}^2) \lesssim K_1^2$ together with triangle inequality imply the desired bound. For the second term, we first notice that $\frac{1}{n_j} \sum_{i \in D_j} E_{ik} = O_p(1)$, and then a similar argument leads to

$$\max_{1 \leq l \leq p} \left\| \frac{1}{n_j} \sum_{i \in D_j^*} [X_{il}\hat{m}^{-j}(X_i) - \mathbb{E}(X_{il} m(X_i))] \right\|$$

$$\leq \max_{1 \leq l \leq p} \left\| \frac{1}{n_j} \sum_{i \in D_j^*} X_{il}(\hat{m}^{-j}(X_i) - m(X_i)) \right\| + \max_{1 \leq l \leq p} \left\| \frac{1}{n_j} \sum_{i \in D_j^*} (X_{il} m(X_i) - \mathbb{E}(X_{il} m(X_i))) \right\|$$

$$\lesssim K_1 c_n + K_1 \sqrt{\frac{\log p}{n}}, \quad (A.35)$$

where we apply the Hoeffding inequality as $|X_{il} m(X_i)| \leq CK_1$. Combining (A.34) and (A.35), we have

$$|I_2| \lesssim \left\| \frac{1}{n_j} \sum_{i \in D_j^*} E_{ik}(\hat{Z}_i - Z_i) \right\|_\infty \|\hat{\Delta}\|_1 \lesssim (K_1 c_n + K_1 \sqrt{\frac{\log p}{n}}) \|\hat{\Delta}\|_1. \quad (A.36)$$
We now consider $I_3$. Recall that Lemma 11 implies $\frac{1}{n}\sum_{i=1}^{n}[X_i^T(\hat{\theta} - \theta^*)]^2 = O_p(K_1^2s(\sigma^2 + \phi^2)\log p).$ Thus,

$$|I_3| \lesssim \frac{1}{n_j} \sum_{i \in D_j^*} [X_i^T(\hat{\theta} - \theta^*)]^2 X_{ik}^2 1/2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2} \lesssim K_1^2 \sqrt{\frac{s(\sigma^2 + \phi^2)\log p}{n}} (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2}. \quad (A.37)$$

Similarly, the Cauchy–Schwarz inequality yields $|I_4| \lesssim \frac{1}{n_j} \sum_{i \in D_j^*} [\beta^T(\hat{Z}_i - Z_i)]^2 1/2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2}$. Moreover,

$$\frac{1}{n_j} \sum_{i \in D_j^*} [\beta^T(\hat{Z}_i - Z_i)]^2 \lesssim \frac{2}{n_j} \sum_{i \in D_j^*} (\beta^T X_i)^2 (\tilde{m}^{-j}(X_i) - m(X_i))^2 + 2 \left( \frac{1}{n_j} \sum_{i \in D_j^*} [\beta^T X_i m(X_i) - \mathbb{E}(\beta^T X_i m(X_i))] \right)^2 \lesssim K_1^2 L_B c_n^2 + (K_1 L_B c_n + K_1 L_B) \sqrt{\frac{\log p}{n}}^2$$

where the last step holds by using a similar argument as in (A.34) and (A.35) together with the fact that $|\beta^T X_i| \leq \|\beta\|_1 \|X_i\|_\infty \leq K_1 L_B$. As a result, we have

$$|I_4| \lesssim (K_1 L_B c_n + K_1 L_B) \sqrt{\frac{\log p}{n}} (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2}.$$  

Collecting the bounds in (A.33), (A.36) and (A.37), we obtain from (A.32) that

$$\hat{\Delta}^T \hat{F} \hat{\Delta} \leq \lambda \|\beta\|_1 - \lambda \|\hat{\beta}\|_1 + t_1 \|\hat{\Delta}\|_1 + t_2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2} \leq \lambda \|\hat{\Delta}_S\|_1 - \lambda \|\hat{\Delta}_{S^C}\|_1 + t_1 \|\hat{\Delta}\|_1 + t_2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2},$$

where $t_1 = C(K_1 c_n + K_1 \sqrt{\frac{\log p}{n}})$ and $t_2 = C[K_1 L_B (c_n + \sqrt{\frac{\log p}{n}}) + K_1^2 \sqrt{\frac{s(\sigma^2 + \phi^2)\log p}{n}}]$ for some sufficiently large constant $C$. By taking $\lambda \geq 2t_1$, we have

$$\hat{\Delta}^T \hat{F} \hat{\Delta} \leq \frac{3}{2} \lambda \|\hat{\Delta}_S\|_1 - \frac{1}{2} \lambda \|\hat{\Delta}_{S^C}\|_1 + t_2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2}. \quad (A.38)$$

In the following, we consider two cases. In case (1): $t_2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2} \leq \lambda \|\hat{\Delta}_S\|_1$, (A.38) further implies

$$\hat{\Delta}^T \hat{F} \hat{\Delta} \leq \frac{5}{2} \lambda \|\hat{\Delta}_S\|_1 - \frac{1}{2} \lambda \|\hat{\Delta}_{S^C}\|_1,$$

which leads to the standard cone condition $\|\hat{\Delta}_{S^C}\|_1 \leq 5 \|\hat{\Delta}_S\|_1$. With lemma 13, we can show that $\|\hat{e}\|_2 \leq \lambda \|\hat{\Delta}_S\|_1 \leq \lambda s_B^{1/2} \|\hat{\Delta}_S\|_2$ and therefore $\|\hat{\Delta}\|_2 \leq \lambda s_B^{1/2}$. Similarly, we can derive $\|\hat{\Delta}\|_1 \leq \lambda s_B$. In case (2): $t_2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2} > \lambda \|\hat{\Delta}_S\|_1$, (A.38) implies

$$\hat{\Delta}^T \hat{F} \hat{\Delta} \leq \frac{3}{2} \lambda \|\hat{\Delta}_S\|_1 + t_2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2} \leq \frac{5}{2} t_2 (\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2},$$

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and therefore $\hat{\Delta}^T \hat{F} \hat{\Delta} \preceq \frac{25}{t_2^2}$. Since $t_2(\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2} \geq \lambda \hat{\Delta}_S^\|1$ holds in case (2), we immediately obtain $\|\hat{\Delta}_S\|_1 \leq \frac{5\lambda}{2X}$. To control $\|\hat{\Delta}_S^\sigma\|_1$, we rely on (A.38) again, which is

$$\frac{1}{2} \lambda \|\hat{\Delta}_S^\sigma\|_1 \leq \frac{3}{2} \lambda \|\hat{\Delta}_S\|_1 + t_2(\hat{\Delta}^T \hat{F} \hat{\Delta})^{1/2}.$$

This leads to $\|\hat{\Delta}_S^\sigma\|_1 \leq 3\|\hat{\Delta}_S\|_1 + \frac{5\lambda}{X} \leq \frac{25\lambda}{2X}$, such that $\|\hat{\Delta}\|_1 \leq t_2^2 / \lambda$. Combining the bounds in these two cases, we derive

$$\|\hat{\Delta}\|_1 \lesssim \lambda s_B + t_2^2 / \lambda,$$

where $\lambda$ is subject to the constraint that $\lambda \geq 2t_1$. To establish a sharp rate of $\|\hat{\Delta}\|_1$, we can further minimize $f(\lambda) = \lambda s_B + \lambda t_2^2 / \lambda$ subject to the constraint $\lambda \geq 2t_1$. Define $\lambda_{\text{opt}} = t_2 / s_B^{1/2}$. When $\lambda_{\text{opt}} \geq 2t_1$, the minimizer of $f(\lambda)$ is $\lambda_{\text{opt}}$ and the resulting minimal value is $f(\lambda_{\text{opt}}) = s_B^{-1/2} t_2$. However, when $\lambda_{\text{opt}} < 2t_1$, by the monotonicity of $f(\lambda)$ the minimal is given by $f(2t_1) \approx t_1 s_B$. Combining these two cases, finally, we obtain the desired rate

$$\|\hat{\Delta}\|_1 \lesssim t_1 s_B + s_B^{1/2} t_2.$$

With a slight modification of the proof (e.g., $\|I_1\| \lesssim K_1 \sqrt{\frac{\log p}{n}} \|\hat{\Delta}\|_1$ still holds uniformly over $1 \leq k \leq p$), we obtain the same rate for $\|\hat{B}_k - B_k\|_1$ uniformly over $1 \leq k \leq p$. This concludes the proof.

Recall that $\hat{Z}_i = X_i \hat{m}^{-j}(X_i) - \hat{\mu}^j$, $Z_i = X_i m(X_i) - \mu$ and $\hat{F} = \frac{1}{n_j} \sum_{i \in D_j} \hat{Z}_i^{\otimes 2}$.

**Lemma 13** (RE condition for $\hat{B}_k$). Assume that the same conditions in Theorem 5 hold. Then with probability tending to 1,

$$\inf_{v \in \mathcal{C}, v \neq 0} \frac{v^T \hat{F} v}{\|v\|_2^2} \geq C,$$

where $\mathcal{C} = \{v \in \mathbb{R}^p : \exists S \subseteq \{1, \ldots, p\}, |S| = s_B, \|v_S^\sigma\|_1 \leq \xi \|v_S\|_1\}$ for some constants $C, \xi > 0$.

**Proof.** We define $F = \frac{1}{n_j} \sum_{i \in D_j} Z_i^{\otimes 2}$. It holds that

$$v^T \hat{F} v = v^T (\hat{F} - F) v + v^T (F - \mathbb{E}(F)) v + v^T \mathbb{E}(F) v$$

$$\geq v^T \mathbb{E}(F) v - \|v^T (\hat{F} - F) v\| - \|v^T (F - \mathbb{E}(F)) v\|.$$

In what follows, we will bound the three terms in the last line one by one. Clearly,

$$v^T \mathbb{E}(F) v \geq C \|v\|_2^2$$

(A.39)

uniformly over $v$, as $\mathbb{E}(F)$ has bounded smallest eigenvalues. For the last term,

$$\|v^T (F - \mathbb{E}(F)) v\| \leq \|v\|_1^2 \|F - \mathbb{E}(F)\|_{\text{max}} \leq s_B (\xi + 1)^2 \|v\|_2^2 \|F - \mathbb{E}(F)\|_{\text{max}} \approx s_B \|v\|_2^2 K_1^2 \sqrt{\frac{\log p}{n}}.$$

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where the second step holds as \( \|v\|_1 \leq (\xi + 1)\|v_S\|_1 \leq (\xi + 1)s_B^{1/2}\|v_S\|_2 \leq (\xi + 1)s_B^{1/2}\|v\|_2 \) and the last step is obtained by the Hoeffding inequality together with the bound \( \|X_i m(X_i)\|_\infty \leq CK_1 \). Under the condition \( s_B K_1^2 \sqrt{\frac{\log p}{n}} = o(1) \), we have

\[
\sup_{v \in C, v \neq 0} \frac{|v^T (F - \mathbb{E}(F))v|}{\|v\|_2^2} = o(1). \tag{A.40}
\]

Now, we focus on the second term \( |v^T (\tilde{F} - F)v| \). To this end, we first note that

\[
|v^T (\tilde{\mu}^j - \mu)| \leq \left| \frac{1}{n_j} \sum_{i \in D_j^*} v^T X_i (\tilde{m}^{-j}(X_i) - m(X_i)) \right| + \left| \frac{1}{n_j} \sum_{i \in D_j^*} v^T (X_i m(X_i) - \mathbb{E}(X_i m(X_i))) \right|
\]

\[
\leq \left| \frac{1}{n_j} \sum_{i \in D_j^*} (v^T X_i)^2 \right|^{1/2} \left| \frac{1}{n_j} \sum_{i \in D_j^*} (\tilde{m}^{-j}(X_i) - m(X_i))^2 \right|^{1/2}
\]

\[
+ \|v\|_1 \left| \frac{1}{n_j} \sum_{i \in D_j^*} (X_i m(X_i) - \mathbb{E}(X_i m(X_i))) \right|_\infty
\]

\[
\lesssim \|v\|_1 K_1 (c_n + \sqrt{\frac{\log p}{n}}), \tag{A.41}
\]

which is implied by the Hoeffding inequality in the last step and \( \|\tilde{m}^{-j} - m\|_2 \lesssim c_n \). In addition,

\[
\frac{1}{n_j} \sum_{i \in D_j^*} (v^T X_i)^2 (\tilde{m}^{-j}(X_i) - m(X_i))^2 \lesssim \|v\|_1^2 K_1^2 c_n^2.
\]

Combined with (A.41), we have

\[
\frac{1}{n_j} \sum_{i \in D_j^*} [v^T X_i (\tilde{m}^{-j}(X_i) - m(X_i)) - v^T (\tilde{\mu}^j - \mu)]^2
\]

\[
\leq \frac{2}{n_j} \sum_{i \in D_j^*} [v^T X_i (\tilde{m}^{-j}(X_i) - m(X_i))]^2 + \frac{2}{n_j} \sum_{i \in D_j^*} [v^T (\tilde{\mu}^j - \mu)]^2
\]

\[
\lesssim \|v\|_1^2 K_1^2 (c_n + \sqrt{\frac{\log p}{n}})^2. \tag{A.42}
\]

An implication of (A.42) is the following inequality

\[
\frac{1}{n_j} \sum_{i \in D_j^*} [v^T X_i (\tilde{m}^{-j}(X_i) + m(X_i)) - v^T (\tilde{\mu}^j + \mu)]^2
\]

\[
\leq \frac{2}{n_j} \sum_{i \in D_j^*} [v^T X_i (\tilde{m}^{-j}(X_i) - m(X_i)) - v^T (\tilde{\mu}^j - \mu)]^2 + \frac{2}{n_j} \sum_{i \in D_j^*} [2v^T X_i m(X_i) - 2v^T \mu]^2
\]

\[
\lesssim \|v\|_1 K_1^2 (c_n + \sqrt{\frac{\log p}{n}})^2 + \|v\|_1^2 K_1^2 \lesssim \|v\|_1^2 K_1^2. \tag{A.43}
\]
Finally, applying Cauchy–Schwarz inequality we can show that

\[
\begin{align*}
|v^T(\hat{F} - F)v| &= \left| \frac{1}{n_j} \sum_{i \in D_j^*} \left[ (v^TX_i\hat{m}^{-j}(X_i) - v^T\tilde{\mu})^2 - (v^TX_im(X_i) - v^T\mu)^2 \right] \right| \\
&= \left| \frac{1}{n_j} \sum_{i \in D_j^*} [v^TX_i(\hat{m}^{-j}(X_i) - m(X_i)) - v^T(\tilde{\mu} - \mu)] [v^TX_i(\hat{m}^{-j}(X_i) + m(X_i)) - v^T(\tilde{\mu} + \mu)] \right| \\
&\leq \left| \frac{1}{n_j} \sum_{i \in D_j^*} [v^TX_i(\hat{m}^{-j}(X_i) - m(X_i)) - v^T(\tilde{\mu}^j - \mu)]^2 \right|^{1/2} \\
&\quad \times \left| \frac{1}{n_j} \sum_{i \in D_j^*} [v^TX_i(\hat{m}^{-j}(X_i) + m(X_i)) - v^T(\tilde{\mu}^j + \mu)]^2 \right|^{1/2} \\
&\lesssim \|v\|^2 K_1^2(c_n + \sqrt{\frac{\log p}{n}}) \lesssim \|v\|^2_2 s_B K_1^2(c_n + \sqrt{\frac{\log p}{n}}),
\end{align*}
\]

where we use (A.42) and (A.43). Therefore, from (A.39), (A.40) and (A.44), we obtain

\[
\inf_{v \in \mathbb{C}, v \neq 0} \frac{v^T\hat{F}v}{\|v\|^2_2} \geq C - o(1).
\]

\[
\square
\]

**B Supplementary Technical Results**

**B.1 Examples of** $\mathbb{E}(f(X) - X^T\theta^\ast)^2 \preceq s$

Assume that the true conditional mean function $f(X)$ has an additive form $f(X) = \sum_{k \in S} f_k(X_k)$ with $\mathbb{E}(f_k(X_k)) = 0$, where $X_k$ is the $k$th component of $X$ and $S$ is a subset of $\{1, ..., p\}$ with $|S| = s$. We further assume that all the covariates $X_1, ..., X_p$ are mutually independent. We have

\[
\mathbb{E}(f(X) - X^T\theta^\ast)^2 = \mathbb{E}\left\{ \sum_{k \in S} (f_k(X_k) - X_k\theta_k^\ast) \right\}^2 \leq \sum_{k \in S} \mathbb{E}(f_k(X_k) - X_k\theta_k^\ast)^2 + \sum_{k \notin S} \mathbb{E}(f_k(X_k) - X_k\theta_k^\ast)^2,
\]

where we use the fact that $\mathbb{E}(f_k(X_k)) = 0$ and $\mathbb{E}(X_k) = 0$. By the definition of $\theta^\ast$, we know that for $k \notin S$, $\theta_k^\ast = 0$. For $k \in S$, $\theta_k^\ast = \text{argmin}_\theta \mathbb{E}(f_k(X_k) - X_k\theta)^2 = \mathbb{E}(f_k(X_k)X_k)/\Sigma_{kk}$ and $\mathbb{E}(f_k(X_k) - X_k\theta_k^\ast)^2 = \mathbb{E}(f_k^2(X_k)) - [\mathbb{E}(f_k(X_k)X_k)]^2/\Sigma_{kk}$ which is typically a constant. For example, if $X_k \sim N(0, 1)$ and $f_k(X_k) = X_k^3$, then $\mathbb{E}(f_k(X_k) - X_k\theta_k^\ast)^2 = 6$. Thus, we have $\mathbb{E}(f(X) - X^T\theta^\ast)^2 = 6s.$

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B.2 Rate of $\hat{\theta}_U$

Recall that the modified Dantzig selector $\hat{\theta}_U$ is defined as

$$\hat{\theta}_U = \arg \min \| \theta \|_1, \quad \text{s.t.} \quad \| \hat{\Sigma}_{n+N} \theta - \frac{1}{n} \sum_{i=1}^n X_i Y_i \|_\infty \leq \lambda_U.$$ 

Assume that Assumption 1 holds. By choosing $\lambda_U \asymp K_1 \sqrt{\frac{(\sigma^2 + \theta^T \Sigma \theta^*) \log p}{n}}$, we obtain that

$$\| \hat{\theta}_U - \theta^* \|_1 \leq O_p \left( s K_1 (\Phi + (\theta^T \Sigma \theta^*)^{1/2}) \sqrt{\frac{\log p}{n}} \right).$$

Under the conditions in our Theorem 2, we have $K_1 = O(1)$. This implies the bound (2.10).

The proof follows from the same argument as in Lemma 11. The only nontrivial step is to bound $\| \hat{\Sigma}_{n+N} \theta - \frac{1}{n} \sum_{i=1}^n X_i Y_i \|_\infty$. Using the triangle inequality, we have

$$\| \hat{\Sigma}_{n+N} \theta - \frac{1}{n} \sum_{i=1}^n X_i Y_i \|_\infty \leq \| \frac{1}{n} \sum_{i=1}^n X_i (Y_i - f(X_i)) \|_\infty + \| \frac{1}{n} \sum_{i=1}^n X_i (f(X_i) - X_i^T \theta^*) \|_\infty + \| (\hat{\Sigma}_n - \Sigma) \theta^* \|_\infty + \| (\hat{\Sigma}_{n+N} - \Sigma) \theta^* \|_\infty.$$ 

We have already derived in (A.15) that,

$$\| \frac{1}{n} \sum_{i=1}^n X_i (Y_i - f(X_i)) \|_\infty \lesssim K_1 \sigma \sqrt{\frac{\log p}{n}}, \quad \| \frac{1}{n} \sum_{i=1}^n X_i (f(X_i) - X_i^T \theta^*) \|_\infty \lesssim K_1 \Phi \sqrt{\frac{\log p}{n}}.$$ 

To control $\| (\hat{\Sigma}_n - \Sigma) \theta^* \|_\infty$, we note that $\| X_i \|_\infty \leq K_1$ and $\mathbb{E}(X_i^T \theta^*)^2 = \theta^T \Sigma \theta^*$. We obtain

$$\| (\hat{\Sigma}_n - \Sigma) \theta^* \|_\infty \lesssim K_1 (\theta^T \Sigma \theta^*)^{1/2} \sqrt{\frac{\log p}{n}},$$

by the Nemirovski moment inequality in Lemma 8 and Markov inequality. The last term $\| (\hat{\Sigma}_{n+N} - \Sigma) \theta^* \|_\infty$ is dominated by $\| (\hat{\Sigma}_n - \Sigma) \theta^* \|_\infty$ and can be ignored. Thus, we obtain

$$\| \hat{\Sigma}_{n+N} \theta - \frac{1}{n} \sum_{i=1}^n X_i Y_i \|_\infty \lesssim K_1 (\Phi + (\theta^T \Sigma \theta^*)^{1/2}) \sqrt{\frac{\log p}{n}}.$$ 

B.3 Sparsity assumption on $B$

We show here the blockwise independence structure in $X$ ensures the sparsity of $B$. We denote the support of function $m$ by $S_m \subseteq \{1, ..., p\}$ which is the index set of all the variables present in $m(\cdot)$. Assume that the predictor variables exhibit block independence with blocks corresponding to the block-diagonal covariance matrix $\Sigma$, and the maximal block-size is equal to $b_{\text{max}}$. Under this assumption, we firstly know that for $1 \leq k \leq p$, if $k \notin S_m$

$$\| \mathbb{E}[(X_m(X) - \mu) X^k m(X)] \|_0 \leq b_{\text{max}}, \quad \text{(B.1)}$$

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where we use $X^k$ to denote the $k$th component of $X$. Otherwise,

$$||E[(Xm(X) - \mu)X^km(X)]||_0 \leq b_{max}|S_m|.$$  \hspace{1cm} (B.2)

Therefore, we can view the covariance matrix of $Xm(X)$ as a different block-diagonal matrix with the same blocks as in $\Sigma$ for those variables not in working model $m$. Moreover, we can claim that $\{E[(Xm(X) - \mu)\otimes^2]\}^{-1}$ presents the same block structure as in covariance matrix of $Xm(X)$.

On the other hand, for $k \notin S_m \cup S_\eta$, where $\eta(X) = f(X) - X^T\theta^*$,

$$||E[(XX^km(X)\eta(X))]||_0 \leq b_{max},$$

and the non-zero elements are within the dependence block of $X^k$. Therefore, given that

$$B_k = \{E[(Xm(X) - \mu)\otimes^2]\}^{-1}E[(XX^km(X)\eta(X))],$$  \hspace{1cm} (B.3)

we know $||B_k||_0 \leq b_{max}$ since $B_{jk}$ is nonzero only when $j$ is in the corresponding dependence block of $X^k$.

For $k \in S_m \cup S_\eta$,

$$||E[(XX^km(X)\eta(X))]||_0 \leq b_{max}|S_m \cup S_\eta|,$$

and by equation B.3 and the block structure of $\{E[(Xm(X) - \mu)\otimes^2]\}^{-1}$, we know

$$||B_k||_0 \leq b_{max}|S_m \cup S_\eta|.$$  \hspace{1cm} (B.4)

Above all, if the supports of working model $m(\cdot)$ and $\eta(\cdot)$, the nonlinear part in $f$ are sparse, the blockwise independence structure of $X$ assumption is sufficient to guarantee the sparsity of $B$.

### B.4 Comparison with related work in Section 3

When the dimension $p$ is fixed and small, Azriel et al. (2016) and Chakrabortty and Cai (2018) investigated how to incorporate the unlabeled data to improve the estimation efficiency for regression coefficients in a working linear regression. In addition to the technical challenges arise from the high dimensionality (e.g., regularization and one-step update), a key difference from the previous works is that our safe semi-supervised approach leads to a more efficient estimator for any linear combination of $\theta^*$. In the following, we briefly summarize their methodologies and explain the differences.

To improve the estimation efficiency for $\theta_j^*$, Azriel et al. (2016) considered the following adjusted linear regression, for any $j \in [p]$

$$\widetilde{Y}_{ij} = \theta_j^* + \phi_j^T U_{ij} + \tilde{\delta}_{ij},$$

where $\widetilde{Y}_{ij} = Y_i \tilde{X}_{ij}$, $U_{ij} = (U_{ij1}, ..., U_{ijp})^T$ with $U_{ijk} = X_{ik} \tilde{X}_{ij}$ for $k \neq j$ and $U_{ijj} = X_{ij} \tilde{X}_{ij} - 1$ and $\tilde{\delta}_{ij}$ is a mean 0 random variable. We use the notation $\tilde{X}_{ij} = (X_{ij} - \gamma_j^T X_{i,-j})/E[(X_{ij} - \gamma_j^T X_{i,-j})^2]$ where $\gamma_j$ is the estimand for the nodewise lasso (3.2). One interesting property of the adjusted linear regression is that the parameter of interest $\theta_j^*$ becomes the intercept parameter, because $E(U_{ij}) = 0$ and $\theta_j^* = E(Y_i \tilde{X}_{ij}) = E(\widetilde{Y}_{ij})$ by the definition of $\widetilde{Y}_{ij}$. Thus, when $p$ is fixed and small, $\theta_j^*$
can be estimated by \( \hat{\theta}_A^j \) the LSE from the adjusted linear regression, where the unlabeled data can help the estimation of \( \gamma_j \) and \( \mathbb{E}[(X_{ij} - \gamma_j^T X_{i,-j})^2] \). Thanks to the orthogonality of \( \tilde{\delta}_{ij} \) and \( U_{ij} \), the asymptotic variance of \( \hat{\theta}_A^j \) is shown to be no greater than \( \hat{\theta}_{LSE}^j \), the \( j \)th component of the standard LSE \( \hat{\theta}_{LSE} = (X^T X)^{-1} X^T Y \); see their Theorem 2. As a result, if the parameter of interest is any component of \( \theta^* \), their estimator provides the safe semi-supervised inference.

However, since the adjusted linear regression is estimated for each \( j \in [p] \) separately, their procedure does not guarantee the orthogonality of \( \tilde{\delta}_{ij} \) and \( U_{ij} \) for any \( j' \neq j \) when the true regression function \( f(X) \) is nonlinear. Therefore, the linear combination of their estimators such as \( \hat{\theta}_A^j + \hat{\theta}_A^{j'} \) may not be more efficient than the standard LSE \( \hat{\theta}_{LSE}^j + \hat{\theta}_{LSE}^{j'} \). Unlike their approach, our estimator is constructed based on the geometric interpretation of estimating functions. The projection theory from estimating functions motivates us to consider the working regression model (3.13), which is different from the adjusted linear regression in Azriel et al. (2016).

Chakrabortty and Cai (2018) proposed a class of Efficient and Adaptive Semi-Supervised Estimators (EASE) which exploit the unlabeled data based on a semi-non-parametric smoothing and refitting estimate of a target imputation function \( \mu(X) \). They mainly focused on the context that \( N \) is much larger than \( n \) and \( p \) is fixed. With an estimated imputation function \( \hat{\mu}(X) \), they derived an initial semi-supervised estimator \( \hat{\theta}_r \) through the estimating equation

\[
\frac{1}{N} \sum_{i=n+1}^{n+N} X_i(\hat{\mu}(X_i) - X_i^T \theta) = 0. \tag{B.4}
\]

The estimator \( \hat{\theta}_r \) attains the semi-parametric efficiency bound when the imputation is sufficient (i.e., the imputation function equals the conditional mean function \( \mu(X) = f(X) \)) or the conditional mean function \( f(X) \) is linear \( f(X) = X^T \theta^* \). As seen in Remark 5, these properties also hold for our efficient semi-supervised estimator \( \hat{\theta}^d \) in (3.1). To ensure the improved efficiency of EASE, they considered a further step of calibration which searched an optimal linear combination of \( \hat{\theta}_r \) and the LSE \( \hat{\theta}_{LSE} \). Their adaptive estimator is defined as \( \hat{\theta}^E = \hat{\theta}_{LSE} + \Delta(\hat{\theta}_r - \hat{\theta}_{LSE}) \), where \( \Delta \) is a diagonal matrix that minimizes the asymptotic variance of \( \hat{\theta}_j^E \) for each \( j \in [p] \). When \( \Delta \) is consistently estimated, \( \hat{\theta}_j^E \) is always no less efficient than the LSE no matter whether the imputation is sufficient or \( f(X) \) is linear. However, by the construction of \( \hat{\theta}^E \), the efficiency improvement is not guaranteed if a linear combination of \( \theta^* \) is considered.

\section{C Supplementary Plots}

This appendix collects additional simulation results. The \( L_2 \) and \( L_1 \) estimation error under Model 1 with \( p = 500 \) and \( n = 200 \) is shown in Figure 6. The length and empirical coverage rate (shown in the number) of 95\% CIs under Model 1 with \( p = 500 \) and \( n = 200 \) is shown in Figure 7. The length and empirical coverage rate (shown in the number) of 95\% CIs under Model 2 with \( p = 200 \) and \( n = 200 \) is shown in Figure 8.

The length and empirical coverage rate (shown in the number) of 95\% CIs under Model 2 with \( p = 200 \) and \( n = 100 \) is shown in Figure 9. As Figure 9 shows, O-SSL does not outperform Dantzig
Figure 6: The $L_2$ and $L_1$ estimation error under Model 1 with $p = 500$ and $n = 200$

Figure 7: The length and empirical coverage rate (shown in the number) of 95% CIs under Model 1 with $p = 500$ and $n = 200$. The top left panel is drawn by averaging over all the covariates not in the support set. The rest are for the coefficients of $X_1$, $X_5$ and $X_6$ in the support set.
Figure 8: The length and empirical coverage rate (shown in the number) of 95% CIs under Model 2 with $p = 200$ and $n = 200$. The top left panel is drawn by averaging over all the covariates not in the support set. The rest are for the coefficients of $X_1$, $X_2$ and $X_6$ in the support set.
Figure 9: The length and empirical coverage rate (shown in the number) of 95% CIs under Model 2 with \( p = 200 \) and \( n = 100 \). The top left panel is drawn by averaging over all the covariates not in the support set. The rest are for the coefficients of \( X_2, X_5 \) and \( X_6 \) in the support set.

any more, but S-SSL still performs better. This agrees with what we expect since the wrong additive model does not fit the conditional mean better than the original linear model. On the other hand, the size of labeled data affects the coverage rate greatly. As we can see with Dantzig, the inference result for \( X_5 \) is unreliable because of a low coverage rate. Although the leverage of unlabeled data helps to alleviate the problem, U-Dantzig results in slightly larger CIs as well. With S-SSL, we can incorporate the unlabeled data without losing efficiency.

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