A zero-estimator approach for estimating the signal level in a high-dimensional model-free setting

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Abstract

We study a high-dimensional regression setting under the assumption of known covariate distribution. We aim at estimating the amount of explained variation in the response by the best linear function of the covariates (the signal level). In our setting, neither sparsity of the coefficient vector, nor normality of the covariates or linearity of the conditional expectation are assumed. We present an unbiased and consistent estimator and then improve it by using a zero-estimator approach, where a zero-estimator is a statistic whose expected value is zero. More generally, we present an algorithm based on the zero estimator approach that in principle can improve any given estimator. We study some asymptotic properties of the proposed estimators and demonstrate their finite sample performance in a simulation study.

Key words and phrases: Linear Projection, Semi-supervised setting, U-statistics, Variance estimation, Zero-estimators.

1 Introduction

In many regression settings, an important goal is to estimate the signal and noise levels, i.e., to quantify the amount of variance in the response variable that can be explained by a set of covariates, versus how much of the variation is left unexplained. When the covariates’ dimension is low and a linear regression model is assumed, the ordinary least squares method can be used to find a consistent estimator for the signal level. However, in a high-dimensional setting, the least squares method breaks down and it becomes more challenging to develop
good estimators without further assumptions. In recent years, several methods have been proposed for estimating the signal level under the assumption that the regression coefficient vector $\beta$ is sparse (Fan et al. (2012); Sun and Zhang (2012); Chatterjee and Jafarov (2013); Verzelen et al. (2018); Cai and Guo (2020)). Other widely-used methods assume some probabilistic structure on $\beta$ (e.g., $\beta$ is Gaussian) and use maximum likelihood to derive consistent estimators of the signal level (Yang et al. (2010); Bonnet et al. (2015)). These methods have been extensively studied in the literature of random-effect models where $\beta$ is treated as random; see de Los Campos et al. (2015) and references therein. However, methods that rely on the assumption that $\beta$ is either sparse or highly structured may not perform well when these assumptions fail to hold. For example, a known problem in genetics is the problem of missing heritability (de Los Campos et al. (2015); Zhu and Zhou (2020)). Heritability is defined as the fraction of the observed outcome (phenotype) that is explained by genetic factors. The term “missing heritability” is traditionally used to describe the gap between heritability estimates from genome-wide-association-studies (GWAS) and the corresponding estimates from family studies. To explain the gap, it has been suggested that some phenotypes are explained by a numerous number of genetic factors that their individual effect is too small to detect, but their collective effect is significant (Yang et al. (2010); Young (2022)). In such a setting, methods that rely on the sparsity assumption may fail to provide accurate estimates.

Rather than assuming sparsity or other structural assumptions on $\beta$, a different approach for estimating the signal level in a high-dimensional setting is to assume some or complete knowledge about the covariate distribution. This can be justified, for example, in the semi-supervised setting when one has access to a large amount of unlabeled (covariate) data without the corresponding labels (responses). When the covariates are assumed independent Gaussian, Dicker (2014) proposed estimators based on the method-of-moments and Janson et al. (2017) used convex optimization techniques. In both methods, the Gaussian assumption was used to show consistency and asymptotic-normality, and it is not clear how robust these methods are when the assumptions are violated. Dropping the Gaussian independent covariate assumption, Livne et al. (2021) proposed a consistent estimator under the assumption that the first two moments of covariates are known. More recently, Chen (2022) proposed an estimator that is consistent and asymptotically-normal when the covariates are independent and the entries of $\beta$ are small and dense.

All of the estimators that we reviewed above were developed under the assumption that the linear model is true, which can be unrealistic in many situations. In this work, we focus our attention on the model-free setting, i.e., no assumptions are made about the relationship between the covariates and the response. Under this setting, Kong and Valiant (2018) proposed
a consistent estimator under some assumptions on the covariance matrix. In this paper we follow the two-stage approach presented in Livne et al. (2021), where an initial estimator is first suggested and then a zero-estimator is used to reduce its variance. Our initial estimator is the same as in Kong and Valiant (2013) and Livne et al. (2021), and the zero estimators we use are tailored to the model-free framework. Furthermore, we provide a general algorithm that, in principle, improve any initial estimator and we also demonstrate the usefulness of the algorithm for several initial estimators.

The rest of this work is organized as follows. In Section 2, we discuss the parameters of interest in a model-free setting under the assumption that the first two moments of the covariates are known. In Section 3, we present our initial estimators and prove that they are consistent under some minimal assumptions. In Section 4, we use the zero-estimator approach to construct two improved estimators and then study some theoretical properties of the improved estimators. Simulation results are given in Section 5. Section 6 demonstrates how the zero-estimator approach can be generalized to other estimators. A discussion is given in Section 7. The proofs are provided in the Appendix.

2 Preliminaries

Let $X \in \mathbb{R}^p$ be a random vector of covariates and let $Y \in \mathbb{R}$ be the response. The conditional mean $E(Y|X)$ is the best predictor in the sense that it minimizes the mean squared error $E\{[Y - g(X)]^2\}$ over all measurable functions $g(X)$ (see Hansen (2022), p. 25). However, the functional form of $E(Y|X)$ is typically unknown and difficult to estimate, especially in a high-dimensional setting. Consequently, we can define the best linear approximation to $E(Y|X)$.

Definition 1. Assume that both $E(Y^2)$, $E(\|X\|^2)$ exist and that the covariance matrix of $X$, denoted by $\Sigma_X$, is invertible. Then, the best linear predictor, $\alpha + \beta^T X$, is defined by the unique $\alpha$ and $\beta$ that minimize the mean squared error

$$
(\alpha, \beta) = \arg \min_{a \in \mathbb{R}, b \in \mathbb{R}^p} E(Y - a - b^T X)^2,
$$

and, by Hansen (2022), pp. 34-36, is given by

$$
\beta = \Sigma_X^{-1}\{E(XY) - E(X)E(Y)\} \quad \text{and} \quad \alpha = E(Y) - \beta^T E(X).
$$

The best linear predictor is essentially the population version of the OLS method. Notice that $\alpha, \beta$ also satisfy $(\alpha, \beta) = \arg \min_{a \in \mathbb{R}, b \in \mathbb{R}^p} E[\{E(Y|X) - a - b^T X\]^2$. It is a model-free quantity, i.e., no specific assumptions are made about the relationship between $X$ and $Y$. In particular, we do not assume that $E(Y|X)$ is linear in $X$. If $E(Y|X)$ happens to be linear, say $E(Y|X) =$
Then the best linear predictor parameters \((\alpha, \beta)\) coincide with the model parameters \((\hat{\alpha}, \hat{\beta})\). However, when \(E(Y|X)\) is not linear, the parameters \(\alpha\) and \(\beta\) are still meaningful: they describe the overall direction of the association between \(X\) and \(Y\) \(\text{(Buja et al. (2019))}\). Hence, Definition 1 is useful since in most cases we have no reason to believe that \(E(Y|X)\) is indeed linear in \(X\).

We now wish to decompose the variance of \(Y\) into signal and noise levels. Let \(\sigma_Y^2\) denote the variance of \(Y\) and define the residual \(\epsilon \equiv Y - \alpha - \beta^T X\). Notice that both \(E(X\epsilon) = 0\) and \(E(\epsilon) = 0\) by construction. Write

\[
\sigma_Y^2 = \text{Var}(\alpha + X^T \beta + \epsilon) = \beta^T \text{Var}(X) \beta + \text{Var}(\epsilon) = \beta^T \Sigma_X \beta + \sigma^2,
\]

where \(\sigma^2 \equiv \text{Var}(\epsilon)\) and \(\Sigma_X \equiv \text{Var}(X)\). Here, the signal level \(\tau^2 \equiv \beta^T \Sigma_X \beta\) can be thought of as the total variance explained by the best linear function of the covariates. The noise level \(\sigma^2\) is the variance left unexplained. Notice that the parameters \(\tau^2, \sigma^2\) and \(\sigma_Y^2\) depend on \(p\) but this is suppressed in the notation.

A common starting point for many works of regression problems is to use strong assumptions about \(E(Y|X)\), and minimal assumptions, if any, about the covariate \(X\). In this work, we take the opposite approach: we make no assumptions about \(E(Y|X)\) but assume we know everything about \(X\) instead. This can be justified, for example, in a semi-supervised setting where, in addition to the labeled data, we also have access to a large amount of unlabeled data; see, for example, the work of Zhang and Bradic \(\text{(2019)}\) who study estimation of the mean and variance of \(Y\) in a semi-supervised, model-free setting. Note that the setting of known-covariate distribution has already been presented and discussed in the context of high-dimensional regression as in Candes et al. \(\text{(2018)}\), Berrett et al. \(\text{(2020)}\) and Wang and Janson \(\text{(2020)}\). Our goal here is to develop good estimators for \(\tau^2\) and \(\sigma^2\) in a model-free setting under the assumption that the distribution of the covariates is known.

Let \((X_1, Y_1), ..., (X_n, Y_n)\) be i.i.d. observations drawn from an unknown distribution where \(X_i \in \mathbb{R}^p\) and \(Y_i \in \mathbb{R}\). Let \((X, Y)\) denote a generic observation from the sample. We assume that \(E(X) \equiv \mu\) is known and also that the variance matrix \(\Sigma_X\) is known and invertible. Linear transformations do not affect the signal and noise levels. Thus, we can apply the transformation \(X \mapsto \Sigma_X^{-1/2}(X - \mu)\) and assume w.l.o.g. that

\[
E(X) = 0 \quad \text{and} \quad \Sigma_X = I.
\]

By (2), \(\sigma_Y^2 = ||\beta||^2 + \sigma^2\), which means that in order to estimate \(\sigma^2\) it is enough to estimate both \(\sigma_Y^2\) and \(\tau^2 \equiv ||\beta||^2\). The variance term \(\sigma_Y^2\) can be easily estimated from the sample. Hence, the main challenge is to derive an estimator for \(\tau^2\).
3 Initial Estimators

In this section, we present our initial estimators for the signal and noise levels, $\tau^2$ and $\sigma^2$. Interestingly, when the linear model is true and $X$ is assumed to be constant, no consistent estimator of $\sigma^2$ exists (Azriel (2019)). However, when $X$ is random, a consistent estimator does exist if $\Sigma$ is known (Verzelen et al. (2018)). The current work goes one step further as we generalize this result without assuming linearity. Indeed, Proposition 2 below demonstrates that by knowing the first and second moments of $X$, it is possible, under some mild assumptions, to construct consistent estimators of $\tau^2$ and $\sigma^2$ in a high-dimensional setting without assuming that $E(Y|X)$ is linear. The estimator we use below was suggested by Kong and Valiant (2018) who provided an upper bound on the variance. Our analysis is more general and we discuss sufficient conditions for consistency.

Let $W_{ij} \equiv X_{ij}Y_i$ for $i = 1, ..., n$, and $j = 1, ..., p$. Notice that

$$E(W_{ij}) = E(X_{ij}Y_i) = E[X_{ij}(\alpha + \beta^TX_i + \varepsilon_i)] = \beta_j,$$

where in the last equality we used (3) and the orthogonality between $X$ and $\varepsilon$. Now, since $\{E(W_{ij})\}^2 = E(W_{ij}^2) - \text{Var}(W_{ij})$, a natural unbiased estimator for $\beta_j^2$ is

$$\hat{\beta}_j^2 = \frac{1}{n} \sum_{i=1}^{n} W_{ij}^2 - \frac{1}{n-1} \sum_{i=1}^{n} (W_{ij} - \bar{W}_j)^2 = \left(\frac{n}{2}\right)^{-1} \sum_{i_1 < i_2}^{n} W_{i_1j}W_{i_2j},$$

where $\bar{W}_j = \frac{1}{n} \sum_{i=1}^{n} W_{ij}$. Thus, an unbiased estimator of $\tau^2$ is given by

$$\hat{\tau}^2 = \sum_{j=1}^{p} \hat{\beta}_j^2 = \left(\frac{n}{2}\right)^{-1} \sum_{i_1 < i_2}^{n} W_{i_1}^TW_{i_2},$$

where $W_i = (W_{i1}, ..., W_{ip})^T$. We call $\hat{\tau}^2$ the \textit{naive estimator}. Notice that $\hat{\tau}^2$ is a U-statistic with the kernel $h(W_1, W_2) = W_1^TW_2$, and thus its variance can be calculated directly by using U-statistic properties (see van der Vaart (2000), Theorem 12.3).

Let $\zeta_1 \equiv \beta^TA\beta - \|\beta\|^4$, $\zeta_2 \equiv \|A\|_F^2 - \|\beta\|^4$, $A \equiv E(WW^T)$ and $\|A\|_F$ denotes the Frobenius norm of $A$. The following proposition calculates the variance of $\hat{\tau}^2$.

\textbf{Proposition 1.} Assuming that $\zeta_1$ and $\zeta_2$ are finite, the variance of the naive estimator $\hat{\tau}^2$ is given by

$$\text{Var}(\hat{\tau}^2) = \frac{4(n-2)}{n(n-1)} \zeta_1 + \frac{2}{n(n-1)} \zeta_2.$$

The next proposition shows that the naive estimator $\hat{\tau}^2$ is consistent under some assumptions.
Proposition 2. Assume that $\frac{\|A\|_F^2}{n^2} \xrightarrow{n \to \infty} 0$, and that $\tau^2$ is bounded. Then,

$$\hat{\tau}^2 - \tau^2 \xrightarrow{p} 0.$$  

Similarly, an estimator for the noise level $\sigma^2$ can be obtained by

$$\hat{\sigma}^2 \equiv \hat{\alpha}_Y^2 - \hat{\tau}^2,$$  \hspace{1cm} (8)

where $\hat{\alpha}_Y \equiv \frac{1}{n-1} \sum_{i=1}^{n} (Y_i - \bar{Y})^2$ is the standard unbiased estimator of $\alpha_Y^2$. Let $\mu_4 \equiv E [(Y - \alpha)^4]$; $\pi = (\pi_1, ..., \pi_p)^T$ where $\pi_j \equiv E [(Y_i - \alpha)^2 W_{ij}]$. The variance of $\hat{\sigma}^2$ is given by the following proposition.

Proposition 3. The variance of $\hat{\sigma}^2$ is

\begin{align*}
\text{Var}(\hat{\sigma}^2) &= \left[ \frac{\hat{\mu}_4}{n} - \frac{(n-3)}{n (n-1)} \alpha_Y^4 \right] + \text{Var}(\hat{\tau}^2) \\
&\quad - \frac{4}{n} (\pi^T \beta - \tau^2 \alpha_Y^2) + \frac{4}{n (n-1)} \sum_{j=1}^{p} \left\{ E[W_{ij}(Y_i - \alpha)] \right\}^2,
\end{align*}

(9)

where $\text{Var}(\hat{\tau}^2)$ is given in (7).

The following result is a corollary of Propositions 2 and 3.

Corollary 1. Assume that $\mu_4$ and $\tau^2$ are bounded and that $\frac{\|A\|_F^2}{n^2} \to 0$. Then,

$$\hat{\sigma}^2 - \sigma^2 \xrightarrow{p} 0.$$  

The condition $\frac{\|A\|_F^2}{n^2} \to 0$ holds in various settings. For example, it can be shown to hold when $p/n^2 \to 0$ and $Y$ is bounded. For more examples and details, see Remark 1 in the Appendix.

4 Reducing Variance Using a Zero Estimator

In this section, we study how the naive estimator $\hat{\tau}^2$, and consequently $\hat{\sigma}^2$, can be improved by using the assumption that the distribution of $X$ is known. We use zero-estimators to construct an improved unbiased estimator of $\tau^2$. This is also known as the method of control variables from the Monte-Carlo literature; see, e.g., Glynn and Szechtman (2002); Lavenberg and Welch (1981). Here, a zero-estimator is defined as a statistic $Z$ such that $E(Z) = 0$. For a given zero-estimator $Z$ and a constant $c$, we define a new estimator $\hat{\tau}^2(Z, c)$ as

$$\hat{\tau}^2(Z, c) = \hat{\tau}^2 - cZ.$$  \hspace{1cm} (10)
For a fixed $c$, notice that $\hat{\tau}^2(Z, c)$ is an unbiased estimator for $\tau^2$. Also notice that for every function $f$ of the covariates $X_1, ..., X_n$, one can always define a zero-estimator

$$Z = f(X_1, \ldots , X_n) - E[f(X_1, \ldots , X_n)].$$

This is possible since we assume that the distribution of the covariates is known and hence $E[f(X_1, \ldots , X_n)]$ is known. The variance of $\hat{\tau}^2(Z, c)$ is

$$\text{Var}[\hat{\tau}^2(Z, c)] = \text{Var}(\hat{\tau}^2) + c^2 \text{Var}(Z) - 2c \text{Cov}(\hat{\tau}^2, Z).$$

Minimizing the variance with respect to $c$ yields the minimizer

$$c^* = \frac{\text{Cov}(\hat{\tau}^2, Z)}{\text{Var}(Z)}. \quad (11)$$

Hence, the corresponding oracle-estimator is

$$\hat{\tau}^2(Z, c^*) = \hat{\tau}^2 - c^*Z.$$

We use the term oracle since the optimal coefficient $c^*$ is an unknown quantity. The variance of the above oracle-estimator is

$$\text{Var}[\hat{\tau}^2(Z, c^*)] = \text{Var}(\hat{\tau}^2) - \frac{[\text{Cov}(\hat{\tau}^2, Z)]^2}{\text{Var}(Z)} = \left(1 - \rho^2_{\hat{\tau}^2, Z}\right) \text{Var}(\hat{\tau}^2), \quad (12)$$

where $\rho_{\hat{\tau}^2, Z}$ is the correlation coefficient between $\hat{\tau}^2$ and $Z$. The term $1 - \rho^2_{\hat{\tau}^2, Z}$ is the factor by which $\text{Var}(\hat{\tau}^2)$ could be reduced if the optimal coefficient $c^*$ was known. Thus, the more correlation there is between the zero-estimator $Z$ and the naive estimator $\hat{\tau}^2$, the greater the reduction in variance.

There are two challenges to be addressed with the above approach. First, one should find a simple zero-estimator $Z$ which is correlated with the naive estimator $\hat{\tau}^2$. Second, the optimal coefficient $c^*$ is an unknown quantity and therefore needs to be estimated.

To address the first challenge, we propose the following zero-estimator

$$Z_g \equiv \bar{g}_n = \frac{1}{n} \sum_{i=1}^{n} g(X_i),$$

where $g(X_i) = \sum_{j<j'} X_{ij}X_{ij'}$. In Remark 2 in the Appendix, we show that the optimal coefficient, with respect to $Z_g$, is

$$c_g^* = \frac{2\beta^T \theta_g}{\text{Var}[g(X)]}, \quad (13)$$

where $\theta_g = E[W g(X)]$. Notice that $\text{Var}[g(X)]$ is a known quantity since the distribution of $g(X)$ is assumed to be known. Hence, the corresponding oracle-estimator is

$$T_g \equiv \hat{\tau}^2(Z_g, c_g^*) = \hat{\tau}^2 - c_g^*Z_g. \quad (14)$$
To address the second challenge, i.e., to estimate the optimal coefficient $c^*_g$, we suggest the following unbiased U-statistic estimator

$$
\hat{c}^*_g = \frac{(n_2)^{-1} \sum_{i_1 \neq i_2} W_{i_1}^TW_{i_2}g(X_{i_2})}{\text{Var}[g(X)]}.
$$

(15)

Thus, the corresponding improved estimator is

$$
T_g \equiv \hat{\tau}^2(Z_g, \hat{c}^*_g) = \hat{\tau}^2 - \hat{c}^*_g Z_g.
$$

(16)

Using the zero-estimator $Z_g$ has a potential drawback. It uses all the $p$ covariates of the vector $X$ regardless of the sparsity level in the data, which can result in some additional variability due to unnecessary estimation. Intuitively, when the sparsity level is high, i.e., only a small number of covariates plays an important role in explaining the response $Y$, it is inefficient to use a zero-estimator that incorporates all the $p$ covariates. In such a setting, it is reasonable to modify the zero-estimator $Z_g$ such that only a small set of covariates will be included, preferably the covariates that capture a significant part of the signal level $\tau^2$. Selecting such a set of covariates can be difficult and one may use a covariate-selection procedure for this purpose.

We call $\delta$ a covariate selection procedure if for every dataset it chooses a subset of indices $S_\delta$ from $\{1, \ldots, p\}$. Different covariate-selection methods exist in the literature (see Oda et al. (2020) and references therein) but these are not a primary focus of this work. For a given selection procedure $\delta$ we modify the estimator $T_g$ such that only the indices in $S_\delta$ will be included in its zero-estimator term. This modified estimator, which is based on a given selection procedure $\delta$, is presented in the algorithm below.

**Algorithm 1:** Proposed estimator for $\tau^2$.

**Input:** A dataset $(X_{n \times p}, Y_{n \times 1})$ and a selection procedure $\delta$.

1. Calculate the naive estimator $\hat{\tau}^2 = (n/2)^{-1} \sum_{i_1 < i_2} W_{i_1}^TW_{i_2}$.

2. Apply procedure $\delta$ to $(X_{n \times p}, Y_{n \times 1})$ to construct the set $S_\delta$.

**Output:** Return the estimator

$$
T_h \equiv \hat{\tau}^2 - \hat{c}^*_h Z_h,
$$

(17)

where $\hat{c}^*_h = \frac{(n/2)^{-1} \sum_{i_1 \neq i_2} W_{i_1}^TW_{i_2}h(X_{i_2})}{\text{Var}[h(X)]}$, $Z_h = \frac{1}{n} \sum_{i=1}^n h(X_i)$ and $h(X_i) = \sum_{j < j' \in S_\delta} X_{ij}X_{ij'}$.

Notice that the estimator $T_g$ defined in (16) is a special case of the estimator $T_h$ defined in Algorithm 1 when $S_\delta = \{1, \ldots, p\}$, i.e., when $\delta$ selects all the $p$ covariates.
Recall that in this work we treat $p$ as a function of $n$, i.e., $p = p_n$ but this is suppressed in the notation. Let $\Theta \equiv \Theta_n \subseteq \{1, \ldots, p\}$ be a deterministic sequence of subsets. In order to analyze the estimator $T_h$ we define a stability property, which is given next.

**Definition 2.** A selection procedure $\delta$ is stable if there exists a deterministic sequence of subsets $\Theta$ such that

$$\lim_{n \to \infty} n[P(S_\delta \neq \Theta)]^{1/2} = 0.$$  

(18)

Definition 2 states that a selection procedure $\delta$ is stable if it is asymptotically close to a deterministic procedure at a suitable rate. The convergence rate of many practical selection procedures is exponential, which is much faster than is required for the condition to hold. For example, the lasso algorithm asymptotically selects the support of $\beta$ at an exponential rate under some assumptions (see Hastie et al. (2015), Theorem 11.3). Notice also that the stability condition holds trivially when $S_\delta = \{1, \ldots, p\}$, i.e., when $\delta$ selects all the $p$ covariates for all $n$.

Define the oracle-estimator $T_h \equiv \hat{\tau}^2 (Z_h, c^*_h)$, where $c^*_h = \frac{\beta^T \theta_h}{\text{Var}[h(X)]}$ and $\theta_h = E[W h(X)]$. Let

$$f(X_i) = \sum_{j < j' \in \Theta} X_{ij} X_{ij'}, \quad T_f \equiv \hat{\tau}^2 (Z_f, c_f^*), \quad T_f \equiv \hat{\tau}^2 (Z_f, c_f^*), \quad c_f^* = \frac{2 \beta^T \theta_f}{\text{Var}[f(X)]},$$

$$\hat{c}_f^* = \frac{2}{n(n-1)} \sum_{i_1 \neq i_2} W_{i_1}^T W_{i_2} f(X_{i_2}), \quad \theta_f = E[W f(X)], \quad Z_f = \frac{1}{n} \sum_{i=1}^n f(X_i),$$

$$B = E[W W^T f(X)], \quad C = E[W W^T f^2(X)].$$

We now prove that the proposed estimator in Algorithm 1 is asymptotically equivalent to its oracle version $T_h$ under some conditions.

**Proposition 4.** Assume that the selection procedure $\delta$ is stable with respect to $\Theta$. Assume also that $n/p$, $\|\beta\|^2$, $\|\theta_f\|^2$, $E[|b|^2]$, and $\frac{E(|b|^2)}{n \text{Var}[f(X)]}$ are bounded, and $\frac{\|A\|^2}{n \text{Var}[f(X)]} \rightarrow 0$, $\frac{\|B\|^2}{n \text{Var}[f(X)]} \rightarrow 0$, and $\frac{\|C\|^2}{(n \text{Var}[f(X)])^2} \rightarrow 0$. In addition, assume that the first four moments of $T_h$, $T_h$, $T_f$, and $T_f$ are bounded. Then,

$$\sqrt{n}[T_h - T_h] \xrightarrow{p} 0.$$  

(20)

Our proof of Proposition 4 shows a slightly stronger result: the proposed estimator $T_h$ is also asymptotically equivalent to $T_f$, the oracle-estimator that originally knows the set of indices $\Theta$.

We now discuss the assumptions of Proposition 4. In Remark 4 several sufficient conditions implying that $\frac{\|A\|^2}{n \text{Var}[f(X)]} \rightarrow 0$ were presented. Similarly, in Remark 5 we show that if the covariates $X_{ij}$, for $j = 1, \ldots, p$, $i = 1, \ldots, n$, and the response $Y$ are bounded, then so is $\frac{E(|b|^2)}{n \text{Var}[f(X)]}$. It is also shown, that if in addition $|\Theta|$ is bounded and $\text{Var}[f(X)]$ is bounded away from zero, then $\frac{\|B\|^2}{n \text{Var}[f(X)]} \rightarrow 0$ and $\frac{\|C\|^2}{(n \text{Var}[f(X)])^2} \rightarrow 0$. Proposition 4 in Livne et al. (2021) shows that
\[ \frac{||\mathbf{B}_j||^2}{\sigma^2 \text{Var}(\hat{f}(\mathbf{X}))} \to 0 \] and \[ \frac{||\mathbf{C}_i||^2}{\text{Var}(\hat{f}(\mathbf{X}))} \to 0 \] hold also when \(|\Theta|\) is unbounded, but with additional conditions on linearity and independence of the covariates. It is also shown there that under those assumptions, \[ \frac{||\mathbf{\theta}_j||^2}{\text{Var}(\hat{f}(\mathbf{X}))} \] is bounded. In simulations, which are not presented here, we observed that these conditions also hold for various non-linear models.

Notice that the zero-estimator \( Z_g \), which is not based on any covariate-selection procedure, is just a special case of \( Z_h \) when \( \delta \) selects all the \( p \) covariates, i.e., \( S_\delta = \{1, \ldots, p\} \). Hence, if the conditions of Proposition 4 hold, then \( \sqrt{n} [\hat{T}_g - T_g] \to_d 0 \), where \( T_g \) and \( \hat{T}_g \) are given in (16) and (14), respectively.

5 Simulations Results

In this section, we illustrate the performance of the proposed estimators using simulations. Specifically, we compare the naive estimator \( \hat{\beta}^2 \) and the improved estimators \( T_g \) and \( T_h \) which are defined in (5), (16), and Algorithm 1, respectively. The code for reproducing the results of this section and the next section (6) is available at [https://t.ly/dwJg](https://t.ly/dwJg).

For demonstration purposes, we consider a setting in which \( K \) entries of the vector \( \beta \) are relatively large (in absolute value), and all other entries are small. The proportion of the signal in those \( K \) entries is defined as the sparsity level of the vector \( \beta \). Next, we study different sparsity levels by defining the following non-linear model,

\[
Y_i = \gamma_{L} \sum_{j \in \Theta} [X_{ij} + \sin(X_{ij})] + \gamma_{S} \sum_{j \not\in \Theta} [X_{ij} + \sin(X_{ij})] + \xi_i, \quad i = 1, \ldots, n, \tag{21}
\]

where \( \gamma_L \equiv \left\{ \frac{\eta^2}{k(1+E[X \sin(X)])} \right\}^{1/2} \), \( \gamma_S \equiv \left\{ \frac{\tau^2(1-\eta)}{(p-k)(1+E[X \sin(X)])\tau^2} \right\}^{1/2} \), and \( \Theta \) is the set of the largest \( K \) entries of the vector \( \beta \). The model has two parameters, \( \tau^2 \) and \( \eta \), that vary across the different simulation scenarios. The covariates were generated from the centered exponential distribution, i.e., \( X_{ij} \sim \text{Exp}(1) - 1 \), \( i = 1, \ldots, n \), \( j = 1, \ldots, p \). The noise level \( \xi_i \) was generated from the standard normal distribution. One can verify that under the above model \( \beta_j^2 = \frac{\eta^2}{K} \) for \( j \in \Theta \), and that \( \beta_j^2 = \frac{\tau^2(1-\eta)}{(p-k)} \) for \( j \not\in \Theta \). Define \( \tau^2_\Theta \equiv \sum_{j \in \Theta} \beta_j^2 \). From the above definitions, it follows that \( \eta = \tau^2_\Theta / \tau^2 \). The parameter \( \eta \) is the proportion of signal that is captured by the set \( \Theta \), which is the sparsity level as defined above. The case of full sparsity, where the entire signal level \( \tau^2 \) comes only from the set \( \Theta \), corresponds to \( \eta = 1 \), and is not assumed here.

We fix \( n = p = 300 \) and \( K = 6 \). For each combination of the parameters \( \tau^2 \in \{1, 2\} \) and \( \eta \in \{0.1, 0.3, 0.5, 0.7, 0.9\} \), we generated 100 independent datasets from model (21) and estimated \( \tau^2 \) using the different estimators. The covariate-selection procedure \( \delta \) that was used in the estimator \( T_h \) is defined in Remark 4 in the Appendix.
Figure 1 plots the RMSE of each estimator as a function of the sparsity level $\eta$ and the signal level $\tau^2$. It is demonstrated that the estimators $\hat{T}_g$ and $\hat{T}_h$ improve (i.e., lower or equal RMSE) the naive estimator in all settings. The improved estimators are complementary to each other, i.e., for small values of $\eta$ the estimator $\hat{T}_g$ performs better than $\hat{T}_h$, and the opposite occurs for large values of $\eta$. This is expected since when the sparsity level $\eta$ is small, the improvement of $\hat{T}_h$ is smaller as it ignores much of the signal that lies outside of the set $\Theta$. On the other hand, when a large portion of the signal $\tau^2$ is captured by only the few covariates in $\Theta$, it is sufficient to make use of only these covariates in the zero-estimator term, and the improvement of $\hat{T}_h$ is greater.

Table 1 shows the RMSE, bias, standard error, and the relative improvement, for the different estimators. It can be observed that the degree of improvements depends on the sparsity level of the data $\eta$. For example, when $\tau^2 = 1$ and sparsity level is low ($\eta = 0.1$), the estimator $\hat{T}_g$ improves the naive estimator by 11%, while the estimator $\hat{T}_h$ presents a similar performance to the naive estimator. On the other hand, when the sparsity level is high ($\eta = 0.9$), the estimator $\hat{T}_h$ improves the naive by 11%, while $\hat{T}_g$ presents a similar performance to the naive estimator, as expected. Notice that when $\tau^2 = 2$ these improvements are even more substantial.

![Figure 1](image.png)  
Figure 1: Root mean square error (RMSE) for the proposed estimators. The x-axis stands for the sparsity level $\eta$. 

Table 1: Summary statistics for the proposed estimators; $n = p = 300$. Bias, standard error (SE), root mean square error (RMSE) and percentage change from the naive estimator (in terms of RMSE) are shown. The table results were computed over 100 simulated datasets for each setting. An estimate for the standard deviation of RMSE ($\hat{\sigma}_{RMSE}$) was calculated using the delta method.

| $\eta$ | $\tau^2$ | Estimator | Bias  | SE    | RMSE  | % Change | $\hat{\sigma}_{RMSE}$ |
|-------|---------|-----------|-------|-------|-------|----------|------------------------|
| 10%   | 1       | $\hat{\tau}^2$ | -0.03 | 0.274 | 0.274 | 0.00     | 0.018                  |
| 10%   | 1       | $T_{\hat{g}}$     | 0.04  | 0.242 | 0.244 | -10.95   | 0.016                  |
| 30%   | 1       | $T_{\hat{h}}$     | -0.03 | 0.274 | 0.274 | 0.00     | 0.017                  |
| 30%   | 1       | $\hat{\tau}^2$    | -0.02 | 0.284 | 0.283 | 0.00     | 0.019                  |
| 30%   | 1       | $T_{\hat{g}}$     | 0.05  | 0.255 | 0.258 | -8.83    | 0.018                  |
| 30%   | 1       | $T_{\hat{h}}$     | 0.00  | 0.282 | 0.28  | -1.06    | 0.017                  |
| 50%   | 1       | $\hat{\tau}^2$    | 0.00  | 0.286 | 0.284 | 0.00     | 0.021                  |
| 50%   | 1       | $T_{\hat{g}}$     | 0.05  | 0.264 | 0.268 | -5.63    | 0.020                  |
| 50%   | 1       | $T_{\hat{h}}$     | 0.02  | 0.277 | 0.276 | -2.82    | 0.017                  |
| 70%   | 1       | $\hat{\tau}^2$    | 0.01  | 0.285 | 0.284 | 0.00     | 0.022                  |
| 70%   | 1       | $T_{\hat{g}}$     | 0.05  | 0.272 | 0.275 | -3.17    | 0.021                  |
| 70%   | 1       | $T_{\hat{h}}$     | 0.04  | 0.265 | 0.267 | -5.99    | 0.017                  |
| 90%   | 1       | $\hat{\tau}^2$    | 0.03  | 0.281 | 0.282 | 0.00     | 0.021                  |
| 90%   | 1       | $T_{\hat{g}}$     | 0.05  | 0.276 | 0.279 | -1.06    | 0.020                  |
| 90%   | 1       | $T_{\hat{h}}$     | 0.07  | 0.242 | 0.25  | -11.35   | 0.015                  |
| 10%   | 2       | $\hat{\tau}^2$    | -0.06 | 0.458 | 0.46  | 0.00     | 0.030                  |
| 10%   | 2       | $T_{\hat{g}}$     | 0.08  | 0.379 | 0.386 | -16.09   | 0.024                  |
| 10%   | 2       | $T_{\hat{h}}$     | -0.05 | 0.457 | 0.458 | -0.43    | 0.029                  |
| 30%   | 2       | $\hat{\tau}^2$    | -0.03 | 0.476 | 0.475 | 0.00     | 0.033                  |
| 30%   | 2       | $T_{\hat{g}}$     | 0.09  | 0.408 | 0.416 | -12.42   | 0.029                  |
| 30%   | 2       | $T_{\hat{h}}$     | -0.01 | 0.469 | 0.466 | -1.89    | 0.029                  |
| 50%   | 2       | $\hat{\tau}^2$    | -0.01 | 0.481 | 0.478 | 0.00     | 0.036                  |
| 50%   | 2       | $T_{\hat{g}}$     | 0.09  | 0.431 | 0.439 | -8.16    | 0.033                  |
| 50%   | 2       | $T_{\hat{h}}$     | 0.03  | 0.458 | 0.457 | -4.39    | 0.028                  |
| 70%   | 2       | $\hat{\tau}^2$    | 0.02  | 0.477 | 0.475 | 0.00     | 0.038                  |
| 70%   | 2       | $T_{\hat{g}}$     | 0.09  | 0.448 | 0.454 | -4.42    | 0.035                  |
| 70%   | 2       | $T_{\hat{h}}$     | 0.08  | 0.429 | 0.433 | -8.84    | 0.026                  |
| 90%   | 2       | $\hat{\tau}^2$    | 0.05  | 0.468 | 0.468 | 0.00     | 0.035                  |
| 90%   | 2       | $T_{\hat{g}}$     | 0.08  | 0.456 | 0.462 | -1.28    | 0.034                  |
| 90%   | 2       | $T_{\hat{h}}$     | 0.12  | 0.376 | 0.392 | -16.24   | 0.023                  |

6 Generalization to Other Estimators

The suggested methodology in this paper is not limited to improving only the naive estimator, but can also be generalized to other estimators. As before, the key idea is to use a zero-estimator that is correlated with an initial estimator of $\tau^2$ in order to reduce its variance.
Unlike the naive estimator $\hat{\tau}^2$, which has by a closed-form expression, other estimators, such as the EigenPrism estimator (Janson et al., 2017), are computed numerically by solving a convex optimization problem. For a given zero-estimator, this makes the task of estimating the optimal-coefficient $c^*$ more challenging than before. To overcome this challenge, we approximate the optimal coefficient $c^*$ using bootstrap samples. This is described in the following algorithm.

**Algorithm 2: Empirical Estimators**

**Input:** A dataset $(X_{n \times p}, Y_{n \times 1})$, an estimation procedure $\tilde{\tau}^2$, and a covariate-selection procedure $\delta$.

1. Apply the procedure $\delta$ to the dataset $(X_{n \times p}, Y_{n \times 1})$ to obtain $S_\delta$.
2. Apply the procedure $\tilde{\tau}^2$ to the dataset.
3. Calculate the zero-estimator $Z_h = \frac{1}{n} \sum_{i=1}^{n} h(X_i)$, where $h(X_i) = \sum_{j < j' \in S_\delta} X_{ij} X_{ij'}$.
4. **Bootstrap step:**
   - Sample $n$ observations at random from $(X_{n \times p}, Y_{n \times 1})$, with replacement, to obtain a bootstrap dataset.
   - Repeat steps 2 and 3 based on the bootstrap dataset.

   The bootstrap step is repeated $M$ times in order to produce $(\tilde{\tau}^2)^{*1}, ..., (\tilde{\tau}^2)^{*M}$ and $Z_{h1}^*, ..., Z_{hM}^*$.

5. Approximate the coefficient $\hat{c}_h^* = \frac{\text{Cov}(\tilde{\tau}^2, Z_h)}{\text{Var}(Z_h)}$ where $\text{Cov}(\cdot)$ denotes the empirical covariance from the bootstrap samples.

**Result:** Return the empirical estimator $T_h^* \equiv \tilde{\tau}^2 - \hat{c}_h^* Z_h$.

In the special case when $\delta$ selects all the $p$ covariates, i.e., $S_\delta = \{1, \ldots, p\}$, we use the notations $Z_g$ and $\hat{c}_g^*$ rather than $Z_h$ and $\hat{c}_h^*$, respectively, i.e., $T_g^* \equiv \tilde{\tau}^2 - \hat{c}_g^* Z_g$.

We illustrate the improvement obtained by Algorithm 2 by choosing $\tilde{\tau}^2$ to be the EigenPrism procedure (Janson et al., 2017), but other estimators can be used as well. We consider the same setting as in Section 5. The number of bootstrap samples is $M = 100$.

The simulation results appear in Table 2 and Figure 2. Both estimators $T_h^*$ and $T_g^*$ show an improvement over the EigenPrism estimator $\tilde{\tau}^2$. The results here are fairly similar to the results shown for the naive estimator in Section 5 with just a smaller degree of improvement.
As before, the improved estimators $T_h$ and $T_g$ are complementary to each other, i.e., for small values of $\eta$ the estimator $T_g$ performs better than $T_h$, and the opposite occurs for large values of $\eta$.

![Figure 2: Root mean square error (RMSE) for the proposed estimators. The x-axis stands for the sparsity level $\eta$.](image)

Figure 2: Root mean square error (RMSE) for the proposed estimators. The x-axis stands for the sparsity level $\eta$. 
Table 2: Summary statistics for the EigenPrism-related estimators; \( n = p = 300 \). Biases, standard errors (SE) and the root mean square errors (RMSE) of the different estimators, computed over 100 independent datasets for each setting. The relative improvement over the EigenPrism estimator \( \tilde{\tau}^2 \) (in terms of RMSE) is also shown. An estimate for the standard deviation of RMSE (\( \hat{\sigma}_{RMSE} \)) was calculated using the delta method.

| \( \eta \) | \( \tau^2 \) | Estimator | Bias | SE    | RMSE  | % Change | \( \hat{\sigma}_{RMSE} \) |
|----------|-----------|-----------|------|-------|-------|----------|----------------|
| 10%      | 1         | \( \tilde{\tau}^2 \) | 0.01 | 0.204 | 0.204 | 0.00     | 0.014         |
| 10%      | 1         | \( T_{\tilde{g}} \) | 0.01 | 0.19  | 0.19  | -6.86    | 0.012         |
| 10%      | 1         | \( T_{\tilde{h}} \) | 0.01 | 0.204 | 0.203 | -0.49    | 0.014         |
| 30%      | 1         | \( \tilde{\tau}^2 \) | 0.01 | 0.202 | 0.201 | 0.00     | 0.014         |
| 30%      | 1         | \( T_{\tilde{g}} \) | 0.01 | 0.195 | 0.194 | -3.48    | 0.014         |
| 30%      | 1         | \( T_{\tilde{h}} \) | 0.01 | 0.201 | 0.201 | 0.00     | 0.014         |
| 50%      | 1         | \( \tilde{\tau}^2 \) | 0.00 | 0.206 | 0.205 | 0.00     | 0.014         |
| 50%      | 1         | \( T_{\tilde{g}} \) | 0.00 | 0.202 | 0.201 | -1.95    | 0.014         |
| 50%      | 1         | \( T_{\tilde{h}} \) | 0.01 | 0.201 | 0.201 | -1.95    | 0.015         |
| 70%      | 1         | \( \tilde{\tau}^2 \) | 0.00 | 0.212 | 0.211 | 0.00     | 0.015         |
| 70%      | 1         | \( T_{\tilde{g}} \) | 0.00 | 0.209 | 0.208 | -1.42    | 0.015         |
| 70%      | 1         | \( T_{\tilde{h}} \) | 0.00 | 0.203 | 0.202 | -4.27    | 0.015         |
| 90%      | 1         | \( \tilde{\tau}^2 \) | -0.01| 0.219 | 0.218 | 0.00     | 0.016         |
| 90%      | 1         | \( T_{\tilde{g}} \) | -0.01| 0.218 | 0.218 | 0.00     | 0.016         |
| 90%      | 1         | \( T_{\tilde{h}} \) | 0.00 | 0.204 | 0.203 | -6.88    | 0.015         |
| 10%      | 2         | \( \tilde{\tau}^2 \) | 0.00 | 0.291 | 0.29  | 0.00     | 0.020         |
| 10%      | 2         | \( T_{\tilde{g}} \) | 0.02 | 0.251 | 0.25  | -13.79   | 0.016         |
| 10%      | 2         | \( T_{\tilde{h}} \) | 0.01 | 0.291 | 0.29  | 0.00     | 0.020         |
| 30%      | 2         | \( \tilde{\tau}^2 \) | 0.03 | 0.279 | 0.279 | 0.00     | 0.019         |
| 30%      | 2         | \( T_{\tilde{g}} \) | 0.03 | 0.258 | 0.258 | -7.53    | 0.018         |
| 30%      | 2         | \( T_{\tilde{h}} \) | 0.03 | 0.276 | 0.276 | -1.08    | 0.019         |
| 50%      | 2         | \( \tilde{\tau}^2 \) | 0.02 | 0.285 | 0.284 | 0.00     | 0.019         |
| 50%      | 2         | \( T_{\tilde{g}} \) | 0.01 | 0.273 | 0.272 | -4.23    | 0.019         |
| 50%      | 2         | \( T_{\tilde{h}} \) | 0.02 | 0.274 | 0.273 | -3.87    | 0.020         |
| 70%      | 2         | \( \tilde{\tau}^2 \) | 0.01 | 0.294 | 0.293 | 0.00     | 0.020         |
| 70%      | 2         | \( T_{\tilde{g}} \) | 0.00 | 0.289 | 0.287 | -2.05    | 0.019         |
| 70%      | 2         | \( T_{\tilde{h}} \) | 0.01 | 0.271 | 0.27  | -7.85    | 0.019         |
| 90%      | 2         | \( \tilde{\tau}^2 \) | -0.01| 0.308 | 0.307 | 0.00     | 0.022         |
| 90%      | 2         | \( T_{\tilde{g}} \) | -0.01| 0.307 | 0.305 | -0.65    | 0.022         |
| 90%      | 2         | \( T_{\tilde{h}} \) | 0.00 | 0.269 | 0.268 | -12.7    | 0.019         |
7 Discussion and Future Work

In this work, we proposed a zero-estimator approach for improving estimation of the signal and noise levels explained by a set of covariates in a high-dimensional regression setting when the covariate distribution is known. We presented theoretical properties of the naive estimator $\hat{\tau}^2$, and the proposed improved estimators $T_h$ and $T_g$. In a simulation study, we demonstrated that the zero-estimator approach leads to a significant reduction in the RMSE. Our method does not rely on sparsity assumptions of the regression coefficient vector, normality of the covariates, or linearity of $E(Y|X)$. The goal in this work is to estimate the signal coming from the best linear function of the covariates, which is a model-free quantity. Our simulations demonstrate that our approach can be generalized to improve other estimators as well.

We suggest the following directions for future work. One natural extension is to relax the assumption of known covariate distribution to allow for a more general setting. This may be studied under the semi-supervised setting where one has access to a large amount of unlabeled data ($N \gg n$) in order to obtain theoretical results as a function of $N$. Another possible future research might be to extend the proposed approach to generalized linear models (GLM) such as logistic and Poisson regression, or survival models.

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8 Appendix

Proof of Proposition \[\square\]

Let \( W_i = (W_{i1}, ..., W_{ip})^T \) and notice that \( \hat{\tau}^2 = \frac{1}{n(n-1)} \sum_{i_1 \neq i_2} \sum_{j=1}^p W_{i1j} W_{i2j} \) is a U-statistic of order 2 with the kernel \( h_r(W_1, W_2) = W_1^T W_2 = \sum_{i=1}^p W_{i1j} W_{i2j} \).

By Theorem 12.3 in \textit{van der Vaart} \[2000\],

\[
\text{Var}(\hat{\tau}^2) = \frac{4(n - 2)}{n(n - 1)} \zeta_1 + \frac{2}{n(n - 1)} \zeta_2,
\]

where \( \zeta_1 \equiv \text{Cov}[h(W_1, W_2), h(W_1, \tilde{W}_2)] \) and \( \zeta_2 \equiv \text{Var}[h(W_1, W_2)] \), and where \( \tilde{W}_2 \) is an independent copy of \( W_2 \).

Define the \( p \times p \) matrix \( A = E(WW^T) \) and notice that

\[
\zeta_1 \equiv \text{Cov}[h(W_1, W_2), h(W_1, \tilde{W}_2)] = \sum_{j,j'} \text{Cov}(W_{1j}, W_{1j'}, \tilde{W}_{2j'}) = \sum_{j,j'} (\beta_j^2 \beta_{j'}^2 E[W_{1j} W_{1j'}] - \beta_j^2 \beta_{j'}^2) = \beta^T A \beta - \|\beta\|^4,
\]

and

\[
\zeta_2 \equiv \text{Cov}[h(W_1, W_2), h(W_1, W_2)] = \sum_{j,j'} \text{Cov}(W_{1j}, W_{1j'}, W_{1j}, \bar{W}_{2j}) = \sum_{j,j'} ((E[W_{1j} W_{1j'}])^2 - \beta_j^2 \beta_{j'}^2) = \|A\|_F^2 - \|\beta\|^4,
\]

where \( \|A\|_F^2 \) is the Frobenius norm of \( A \). Thus, \( \square \) follows from (22).

\[\square\]

Proof of Proposition \[\square\]

Since \( \hat{\tau}^2 \) is an unbiased estimator of \( \tau^2 \), then it is enough to prove that \( \text{Var}[\hat{\tau}^2] \xrightarrow{n \to \infty} 0 \). By \( \square \) it is enough to require that \( \frac{\beta^T A \beta}{n} \xrightarrow{n \to \infty} 0 \) and \( \frac{\|A\|_F^2}{n} \xrightarrow{n \to \infty} 0 \). The latter is assumed and we now show that the former also holds true.

Let \( \lambda_1 \geq ... \geq \lambda_p \) be the eigenvalues of \( A \) and notice that \( A \) is symmetric. Thus,

\[
\frac{1}{n^2} (\lambda_1 A)^2 \leq \frac{1}{n^2} \sum_{j=1}^p \lambda_j^2 A = \frac{1}{n^2} \text{tr}(A^2) = \frac{1}{n^2} \|A\|_F^2.
\]

Since we assume that \( \frac{\|A\|_F^2}{n} \xrightarrow{n \to \infty} 0 \), we can conclude that \( \frac{\lambda_1 A}{n} \xrightarrow{n \to \infty} 0 \). Now, recall that the maximum of the quadratic form \( a^T A a \) satisfies \( \lambda_1 = \max_a a^T A a \). Hence,

\[
\frac{1}{n} a^T A \beta = \frac{1}{n} \|\beta\|^2 \left( \frac{\beta}{\|\beta\|} \right)^T \frac{\beta}{\|\beta\|} = \frac{1}{n} \|\beta\|^2 \lambda_1 = \frac{1}{n} \tau_n^2 \xrightarrow{n \to \infty} 0,
\]

where the last limit follows from the assumption that \( \tau^2 = O(1) \), and from the fact that \( \frac{\lambda_1}{n} \xrightarrow{n \to \infty} 0 \).

We conclude that \( \text{Var}[\hat{\tau}^2] \xrightarrow{n \to \infty} 0 \). \( \square \)
Proof of Proposition 3.

Recall that (8) states that \( \hat{\sigma}^2 \equiv \hat{\sigma}_{\bar{Y}}^2 - \hat{\tau}^2 \). Thus,

\[
\text{Var} \left( \hat{\sigma}^2 \right) = \text{Var} \left( \hat{\tau}^2 \right) + \text{Var} \left( \hat{\sigma}_{\bar{Y}}^2 \right) - 2 \text{Cov} \left( \hat{\sigma}_{\bar{Y}}^2, \hat{\tau}^2 \right). \tag{23}
\]

The variance of \( \hat{\tau}^2 \) is given in (9). By standard U-statistic calculations (see e.g., Example 1.8 in Bose and Chatterjee (2018)), the variance of \( \hat{\sigma}_{\bar{Y}}^2 \) is

\[
\text{Var}(\hat{\sigma}_{\bar{Y}}^2) = \frac{4(n-2)}{n(n-1)} \psi_1 + \frac{2}{n(n-1)} \psi_2,
\]

where \( \psi_1 \equiv \frac{\mu_4 - \sigma^4}{4} \) and \( \psi_2 \equiv \frac{\mu_4 + \sigma^4}{2} \). This can be further simplified to obtain

\[
\text{Var} \left( \hat{\sigma}_{\bar{Y}}^2 \right) = \frac{1}{n} \mu_4 - \left( \frac{n-3}{n(n-1)} \right) \sigma^4. \tag{24}
\]

We now calculate the covariance between and \( \hat{\sigma}_{\bar{Y}}^2 \) and \( \hat{\tau}^2 \). Write,

\[
\text{Cov} \left( \hat{\sigma}_{\bar{Y}}^2, \hat{\tau}^2 \right) = \text{Cov} \left[ \frac{1}{n(n-1)} \sum_{i_1 \neq i_2} (Y_{i_1} - Y_{i_2})^2 / 2, \frac{1}{n(n-1)} \sum_{j=1}^p \sum_{i_1 \neq i_2} W_{i_1j}W_{i_2j} \right]
\]

\[
= \frac{1}{2n^2(n-1)^2} \sum_{j=1}^p \sum_{i_1 \neq i_2} \sum_{i_3 \neq i_4} \text{Cov} \left[ W_{i_1j}W_{i_2j}, (Y_{i_1} - Y_{i_2})^2 \right].
\]

The covariance above is different from zero either when one of \( \{i_1, i_2\} \) is equal to one of \( \{i_3, i_4\} \), or when \( \{i_1, i_2\} \) is equal to \( \{i_3, i_4\} \). There are \( 4n(n-1)(n-2) \) quadruples \( \{i_1, i_2, i_3, i_4\} \) for the first case, and \( 2n(n-1) \) for the second case.

Therefore,

\[
\text{Cov} \left( \hat{\sigma}_{\bar{Y}}^2, \hat{\tau}^2 \right) = \frac{2(n-2)}{n(n-1)} \sum_{j=1}^p \text{Cov} [W_{i_1j}W_{i_2j}, (Y - Y_3)^2] + \frac{1}{n(n-1)} \sum_{j=1}^p \text{Cov} [W_{i_1j}W_{i_2j}, (Y_1 - Y_2)^2]. \tag{25}
\]

The first covariance term in (25) is

\[
\text{Cov} [W_{i_1j}W_{i_2j}, (Y_1 - Y_3)^2] = E \left[ (W_{i_1j}W_{i_2j}) (Y_1 - Y_3)^2 - 2(Y_1 - Y_3) \right] \]

\[
= E \left[ (W_{i_1j}W_{i_2j} - \beta^2) [(Y_1 - Y_3)^2 - 2(Y_1 - Y_3)] \right]
\]

\[
= E \left[ (W_{i_1j}W_{i_2j} - \beta^2) ([Y_1 - \alpha - (Y_3 - \alpha)]^2 - 2(Y_1 - \alpha - (Y_3 - \alpha))] \right]
\]

\[
= E \left[ (W_{i_1j}W_{i_2j} - \beta^2) ([Y_1 - \alpha - Y_3]^2 - \beta^2 \sigma^2) \right] - 2E[(Y_1 - \alpha)(Y_3 - \alpha) + (Y_3 - \alpha)^2 - \sigma^2]
\]

\[
= E \left[ (W_{i_1j}W_{i_2j} - \beta^2) (Y_1 - \alpha)^2 - \sigma^2 \right] - 2E[(Y_1 - \alpha)^2 - \sigma^2]
\]

\[
= E \left[ (W_{i_1j}W_{i_2j} - \beta^2) (Y_1 - \alpha)^2 - \beta^2 \sigma^2 \right].
\]

The second covariance term of (25) is

\[
\text{Cov} \left[ W_{i_1j}W_{i_2j}, (Y_1 - Y_2)^2 \right] = E \left[ (W_{i_1j}W_{i_2j} - E(W_{i_1j}W_{i_2j})) (Y_1 - Y_2)^2 - E \left( (Y_1 - Y_2)^2 \right) \right]
\]

\[
= E \left\{ (W_{i_1j}W_{i_2j} - \beta^2) \left( (Y_1 - Y_2)^2 - 2 \sigma^2 \right) \right\}
\]

\[
= E \left\{ (W_{i_1j}W_{i_2j} - \beta^2) \left( (Y_1 - Y_2)^2 - 2 \sigma^2 \right) \right\}
\]

\[
= E \left\{ (W_{i_1j}W_{i_2j} - \beta^2) \left( (Y_1 - Y_2)^2 - 2 \sigma^2 \right) \right\}
\]

\[
= E \left\{ (W_{i_1j}W_{i_2j} - \beta^2) \left( (Y_1 - Y_2)^2 - 2 \sigma^2 \right) \right\}
\]

\[
= 2E \left\{ (Y_1 - \alpha)^2 (W_{i_1j} - \beta_1) \beta_2 - \sigma^2 \beta^2 \right\} - 2E [W_{i_1j} (Y_1 - \alpha) W_{i_2j} (Y_2 - \alpha)]
\]

\[
= 2E \left\{ (Y_1 - \alpha)^2 W_{i_1j} \beta_3 - \sigma^2 \beta^2 \right\} - 2E \left[ W_{i_1j} (Y_1 - \alpha) W_{i_2j} (Y_2 - \alpha) \right]
\]

\[
= 2E \left\{ (Y_1 - \alpha)^2 W_{i_1j} \beta_3 - 2 \sigma^2 \beta^2 - 2E [W_{i_1j} (Y_1 - \alpha)]^2 \right\}.
\]
Hence, by (25) we have
\[
\text{Cov} \left( \hat{\sigma}^2, \hat{\tau}^2 \right) = \frac{2(n-2)}{n(n-1)} \sum_{j=1}^{p} \left\{ E \left[ W_{ij} (Y_1 - \alpha)^2 \right] \beta_j - \beta_j^2 \sigma_j^2 \right\} + \frac{1}{n(n-1)} \sum_{j=1}^{p} \left\{ 2E \left[ (Y_1 - \alpha)^2 W_{ij} \right] \beta_j - 2\sigma_j^2 \beta_j^2 - 2 \{ E \left[ W_{ij} (Y_1 - \alpha) \right] \}^2 \right\},
\]
which can be further simplified as
\[
\text{Cov} \left( \hat{\sigma}^2, \hat{\tau}^2 \right) = \frac{2}{n} \left( \pi^T \beta - \tau^2 \sigma^2 \right) - \frac{2}{n(n-1)} \sum_{j=1}^{p} \left\{ E \left[ W_{ij} (Y_1 - \alpha) \right] \right\}^2,
\]
where \( \pi = (\pi_1, \ldots, \pi_p)^T \) and \( \pi_j = E \left[ (Y_1 - \alpha)^2 W_{ij} \right] \).

Plugging (24) and (26) into (23) leads to (9).

\[\blacksquare\]

**Proof of Corollary 1**

Since \( \hat{\sigma}^2 \) is an unbiased estimator of \( \sigma^2 \), it is enough to prove that \( \text{Var}(\hat{\sigma}^2) \xrightarrow{n \to \infty} 0 \). Recall that \( \hat{\sigma}^2 = \hat{\sigma}^2 - \hat{\tau}^2 \). It follows that \( \text{Var}(\hat{\sigma}^2) \leq 2\text{Var}(\hat{\sigma}^2) + 2\text{Var}(\hat{\tau}^2) \). Thus, it is enough to prove that \( \text{Var}(\hat{\sigma}^2) \xrightarrow{n \to \infty} 0 \) and \( \text{Var}(\hat{\tau}^2) \xrightarrow{n \to \infty} 0 \). The former requires, by (24), the assumption that \( \mu_4 \) is bounded and the latter holds true by Proposition 2.

**Remark 1.** The condition \( \frac{\|A\|_F^2}{n^2} \to 0 \) holds in the homoskedastic linear model with the additional assumption that the columns of \( X \) are independent (Livne et al. [2021], Proposition 2). We now show two more examples where the condition \( \frac{\|A\|_F^2}{n^2} \to 0 \) holds without assuming linearity.

1) We show that if \( p/n^2 \to 0 \) and \( Y^2 \leq C \) for some constant \( C \), then \( \frac{\|A\|_F^2}{n^2} \to 0 \). For \( a \in \mathbb{R}^p \) we have,

\[
a^T A a = a^T E \left( XW^T \right) a = E \left( a^T XW^T a \right) = E \left[ (a^T X)^2 \right] \\
= E \left[ \left( \sum_{j=1}^{p} a_j X_{ij} \right)^2 \right] \leq CE \left[ \left( \sum_{j=1}^{p} a_j X_{ij} \right)^2 \right] \\
= C \left( \sum_{j=1}^{p} a_j^2 E \left( X_{ij}^2 \right) \right) + CE \left( \sum_{j \neq j'} a_j a_{j'} E \left( X_{ij} X_{ij'} \right) \right) \\
= C \|a\|^2,
\]

where the last equality follows from \( \Sigma = I \). Now, let \( \lambda_1 A \geq \lambda_2 A \geq \ldots \geq \lambda_p A \) be the eigenvalues of \( A \), and recall that the extrema of the quadratic form \( a^T A a \) satisfies \( \lambda_1 A = \max_a a^T A a \), and hence by (24) we have \( \lambda_1 \leq C \). Now, since \( p/n^2 \to 0 \) by assumption, it follows that

\[
\frac{\|A\|_F^2}{n^2} = \frac{\text{trace} \left( A^2 \right)}{n^2} = \frac{\sum_{j=1}^{p} \lambda_j^2 A}{n^2} \leq \frac{p \lambda_1^2 A}{n^2} \leq \frac{p C^2}{n^2} \to 0.
\]

2) We show that if \( p/n^2 \to 0 \), \( E(Y^4), E(X_{ij}^4) \leq C \) for \( j = 1, \ldots, p \) and \( C \geq 1 \), and the columns of \( X \) are independent,
then \(\frac{\|A\|^2}{n^2}\) → 0. For \(a \in \mathbb{R}^p\) we have by Cauchy–Schwarz,

\[
a^T A a = E \left[ Y^2 \left( \sum_{j=1}^p a_j X_{ij} \right)^2 \right] \leq \left[ E \left( Y_i^4 \right) \right]^{1/2} \left\{ E \left( \sum_{j=1}^p a_j X_{ij} \right)^2 \right\}^{1/2}
\]

\[
\leq C^{1/2} \left\{ \sum_{i_1 \neq i_2 \neq i_3} a_{i_1} a_{i_2} a_{i_3} E \left( X_{i_1} X_{i_2} X_{i_3} X_{i_4} \right) \right\}^{1/2}
\]

\[
\leq C^{1/2} \left\{ \sum_{j=1}^p a_j^4 E \left( X_{ij}^4 \right) + \sum_{j \neq j'} a_j^2 a_{j'}^2 E \left( X_{ij}^2 \right) E \left( X_{ij'}^2 \right) \right\}^{1/2}
\]

\[
\leq C \left\{ \sum_{j=1}^p a_j^4 + \sum_{j \neq j'} a_j^2 a_{j'}^2 \right\}^{1/2}
\]

Notice that since that the columns of \(X\) are independent, the expectation \(E \left( X_{i_1} X_{i_2} X_{i_3} X_{i_4} \right) \) is not zero (up to permutation) when \(j_1 = j_2\) and \(j_3 = j_4\) or when \(j_1 = j_2 = j_3 = j_4\). Also notice we obtained the same result as in (27), and hence \(\frac{\|A\|^2}{n^2}\) → 0 follows by the same arguments as in the previous example.

**Remark 2. Calculations for Equation (13)**

Write,

\[
\text{Cov} \left( \hat{\beta}^2, Z_q \right) = \text{Cov} \left( \frac{1}{n(n-1)} \sum_{i_1 \neq i_2} \sum_{j=1}^p W_{i_1,j} W_{i_2,j} - \frac{1}{n} \sum_{i=1}^n g(X_i) \right)
\]

\[
= \frac{1}{n^2(n-1)} \sum_{i_1 \neq i_2} \sum_{j=1}^p \sum_{i=1}^n E \left( W_{i_1,j} W_{i_2,j} g(X_i) \right)
\]

\[
= \frac{2}{n^2(n-1)} \sum_{i_1 \neq i_2} \sum_{j=1}^p E \left( W_{i_1,j} g_{i_1} \right) E \left( W_{i_2,j} \right)
\]

\[
= \frac{2}{n} \hat{\beta}^T \theta_q,
\]

where \(\theta_q = E \left[ W g(X) \right]\). Also notice that \(\text{Var} \left( Z_q \right) = \frac{1}{n} \sum_{i=1}^n \text{Var} \left( g(X_i) \right) = \frac{\text{Var} \left( g(X) \right)}{n}\). Thus, by (11) we get

\[
c_q = \frac{\text{Cov} \left( \hat{\beta}^2, Z_q \right)}{\text{Var} \left( Z_q \right)} = \frac{2 \hat{\beta}^T \theta_q}{\text{Var} \left( g(X) \right)}
\]

**Proof of Proposition (4)**

We wish to prove that \(\sqrt{n} \left( T_h - T_h^* \right) \xrightarrow{p} 0\). Write,

\[
\sqrt{n} \left( T_h - T_h^* \right) = \sqrt{n} \left[ \left( T_h - T_f \right) + \left( T_f - T_h^* \right) \right].
\]

Thus, we need to show that

\[
\sqrt{n} \left( T_h - T_f \right) \xrightarrow{p} 0,
\]

(29)

\[
\sqrt{n} \left( T_f - T_h^* \right) \xrightarrow{p} 0\),
\]

(30)

\[
\sqrt{n} \left( T_f - T_h^* \right) \xrightarrow{p} 0,
\]

(31)
The proofs of (29) and (30) are essentially the same as the proof of Proposition 5 in Livne et al. (2021). This is true since \( h(X)1_A = f(X)1_A \), where \( A \) denotes the event that the selection procedure \( \delta \) perfectly selects the set \( \Theta \), i.e., \( A \equiv \{ S_\delta = \Theta \} \), and \( 1_A \) denotes the indicator of \( A \).

We now wish to prove (31). Write,

\[
\sqrt{n} \left[T_\delta - T_f\right] = \sqrt{n} \left[\hat{\theta}^2 - \hat{\theta}_f^2 Z_f - (\hat{\theta}^2 - \hat{\theta}_f^2 Z_f)\right] = \sqrt{n}Z_f(\hat{\theta}_f - \hat{\theta}_f).
\]

By Markov and Cauchy-Schwarz inequalities, it is enough to show that

\[
P \left( \left| \sqrt{n}Z_f(\hat{\theta}_f - \hat{\theta}_f) \right| > \varepsilon \right) \leq \frac{E \left\{ \sqrt{n}Z_f(\hat{\theta}_f - \hat{\theta}_f) \right\}^2}{\varepsilon} \leq \frac{nE(Z_f^2)E((\hat{\theta}_f - \hat{\theta}_f)^2)}{\varepsilon} \to 0.
\]

Notice that \( E(Z_f^2) = \text{Var}(Z_f) = \frac{\text{Var}[f(X)]}{n} \) and \( E((\hat{\theta}_f - \hat{\theta}_f)^2) = \text{Var}(\hat{\theta}_f) \), where by (19) we have

\[
\hat{\theta}_f = \frac{\sum_{i_1 \neq i_2} W_{i_1}^2 W_{i_2} f(X_{i_2})}{\text{Var}[f(X)]} \equiv \frac{U}{\text{Var}[f(X)]}.
\]

Hence, it enough to show that

\[
\frac{\text{Var}(U)}{\text{Var}[f(X)]} \to 0. \tag{32}
\]

The variance of \( U \) is

\[
\text{Var}(U) = \text{Var} \left[ \frac{2}{n(n-1)} \sum_{i_1 \neq i_2} \sum_{j=1}^{p} W_{i_1} W_{i_2} f(X_{i_2}) \right]
\]

\[
= \frac{4}{n^2(n-1)^2} \sum_{j,j' = 1}^{p} \sum_{i_1 \neq i_2, i_1 \neq i_3} \text{Cov}[W_{i_1} W_{i_2} f(X_{i_2}), W_{i_3} W_{i_4} f(X_{i_4})]. \tag{33}
\]

The covariance in (33) is different from zero in the following two cases:

1. When \( \{i_1, i_2\} \) is equal to \( \{i_3, i_4\} \).

2. When one of \( \{i_1, i_2\} \) equals to \( \{i_3, i_4\} \) while the other is different.

The first condition includes two different sub-cases and each of those consists of \( n(n-1) \) quadruples \((i_1, i_2, i_3, i_4)\) that satisfy the condition. Similarly, the second condition above includes four different sub-cases and each of those consists of \( n(n-1)(n-2) \) quadruples that satisfy the condition.

We now calculate the covariance for all these six sub-cases.

(1) The covariance when \( i_1 = i_3, i_2 = i_4 \) is

\[
\text{Cov}[W_{i_1} W_{i_2} f(X_{i_2}), W_{i_3} W_{i_4} f(X_{i_4})] = E(W_{i_1} W_{i_2} f^2(X_{i_2})) - E(W_{i_1} W_{i_2} f(X_{i_2})) E(W_{i_3} W_{i_4} f(X_{i_4})) - E(W_{i_1} W_{i_2} f(X_{i_2})) E(W_{i_3} W_{i_4} f(X_{i_4}))
\]

\[
= E(W_{i_1} W_{i_2} f(X_{i_2})) E(W_{i_3} W_{i_4} f^2(X_{i_4}) - \beta_{j,j'} \theta_{j,j'} \theta_{j',j'}),
\]

where recall that \( b \equiv W_f(X) \). Thus, we define

\[
\delta_1 \equiv \sum_{j,j'} \left( E(W_{i_1} W_{i_2} f(X_{i_2})) E(W_{i_3} W_{i_4} f^2(X_{i_4}) - \beta_{j,j'} \theta_{j,j'} \theta_{j',j'}) \right) = E(b^T A b) - (\theta^T \theta)^2. \tag{34}
\]
(2) The covariance when $i_1 = i_4, i_2 = i_3$ is

$$\text{Cov} [W_{i_1}W_{i_2}f(X_{i_2}), W_{i_2}W_{i_3}f(X_{i_3})] = E [W_{i_1}W_{i_2}f(X_{i_2})] E [W_{i_2}W_{i_3}f(X_{i_3})]$$

$$- E(W_{i_1})E [W_{i_2}f(X_{i_2})] E (W_{i_3}f(X_{i_3}))$$

$$= \{E [W_{i_1}W_{i_2}f(X_i)] \}^2 - \beta_j \beta_{j'} \theta_f \theta_{f'}.$$

Thus, we define

$$\delta_2 \equiv \sum_{j,j'} \left\{ [E(W_{i_1}W_{i_2}f(X_i))]^2 - \beta_j \beta_{j'} \theta_f \theta_{f'} \right\} = \|\mathbf{B}\|_F^2 - (\beta^T \theta_f)^2,$$  \hspace{1cm} (35)

where $\mathbf{B} \equiv E (W W^T f(X))$.

(3) Similarly, when $i_1 = i_3, i_2 \neq i_4$ we have

$$\delta_3 \equiv \sum_{j,j'} \left\{ [E(W_{i_1}W_{i_2}f(X_i))] \theta_f \theta_{f'} - \beta_j \beta_{j'} \theta_f \theta_{f'} \right\} = \theta_j^T \mathbf{A} \theta_{f} - (\beta^T \theta_f)^2.$$  \hspace{1cm} (36)

(4)-(5) When $i_1 = i_4, i_2 \neq i_3$ or when $i_2 = i_3, i_1 \neq i_4$ we have

$$\delta_4 = \delta_5 \equiv \sum_{j,j'} \left\{ \beta_j \beta_{j'} E [W_{i_1}W_{i_2}f(X_i)] - \beta_j \beta_{j'} \theta_f \theta_{f'} \right\} = \beta^T \mathbf{B} \beta_f - (\beta^T \theta_f)^2.$$  \hspace{1cm} (37)

(6) When $i_2 = i_4, i_1 \neq i_3,

$$\delta_6 \equiv \sum_{j,j'} \left\{ \beta_j \beta_{j'} E [W_{i_1}W_{i_2}f^2(X_i)] - \beta_j \beta_{j'} \theta_f \theta_{f'} \right\} = \beta^T \mathbf{C} \beta_f - (\beta^T \theta_f)^2,$$

where $\mathbf{C} = E (W W^T f^2(X))$. Thus, plugging-in (34) - (38) into (33) gives

$$\text{Var}(U) = 4 \left\{ \frac{1}{n (n-1)} (\delta_1 + \delta_2) + \frac{(n-2)}{n (n-1)} (\delta_3 + \delta_4 + \delta_5 + \delta_6) \right\}.$$  \hspace{1cm} (39)

Recall that we wish to show that $\frac{\text{Var}(U)}{\text{Var}[f(X)]} \to 0$. Thus, it is enough to show that

$$\frac{(\delta_1 + \delta_2)}{n \text{Var}[f(X)]} \to 0,$$ \hspace{1cm} (40)

and

$$\frac{(\delta_1 + \delta_4 + \delta_5 + \delta_6)}{n \text{Var}[f(X)]} \to 0.$$ \hspace{1cm} (41)

Consider $\delta_1$. For any square matrix $\mathbf{M}$, we denote $\lambda_{1 \mathbf{M}}$ to be the largest eigenvalue of $\mathbf{M}$. Write,

$$\frac{\delta_1}{n \text{Var}[f(X)]} \leq \frac{E (\theta_f^T \mathbf{A} \theta_f)}{n \text{Var}[f(X)]} \leq \frac{\lambda_{1 \mathbf{A}}}{n} \frac{E (\|b\|^2)}{n \text{Var}[f(X)]} \leq \sqrt{\frac{\|\mathbf{A}\|_F^2}{n^2}} \frac{E (\|b\|^2)}{n \text{Var}[f(X)]} \to 0,$$

where the last inequality holds since we assume that $\frac{\|\mathbf{A}\|_F^2}{n^2} \to 0$ and $\frac{E (\|b\|^2)}{n \text{Var}[f(X)]}$ is bounded. Similarly,

$$\frac{\delta_2}{n \text{Var}[f(X)]} \leq \frac{\|\mathbf{B}\|_F^2}{n \text{Var}[f(X)]} \to 0,$$

where $\frac{\|\mathbf{B}\|_F^2}{n \text{Var}[f(X)]} \to 0$ by assumption.

Consider now $\delta_3$. Write,

$$\frac{\delta_3}{n \text{Var}[f(X)]} \leq \frac{\theta_f^T \mathbf{A} \theta_f}{n \text{Var}[f(X)]} \leq \frac{\lambda_{1 \mathbf{A}}}{n} \frac{\|\theta_f\|^2}{\text{Var}[f(X)]} \leq \sqrt{\frac{\|\mathbf{A}\|_F^2}{n^2}} \frac{\|\theta_f\|^2}{n \text{Var}[f(X)]} \to 0,$$
where the above holds since we assume that $\frac{\|g\|^2}{\text{Var}[f(X)]}$ is bounded and $\sqrt{n} \frac{\|A\|^2}{n^2} \to 0$.

Recall that $\delta_4 = \delta_6$. By the Cauchy–Schwarz inequality and the inequality of arithmetic means we have

$$
\frac{\delta_4}{n \text{Var}[f(X)]} \leq \frac{\beta^T \theta}{n \text{Var}[f(X)]} \leq \frac{\lambda_1 \|B\|}{n \text{Var}[f(X)]} \leq \sqrt{\frac{\|B\|^2}{2 (n^2 \text{Var}[f(X)])}} \to 0,
$$

where the expression in (42) converges to zero by similar arguments as shown above.

Similarly for $\delta_6$,

$$
\frac{\delta_6}{n \text{Var}[f(X)]} \leq \frac{\beta^T C \beta}{n \text{Var}[f(X)]} \leq \frac{\lambda_1 C}{n \text{Var}[f(X)]} \leq \sqrt{\frac{\|C\|^2}{2 (n^2 \text{Var}[f(X)])}} \|\beta\|^2 \to 0,
$$

where $\frac{\|C\|^2}{(n \text{Var}[f(X)])^2} \to 0$ and $\tau^2 \equiv \|\beta\|^2 = O(1)$ by assumptions. Hence, (42) follows. This completes the proof that

$$
\sqrt{n} \left[ T_h - T_h \right] \to 0.
$$

Remark 3. We first show that if $Y^2$ and $X^2_{ij}$ are bounded for all $j = 1, ..., p$, $i = 1, ..., n$ and $p/n = O(1)$, then $\frac{E(|b|^2)}{n \text{Var}[f(X)]}$ is bounded. Let $C$ be the upper bound of the maximum of $Y^2$ and $X^2_{ij}$, for $j = 1, ..., p$ and $i = 1, ..., n$. Then,

$$
\frac{E \left( \|b\|^2 \right)}{n \text{Var}[f(X)]} = \frac{\sum_{j=1}^{p} E (b_j^2)}{n \text{Var}[f(X)]} = \frac{\sum_{j=1}^{p} E \left[ X^2_{ij} Y^2 f^2 (X) \right]}{n \text{Var}[f(X)]} \leq \frac{C^2 p E \left[ f^2 (X) \right]}{n \text{Var}[f(X)]} = \frac{C^2 p}{n} = O(1),
$$

where notice that we used the assumption that $p/n = O(1)$.

We now show that under the same assumptions as above, together with the assumptions that $\Theta$ is bounded and $\text{Var}[f(X)] \geq c > 0$, then $\frac{\|B\|^2}{n \text{Var}[f(X)]} \to 0$. Recall that $f (X) = \sum_{j<j'} X_{ij} X_{i'j'}$. Notice that when $\Theta$ is bounded, and when the covariates $X_{ij}$, $i = 1, ..., n$, $j = 1, ..., p$ are bounded, then so is $f (X)$. Let $C$ be the upper bound of $|f(X)|$. Similarly to (27), for $a \in \mathbb{R}^p$, we have

$$
a^T B a = E \left[ a^T W W^T a f (X) \right] \leq E \left[ |f (X)| \left( a^T W \right)^2 \right] \leq CE \left( \left( a^T XY \right)^2 \right)
$$

$$
= CE \left[ \left( \sum_{j=1}^{p} a_j X_j \right)^2 \right] \leq C^2 E \left[ \left( \sum_{j=1}^{p} a_j X_j \right)^2 \right]
$$

$$
= C^2 \sum_{j \neq j'} a_j a_{j'} E \left( X_j X_{j'} \right) + C^2 \sum_{j=1}^{p} a_j^2 E \left( X_j^2 \right) = C^2 \|a\|^2.
$$

It follows that $\frac{\lambda_1 B}{\|B\|^2} = C^2$, and by a similar argument as in (28) we conclude that

$$
\frac{\|B\|^2}{n^2 \text{Var}[f(X)]} \leq \frac{\|B\|^2}{n^2 \text{Var}[f(X)]} \leq \frac{p \lambda_1^2 B}{n^2 \text{Var}[f(X)]} \leq \frac{p C^4}{n^2 c} \to 0,
$$

where recall we assume that $n/p = O(1)$. A similar argument can be used to show that under the above conditions, $\frac{\|C\|^2}{(n \text{Var}[f(X)])^2} \to 0$. 

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Remark 4. We use the following simple selection algorithm \( \delta \):

**Algorithm 3: Covariate selection \( \delta \)**

**Input:** A dataset \((X_{n \times p}, Y_{n \times 1})\).

1. Calculate \( \hat{\beta}^2_1, \ldots, \hat{\beta}^2_p \) where \( \hat{\beta}^2_j \) is given in (5) for \( j = 1, \ldots, p \).

2. Calculate the differences \( \lambda_j = \hat{\beta}^2_j - \hat{\beta}^2_{(j-1)} \) for \( j = 2, \ldots, p \) where \( \hat{\beta}^2_{(1)} < \hat{\beta}^2_{(2)} < \ldots < \hat{\beta}^2_{(p)} \) denotes the order statistics.

3. Select the covariates \( S_\delta = \{ j : \hat{\beta}^2_{(j)} > \hat{\beta}^2_{(j^*)} \} \), where \( j^* = \arg \max_j \lambda_j \).

**Result:** Return \( S_\delta \).

The algorithm above finds the largest gap between the ordered estimated squared coefficients and then uses this gap as a threshold to select a set of coefficients \( S_\delta \subset \{1, \ldots, p\} \). The algorithm works well in scenarios where a relatively large gap truly separates between larger coefficients and the smaller coefficients of the vector \( \beta \).
