Improved Estimators for Semi-supervised High-dimensional Regression Model

Ilan Livne, David Azriel, Yair Goldberg

Technion - Israel Institute of Technology

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Abstract

We study a linear high-dimensional regression model in a semi-supervised setting, where for many observations only the vector of covariates $X$ is given with no responses $Y$. We consider a linear regression model but do not make any sparsity assumptions on the vector of coefficients, and aim at estimating $\text{Var}(Y|X)$. We propose an estimator, which is unbiased, consistent, and asymptotically normal. This estimator can be improved by adding zero-estimators arising from the unlabeled data. Adding zero-estimators does not affect the bias and potentially can reduce the variance. We further illustrate our approach for other estimators, and present an algorithm that improves estimation for any given variance estimator. Our theoretical results are demonstrated in a simulation study.

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

1 Introduction

High-dimensional data analysis, where the number of predictors is larger than the sample size, is a topic of current interest. In such settings, an important goal is to estimate the signal level $\tau^2$ and the noise level $\sigma^2$, i.e., to quantify how much variation in the response variable can be explained by the predictors, versus how much of the variation is left unexplained. For example, in disease classification using DNA microarray data, where the number of potential predictors, say the genotypes, is enormous per each individual, one may wish to understand how disease risk is associated with genotype versus environmental factors.
Estimating the signal and noise levels is important even in a low-dimensional setting. In particular, a statistical model partitions the total variability of the response variable into two components: the variance of the fitted model $\tau^2$, and the variance of the residuals $\sigma^2$. This partition is at the heart of techniques such as ANOVA and linear regression, where $\tau^2$ and $\sigma^2$ might also be commonly referred to as explained versus unexplained variation, or between treatments versus within treatments variation. Moreover, in model selection problems, $\tau^2$ and $\sigma^2$ may be required for computing popular statistics, such as Cp, AIC, BIC and $R^2$. Both $\tau^2$ and $\sigma^2$ are also closely related to other important statistical problems, such as genetic heritability and signal detection. Hence, developing good estimators for these quantities is a desirable goal.

When the number of covariates $p$ is much smaller than the number of observations $n$, and a linear model is assumed, the ordinary least squares (henceforth, OLS) method provides us straightforward estimators for $\tau^2$ and $\sigma^2$. However, when $p > n$, it becomes more challenging to perform inference on $\tau^2$ and $\sigma^2$ without further assumptions, such as sparsity of the coefficients. In practice, the sparsity assumption may be unrealistic for some areas of interest. In this case, considering only a small number of significant coefficient can lead to biases and inaccuracies. One relevant example is the problem of missing heritability, i.e., the gap between heritability estimates from genome-wide-association-studies (GWAS) and the corresponding estimates from twin studies. For example, by 2010, GWAS studies had identified a relatively small number of covariates that collectively explained around 5% of the total variations in the trait height, which is a small fraction compared to 80% of the total variations that were explained by twin studies (Eichler et al., 2010). Identifying all the GWAS covariates affecting a trait, and measuring how much variation they capture, is believed to bridge a significant fraction of the heritability gap. With that in mind, methods that heavily rely on the sparsity assumption may underestimate $\tau^2$ by their nature. We show in this work that in the semi-supervised setting, in which for many observations only the covariates $X$ are given with no responses $Y$, one may consistently estimate the heritability without sparsity assumptions. We use the term semi-supervised setting to describe a setting in which the distribution of $X$ is known. The setting where the distribution of $X$ is only partially known is not part of this work.

Estimating $\tau^2$ and $\sigma^2$ in a high-dimensional regression setting is generally a challenging problem. As mentioned above, the sparsity assumption, which means that only a relatively small number of predictors are relevant, plays an important role in this context. Fan et al. (2012) introduced a refitted cross validation method for estimating $\sigma^2$. Their method includes a two-staged procedure where a variable-selection technique is performed in the first stage, and OLS is used to estimate $\sigma^2$ in the second stage. Sun and Zhang (2012) introduced the scaled lasso algorithm that jointly estimates the noise level and the regression coefficients by
an iterative lasso procedure. Both works provide asymptotic distributional results for their estimators and prove consistency under several assumptions including sparsity. In the context of heritability estimation, Gorfine et al. (2017) presented the HERRA estimator, which is based on the above methods and is also applicable to time-to-event outcomes, in addition to continuous or dichotomous outcomes. Another recent related work is Cai and Guo (2020) that considers, as we do here, a semi-supervised learning setting. In their work, Cai and Guo proposed the CHIVE estimator of $\tau^2$, which integrates both labelled and unlabelled data and works well when the model is sparse. They characterize its limiting distribution and calculate confidence intervals for $\tau^2$. For more related works, see the literature review of Cai and Guo (2020).

Rather than assuming sparsity, or other structural assumptions on the coefficient vector $\beta$, a different approach for high-dimensional inference is to assume some knowledge about the covariates distribution. Dicker (2014) uses the method-of-moments to develop several asymptotically-normal estimators of $\tau^2$ and $\sigma^2$, when the covariates are assumed to be Gaussian. Schwartzman et al. (2019) proposed the GWASH estimator for estimating heritability, which is essentially a modification of one of Dicker’s estimators where the columns of $X$ are standardized. Unlike Dicker, the GWASH estimator can also be computed from typical summary statistics, without accessing the original data. Janson et al. (2017) proposed the EigenPrism procedure to estimate $\tau^2$ and $\sigma^2$. Their method, which is based on singular value decomposition and convex optimization techniques, provides estimates and confidence intervals for normal covariates.

In this paper we introduce a naive estimator of $\tau^2$ and show that it is asymptotically equivalent to Dicker’s estimators when the covariates are normal, an assumption which is relaxed in this work. The naive estimator is also a U-statistic and asymptotically normal. U-statistics can be typically used to obtain uniformly minimum variance unbiased estimators (UMVUE). However, when moments restrictions exist, U-statistics are no longer UMVUE, as shown by Hoeffding (1977). Under the assumed semi-supervised setting, the distribution of $X$ is known (and hence, moments of $X$ are known). Thus, the naive estimator is not UMVUE and it potentially can be improved. We demonstrate how its variance can be reduced by using zero-estimators that incorporate the additional information from the unlabelled data.

The contribution of this paper is threefold. First, we propose a novel approach for improving initial estimators of the signal level $\tau^2$ in the semi-supervised setting without assuming sparsity or normality of the covariates. The key idea of this approach is to use zero-estimators that are correlated with the initial estimator of $\tau^2$ in order to reduce variance without introducing extra bias. Second, we define a new notion of optimality with respect to a linear family of zero-estimators. This allows us to suggest a necessary and sufficient condition for identifying optimal oracle-estimators. We use the term oracle to point out that the specific coefficients
that compose the optimal linear combination of zero-estimators are dependent on the unknown parameters. Third, we suggest two estimators that successfully improve initial estimators of $\tau^2$. We discuss in detail the improvement of the naive estimator and also apply our approach to other estimators. Thus, in fact, we provide an algorithm that has the potential to improve any given estimator of $\tau^2$.

The rest of this work in organized as follows. In Section 2 we describe our setting and introduce the naive estimator. In Section 3 we introduce the zero-estimator approach and suggest a new notion of optimality with respect to linear families of zero-estimators. An optimal oracle estimator of $\tau^2$ is also presented. In Section 4 we apply the zero-estimator approach to improve the naive estimator. We 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, while the proofs are provided in the Appendix.

2 The Naive Estimator

2.1 Preliminaries

We begin with describing our setting and assumptions. Let $(X_1, Y_1), \ldots, (X_n, Y_n)$ be i.i.d. observations drawn from some unknown distribution where $X_i \in \mathbb{R}^p$ and $Y_i \in \mathbb{R}$. We consider a semi-supervised setting, where we have access to infinite i.i.d. observations of the covariates. Thus, we essentially assume we know the covariate distribution. Notice that the assumption of known covariate distribution has already been presented and discussed in the context of high-dimension regression (e.g. Candes et al. 2017 and Janson et al. 2017) without using the term “semi-supervised learning”.

For $i = 1, \ldots, n$ we consider the the linear model

$$Y_i = \beta^T X_i + \epsilon_i,$$

where $E(\epsilon_i|X_i) = 0$ and $E(\epsilon_i^2|X_i) = \sigma^2$. We also assume that the intercept term is zero, which can be achieved in practice by centering the $Y$’s. Let $(X, Y)$ denote a generic observation and let $\sigma_Y^2$ denote the variance of $Y$. Notice that it can be decomposed into signal and noise components,

$$\sigma_Y^2 = \text{Var}(X^T \beta + \epsilon) = \beta^T \text{Cov}(X) \beta + \text{Var}(\epsilon) = \beta^T \Sigma \beta + \sigma^2;$$

where $\text{Var}(\epsilon) = E(\epsilon^2) = \sigma^2$ and $\text{Cov}(X) = \Sigma$. 


The signal component $\tau^2 \equiv \beta^T \Sigma \beta$ can be thought of as the total variance explained by the best linear function of the covariates, while the noise component $\sigma^2$ can be thought of as the variance left unexplained. We assume that $E(X) \equiv \mu$ are known and also that $\Sigma$ is invertible. Therefore, we can apply the linear transformation $X \mapsto \Sigma^{-1/2}(X - \mu)$ and assume w.l.o.g. that $\mu = 0$ and $\Sigma = I$. It follows by (2) that $\sigma_Y^2 = \|\beta\|^2 + \sigma^2$, which implies that in order to evaluate $\sigma^2$, it is enough to estimate both $\sigma_Y^2$ and $\|\beta\|^2$. The former can be easily evaluated from the sample, and the main challenge is to derive an estimator for $\|\beta\|^2$ in the high-dimensional setting.

### 2.2 A Naive Estimator

In order to find an unbiased estimator for $\|\beta\|^2 = \sum_{j=1}^p \beta_j^2$ we first consider the estimation of $\beta_j^2$ for each $j$. A straightforward approach is given as follows: Let $W_{ij} \equiv X_{ij}Y_i$ for $i = 1, ..., n$, and $j = 1, ..., p$. Notice that

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

Now, since $\{E(W_{ij})\}^2 = E(W_{ij}^2) = \text{Var}(W_{ij})$, a natural unbiased estimator for $\beta_j^2$ is

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

where $\bar{W}_j = \frac{1}{n} \sum_{i=1}^n W_{ij}$. Thus, unbiased estimates of $\tau^2 \equiv \|\beta\|^2$ and $\sigma^2$ are given by

$$\hat{\tau}^2 = \sum_{j=1}^p \hat{\beta}_j^2 = \frac{1}{n(n-1)} \sum_{j=1}^p \sum_{i_1 \neq i_2}^n W_{i_1j}W_{i_2j}, \quad \hat{\sigma}^2 = \hat{\sigma}_Y^2 - \hat{\tau}^2,$$

where $\hat{\sigma}_Y^2 = \frac{1}{n} \sum_{i=1}^n (Y_i - \bar{Y})^2$. We use the term Naive to describe $\hat{\tau}^2$ since its construction is relatively simple and straightforward. The Naive estimator was also discussed by Kong and Valiant (2018). A similar estimator was proposed by Dicker (2014). Specifically, let

$$\hat{\tau}^2_{\text{Dicker}} = \frac{\|X^T Y\|^2 - p\|Y\|^2}{n(n + 1)}$$

where $X$ is the $n \times p$ design matrix and $Y = (Y_1, ..., Y_n)^T$. The following lemma shows that $\hat{\tau}^2$ and $\hat{\tau}^2_{\text{Dicker}}$ are asymptotically equivalent under some conditions.

**Lemma 1.** Assume the linear model in (1) and $X_i \overset{i.i.d.}{\sim} N(0, I)$, and that $\varepsilon_1, \ldots, \varepsilon_n \sim N(0, \sigma^2)$. When $\tau^2 + \sigma^2$ is bounded and $p/n$ converges to a constant, then,

$$\sqrt{n}(\hat{\tau}^2 - \hat{\tau}^2_{\text{Dicker}}) \overset{p}{\to} 0.$$
Note that in this paper we are interested in a high-dimensional regression setting and therefore we study the limiting behaviour when $n$ and $p$ go together to $\infty$. Using Corollary 1 from Dicker (2014), which computes the asymptotic variance of $\hat{\tau}^2_{Dicker}$, and the above lemma, we obtain the following corollary.

**Corollary 1.** Under the assumptions of Lemma 1

$$\sqrt{n} \left( \frac{\hat{\tau}^2 - \tau^2}{\psi} \right) \xrightarrow{D} N(0,1),$$

where $\psi = 2 \left\{ 1 + \frac{2}{n} \right\} \left( \sigma^2 + \tau^2 \right)^2 - \sigma^4 + 3\tau^4$.  

The variance of the naive estimator $\hat{\tau}^2$ under model (1) (without assuming normality) is given by the following proposition.

**Proposition 1.** Assume model (1) and additionally that $\beta^T A \beta$ and $\|A\|_F^2$ are finite. Then,

$$\text{Var}(\hat{\tau}^2) = \frac{4(n-2)}{n(n-1)} \left[ \beta^T A \beta - \|\beta\|^4 \right] + \frac{2}{n(n-1)} \left[ \|A\|_F^2 - \|\beta\|^4 \right],$$

where $A = E(W_i W_i^T)$ and $\|A\|_F^2$ denoted the Frobenius norm of $A$.

The following proposition shows that the naive estimator is consistent under some minimal assumptions.

**Proposition 2.** Assume model (1) and additionally that $\tau^2 + \sigma^2 = O(1)$ and $\frac{\|A\|_F^2}{n^2} \rightarrow 0$. Then, $\hat{\tau}^2$ is consistent. Moreover, when the columns of $X$ are independent and both $p/n$ and $E(X_{ij}^4)$ are bounded, then $\frac{\|A\|_F^2}{n^2} \rightarrow 0$ holds and $\hat{\tau}^2$ is $\sqrt{n}$-consistent.

## 3 Oracle Estimator

In this section we introduce the zero-estimator approach and study how it can be used to improve the naive estimator. In Section 3.1 we present the zero-estimator approach and an illustration of this approach is given in Section 3.2. Section 3.3 introduces a new notion of optimality with respect to linear families for zero-estimators. We then find an optimal oracle estimator of $\tau^2$ and calculate its improvement over the naive estimator.

### 3.1 The Zero-Estimator Approach

We describe the approach in general terms. Consider a random variable $V \sim P$, where $P$ belongs to a family of distributions $\mathcal{P}$. Let $g(V)$ be a zero-estimator, i.e., $E_P[g(V)] = 0$ for
all $P \in \mathcal{P}$. Let $T(V)$ be an unbiased estimator of a certain quantity of interest $\theta$. Then, the statistic $U_c(V)$, defined by $U_c(V) = T(V) - cg(V)$ for a fixed constant $c$, is also an unbiased estimator of $\theta$. The variance of $U_c(V)$ is

$$\text{Var}[U_c(V)] = \text{Var}[T(V)] + c^2\text{Var}[g(V)] - 2c \cdot \text{Cov}[T(V), g(V)].$$

Minimizing $\text{Var}[U_c(V)]$ with respect to $c$ yields the minimizer

$$c^* = \frac{\text{Cov}[T(V), g(V)]}{\text{Var}[g(V)]}.$$  

(7)

Notice that $\text{Cov}[T(V), g(V)] \neq 0$ implies $\text{Var}[U_{c^*}(V)] < \text{Var}(T(V))$. In other words, by combining a correlated unbiased estimator of zero with the initial unbiased estimator of $\theta$, one can lower the variance. Note that plugging $c^*$ in (6) reveals how much variance can be potentially reduced,

$$\text{Var}[U_{c^*}(V)] = \text{Var}[T(V)] - [c^*]^2\text{Var}[g(V)]$$

$$= \text{Var}[T(V)] - \frac{\{\text{Cov}[T(V), g(V)]\}^2}{\text{Var}[g(V)]} = (1 - \rho^2)\text{Var}[T(V)],$$

(8)

where $\rho$ is the correlation coefficient between $T(V)$ and $g(V)$. Therefore, it is best to find an unbiased zero-estimator $g(V)$ which is highly correlated with $T(V)$, the initial unbiased estimator of $\theta$. It is important to notice that $c^*$ is an unknown quantity and, therefore, $U_{c^*}$ is not a statistic. However, in practice, one can estimate $c^*$ by some $\hat{c}^*$ and use the approximation $U_{\hat{c}^*}$ instead.

### 3.2 Illustration of the Zero-Estimator Approach

The following example illustrates how the zero-estimator approach can be applied to improve the naive estimator $\hat{\tau}^2$ in the simple linear model setting.

**Example 1** ($p = 1$). Assume model (1) with $X \sim N(0, 1)$. By (8), we wish to find a zero-estimator $g(X)$ which is correlated with $\hat{\tau}^2$. Consider the estimator $U_c = \hat{\tau}^2 + cg(X)$, where $g(X) \equiv \frac{1}{n} \sum_{i=1}^{n} (X_i^2 - 1)$ and $c$ is a fixed constant. The variance of $U_c$ is minimized by $c^* = -2\beta^2$ and one can verify that $\text{Var}(U_{c^*}) = \text{Var}(\hat{\tau}^2) - \frac{8}{n} \beta^4$. For more details see Remark 3 in the Appendix.

The above example illustrates the potential of using additional information that exists in the semi-supervised setting to lower the variance of the initial Naive estimator $\hat{\tau}^2$. However, it also raises the question: Can we achieve a lower variance by adding different zero-estimators? One might attempt to reduce the variance by adding zero-estimators such as $g_k(X) \equiv \frac{1}{n} \sum_{i=1}^{n} X_i^k -$
3.3 Optimal Oracle Estimator

We now define a new oracle unbiased estimator of \( \tau^2 \) and prove that under some regularity assumptions this estimator is optimal with respect to a family of zero-estimators. Here, optimality means that the variance cannot be further reduced by including additional zero-estimators of that given family. We now specifically define our notion of optimality in a general setting.

**Definition 1.** Let \( T \) be an unbiased estimator of \( \theta \) and let \( g_1, g_2, \ldots \) be a sequence of zero-estimators, i.e., \( E_\theta(g_i) = 0 \) for \( i \in \mathbb{N} \) and for all \( \theta \). Let \( G = \left\{ \sum_{k=1}^{m} c_k g_k : c_k \in \mathbb{R}, m \in \mathbb{N} \right\} \) be a family of zero-estimators. For a zero-estimator \( g^* \in G \), we say that \( R^* = T + g^* \) is an optimal oracle estimator (OOE) of \( \theta \) with respect to \( G \) iff \( \text{Var}_\theta[R^*] = \text{Var}_\theta[T + g^*] \leq \text{Var}_\theta[T + g] \) for all \( g \in G \) and for all \( \theta \).

We use the term oracle since \( g^* = \sum_{k=1}^{m} c_k^* g_k \) for some optimal coefficients \( c_1^*, ..., c_m^* \), which are a function of the unknown parameter \( \theta \). The following theorem suggests a necessary and sufficient condition for obtaining an OOE.

**Theorem 1.** Let \( g_m = (g_1, ..., g_m)^T \) be a vector of zero-estimators and assume the covariance matrix \( M = \text{Var}[g_m] \) is positive definite for every \( m \). Then, \( R^* \) is an optimal oracle estimator (OOE) with respect to the family of zero-estimator \( G \) iff \( R^* \) is uncorrelated with every zero-estimator \( g \in G \), i.e., \( \text{Cov}_\theta[R^*, g] = 0 \) for all \( g \in G \) and for all \( \theta \).

Returning to our setting, define the following oracle estimator

\[
T_{\text{oracle}} = \hat{\tau}^2 - 2 \sum_{j=1}^{p} \sum_{j' = 1}^{p} \psi_{jj'},
\]

where \( \psi_{jj'} = \beta_j \beta_{j'} h_{jj'} \) and \( h_{jj'} = \frac{1}{n} \sum_{i=1}^{n} [X_{ij} X_{ij'} - E(X_{ij} X_{ij'})] \), and let the \( G \) be the family of zero-estimators of the form \( g_{k_1...k_p} = \frac{1}{n} \sum_{i=1}^{n} [X_{i1}^{k_1} \cdot \ldots \cdot X_{ip}^{k_p} - E(X_{i1}^{k_1} \cdot \ldots \cdot X_{ip}^{k_p})] \), where \( (k_1, ..., k_p) \in \{0, 1, 2, 3, ..., p \}^p \equiv \mathbb{N}_0^p \). The following proposition shows that \( T_{\text{oracle}} \) is an OOE with respect to \( G \).

**Theorem 2 (General \( p \)).** Assume model (1) and additionally that \( X \) has moments of all orders. Then, the oracle estimator \( T_{\text{oracle}} \) defined in (9) is an OOE of \( \tau^2 \) with respect to \( G \).
Remark 1. For the proof of Theorem 2 and Proposition 1, homoscedasticity of $\epsilon$ is not required.

We now compute the variance reduction of $T_{\text{oracle}}$ with respect to the naive estimator. The following statement is a corollary of Proposition 1.

**Corollary 2.** Assume model (1) and additionally that the columns of $X$ are independent. Then,

\[
\text{Var}(T_{\text{oracle}}) = \text{Var}(\hat{\tau}^2) - \frac{4}{n} \left\{ \sum_{j=1}^{p} \beta_j^4 E(X_{ij}^4 - 1) + 2 \sum_{j \neq j'} \beta_j^2 \beta_{j'}^2 \right\}. \tag{10}
\]

Moreover, in the special case where $X_{i} \sim N(0, I)$. Then, Rewriting (10) yields

\[
\text{Var}(T_{\text{oracle}}) = \text{Var}(\hat{\tau}^2) - \frac{8}{n} \tau^4. \tag{11}
\]

Notice that by Cauchy–Schwarz inequality, since $E(X^2) = 1$ then $E(X^4) \geq 1$, and therefore $\text{Var}(T_{\text{oracle}}) < \text{Var}(\hat{\tau}^2)$. The following example provides intuition about the improvement of $\text{Var}(T_{\text{oracle}})$ over $\text{Var}(\hat{\tau}^2)$.

**Example 2.** Consider a setting where $n = p; \tau^2 = \sigma^2 = 1$ and $X_{i} \sim N(0, I)$. In this case, one can verify by (1) that $\text{Var}(\hat{\tau}^2) = \frac{20}{n} + O(n^{-2})$ and therefore $\text{Var}(T_{\text{oracle}}) = \frac{12}{n} + O(n^{-2})$. In other words: the optimal oracle estimator $T_{\text{oracle}}$ reduces (asymptotically) the variance of the naive estimator by 40%. Moreover, when $p/n$ converges to zero, the reduction is 66%. See Remark 4 in the Appendix for more details about the relative improvement of the optimal oracle estimator.

## 4 Proposed Estimators

In this section we show how to use the zero-estimator approach to derive improved estimators over $\hat{\tau}^2$. In Section 4.1 we show that estimating all $p^2$ optimal coefficients given in (9) may introduce too much variance. Therefore, Sections 4.2 and 4.3 introduce alternative methods to reduce the number of zero-estimators used in estimation.

### 4.1 The cost of estimation

The optimal oracle estimator defined in (11) is based on adding $p^2$ zero-estimators. Therefore, it is reasonable to suggest and study the following estimator instead of the oracle one:

\[
T = \hat{\tau}^2 - 2 \sum_{j=1}^{p} \sum_{j'=1}^{p} \hat{\psi}_{jj'},
\]
where
\[ \hat{\psi}_{jj} = \frac{1}{n(n-1)(n-2)} \sum_{i_1 \neq i_2 \neq i_3} W_{i_1j} W_{i_2j'} [X_{i_1j} X_{i_3j'} - E(X_{i_1j} X_{i_3j'})], \]
is a U-statistics estimator of \( \hat{\psi}_{jj} \equiv \beta_j \beta_{j'} h_{jj'} \). Notice that \( E(\hat{\psi}_{jj}) = 0 \) and that for \( i_1 \neq i_2 \) we have \( E(W_{i_1j} W_{i_2j'}) = \beta_j \beta_{j'} \); thus, \( T \) is an unbiased estimator of \( \tau^2 \) and we wish to check it reduces the variance of naive estimator \( \hat{\tau}^2 \). This is described in the following proposition.

**Proposition 3.** Assume model (1) and additionally that \( \tau^2 + \sigma^2 = O(1) \); \( E(X_i^4) \leq C \) for some positive constant \( C \), and \( p/n = O(1) \). Then,

\[ \text{Var}(T) = \text{Var}(T_{\text{oracle}}) + \frac{8 p^2 \sigma_Y^4}{n^3} + O(n^{-2}) \]

\[ = \text{Var}(\hat{\tau}^2) - \frac{4}{n} \sum_{j=1}^p \beta_j^4 \left[ E(X_i^4) - 1 \right] + \frac{8 p^2 \sigma_Y^4}{n^3} + O(n^{-2}), \]

where \( \sigma_Y^2 \equiv \tau^2 + \sigma^2 \).

Note that the second equation in (12) follows from (10). To build some intuition, consider the case when \( X_i \stackrel{i.i.d.}{\sim} N(0, I) \) and \( p = n \). Then, the last equation can be rewritten as

\[ \text{Var}(T) = \text{Var}(\hat{\tau}^2) + \frac{8}{n} (2\tau^2\sigma^2 + \sigma^4) + O(n^{-2}). \]

Notice that the term \( \frac{8}{n} (2\tau^2\sigma^2 + \sigma^4) \) in (13) reflects the additional variability that comes with the attempt at estimating all \( p^2 \) optimal coefficients. Therefore, the estimator \( T \) fails to improve the naive estimator \( \hat{\tau}^2 \) and a similar result holds for \( p/n \to c \) for some positive constant \( c \). Thus, alternative ways that improve the naive estimator are warranted, which are discussed next.

### 4.2 Improvement with a single zero-estimator

A simple way to improve the naive estimator is by adding only a single zero-estimator. More specifically, let \( U_{c^*} = \hat{\tau}^2 - c^* g_n \) where \( c^* = \frac{\text{Cov}[\hat{\tau}^2, g_n]}{\text{Var}[g_n]} \) and \( g_n \) is some zero-estimator. By (8) we have

\[ \text{Var}[U_{c^*}] = \text{Var}(\hat{\tau}^2) - \frac{\{\text{Cov}[\hat{\tau}^2, g_n]\}^2}{\text{Var}[g_n]}. \]

Notice that \( U_{c^*} \) is an oracle estimator and thus \( c^* \) needs to be estimated in order to eventually construct a non-oracle estimator. Let \( g_n = \frac{1}{n} \sum_{i=1}^n g_i \) be the sample mean of some zero estimators \( g_1, ..., g_n \). By (10), it can be shown that

\[ c^* = \frac{2 \sum_{j=1}^p \beta_j \theta_j}{\text{Var}(g_i)}, \]

where
\[ \hat{\psi}_{jj} = \frac{1}{n(n-1)(n-2)} \sum_{i_1 \neq i_2 \neq i_3} W_{i_1j} W_{i_2j'} [X_{i_1j} X_{i_3j'} - E(X_{i_1j} X_{i_3j'})], \]
where $\theta_j \equiv E(S_{ij})$ and $S_{ij} = W_{ij}g_i$. Notice that $\text{Var}(g_i)$ does not depend on $i$. Derivation of (15) can be found in Remark 5 in the Appendix. Here, we specifically chose $g_i = \sum_{j < j'} X_{ij} X_{ij'}$ as it worked well in the simulations but we do not argue that this is the best choice. Let $T_{c^*} = \hat{\tau}^2 - c^*g_n$ denote the oracle estimator for the specific choice of $g_n$, and where $c^*$ is given in (15). Notice that by (14) we have

$$
\text{Var}(T_{c^*}) = \text{Var}(\hat{\tau}^2) - \Delta_n^2 p \sum_{j=1}^p \beta_j^2 \theta_j^2 n \text{Var}(g_i).
$$

(16)

The following example demonstrates the improvement of $\text{Var}(T_{c^*})$ over $\text{Var}(\hat{\tau}^2)$.

**Example 3** (Example 2 - continued). Consider a setting where $n = p$; $\tau^2 = \sigma^2 = 1$; $X_i \sim N(0, I)$ for $j = 1, \ldots, p$. Notice that this is an extreme non-sparse settings since the signal level $\tau^2$ is uniformly distributed across all $p$ covariates. In this case one can verify that $\text{Var}(T_{c^*}) = \frac{12}{n} + O(n^{-2})$, which is approximately 40% improvement over the naive estimator variance (asymptotically). For more details see Remark 6 in the Appendix.

In the view of (15), a straightforward U-statistic estimator for $c^*$ is

$$
\hat{c}^* = \frac{2}{n(n-1)} \sum_{i \neq j}^p \sum_{j=1}^p W_{ij} S_{ij} \frac{1}{\text{Var}(g_i)},
$$

(17)

where $\text{Var}(g_i)$ is assumed known as it depends only on the marginal distribution of $X$. Thus, we suggest the following estimator

$$
T_{c^*} = \hat{\tau}^2 - \hat{c}^* g_n,
$$

(18)

and prove that $T_{c^*}$ and $T_{c^*}$ are asymptotically equivalent under some conditions.

**Proposition 4.** Assume model (1) and additionally that $\tau^2 + \sigma^2$ and $p/n$ are $O(1)$. Also, for every $j_1, j_2, j_3, j_4$ assume that $E(X_{i,j_1}^2 X_{i,j_2}^2 X_{i,j_3}^2 X_{i,j_4}^2)$ is bounded and that the columns of the design matrix $X$ are independent. Then, $\sqrt{n} \left[ T_{c^*} - T_{c^*} \right] \overset{p}{\to} 0$.

We note that the requirement that the columns of $X$ be independent can be relaxed to some form of weak dependence.

### 4.3 Improvement by selecting small number of covariates

Rather than using a single zero-estimator to improve the naive estimator, we now consider estimating a small number of coefficients of $T_{\text{ oracle}}$. Recall that $T_{\text{ oracle}}$ is based on adding $p^2$ zero estimators to the naive estimator. This estimation comes with high cost in terms of
additional variability as shown is (13). Therefore, it is reasonable to use only a small number of zero estimators. Specifically, let $\mathbf{B} \subset \{1, ..., p\}$ be a fixed set of some indices such that $|\mathbf{B}| \ll p$ and consider the estimator

$$T_{\mathbf{B}} = \hat{\tau}^2 - 2 \sum_{j,j' \in \mathbf{B}} \hat{\psi}_{jj'}.$$  \hfill (19)

By the same argument as in Proposition 3 we now have

$$\text{Var} (T_{\mathbf{B}}) = \text{Var} (\hat{\tau}^2) - \frac{4}{n} \left\{ \sum_{j \in \mathbf{B}} \beta_j^4 [E (X_j^4) - 1] + 2 \sum_{j \neq j' \in \mathbf{B}} \beta_j^2 \beta_j'^2 \right\} + O \left( n^{-2} \right). \hfill (20)$$

Also notice that when $X_i \overset{i.i.d}{\sim} N (0, \mathbf{I})$, (20) can be rewritten as

$$\text{Var} (T_{\mathbf{B}}) = \text{Var} (\hat{\tau}^2) - \frac{8}{n} \tau_{\mathbf{B}}^2 + O (n^{-2}). \hfill (21)$$

where $\tau_{\mathbf{B}}^2 = \sum_{j \in \mathbf{B}} \beta_j^2$. Thus, if $\tau_{\mathbf{B}}^2$ is sufficiently large, one can expect a significant improvement over the naive estimator by using a small number of zero-estimators. For example, when $\tau_{\mathbf{B}}^2 = 0.5$; $p = n$; $\tau^2 = \sigma^2 = 1$, then $T_{\mathbf{B}}$ reduces the Var($\hat{\tau}^2$) by 10%. For more details see Remark 7 in the Appendix.

Notice that we do not assume sparsity of the coefficients. The sparsity assumption essentially ignores covariates that do not belong to the set $\mathbf{B}$. When $\beta_j$’s for $j \notin \mathbf{B}$ contribute much to the signal level $\tau^2 \equiv \| \beta \|^2$, the sparse approach leads to disregarding a significant portion of the signal, while our estimators do account for this as all $p$ covariates are used in $\hat{\tau}^2$.

The following example illustrates some key aspects of our proposed estimators.

**Example 4** (Example 3 - continued). Let $n = p$; $\tau^2 = \sigma^2 = 1$ and $X_i \overset{i.i.d}{\sim} N (0, \mathbf{I})$. Consider the following two extreme scenarios:

1. **non-sparse setting**: The signal level $\tau^2$ is uniformly distributed over all $p$ covariates, i.e., $\beta_j^2 = \frac{1}{p}$ for all $j = 1, ..., p$.

2. **Sparse setting**: the signal level $\tau^2$ is "point mass" distributed over the set $\mathbf{B}$, i.e., $\tau_{\mathbf{B}}^2 = \tau^2$.

Two interesting key points:

1. In the first scenario the estimator $T_{\mathbf{B}}$ has the same asymptotic variance as $\hat{\tau}^2$, while the estimator $T_c$ reduces the variance by approximately 40%.

2. In the second scenario the variance reduction of $T_{\mathbf{B}}$ is approximately 40%, while $T_c$ has the same asymptotic variance as $\hat{\tau}^2$. 

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Interestingly, in this example, the OOE estimator $T_{\text{oracle}}$ asymptotically improves the naive by 40% regardless of the scenario choice, as shown by (11). For more details see Remark 8 in the Appendix.

A desirable set of indices $B$ contains relatively small amount of covariates that capture a significant part of the signal level $\tau^2$. There are different methods to choose the covariates that will be included in $B$, but these are not a primary focus of this work. For more information about covariate selection methods see Zambom and Kim (2018) and Oda et al. (2020) and references therein. In Section 5 below we work with a certain selection algorithm defined there.

We call $\delta$ a covariate selection algorithm if for every dataset $(X_{n \times p}, Y_{n \times 1})$ it chooses a subset of indices $B_{\delta}$ from $\{1, \ldots, p\}$. Our proposed estimator for $\tau^2$, which is based on selecting small number of covariates, is given in Algorithm 1.

### Algorithm 1: Proposed Estimator based on covariate selection

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

1. Calculate the naive estimator $\hat{\tau}^2 = \frac{1}{n(n-1)} \sum_{j=1}^{p} \sum_{i=1, i \neq i_j}^{n} W_{i_1 j}W_{i_2 j}$, where $W_{i j} = X_{i j}Y_i$.

2. Apply algorithm $\gamma$ to $(X, Y)$ to construct $B_{\gamma}$.

3. Calculate the zero-estimator terms:

   $\hat{\psi}_{jj'} \equiv \frac{2}{n(n-1)(n-2)} \sum_{i_1 \neq i_2 \neq i_3} W_{i_1 j}W_{i_2 j'} [X_{i_3 j}X_{i_3 j'} - E(X_{i_3 j}X_{i_3 j'}),$

   for all $j, j' \in B_{\gamma}$.

**Result:** Return $T_\gamma = \hat{\tau}^2 - \sum_{j, j' \in B_{\gamma}} \hat{\psi}_{jj'}$.

Some asymptotic properties of $T_\gamma$ are given by the following proposition.

**Proposition 5.** Assume there is a set $B \equiv \{j : \beta_j^2 > b\}$ where $b$ is a positive constant, such that $|B| = p_0$ where $p_0$ is a fixed constant. Also assume that $\lim_{n \to \infty} n [P \{B \neq B\}]^{1/2} = 0$, and that $E(T_\gamma^4)$ and $E(T_B^3)$ are bounded. Then,

$$\sqrt{n}(T_\gamma - T_B) \xrightarrow{p} 0.$$  

Notice that the requirement $\lim_{n \to \infty} n [P \{B_{\gamma} \neq B\}]^{1/2} = 0$ is stronger than just consistency.  

**Remark 2 (Practical considerations).** Some cautions regarding the estimator $T_\gamma$ need to be considered in practice. When $n$ is insufficiently large, then $B_\gamma$ might be different than $B$ and Proposition 5 no longer holds. Specifically, let $S \cap B_\gamma$ and $B \cap S_\gamma$ be the set of false positive and false negative errors, respectively, where $S = \{1, \ldots, p\} \setminus B$ and $S_\gamma = \{1, \ldots, p\} \setminus B_\gamma$. While false
negatives merely result in not including some potential zero-estimator terms in our proposed estimator, false positives can lead to a substantial bias. This is true since the expected value of a post-selected zero-estimator is not necessarily zero anymore. A common approach to overcome this problem is to randomly split the data into two parts where the first part is used for covariate selection and the second part is used for evaluation of the zero-estimator terms.

4.4 Estimating the variance of the proposed estimators

We now suggest estimators for \( \text{Var}(\hat{\tau}^2) \), \( \text{Var}(T_\gamma) \) and \( \text{Var}(T_{\hat{\nu}}) \). Let

\[
\text{Var}(\hat{\tau}^2) = \frac{4}{n} \left[ \frac{(n-2)}{(n-1)} \left[ \hat{\sigma}_N^2 \hat{\tau}^2 + \hat{\tau}_c^4 \right] + \frac{1}{2(n-1)} \left( p\hat{\sigma}_N^4 + 4\hat{\sigma}_N^2 \hat{\tau}_c^2 + 3\hat{\tau}_c^4 \right) \right],
\]

where \( \hat{\sigma}_N^2 = \frac{1}{n-1} \sum_{i=1}^{n} (Y_i - \bar{Y})^2 \), and \( \hat{\sigma}_N^4 = (\hat{\sigma}_N^2)^2 \). The following proposition shows that \( \text{Var}(\hat{\tau}^2) \) is consistent under some conditions.

Proposition 6. Assume model (1) and additionally that \( \tau^2 + \sigma^2 = O(1) \), \( X_i \overset{i.i.d.}{\sim} N(0, I) \) and \( p/n = O(1) \). Then,

\[
n \left[ \text{Var}(\hat{\tau}^2) - \text{Var}(\tau^2) \right] \xrightarrow{p} 0.
\]

Consider now \( \text{Var}(T_\gamma) \) and let \( \text{Var}(T_\gamma) = \text{Var}(\hat{\tau}^2) - \frac{8}{n} \hat{\tau}_c^4 \hat{\beta}_c^4 \), where \( \hat{\tau}_c^2 = \sum_{j \in B_c} \hat{\beta}_j^2 \) and \( \hat{\tau}_c^4 = (\hat{\tau}_c^2)^2 \). The following propositions shows that \( \text{Var}(T_\gamma) \) is consistent.

Proposition 7. Under the assumptions of Propositions 5 and 6

\[
n \left[ \text{Var}(T_\gamma) - \text{Var}(T_\gamma) \right] \xrightarrow{p} 0.
\]

When normality of the covariates is not assumed, we suggest the following estimators:

\[
\text{Var}(\hat{\tau}^2) = \frac{4}{n} \left[ \frac{(n-2)}{(n-1)} \left[ \hat{\beta}^T A \beta - ||\beta||^4 \right] + \frac{2}{n} \left[ \frac{||A||^2_F - ||\beta||^4}{n-1} \right] \right];
\]

\[
\text{Var}(T_\gamma) = \text{Var}(\hat{\tau}^2) - \frac{4}{n} \left\{ \sum_{j \in B_c} \hat{\beta}_j^4 \left[ E(X_{1j}^4) - 1 \right] + 2 \sum_{j \neq j' \in B_c} \hat{\beta}_j^2 \hat{\beta}_j'^2 \right\};
\]

and

\[
\text{Var}(T_{\hat{\nu}}) = \text{Var}(\hat{\tau}^2) - \frac{2}{n(n-1)} \sum_{i \neq i' \in [1:2]} \sum_{j=1}^{P} W_{i,j} S_{ij} \left[ \frac{1}{n(n-1)} \sum_{i \neq i' \in [1:2]} W_{i,j} S_{ij} \right]^2,
\]

where \( \hat{\beta}^T A \beta = \frac{1}{n(n-1)} \sum_{i_1 \neq i_2 \neq i_3} W_{i_1} (W_{i_2} W_{i_3}^T) W_{i_3} \), \( ||A||^2_F = \frac{1}{n(n-1)} \sum_{i \neq i' \in [1:2]} (W_{i,i}^T W_{i,i'})^2 \); \( ||\beta||^4 = \frac{1}{n(n-1)} \sum_{i_1 \neq i_2 \neq i_3} W_{i,i}^T W_{i,i'}^2 \) are all U-statistics estimators, and \( \hat{\beta}_j^2 \) is given by (3). Although we do not provide here formal proofs, our simulations support that these estimators are consistent under the same assumptions of Proposition 3.
5 Simulations Results

We now provide a simulation study to illustrate our estimators performance. We compare the different estimators that were discussed earlier in this work:

- The naive estimator $\hat{\tau}^2$ which is given in (4).
- The optimal oracle estimator $T_{\text{oracle}}$ which is given in (9).
- The estimator $T_{c^*}$ which is based on adding a single zero-estimator and is given in (18).
- The estimator $T_{\gamma}$ which is based on selecting a small number of covariates and is given by Algorithm 1. Details about the specific selection algorithm we used can be found in Remark 9 in Appendix.

An additional estimator we include in the simulation study is the PSI (Post Selective Inference), which was calculated using the estimateSigma function from the selectiveInference R package. The PSI estimator is based on the LASSO method which assumes sparsity of the coefficients and therefore ignores small coefficients.

We fix $\beta_j^2 = \frac{\tau^2}{B}$ for $j = 1, \ldots, 5$, and $\beta_j^2 = \frac{\tau^2 - \tau^2_{B}}{p-B}$ for $j = 6, \ldots, p$, where $\tau^2$ and $\tau^2_{B}$ vary among different scenarios. The number of observations and covariates is $n = p = 400$, and the residual variance is $\sigma^2 = 1$. For each scenario, we generated 100 independent datasets and estimated $\tau^2$ by using the different estimators. Boxplots of the estimates are plotted in Figure 1 and results of the RMSE are given in Table 1. Code for reproducing the results is available at https://git.io/Jt6bC.

Figure 1 demonstrates that:

- Both of the proposed estimators demonstrate an improvement over the naive estimator in terms of RMSE. For example, when $\tau^2 = 1$ and $\tau^2_{B} = 1/3$, the Single estimator $T_{c^*}$ improve the naive estimator by 17% and when $\tau^2_{B} = 2/3$, the Selection estimator $T_{\gamma}$ improves the naive by 15%. When $\tau^2 = 2$ these improvements are even more substantial.
- As already been suggested in Example 4, the Selection estimator $T_{\gamma}$ works well when $\tau^2_{B}$ is large while the Single estimator $T_{c^*}$ works well when $\tau^2_{B}$ is small.
- The PSI estimator is biased in a non-sparse setting. For example, when $\tau^2_{B} = 1/3$ the PSI has larger RMSE than the proposed estimators. When $\tau^2_{B} = 0.99$ the PSI has low bias therefore and low RMSE. This is not surprising since the PSI estimator is based on the LASSO method which is known to work well when the true model that generates the data is sparse.

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Figure 1: Boxplots representing the estimators distribution. The x-axis stands for $\tau^2_B$. The red dashed is the true value of $\tau^2$. 
Table 1: Summary statistics. An estimate for the standard deviation of RMSE ($\hat{\sigma}_{RMSE}$) was calculated using the delta method. The estimator with the lowest RMSE (excluding the oracle) is in bold.

| $\tau^2_B$ | $\tau^2$ | $n$ | Estimator | Mean | Bias | SE  | RMSE | $1000 \cdot \hat{\sigma}_{RMSE}$ |
|------------|----------|-----|-----------|------|------|-----|------|----------------------------------|
| 33%        | 1        | 400 | Naive     | 1.02 | -0.02| 0.258| 0.258| 19                               |
| 33%        | 1        | 400 | Selection | 1.02 | -0.02| 0.245| 0.244| 18                               |
| 33%        | 1        | 400 | Single    | 0.99 | 0.01 | 0.214| 0.213| 14                               |
| 33%        | 1        | 400 | OOE       | 1.02 | -0.02| 0.193| 0.193| 14                               |
| 33%        | 1        | 400 | PSI       | 0.74 | 0.26 | 0.221| 0.341| 20                               |
| 66%        | 1        | 400 | Naive     | 1.02 | -0.02| 0.259| 0.259| 21                               |
| 66%        | 1        | 400 | Selection | 1.02 | -0.02| 0.22 | 0.219| 18                               |
| 66%        | 1        | 400 | Single    | 1    | 0    | 0.234| 0.233| 18                               |
| 66%        | 1        | 400 | OOE       | 1.02 | -0.02| 0.185| 0.185| 15                               |
| 66%        | 1        | 400 | PSI       | 0.84 | 0.16 | 0.172| 0.231| 13                               |
| 99%        | 1        | 400 | Naive     | 1.02 | -0.02| 0.261| 0.261| 28                               |
| 99%        | 1        | 400 | Selection | 1.01 | -0.01| 0.172| 0.171| 13                               |
| 99%        | 1        | 400 | Single    | 1.01 | -0.01| 0.254| 0.253| 28                               |
| 99%        | 1        | 400 | OOE       | 1.02 | -0.02| 0.17 | 0.171| 15                               |
| 99%        | 1        | 400 | PSI       | 0.98 | 0.02 | 0.157| 0.157| 14                               |
| 33%        | 2        | 400 | Naive     | 2.02 | -0.02| 0.436| 0.435| 33                               |
| 33%        | 2        | 400 | Selection | 2.02 | -0.02| 0.411| 0.41  | 30                               |
| 33%        | 2        | 400 | Single    | 1.96 | 0.04 | 0.342| 0.342| 22                               |
| 33%        | 2        | 400 | OOE       | 2.02 | -0.02| 0.286| 0.286| 21                               |
| 33%        | 2        | 400 | PSI       | 1.65 | 0.35 | 0.395| 0.529| 32                               |
| 66%        | 2        | 400 | Naive     | 2.03 | -0.03| 0.443| 0.441| 38                               |
| 66%        | 2        | 400 | Selection | 2.02 | -0.02| 0.362| 0.36  | 30                               |
| 66%        | 2        | 400 | Single    | 1.98 | 0.02 | 0.393| 0.392| 30                               |
| 66%        | 2        | 400 | OOE       | 2.02 | -0.02| 0.274| 0.273| 22                               |
| 66%        | 2        | 400 | PSI       | 1.74 | 0.26 | 0.268| 0.375| 24                               |
| 99%        | 2        | 400 | Naive     | 2.02 | -0.02| 0.46 | 0.458| 51                               |
| 99%        | 2        | 400 | Selection | 2    | 0    | 0.267| 0.265| 20                               |
| 99%        | 2        | 400 | Single    | 2    | 0    | 0.446| 0.443| 50                               |
| 99%        | 2        | 400 | OOE       | 2.02 | -0.02| 0.251| 0.25  | 22                               |
| 99%        | 2        | 400 | PSI       | 1.97 | 0.03 | 0.243| 0.243| 20                               |

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. The key is to add zero-estimators that are highly correlated with our initial estimator of $\tau^2$; see Equation (8). Unlike the naive es-
timator, which is represented by a closed-form expression, other common estimators, such as the EigenPrism estimator [Janson et al., 2017], are computed numerically and do not have a closed-form representation. That makes the task of finding optimal zero-estimators somewhat more challenging since the zero-estimators’ coefficients also need to be computed numerically. A comprehensive theory that generalizes the zero-estimate approach to other estimators, other than the naive, is beyond the scope of this work. However, here we present a general algorithm that achieves improvement without claiming optimality. The algorithm is based on adding a single zero-estimator as in Section 4.2. The algorithm below approximates the optimal-oracle coefficient $c^*$ given in (7) from bootstrap samples and then, returns a new estimator that is composed of both the initial estimator of $\tau^2$ and a single zero-estimator.

**Algorithm 2: Empirical Estimator**

**Input:** A dataset $(X, Y)$, an initial estimator $\tilde{\tau}^2$, and a selection algorithm $\gamma$.

1. Calculate an initial estimator $\tilde{\tau}^2$ of $\tau^2$.

2. **Bootstrap step:**
   - Resample with replacement $n$ observations from $(X, Y)$.
   - Calculate the initial estimator $\tilde{\tau}^2$ of $\tau^2$.
   - Calculate the zero-estimator $g_n = \frac{1}{n} \sum_{i=1}^{n} g_i$ where $g_i = \sum_{j<j'} X_{ij}X_{ij'}$.

   This procedure is repeated $B$ times in order to produce $(\tilde{\tau}^2)^1, \ldots, (\tilde{\tau}^2)^B$ and $g_n^1, \ldots, g_n^B$.

3. Approximate the coefficient $c^*$ by

   $$\hat{c}^* = \frac{\text{Cov}(\tilde{\tau}^2, g_n)}{\text{Var}(g_n)}$$

   where $\text{Cov}(\cdot)$ denotes the empirical covariance from the bootstrap samples, and $\text{Var}(g_n)$ is known by the semi-supervised setting.

**Result:** Return the empirical estimator $T_{emp} = \tilde{\tau}^2 - \hat{c}^* g_n$.

We now demonstrate the performance of the empirical estimator given by Algorithm 2 together with two initial estimators mentioned earlier: The EigenPrism [Janson et al., 2017] and the PSI which is described in Taylor and Tibshirani (2018) and was used in Section 5. We consider the same setting as in Section 5. Results are given in Tables 2-3 and the code for reproducing the results is available at [https://git.io/Jt6bC](https://git.io/Jt6bC).

Tables 2-3 demonstrate that the standard error of the empirical estimators is equal to or lower than the standard error of the initial estimators, and as $\tau^2$ increases, the improvement over
the initial estimators is more substantial. As in Section 5, the single zero-estimator approach works especially well when \( \tau_B^2 \) is small; otherwise, there is a small or no improvement, but also no additional variance or bias is introduced. This highlights the fact that the zero-estimator approach is not limited to improving only the naive estimator but rather has the potential to improve other estimators as well.

Table 2: Summary statistics equivalent to Table 1 for the EigenPrism estimator.

| \( \tau_B^2 \) | \( \tau^2 \) | \( n \) | Estimator       | Mean | Bias  | SE   | RMSE | 1000 \cdot \sigma_{RMSE} |
|----------------|------------|------|----------------|------|-------|------|------|----------------------------|
| 33%            | 1          | 400  | Eigenprism     | 1.01 | -0.01 | 0.167| 0.166| 13                          |
| 33%            | 1          | 400  | Empirical Eigen| 1.01 | -0.01 | 0.164| 0.163| 15                          |
| 66%            | 1          | 400  | Eigenprism     | 1.01 | -0.01 | 0.17  | 0.17 | 15                          |
| 66%            | 1          | 400  | Empirical Eigen| 1.01 | -0.01 | 0.164| 0.163| 15                          |
| 99%            | 1          | 400  | Eigenprism     | 1.01 | -0.01 | 0.175| 0.174| 15                          |
| 99%            | 1          | 400  | Empirical Eigen| 1.01 | -0.01 | 0.175| 0.174| 15                          |
| 33%            | 2          | 400  | Eigenprism     | 2.01 | -0.01 | 0.245| 0.243| 18                          |
| 33%            | 2          | 400  | Empirical Eigen| 2.01 | -0.01 | 0.247| 0.246| 19                          |
| 66%            | 2          | 400  | Eigenprism     | 2    | 0     | 0.208| 0.207| 19                          |
| 66%            | 2          | 400  | Empirical Eigen| 2    | 0     | 0.231| 0.23  | 24                          |
| 99%            | 2          | 400  | Eigenprism     | 2    | 0     | 0.259| 0.257| 23                          |
| 99%            | 2          | 400  | Empirical Eigen| 2    | 0     | 0.259| 0.257| 23                          |

Table 3: Summary statistics equivalent to Table 1 for the PSI estimator.

| \( \tau_B^2 \) | \( \tau^2 \) | \( n \) | Estimator      | Mean  | Bias  | SE   | RMSE  | 1000 \cdot \sigma_{RMSE} |
|----------------|------------|------|----------------|-------|-------|------|-------|----------------------------|
| 33%            | 1          | 400  | PSI            | 0.74  | 0.26  | 0.221| 0.341 | 20                          |
| 33%            | 1          | 400  | Empirical PSI  | 0.73  | 0.27  | 0.21 | 0.339 | 19                          |
| 66%            | 1          | 400  | PSI            | 0.84  | 0.16  | 0.172| 0.231 | 13                          |
| 66%            | 1          | 400  | Empirical PSI  | 0.84  | 0.16  | 0.163| 0.227 | 12                          |
| 99%            | 1          | 400  | PSI            | 0.98  | 0.02  | 0.157| 0.157 | 14                          |
| 99%            | 1          | 400  | Empirical PSI  | 0.98  | 0.02  | 0.155| 0.155 | 13                          |
| 33%            | 2          | 400  | PSI            | 1.65  | 0.35  | 0.395| 0.529 | 32                          |
| 33%            | 2          | 400  | Empirical PSI  | 1.63  | 0.37  | 0.355| 0.51  | 31                          |
| 66%            | 2          | 400  | PSI            | 1.74  | 0.26  | 0.268| 0.375 | 24                          |
| 66%            | 2          | 400  | Empirical PSI  | 1.73  | 0.27  | 0.251| 0.371 | 24                          |
| 99%            | 2          | 400  | PSI            | 1.97  | 0.03  | 0.243| 0.243 | 20                          |
| 99%            | 2          | 400  | Empirical PSI  | 1.97  | 0.03  | 0.237| 0.238 | 19                          |

7 Discussion

This paper presents a new approach for improving estimation of the explained variance \( \tau^2 \) of a high-dimensional regression model in a semi-supervised setting without assuming sparsity. The
key idea is to use zero-estimator that is correlated with the initial unbiased estimator of $\tau^2$ in order to lower its variance without introducing additional bias. The semi-supervised setting, where the number of observations is much greater than the number of responses, allows us to construct such zero-estimators. We introduced a new notion of optimality with respect to zero-estimators and presented an oracle-estimator that achieves this type of optimality. We proposed two different (non-oracle) estimators that showed a significant reduction, but not optimal, in the asymptotic variance of the naive estimator. Our simulations showed that our approach can be generalized to other types of initial estimators other than the naive estimator.

Many open questions remain for future research. While our proposed estimators improved the naive estimator, it did not achieve the optimal improvement of the oracle estimator. Thus, it remains unclear if and how one can achieve optimal improvement. Moreover, in this work, strong assumption was made about the unsupervised data size, i.e., $N = \infty$. Thus, generalizing the suggested approach by relaxing this assumption to allow for a more general setting with finite $N \gg n$ is a natural direction for future work. A more ambitious future goal would be to extend the suggested approach to generalized linear models (GLM), and specifically to logistic regression. In this case, the concepts of signal and noise levels are less clear and are more challenging to define.

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8 Appendix

Proof of Lemma \[21\]

Notice that \( \mathbf{X}^T \mathbf{Y} = \left( \sum_{i=1}^{n} W_{i1}, \ldots, \sum_{i=1}^{n} W_{ip} \right)^T \) where \( \mathbf{X} \) is the \( n \times p \) design matrix and \( \mathbf{Y} = (Y_1, \ldots, Y_n)^T \). Thus, the naive estimator can be also written as

\[
\hat{\tau}^2 = \frac{1}{n(n-1)} \sum_{i_1 \neq i_2} \sum_{j=1}^{p} W_{i_1j} W_{i_2j} = \frac{\| \mathbf{X}^T \mathbf{Y} \|^2 - \sum_{j=1}^{p} \sum_{i=1}^{n} W_{ij}^2}{n(n-1)}.
\]

The Dicker estimate for \( \tau^2 \) is given by \( \hat{\tau}_{\text{Dicker}}^2 = \frac{\| \mathbf{X}^T \mathbf{Y} \|^2 - p\| \mathbf{Y} \|^2}{n(n+1)} \). We need to prove that root-\( n \) times the difference between the estimators converges in probability to zero, i.e., \( \sqrt{n}(\hat{\tau}_{\text{Dicker}}^2 - \tau^2) \to 0 \). We have,

\[
\sqrt{n}(\hat{\tau}_{\text{Dicker}}^2 - \tau^2) = \sqrt{n} \left( \frac{\| \mathbf{X}^T \mathbf{Y} \|^2 - p\| \mathbf{Y} \|^2}{n(n+1)} - \frac{\| \mathbf{X}^T \mathbf{Y} \|^2 - \sum_{j=1}^{p} \sum_{i=1}^{n} W_{ij}^2}{n(n-1)} \right)
= \sqrt{n} \left( \frac{\sum_{j=1}^{p} \sum_{i=1}^{n} W_{ij}^2}{n(n-1)} - \frac{p\| \mathbf{Y} \|^2}{n(n+1)} - \frac{2\| \mathbf{X}^T \mathbf{Y} \|^2}{n(n-1)(n+1)} \right)
\]

We start with the first term,

\[
n^{-1.5} \left( \sum_{j=1}^{p} \sum_{i=1}^{n} W_{ij}^2 - p\| \mathbf{Y} \|^2 \right) = n^{-1.5} \left( \sum_{j=1}^{p} \sum_{i=1}^{n} Y_{ij}^2 W_{ij}^2 - p \sum_{i=1}^{n} Y_{i}^2 \right)
= n^{-1.5} \left( \sum_{i=1}^{n} Y_{i}^2 \sum_{j=1}^{p} W_{ij}^2 - p \sum_{i=1}^{n} Y_{i}^2 \right)
= n^{-0.5} \sum_{i=1}^{n} Y_{i}^2 \left[ \frac{1}{n} \sum_{j=1}^{p} (X_{ij}^2 - 1) \right] \equiv n^{-0.5} \sum_{i=1}^{n} \omega_i \tag{25}
\]

where \( \omega_i = Y_{i}^2 \left[ \frac{1}{n} \sum_{j} (X_{ij}^2 - 1) \right] \). Notice that \( \omega_i \) depends on \( n \) but this is suppressed in the notation. In order to show that \( n^{-0.5} \sum_{i=1}^{n} \omega_i \to 0 \), it is enough to show that \( E \left( n^{-0.5} \sum_{i=1}^{n} \omega_i \right) \to 0 \) and \( \text{Var} \left( n^{-0.5} \sum_{i=1}^{n} \omega_i \right) \to 0 \). Moreover, since \( E \left( n^{-0.5} \sum_{i=1}^{n} \omega_i \right) = \sqrt{n} E(\omega_i) \) and \( \text{Var} \left( n^{-0.5} \sum_{i=1}^{n} \omega_i \right) = \text{Var}(\omega_i) = E(\omega_i^2) - [E(\omega_i)]^2 \), it is enough to show that \( \sqrt{n} E(\omega_i) \) and \( E(\omega_i^2) \) converge to zero.

Consider now \( \sqrt{n} E(\omega_i) \). By \( \tag{23} \) we have

\[
\sum_{i=1}^{n} \omega_i = \frac{1}{n} \left[ \sum_{j=1}^{p} \sum_{i=1}^{n} W_{ij}^2 - p\| \mathbf{Y} \|^2 \right].
\]

Taking expectation of both sides,

\[
\sum_{i=1}^{n} E(\omega_i) = \frac{1}{n} \left[ \sum_{j=1}^{p} \sum_{i=1}^{n} E(W_{ij}^2) - pE(\| \mathbf{Y} \|^2) \right].
\]
Now, notice that

\[ E(W_{ij}^2) = E[X_i^2(\beta^T X + \epsilon)^2] = \|\beta\|^2 + \sigma^2 + 3\beta_i^2 |E(X_{ij}^4) - 1| = \tau^2 + \sigma^2 + 2\beta_i^2. \]  

(26)

Also notice that \( Y_i^2 / (\sigma^2 + \tau^2) \sim \chi^2_1 \), and hence \( E(\|Y\|^2) = n(\tau^2 + \sigma^2) \). Therefore,

\[
nE(\omega_i) = \frac{1}{n} \left[ \sum_{j=1}^{p} \sum_{i=1}^{n} \left( \tau^2 + \sigma^2 + 2\beta_i^2 \right) - pn \left( \tau^2 + \sigma^2 \right) \right] = \frac{1}{n} \left[ \sum_{i=1}^{n} \left[ p \left( \tau^2 + \sigma^2 \right) + 2\sigma^2_1 - pn \left( \tau^2 + \sigma^2 \right) \right] = 2\tau^2 \]
\]

which implies that \( \sqrt{n}E(\omega_i) = \frac{2\tau}{\sqrt{n}} \to 0 \).

Consider now \( E(\omega_i^2) \). By Cauchy-Schwartz,

\[
E(\omega_i^2) = E \left[ \left( \frac{Y_i}{\sum_j V_{ij}^2} \right)^4 \right] = \left[ E \left( \frac{Y_i}{\sum_j V_{ij}^2} \right)^2 \right]^{1/2} \left[ E \left( \left| \frac{Y_i}{\sum_j V_{ij}^2} \right|^4 \right) \right]^{1/2} \leq \left\{ E \left( \frac{Y_i}{\sum_j V_{ij}^2} \right)^2 \right\}^{1/2} \left\{ E \left( \left| \frac{Y_i}{\sum_j V_{ij}^2} \right|^4 \right) \right\}^{1/2} \leq C_2p, \]

for a positive constant \( C_1 \). In the second case we have \( E(V_{i1}^2 V_{j2} V_{j3} V_{j4}) \) is not 0 when \( j_1 = j_3 \) and \( j_2 = j_4 \) (up to permutations) or when all terms are equal. In the first case we have

\[
\sum_{j \neq j'} E(V_{i1}^2 V_{j2}^2) = \sum_{j \neq j'} \left[ E \left( \frac{Y_i}{\sum_j V_{ij}^2} \right)^2 \right] = p(p-1) \left[ E \left( \left| \frac{Y_i}{\sum_j V_{ij}^2} \right|^2 \right) \right] \leq C_1p^2, \]

for a positive constant \( C_2 \). Hence, as \( p \) and \( n \) have the same order of magnitude, we have

\[
\left\{ E \left( \left( \frac{n-1}{\sum_j V_{ij}^2} \right)^4 \right) \right\}^{1/2} = \left\{ n^{-4} \sum_{j_1,j_2,j_3,j_4} E(V_{i1} V_{j2} V_{j3} V_{j4}) \right\}^{1/2} \leq \left( n^{-4} \cdot O(p^2) \right)^{1/2} \leq K/n, \]

which implies \( E(\omega_i^2) \leq K_1/n \to 0 \), where \( K \) and \( K_1 \) are positive constants. This completes the proof that

\[
n^{-1.5} \left( \sum_{i=1}^{n} \sum_{j=1}^{p} W_{ij}^2 - p\|Y\|^2 \right) \overset{p}{\to} 0. \]

We now move to prove that \( n^{-2.5} \left( \|X^T Y\|^2 \right) \overset{p}{\to} 0 \). By Markov’s inequality, for \( \epsilon > 0 \)

\[
P \left( n^{-2.5} \|X^T Y\|^2 > \epsilon \right) \leq n^{-2.5} E \left( \|X^T Y\|^2 \right) / \epsilon. \]

Thus, it is enough to show that \( n^{-2}E \left( \|X^T Y\|^2 \right) \) is bounded. Notice that

\[
E \left( \|X^T Y\|^2 \right) = \sum_{i_1,i_2,j=1}^{p} E \left( W_{i_1,j} W_{i_2,j} \right) = \sum_{i=1}^{n} \sum_{j=1}^{p} E \left( W_{ij}^2 \right) + \sum_{i \neq i_2} E \left( W_{i1,j} W_{i2,j} \right) \]
\[
= \sum_{i=1}^{n} \sum_{j=1}^{p} \left( \tau^2 + \sigma^2 + 2\beta_i^2 \right) + \sum_{i \neq i_2} \sum_{j=1}^{p} \beta_i^2 = n \left[ p \left( \tau^2 + \sigma^2 \right) + 2\sigma^2_1 \right] + n(n-1) \tau^2 \]
\[
= n \left[ p \left( \tau^2 + \sigma^2 \right) + (n+1) \tau^2 \right].
\]
where we used (26) in the third equality. Therefore, \( n^{-2}E \left( \|XX^TYY^T\|^2 \right) = n^{-1} \left[ p \left( \sigma^2 + \tau^2 \right) + (n + 1) \tau^2 \right] \). Since \( p \) and \( n \) have the same order of magnitude and \( \tau^2 - \sigma^2 \) is bounded by assumption, then \( n^{-2}E \left( \|XX^TYY^T\|^2 \right) \) is also bounded. This completes the proof of \( n^{-2.5} \left( \|XX^TYY^T\|^2 \right) \overset{p}{\rightarrow} 0 \) and hence \( \sqrt{n} \left( \tau_Dicker - \tau^2 \right) \overset{p}{\rightarrow} 0 \).

\[ \text{Proof of Corollary 1} \]
According to Corollary 1 in Dicker (2014), we have
\[
\sqrt{n} \left( \tau_Dicker - \tau^2 \right) \overset{\psi}{\rightarrow} N(0,1),
\]
where \( \psi = 2 \left( 1 + \frac{p}{n} \right) \left( \sigma^2 + \tau^2 \right)^2 - \sigma^4 + 3\tau^4 \), given that \( p/n \) converges to a constant. Therefore, we can write
\[
\sqrt{n} \left( \tau^2 - \tau \right) = \frac{1}{\psi} \left( \sqrt{n} \left( \tau^2 - \tau_Dicker \right) + \sqrt{n} \left( \tau_Dicker - \tau^2 \right) \right),
\]
and obtain \( \sqrt{n} \left( \tau^2 - \tau \right) \overset{\psi}{\rightarrow} N(0,1) \) by Slutsky’s theorem.

\[ \text{Proof of Proposition 1} \]
Let \( W = (W_1, ..., W_p)^T \) and notice that \( \hat{\tau}^2 = \frac{1}{n(n-1)} \sum_{i \neq j} \sum_{i,j} W_{ij}W_{ij} \) is a U-statistic of order 2 with the kernel \( h(w_1, w_2) = w_1 \cdot w_2 = \sum_{j=1}^{p} w_{1j}w_{2j} \), where \( w_i \in \mathbb{R}^p \).

By Theorem 12.3 in van der Vaart (2000),
\[
\text{Var} \left( \hat{\tau}^2 \right) = \frac{4(n-2)}{n(n-1)} \zeta_1 + \frac{2}{n(n-1)} \zeta_2, \tag{27}
\]
where \( \zeta_1 = \text{Cov} \left[ h(W_1, W_2), h(W_1, \tilde{W}_2) \right] \) and \( \zeta_2 = \text{Cov} \left[ h(W_1, W_2), h(W_1, W_2) \right] \) where \( \tilde{W}_2 \) is an independent copy of \( W_2 \). Now, let \( A = E \left( W, W^T \right) \) be a \( p \times p \) matrix and notice that
\[
\zeta_1 = \text{Cov} \left[ h(W_1, W_2), h(W_1, \tilde{W}_2) \right] = \sum_{j,j'} \text{Cov} \left( W_{ij}W_{ij'}, \tilde{W}_{ij'} \right) = \sum_{j,j'} \left( \beta_j \beta_{j'} E \left[ W_{ij}W_{ij'} \right] - \beta_j^2 \beta_{j'}^2 \right) = \beta^T A \beta - \| \beta \|^4
\]
and
\[
\zeta_2 = \text{Cov} \left[ h(W_1, W_2), h(W_1, W_2) \right] = \sum_{j,j'} \text{Cov} \left( W_{ij}W_{ij'}, W_{ij}W_{ij'} \right) = \sum_{j,j'} \left( E \left[ W_{ij}W_{ij'} \right] \right)^2 - \beta_j^2 \beta_{j'}^2 = \|A\|^2_F - \| \beta \|^4,
\]
where \( \|A\|^2_F \) is the Frobenius norm of \( A \). Thus, by rewriting (27) the variance of the naive estimator is given by
\[
\text{Var} \left( \hat{\tau}^2 \right) = \frac{4(n-2)}{n(n-1)} \left[ \beta^T A \beta - \| \beta \|^4 \right] + \frac{2}{n(n-1)} \left[ \|A\|^2_F - \| \beta \|^4 \right]. \tag{28}
\]

\[ \text{Proof of Proposition 2} \]
Notice that \( \hat{\tau}^2 \) is consistent if \( \text{Var}[\hat{\tau}^2] \overset{n \to \infty}{\longrightarrow} 0 \) since \( \hat{\tau}^2 \) is unbiased. Thus, by (28) it is enough to require that
\[
\frac{\beta^T A \beta - \| \beta \|^4}{n(n-1)} \overset{n \to \infty}{\longrightarrow} 0.
\]
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 \(\lambda_1 \geq \ldots \geq \lambda_p\) be the eigenvalues of \(A\) and notice that \(A\) is symmetric. We have that \(n^{-2} \sum_{j=1}^n \lambda_j^2 \leq n^{-2} \sum_{j=1}^n \lambda_j^2 = n^{-2} \text{tr}(A^2) = n^{-2} \|A\|_F^2\) and therefore (iii) implies that \(\frac{A}{n} \xrightarrow{n \to \infty} 0\). Now, \(\frac{1}{n} \beta^T \mathbf{A}\beta \equiv \frac{1}{n} \|\beta\|^2 ((\mathbf{A} / \sqrt{n})^T \mathbf{A} / \sqrt{n}) \leq \frac{1}{n} \|\beta\|^2 \lambda_1 \xrightarrow{n \to \infty} 0\), where the last limit follows from the assumption that \(\tau^2 = O(1)\), and from the fact that \(\frac{A}{n} \xrightarrow{n \to \infty} 0\). We conclude that \(\text{Var}(\hat{\beta}^2) \xrightarrow{n \to \infty} 0\).

We now prove the moreover part, that is, independence of the columns of \(X\) implies that \(\frac{\|A\|_F^2}{n} \xrightarrow{n \to \infty} 0\). By definition we have \(\|A\|_F^2 = \sum_{j,j'}(E(W_{ij}W_{ij'}))\). Notice that when \(j = j'\) we have,

\[
E(W_{ij}^2) = E\left(X_{ij}^2Y_{ij}^2\right) = E\left(X_{ij}^2\left[\beta^T X_i + \varepsilon_i\right]^2\right) = E\left(X_{ij}^2 \left[\sum_{k,k'} \beta_k \beta_{k'} X_{ik} X_{ik'} + 2\beta^T X_i \varepsilon_i + \varepsilon_i^2\right]\right)
\]

\[
= E\left(X_{ij}^2 \sum_{k,k'} \beta_k \beta_{k'} X_{ik} X_{ik'}\right) + 0 + E\left(X_{ij}^2 \varepsilon_i\right)
\]

\[
= E\left(X_{ij}^2 \sum_{k=1}^p \beta_k^2 X_{ik}^2\right) + E\left(X_{ij}^2 \sum_{k \neq k'} \beta_k \beta_{k'} X_{ik} X_{ik'}\right) + \sigma^2 E\left(X_{ij}^2\right)
\]

\[
= \beta_j^2 E\left(X_{ij}^2\right) + \sum_{k \neq j} \beta_k^2 E\left(X_{ij}^2\right) + \sigma^2
\]

Notice that \(E\left(X_{ij}^2 \sum_{k \neq k'} \beta_k \beta_{k'} X_{ik} X_{ik'}\right) = 0\) follows from the assumptions that the columns of \(X\) are independent and \(E(X_{ij}) = 0\) for each \(j\). Also notice that in the third row we used the assumption that \(E(\varepsilon_i^2 | X_i) = \sigma^2\).

Similarly, when \(j \neq j'\),

\[
E(W_{ij}W_{ij'}) = E\left(X_{ij}X_{ij'}Y_{ij}^2\right) = E\left[X_{ij}X_{ij'}\left(\beta^T X_i + \varepsilon_i\right)^2\right] = E\left[X_{ij}X_{ij'}\left(\beta^T X_i + \varepsilon_i\right)^2\right]
\]

\[
= E\left[X_{ij}X_{ij'} \left(\sum_{k,k'} \beta_k \beta_{k'} X_{ik} X_{ik'} + 2\beta^T X_i \varepsilon_i + \varepsilon_i^2\right)\right]
\]

\[
= E\left[X_{ij}X_{ij'} \sum_{k,k'} \beta_k \beta_{k'} X_{ik} X_{ik'}\right] + 0 + E\left(X_{ij}X_{ij'} \varepsilon_i^2\right)
\]

\[
= 2\beta_j \beta_{j'} E\left(X_{ij}^2X_{ij'}^2\right) + 0 + E\left(X_{ij}X_{ij'}\right) E\left(\varepsilon_i^2\right) = 2\beta_j \beta_{j'} E\left(X_{ij}^2\right) E\left(X_{ij'}^2\right) = 2\beta_j \beta_{j'}.
\]

This can be written more compactly as

\[
E(W_{ij}W_{ij'}) = \begin{cases} 2\beta_j \beta_{j'}, & j \neq j' \\ \sigma_j^2 + \beta_j^2 [E(X_{ij}^2) - 1], & j = j' \end{cases}
\]

where \(\sigma_j^2 = \|\beta\|^2 + \sigma^2\). Therefore,

\[
\frac{\|A\|_F^2}{n} = 4 \sum_{j \neq j'} \beta_j^2 \beta_{j'}^2 + \sum_j \left(\sigma_j^2 + \beta_j^2 [E(X_{ij}^2) - 1]\right)^2 \leq 4\|\beta\|^4 + \sum_j \left(\sigma_j^2 + \beta_j^2 [E(X_{ij}^2) - 1]\right)^2 + 2\sigma_j^2 \beta_j^2 [E(X_{ij}^2) - 1]
\]

\[
= p\sigma_j^4 + O(1).
\]

where the last equality holds since \(\sigma_j^2 = \tau^2 + \sigma^2 = O(1),\ E(X_{ij}^2) = O(1)\) and by the Cauchy–Schwarz inequality we have \(\sum_j \beta_j^4 \leq \sum_{j,j'} \beta_j^2 \beta_{j'}^2 = \|\beta\|^4 = O(1)\). Now since \(p/n = O(1)\) then \(\frac{\|A\|_F^2}{n} \to 0\) and we conclude that \(\text{Var}(\hat{\tau}^2) = O(n)\), i.e., \(\hat{\tau}^2\) is \(\sqrt{n}\)-consistent.
Remark 3. Calculations for Example 7

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

\[ = \frac{2}{n^2 (n-1)} \sum_{i_1<i_2} \sum_{i=1}^n \text{Cov} \left( X_{i_1} Y_{i_1} X_{i_2} Y_{i_2}, X_i^2 \right) \]

\[ = \frac{2}{n^2 (n-1)} \sum_{i_1<i_2} \sum_{i=1}^n \left[ E \left( X_{i_1} Y_{i_1} X_{i_2} Y_{i_2} X_i^2 \right) - \beta^2 \right] \]

\[ = \frac{4}{n^2 (n-1)} \sum_{i_1<i_2} \left[ E \left( X_{i_1} Y_{i_1} X_{i_2} Y_{i_2} \right) - \beta \right] \]

\[ = \frac{4\beta}{n^2 (n-1)} \frac{n(n-1)}{2} \left[ E \left( X_{i_1} Y_{i_1} \right) - \beta \right] \]

\[ = \frac{2\beta}{n} \left[ E \left( X^3 Y \right) - \beta \right], \]

where in the third equality we used \( E(X_i^2) = 1 \) and \( E(X_i Y_i) \equiv \beta \). In the fourth equality the expectation is zero for all \( i \neq i_1, i_2 \). Now, since \( X \sim N(0, 1) \) and \( E(\epsilon | X) = 0 \), then

\[ E \left( X^3 Y \right) = E \left( X^3 (\beta X + \epsilon) \right) = \beta E \left( X^4 \right) = 3\beta. \]

Therefore, \( \text{Cov}[\hat{\beta}^2, g(X)] = \frac{4\beta^2}{n} \). Notice that

\[ \text{Var} [g(X)] = \text{Var} \left[ \frac{1}{n} \sum_{i=1}^n (X_i^2 - 1) \right] = \frac{1}{n} \left[ E \left( X^4 \right) - E \left( X^2 \right)^2 \right] = \frac{2}{n}. \]

Therefore, by (7) we get \( \epsilon^* = -2\beta \hat{\beta} \hat{X} \). Plugging-in \( \epsilon^* \) back in (8) yields \( \text{Var}(\hat{\epsilon} \epsilon^*) = \text{Var}(\hat{\tau}^2) - \frac{2}{5}\beta^4 \).

Proof of Theorem 7

1. We now prove the first direction: OOE \( \Rightarrow \text{Cov}[R^*, g] = 0 \) for all \( g \in \mathcal{G} \).

Let \( R^* \equiv T + g^* \) be an OOE for \( \theta \) with respect to the family of zero-estimators \( \mathcal{G} \). By definition, \( \text{Var}[R^*] \leq \text{Var}[T + g] \) for all \( g \in \mathcal{G} \). For every \( g = \sum_{k=1}^m c_k g_k \), define \( \tilde{g} \equiv g - g^* = \sum_{k=1}^m (c_k - c_k^*) g_k = \sum_{k=1}^m \tilde{c}_k g_k \) for some fixed \( m \), and note that \( \tilde{g} \in \mathcal{G} \). Then,

\[ \text{Var}[R^*] \leq \text{Var}[T + g] = \text{Var}[T + g^* + \tilde{g}] = \text{Var}[R^* + \sum_{k=1}^m \tilde{c}_k g_k] \]

\[ = \text{Var}[R^*] + 2 \sum_{k=1}^m \tilde{c}_k \cdot \text{Cov}[R^*, g_k] + \text{Var}[\sum_{k=1}^m \tilde{c}_k g_k]. \]

Therefore, for all \((\tilde{c}_1, \ldots, \tilde{c}_m)\),

\[ 0 \leq 2 \sum_{k=1}^m \tilde{c}_k \cdot \text{Cov}[R^*, g_k] + \text{Var}[\sum_{k=1}^m \tilde{c}_k g_k], \]

which can be represented compactly as

\[ 0 \leq -2\tilde{c}^T b + \text{Var}[\tilde{c}^T g_m] = -2\tilde{c}^T b + \tilde{c}^T M \tilde{c} \equiv f(\tilde{c}), \]

where \( b = -(\text{Cov}[R^*, g_1], ..., \text{Cov}[R^*, g_m])^T, g_m = (g_1, ..., g_m)^T, M = \text{Cov}[g_m] \) and \( \tilde{c} \equiv (\tilde{c}_1, ..., \tilde{c}_m)^T \). Notice that \( f(\tilde{c}) \) is a convex function in \( \tilde{c} \) that satisfies \( f(\tilde{c}) \geq 0 \) for all \( \tilde{c} \). Differentiate \( f(\tilde{c}) \) in order to find its minimum

\[ \nabla f(\tilde{c}) = -2b + 2M \tilde{c} = 0. \]
Assuming $M$ is positive definite and solving for $\tilde{c}$ yields the minimizer $\tilde{c}_{\text{min}} = M^{-1}b$. Plug-in $\tilde{c}_{\text{min}}$ in the (32) yields

$$f(\tilde{c}_{\text{min}}) \equiv -2(M^{-1}b)^Tb + (M^{-1}b)^TM(M^{-1}b) = -b^TM^{-1}b \geq 0. \quad (33)$$

Since, by assumption, $M$ is positive definite, so is $M^{-1}$, i.e., $b^TM^{-1}b > 0$ for all non-zero $b \in \mathbb{R}^m$. Thus, (33) is satisfied only if $b \equiv 0$, i.e., $\text{Cov}[R^*, g_0] = 0$ which also implies $\text{Cov}[R^*, \sum_{i=1}^m c_ig_i] = 0$ for any $c_1, \ldots, c_m \in \mathbb{R}$. Therefore, $\text{Cov}[R^*, g] = 0$ for all $g \in \mathcal{G}$.

2. We now prove the other direction: if $R^*$ is uncorrelated with all zero-estimators of a given family $\mathcal{G}$ then it is an OOE. Let $R^* = T + g^*$ and $R \equiv T + g$ be unbiased estimators of $\theta$, where $g^*, g \in \mathcal{G}$. Define $\tilde{g} \equiv R^* - R = g^* - g$ and notice that $\tilde{g} \in \mathcal{G}$. Since by assumption $R^*$ is uncorrelated with $\tilde{g}$,

$$0 = \text{Cov}[R^*, \tilde{g}] \equiv \text{Cov}[R^*, R^* - R] = \text{Var}[R^*] - \text{Cov}[R^*, R],$$

and hence $\text{Var}[R^*] = \text{Cov}[R^*, R]$. By the Cauchy–Schwarz inequality, $(\text{Cov}[R^*, R])^2 \leq \text{Var}[R^*] \text{Var}[R]$, we conclude that $\text{Var}[R^*] \leq \text{Var}[R] = \text{Var}[T + g]$ for all $g \in \mathcal{G}$.

**Proof of Theorem 2**

We start by proving Theorem 2 for the special case of $p = 2$ and then generalize for $p > 2$. By Theorem 1 we need to show that $\text{Cov}(\text{Torace}, g_{k_1k_2}) = 0$ for all $(k_1, k_2) \in \mathbb{N}_0^2$ where $g_{k_1k_2} = \frac{1}{n} \sum_{i=1}^n \left[ X_{i1}^k X_{i2}^k - E(X_{i1}^k X_{i2}^k) \right]$. Write,

$$\text{Cov}(\text{Torace}, g_{k_1k_2}) = \text{Cov}\left(\tilde{\tau}^2 - 2 \sum_{j=1}^2 \sum_{j' = 1}^2 \psi_{jj'}, g_{k_1k_2}\right) = \text{Cov}\left(\tilde{\tau}^2, g_{k_1k_2}\right) - 2 \sum_{j=1}^2 \sum_{j' = 1}^2 \text{Cov}(\psi_{jj'}, g_{k_1k_2}).$$

Thus, we need to show that

$$\text{Cov}\left(\tilde{\tau}^2, g_{k_1k_2}\right) = 2 \sum_{j=1}^2 \sum_{j' = 1}^2 \text{Cov}(\psi_{jj'}, g_{k_1k_2}). \quad (34)$$

We start with calculating the LHS of (34), namely $\text{Cov}(\tilde{\tau}^2, g_{k_1k_2})$. Recall that $\tilde{\tau}^2 \equiv \hat{\beta}_1^2 + \hat{\beta}_2^2$ and therefore $\text{Cov}[\tilde{\tau}^2, g_{k_1k_2}] = \text{Cov}(\hat{\beta}_1^2, g_{k_1k_2}) + \text{Cov}(\hat{\beta}_2^2, g_{k_1k_2})$. Now, for all $(k_1, k_2) \in \mathbb{N}_0^2$, we have

$$\text{Cov}(\hat{\beta}_1^2, g_{k_1k_2}) \equiv \text{Cov}\left(\frac{2}{n(n-1)} \sum_{i_1 < i_2} W_{i1}W_{i2} \frac{1}{n} \sum_{i=1}^n (X_{i1}^{k_1} X_{i2}^{k_2} - E[X_{i1}^{k_1} X_{i2}^{k_2}])\right)$$

$$= \frac{2}{n^2(n-1)} \sum_{i_1 < i_2} \sum_{i=1}^n \text{Cov}(X_{i1}^1 Y_{i1} X_{i2} X_{i1}^{k_2} X_{i2}^{k_2})$$

$$= \frac{2}{n^2(n-1)} \sum_{i_1 < i_2} \sum_{i=1}^n \left( E[X_{i1}^1 Y_{i1} X_{i2} X_{i1}^{k_2} X_{i2}^{k_2}] - \beta_1^2 E[X_{i1}^{k_1} X_{i2}^{k_2}] \right)$$

$$= \frac{4}{n^2(n-1)} \sum_{i_1 < i_2} \left( E[X_{i1}^1 Y_{i1} X_{i2} X_{i1}^{k_2} X_{i2}^{k_2}] - \beta_1^2 E[X_{i1}^{k_1} X_{i2}^{k_2}] \right)$$

$$= \frac{4}{n^2(n-1)} \sum_{i_1 < i_2} \left( E[X_{i1}^{k_1+1} Y_{i1} X_{i2}^{k_2}] E[X_{i2} Y_{i1}^2] - \beta_1^2 E[X_{i1}^{k_1} X_{i2}^{k_2}] \right)$$

$$= \frac{4}{n^2(n-1)} \sum_{i_1 < i_2} \left( E[X_{i1}^{k_1+1} Y_{i1} X_{i2}^{k_2}] E[X_{i2} Y_{i1}^2] - \beta_1^2 E[X_{i1}^{k_1} X_{i2}^{k_2}] \right)$$

$$= \frac{4}{n^2(n-1)} \sum_{i_1 < i_2} \frac{n(n-1)}{2} \left( E[X_{i1}^{k_1+1} Y_{i1} X_{i2}^{k_2}] E[X_{i2} Y_{i1}^2] - \beta_1^2 E[X_{i1}^{k_1} X_{i2}^{k_2}] \right)$$

$$= \frac{2}{n} \left( E[X_{i2}^{k_1+1} Y_{i1} X_{i2}^{k_2}] \beta_1 - \beta_1^2 E[X_{i1}^{k_1} X_{i2}^{k_2}] \right).$$

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where the calculations can be justified by similar arguments to those presented in (31). We shall use the following notation:

\[
A \equiv E \left[ X_{11}^{k_1+1} X_{12}^{k_2} \right] \\
B \equiv E \left[ X_{11}^{k_1+1} X_{12}^{k_2+1} \right] \\
C \equiv E \left[ X_{11}^{k_1} X_{12}^{k_2} \right] \\
D \equiv E \left[ X_{11}^{k_1} X_{12}^{k_2+2} \right].
\]

Notice that \( A, B, C \) and \( D \) are functions of \((k_1, k_2)\) but this is suppressed in the notation. Write,

\[
E[X_{11}^{k_1+1} X_{12}^{k_2} Y_1] = E[X_{11}^{k_1+1} X_{12}^{k_2} (\beta_1 X_{11} + \beta_2 X_{12} + \epsilon_1)]
= \beta_1 E[X_{11}^{k_1+2} X_{12}^{k_2}] + \beta_2 E[X_{11}^{k_1+1} X_{12}^{k_2+1}] = \beta_1 A + \beta_2 B.
\]

Thus, rewrite (35) and obtain

\[
\text{Cov}[\beta_1^2, g_{k_1 k_2}] = \frac{2}{n} \left( [\beta_1 A + \beta_2 B] \beta_1 - \beta_1^2 C \right). \tag{36}
\]

Similarly, by symmetry,

\[
\text{Cov}[\beta_2^2, g_{k_1 k_2}] = \frac{2}{n} \left( [\beta_2 D + \beta_1 B] \beta_2 - \beta_1^2 C \right). \tag{37}
\]

Using (36) and (37) we get

\[
\text{Cov}[\hat{\beta}_1^2, g_{k_1 k_2}] = \text{Cov}(\beta_1^2, g_{k_1 k_2}) + \text{Cov}(\beta_2^2, g_{k_1 k_2})
= \frac{2}{n} \left( [\beta_1 A + \beta_2 B] \beta_1 - \beta_1^2 C + [\beta_2 D + \beta_1 B] \beta_2 - \beta_1^2 C \right)
= \frac{2}{n} \left( \beta_1^2 A + \beta_2^2 D + 2\beta_1 \beta_2 B - C (\beta_1^2 + \beta_2^2) \right) \tag{38}
= \frac{2}{n} (L_1 + L_2 - L_3).
\]

We now move to calculate the RHS of (34), namely \( \sum_{j=1}^{2} \sum_{j'=1}^{2} \text{Cov}(\psi_{jj'}, g_{k_1 k_2}) \). First, recall that \( h_{jj} \equiv \frac{1}{n} \sum_{i=1}^{n} [X_{ij} X_{ij'} - E(X_{ij} X_{ij'})] \)
and \( h_{k_1 k_2} \equiv \frac{1}{n} \sum_{i=1}^{n} \left[ X_{11}^{k_1} X_{12}^{k_2} - E \left( X_{11}^{k_1} X_{12}^{k_2} \right) \right] \) where \((k_1, k_2)\) \( \in \mathbb{N}_0^k \). Hence, \( h_{11} \equiv \frac{1}{n} \sum_{i=1}^{n} (X_{11}^2 - 1) \) which by definition is also equal to \( g_{20} \). Similarly, we have \( h_{12} = h_{21} = \frac{1}{n} \sum_{i=1}^{n} (X_{11} X_{12}) = g_{11} \) and \( h_{22} = \frac{1}{n} \sum_{i=1}^{n} (X_{12}^2 - 1) = g_{02} \). Thus,

\[
\sum_{j=1}^{2} \sum_{j'=1}^{2} \text{Cov}(\psi_{jj'}, g_{k_1 k_2}) = \sum_{j=1}^{2} \sum_{j'=1}^{2} \beta_j \beta_{j'} \text{Cov}(h_{jj'}, g_{k_1 k_2})
= \beta_{11}^2 \text{Cov}(h_{11}, g_{k_1 k_2}) + 2\beta_{11} \beta_{12} \text{Cov}(h_{12}, g_{k_1 k_2}) + \beta_{12}^2 \text{Cov}(h_{22}, g_{k_1 k_2})
= \beta_{11}^2 \text{Cov}(g_{20}, g_{k_1 k_2}) + 2\beta_{11} \beta_{12} \text{Cov}(g_{11}, g_{k_1 k_2}) + \beta_{12}^2 \text{Cov}(g_{02}, g_{k_1 k_2}). \tag{39}
\]

Now, observe that for every \((k_1, k_2, d_1, d_2) \in \mathbb{N}_0^d \),

\[
\text{Cov}[g_{k_1 k_2}, g_{d_1 d_2}] = \text{Cov} \left( \frac{1}{n} \sum_{i=1}^{n} [X_{11}^{k_1} X_{12}^{k_2} - E(X_{11}^{k_1} X_{12}^{k_2})], \frac{1}{n} \sum_{i=1}^{n} [X_{11}^{d_1} X_{12}^{d_2} - E(X_{11}^{d_1} X_{12}^{d_2})] \right)
= n^{-2} \sum_{i=1}^{n} \sum_{i=1}^{n} \left( E[X_{11}^{k_1} X_{12}^{k_2} X_{11}^{d_1} X_{12}^{d_2}] - E[X_{11}^{k_1} X_{11}^{d_1}] E[X_{12}^{k_2} X_{12}^{d_2}] \right) \tag{40}
= \frac{1}{n} \left( E[X_{11}^{k_1+d_1} X_{12}^{k_2+d_2}] - E[X_{11}^{k_1} X_{12}^{k_2}] E[X_{11}^{d_1} X_{12}^{d_2}] \right),
\]

where the third equality holds since the terms with \( i_1 \neq i_2 \) vanish. It follows from (40) that

\[
\text{Cov}[g_{k_1 k_2}, g_{20}] = \frac{1}{n} \left( E[X_{11}^{k_1+2} X_{12}^{k_2}] - E[X_{11}^{k_1} X_{12}^{k_2}] \right) = \frac{1}{n} (A - C),
\]

\[
\text{Cov}[g_{k_1 k_2}, g_{11}] = \frac{1}{n} E[X_{11}^{k_1+1} X_{12}^{k_2+1}] = \frac{A}{n},
\]

\[
\text{Cov}[g_{k_1 k_2}, g_{02}] = \frac{1}{n} \left( E[X_{11}^{k_1} X_{12}^{k_2+2}] - E[X_{11}^{k_1} X_{12}^{k_2}] \right) = \frac{1}{n} (D - C). \]
Therefore, rewrite (39) to get
\[
2 \sum_{j=1}^{2} \sum_{j'=1}^{2} \text{Cov} (\psi_{jj'}, g_{k_1k_2}) = \frac{2}{n} \left[ \sum_{j=1}^{L_1} \left( \beta_1^2 A + \beta_2^2 D + 2\beta_1\beta_2 B - C \left( \beta_1^2 + \beta_2^2 \right) \right) \right] = \frac{2}{n} (L_1 + L_2 - L_3) \quad (41)
\]
which is exactly the same expression as in (35). Hence, equation (41) follows which completes the proof of Theorem 2 for \( p = 2 \).

We now generalize the proof for \( p > 2 \). Similarly to (41) we want to show that
\[
\text{Cov} \left( \hat{\tau}^2, g_{k_1...k_p} \right) = 2 \sum_{j=1}^{p} \sum_{j'=1}^{p} \text{Cov} \left( \psi_{jj'}, g_{k_1...k_p} \right).
\quad (42)
\]

We begin by calculating the LHS of (42), i.e., the covariance between \( \hat{\tau}^2 \) and \( g_{k_1...k_p} \). By the same type of calculations as in (39), for all \((k_1,...,k_p) \in \mathbb{N}_0^p\) we have
\[
\text{Cov} \left[ \hat{\tau}^2, g_{k_1,...,k_p} \right] = \frac{2}{n} \left\{ \beta_j E \left( X_{ijj}^{k_1+2} \prod_{m \neq j} X_{1m}^{k_m} \right) + \sum_{j \neq j'} \beta_{jj'} \left( X_{ijj}^{k_{j'}+1} \prod_{m \neq j'} X_{0m}^{k_m} \right) \right\} \quad (43)
\]
Summing the above expressions for \( j = 1, \ldots, p \), yields
\[
\text{Cov} \left[ \hat{\tau}^2, g_{k_1,...,k_p} \right] = \sum_{j=1}^{p} \text{Cov} \left[ \hat{\tau}^2, g_{k_1,...,k_p} \right] = \sum_{j=1}^{p} \beta_j \left( X_{ijj}^{k_1+1} \prod_{m \neq j} X_{1m}^{k_m} \right) - \frac{2}{n} (L_1 + L_2 - L_3),
\]
where \( L_1, L_2 \) and \( L_3 \) are just a generalization of the notation given in (35). Again, notice that \( L_1, L_2 \) and \( L_3 \) are functions of \( k_1, ..., k_p \) but this is suppressed in the notation.

We now move to calculate the RHS of (42), namely \[ 2 \sum_{j=1}^{p} \sum_{j'=1}^{p} \text{Cov} \left( \psi_{jj'}, g_{k_1...k_p} \right) \]. Since \( \psi_{jj'} = \beta_j \beta_{jj'}h_{jj'} \) we have
\[
\sum_{j=1}^{p} \sum_{j'=1}^{p} \text{Cov} \left( \psi_{jj'}, g_{k_1...k_p} \right) = \sum_{j=1}^{p} \sum_{j'=1}^{p} \beta_j \beta_{jj'} \text{Cov} \left( h_{jj'}, g_{k_1...k_p} \right). \quad (44)
\]
Again, notice the relationship between \( h_{jj'} \) and \( g_{k_1...k_p} \) : when \( j = j' \) we have \( h_{jj} \equiv \frac{1}{n} \sum_{i=1}^{n} (X_{ij}^2 - 1) = g_{0...0} \) (i.e., the \( j \)-th entry is 2 and all others are 0), and for \( j \neq j' \) we have \( h_{jj'} \equiv \frac{1}{n} \sum_{i=1}^{n} X_{ij}X_{ij'} = g_{0...1...0} \) (i.e., the \( j \)-th and \( j' \)-th entries are 1 and all other entries are 0). Hence,
\[
\sum_{j=1}^{p} \sum_{j'=1}^{p} \text{Cov} \left( \psi_{jj'}, g_{k_1...k_p} \right) = \sum_{j=1}^{p} \sum_{j'=1}^{p} \beta_j \beta_{jj'} \text{Cov} \left( h_{jj'}, g_{k_1...k_p} \right) = \sum_{j=1}^{p} \beta_j^2 \text{Cov} \left( g_{0...0}, g_{k_1...k_p} \right) + \sum_{j \neq j'} \beta_j \beta_{jj'} \text{Cov} \left( g_{0...1...0}, g_{k_1...k_p} \right). \quad (45)
\]
Now, similar to (10), for all pairs of index vectors \((k_1, \ldots, k_p) \in \mathbb{N}_0^p\), and \((k'_1, \ldots, k'_p) \in \mathbb{N}_0^p\)

\[
\text{Cov} \left( g_{k_1, \ldots, k_p}, g_{k'_1, \ldots, k'_p} \right) = \frac{1}{n} \left\{ E \left( \prod_{j=1}^p X_{1j}^{k_j+k'_j} \right) - E \left( \prod_{j=1}^p X_{1j}^{k_j} \right) E \left( \prod_{j=1}^p X_{1j}^{k'_j} \right) \right\} \tag{46}
\]

This implies that

\[
\text{Cov} \left[ g_{0, \ldots, 0}, g_{k_1, \ldots, k_p} \right] = \frac{1}{n} \left[ E \left( X_{1j}^{k_j+2} \prod_{m \neq j} X_{1m}^{k_m} \right) - E \left( \prod_{j=1}^p X_{1j}^{k_j} \right) \right]
\]

and

\[
\text{Cov} \left[ g_{0, \ldots, 1, \ldots, 0}, g_{k_1, \ldots, k_p} \right] = \frac{1}{n} E \left( X_{1j}^{k_j+1} X_{1j'}^{k_{j'}+1} \prod_{m \neq j, j'} X_{1m}^{k_m} \right).
\]

Hence, rewrite (15) to see that

\[
2 \sum_{j=1}^p \sum_{j'=1}^p \text{Cov} \left( \psi_{jj'}, g_{k_1, \ldots, k_p} \right) = 2 \sum_{j=1}^p \beta_j^2 \text{Cov} \left( g_{0, \ldots, 0}, g_{k_1, \ldots, k_p} \right) + 2 \sum_{j \neq j'} \beta_j \beta_{j'} \text{Cov} \left( g_{0, \ldots, 0}, g_{k_1, \ldots, k_p} \right)
\]

\[
= \frac{2}{n} \sum_{j=1}^p \beta_j^2 \left[ E \left( X_{1j}^{k_j+2} \prod_{m \neq j} X_{1m}^{k_m} \right) - E \left( \prod_{j=1}^p X_{1j}^{k_j} \right) \right] + \frac{2}{n} \sum_{j \neq j'} \beta_j \beta_{j'} E \left( X_{1j}^{k_j+1} X_{1j'}^{k_{j'}+1} \prod_{m \neq j, j'} X_{1m}^{k_m} \right)
\]

which is exactly the same expression as in (13). Hence, equation (12) follows which completes the proof of Theorem 2. □

**Proof of Corollary 2**

Write,

\[
\text{Var} \left( T_{\text{oracle}} \right) = \text{Var} \left( \hat{r}^2 - 2 \sum_{j,j'} \psi_{jj'} \right) = \text{Var} \left( \hat{r}^2 \right) - 4 \sum_{j,j'} \beta_j \beta_{j'} \text{Cov} \left( \hat{r}^2, h_{jj'} \right) + 4 \text{Var} \left( \sum_{j,j'} \psi_{jj'} \right). \tag{48}
\]

Consider \( \sum_{j,j'} \beta_j \beta_{j'} \text{Cov} \left( \hat{r}^2, h_{jj'} \right) \). We have

\[
\sum_{j,j'} \beta_j \beta_{j'} \text{Cov} \left( \hat{r}^2, h_{jj'} \right) = \sum_{j=1}^p \beta_j^2 \text{Cov} \left( \hat{r}^2, h_{jj} \right) + \sum_{j \neq j'} \beta_j \beta_{j'} \text{Cov} \left( \hat{r}^2, h_{jj'} \right)
\]

\[
= \sum_{j=1}^p \beta_j^2 \text{Cov} \left( \hat{r}^2, g_{0, \ldots, 0} \right) + \sum_{j \neq j'} \beta_j \beta_{j'} \text{Cov} \left( \hat{r}^2, g_{0, \ldots, 1, \ldots, 0} \right)
\]

\[
= \sum_{j=1}^p \beta_j^2 \left[ \frac{2\beta_j^2}{n} \left( E \left( X_{1j}^2 \right) - 1 \right) \right] + \sum_{j \neq j'} \beta_j \beta_{j'} \left[ \frac{4}{n} \beta_j \beta_{j'} \right]
\]

\[
= \frac{2}{n} \sum_{j=1}^p \beta_j^4 \left[ E \left( X_{1j}^4 \right) - 1 \right] + \frac{4}{n} \sum_{j \neq j'} \beta_j^2 \beta_{j'}^2
\]

where the second and third equality are justified by (15) and (13) respectively. Consider now \( \text{Var} \left( \sum_{j,j'} \psi_{jj'} \right) \). Write,

\[
\text{Var} \left( \sum_{j,j'} \psi_{jj'} \right) = \text{Cov} \left( \sum_{j,j'} \beta_j \beta_{j'} h_{jj'}, \sum_{j,j'} \beta_j \beta_{j'} h_{jj'} \right)
\]

\[
= \sum_{j_1,j_2,j_3,j_4} \beta_{j_1} \beta_{j_2} \beta_{j_3} \beta_{j_4} \text{Cov} \left( h_{j_1,j_2}, h_{j_3,j_4} \right)
\]

\[
= \frac{1}{n^2} \sum_{j_1,j_2,j_3,j_4} \beta_{j_1} \beta_{j_2} \beta_{j_3} \beta_{j_4} \sum_{i_1,i_2} \text{Cov} \left( X_{i_1,j_1} X_{i_2,j_2}, X_{i_3,j_3} X_{i_4,j_4} \right)
\]

\[
= \frac{1}{n^2} \sum_{j_1,j_2,j_3,j_4} \beta_{j_1} \beta_{j_2} \beta_{j_3} \beta_{j_4} \left[ E \left( X_{i_1,j_1} X_{i_2,j_2} X_{i_3,j_3} X_{i_4,j_4} \right) - E \left( X_{i_1,j_1} X_{i_2,j_2} \right) E \left( X_{i_3,j_3} X_{i_4,j_4} \right) \right]
\]

\[
= n^{-2} \sum_{j_1,j_2,j_3,j_4} \beta_{j_1} \beta_{j_2} \beta_{j_3} \beta_{j_4} \sum_{i_1} E \left( X_{i_1,j_1} X_{i_2,j_2} X_{i_3,j_3} X_{i_4,j_4} \right) - E \left( X_{i_1,j_1} X_{i_2,j_2} \right) E \left( X_{i_3,j_3} X_{i_4,j_4} \right)
\]

\[
= \frac{1}{n} \sum_{j_1,j_2,j_3,j_4} \beta_{j_1} \beta_{j_2} \beta_{j_3} \beta_{j_4} \left[ E \left( X_{i_1,j_1} X_{i_2,j_2} X_{i_3,j_3} X_{i_4,j_4} \right) - E \left( X_{i_1,j_1} X_{i_2,j_2} \right) E \left( X_{i_3,j_3} X_{i_4,j_4} \right) \right],
\]

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where the fifth equality holds since the summand is 0 for all \( i_1 \neq i_2 \). The summation is not zero in only three cases:

1) \( j_1 = j_4 \neq j_2 = j_3 \)
2) \( j_1 = j_3 \neq j_2 = j_4 \)
3) \( j_1 = j_2 = j_3 = j_4 \).

For the first two cases the summation equals \( \frac{1}{n} \sum_{j \neq j'} \beta_j^2 \beta_{j'}^2 \). For the third case the summation equals to \( \frac{1}{n} \sum_{j=1}^{n} \beta_j^4 \left[ E \left( X_{i_j}^4 - 1 \right) \right] \).

Overall we have

\[
\text{Var} \left( \sum_{j,j'} \psi_{jj'} \right) = \frac{1}{n} \sum_{j,j'} \beta_j^2 \beta_{j'}^2 + \frac{1}{n} \sum_{j,j'} \beta_j^2 \beta_{j'}^2 + \frac{1}{n} \sum_{j=1}^{n} \beta_j^4 \left[ E \left( X_{i_j}^4 - 1 \right) \right].
\]

Rewrite (5) to get

\[
\text{Var} (T_{\text{oracle}}) = \text{Var} \left( \hat{\tau}^2 \right) - 4 \sum_{j,j'} \beta_j \beta_{j'} \text{Cov} \left( \hat{\tau}^2, h_{jj'} \right) + 4 \text{Var} \left( \sum_{j,j'} \psi_{jj'} \right)
\]

\[
= \text{Var} \left( \hat{\tau}^2 \right) - 4 \left( \sum_{j=1}^{p} \beta_j^4 \left[ E \left( X_{i_j}^4 - 1 \right) \right] \right) + \frac{8}{n - 1} \left( \sum_{j=1}^{n} \beta_j^2 \right)^2
\]

\[
= \text{Var} \left( \hat{\tau}^2 \right) - 4 \left( \sum_{j=1}^{p} \beta_j^4 \left[ E \left( X_{i_j}^4 - 1 \right) \right] \right) + \frac{8}{n - 1} \left( \sum_{j=1}^{n} \beta_j^2 \right)^2 \left( 4 \sigma_Y^2 + 3 \tau^2 \right)
\]

\[
= \text{Var} \left( \hat{\tau}^2 \right) - 4 \left( \sum_{j=1}^{p} \beta_j^4 \left[ E \left( X_{i_j}^4 - 1 \right) \right] \right) + \frac{8}{n - 1} \left( \sum_{j=1}^{n} \beta_j^2 \right)^2 \left( 4 \sigma_Y^2 + 3 \tau^2 \right)
\]

\[
\text{Var}(\hat{\tau}^2) = \frac{20}{n} + O(n^{-2}),
\]

and \( \text{Var}(T_{\text{oracle}}) = \text{Var}(\hat{\tau}^2) - \frac{8}{n} \tau^4 = \frac{12}{n} + O(n^{-2}) \) by (11). More generally, the asymptotic improvement of \( T_{\text{oracle}} \) over the naïve estimator is:

\[
\lim_{n,p \to \infty} \frac{\text{Var}(\hat{\tau}^2) - \text{Var}(T_{\text{oracle}})}{\text{Var}(\hat{\tau}^2)} = \lim_{n,p \to \infty} \frac{4 \left( \frac{n-2}{n-1} \sigma_Y^2 \tau^2 + \tau^4 \right)}{2 \sigma_Y^4 + 3 \tau^2}
\]

\[
= \frac{2}{3 \tau^2} = \frac{40\%}{2 \tau^2}
\]

where we used the fact that \( \sigma_Y^2 = \tau^2 + \sigma^2 = 2 \tau^2 \) in the second equality. Now, notice that when \( p = n \) then the reduction is \( \frac{2}{2 + 2} = 40\% \) and when \( p/n \) converges to zero, the reduction is 66%.

**Proof of Proposition 3**

Write,

\[
\text{Var} (T) = \text{Var} \left( \hat{\tau}^2 - 2 \sum_{j=1}^{p} \sum_{j'=1}^{p} \hat{\psi}_{jj'} \right)
\]

\[
= \text{Var} \left( \hat{\tau}^2 \right) - 4 \text{Cov} \left( \hat{\tau}^2, \sum_{j=1}^{p} \sum_{j'=1}^{p} \hat{\psi}_{jj'} \right) + 4 \text{Var} \left( \sum_{j=1}^{p} \sum_{j'=1}^{p} \hat{\psi}_{jj'} \right).
\]

31
We start with calculating the middle term. Let \( p_n(k) \equiv n(n-1)(n-2) \cdots (n-k) \). Write,

\[
\text{Cov}(\hat{\tau}^2, \sum_{j=1}^{p} \sum_{j'=1}^{p} \hat{\psi}_{jj'}) = \text{Cov}\left( \frac{1}{n(n-1)} \sum_{i_1 \neq j_2, j_3} \sum_{j=1}^{p} W_{i_1 j} W_{i_2 j_3} \left[ X_{i_1, j} X_{i_2, j_3} - E(X_{i_1, j} X_{i_2, j_3}) \right] \right)
\]

\[
= C_n \sum_{i=1}^{p} \sum_{j=1}^{p} \text{Cov} \left( W_{i_1 j} W_{i_2 j_3} \left[ X_{i_1, j} X_{i_2, j_3} - E(X_{i_1, j} X_{i_2, j_3}) \right] \right), \tag{52}
\]

where \( C_n \equiv \frac{1}{p_n(3) p_n(2)} \), \( I \) is the set of all quintuples of indices \( (i_1, i_2, i_3, i_4, i_5) \) such that \( i_1 \neq i_2 \) and \( i_3 \neq i_4 \neq i_5 \), and \( J \) is the set of all triples of indices \( (j_1, j_2, j_3) \). For the set \( I \), there are \( \binom{5}{3} \cdot 3 \cdot 6 \) different cases to consider when one of \( \{i_1, i_2\} \) is equal to one of \( \{i_3, i_4, i_5\} \), and an additional \( \binom{2}{1} \cdot 3 \cdot 6 = 6 \) cases to consider when two of \( \{i_1, i_2\} \) are equal to two of \( \{i_3, i_4, i_5\} \). Similarly, for the set \( J \) there are three cases to consider when only two indices of \( \{j_1, j_2, j_3\} \) are equal to each other, \( e.g., j_1 = j_2 \neq j_3 \); one case to consider when no pair of indices is equal to each other and; one case to consider when all three indices are equal. Thus, there are total of \((6+6) \times (3+1+1) = 60 \) cases to consider. Here we demonstrate only one such case. Let \( I_1 = \{(i_1, \ldots, i_5) : i_1 = i_5 \neq i_2 \neq i_3 \neq i_4\} \) and \( J_1 = \{(j_1, j_2, j_3) : j_1 = j_2 = j_3\} \).

Write,

\[
C_n \sum_{i=1}^{p} \sum_{j=1}^{p} \text{Cov} \left( W_{i_1, j} W_{i_2, j_3} \left[ X_{i_1, j} X_{i_2, j_3} - E(X_{i_1, j} X_{i_2, j_3}) \right] \right)
\]

\[
= C_n \sum_{i=1}^{p} \sum_{j=1}^{p} \text{Cov} \left( W_{i_1, j} W_{i_2, j_3} \left[ X_{i_1, j} X_{i_2, j_3} - E(X_{i_1, j} X_{i_2, j_3}) \right] \right) \tag{53}
\]

Now, notice that

\[
E \left[ X_{i_1} \left( X_{i_2} - 1 \right) \right] = E \left[ X_{i_1} Y_j \left( X_{i_2} - 1 \right) \right] = E \left[ X_{i_1} Y_j \left( \beta_x^T X + \epsilon_i \right) \right] - \beta_j
\]

\[
= \beta_j E \left( X_{i_1}^3 \right) - \beta_j
\]

\[
= \beta_j [E(X_{i_1}^4) - 1]. \tag{54}
\]

Rewrite \(53\) to get

\[
C_n \sum_{i=1}^{p} \sum_{j=1}^{p} \beta_j^4 \left[ W_{i_1, j} \left( X_{i_2} - 1 \right) \right] = C_n \sum_{i=1}^{p} \sum_{j=1}^{p} \beta_j^4 \left[ \beta_j [E(X_{i_1}^4) - 1] \right]
\]

\[
= \frac{p_n(3)}{p_n(1) \cdot p_n(2)} \sum_{j=1}^{p} \beta_j^4 [E(X_{i_2}^4) - 1]
\]

\[
= \frac{(n-3)}{n(n-1)} \sum_{j=1}^{p} \beta_j^4 [E(X_{i_2}^4) - 1]
\]

\[
= \frac{1}{n} \sum_{j=1}^{p} \beta_j^4 [E(X_{i_2}^4) - 1] + O(n^{-2}),
\]

where we used \(54\) to justify the first equality. By the same type of calculation, one can compute the covariance in \(52\) over all 60 and obtain that

\[
\text{Cov}(\hat{\tau}^2, \sum_{j=1}^{p} \sum_{j'=1}^{p} \hat{\psi}_{jj'}) = \frac{2}{n} \left( \sum_{j=1}^{p} \beta_j^4 \left[ E \left( X_{i_1}^4 - 1 \right) \right] + 2 \sum_{j \neq j'} \beta_j^2 \beta_j^2 \right) + O \left( n^{-2} \right). \tag{55}
\]
We now move to calculate the last term of (51). Recall that

\[ \hat{\psi}_{jj'} = \frac{1}{n (n-1) (n-2)} \sum_{i_1 \neq i_2 \neq i_3} W_{i_1 j} W_{i_2 j'} [X_{i_3 j} X_{i_3 j'} - E(X_{i_3 j} X_{i_3 j'})]. \]

Therefore,

\[
\text{Var}(\sum_{j=1}^p \sum_{j'=1}^p \hat{\psi}_{jj'}) = \sum_j \text{Cov} \left( \hat{\psi}_{j_1 j_2}, \hat{\psi}_{j_3 j_4} \right) \\
= \frac{1}{[n (n-1) (n-2)]^2} \sum_j \text{Cov} \left( \sum_{i_1 \neq i_2 \neq i_3} W_{i_1 j_1} W_{i_2 j_2} X_{i_3 j_1} X_{i_3 j_2}, \sum_{i_1 \neq i_2 \neq i_3} W_{i_1 j_2} W_{i_2 j_4} X_{i_3 j_3} X_{i_3 j_4} \right) \\
= \frac{1}{3^4} (2) \sum_j \sum_i \text{Cov} \left( W_{i_1 j_1} W_{i_2 j_2} X_{i_3 j_1} X_{i_3 j_2}, W_{i_4 j_3} W_{i_5 j_4} X_{i_6 j_3} X_{i_6 j_4} \right),
\]

where \( J \) is now defined to be the set of all quadruples \((j_1, j_2, j_3, j_4)\), and \( I \) is now defined to be the set of all sextuples \((i_1, ..., i_6)\) such that \(i_1 \neq i_2 \neq i_3 \neq i_4 \neq i_5 \neq i_6\). For the set \( I \), there are three different cases to consider: (1) when one of \( \{i_1, i_2, i_3\} \) is equal to one of \( \{i_4, i_5, i_6\} \); (2) when two of \( \{i_1, i_2, i_3\} \) are equal to two of \( \{i_4, i_5, i_6\} \); and (3) when \( \{i_1, i_2, i_3\} \) are equal to \( \{i_4, i_5, i_6\} \). There are \( \binom{6}{3} \cdot 3 = 9 \) options for the first case, \( \binom{6}{3} \cdot 3! = 18 \) for the second case, and \( \binom{6}{3} \cdot 3! = 6 \) options for the third case. For the set \( J \), there are five different cases to consider: (1) when there is only one pair of equal indices (e.g., \( j_1 = j_2 \neq j_3 \neq j_4 \)); (2) when there are two pairs of equal indices (e.g., \( j_1 = j_2 \neq j_3 = j_4 \)); (3) when only three indices are equal (e.g., \( j_1 = j_2 = j_3 \neq j_4 \)); (4) when all four indices are equal; and (5) all four indices are different from each other. Note that there are \( \binom{4}{2} = 6 \) combinations for the first case, \( \binom{4}{2} = 6 \) for the second case, \( \binom{4}{3} = 4 \) combinations for the third case, and a single combination for each of the last two cases. Thus, there are total of \((9 + 18 + 6) \times (6 + 6 + 4 + 1 + 1) = 594\) Again we demonstrate only one such calculation. Let \( I_2 = \{(i_1, ..., i_6) : i_1 = i_2 = i_3 = i_5 = i_6\} \) and \( I_2 = \{(j_1, j_2, j_3, j_4) : j_1 = j_3 \neq j_2 = j_4\} \). In the view of (51),

\[
p_n^{-2} (2) \sum_{j_2} \sum_{j_2} \text{Cov} \left( W_{i_1 j_1} W_{i_2 j_2} X_{i_3 j_1} X_{i_3 j_2}, W_{i_4 j_3} W_{i_5 j_4} X_{i_6 j_3} X_{i_6 j_4} \right) = \\
p_n^{-2} (2) \sum_{j_2} \sum_{j_2} \text{Cov} \left( W_{i_1 j_1} W_{i_2 j_2} X_{i_3 j_1} X_{i_3 j_2}, W_{i_1 j_1} W_{i_2 j_2} X_{i_3 j_3} X_{i_3 j_4} \right) \\
= p_n^{-2} (2) \sum_{j_2} \sum_{j_2} E \left( W_{i_1 j_1} \right) E \left( W_{i_2 j_2} \right) E \left( X_{i_3 j_1} \right) E \left( X_{i_3 j_2} \right) \\
= p_n^{-2} (2) \sum_{j_2} \sum_{j_2} \left( \sigma_{i_1}^2 + \beta_{i_1}^2 \left( \text{Var} \left( X_{i_3 j_1} \right) - 1 \right) \right) \left( \sigma_{i_2}^2 + \beta_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_2} \right) - 1 \right) \right) \\
\leq p_n^{-2} (2) \sum_{j_2} \sum_{j_2} \left( \sigma_{i_1}^2 + \beta_{i_1}^2 \left( \text{Var} \left( X_{i_3 j_1} \right) - 1 \right) \right) \left( \sigma_{i_2}^2 + \beta_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_2} \right) - 1 \right) \right) \\
= p_n^{-1} (2) \sum_{j_1 \neq j_2} \left[ \sigma_{i_1}^2 + \sigma_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_1} \right) - 1 \right) \right] \left( \beta_{i_1}^2 + \beta_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_2} \right) - 1 \right) \right) \\
\leq p_n^{-1} (2) \left[ (p - 1) \sigma_{i_1}^2 + \sigma_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_1} \right) - 1 \right) \right] \left( \beta_{i_1}^2 + \beta_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_2} \right) - 1 \right) \right) \\
\leq p_n^{-1} (2) \left[ (p - 1) \sigma_{i_1}^2 + \sigma_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_1} \right) - 1 \right) \right] \left( \beta_{i_1}^2 + \beta_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_2} \right) - 1 \right) \right) \\
\leq p_n^{-1} (2) \left[ (p - 1) \sigma_{i_1}^2 + \sigma_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_1} \right) - 1 \right) \right] \left( \beta_{i_1}^2 + \beta_{i_2}^2 \left( \text{Var} \left( X_{i_3 j_2} \right) - 1 \right) \right),
\]

where the fourth equality we use \( E \left( W_{i_1 j_1} \right) = \sigma_{i_1}^2 + \beta_{i_1}^2 \left( \text{Var} \left( X_{i_3 j_1} \right) - 1 \right) \), which is given by (20), and in the fifth equality we used the assumption that \( E(X_{i_3 j_i}^2) \leq C \) for some positive \( C \). Since we assume \( p/n = O(1) \), the above expression can be further simplified to \( \frac{p \sigma_{i_1}^2}{n} + O \left( \frac{1}{n^2} \right) \).
By the same type of calculation, one can compute the covariance in (56) over all 594 cases and obtain that
\[
\text{Var}\left(\sum_{j=1}^{p} \sum_{j' \neq 1} \psi_{jj'}\right) = \frac{1}{n} \left\{ \sum_{j=1}^{p} \beta_{j}^{4} \left[ E \left( X_{1j}^{4} - 1 \right) \right] + 2 \sum_{j \neq j'} \beta_{j}^{2} \beta_{j'}^{2} \right\} + \frac{2p^{2} \sigma_{y}^{4}}{n^{3}} + O \left( n^{-2} \right).
\] (57)

Lastly, plug-in (55) and (57) into (53) to get
\[
\text{Var}(T) = \text{Var}\left(\hat{\tau}^{2}\right) - 4\text{Cov}\left(\hat{\tau}^{2}, \sum_{j=1}^{p} \sum_{j' \neq 1} \hat{\psi}_{jj'}\right) + 4\text{Var}\left(\sum_{j=1}^{p} \sum_{j' \neq 1} \hat{\psi}_{jj'}\right)
\]
\[
= \text{Var}\left(\hat{\tau}^{2}\right) - 4 \left( \frac{2}{n} \left\{ \sum_{j=1}^{p} \beta_{j}^{4} \left[ E \left( X_{1j}^{4} - 1 \right) \right] + 2 \sum_{j \neq j'} \beta_{j}^{2} \beta_{j'}^{2} \right\} \right)
\]
\[
+ 4 \left( \frac{1}{n} \left\{ \sum_{j=1}^{p} \beta_{j}^{4} \left[ E \left( X_{1j}^{4} - 1 \right) \right] + 2 \sum_{j \neq j'} \beta_{j}^{2} \beta_{j'}^{2} \right\} + \frac{2p^{2} \sigma_{y}^{4}}{n^{3}} \right) + O \left( n^{-2} \right)
\]
\[
= \text{Var}\left(\hat{\tau}^{2}\right) - \frac{4}{n} \left\{ \sum_{j=1}^{p} \beta_{j}^{4} \left[ E \left( X_{1j}^{4} - 1 \right) \right] + 2 \sum_{j \neq j'} \beta_{j}^{2} \beta_{j'}^{2} \right\} + \frac{8p^{2} \sigma_{y}^{4}}{n^{3}} + O(n^{-2})
\]
\[
= \text{Var}(T_{\text{oracle}}) + \frac{4p^{2} \sigma_{y}^{4}}{n^{3}} + O \left( n^{-2} \right),
\]
where the last equality holds by (11).

\textbf{Remark 5. Calculations for equation (15)}

Write,
\[
\text{Cov}\left(\hat{\tau}^{2}, g_{n}\right) = \text{Cov}\left(\frac{1}{n(n-1)} \sum_{i_{1} \neq i_{2}} \sum_{j=1}^{p} W_{i_{1}j} W_{i_{2}j}, \frac{1}{n} \sum_{i=1}^{n} g_{i}\right)
\]
\[
= \frac{1}{n^{2}(n-1)} \sum_{i_{1} \neq i_{2}} \sum_{j=1}^{p} E \left( W_{i_{1}j} W_{i_{2}j} g_{i}\right)
\]
\[
= \frac{2}{n^{2}(n-1)} \sum_{i_{1} \neq i_{2}} \sum_{j=1}^{p} E \left( W_{i_{1}j} g_{i}\right) E \left( W_{i_{2}j}\right)
\]
\[
= \frac{2}{n^{2}(n-1)} \sum_{i_{1} \neq i_{2}} \sum_{j=1}^{p} E \left( W_{i_{1}j} g_{i}\right) E \left( S_{ij}\right)
\]
\[
= \frac{2}{n} \sum_{j=1}^{p} E \left( S_{ij}\right) \beta_{j},
\]
where $S_{ij} \equiv W_{ij} g_{i}$. Also notice that $\text{Var}(g_{n}) = \text{Var}\left(\frac{1}{n} \sum_{i=1}^{n} g_{i}\right) = \frac{\text{Var}(g_{i})}{n}$. Thus, by (17) we get
\[
c^{*} = \frac{\text{Cov}\left(\hat{\tau}^{2}, g_{n}\right)}{\text{Var}(g_{n})} = \frac{2}{n} \sum_{j=1}^{p} E \left( S_{ij}\right) \beta_{j}
\]

\textbf{Remark 6. Calculations for Example (16)}

In order to calculate $\text{Var}(T_{c^{*}})$ we need to calculate the numerator and denominator of (16). Consider first $\theta_{j} \equiv E(S_{ij})$.

Write,
\[
\theta_{j} = E(S_{ij}) = E(X_{ij}Y_{i}g_{i}) = E(X_{ij} \left( \beta^{T}X_{i} + e_{i}\right) g_{i})
\]
\[
E \left( X_{ij} \left( \sum_{m=1}^{k} \beta_{m}X_{im} + e_{i}\right) \sum_{k' < k'} X_{ik}X_{ik'}\right) = \sum_{m=1}^{p} \sum_{k < k'} \beta_{m} E \left( X_{ij}X_{im}X_{ik}X_{ik'}\right)
\]
where in the last equality we used the assumption that $E(e|X) = 0$. Since the columns of $X$ are independent, the summation is not zero (up to permutations) when $j = k$ and $m = k'$. In this case we have
\[
\theta_{j} = \sum_{m=1}^{p} \sum_{k < k'} \beta_{m} E \left( X_{ij}X_{im}X_{ik}X_{ik'}\right) = \sum_{m \neq j} \beta_{m} E \left( X_{ij}^{2}X_{im}^{2}\right) = \sum_{m \neq j} \beta_{m} E \left( X_{ij}^{2}\right) E \left( X_{im}^{2}\right) = \sum_{m \neq j} \beta_{m}.
\]
Notice that in the forth equality we used the assumption that \( E(X_{ij}^2) = 1 \) for all \( j = 1, ..., p \). Thus,

\[
\sum_{j=1}^{p} \beta_j E(S_{ij}) = \sum_{j=1}^{p} \beta_j \sum_{m \neq j}^{p} \beta_m = \sum_{j=1}^{p} \beta_j \left( \sum_{m=1}^{p} \beta_m - \beta_j \right) = \left( \sum_{j=1}^{p} \beta_j \right)^2 - \sum_{j=1}^{p} \beta_j^2 = \left( \sum_{j=1}^{p} \beta_j \right)^2 - \tau^2. \tag{58}
\]

plug-in \( \tau^2 = 1 \) and \( \beta_j = \frac{1}{\sqrt{n}} \) to get the numerator of (60):

\[
\left[ 2 \sum_{j=1}^{p} \beta_j E(S_{ij}) \right]^2 = 4 \left[ \left( \sum_{j=1}^{p} \beta_j \right)^2 - \tau^2 \right]^2 = 4 \left( \frac{1}{\sqrt{n}} \right)^2 - 1 \right]^2 = 4(\tau^2 - 1)^2.
\]

Consider now the denominator of (60). Write,

\[
\text{Var} (g_i) = E \left( g_i^2 \right) = E \left( \sum_{j<j'} X_{ij} X_{i'j'} \right)^2 = \sum_{j_1<j_2,j_3<j_4} E \left( X_{ij_1} X_{ij_2} X_{i'j_3} X_{i'j_4} \right).
\]

Since we assume that the columns of \( X \) are independent, the summation is not zero when \( j_1 = j_3 \) and \( j_2 = j_4 \). Thus,

\[
\text{Var} (g_i) = \sum_{j_1<j_2} E \left( X_{ij_1} X_{ij_2} \right) = \sum_{j_1<j_2} E \left( X_{ij_1} \right) E \left( X_{ij_2} \right) = p(p-1)/2. \tag{59}
\]

Notice that we used the assumption that since we assume that \( \Sigma = I \) in the last equality. Now, recall by (59) that \( \text{Var} (\hat{\tau}^2) = \frac{20}{n} + O \left( \frac{1}{n^2} \right) \). Therefore, we have

\[
\text{Var}(T_{\hat{\tau}}) = \text{Var} (\hat{\tau}^2) - \frac{\left[ 2 \sum_{j=1}^{p} \beta_j E(S_{ij}) \right]^2}{n \text{Var} (g_i)} = \frac{20}{n} + O \left( \frac{1}{n^2} \right) - \frac{4(p-1)^2}{p(p-1)/2} = \frac{12}{n} + O \left( \frac{1}{n^2} \right), \tag{60}
\]

where we used the assumption that \( n = p \) in the last equality.

**Proof of Proposition 4**

We need to prove that \( \sqrt{n} \left[ T_{\hat{\tau}} - T_{\hat{\tau}} \right] \xrightarrow{d} 0 \). Write,

\[
\sqrt{n} \left[ T_{\hat{\tau}} - T_{\hat{\tau}} \right] = \sqrt{n} \left[ \hat{\tau}^2 - \hat{\tau}^2 \right] = \sqrt{n} \left( \hat{\tau}^2 - \tau^2 \right).
\]

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

\[
p \left\{ \left\lvert \sqrt{n} \text{Var} (\hat{\tau}^2) \right\rvert > \varepsilon \right\} \leq E \left\{ \left\lvert \sqrt{n} \text{Var} (\hat{\tau}^2) \right\rvert \right\} \leq \sqrt{n} E(\hat{\tau}^2) E \left( \left( \hat{\tau}^2 - \tau^2 \right)^2 \right) \xrightarrow{p} 0.
\]

Since \( E(\hat{\tau}^2) = \frac{\text{Var}(g_i)}{n} \) and \( E(\left( \hat{\tau}^2 - \tau^2 \right)^2) = \text{Var}(\hat{\tau}^2) \), it enough to show that \( \text{Var}(g_i) \text{Var}(\hat{\tau}^2) \to 0 \). Notice that by (57) we have

\[
\text{Var} (g_i) \text{Var}(\hat{\tau}^2) = \frac{\text{Var} (U)}{\text{Var} (g_i)} \tag{61}
\]

where \( U \equiv 2 \sum_{ij \neq i'j'} W_{ij} S_{ij} \), is a U-statistic of order 2 with the kernel \( (W_1, S_2) = W_1^T S_2 = \sum_{j=1}^{P} W_{ij} S_{ij} \). By Theorem 12.3 in van der Vaart (2000), the variance of \( U \)

\[
\text{Var} (U) = \frac{4(n-2)}{n(n-1)} \delta_1 + \frac{2}{n(n-1)} \delta_2, \tag{62}
\]

where \( \delta_1 = \text{Cov} \left[ h \left( W_1, S_2 \right), h \left( W_1, S_2 \right) \right] \) and \( \delta_2 = \text{Cov} \left[ h \left( W_1, S_2 \right), h \left( W_1, S_2 \right) \right] \). Consider now the denominator of (61). Write,

\[
\text{Var} (g_i) = E \left( g_i^2 \right) = E \left( \sum_{j<j'} X_{ij} X_{ij'} \right)^2 = \sum_{j_1<j_2,j_3<j_4} E \left( X_{ij_1} X_{ij_2} X_{ij_3} X_{ij_4} \right).
\]
Since we assume that the columns of $X$ are independent, the summation is not zero when $j_1 = j_3$ and $j_2 = j_4$. Thus,

$$\text{Var}(g_i) = \sum_{j_1 < j_2} E\left(X_{j_1j_2}^2\right) = \sum_{j_1 < j_2} E\left(X_{j_1j_2}^2\right) = p(p-1)/2. \tag{63}$$

Notice that since we assume that $\Sigma = \mathbf{I}$ then $E(X_{ij}^2) = 1$ for all $i = 1, ..., n$ and $j = 1, ..., p$. Now, since we assume that $n/p = O(1)$, by (61) and (62) it is enough to prove that $\frac{A}{n} \rightarrow 0$ and $\frac{\delta}{n} \rightarrow 0$.

Consider first $\frac{A}{n}$. Write,

$$\delta_1 = \text{Cov}\left[h\left(W_1, S_2\right), h\left(W_1, S_2\right)\right] = \text{Cov}\left[\sum_{j=1}^{p} W_{1j} S_{2j}, \sum_{j=1}^{p} W_{1j} \bar{S}_{2j}\right] = \sum_{j,j'} \{E(W_{1j} W_{1j'}) \theta_j \theta_{j'} - \beta_j \beta_{j'} \theta_j \theta_{j'}\} = \theta^T \mathbf{A} \theta - \left(\sum_{j=1}^{p} \beta_j \beta_j\right),$$

where $\theta_j \equiv E(S_{ij})$, $\theta = (\theta_1, ..., \theta_p)^T$, $A = E(\mathbf{W W}^T)$ and $W = (W_{11}, ..., W_{1p})$. Thus, we need to show that $\frac{\theta^T \mathbf{A} \theta}{n} \rightarrow 0$.

Let $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_p$ be the eigenvalues of $A$. Notice that $\lambda_1^2 = \sum_{j=1}^{p} \lambda_j^2 = \text{trace}(A^2) = ||A||^2_F$, and since by Corollary 2 we have $\frac{||A||^2_F}{n} \rightarrow 0$ then also $\frac{\theta^T \mathbf{A} \theta}{n} \rightarrow 0$. Now, since max$_{\theta \in \mathbb{R}^p}$ $\left(\frac{\theta^T \mathbf{A} \theta}{||\theta||^2}\right) = \lambda_1$ then $\frac{\theta^T \mathbf{A} \theta}{n} = \frac{1}{n} ||\theta||^2 \cdot \left(\frac{\theta^T \mathbf{A} \theta}{||\theta||^2}\right) \leq \frac{1}{n} ||\theta||^2 \cdot \lambda_1$. Thus, it is enough to show that $\frac{||\theta||^2}{n}$ is bounded. Write,

$$\theta_j \equiv E(S_{ij}) = E(X_{ij} Y_i g_i) = E(X_{ij} (\beta^T X_i + \varepsilon_i) g_i) = E\left(X_{ij} \left(\sum_{m=1}^{p} \beta_m X_{im} + \varepsilon_{i}\right) X_{ik} X_{ik'}\right) = \sum_{m=1}^{p} \sum_{k<k'} \beta_m E(X_{ij} X_{im} X_{ik} X_{ik'})$$

where in the last equality we used the assumption that $E(\varepsilon|X) = 0$. Since we assume that the columns of $X$ are independent, the summation is not zero (up to permutations) when $j = k$ and $m = k'$. In this case we have by Cauchy–Schwarz

$$\theta_j = \sum_{m=1}^{p} \sum_{k<k'} \beta_m E(X_{ij} X_{im} X_{ik} X_{ik'}) = \sum_{m \neq j}^{p} \beta_m E\left(X_{ij}^2\right) = \sum_{m \neq j}^{p} \beta_m E\left(X_{ij}^2\right) = \sum_{m \neq j}^{p} \beta_m \leq \sqrt{p} ||\beta||.$$

Notice that in the forth equality we used the assumption that $E(X_{ij}^2) = 1$ for all $i = 1, ..., n$ and $j = 1, ..., p$. Thus $||\theta||^2 = \sum_{j=1}^{p} \theta_j^2 \leq \sum_{j=1}^{p} (p||\beta||^2) = p^2 \tau^2 = O(p^2)$. Since we assume that $p/n = O(1)$, then $\frac{||\theta||^2}{n}$ is indeed bounded.

Consider now $\frac{\delta}{n}$. Write,

$$\delta_2 = \text{Cov}\left[h\left(W_1, S_2\right), h\left(W_1, S_2\right)\right] = \text{Cov}\left[\sum_{j=1}^{p} W_{1j} S_{2j}, \sum_{j=1}^{p} W_{1j} \bar{S}_{2j}\right] = \sum_{j,j'} \{E(W_{1j} W_{1j'}) E(S_{2j} S_{2j'}) - \beta_j \beta_{j'} \theta_j \theta_{j'}\}$$

Since $p/n = O(1)$ by assumption, it is enough to show that $\eta \equiv \sum_{j,j'} E(W_{1j} W_{1j'}) E(S_{2j} S_{2j'}) = O(p^3)$. Write,

$$\sum_{j,j'} E(W_{1j} W_{1j'}) E(S_{2j} S_{2j'}) = \sum_{j,j'} E(W_{1j} W_{1j'}) E(W_{1j} W_{2j'} g_i^2)$$

$$= \sum_{j,j'} E\left(X_{ij} X_{ij} Y_i^2\right) E\left[X_{2j} X_{2j'} Y_i^2 \left(\sum_{k<k'} X_{2k} X_{2k'}\right)^2\right]$$

$$= \sum_{j,j'} E\left(X_{ij} X_{ij} Y_i^2\right) E\left[X_{2j} X_{2j'} Y_i^2 \sum_{k_1<k_2} \sum_{k_3<k_4} X_{2k_1} X_{2k_2} X_{2k_3} X_{2k_4}\right]$$

$$= \sum_{j_1,j_2} \sum_{k_1<k_2} \sum_{k_3<k_4} E\left(X_{ij_1} X_{ij_2} Y_i^2\right) E\left(X_{2j_1} X_{2j_2} Y_i^2 X_{2k_1} X_{2k_2} X_{2k_3} X_{2k_4}\right).$$
Plug-in $Y = \beta^T X + \epsilon$ to get

$$
\eta = \sum_{j_1,j_2} \sum_{k_1<k_2<k_3<k_4} E \left( X_{j_11} X_{j_22} Y_{1j_3}^2 \right) E \left( X_{j_21} X_{j_22} Y_{1j_3}^2 X_{2k_1} X_{2k_2} X_{2k_3} X_{2k_4} \right) 
$$

$$
= \sum_{j_1,j_2} \sum_{k_1<k_2<k_3<k_4} E \left[ X_{j_11} X_{j_22} \left( \beta^T X_1 + \epsilon_1 \right)^2 \right] E \left[ X_{j_21} X_{j_22} \left( \beta^T X_2 + \epsilon_2 \right)^2 X_{2k_1} X_{2k_2} X_{2k_3} X_{2k_4} \right] 
$$

$$
= \sum_{j_1,j_2} \sum_{k_1<k_2<k_3<k_4} E \left[ X_{j_11} X_{j_22} \left( \sum_{j,j'} \beta_{jj'} \epsilon_{1j} \epsilon_{1j'} \right) \right] E \left[ X_{j_21} X_{j_22} \left( \sum_{j,j'} \beta_{jj'} \epsilon_{2j} \epsilon_{2j'} + \epsilon_2^2 \right) X_{2k_1} X_{2k_2} X_{2k_3} X_{2k_4} \right] 
$$

$$
= \sum_{j_1,j_2} \sum_{j_3,j_4} \sum_{k_1<k_2<k_3<k_4} \sum_{j_1,j_2} \sum_{k_1<k_2<k_3<k_4} \sum_{j_3,j_4} \beta_{jj_1} \beta_{jj_2} \beta_{jj_3} \beta_{jj_4} E \left( X_{j_11} X_{j_22} X_{j_33} X_{j_44} \right) E \left( X_{j_21} X_{j_22} X_{j_33} X_{j_44} \right) 
$$

$$
+ \sigma^4 \sum_{j_1,j_2} \sum_{k_1<k_2<k_3<k_4} E \left( X_{j_11} X_{j_22} \right) E \left( X_{j_21} X_{j_22} X_{2k_1} X_{2k_2} X_{2k_3} X_{2k_4} \right),
$$

where in the forth equality we used the assumption that $E(\epsilon^2 | x) = \sigma^2$. Now, notice that:

- $L_1$ is not zero (up to permutation) when $j_1 = j_2$ and $j_3 = j_4$.
- $L_2$ is not zero (up to permutation) when $j_1 = j_2; j_3 = j_5; k_1 = k_3; k_2 = k_4$.
- $L_3$ is not zero when $j_1 = j_2$
- $L_4$ is not zero (up to permutation) when $j_1 = j_2; j_3 = k_3; k_2 = k_4$.

Putting it all together to get

$$
\eta = \sum_{j_1,j_2} \sum_{j_3,j_4} \sum_{k_1<k_2} \beta_{jj_1} \beta_{jj_2} E \left( X_{j_11} X_{j_22} X_{j_33} X_{j_44} \right) E \left( X_{j_21} X_{j_22} X_{j_33} X_{j_44} \right) + \sigma^4 \sum_{j_1,j_2} \sum_{k_1<k_2} E \left( X_{j_11} \right) E \left( X_{j_21} X_{j_22} X_{2k_1} X_{2k_2} \right).
$$

Since we assume that $E \left( X_{j_11} X_{j_22} X_{j_33} X_{j_44} \right) = O(1)$ for every $j_1, j_2, j_3, j_4$, all the expectations above are also $O(1)$. Also recall that $\tau^2 + \sigma^2 = O(1)$, and $\sum_{j_3,j_4} \beta_{jj_3} \beta_{jj_4} = \tau^4 = O(1)$. Thus, we obtain that $\eta = O(p^3)$. This completes the proof that $\sqrt{n} \left[ T_{B^*} - T_{B} \right] \xrightarrow{p} 0$.

**Remark 7.** We now calculate the asymptotic improvement of $T_B$ over the naive estimator. For simplicity, consider the case when $\tau^2 = \sigma^2 = 1$. Recall the variance of $\hat{\tau}^2$ and $T_B$ given in (4) and (29), respectively. Write,

$$
\lim_{n,p \to \infty} \frac{\text{Var} \left( \hat{\tau}^2 \right) - \text{Var} \left( T_B \right)}{\text{Var} \left( \hat{\tau}^2 \right)} = \lim_{n,p \to \infty} \frac{8\tau^4/n + \frac{1}{2n(1-\frac{1}{n})} \left( \sigma^2 \tau^2 + \sigma^4 \right)}{3\tau^4 + 4\tau^2} = \frac{0.5}{2n(1-\frac{1}{n})}.
$$

where we used (4) in the first equality, and the fact that $\sigma^2 = 2\tau^2 = 2$ in the second equality. Now, notice that when $p = n$ and $\tau_B^4 = 0.5$ then the reduction is $\frac{0.5}{3+2} = 10\%$ and when $p/n$ converges to zero, the reduction is 16%.

**Remark 8.** *Calculations for Example 4*

Consider the first scenario where $\beta_{jj}^2 = \frac{1}{p}$. Recall that we assume that the set $B$ is a fixed set of indices such that $|B| \ll p$.

Therefore, we have $\tau^2_B = \sum_{j \in B} \beta_{jj}^2 = O \left( \frac{1}{p} \right)$. Now, by (29) we have $\text{Var} \left( T_B \right) = \text{Var} \left( \hat{\tau}^2 \right) - \frac{2\tau^2}{n} + O(n^{-2})$ and by Remark 7 we have $\text{Var} \left( \hat{\tau}^2 \right) = \frac{20}{n} + O(n^{-2})$. Using the assumption that $n = p$ we can conclude that $\text{Var} \left( T_B \right) = \frac{20}{n} + O \left( \frac{1}{p} \right)$. Hence,
in this scenario, $T_B$ and the naive estimator have the same asymptotic variance. In contrast, recall that in Example 3 we showed that the asymptotic variance of $T_{\gamma}$ is 40% lower than the variance of the naive estimator.

Consider now the second scenario where $\hat{\tau}_{AB}^2 = \tau^2 = 1$. By (21) we have

$$\text{Var}(T_B) = \text{Var}(\hat{\tau}^2) - \frac{8}{n} \frac{4}{T_B} + O(n^{-2}) = \frac{12}{n} + O(n^{-2}).$$

Hence, in this scenario the asymptotic variance of $T_B$ is 40% smaller than the variance of the naive estimator. Consider now $\text{Var}(T_{\gamma})$. By Cauchy–Schwarz inequality

$$\left(\sum_{j=1}^{p} \beta_j \theta_j \right)^2 \leq \sum_{j=1}^{p} \beta_j^2 \cdot |B| = \hat{\tau}_{AB}^2 |B| = O(1),$$

where the last equality holds since we assume that $B \subset \{1, ..., p\}$ be a fixed set of some indices such that $|B| \ll p$. Now, By (55) we have

$$\sum_{j=1}^{p} \beta_j \theta_j = \left(\sum_{j=1}^{p} \beta_j \right)^2 - \tau^2 = \left(\sum_{j \in B} \beta_j + \sum_{j \notin B} \beta_j \right)^2 - \hat{\tau}_{AB}^2 \leq |B| - 1 = O(1).$$

Now, recall that $\text{Var}(\hat{\tau}^2) = \frac{20}{n} + O\left(\frac{1}{n^2}\right)$ and $\text{Var}(g_j) = p(p-1)/2$ by (50) and (59) respectively. Therefore, we have

$$\text{Var}(T_{\gamma}) = \text{Var}(\hat{\tau}^2) - \frac{2}{n \text{Var}(g_j)} \left(\frac{\frac{p}{\text{Var}(g_j)} \beta_j \theta_j}{n} \right)^2 = \frac{20}{n} + O\left(\frac{1}{n^2}\right) - O\left(\frac{1}{np^2}\right) = \frac{20}{n} + O\left(\frac{1}{n^2}\right).$$

Hence, in this scenario, $T_{\gamma}$ and the naive estimator have the same asymptotic variance.

Lastly, recall that in Example 2 we already showed that, asymptotically, the variance of $T_\text{oracle}$ (i.e., the optimal oracle estimator) is 40% lower than the naive variance (without any assumptions about the structure of the coefficient vector $\beta$).

**Proof of Proposition 5**

In order to prove that $\sqrt{n} (T_{\gamma} - T_B) \xrightarrow{d} 0$, it is enough to show that

$$E \left\{ \sqrt{n} (T_{\gamma} - T_B) \right\} \to 0,$$

$$\text{Var} \left\{ \sqrt{n} (T_{\gamma} - T_B) \right\} \to 0.$$  

(64)  

(65)

We start with the first equation. Let $A$ denote the event that the selection algorithm $\gamma$ perfectly identifies the set of large coefficients, i.e., $A = \{B_\gamma = B\}$. Let $p_A \equiv P(A)$ denote the probability that $A$ occurs, and let $1_A$ denote the indicator of $A$. Notice that $E(T_B) = \tau^2$ and $T_\gamma 1_A = T_B 1_A$. Thus,

$$E \left\{ \sqrt{n} (T_{\gamma} - T_B) \right\} = \sqrt{n} \left[ E(T_{\gamma}) - \tau^2 \right] = \sqrt{n} \left[ E \left( T_{\gamma} (1 - 1_A) \right) + E \left( T_\gamma 1_A \right) - \tau^2 \right]$$

$$= \sqrt{n} E \left( T_{\gamma} (1 - 1_A) \right) + \sqrt{n} E \left( T_B 1_A \right) - \tau^2,$$

(66)

where the last equality holds since $T_\gamma 1_A = T_B 1_A$. For the convenience of notation, let $C$ be an upper bound of the maximum over all first four moments of $T_\gamma$ and $T_B$, and consider the first term of (66). By the Cauchy–Schwarz inequality,

$$\sqrt{n} E \left[ T_\gamma (1 - 1_A) \right] \leq \sqrt{n} \left\{ E \left[ T_\gamma^2 \right] \right\}^{1/2} \left\{ E \left[ (1 - 1_A)^2 \right] \right\}^{1/2} \leq \sqrt{n} C^{1/2} \left( 1 - p_A \right)^{1/2} \to 0,$$

(67)

where the last inequality holds since $\lim_{n \to \infty} n \left( 1 - p_A \right)^{1/2} = 0$ by assumption. We now consider the second term of (66).

Write,

$$\sqrt{n} \left[ E \left( T_B 1_A \right) - \tau^2 \right] = \sqrt{n} E \left( T_B 1_A - T_B \right) = -\sqrt{n} E \left[ T_B (1 - 1_A) \right],$$

(68)
and notice that by the same type of argument as in (64) we have $\sqrt{n}E[T_B (1 - 1_A)] \to 0$. This completes the proof of (63).

We now move to show that $\text{Var} \{\sqrt{n}(T_\gamma - T_B)\} \to 0$. Write,

$$\text{Var} \{\sqrt{n}(T_\gamma - T_B)\} = n \text{Var} (T_\gamma - T_B)$$

$$= n \left\{ \text{Var} (T_\gamma) + \text{Var} (T_B) - 2 \text{Cov} (T_\gamma, T_B) \right\}$$

$$= n \left\{ E\left(T_\gamma^2\right) - [E(T_\gamma)]^2 + E\left(T_B^2\right) - \tau^4 - 2 \left[ E(T_\gamma T_B) - E(T_\gamma) \tau^2 \right] \right\}$$

$$= n \left\{ E\left(T_\gamma^2\right) - E(T_\gamma T_B) + E\left(T_B^2\right) - E(T_\gamma T_B) + E(T_\gamma) \left[ \tau^2 - E(T_\gamma) \right] - \tau^2 \left[ \tau^2 - E(T_\gamma) \right] \right\}$$

$$= n \left\{ \frac{E\left(T_\gamma^2\right) - E(T_\gamma T_B)}{\hat{\theta}_1} + \frac{E\left(T_B^2\right) - E(T_\gamma T_B)}{\hat{\theta}_2} - \left[ \tau^2 - E(T_\gamma) \right]^2 \right\}.$$

Thus, it is enough to show that $n\theta_1 \to 0$, $n\theta_2 \to 0$ and $n\theta_3 \to 0$.

We start with showing that $n\theta_1 \to 0$. Notice that $T_B^2 1_A = T_B T_\gamma 1_A = T_\gamma^2 1_A$. Thus,

$$n\theta_1 = n \left\{ E\left(T_\gamma^2\right) - E(T_\gamma T_B) \right\}$$

$$= n \left\{ E\left(T_\gamma^2\right) - E(T_\gamma T_B (1 - 1_A)) - E(T_\gamma T_B 1_A) \right\}$$

$$= n \left\{ E\left(T_\gamma^2\right) - E(T_\gamma T_B (1 - 1_A)) - E(T_\gamma 1_A) \right\}$$

$$= n \left\{ E\left[T_\gamma^2 (1 - 1_A)\right] - E[T_\gamma T_B (1 - 1_A)] \right\}.$$

Now, notice that $n(E\left[T_\gamma^2 (1 - 1_A)\right]) \to 0$ by similar arguments as in (63), with a slight modification of using the existence of the fourth moments of $T_\gamma$ and $T_B$, rather than the second moments. Also, by Cauchy–Schwarz inequality we have,

$$nE[T_\gamma T_B (1 - 1_A)] \leq n\left\{ E\left(T_\gamma^2 T_B^2\right) \right\}^{1/2} \left\{ E\left[(1 - 1_A)^2\right] \right\}^{1/2}$$

$$\leq n\left\{ E\left(T_\gamma^2\right) E\left(T_B^2\right) \right\}^{1/4} \{1 - p_A\}^{1/2}$$

$$\leq n C^{1/2} \{1 - p_A\}^{1/2} \to 0,$$

where $C$ is an upper bound of the maximum over all first four moments of $T_\gamma$ and $T_B$. Therefore, $n\theta_1 \to 0$.

Consider now $n\theta_2$. Write,

$$n\theta_2 = n \left\{ E\left(T_B^2\right) - E(T_\gamma T_B) \right\}$$

$$= n \left\{ E\left(T_B^2\right) - E[T_\gamma T_B (1 - 1_A)] - E(T_\gamma T_B 1_A) \right\}$$

$$= n \left\{ E\left(T_B^2\right) - E[T_\gamma T_B (1 - 1_A)] - E(T_\gamma^2 1_A) \right\}$$

$$= n \left\{ E\left[T_B^2 (1 - 1_A)\right] - E[T_\gamma T_B (1 - 1_A)] \right\} \to 0,$$

and notice that the last equation follows by similar arguments.
Consider now \( n \theta_3 \). Write,

\[
n \theta_3 = n \left[ E \left( T_B \right) - E \left( T_\gamma \right) \right]
\]

\[
= n \left[ E \left[ T_B \left( 1 - 1_{A} \right) + T_B 1_{A} \right] - E \left( T_\gamma \right) \right]
\]

\[
= n \left\{ E \left[ T_B \left( 1 - 1_{A} \right) \right] + E \left( T_B 1_{A} - T_\gamma \right) \right\}
\]

\[
= n \left\{ E \left[ T_B \left( 1 - 1_{A} \right) \right] + E \left( T_\gamma 1_{A} - T_\gamma \right) \right\}
\]

\[
= n \left\{ E \left[ T_B \left( 1 - 1_{A} \right) \right] - E \left[ T_\gamma \left( 1 - 1_{A} \right) \right] \right\} \to 0.
\]

where the last equation follows by similar arguments as in (64). This completes the proof of (65) and we conclude that

\( \sqrt{n} \left( T_\gamma - T_B \right) \xrightarrow{p} 0. \)

\[
\text{Proof of Proposition 6}
\]

We wish to prove that

\[
\text{Proof of Proposition 7}
\]

We now move to prove that

\[
\frac{n}{\sqrt{p}} \left[ \text{Var} \left( \hat{T}_2 \right) - \text{Var} \left( \hat{T}_2 \right) \right] \xrightarrow{p} 0.
\]

Recall by (5) that

\[
\text{Proof of Proposition 7}
\]

We wish to prove that

\[
n \left[ \text{Var} \left( \hat{T}_2 \right) - \text{Var} \left( \hat{T}_2 \right) \right] \xrightarrow{p} 0.
\]

(69)

Now, as we assumed standard Gaussian covariates, one can verify that

\[
\hat{\beta}^T A \beta - \| \beta \|^4 = \text{Var} \left( \hat{T}_2 \right) - \| \beta \|^4 = \sigma_2^2 + 4 \sigma_2^2 \tau^2 + 3 \tau^4.
\]

Thus, in this case we can write

\[
\text{Var} \left( \hat{T}_2 \right) = \frac{4}{n} \left[ \frac{(n-2)}{n-1} \left( \sigma_2^2 + 2 \tau^4 \right) \right],
\]

(70)

In order to prove that (69) holds, it is enough to prove the consistency of \( \hat{\sigma}_2^2 \) and \( \hat{\tau}_2^2 \). Consistency of the sample variance \( \hat{\sigma}_2^2 \)

is a standard result, and since \( \hat{\sigma}_2^2 \) is an unbiased estimator, it is enough to show that its variance converges to zero as

\( n \to \infty. \) Since we assume \( \hat{\sigma}_2^2 + \sigma_2^2 = O(1) \) and \( p/n = O(1), \) we have by (69) that \( \text{Var}(\hat{T}_2) \to 0, \) and (69) follows.

\[
\text{Proof of Proposition 7}
\]

We now move to prove that

\[
n \left[ \text{Var} \left( T_\gamma \right) - \text{Var} \left( T_\gamma \right) \right] \xrightarrow{p} 0.
\]

(71)

Recall that by Proposition 5 we have \( \lim_{n \to \infty} n \left[ \text{Var} \left( T_B \right) - \text{Var} \left( T_\gamma \right) \right] = 0. \) Hence, it is enough to show that

\[
n \left[ \text{Var} \left( T_\gamma \right) - \text{Var} \left( T_B \right) \right] \xrightarrow{p} 0.
\]

Since we assume \( X_i \stackrel{i.i.d.}{\sim} N(0, I) \) then by (28) we have \( \text{Var}(T_B) = \text{Var}(\hat{\tau}_2) - \frac{\sigma_2^2}{p} \hat{\tau}_2^2 + O(n^{-2}). \) Recall that by definition we have \( \text{Var}(T_\gamma) = \text{Var}(\hat{T}_2) - \frac{\sigma_2^2}{p} \hat{\tau}_2^2. \) Also recall that \( \text{Var}(\hat{T}_2) \) is consistent by Proposition 6. Thus, it is enough to prove that \( \hat{\tau}_2^2 - \tau_2^2 \xrightarrow{p} 0. \) Now, since we assumed that \( n \left[ P \left( \{ \mathbf{B}_j \neq \mathbf{B} \} \right) \right]^{1/2} \xrightarrow{n \to \infty} 0 \) then clearly \( P \left( \mathbf{B}_j = \mathbf{B} \right) \xrightarrow{n \to \infty} 1. \) Thus, it is enough to show that \( \hat{\tau}_2^2 - \tau_2^2 \xrightarrow{p} 0. \) Recall that \( E(\hat{\tau}_j^2) = \tau_j^2 \) for \( j = 1, \ldots, p \) and notice that \( \text{Var}(\hat{\tau}_j^2) \xrightarrow{n \to \infty} 0 \) by similar arguments that were used to derive (5). Hence, we have \( \hat{\tau}_j^2 - \tau_j^2 \xrightarrow{p} 0. \) Since we assumed that \( \mathbf{B} \) is finite, we have

\[
\hat{\tau}_2^2 - \tau_2^2 = \sum_{j \in \mathbf{B}} (\hat{\tau}_j^2 - \tau_j^2) \xrightarrow{p} 0,
\]

and (71) follows.
Remark 9. We use the following simple selection algorithm $\gamma$:

**Algorithm 3: Covariate selection $\gamma$**

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

1. Calculate $\hat{\beta}_1^2, ..., \hat{\beta}_p^2$ where $\hat{\beta}_j^2$ is given in (3) for $j = 1, ..., p$.

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

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

**Result:** Return $B_\gamma$.

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 $B_\gamma \subset \{ 1, ..., p \}$. The algorithm works well in scenarios where a relatively large gap truly separates between larger coefficients and the smaller coefficients of the vector $\beta$. 
Ilan Livne (ilan.livne@campus.technion.ac.il)
David Azriel (davidazr@technion.ac.il)
Yair Goldberg (yairgo@technion.ac.il)

The Faculty of Industrial Engineering and Management, Technion.