We study the benign overfitting theory in the prediction of the conditional average treatment effect (CATE), with linear regression models. As the development of machine learning for causal inference, a wide range of large-scale models for causality are gaining attention. One problem is that suspicions have been raised that the large-scale models are prone to overfitting to observations with sample selection, hence the large models may not be suitable for causal prediction. In this study, to resolve the suspicious, we investigate on the validity of causal inference methods for overparameterized models, by applying the recent theory of benign overfitting (Bartlett et al., 2020). Specifically, we consider samples whose distribution switches depending on an assignment rule, and study the prediction of CATE with linear models whose dimension diverges to infinity. We focus on two methods: the T-learner, which based on a difference between separately constructed estimators with each treatment group, and the inverse probability weight (IPW)-learner, which solves another regression problem approximated by a propensity score. In both methods, the estimator consists of interpolators that fit the samples perfectly. As a result, we show that the T-learner fails to achieve the consistency except the random assignment, while the IPW-learner converges the risk to zero if the propensity score is known. This difference stems from that the T-learner is unable to preserve eigenspaces of the covariances, which is necessary for benign overfitting in the overparameterized setting. Our result provides new insights into the usage of causal inference methods in the overparameterized setting, in particular, doubly robust estimators.
there has been a lot of interest in how to train models given high-dimensional data and models (Belloni et al., 2011, 2014; Candes and Tao, 2007; Moon et al., 2007; Sun and Zhang, 2012; Song et al., 2015). Especially, several machine learning studies estimate and predict CATE using large-scale flexible models such as neural networks (Johansson et al., 2016; Shalit et al., 2017; Yao et al., 2018; Atan et al., 2018; Farrell et al., 2020).

Despite the developments, the validity of CATE prediction using large-scale models is still an ongoing issue. When the data are not perfectly observed, as in the CATE problem, the flexible models is more likely to overfit the observations. Künzel et al. (2019) points out the possibility of overfitting of a method for CATE prediction. For ordinary regression problems without no treatment effects, new various theories for overparameterized models have emerged such as the benign overfitting (Bartlett et al., 2020); that is, a prediction error can be sufficiently small, even though the predictor overfits training data by numerous parameters greater than the sample size. However, it is not clear whether the recent overparameterization theory are applicable to the problems of CATE prediction.

In this study, we investigate CATE prediction with linear regression models whose number of parameter is larger than the number of observations by following Bartlett et al. (2020). Specifically, we consider the excess risk of two standard prediction methods: the T-learner (Künzel et al., 2019) and inverse probability weight (IPW)-learner with linear regression models. The T-learner separately constructs the interpolating estimator of each treatment effect. The IPW-learner first approximates a response variable of the CATE problem by using treatment assignment probability, called the propensity score, then develops prediction for the approximated response. For both methods, we derive the upper and lower bounds on the excess risk of CATE prediction and then investigate the conditions under which the upper bound goes to zero.

As a result, we find that the design of the treatment assignment plays an important role in benign overfitting. For the T-learner case, when the treatment assignment does not depend on the covariates, which is standard in randomized controlled trials (RCTs), the prediction risk goes to zero under the same conditions as in Bartlett et al. (2020). In contrast, when the treatment assignment depends on the covariates owing to the selection bias, the convergence of the risk is not guaranteed. This result is consistent with the previous works (Künzel et al., 2019; Nie and Wager, 2020), which claims the danger of overfitting of the T-learner. For the IPW-learner case, on the other hand, the prediction risk converges to zero, regardless of the assignment rule. These results give implications for CATE prediction of overparameterization, and also provide insights into the use of other methods. For example, when using the two-step algorithms, such as doubly robust method (Chernozhukov et al., 2018; Kennedy, 2020) and R-learner (Nie and Wager, 2020), our result implies the importance of correctly estimating IPW in the first stage nuisance parameter estimation instead of using the T-learner.

**Related work.** There is a rich literature on the overparameterized setting. The most closest theory to our work is the benign overfitting in linear regression Bartlett et al. (2020), which reveals a sufficient condition under which the prediction risk converges to zero with the overparameterized linear model. Subsequent to Bartlett et al. (2020), the framework is extended to ridge regression (Tsigler and Bartlett, 2020), multiclass classification (Wang et al., 2021), and a max-margin classifier (Cao et al., 2021). Koehler et al. (2021) reveals a connection between benign overfitting and the notion of uniform convergence. For other studies studies on overparameterization, numerous works study the precious asymptotics of overparameterized models by using the random matrix theory. Muthukumar et al. (2019); Hastie et al. (2019); Dobriban and Wager (2018) consider linear regression or shallow neural networks, Dobriban and Wager (2018); Wu and Xu (2020) study a ridge regression problem, and Chatterji and Long (2021) studies a binary classification problem, Belkin et al. (2018, 2019); Liang and Rakhlin (2020) study interpolating kernel methods.

CATE prediction has also been proposed using kernel-based methods (Fan and Zhang, 2008), Gaussian processes (Alaa and van der Schaar, 2017, 2018), generative adversarial nets (Yoon et al., 2018), boosting, tree-based methods (Zeileis and Hothorn, 2008; Su et al., 2009; Imai and Strauss, 2011; Kang et al., 2012; Lipkovich et al., 2011; Loh et al., 2012; Wager and Athey, 2018; Athey et al., 2019; Chatla and Shmueli, 2020), nearest neighbor matching, series estimation, and Bayesian additive regression trees (Hill, 2011). Gunter et al. (2011); Imai and Strauss (2011); Imai and Ratkovic (2013) formulate the CATE estimation problem as a variable selection problem. Cai and Guo (2017); Cai et al. (2021) study confidence intervals for high-dimensional cases. As a unifying framework, Künzel et al. (2019) introduces meta-learners, such as the T-learner and X-learner. Other various methods have also been proposed (Li and Fu, 2017; Kallus, 2017; Powers et al., 2017; Subbaswamy and Saria, 2018; Zhao, 2019; Hahn et al., 2020; Nie and Wager, 2020; Kennedy, 2020).

**Notation.** We define a (potentially infinite-dimensional) Hilbert space \( \mathbb{H} \) with a norm \( \| \cdot \| \). For two vectors \( z, z' \in \mathbb{H} \), \( z^\top z' \) denotes an inner product between \( z \) and \( z' \), and \( z z^\top \) denotes a tensor product. For an operator \( \Sigma : \mathbb{H} \to \mathbb{H} \), we use \( \mu_1(\Sigma) \geq \mu_2(\Sigma) \geq \cdots \) to denote the eigenvalues of \( \Sigma \) in descending order, and we denote the operator norm of \( \Sigma \) by \( \| \Sigma \| \). We use \( I \) to denote the identity operator on \( \mathbb{H} \) and \( I_n \) to denote the \( n \times n \) identity matrix. For an event \( E \), \( 1\{E\} \) is an indicator function, which is 1 if \( E \) is true, and 0 if \( E \) is false. For a sequence \( \{a_n\}_n \), \( O(a_n) \) and
\(o(a_n)\) denote Landau’s big and small o notation, and \(O_P(a_n)\) and \(o_P(a_n)\) denote its probabilistic version. We write \(a_n = \Omega(b_n)\) for \(\limsup_{n \to \infty} |a_n/b_n| > 0\), and \(a_n = \omega(b_n)\) for \(\limsup_{n \to \infty} |a_n/b_n| = \infty\). Also, \(a_n = \Theta(b_n)\) means that both of \(a_n = O(b_n)\) and \(a_n = \Omega(b_n)\) hold.

2 Setting: Linear Regression and Prediction for CATE

2.1 Conditional Average Treatment Effect

We introduce the notion of conditional average treatment effect (CATE). Suppose that there are two treatments \(\varepsilon\), where \(\varepsilon\) takes \(\{1, 0\}\), two treatments \(\varepsilon = 1\) corresponds to the active treatment, and treatment \(\varepsilon = 0\) corresponds to the control treatment. We have access to \(n\) training examples \(\{(x_i, d_i, y_{i1}, y_{i0})\}_{i=1}^n\), each of which consists of a covariate \(x_i\) from \(\mathbb{H}\), a treatment indicator \(d_i \in \{1, 0\}\), and a real-valued response variable \(y_{i\varepsilon}\), and the examples are independent and identical copies of a jointly random element \((x, d, y_1, y_0) \sim P\) from the population distribution \(P\). \(p(d = a|x)\) denotes the probability that an individual with covariate \(x\) receives treatment \(a \in \{1, 0\}\), which is called the propensity score. We then posit the existence of potential outcome random variables \(y_{1}\) and \(y_{0}\) corresponding respectively to the response subject would have experienced with and without treatment. By using the potential outcomes, the response variable \(y\) can be written as

\[y = \mathbb{1}[d = 1]y_1 + \mathbb{1}[d = 0]y_0.\]

We define the CATE at \(x\) as

\[\tau^*(x) = \mathbb{E}(y_1|x) - \mathbb{E}(y_0|x)\]

The main difficulty is that we can only observe a realized one of the two potential outcomes \(y_a\) if \(d = a\) for \(a \in \{0, 1\}\) from the given training example; thus, the model cannot be directly learned by minimizing the corresponding empirical risk.

2.2 Linear Regression Model for Potential Outcomes

In this study, we consider a linear model for the potential outcome variables \(y_a, a \in \{0, 1\}\), then study the prediction of \(\tau^*(x)\). For each \(a \in \{0, 1\}\), suppose that there exists a true parameter vector \(\theta^*_a \in \mathbb{H}\) such that the variables \(x\) and \(y_a\) follows the following linear model

\[y_a = (\theta^*_a)^\top x + \varepsilon_a,\]

where \(\varepsilon_a\) is an independent noise variable whose mean is zero and variance is finite. Note that \(\varepsilon_0\) and \(\varepsilon_1\) are independent to each other. Note that \(\theta^*_a\) is the optimal parameter for predicting \(y_a\) without the selection, that is, \(\mathbb{E}(y_a - x^\top \theta_a)^2 = \min_{\theta \in \mathbb{H}} \mathbb{E}(y_a - x^\top \theta)^2\) holds.

For each \(a \in \{0, 1\}\), we give the following notations. We define a population covariance operator \(\Sigma = \mathbb{E}[xx^\top]\), and a covariance operator with the selection assignment \(\Sigma_a \in \mathbb{E}[\mathbb{1}[d = a]xx^\top] = \mathbb{E}[p(d = a|x)xx^\top]\). We consider an empirical potential outcome \(y_{a,i}\) corresponding \(y_i\) for \(i = 1, \ldots, n\), and also define an empirical vector \(y_a \in \mathbb{R}^n\) whose \(i\)-th entry is \(\mathbb{1}[d_i = a]y_{i}\), and a vector \(\varepsilon_a \in \mathbb{R}^n\) whose \(i\)-th entry \(\varepsilon_{a,i} = \mathbb{1}[d_i = a] \varepsilon_{a,i}\), where \(\varepsilon_{a,i} = (y_{a,i} - (\theta^*_a)^\top x_i)\). Following Bartlett et al. (2020), we use the infinite matrix notation: \(X_a\) denotes a linear map from \(\mathbb{H}\) to \(\mathbb{R}^n\) corresponding to \((\mathbb{1}[d_1 = a]x_1^\top, \ldots, \mathbb{1}[d_n = a]x_n^\top)^\top\); so that, \(X_a\) has its \(i\)-th component as \(\mathbb{1}[d_i = a]x_i^\top \theta\) for \(\theta \in \mathbb{H}\). We use the similar notation for the linear map \(X_a^\top\) from \(\mathbb{R}^n\) to \(\mathbb{H}\). Let us also define the linear map \(X = X_1 + X_0\) from \(\mathbb{H}\) to \(\mathbb{R}^n\); that is, it corresponds to \(x_1, \ldots, x_n \in \mathbb{H}\). We also define \(X^\top = X_1^\top + X_0^\top\).

2.3 Excess Prediction Risk for CATE

Given the observations \(\{(x_i, d_i, y_{i1}, y_{i0})\}_{i=1}^n\), we consider an estimator which returns parameter \(\hat{\theta} \in \mathbb{H}\). Then, we predict the CATE given covariate \(x \in \mathbb{H}\) as \(x^\top \hat{\theta}\). We measure the predictive performance of this estimator by using the excess risk.

**Definition 2.1 (Excess risk).** The excess risk of the estimator is defined as

\[R(\hat{\theta}) := \mathbb{E}_{x,y} \left[ (\hat{y} - y)^2 - (\hat{y} - x^\top \theta^*_a)^2 \right],\]

where \(\hat{y} = y_1 - y_0, \theta^* = \theta^*_1 - \theta^*_0,\) and \(\mathbb{E}_{x,y}\) denotes the conditional expectation given all random quantities other than \(x, y_1, y_0\) (in this case, given the estimate \(\hat{\theta}\)).

This risk is used to predict the difference between the two groups to differentiate them from the treatment. In the ordinary regression case, such as the excess risk defined in Bartlett et al. (2020), the differences, \(y_1 - y_0\) and \(\theta^*_1 - \theta^*_0\), are not included.
2.4 Assumption

To study the prediction risk, we need to make regular assumptions.

**Assumption 2.2 (Basic).** The following conditions hold:

1. $x$ and $y_a$ are mean zero for $a \in \{0, 1\}$;
2. there exists an $\mathbb{H}$-valued random element $z$ which is conditionally $\sigma^2_z$-sub-Gaussian with $\sigma_z$, which means $\mathbb{E}\left[\exp(\lambda^\top z)\right] \leq \exp(\sigma^2_z \|\lambda\|^2/2)$ for all $\lambda \in \mathbb{H}$, and it satisfies $x = \Sigma^{1/2} z$.
3. For $a \in \{0, 1\}$, $\varepsilon_a$ is sub-Gaussian and has positive conditional variance, that is, there exist $\sigma^2_y, \sigma^2 > 0$ such that $\mathbb{E}\left[\exp(\lambda^\top \varepsilon_a)|x\right] \leq \exp(\sigma^2_y \lambda^2/2)$ for any $\lambda \in \mathbb{R}$ and $\mathbb{E}[\varepsilon_a^2|x] \geq \sigma^2$.
4. almost surely, for each $a \in \{0, 1\}$, the projection of the data $X_a$ on the space orthogonal to any eigenvector of $\Sigma_a$ spans a space of dimension $n$.

Assumption 2.2 is a common setting in linear regression. For example, Assumption 2.2 is satisfied if $x$ and $y_a$ are jointly Gaussian with zero mean and $\text{rank}(\Sigma) > n$ (Bartlett et al., 2020).

**Assumption 2.3 (Unconfoundedness).** The treatment assignment $d$ is independent of the potential outcomes for $\{y_1, y_0\}$ conditional on $x$:

$$\{y_1, y_0\} \perp d \mid x.$$

Assumption 2.3 expresses a natural setting wherein the assignment is independent of the output conditioned on the covariates. This is the standard approach in treatment effect prediction (Rosenbaum and Rubin, 1983).

**Assumption 2.4 (Overlap of assignment support).** For some $0 < \varphi < 0.5$ and all $x \in \mathbb{H}$,

$$\varphi < p(d = 1|x) < 1 - \varphi.$$

Assumption 2.4 allows us to avoid overlap in treatment assignments. The situation where no covariates are selected at all can also be avoided. By this assumption, we can guarantee the identifiability of the assignment and the parameters (Imbens and Rubin, 2015).

3 Predictors with Interpolation

We can construct specific method to predict the CATE $\tau^*(x)$ with linear models in several ways. In this study, we consider the following two prediction methods: the T-learner and IPW-learner.

**The T-learner:** This method consists of a two-step procedure: in the first stage, we estimate the parameters of linear regression models for $\mathbb{E}[y_1|x]$ and $\mathbb{E}[y_0|x]$, separately; then, in the second stage, we predict the CATE by the difference of the two estimators.

**The IPW-learner:** This approach utilizes a propensity score $p(d = 1|x)$ to constructs an conditionally unbiased estimator of $\tau^*(x_i)$ by using $y_i$ and $d_i$; then, constructs a predictor by regressing the unbiased estimator on the covariates $x$.

3.1 The T-learner

In the first stage, we estimate $\theta^*_a$ for each $a \in \{0, 1\}$ separately. We consider an interpolating estimator, which can fit the data perfectly when the dimension of $x$ is larger than the sample size $n$; that is an interpolating estimator $\hat{\theta}_a$ satisfies $X_a \hat{\theta}_a = y_a$ when $\mathbb{H} = \mathbb{R}^p$, where $p > n$. Specifically, we define the interpolating estimator for each $a \in \{0, 1\}$ as

$$\hat{\theta}_a = \arg \min_{\theta} \left\{ ||\theta||^2 : X_a^\top X_a \theta = X_a^\top y_a \right\} = \left(X_a^\top X_a\right)^{-1} X_a^\top y_a = X_a^\top (X_a X_a^\top)^{-1} y_a,$$

where $(X_a X_a^\top)^{-1}$ denotes the pseudoinverse of the bounded linear operator $X_a^\top X_a$ (for infinite-dimensional $\mathbb{H}$, the existence of the pseudoinverse is guaranteed because $X_a^\top X_a$ is bounded and has a closed range; see Desoer and Whalen (1963)). When $\mathbb{H}$ has dimension $p$ with $p < n$ and $X_a$ has rank $p$, there is a unique solution to the normal equations. On the contrary, the condition 2.2 in Assumption 2.2 implies that we can find many solutions $\theta \in \mathbb{H}$ to the normal equations that achieve $X_a \theta = y_a$. Hence, in this case, the minimum norm solution is given by $\hat{\theta}_a = X_a^\top (X_a X_a^\top)^{-1} y_a$.

In the second stage, we define a difference of the above estimators as $\tilde{\theta}_{\text{T-learner}} := \tilde{\theta}_1 - \tilde{\theta}_0$. Then, we predict the CATE $\tau^*(x)$ by

$$\hat{\tau}_{\text{T-learner}}(x) = x^\top \tilde{\theta}_{\text{T-learner}} = x^\top (\hat{\theta}_1 - \hat{\theta}_0).$$
This approach of taking the difference between separate estimators from different treatment groups is a commonly considered method in causal inference without overparameterization. This approach is named “T”-learner after the Two separate models used.

3.2 The IPW-learner with Known Propensity Score

We utilize an approach to correct shift of distributions of the observed and population covariates. Suppose that the population covariates are $y_1, \ldots, y_n$.

We derive our main result on the excess risk of the predictor. At the first step, we derive an upper bound of the risk, where the minimum of the empty set is defined as $\infty$.

This approach of taking the difference between separate estimators from different treatment groups is a commonly considered method in causal inference without overparameterization. This approach is named “T”-learner after the Two separate models used.

4 Excess Risk Bounds and Benign Overfitting in the T-learner

4.1 Effective Rank and Related Notion

To develop an upper bound of the risk of the T-learner, we define a notion of the effective rank to describe the benign overfitting, by following Bartlett et al. (2020).

Definition 4.1 (Effective Ranks). For a covariance operator $\Sigma$, define $\lambda_i = \mu_i(\Sigma)$ for $i = 1, 2, \ldots$. If $\sum_{i=1}^{\infty} \lambda_i < \infty$ and $\lambda_{k+1} > 0$ for $k \geq 0$, define

$$r_k(\Sigma) = \sum_{i \geq k} \lambda_i, \quad \text{and} \quad R_k(\Sigma) = \left( \frac{\sum_{i \geq k} \lambda_i}{\sum_{i \geq k} \lambda_i^2} \right)^2.$$

The effective rank is a measure of the complexity of covariances, using a tail of eigenvalues of the covariance matrix. It is used in the analysis of random matrices, such as in Koltchinskii and Lounici (2017), to represent the benign overfitting of ordinary linear regression.

Further, with a given $n \in \mathbb{N}$ and a constant $b > 0$, we define the following number of eigenvalues of the covariance operator $\Sigma$ which has a sufficiently large volume:

$$k^* = k^*_n \equiv \min \{ k \geq 0 : r_k(\Sigma) \geq bn \},$$

where the minimum of the empty set is defined as $\infty$. This notation is a continuation of the one used in Bartlett et al. (2020). The constant $b$ will be specified in theorems.

Also, with a given $n \in \mathbb{N}$, $\delta \in (0, 1)$ and a covariance operator $\Sigma$, we define the following terms

$$B_{n,\delta}(\Sigma) = \|\Sigma\| \max \left\{ \frac{r_0(\Sigma)}{n}, \frac{\log(\delta^{-1})}{n}, \frac{\log(\delta^{-1})}{n} \right\}, \quad \text{and} \quad \mathcal{V}_n(\Sigma) = \sigma^2 \left( \frac{k^*_n}{n} + \frac{n}{R_{k^*_n}(\Sigma)} \right).$$

These terms are used to describe the excess risk. In general, while $B_{n,\delta}(\Sigma)$ corresponds to a bias, $\mathcal{V}_n(\Sigma)$ relates to the variance of the prediction. How the aforementioned describe the error is explained by the following theorem.

4.2 Upper Bound

We derive our main result on the excess risk of the predictor. At the first step, we derive an upper bound of the risk, which is decomposed into bias and variance related terms. For $a \in \{0, 1\}$, we define $P_a = (X_aX_a^\top)^{-1}X_a$, and a projection operator to a complement space of $X_a$ as $\Pi_a := I - X_a^\top(X_aX_a^\top)^{-1}X_a$. 


Lemma 4.2 (Basic decomposition). The following inequality holds:

\[ R(\tilde{\theta}^{T}\text{-learner}) \leq \sum_{a \in \{0,1\}} (2\theta_a^* \Sigma A \theta_a^* + 2\tilde{\epsilon}_a^T \Sigma A \tilde{\epsilon}_a + 2\theta_a^T D_{a,1-a} \xi_1) - 2\theta_1^T \Sigma A \xi_1 - 2\epsilon_1^T F_{1,0} \epsilon_0, \]

where \( B_a = \Sigma A^\top \Sigma A \), \( B_{1,0} = \Sigma A^\top \Sigma A \), \( C_a = \Sigma A^\top \Sigma A \), \( D_{a,1-a} = \Sigma A^\top \Sigma A \), and \( F_{1,0} = \Sigma A^\top \Sigma A \).

The terms \( 2\theta_a^* \Sigma A \theta_a^* \) and \( \tilde{\epsilon}_a^T \Sigma A \tilde{\epsilon}_a \) mean bias and variance of the error by \( \tilde{\theta}_a \) for each \( a \in \{0,1\} \). In contrast, the rest of the terms \( \theta_a^T D_{a,1-a} \tilde{\epsilon}_1 \), \( \theta_1^T \Sigma A \xi_1 \), and \( \epsilon_1^T F_{1,0} \epsilon_0 \) denote the cross effects between \( \theta_1 \) and \( \theta_0 \). These items are specific to our setting.

By using the decomposition and the effective rank and notations, we present the following upper bound on the excess risk in the following theorem:

Theorem 4.3 (Upper bounds for the T-leaner in overparameterized models). For any \( \sigma_x \) there are \( b, c, c_1 > 1 \) for which the following holds. Consider a linear regression problem from Section 2.2 and suppose that Assumption 2.2, 2.3, and 2.4 hold. Suppose \( \delta \) and \( \sigma \) are such that \( \sigma < 1 \) with \( \log(1/\delta) \leq n/c \). If \( k^* \leq n/c_1 \), then the excess risk (Definition 2.1) of the predictor in (1) satisfies with probability at least \( 1 - \delta \):

\[
R(\tilde{\theta}^{T}\text{-learner}) \leq \sum_{a \in \{0,1\}} (c||\theta_a^*||^2 B_{n,a}(\Sigma_a) + ||\Sigma - \zeta_a^* \Sigma_a|| ||\theta_a^*||^2) + c||\theta_1^*|| ||\theta_0^*|| B_{n,a}(\Sigma_a)
+ c \log(\delta^{-1}) \left\{ V_n(\Sigma) + (||\theta_1^*|| + ||\theta_0^*||) \sqrt{V_n(\Sigma)} \right\},
\]

where \( \zeta_a^* = \arg\min_{\zeta \in \mathbb{R}^{+}} ||\Sigma - \zeta \Sigma_a||. \)

We obtain the following three implications from this result. (i) Regarding the bias terms, all the covariances \( \Sigma, \Sigma_1, \) and \( \Sigma_2 \) affect the upper bound. This means that if, for example, the treatment assignment significantly increases the effective rank of the covariance \( \Sigma_1 \) for the particular treatment group, it prevents this upper bound from being reduced to zero. (ii) The variance terms depend only on the covariance \( \Sigma \) of the population distribution and are unaffected by the covariance of each treatment group. This result contrasts with that of bias. (iii) Importantly, deviations of the covariance \( ||\Sigma - \zeta^* \Sigma_a|| \) appear in the bound. This means that if the covariance \( \Sigma_a \) of each treatment group \( a \in \{0,1\} \) has an eigenspace that is largely different from the covariance \( \Sigma \) of the population distribution, a non-negligible error will occur. This item has important implications for predicting treatment effects.

4.2.1 Difference from Ordinary Linear Regression in Bartlett et al. (2020)

For the ordinary regression without treatment effects, Bartlett et al. (2020) shows that an interpolating estimator has the following upper bound on the excess risk:

\[
c||\theta^*||^2 B_{n,a}(\Sigma) + c \log(\delta^{-1}) V_n(\Sigma),
\]

where \( \theta^* \in \mathbb{H} \) is a true parameter for the linear regression model. Our derived upper bound differs from that of Bartlett et al. (2020) in several aspects. First, there is a deviation of the covariance, \( ||\Sigma - \zeta^* \Sigma_a|| \). This term is due to the change in the distribution by the treatment assignment. Second, because of the cross terms from the different control groups; that is, \( \theta_1, \theta_0, \epsilon_1, \) and \( c_0 \), the terms \( c||\theta_1^*|| ||\theta_0^*|| B_{n,a}(\Sigma) \) and \( c(||\theta_1^*|| + ||\theta_0^*||) \log(1/\delta) \sqrt{V_n(\Sigma)} \) appear. Especially, the first difference is critical because it restricts the problem instances where benign overfitting occurs.

This difference indicates that, unlike the ordinary linear regression, the CATE prediction requires additional conditions in the overparameterization scheme. In the next section, we discuss the conditions for benign overfitting.

Remark (Excess risk lower bounds under overparameterized models). For the readers’ reference, we also remark the lower bound of the excess risk. For any \( \sigma_x \) there are \( b, c, c_1 > 1 \) for which the following holds. Consider a linear regression problem from Section 2.2 and suppose that Assumption 2.2, 2.3, and 2.4 hold. If \( k^* \geq n/c_1 \), then \( \mathbb{E} R(\tilde{\theta}) \geq \sigma^2/c. \) Otherwise,

\[
\mathbb{E} R(\tilde{\theta}^{T}\text{-learner}) \geq -c||\theta_1^*|| ||\theta_0^*|| B_n(\Sigma) + c^{-1} V_n(\Sigma),
\]

where \( B_n(\Sigma) = \int_0^1 B_{n,a}(\Sigma) d\delta. \) Unlike the lower bound shown in Bartlett et al. (2020), this lower bound does not give much information owing to the negative term \( -c||\theta_1^*|| ||\theta_0^*|| B_n(\Sigma). \)
4.3 Conditions for Benign Overfitting

We discuss the conditions for the convergence of the derived upper bound to zero, which is referred to as benign overfitting. For \( \Sigma \), we consider the following two cases. In the first case, \( \Sigma \) is a fixed operator between infinite-dimensional Hilbert spaces. In the second case, \( \Sigma \) can change with \( n \). For the latter case, we denote \( \Sigma \) by \( \Sigma_n \) to represent the dependency (resp. \( \Sigma_a \) by \( \Sigma_{a,n} \) for \( a \in \{0,1\} \)). Without loss of generality, in the following discussion, we may assume that \( \|\Sigma\| = 1 \).

In the latter case, for an ordinary linear regression case without treatment effects, Bartlett et al. (2020) reveals that benign overfitting occurs when a sequence of covariance operators \( \Sigma_n \) satisfies

\[
\lim_{n \to \infty} r_0(\Sigma_n) = \lim_{n \to \infty} \frac{k_n^a}{n} = \lim_{n \to \infty} \frac{n}{R_{k,n^*}(\Sigma_n)} = 0.
\]

Bartlett et al. (2020) further analyzes the conditions for the upper bound to go to zero in their Theorem 2. If (5) holds, both \( B_{n,\delta}(\Sigma) \) and \( V_n(\Sigma) \) in (4) obviously converge to zero as \( \delta \to 1 \).

To describe the situation where the benign overfitting occurs, we summarize desirable properties of covariance operators \( \Sigma \) as follow. Here, we consider both the case (a) where \( \Sigma \) is independent of \( n \), and the case (b) where \( \Sigma = \Sigma_n \) depends on \( n \) and the dimension of \( \Sigma_n \) increases with \( n \). These properties are developed by Bartlett et al. (2020).

**Definition 4.4 (Benign covariance).** We call a covariance matrix \( \Sigma \) is benign, if it satisfies either of the followings:

1. \( \Sigma \) is a fixed operator between infinite-dimensional spaces, and for some \( \beta > 0 \) it satisfies
   \[
   \mu_k(\Sigma) = k^{-\alpha} \ln^{-\beta}(k + 1),
   \]
   \[
   (b) \Sigma = \Sigma_n \text{ depends on } n, \text{ and satisfies the following with } \gamma_k = \Theta(\exp(-k/\tau)) \text{ for all } k \in \mathbb{N}:
   \mu_k(\Sigma_n) = (\gamma_k + \epsilon_n) \cdot \mathbb{I}\{k \leq p_n\}.
   \]

This condition concerns the covariance \( \Sigma \) of the population distribution, which also evaluates the covariance \( \Sigma_n \) of each treatment group \( a \in \{0,1\} \).

**Lemma 4.5.** If \( \Sigma \) is a benign covariance, we have \( \max_{a \in \{0,1\}} r_0(\Sigma_a) = o(n) \).

In CATE prediction, in addition to the abovementioned condition, we need conditions:

**Assumption 4.6 (Coherent covariance).** The following equality holds:

\[
\min_{\zeta \in \mathbb{R}^n} \|\Sigma - \zeta \Sigma_1\| = \min_{\zeta \in \mathbb{R}^n} \|\Sigma - \zeta \Sigma_0\| = 0.
\]

This condition is satisfied when the eigenspace of the covariance \( \Sigma_n \) of each assigned group coincides with the eigenspace of the covariance \( \Sigma \) of the population distribution. In other words, intuitively, the assignment rule must not change the data structure of the observation.

Then, combining Theorem 2 of Bartlett et al. (2020) and our new conditions (6), we summarize the conditions for the benign overfitting in the following theorem.

**Theorem 4.7 (Benign overfitting in the T-learner).** Suppose assumptions in Theorem 4.3 holds. Also, suppose that \( \Sigma \) is a benign covariance as Definition 4.4, and Assumption 4.6 holds. Then,

\[
R(\hat{\theta}_T) = o_p(1), \quad (n \to \infty),
\]

if and only if \( \alpha = 1 \) and \( \beta > 1 \) (case (a) in Definition 4.4), or \( p_n = \omega(n) \) and \( ne^{-o(n)} = \epsilon np_n = o(n) \) (case (b) in Definition 4.4).

Further, if we have \( p_n = \Omega(n) \) and \( \epsilon np_n = ne^{-o(n)} \) in the case (b) in Definition 4.4, we obtain

\[
R(\hat{\theta}_T) = O_p \left( \frac{\epsilon np_n + 1}{n} + \frac{\ln(n/\epsilon np_n)}{n} + \max \left\{ \frac{1}{n}, \frac{n}{p_n} \right\} \right).
\]

Except for the conditions (6), the statements are the identical to Theorem 2 in Bartlett et al. (2020). Therefore, in CATE prediction, it is important to determine whether (6) is satisfied or not. (6) is more problematic because the term does not usually go to zero even if we put some conditions on the eigenvalues. To consider which cases satisfy (6), we divide the problem instances into two situations: cases under RCTs and selection bias.
4.4 Benign Overfitting in Randomized Control and Sample Selection

Randomized Control Trial (RCT) : When we consider RCTs; that is, when a treatment assignment does not depend on covariates, we can simplify the covariance $\Sigma_a$ for each treatment group simpler. If the variable $d$ for the treatment assignment does not depend on $x$, then for each $a \in \{0, 1\}$, we have

$$\Sigma_a = \mathbb{E}[[d = a]xx^T] = p(d = a)\mathbb{E}[xx^T] = p(d = a)\Sigma.$$

Then, for $a \in \{0, 1\}$, we have $\min_{\zeta \in \mathbb{R}^+} ||\Sigma - \zeta \Sigma_a|| = ||\Sigma - 1/p(d = a)\Sigma_a|| = 0$ holds. This is a situation that standard RCTs satisfy, whereby we randomly assign treatments independently from the covariates. In addition, we also have $r_0(\Sigma_a) = p(d = a)r_0(\Sigma)$. Hence, the following statement holds without a proof.

**Proposition 4.8.** Suppose that the propensity score does not depend on the covariates; that is $p(d = a|x) = p(d = a)$. Then, Assumption 2.4 holds.

Therefore, when predicting the CATE on data collected by RCTs, the excess prediction risk converges to zero under the same conditions for linear regression discussed in Bartlett et al. (2020).

Selection Bias : If there is a selection bias in the sense that the treatment assignment depends on the covariate $x$, the conditions under which benign overfitting occurs are severe. Under selection bias, the covariance $\Sigma_a$ for each treatment group $a \in \{0, 1\}$ is given as $\Sigma_a = \mathbb{E}_a[\mathbb{E}[p(d = a|x)x|x^T|x]]$. This disallows us from decomposing $\Sigma_a$ into $p(d = a|x)$ and $\Sigma$. Therefore, we cannot make the deviation $\min_{\zeta \in \mathbb{R}^+} ||\Sigma - \zeta \Sigma_a||$ zero.

5 Excess Risk Bounds and Benign Overfitting in the IPW-learner

First, to evaluate the IPW-learner, we define a new excess risk as

$$\hat{R}(\theta) := \mathbb{E}_{x,y}\left[(\hat{y} - x^T \theta)^2 - (\hat{y} - x^T \theta^*)^2\right].$$

Importantly, this new risk is same to the risk given in Definition 2.1.

**Lemma 5.1.** For any $\theta \in \mathbb{H}$, we have $R(\theta) = \hat{R}(\theta)$.

Next, when using the IPW estimator, we confirm that Assumptions 1, 3, and 4 in Definition 1 of Bartlett et al. (2020) can be replaced as follows.

**Lemma 5.2 (Basic assumptions in the IPW-learner).** Under Assumptions 2.2–2.4, the following hold:

1’ $x$ and $\hat{y}$ are mean zero;

2’ the conditional noise variance is bounded below by some constant $\tilde{\sigma}^2$: $\mathbb{E}[(\hat{y} - x^T \theta^*)^2|x] \geq \tilde{\sigma}^2$.

3’ $\hat{y} - x^T \theta^*$ is $\tilde{\sigma}^2$-sub-Gaussian, conditionally on $x$, that is for all $\lambda \in \mathbb{R}$, $\mathbb{E}[\exp(\lambda(\hat{y} - x^T \theta^*))|x] \leq \exp(\tilde{\sigma}^2 \lambda^2/2)$.

Since the statements in Lemma 5.2 correspond to Assumptions 1, 3, and 4 in Definition 1 in Bartlett et al. (2020), we can directly apply Theorem 1 of Bartlett et al. (2020) to obtain the following result by combining them with Assumptions 2.2.

**Theorem 5.3 (Excess risk upper bounds in IPW-learner).** For any $\sigma_\theta$, there are $h, c, c_1 > 1$ for which the following holds. Consider a linear regression problem from Section 2.2 and suppose that Assumption 2.2, 2.3, and 2.4, hold. Suppose $\delta < 1$ with $\log(1/\delta) < n/c$. If $k^* < n/c_1$, then the excess risk (Definition 2.1) of the predictor in (3) satisfies

$$R(\hat{\theta}_{\text{IPW-learner}}) \leq c||\theta^*\|^2B_{n,\lambda}(\Sigma) + c\log(1/\delta)V_n(\Sigma).$$

with probability at least $1 - \delta$.

Thus, the upper bound has the same form as that of Bartlett et al. (2020), although some constant terms are affected by the construction of the IPW estimator. As presented in Bartlett et al. (2020), if (5) is satisfied, the upper bound goes to zero. This means that this upper bound goes to zero under the same condition as that in Bartlett et al. (2020).

**Theorem 5.4 (Benign overfitting in IPW-learner).** Suppose that the assumptions in Theorem 5.3 hold. Also, suppose that $\Sigma$ is a benign covariance as Definition 4.4. Then, we have

$$R(\hat{\theta}_{\text{IPW-learner}}) = o_p(1), \ (n \to \infty),$$

if and only if $\alpha = 1$ and $\beta > 1$ (case (a) in Definition 4.4), or $p_n = \omega(n)$ and $ne^{-o(n)} = \epsilon_np_n = o(n)$ (case (b) in Definition 4.4).
Further, if we have $p_n = \Omega(n)$ and $\epsilon_n p_n = ne^{-o(n)}$ the case (b) in Definition 4.4), we obtain

$R(\hat{\theta}_{\text{IPW-learner}}) = O_p\left(\frac{\epsilon_n p_n + 1}{n} + \frac{\ln(n/\epsilon_n p_n)}{n} + \max\left\{\frac{1}{n}, \frac{n}{p_n}\right\}\right)$. 

In this result, unlike the case where we use the T-learner, the upper bound goes to zero for both cases with RCTs and selection bias. This is because the deviation term $\|\Sigma - \zeta^*\Sigma_a\|$ in Theorem 4.3 does not appear when using the IPW-learner.

6 Discussion

6.1 CATE Estimation in Non-overparametrized Setting

When the model is not overparametrized, both the T-learner and IPW-learner have a risk converges to zero as $n \to \infty$ (Abrevaya et al., 2015). This fact is contrasive to our results with overparameterization, especially for the case of the T-learner. This result implies the potential danger of using the T-learner in large-scale models.

6.2 Application to Doubly Robust Estimator

The doubly robust estimator (Porter et al., 2011; Funk et al., 2011; Foster and Syrgkanis, 2019; Kennedy, 2020) is another common choice for the CATE prediction. An advantage of the double robust estimator is that an asymptotic variance of the estimator is semiparametric efficient; that is, the asymptotic variance achieves its lower bound (Hahn, 1998; Chernozhukov et al., 2018). However, some problems appear in the overparameterization setting, when this method estimates an conditional outcome $E[y_{a,i}|x_i]$ as preparation. Specifically, according to our results, the T-learner is not guaranteed to be valid to estimate the outcome under overparameterization. Even if the IPW-learner is used, we need the correct propensity score. Unless these issues are resolved, it is difficult to utilize the doubly robust estimator with overparameterization.

6.3 Implications for Applications

Our result implies the importance of bias correction methods. When data is collected via RCTs, we recommend the usual method, such as performing regressions for each assigned group like the T-learner. In contrast, if there is selection bias, we recommend to achieve a correct assigned probability and utilize the IPW-learner.

7 Conclusion

We investigate the necessary conditions for benign overfitting in CATE prediction using a linear regression model. For predicting the CATE, we consider two methods: the T-learner and IPW learner. When the treatment assignment $d$ does not depend on the covariates, both the T-learner and IPW-learner with interpolating prediction rule show benign-overfitting. However, when the treatment assignment $d_i$ depends on the covariates, the excess risk of the T-learner does not converge to zero, while that of the IPW-learner converges. Thus, this paper shows the situation in which CATE prediction with an overparameterized model works.

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A Auxiliary Results from Bartlett et al. (2020) and Vershynin (2018)

Proposition A.1 (Lemma S.2 in Bartlett et al. (2020)). Consider random variables $\epsilon_1, \ldots, \epsilon_n$, conditionally independent given $X$ and conditionally $\sigma^2$-sub-Gaussian, that is, for all $\lambda \in \mathbb{R}$,
\[
\mathbb{E}[\exp(\lambda \epsilon_i) | X] \leq \exp(\sigma^2 \lambda^2 / 2).
\]
Suppose that, given $X$, $M \in \mathbb{R}^{n \times n}$ is a.s. positive semidefinite. Then a.s. on $X$, with conditional probability at least $1 - \exp(-t)$,
\[
\epsilon^\top M \epsilon \leq \sigma^2 \text{tr}(M) + 2\sigma^2 \|M\| t + 2\sigma^2 \sqrt{\|M\|^2 t^2 + \text{tr}(M^2) t}.
\]

Proposition A.2 (Lemma S.3 in Bartlett et al. (2020)). Suppose $k < n$, $A \in \mathbb{R}^{n \times n}$ is an invertible matrix, and $Z \in \mathbb{R}^{n \times k}$ is such that $ZZ^\top + A$ is invertible. Then
\[
ZZ^\top + A = (I + Z^\top A^{-1} Z)^{-1} ZZ^\top A^{-1} Z (I + Z^\top A^{-1} Z)^{-1}.
\]

Proposition A.3 (Bernstein’s inequality, Lemma S.5 in Bartlett et al. (2020)). There is a universal constant $c$ such that, for any independent, zero mean, sub-Gaussian random variables $\xi_1, \ldots, \xi_N$, any $a = (a_1, \ldots, a_N) \in \mathbb{R}^n$, and any $t \geq 0$,
\[
\mathbb{P}\left(\sum_{i=1}^N a_i \xi_i > t\right) \leq 2 \exp\left(-c \min\left(\frac{t^2}{\sigma^2 \sum_{i=1}^N a_i^2}, \frac{t}{\sigma \max_{1 \leq i \leq N} a_i}\right)\right).
\]

Proposition A.4 (Corollary S.6 in Bartlett et al. (2020)). There is a universal constant $c$ such that for any non-increasing sequence $\{\lambda_i\}_{i=1}^{\infty}$ of non-negative numbers such that $\sum_{i=1}^{\infty} \lambda_i < \infty$, and any independent, centered, sub-Gaussian random variables $\{\xi_i\}_{i=1}^{\infty}$, any $x > 0$, with probability at least $1 - 2e^{-x}$
\[
\sum_{i=1}^{\infty} \lambda_i \xi_i \leq c \sigma \max\left(x \lambda_1, \sqrt{x \sum_{i=1}^{\infty} \lambda_i^2}\right).
\]

Proposition A.5 ($\epsilon$-net argument, Lemma S.8 in Bartlett et al. (2020)). Suppose $A \in \mathbb{R}^{n \times n}$ is a symmetric matrix, and $\mathcal{N}_\epsilon$ is an $\epsilon$-net on the unit sphere $S^{n-1}$ in the Euclidean norm, where $\epsilon < \frac{1}{2}$. Then
\[
\|A\| \leq (1 - \epsilon)^{-2} \max_{x \in \mathcal{N}_\epsilon} |x^\top Ax|.
\]

Proposition A.6 (General Hoeffding inequality, Theorem 2.6.3 in Vershynin (2018)). There is a universal constant $c$ such that, for any independent, mean zero, sub-Gaussian random variables $\xi_1, \ldots, \xi_N$, any $a = (a_1, \ldots, a_N) \in \mathbb{R}^n$, and any $t \geq 0$,
\[
\mathbb{P}\left(\sum_{i=1}^N a_i \xi_i > t\right) \leq 2 \exp\left(-c \min\left(\frac{t^2}{\sigma^2 \sum_{i=1}^N a_i^2}, \frac{t}{\sigma \max_{1 \leq i \leq N} a_i}\right)\right).
\]

Corollary A.7. There is a universal constant $c$ such that for any non-increasing sequence $\{\lambda_i\}_{i=1}^{\infty}$ of non-negative numbers such that $\sum_{i=1}^{\infty} \lambda_i < \infty$, and any independent, centered, sub-Gaussian random variables $\{\xi_i\}_{i=1}^{\infty}$, and any $x > 0$, with probability at least $1 - 2e^{-x}$
\[
\sum_{i=1}^{\infty} \lambda_i \xi_i \leq c \sigma \sqrt{x \sum_{i=1}^{\infty} \lambda_i^2}.
\]

B Proof of Lemma I.1

Proof. First, as in the proof of Bartlett et al. (2020), we have
\[
R(\theta^\text{learner}) = \mathbb{E}_{x,y} [\hat{y} - x^\top \hat{\theta}]^2 = \mathbb{E}_x [x^\top (\theta^* - \hat{\theta})]^2.
\]
We can decompose $\mathbb{E}_x [x^\top (\theta^* - \hat{\theta})]^2$ as
\[
\mathbb{E}_x [x^\top (\theta^* - \hat{\theta})]^2 = \mathbb{E}_x [(x^\top (\theta^* - \hat{\theta}) - x^\top (\theta^*_1 - \hat{\theta}) + x^\top (\theta^*_1 - \hat{\theta}) - x^\top (\theta^*_0 - \hat{\theta})]^2
\]
\[
= \mathbb{E}_x [(x^\top (\theta^*_1 - \hat{\theta}) - x^\top (\theta^*_0 - \hat{\theta})|^2 + \mathbb{E}_x [(x^\top (\theta^*_0 - \hat{\theta})^2) - 2 \mathbb{E}_x [((\theta^*_1 - \hat{\theta})^\top x)(x^\top (\theta^*_0 - \hat{\theta}))]].
\]

Excess risk of $y_1$. Excess risk of $y_0$. Excess risk incurred by the difference between $y_1$ and $y_0$. 

13
In Lemma 2 of Bartlett et al. (2020), by using Lemma S.2 and S.18 of Bartlett et al. (2020), the authors show

\[
\mathbb{E}_x \left[ \left( x^T (\theta_1^* - \hat{\theta}_1) \right)^2 \right] \leq 2 \theta_1^T B_1 \theta_1^* + 2 \epsilon_1^T C_1 \epsilon_1,
\]

\[
\mathbb{E}_{x, \epsilon} \left[ \left( x^T (\theta_1^* - \hat{\theta}_1) \right)^2 \right] \geq \theta_1^T B_1 \theta_1^* + \sigma_1^2 \text{tr}(C_1),
\]

\[
\mathbb{E}_x \left[ \left( x^T (\theta_0^* - \hat{\theta}_0) \right)^2 \right] \leq 2 \theta_0^T B_0 \theta_0^* + 2 \epsilon_0^T C_0 \epsilon_0,
\]

\[
\mathbb{E}_{x, \epsilon} \left[ \left( x^T (\theta_0^* - \hat{\theta}_0) \right)^2 \right] \geq \theta_0^T B_0 \theta_0^* + \sigma_0^2 \text{tr}(C_0).
\]

Our remaining task is to consider the bound of \( \left( \theta_1^* - \hat{\theta}_1 \right)^T \left( \theta_0^* - \hat{\theta}_0 \right) \), which is decomposed as

\[
\mathbb{E}_x \left[ \left( \left( \theta_1^* - \hat{\theta}_1 \right)^T x \right) \left( \theta_0^* - \hat{\theta}_0 \right) \right] = \mathbb{E}_x \left[ \left( \theta_1^T (I - X_1^T X_1^*)^{-1} X_1 - \epsilon_1^T (X_1^*)^{-1} X_1 x \right) \left( \theta_0^* - \hat{\theta}_0 \right) \right]
\]

\[
= \left( \theta_1^T (I - X_1^T X_1^*)^{-1} X_1 \right) \Sigma (I - X_0^T X_0^*)^{-1} X_0 \theta_0^* - \epsilon_1^T (X_1^*)^{-1} X_1 \Sigma (I - X_0^T X_0^*)^{-1} X_0 \theta_0^* + \epsilon_1^T (X_1^*)^{-1} X_1 \Sigma (I - X_0^T X_0^*)^{-1} X_0 \theta_0^*.
\]

Therefore, \( \mathbb{E}_x \left[ \left( \left( \theta_1^* - \hat{\theta}_1 \right)^T x \right) \left( \theta_0^* - \hat{\theta}_0 \right) \right] = \theta_1^T B_1 \theta_1^* - \theta_1^T D \epsilon_0 - \epsilon_1^T E \theta_0^* + \epsilon_1^T F \epsilon_0 \), and \( \mathbb{E}_{x, \epsilon} \left[ \left( \theta_1^* - \hat{\theta}_1 \right)^T x \left( \theta_0^* - \hat{\theta}_0 \right) \right] = \theta_1^T B_{1,0} \theta_0^*.
\]

Thus, we obtain the upper bound as

\[
R(\hat{\theta}^{T\text{-learner}}) \leq 2 \theta_1^T B_1 \theta_1^* + 2 \epsilon_1^T C_1 \epsilon_1 + 2 \theta_0^T B_0 \theta_0^* + 2 \epsilon_0^T C_0 \epsilon_0 - 2 \theta_1^T B_{1,0} \theta_0^* + 2 \epsilon_1^T E \theta_0^* + 2 \epsilon_1^T F \epsilon_0 - 2 \epsilon_1^T G \epsilon_0
\]

and the lower bound as

\[
\mathbb{E}_{x, \epsilon} \left[ R(\hat{\theta}^{T\text{-learner}}) \right] \geq \theta_1^T B_1 \theta_1^* + \sigma_1^2 \text{tr}(C_1) + \theta_0^T B_0 \theta_0^* + \sigma_0^2 \text{tr}(C_0) - 2 \epsilon_1^T B_{1,0} \theta_0^*.
\]

\[\square\]

C Proof of Lemma I.2

**Proof.** We consider only the case \( a = 1 \). The case \( a = 0 \) can be proved in the same way. Note that

\[
(I - X_1^T (X_1 X_1^T)^{-1} X_1) X_1^T = X_1^T - X_1^T (X_1 X_1^T)^{-1} (X_1 X_1^T) = 0.
\]

Moreover, for any \( v \) in the orthogonal complement to the span of the columns of \( X_1^T \),

\[
(I - X_1^T (X_1 X_1^T)^{-1} X_1) v = v.
\]

Thus,

\[
\|I - X_1^T (X_1 X_1^T)^{-1} X_1\| \leq 1.
\]

Given \( \zeta^* = \arg \min_{\zeta \in \mathbb{R}^+} \| \Sigma - \zeta \Sigma_0 \| \), we apply (7) to write

\[
\theta_1^T B_1 \theta_1^* = \theta_1^T (I - X_1^T (X_1 X_1^T)^{-1} X_1) \Sigma (I - X_1^T (X_1 X_1^T)^{-1} X_1) \theta_1^*
\]

\[
= \theta_1^T (I - X_1^T (X_1 X_1^T)^{-1} X_1) \left( \zeta^* \Sigma_1 - \zeta^* \frac{1}{n} X_1^T X_1 \right) (I - X_1^T (X_1 X_1^T)^{-1} X_1) \theta_1^*
\]

\[
+ \theta_1^T (I - X_1^T (X_1 X_1^T)^{-1} X_1) (\Sigma - \zeta^* \Sigma_1) (I - X_1^T (X_1 X_1^T)^{-1} X_1) \theta_1^*.
\]
Combining with (8) shows that

\[ \theta_1^* \top B_1 \theta_1^* \leq \zeta \left\| \Sigma_1 - \frac{1}{n} X_1 \top X_1 \right\| \left\| \theta_1^* \right\|^2 + \| \Sigma - \zeta \Sigma_1 \| \left\| \theta_1^* \right\|^2. \]

Thus, due to Theorem 9 in Koltchinskii and Lounici (2017), there is an absolute constant \( c \) such that for any \( t > 1 \) with probability at least \( 1 - \exp(-t) \),

\[ \theta_1^* \top B_1 \theta_1^* \leq c \| \theta_1^* \|^2 \| \Sigma_1 \| \max \left\{ \sqrt{\frac{r(\Sigma_1)}{n}}, \frac{r(\Sigma_1)}{n}, \frac{t}{n} \right\} + \| \Sigma - \zeta \Sigma_1 \| \left\| \theta_1^* \right\|^2, \]

where

\[ r(\Sigma_1) := \frac{(\mathbb{E} || x ||^2)^2}{\| \Sigma_1 \|} \leq \frac{\text{tr}(\Sigma_1)}{\| \Sigma_1 \|} = \frac{1}{\lambda_1} \sum_i \lambda_i = r_0(\Sigma_1). \]

Since \( 1 < t < n \) implies \( \sqrt{\frac{t}{n}} > \frac{1}{n} \),

\[ \theta_1^* \top B_1 \theta_1^* \leq c \| \theta_1^* \|^2 \| \Sigma_1 \| \max \left\{ \sqrt{\frac{r(\Sigma_1)}{n}}, \frac{r(\Sigma_1)}{n}, \sqrt{\frac{t}{n}} \right\} + \| \Sigma - \zeta \Sigma_1 \| \left\| \theta_1^* \right\|^2, \]

\[ \square \]

D

**Proof of Lemma 1.3**

*Proof.* Recall that

\[ B_{1,0} = (I - X_1 \top (X_1 X_1 \top)^{-1} X_1) \Sigma (I - X_0 \top (X_0 X_0 \top)^{-1} X_0) \]

Now we can apply (7) to write

\[ \theta_1^* \top B_{1,0} \theta_1^* \]

\[ = \theta_1^* \left( I - X_1 \top (X_1 X_1 \top)^{-1} X_1 \right) \Sigma \left( I - X_0 \top (X_0 X_0 \top)^{-1} X_0 \right) \theta_1^* \]

\[ = \theta_1^* \left( I - X_1 \top X_1 \right) \Sigma \left( I - X_0 \top X_0 \right) \theta_1^* + \frac{1}{n} X_0 \top X_1 \theta_1^* \]

where \( X_1 \top X = X_1 \top X_1 + X_1 \top X_0 + X_0 \top X_1 + X_0 \top X_0 \). Here, note that \( X_0 \top X_1 = 0 \). Combining with (8) shows that

\[ \theta_1^* \top B_{1,0} \theta_1^* \leq \left\| \Sigma - \frac{1}{n} X_1 \top X \right\| \left\| \theta_1^* \right\| \left\| \theta_1^* \right\| \]

Thus, due to Theorem 9 in Koltchinskii and Lounici (2017), there is an absolute constant \( c \) such that for any \( t > 1 \) with probability at least \( 1 - \exp(-t) \),

\[ \left| 2 \theta_1^* \top B_{1,0} \theta_1^* \right| \leq c \| \theta_1^* \| \| \theta_1^* \| \| \Sigma \| \max \left\{ \sqrt{\frac{r(\Sigma)}{n}}, \frac{r(\Sigma)}{n}, \frac{t}{n} \right\}, \]

where

\[ r(\Sigma) := \frac{(\mathbb{E} || x ||^2)^2}{\| \Sigma \|} \leq \frac{\text{tr}(\Sigma)}{\| \Sigma \|} = \frac{1}{\lambda_1} \sum_i \lambda_i = r_0(\Sigma). \]

\[ \square \]
E Proof of Lemma I.5

We use the fact $X_1 \Sigma X_0^\top = 0$ and compute the term as

$$D = (I - X_1^\top (X_1 X_1^\top)^{-1} X_1) \Sigma X_0^\top (X_0 X_0^\top)^{-1} = \Sigma X_0^\top (X_0 X_0^\top)^{-1}$$

**Lemma E.1.** For each $a \in \{0, 1\}$, consider random variables $\varepsilon_a = (\varepsilon_{a,1}, \ldots, \varepsilon_{a,n})$, conditionally independent given $X_a$ and conditionally $\sigma^2$ sub-Gaussian, that is, for all $\lambda \in \mathbb{R}$,

$$\mathbb{E} [\exp (\lambda \varepsilon_{a,i}) | X_a] \leq \exp (\sigma^2 \lambda^2 / 2).$$

Then a.s. on $X_1$ and $X_0$, with conditional probability at least $1 - \exp(-t)$,

$$\lambda_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1} \varepsilon_0 < \sqrt{2t \sigma^2 \| \lambda_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1} \|_2^2}.$$

Similarly, a.s. on $X_1$ and $X_0$, with conditional probability at least $1 - \exp(-t)$,

$$\varepsilon_1 (X_1 X_1^\top)^{-1} X_1 \Sigma \theta_0^* < \sqrt{2t \sigma^2 \| \lambda_1^\top \Sigma X_1^\top (X_1 X_1^\top)^{-1} \|_2^2}.$$

**Proof.** We only prove the first statement. The second statement can be shown in the same way.

For any $v = (v_1, ..., v_n) \in \mathbb{R}_+^n$, the following inequality holds:

$$\mathbb{E} [\exp (v^\top \varepsilon_a) | X_a] = \prod_{i=1}^n \mathbb{E} [\exp (v_i \varepsilon_{a,i}) | X_a]$$

$$\leq \prod_{i=1}^n \exp (\sigma^2 v_i^2 / 2) = \exp \left( \sigma^2 \sum_{i=1}^n v_i^2 / 2 \right) = \exp \left( \sigma^2 \| v \|_2^2 / 2 \right).$$

By replacing $v$ with $\lambda \theta_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1}$ and using Chernoff bound (Section 2.2, Boucheron et al., 2004), for any $s \geq 0$,

$$\theta_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1} \varepsilon > s$$

for $\lambda \geq 0$ with probability at most

$$\frac{\mathbb{E} [\exp (v^\top \varepsilon_a) | X_a]}{\exp (-\lambda s)} \leq \exp \left( \lambda^2 \sigma^2 \| \theta_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1} \|_2^2 / 2 - \lambda s \right)$$

almost surely conditional on $X_1$ and $X_0$. Letting

$$\lambda = \frac{s}{\sigma^2 \| \theta_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1} \|_2^2}$$

gives the bound

$$\exp \left( - \frac{s^2}{2 \sigma^2 \| \theta_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1} \|_2^2} \right).$$

Then, letting $t = \frac{s^2}{2 \sigma^2 \| \theta_1^\top \Sigma X_0^\top (X_0 X_0^\top)^{-1} \|_2^2}$, we complete the proof.

\[\square\]

F Related Results in Section I.3

**Corollary F.1** (Refinement of Corollary S.7 in Bartlett et al. (2020)). Suppose $z \in \mathbb{R}^n$ is a random vector with independent $\sigma^2$ sub-Gaussian coordinates with unit variances, $L$ is a random subspace of $\mathbb{R}^n$ of codimension $k$, and $L$ is independent of $z$. Then for some universal constants $c_1, c_2$ and any $t > 0$, with probability at least $1 - 3 \exp(-t)$,

$$\|z\|^2 \leq n + c_1 (t + \sqrt{nt}),$$

$$\|\Pi_L z\|^2 \geq n - c_2 (k + t + \sqrt{nt}),$$

where $\Pi_L$ is the orthogonal projection on $L$. 

16
\textbf{Proof.} First, note that $z$ can have non-zero mean. Therefore, we consider centralizing it as $\tilde{z} = z - \mathbb{E}[z]$. We can apply Corollary S.7 in Bartlett et al. (2020) to $\tilde{z}$. Then, for any $t > 0$, with probability at least $1 - 2\exp(-t)$,
\[
\|\tilde{z}\|^2 \leq n + a'(t + \sqrt{n}t),
\]
where $a'$ is a constant. Therefore,
\[
\|z\|^2 \leq \|z - \mathbb{E}[z]\|^2 + \|\mathbb{E}[z]\|^2 \leq \|\mathbb{E}[z]\|^2 + n + a(t + \sqrt{n}t) \leq n + a(t + \sqrt{n}t).
\]
Similarly, for any $t > 0$, with probability at least $1 - \exp(-t)$,
\[
\|\Pi_L \tilde{z}\|^2 \geq n - a(2k + 4t + c \max(t, \sqrt{n}t)).
\]
We also have
\[
\|\Pi_L \mathbb{E}[z]\|^2 + \|\Pi_L z\|^2 \geq \|\Pi_L \tilde{z}\|^2.
\]
Therefore, with probability at least $1 - 3\exp(-t)$
\[
\|z\|^2 \leq n + c_1 \max(t, \sqrt{n}t),
\]
\[
\|\Pi_L z\|^2 \geq \|\tilde{z}\|^2 - \sigma^2(2k + 4t) - \|\Pi_L \mathbb{E}[z]\|^2 \\
\geq n - c_2(2k + 4t + c \max(t, \sqrt{n}t)).
\]
\hfill \Box

\section{Proof of Lemma 5.2}

\textbf{Proof.} First, we have
\[
\hat{y} = \frac{1[d = 1]y_1}{p(d = 1|x)} + \frac{1[d = 0]y_0}{p(d = 0|x)}
\]
From Assumptions 2.4,
\[
\mathbb{E}[\hat{y}] = \mathbb{E}\left[\frac{1[d = 1]y_1}{p(d = 1|x)} - \frac{1[d = 0]y_0}{p(d = 0|x)}\right] = \mathbb{E}\left[\frac{p(d = 1|x)\mathbb{E}[y_1|x] - p(d = 0|x)\mathbb{E}[y_0|x]}{p(d = 1|x)}\right] = \mathbb{E}[y_1] - \mathbb{E}[y_0].
\]
From Assumption 2.2, $\mathbb{E}[y_1] = \mathbb{E}[y_0] = 0$. Therefore, $\mathbb{E}[\hat{y}] = 0$. Thus, Statement 1' holds.

The conditional noise variance can be written as
\[
\mathbb{E}\left[ (\hat{y} - x^\top \theta^*)^2 | x \right] \\
= \mathbb{E}\left[ (\hat{y}^2) | x \right] - (x^\top \theta^*)^2 \\
= \mathbb{E}\left[ \frac{1[d = 1]y_1^2}{p^2(d = 1|x)} + \frac{2[1[d = 1]1[d = 0]y_1y_0}{p(d = 1|x)p(d = 0|x)} + \frac{1[d = 0]y_0^2}{p^2(d = 0|x)} | x \right] - \left(\tau^*(x)\right)^2 \\
= \frac{p(d = 1|x)\mathbb{E}\left[y_1^2 | x\right]}{p^2(d = 1|x)} + \frac{p(d = 0|x)\mathbb{E}\left[y_0^2 | x\right]}{p^2(d = 0|x)} - \left(\tau^*(x)\right)^2 \\
= \mathbb{E}\left[y_1^2 | x\right] + \frac{\mathbb{E}\left[y_0^2 | x\right]}{p(d = 0|x)} - \left(x^\top \theta_1^* - x^\top \theta_0^*\right)^2 \\
\geq \mathbb{E}\left[y_1^2 | x\right] + \frac{\mathbb{E}\left[y_0^2 | x\right]}{p(d = 0|x)} - \left(x^\top \theta_1^*\right)^2 - \left(x^\top \theta_0^*\right)^2 \\
= \mathbb{E}\left[y_1^2 | x\right] + \frac{\mathbb{E}\left[y_0^2 | x\right]}{p(d = 0|x)} - \mathbb{E}[y_1^2 | x] - \mathbb{E}[y_0^2 | x] + \mathbb{E}[y_1^2 | x] - \mathbb{E}[y_0^2 | x] - \left(x^\top \theta_1^*\right)^2 - \left(x^\top \theta_0^*\right)^2 \\
= \mathbb{E}\left[(1 - p(d = 1|x))y_1^2 | x\right] + \frac{(1 - p(d = 0|x))\mathbb{E}\left[y_0^2 | x\right]}{p(d = 0|x)} + \mathbb{E}\left[(y_1 - x^\top \theta_1^*)^2 | x\right] + \mathbb{E}\left[(y_0 - x^\top \theta_0^*)^2 | x\right] \\
\geq 2\sigma^2,
\]
where we use \( \mathbb{E}[y|x] = x^\top \theta^* = \tau^*(x) \), \( \mathbb{I}[d = 1]|d = 0] = 0, \) and \( \mathbb{E}[(y_a - x^\top \theta_a^*)^2|x] \geq \sigma^2 \) (from Assumption 2.2). Thus, Statement 3' holds.

Proposition 2.5.2 in Vershynin (2018) states that for a random variable \( R \), \( \mathbb{E}([\exp(R^2)]) < \infty \) is equivalent to \( R \) being a sub-Gaussian random variable. Here, from Assumption 2.4 \((1/p(d = a|x) < \infty)\),

\[
\mathbb{E}\left[ \exp\left( (\hat{y} - x^\top \theta^*)^2 \right) \right]
\]
\[
= \mathbb{E}\left[ \exp\left( \left( \frac{\mathbb{I}[d = 1]y_1}{p(d = 1|x)} - \frac{\mathbb{I}[d = 0]y_0}{p(d = 0|x)} - x^\top \theta^* \right)^2 \right) \middle| x \right]
\]
\[
= \mathbb{E}\left[ \exp\left( \left( \frac{\mathbb{I}[d = 1]y_1}{p(d = 1|x)} - \frac{\mathbb{I}[d = 0]y_0}{p(d = 0|x)} \right) + \frac{\mathbb{I}[d = 1]x^\top \theta_a^*}{p(d = 1|x)} + \frac{\mathbb{I}[d = 0]x^\top \theta_0^*}{p(d = 0|x)} \right)^2 \middle| x \right]
\]
\[
\leq \mathbb{E}\left[ \exp\left( \sum_a \left( \frac{\mathbb{I}[d = a](y_a - x^\top \theta_a^*)}{p(d = a|x)} \right)^2 + \sum_a \left( \frac{\mathbb{I}[d = a]x^\top \theta_0^* - x^\top \theta_a^*}{p(d = a|x)} \right)^2 \right) \middle| x \right] \leq \infty,
\]

where we also assume that \( y_a - x^\top \theta_a^* \) is \( \sigma_a^2 \)-sub-Gaussian, conditionally on \( x \). Thus, \( \hat{y} - x^\top \theta^* \) is also sub-Gaussian, and Statement 4' holds.

\[\square\]

### Proof of Lemma 3.1

**Proof.**

\[
\mathbb{E}[\hat{y}_i|x] = \mathbb{E}\left[ \frac{\mathbb{I}[d_i = 1]y_i}{p(d = 1|x)} - \frac{\mathbb{I}[d_i = 0]y_0}{1 - p(d = 1|x)} \right] = \mathbb{E}\left[ \frac{\mathbb{I}[d_i = 1]|y_{1,i},x|}{p(d = 1|x)} - \frac{\mathbb{I}[d_i = 0]|y_{0,i},x|}{1 - p(d = 1|x)} \right]
\]
\[
= \frac{\mathbb{E}[|y_{1,i},x|]}{p(d = 1|x)} - \frac{\mathbb{E}[|y_{0,i},x|]}{1 - p(d = 1|x)} = \mathbb{E}[|y_{1,i}|x] - \mathbb{E}[|y_{0,i}|x] = \tau^*(x)
\]

\[\square\]

### I Proof of Theorem 4.3

This section provides the proof of Theorem 4.3. In Lemma I.1, we first decompose the excess risk. Then, the following lemmas (Lemma I.2–I.6) show the upper or lower bounds of each decomposed term. The proof of each lemma is provided in Sections I.2–I.5. Combining these bounds, Section I.6 completes the proof.

#### I.1 Basic Decomposition of the Excess Risk and Associated Lemmas

First, we decompose the upper and lower bounds of the excess risk into several terms that can be bounded.

**Lemma I.1** (Full version of Lemma 4.2).

\[
R(\hat{\theta}^{T-learner}) = \mathbb{E}_x \left[ (x^\top(\theta^*_1 - \hat{\theta}_1))^2 \right] + \mathbb{E}_x \left[ (x^\top(\theta_a^*_0 - \hat{\theta}_0))^2 \right] - 2\mathbb{E}_x \left[ (\theta_a^*_1 - \hat{\theta}_1)^\top x_i \right] \left( (x_i^\top \theta_a^*_0 - \hat{\theta}_0) \right)
\leq 2\theta_1^T B_1 \theta_1^* + 2\varepsilon_1^T C_1 \varepsilon_1 + 2\theta_a^T B_0 \theta_a^* + 2\varepsilon_a^T C_0 \varepsilon_0 - 2\theta_1^T B_1 \theta_0^* + 2\theta_a^T D \varepsilon_0 + 2\varepsilon_1^T E \theta_0^* - 2\varepsilon_1^T F \varepsilon_0. \quad (9)
\]
and
\[
\mathbb{E}_{\varepsilon, \xi} \left[ R(\hat{\theta}^{T\text{-learner}}) \right] \geq \theta_1^*^T B_1 \theta_1^* + \sigma_1^2 \text{tr}(C_1) + \theta_0^T B_0 \theta_0^* + \sigma_1^2 \text{tr}(C_0) - 2\theta_1^*^T B_{1,0} \theta_0^*,
\] (10)
where
\[
B_1 = (I - X_1^T (X_1 X_1^T)^{-1} X_1) \Sigma (I - X_1^T (X_1 X_1^T)^{-1} X_1)
\]
\[
B_0 = (I - X_0^T (X_0 X_0^T)^{-1} X_0) \Sigma (I - X_0^T (X_0 X_0^T)^{-1} X_0)
\]
\[
B_{1,0} = (I - X_1^T (X_1 X_1^T)^{-1} X_1) \Sigma (I - X_0^T (X_0 X_0^T)^{-1} X_0)
\]
\[
C_1 = (X_1 X_1^T)^{-1} X_1 \Sigma X_1^T (X_1 X_1^T)^{-1}
\]
\[
C_0 = (X_0 X_0^T)^{-1} X_0 \Sigma X_0^T (X_0 X_0^T)^{-1}
\]
\[
D = (I - X_1^T (X_1 X_1^T)^{-1} X_1) \Sigma X_0^T (X_0 X_0^T)^{-1}
\]
\[
E = (X_1 X_1^T)^{-1} X_1 \Sigma (I - X_0^T (X_0 X_0^T)^{-1} X_0)
\]
\[
F = (X_1 X_1^T)^{-1} X_1 \Sigma X_0^T (X_0 X_0^T)^{-1}
\]
The proof is shown in Appendix B.

In the upper bound (9), $2\theta_1^T B_1 \theta_1^*$ and $2\theta_0^T B_0 \theta_0^*$ correspond to the biases in predicting $y_1$ and $y_0$, respectively; $2\varepsilon_1^T C_1 \varepsilon_1$ and $2\varepsilon_0^T C_0 \varepsilon_0$ correspond to the variances in predicting $y_1$ and $y_0$, respectively; $-2\theta_1^T B_{1,0} \theta_0^* + 2\theta_0^T D \varepsilon_0 + 2\varepsilon_1^T E \theta_0^* - 2\varepsilon_1^T F \varepsilon_0$ appear from the cross term of $\hat{\theta}_1$ and $\theta_0$. In the lower bound (10), some terms used in the upper bound vanish owing to the independency of the error terms among the treatments.

Next, we consider bounding each term in (9) and (10). Here, we use the properties that
\[
X_0 X_1^T = 0,
\]
and for a matrix $M \in \mathbb{R}^{n \times n}$,
\[
X_0 M X_1^T = 0,
\]
where $0$ is a $n \times n$ zero matrix.

**Lemma 1.2** (Upper bounds regarding the terms including $B_1$ and $B_0$). For each $a \in \{0, 1\}$, there exists a constant $c$ that depends only on $\sigma_x$, such that for any $1 < t < n$, with probability at least $1 - \exp(-t)$,
\[
\theta_a^*^T B_a \theta_a^* \leq c \|\theta_a^*\|^2 \|\Sigma_a\| \max \left\{ \sqrt{\frac{r_0(\Sigma_a)}{n}}, \frac{r_0(\Sigma_a)}{n}, \sqrt{\frac{t}{n}} \right\} + \|\Sigma - \zeta_a^* \Sigma_a\| \|\theta_a^*\|^2,
\]
where $\zeta_a^* = \arg\min_{\zeta \in \mathbb{R}^+} \|\Sigma - \zeta \Sigma_a\|$. The proof is shown in Appendix C.

**Lemma 1.3** (Upper and Lower bounds regarding the term including $B_{1,0}$). There is a constant $c$ that depends only on $\sigma_x$ such that for any $1 < t < n$, with probability at least $1 - \exp(-t)$,
\[
\left| 2\theta_1^T B_{1,0} \theta_0^* \right| \leq c \|\theta_1^*\| \|\theta_0^*\| \|\Sigma\| \max \left\{ \sqrt{\frac{r_0(\Sigma)}{n}}, \frac{r_0(\Sigma)}{n}, \sqrt{\frac{t}{n}} \right\}
\]
The proof is shown in Appendix D.

**Lemma 1.4** (Upper bounds regarding the terms including $C_1$ and $C_0$). Suppose that, given $X_1$ and $X_0$, $C_1$ and $C_0$ are a.s. positive semidefinite. Then a.s. on $X_1$ and $X_0$, with conditional probability at least $1 - 2 \exp(-t)$,
\[
\varepsilon_1^T C_1 \varepsilon_1 \leq c_0 \sigma^2 \text{tr}(C_1) \quad \varepsilon_0^T C_0 \varepsilon_0 \leq c_1 \sigma^2 \text{tr}(C_0)
\]

**Proof.** From Proposition A.1 (Lemma S.2 in Bartlett et al. (2020)), since $\|C_a\| \leq \text{tr}(C_a)$ and $\text{tr}(C_a^2) \leq \text{tr}(C_a)^2$ for $a \in \{0, 1\}$, with probability at least $1 - \exp(-t)$,
\[
\varepsilon_a^T C_a \varepsilon_a \leq \sigma^2 \text{tr}(C_a)(2t + 1) + 2\sigma^2 \sqrt{\text{tr}(C_a)^2(t^2 + t)} \leq (4t + 2)\sigma^2 \text{tr}(C_a)
\]

\[\square\]
Lemma I.5 (Upper bounds regarding the terms including \(D\) and \(E\)). Almost surely on \(X_1\) and \(X_0\), with conditional probability at least \(1 - \exp(-t)\),
\[
\theta_1^T \Sigma X_0^T (X_0 X_0^T)^{-1} \varepsilon_0 < \sqrt{2t \sigma^2 \| \theta_1^T \Sigma X_0^T (X_0 X_0^T)^{-1} \|_2^2}.
\]
Similarly, a.s. on \(X_1\) and \(X_0\), with conditional probability at least \(1 - \exp(-t)\),
\[
\varepsilon_1 (X_1 X_1^T)^{-1} X_1 \Sigma \theta_0^T < \sqrt{2t \sigma^2 \| \theta_0^T \Sigma X_1^T (X_1 X_1^T)^{-1} \|_2^2}.
\]

The proof is shown in Appendix E.

Lemma I.6 (Equality regarding the term including \(F\)).
\[
\varepsilon_1^T F \varepsilon_0 = 0
\]

Lemma I.6 holds from \(X_1 \Sigma X_0^T = 0\).

\[\text{I.2 Concentration Inequalities for the Upper and Lower Bounds of } \text{tr}(C_a)\]

To show the upper and lower bounds of \(\text{tr}(C_a)\) for each \(a \in \{1, 0\}\) in Sections I.3 and I.4, we present the associated lemmas in this section.

Lemma I.7 (From Lemma 3 in Bartlett et al. (2020)). Consider a covariance operator \(\Sigma\) with \(\lambda_i = \mu_i(\Sigma)\) and \(\lambda_n > 0\). Write its spectral decomposition \(\Sigma = \sum_j \lambda_j v_j v_j^T\), where the orthonormal \(v_{a,j} \in \mathbb{H}\) are the eigenvectors corresponding to the \(\lambda_j\). For \(i\) with \(\lambda_i > 0\), define \(z_i = X v_i / \sqrt{\lambda_i}\) and \(z_{a,i} = X_a v_i / \sqrt{\lambda_i}\). Then
\[
\text{tr}(C_a) = \sum_i \left[ \lambda_i^2 z_{a,i}^T \left( \sum_j \lambda_j z_{a,j} z_{a,j}^T \right)^{-2} z_{a,i} \right],
\]
and these \(z_{a,i} \in \mathbb{R}^n\) satisfies that for all \(\lambda \in \mathbb{H}\),
\[
\mathbb{E}[\exp(\lambda^T z_{a,i})] \leq c \exp(d - 1) \exp(\sigma^2 \| \lambda \|^2 / 2) + c(d = 0),
\]
where \(\frac{p(d=1)}{p(d=0)} \leq c\). Furthermore, for any \(i\) with \(\lambda_i > 0\), we have
\[
\lambda_i^2 z_{a,i}^T \left( \sum_j \lambda_j z_{a,j} z_{a,j}^T \right)^{-2} z_{a,i} = \frac{\lambda_i^2 z_{a,i} G_{a,-i}^{-1} z_{a,i}}{(1 + \lambda_i z_{a,i} G_{a,-i}^{-1} z_{a,i})^2},
\]
where \(G_{a,-i} = \sum_{j \neq i} \lambda_j z_{a,j} z_{a,j}^T\).

The weighted sum of outer products of these sub-Gaussian vectors plays a central role in the rest of the proof. Define
\[
G_a = \sum_i \lambda_i z_{a,i} z_{a,i}^T, \quad G_{a,-i} = \sum_{j \neq i} \lambda_j z_{a,j} z_{a,j}^T, \quad G_{a,k} = \sum_{i > k} \lambda_i z_{a,i} z_{a,i}^T,
\]
where recall that \(z_{a,i} \in \mathbb{R}^n\) are defined in Lemma I.7. Note that the vector \(z_{a,i}\) is independent of the matrix \(G_{a,-i}\); therefore, in the last part of Lemma I.7, all the random quadratic forms are independent of the points where those forms are evaluated.

The next step is to replace Lemma 4 in Bartlett et al. (2020) by showing that eigenvalues of \(G_a\), \(G_{a,-i}\) and \(G_{a,k}\) are concentrated.

Lemma I.8. There is a universal constant \(c\) such that with probability at least \(1 - 2 \exp(-n/c)\),
\[
\frac{1}{c} \sum_i \lambda_i - c \lambda_1 n \leq \mu_n(G_a) \leq \mu_1(G_a) \leq c \left( \sum_i \lambda_i + \lambda_1 \right).
\]

Proof. First, we develop a probabilistic bound on \(|v^T G_a v - \sum \lambda_i|\) for any \(v \in \mathbb{R}^n\), by applying the Bernstein inequality for a weighted sum of centered sub-exponential random variables (Proposition A.4). To this end, we confirm that \(v^T G_a v\) is a sub-exponential random variable.
We fix $v \in \mathbb{R}^n$ and rewrite $v^\top G_a v$ as

$$v^\top G_a v = \sum_i \lambda_i (v^\top z_{a,i})^2,$$

then study its centered element $(v^\top z_{a,i})^2 - \mathbb{E}[(v^\top z_{a,i})^2]$. We note that for a random variable $R$, $\mathbb{E}[\exp(R^2)] < \infty$ implies that $R$ is a sub-Gaussian random variable (Proposition 2.5.2 in Vershynin (2018)). For any $i$, we have

$$\mathbb{E} \left[ \exp \left( (\sqrt{\lambda_i} v^\top z_{a,i})^2 \right) \right] \leq \mathbb{E} \left[ \exp \left( (\sqrt{\lambda_i} v^\top z_{a,i})^2 \right) \right] \leq \mathbb{E} \left[ \exp \left( (\lambda_i v^\top x)^2 \right) \right] < \infty.$$

The last inequality follows the assumption on the sub-Gaussian property of $x$. Then, we use Proposition 2.5.2 in Vershynin (2018) again and find that $v^\top z_{a,i}$ is a sub-Gaussian random variable. Furthermore, because a random variable $R$ is sub-Gaussian if and only if $R^2$ is sub-exponential (Lemma 2.7.6 in Vershynin (2018)), we find that $(v^\top z_{a,i})^2$ is a sub-exponential random variable. Because a centered sub-exponential random variable is also sub-exponential (Exercise 2.7.10 in Vershynin (2018)), $(v^\top z_{a,i})^2 - \mathbb{E}[(v^\top z_{a,i})^2]$ is a sub-exponential random variable.

We study the centered version of $\alpha v^\top G_a v$ for a fixed $\alpha \in \mathbb{R}$ using the above result. The sub-exponential random variable $\alpha v^\top G_a v$ has the mean

$$\alpha \mathbb{E} \left[ \sum_i \lambda_i (v^\top \mathbb{I}[d_i = a] z_i)^2 \right] = \alpha \sum_i \lambda_i \mathbb{E} \left[ p(a|z_i) v^\top z_i z_i^\top v \right],$$

and from Lemma 2.7.10 in Vershynin (2018), $\alpha v^\top G_a v - \alpha \mathbb{E}[\sum_i \lambda_i (v^\top \mathbb{I}[d_i = a] z_i)^2]$ is a centered sub-exponential random variable, which is equal to

$$\alpha v^\top G_a v - \alpha \mathbb{E} \left[ \sum_i \lambda_i (v^\top \mathbb{I}[d_i = a] z_i)^2 \right] = \alpha v^\top G_a v - \alpha \sum_i \lambda_i \mathbb{E} \left[ p(a|z_i) v^\top z_i z_i^\top v \right] = \sum_i \lambda_i \left( (v^\top \mathbb{I}[d_i = a] z_i)^2 - \alpha \mathbb{E} \left[ p(a|z_i) v^\top z_i z_i^\top v \right] \right).$$

Let $\alpha = \frac{\sum_i \lambda_i \mathbb{E} \left[ p(a|z_i) v^\top z_i z_i^\top v \right]}{\sum_i \lambda_i}$, which is positive and finite because the eigenvalue $\lambda_i$ and $\mathbb{E} \left[ p(a|z_i) v^\top z_i z_i^\top v \right]$ are non-negative and $p(a|z_i) > 0$.

Then, because $\alpha v^\top G_a v - \sum_i \lambda_i$ is a centered sub-exponential random variable, Proposition A.4 (Corollary S.6, Bartlett et al., 2020) yields that for some constant $c_2$ with probability at least $1 - 2 \exp(-t)$,

$$\left| \alpha v^\top G_a v - \sum_i \lambda_i \right| \leq c_2 \max \left\{ \lambda_1 t, \sqrt{t \sum \lambda_i^2} \right\}. \tag{11}$$

Then, for a fixed vector $\hat{v} = \sqrt{\alpha} v$,

$$\left| \hat{v}^\top G_a \hat{v} - \sum_i \lambda_i \right| \leq c_2 \max \left\{ \lambda_1 t, \sqrt{t \sum \lambda_i^2} \right\}.$$

We also denote $\hat{v}$ by $v$ for brevity.

Second, we improve the above inequality using a uniform bound technique by following the proof of Theorem 4.4.5 in Vershynin (2018). Let $\mathcal{N}$ be a $\frac{1}{t}$-net on the sphere $S^{n-1}$ with respect to the Euclidean distance such that $|\mathcal{N}| \leq 9^n$. We can find such $\frac{1}{t}$-net from Corollary 4.2.13. Then, from the union bound over the elements of $\mathcal{N}$, for every $v \in \mathcal{N}$,

$$P \left( \left| v^\top G_a v - \sum_i \lambda_i \right| \geq c_1 \max \left\{ \lambda_1 t, \sqrt{t \sum \lambda_i^2} \right\} \right) \leq \sum_{v \in \mathcal{N}} P \left( \left| v^\top G_a v - \sum_i \lambda_i \right| \geq c_1 \max \left\{ \lambda_1 t, \sqrt{t \sum \lambda_i^2} \right\} \right) \leq 9^n \cdot 2 \exp(-t).$$

21
Therefore, we see that with probability $1 - 2 \exp(-t)$, every $v \in \mathcal{N}$ satisfies
\[
\left| v^\top G_a v - \sum_i \lambda_i \right| \leq c_1 \max \left\{ \lambda_1 (t + n \log(9)), \sqrt{(t + n \log(9)) \sum \lambda_i^2} \right\}. \tag{12}
\]

From Proposition A.5 Bartlett et al. (Lemma S.8, 2020), with probability at least $1 - 2 \exp(-t)$,
\[
\left\| G_a - I_n \sum_i \lambda_i \right\| \leq c_2 \left( \lambda_1 (t + n \log(9)) + \sqrt{(t + n \log(9)) \sum \lambda_i^2} \right).
\]

When $t < n/c_3$, we can write $t + n \log(9) \leq c_4 n$, and we have
\[
\lambda_1 (t + n \log(9)) + \sqrt{(t + n \log(9)) \sum \lambda_i^2} \\
\leq c_4 \left( \lambda_1 n + \sqrt{n \sum \lambda_i^2} \right) \tag{13} \\
\leq c_4 \lambda_1 n + \sqrt{\left( c_4^2 \lambda_1 n \right) \sum \lambda_i} \\
\leq c_4 \lambda_1 n + \frac{1}{2} \left( c_4^2 \lambda_1 n \right) + \frac{1}{2} \left( \sum \lambda_i \right) \\
\leq c_5 \lambda_1 n + \frac{1}{2c_2} \sum \lambda_i. \tag{14}
\]

Here, we use the inequality of arithmetic and geometric means.

Finally, we derive the desired upper bound on $\mu_1(G_a)$ and lower bound on $\mu_n(G_a)$. By the definition of a spectral norm, we have
\[
\left\| G_a - I_n \sum_i \lambda_i \right\| = \mu_1 \left( G_a - I_n \sum_i \lambda_i \right).
\]

For some constant $c_6 > 0$, from (14), $\lambda_1 (t + n \log(9)) + \sqrt{(t + n \log(9)) \sum \lambda_i^2} \leq c_5 \lambda_1 n + \frac{1}{2c_2} \sum \lambda_i$ implies the upper bound
\[
\mu_1(G_a) \leq c_6 \left( \sum_i \lambda_i + \lambda_1 n \right).
\]

Let $v$ be an eigenvector corresponding to $\mu_n(G_a)$. Then, by definition and from (12) and (13), with probability at least $1 - 2 \exp(-t)$,
\[
\left| v^\top G_a v - \sum_i \lambda_i \right| = \left| \mu_n(G_a) - \sum_i \lambda_i \right| \\
\leq c_1 \max \left\{ \lambda_1 (t + n \log(9)), \sqrt{(t + n \log(9)) \sum \lambda_i^2} \right\} \\
\leq c_4 \lambda_1 n + c_4 \sqrt{n \sum \lambda_i^2} \\
\leq c_4 \lambda_1 n + c_4 \sqrt{n \lambda_1 \sum \lambda_i}.
\]

Using the inequality of arithmetic and geometric means, this implies the following lower bound
\[
\mu_n(G_a) \geq \sum_i \lambda_i - c_4 \lambda_1 n - \frac{c_4}{2} \lambda_1 - \frac{c_4}{2} \sum \lambda_i.
\]

Therefore, by appropriately choosing the constant, we conclude the proof.
By applying a similar step in the proof of Lemma I.8 for \( i > k \) and any \( k \geq 0 \), we also obtain the following corollary.

**Corollary I.9.** There is a universal constant \( c \) such that for any \( k \geq 0 \) with probability at least \( 1 - 2 \exp(-n/c) \),

\[
\frac{1}{c} \sum_{i > k} \lambda_i - c\lambda_{k+1} n \leq \mu_n(G_{a,k}) \leq \mu_1(G_{a,k}) \leq c \left( \sum_{j > k} \lambda_j + \lambda_{k+1} n \right).
\]

Then, by using Lemma I.9 instead of Lemma 4 in Bartlett et al. (2020), we obtain the following lemma corresponding to Lemma 5 in Bartlett et al. (2020).

**Lemma I.10 (From Lemma 5 in Bartlett et al. (2020)).** There are constants \( b, c \geq 1 \) such that for any \( k \geq 0 \), with probability at least \( 1 - 2e^{-n/c} \),

1. for all \( i \geq 1 \),

\[
\mu_{k+1}(G_{a,-i}) \leq \mu_{k+1}(G_a) \leq \mu_1(G_{a,k}) \leq c \left( \sum_{j > k} \lambda_j + \lambda_{k+1} n \right),
\]

2. for all \( 1 \leq i \leq k \),

\[
\mu_n(G_a) \geq \mu_n(G_{a,-i}) \geq \mu_n(G_{a,k}) \geq \frac{1}{c} \sum_{j > k} \lambda_j - c\lambda_{k+1} n,
\]

3. if \( r_k(\Sigma) \geq bn \), then

\[
\frac{1}{c} \lambda_{k+1} r_k(\Sigma) \leq \mu_n(G_{a,k}) \leq \mu_1(G_{a,k}) \leq c\lambda_{k+1} r_k(\Sigma).
\]

**Proof.** We provide some inequalities as preparation. From Lemma I.9, with probability at least \( 1 - 2 \exp(-n/c_1) \), the following inequalities hold:

\[
\frac{1}{c_1} \sum_{j > k} \lambda_j - c_1 \lambda_{k+1} n \leq \mu_n(G_{a,k}) \leq \mu_1(G_{a,k}) \leq c_1 \left( \sum_{j > k} \lambda_j + \lambda_{k+1} n \right).
\]  \( (15) \)

Here, the matrix

\[
G_a - G_{a,k} = \sum_i \lambda_i z_{a,i}z_{a,i}^\top - \sum_{i > k} \lambda_i z_{a,i}z_{a,i}^\top = \sum_{i < k} \lambda_i z_{a,i}z_{a,i}^\top
\]
ranks at most \( k \) because it is the sum of \( k \) matrices of rank 1. Thus, there is a linear space \( \mathcal{L} \) of dimension \( n - k \) such that, for all \( v \in \mathcal{L} \),

\[
v^\top G_a v = v^\top G_{a,k} v \leq \mu_1(G_{a,k}) \|v\|^2 \]

and, therefore, we have

\[
\mu_{k+1}(G_a) \leq \mu_1(G_{a,k}).
\]  \( (16) \)

We show the first statement. Because \( G_a \succeq G_{a,-i} \) holds for any \( i \), Lemma S.11 in Bartlett et al. (2020) gives \( \mu_j(G_{a,-i}) \leq \mu_j(G_a) \) for all \( i \) and \( j \). Hence, by combining this inequality with (15) and (16), the first statement holds.

For the second statement, for \( i \leq k \), \( G_{a,k} \succeq G_{a,-i} \), all the eigenvalues of \( G_{a,-i} \) are lower bounded by \( \mu_n(G_{a,k}) \). Thus, with (15) and (16), the second statement holds.

Finally, for the third statement, if \( r_k(\Sigma) \geq bn \),

\[
\sum_{j > k} \lambda_j + \lambda_{k+1} n = \lambda_{k+1} r_k(\Sigma) + \lambda_{k+1} n \leq \left( 1 + \frac{1}{b} \right) \lambda_{k+1} r_k(\Sigma),
\]

\[
\frac{1}{c_1} \sum_{j > k} \lambda_j - c_1 \lambda_{k+1} n = \frac{1}{c_1} \lambda_{k+1} r_k(\Sigma) - c_1 \lambda_{k+1} n \geq \left( \frac{1}{c_1} - \frac{c_1}{b} \right) \lambda_{k+1} r_k(\Sigma).
\]

Choosing \( b > c_1^2 \) and \( c > \max\{c_1 + 1/c_1, (1/c_1 - c_1/b)^{-1}\} \) and (15) give the third claim of the lemma.  \( \square \)
I.3 Upper Bound on $\text{tr}(C_a)$

Lemma I.10 gives the following upper bound on $\text{tr}(C_a)$, which corresponds to Lemma 6 in Bartlett et al. (2020).

**Lemma I.11.** There are constants $b, c \geq 1$ such that if $0 \leq k \leq n/c$, $r_k(\Sigma) \geq bn$, and $m \leq k$ then with probability at least $1 - 7e^{-n/c}$,

$$\text{tr}(C_a) \leq c \left( \frac{m}{n} + n \frac{\sum_{i>m} \lambda_i^2}{(\lambda_{k+1} r_k(\Sigma))^2} \right).$$

**Proof.** Fix $b$ as in Lemma I.10. By Lemma I.7,

$$\text{tr}(C_a) = \sum_i \lambda_i^2 z_{a,i}^T G_a^{-1} z_{a,i}$$

$$= \sum_{i=1}^m \lambda_i^2 z_{a,i}^T G_a^{-1} z_{a,i} + \sum_{i>m} \lambda_i^2 z_{a,i}^T G_a^{-1} z_{a,i}', \quad (17)$$

First, we consider bounding the first term: the sum up to $m$. If $r_k(\Sigma) \geq bn$, Lemma I.10 shows that with probability at least $1 - 2e^{-n/c_1}$, for all $i \leq k$, we have an upper bound on $\mu_n(G_{a,-i})$:

$$\mu_n(G_{a,-i}) \geq \lambda_{k+1} r_k(\Sigma) / c_1;$$

for all $i$, we have a lower bound on on $\mu_n(G_{a,-i})$:

$$\mu_{k+1}(G_{a,-i}) \leq c_1 \lambda_{k+1} r_k(\Sigma).$$

The lower bound on $\mu_n(G_{a,-i})$ implies that for all $z \in \mathbb{R}^n$ and $1 \leq i \leq m$,

$$z^T G_{a,-i}^{-1} z \geq \frac{c_1^2 \|z\|^2}{(\lambda_{k+1} r_k(\Sigma))^2},$$

and the upper bound on $\mu_{k+1}(G_{a,-i})$ gives

$$z^T G_{a,-i}^{-1} z \geq (\Pi_{\mathcal{L}_i} z)^T G_{a,-i}^{-1} \Pi_{\mathcal{L}_i} z \geq \frac{\|\Pi_{\mathcal{L}_i} z\|^2}{c_1 \lambda_{k+1} r_k(\Sigma)},$$

where $\mathcal{L}_i$ is the span of the $n-k$ eigenvectors of $G_{a,-i}$ corresponding to the smallest $n-k$ eigenvalues. Recall that $\Pi_{\mathcal{L}}$ is the orthogonal projection on $\mathcal{L}$. Then, for $i \leq m$,

$$\frac{\lambda_i^2 z_{a,i}^T G_{a,-i}^{-1} z_{a,i}}{(1 + \lambda_i z_{a,i}^T G_{a,-i}^{-1} z_{a,i})^2} \leq \frac{\|z_{a,i}\|^2}{(\lambda_{k+1} r_k(\Sigma))^2} \leq c_4 \|\Pi_{\mathcal{L}_i} z_{a,i}\|^4. \quad (18)$$

Next, we apply Corollary F.1 $m$ times, together with a union bound, to show that with probability at least $1 - 3 \exp(-t)$, for all $1 \leq i \leq m$ and constants $u_1, u_2$,

$$\|z_{a,i}\|^2 \leq n + u_1 (t + \ln k + \sqrt{n(t + \ln k)}) \leq c_2 n, \quad (19)$$

$$\|\Pi_{\mathcal{L}_i} z_{a,i}\|^2 \geq n - u_2 (k + t + \log k + \sqrt{n(t + \ln k)}) \geq n/c_3, \quad (20)$$

provided that $t < n/c_0$ and $c > c_0$ for some sufficiently large $c_0$ (note that $c_2$ and $c_3$ only depend on $c_0$, $a$ and $\sigma_x$, and we can still take $c$ to be sufficiently large at the end without changing $c_2$ and $c_3$). Combining (18), (19), and (20), with probability at least $1 - 5e^{-n/c_0}$,

$$\frac{\lambda_i^2 z_{a,i}^T G_{a,-i}^{-1} z_{a,i}}{(1 + \lambda_i z_{a,i}^T G_{a,-i}^{-1} z_{a,i})^2} \leq \frac{c_4}{n}.$$  

Then, we have

$$\sum_{i=1}^m \frac{\lambda_i^2 z_{a,i}^T G_{a,-i}^{-1} z_{a,i}}{(1 + \lambda_i z_{a,i}^T G_{a,-i}^{-1} z_{a,i})^2} \leq \frac{c_4 m}{n}. \quad (18')$$

Second, consider bounding the second sum in (17); that is,

$$\sum_{i>m} \lambda_i^2 z_{a,i}^T G_{a,-i}^{-1} z_{a,i}$$


Lemma I.10 shows that, on the same high probability event that we consider in bounding the first half of the sum, \( \mu_n(G_a) \geq \lambda_{k+1} r_k(\Sigma)/c_1 \). Hence,

\[
\sum_{i > m} \lambda_i^2 z_{a,i}^\top G_a^{-2} z_{a,i} \leq c_1^2 \sum_{i > m} \lambda_i^2 \| z_{a,i} \|^2 / (\lambda_{k+1} r_k(\Sigma))^2.
\]

Note that \( \sum_{i > m} \lambda_i^2 \| z_{a,i} - \mathbb{E}[z_{a,i}] \|^2 \) is the weighted sum of the centered sub-exponential random variables, with the weights given by \( \lambda_i^2 \) in blocks of size \( n \). Then, using Proposition A.4, we can bound \( \sum_{i > m} \lambda_i^2 \| z_{a,i} - \mathbb{E}[z_{a,i}] \|^2 \). Thus, Proposition A.4 implies that with probability at least \( 1 - 2 \exp(-t) \), for some constants \( c_3, c_4, c_5 \),

\[
\sum_{i > m} \lambda_i^2 \| z_{a,i} \|^2 = \sum_{i > m} \lambda_i^2 \| z_{a,i} - \mathbb{E}[z_{a,i}] + \mathbb{E}[z_{a,i}] \|^2 \\
\leq 2 \sum_{i > m} \lambda_i^2 \| z_{a,i} - \mathbb{E}[z_{a,i}] \|^2 + 2 \sum_{i > m} \lambda_i^2 \| \mathbb{E}[z_{a,i}] \|^2 \\
\leq c_3 n \sum_{i > m} \lambda_i^2 + c_4 \max \left( \lambda_{m+1}^2, \sqrt{\frac{\lambda_i^2 n}{\lambda_i^2}} \right) \\
\leq c_3 n \sum_{i > m} \lambda_i^2 + c_4 \max \left( t \sum_{i > m} \lambda_i^2, \sqrt{\lambda_i^2} \right) \\
\leq c_5 n \sum_{i > m} \lambda_i^2,
\]

because \( t < n/c_0 \) and \( \mathbb{E}[z_{a,i}] \) is a constant \( n \)-dimensional vector. Combining the above gives

\[
\sum_{i > m} \lambda_i^2 z_{a,i}^\top G_a^{-2} z_{a,i} \leq c_6 n \frac{\sum_{i > m} \lambda_i^2}{(\lambda_{k+1} r_k(\Sigma))^2}.
\]

Finally, putting both parts together and taking \( c > \max\{c_0, c_4, c_5\} \) gives the lemma.

\[
\square
\]

I.4 Lower Bound on \( \text{tr}(C_a) \)

Next, we derive the lower bound on \( \text{tr}(C_a) \). We restate Lemma 8 and 9 in Bartlett et al. (2020) as follows:

**Lemma I.12.** There is a constant \( c \) such that for any \( i \geq 1 \) with \( \lambda_i > 0 \), and any \( 0 \leq k \leq n/c \), with probability at least \( 1 - 5e^{-n/c} \),

\[
\lambda_i^2 z_i^\top G_a^{-2} z_i / (1 + \lambda_i z_i^\top G_a^{-1} z_i)^2 \geq \frac{1}{cn} \left( 1 + \sum_{j > k} \lambda_j + n \lambda_{k+1} \right) \lambda_i^2 .
\]

**Lemma I.13.** Suppose \( n \leq \infty \) and \( \{\eta_i\}_{i=1}^n \) is a sequence of non-negative random variables, \( \{t_i\}_{i=1}^n \) is a sequence of non-negative real numbers (at least one of which is strictly positive) such that for some \( \delta \in (0, 1) \) and any \( i \leq n \), \( \Pr(\eta_i > t_i) \geq 1 - \delta \). Then

\[
\Pr \left( \sum_{i=1}^n \eta_i \geq \frac{1}{2} \sum_{i=1}^n t_i \right) \geq 1 - 2\delta.
\]

We can show these lemmas as well as those in Bartlett et al. (2020) by replacing Corollary 1 in Bartlett et al. (2020) with Corollary F.1.

From Lemmas I.7, I.12 and I.13, we can obtain the following lemma corresponding to Lemma 10 in Bartlett et al. (2020).

**Lemma I.14.** There are constants \( c \) such that for any \( 0 \leq k \leq n/c \) and any \( b > 1 \) with probability at least \( 1 - 10e^{-n/c} \),

1. If \( r_k(\Sigma) < bn \), then \( \text{tr}(C_a) \geq \frac{k+1}{cb^2 n} \).
2. If \( r_k(\Sigma) \geq bn \), then
\[
\text{tr}(C_{a}) \geq \frac{1}{cb} \min_{m \leq k} \left( \frac{m}{n} + \frac{b^2 n \sum_{i>m} \lambda_i^2}{(\lambda_{k+1} r_k(\Sigma))^2} \right).
\]

In particular, if all choices of \( k \leq n/c \) give \( r_k(\Sigma) < bn \), then \( r_{n/c}(\Sigma) < bn \) implies that with probability at least \( 1 - 10e^{-n/c} \), \( \text{tr}(C_{a}) = \Omega_{\sigma_x}(1) \).

We can show the lemma as well as Lemma 10 in Bartlett et al. (2020) by replacing Lemmas 3, 8, and 9 in Bartlett et al. (2020) with Lemmas I.7, I.12 and I.13.

### I.5 Upper Bounds regarding \( \| \theta_a^T \Sigma X_0^T (X_0 X_0^T)^{-1} \|_2 \) and \( \| \theta_0^T \Sigma X_1^T (X_1 X_1^T)^{-1} \|_2 \)

Next, we show the upper bounds of \( \| \theta_a^T \Sigma X_0^T (X_0 X_0^T)^{-1} \|_2 \) and \( \| \theta_0^T \Sigma X_1^T (X_1 X_1^T)^{-1} \|_2 \). The proof uses the result presented in Section I.3.

**Lemma I.15.** For each \( a \in \{1, 0\} \), there are constants \( b, c \geq 1 \) such that if \( 0 \leq k \leq n/c \), \( r_k(\Sigma) \geq bn \), and \( m \leq k \) then with probability at least \( 1 - 7e^{-n/c} \),
\[
\| \theta_a^T \Sigma X_{1-a}^T (X_{1-a} X_{1-a}^T)^{-1} \|_2 \leq c \| \theta_0^T \|_2 \sqrt{\left( \frac{m}{n} + \frac{\sum_{i>m} \lambda_i^2}{(\lambda_{k+1} r_k(\Sigma))^2} \right)}.
\]

**Proof.** We consider a case with \( a = 1 \). We can also show another case with \( a = 0 \).

By applying a step similar to that used in Lemma I.7, we decompose the target value as
\[
\| \theta_1^T \Sigma X_0^T (X_0 X_0^T)^{-1} \|_2 \leq \| \theta_1^T \sum_i \lambda_i \sqrt{\lambda_i} v_i z_{0,i}^T \left( \sum_j \lambda_j z_{0,j} z_{0,j}^T \right) \|_2 \leq \| \theta_1^T \sum_i \lambda_i \sqrt{\lambda_i} v_i z_{0,i} \left( \lambda_j z_{0,j} z_{0,j}^T + G_{0,-j} \right)^{-1} \|_2.
\]

The Sherman–Morrison–Woodbury formula gives
\[
(\lambda_i z_{0,i} z_{0,i}^T + G_{0,-i})^{-1} = G_{0,-i}^{-1} - G_{0,-i}^{-1} (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i})^{-1} z_{0,i}^T \sqrt{\lambda_i} G_{0,-i}^{-1}.
\]

Therefore,
\[
\sqrt{\lambda_i} v_i z_{0,i} \left( \lambda_i z_{0,i} z_{0,i}^T + G_{0,-i} \right)^{-1} = \sqrt{\lambda_i} v_i \left( G_{0,-i}^{-1} - G_{0,-i}^{-1} (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i})^{-1} z_{0,i}^T \sqrt{\lambda_i} G_{0,-i}^{-1} \right)
\]
\[
= v_i \left( z_{0,i}^T \sqrt{\lambda_i} G_{0,-i}^{-1} - z_{0,i}^T \lambda_i z_{0,i} (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i})^{-1} \right) z_{0,i}^T \sqrt{\lambda_i} G_{0,-i}^{-1}
\]
\[
= v_i \left( 1 - z_{0,i}^T G_{0,-i}^{-1} \lambda_i z_{0,i} (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i})^{-1} \right) z_{0,i}^T \sqrt{\lambda_i} G_{0,-i}^{-1}
\]
\[
= v_i \left( 1 + \lambda_i z_{0,i} G_{0,-i} z_{0,i} \right)^{-1} z_{0,i}^T \sqrt{\lambda_i} G_{0,-i}^{-1}.
\]

In this study, we use \( 1 - z_{0,i}^T G_{0,-i}^{-1} \lambda_i z_{0,i} (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i})^{-1} \) because
\[
(1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i}) (1 - z_{0,i}^T G_{0,-i}^{-1} \lambda_i z_{0,i} (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i})^{-1})
\]
\[
= (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i}) - (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i}) \left( z_{0,i}^T G_{0,-i}^{-1} \lambda_i z_{0,i} (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i})^{-1} \right)
\]
\[
= (1 + \lambda_i z_{0,i}^T G_{0,-i}^{-1} z_{0,i}) - z_{0,i}^T G_{0,-i} \lambda_i z_{0,i} = 1.
\]
Thus, we have

$$
\|\theta_1^* \Sigma X_0^T (X_0 X_0^T)^{-1}\|_2 \\
= \sqrt{\theta_1^* \Sigma X_0^T (X_0 X_0^T)^{-2} X_0 \Sigma} \\
\leq \sqrt{\|\theta_1^*\|_2^2 \|\Sigma X_0^T (X_0 X_0^T)^{-2} X_0 \Sigma\|} \\
\leq \sqrt{\|\theta_1^*\|_2^2 \text{tr} (\Sigma X_0^T (X_0 X_0^T)^{-2} X_0 \Sigma)}.
$$

Then, because $X_0 X_0^T = \sum_i \lambda_i z_{0,i} z_{0,i}^T$ and $X_0 \Sigma = \sum_i \lambda_i \sqrt{\lambda_i} z_{0,i} v_i^T$ from $X_0 z_{0,i} = X_0 v_i$ and $\Sigma = \sum_i \lambda_i v_i v_i^T$,

$$
\text{tr} (\Sigma X_0^T (X_0 X_0^T)^{-2} X_0 \Sigma) \\
= \text{tr} \left( \left( \sum_j \lambda_j z_{0,j} z_{0,j}^T \right)^{-2} \left( \sum_i \lambda_i z_{0,i} v_i^T \right)^2 \left( \sum_i \lambda_i z_{0,i} v_i^T \right)^{-2} \sum_i \lambda_i z_{0,i} z_{0,i}^T \right) \\
= c \left( \sum_i \lambda_i^2 z_{0,i} z_{0,i}^T \left( \sum_j \lambda_j z_{0,j} z_{0,j}^T \right)^{-2} \sum \lambda_i z_{0,i} z_{0,i}^T \right) \\
= c \sum_i \lambda_i^2 z_{0,i} \left( \sum_j \lambda_j z_{0,j} z_{0,j}^T \right)^{-2} \sum \lambda_i z_{0,i} z_{0,i}^T,
$$

where we use $v_i^T v_i = 1$ and $\text{max}_i \lambda_i \leq c$ for some constant $c > 0$. Then, by applying the same step in the proof of Lemma I.11 to $\sum_i \lambda_i^2 z_{0,i} \left( \sum_j \lambda_j z_{0,j} z_{0,j}^T \right)^{-2} \sum \lambda_i z_{0,i} z_{0,i}^T$,

$$
\|\theta_1^* \Sigma X_0^T (X_0 X_0^T)^{-1}\|_2 \\
\leq \sqrt{\|\theta_1^*\|_2^2 \text{tr} (\Sigma X_0^T (X_0 X_0^T)^{-2} X_0 \Sigma)} \\
\leq c\|\theta_1^*\|_2^2 \sqrt{\frac{m}{n} + \frac{\sum_{i > m} \lambda_i^2}{(\lambda_{k+1} r_k(\Sigma))^2}}.
$$

This concludes the proof.

\[\square\]

### I.6 Final Step for Proof of the Upper Bound

To complete the proof of Theorem 4.3, we combine Lemmas I.2–I.16 with Lemma I.1. We set $b$ in Lemmas I.14–I.15 and Theorem 4.3 to the constant $b$ from Lemma I.11. Let $c_1$ be the maximum of the constants $c$ from Lemmas I.14 and I.11.

By using Lemma I.14, we consider the lower bound based on the value of $k$. If there is no $k \leq n/c$ such that $r_k(\Sigma) \geq bn$, then Lemma I.14 implies that $\text{tr}(C_k) \geq \frac{k+1}{\delta \sigma^2 n^2}$. Then, by combining it with Lemmas I.1 and I.4, we can obtain the lower bound of the expected excess risk as $\Omega(\sigma^2)$, which proves the first lower bound of Theorem 4.3 for large $k^*$: suppose $\delta < 1$ with $\log(1/\delta) < n/c$. If $k^* \geq n/c_1$, then

$$
\text{EER}(\theta) \geq \sigma^2/c.
$$

If there exist some $k \leq n/c$ such that $r_k(\Sigma) \geq bn$, then from Lemmas I.11 and I.14, the upper and lower bounds of Lemmas I.11 and I.14 regarding the terms, including $C_1$ and $C_0$, are constant multiples of

$$
\min_{m \leq k} \frac{m}{n} + \frac{\sum_{i > m} \lambda_i^2}{(\lambda_{k+1} r_k(\Sigma))^2};
$$


from Lemmas I.5 and I.15, the upper and lower bounds regarding the term, including $D$ and $E$, are also constant multiples of

$$\min_{m \leq k} \sqrt{\frac{m}{n} + \frac{n}{(\lambda_{k+1} r_k(\Sigma))^2}};$$

Note that by Lemma I.10, for any qualifying value of $k$, the smallest eigenvalue of $G_a$ is within a constant factor of $\lambda_{k+1} r_k(\Sigma)$. Thus, any two choices of $k$ satisfying $k \leq n/c$ and $r_k(\Sigma) \geq bn$ must have values of $\lambda_{k+1} r_k(\Sigma)$ within constant factors. The smallest such $k$ simplifies the bound on $\text{tr}(C)$, as the following proposition in Bartlett et al. (2020) shows.

**Proposition I.16 (Lemma 11 in Bartlett et al. (2020)).** For any $b \geq 1$ and $k^* := \min\{k : r_k(\Sigma) \geq bn\}$, if $k^* < \infty$, we have

$$\min_{m \leq k^*} \left( \frac{m}{bn} + \frac{bn \sum_{i > m} \lambda_i^2}{(\lambda_{k^*+1} r_{k^*}(\Sigma))^2} \right) = \frac{k^*}{bn} + \frac{bn \sum_{i > k^*} \lambda_i^2}{(\lambda_{k^*+1} r_{k^*}(\Sigma))^2} = \frac{k^*}{bn} + \frac{R_{k^*}(\Sigma)}{n}.$$ 

By Proposition I.16, the lower bound is within a constant factor of $\frac{k^*}{n} + \frac{n}{R_{k^*}(\Sigma)}$.

Taking $c$ sufficiently large, and combining these results with Lemma I.1 and the upper bound on the term $\theta^* \Sigma \theta^*$ in Lemma I.3 completes the proofs of Theorems 4.3 and 5.3.

### J Proof of Lemma 5.1

**Proof.** We show that $R(\theta) - \hat{R}(\theta) = 0$ as

$$R(\hat{\theta}^{\text{IPW-learner}}) - \hat{R}(\theta^{\text{IPW-learner}}) = E_{x,y}[(\hat{y} - x^T \theta)^2 - (\hat{y} - x^T \theta^*)^2] - E_{x,y}[(\hat{y} - x^T \theta)^2 - (\hat{y} - x^T \theta^*)^2]$$

$$= E_{x,y}[(\hat{y} - \hat{y} + \hat{y} - x^T \theta)^2 - (\hat{y} + \hat{y} - x^T \theta^*)^2] - E_{x,y}[(\hat{y} - x^T \theta)^2 - (\hat{y} - x^T \theta^*)^2]$$

$$= E_{x,y}[(\hat{y} - \hat{y})^2 + 2(\hat{y} - \hat{y}) (\hat{y} - x^T \theta) - (\hat{y} - \hat{y})^2 - 2(\hat{y} - \hat{y}) (\hat{y} - x^T \theta^*)]$$

$$= 2E_{x,y}[(\hat{y} - \hat{y}) (x^T (\theta^* - \theta))]$$

$$= 2E_x \left[ E_y \left[ \hat{y} - \hat{y}|x \right] (x^T (\theta^* - \theta)) \right]$$

$$= 2E_x \left[ E \left[ \tau^*(x) - \tau^*(x) \right] (x^T (\theta^* - \theta)) \right]$$

$$= 0.$$ 

Here, we used

$$E \left[ \hat{y}|x \right] = E \left[ y_1 - y_0|x \right] = \tau^*(x).$$

### K Proof of Theorem 5.3

**Proof.** Because Statements 1’, 3’, and 4’ in Lemma 5.2 correspond to Assumptions 1, 3, and 4 in Definition 1 in Bartlett et al. (2020), by combining them with 2 and 5 in Assumptions 2.2, we can directly apply Theorem 1 of Bartlett et al. (2020) to obtain the following result.

**Corollary K.1 (Excess risk upper bounds in the IPW-learner).** For any $\sigma_z$ there are $b, c, c_1 > 1$ for which the following holds. Consider a linear regression problem from Section 2.2 and suppose that Assumption 2.3, 2.4, and 2.2 hold. Suppose $\delta < 1$ with $\log(1/\delta) < n/c$. If $k^* < n/c_1$, then the excess risk (Definition 2.1) of the predictor in (1) satisfies

$$\hat{R}(\hat{\theta}^{\text{IPW-learner}}) \leq c\|\theta^*\|^2 E_{n,\delta}(\Sigma) + c \log(1/\delta) \nu_n(\Sigma),$$

with probability at least $1 - \delta$. 

28
Proof. In Definition 1 of Bartlett et al. (2020), we replace Assumptions 1, 3, and 4 with Statements 1’, 3’, and 4’ in Lemma 5.2. Then, we can define a linear regression problem under these assumptions. Therefore, we can directly apply Theorem 1 in Bartlett et al. (2020) to obtain the upper bound of the new excess risk $\tilde{R}(\theta)$.

□

By combining this corollary with Lemma 5.1, we obtain the statement.

□

L Proof of Theorem 4.7

We firstly develop the following lemma on the eigenvalues of $\Sigma_a$.

Lemma L.1 (Lemma 4.5). If $\Sigma$ is a benign covariance, we have

$$\max_{a \in \{0, 1\}} \sum_{k=1}^{\infty} \mu_k(\Sigma_a) = o(n)$$

(21)

Proof. Since $\sum_{k=1}^{\infty} \mu_k(\Sigma) = o(n)$ holds for the benign covariance $\Sigma$, showing the positive definiteness of $\Sigma - \Sigma_a$ is sufficient to achieve the statement.

Take $z \in \mathbb{H}$ arbitrary such that $\|z\| = 1$.

$$z^T(\Sigma - \Sigma_a)z = z^T \mathbb{E}[(1 - 1[d = a])xx^T]z$$

$$= z^T \mathbb{E}_x[\mathbb{E}_d[1 - 1[d = a]|x]xx^T]z$$

$$= z^T \mathbb{E}_x[(1 - p(d = a|x))xx^T]z.$$ 

Since $xx^T$ is a positive semi-definite operator, we obtain

$$z^T(1 - p(d = a|x))xx^T z \geq z^T(1 - \varphi)xx^T z.$$ 

Hence, we have

$$z^T \mathbb{E}_x[(1 - p(d = a|x))xx^T]z \geq (1 - \varphi)z^T \mathbb{E}[xx^T]z = (1 - \varphi)z^T \Sigma z > 0.$$ 

The last inequality follows the positive definiteness of $\Sigma$ and Assumption 2.4.

□

M Proof of Theorem 5.4

Proof. We obtain the statement by combining Theorem 5.3 and Theorem 6 in Bartlett et al. (2020).

□