Towards R-learner of conditional average treatment effects with a continuous treatment: T-identification, estimation, and inference

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Abstract

The R-learner has been popular in causal inference as a flexible and efficient meta-learning approach for heterogeneous treatment effect estimation. In this article, we show the identifiability transition of the generalized R-learning framework from a binary treatment to continuous treatment. To resolve the non-identification issue with continuous treatment, we propose a novel identification strategy named T-identification, acknowledging the use of Tikhonov regularization rooted in the nonlinear functional analysis. Following the new identification strategy, we introduce an ℓ2-penalized R-learner framework to estimate the conditional average treatment effect with continuous treatment. The new R-learner framework accommodates modern, flexible machine learning algorithms for both nuisance function and target estimand estimation. Asymptotic properties are studied when the target estimand is approximated by sieve approximation, including general error bounds, asymptotic normality, and inference. Simulations illustrate the superior performance of our proposed estimator. An application of the new method to the medical information mart for intensive care data reveals the heterogeneous treatment effect of oxygen saturation on survival in sepsis patients.

Keywords. Causal estimation and inference; Empirical risk minimization; Low rank matrix; The method of sieves.

1 Introduction

Estimating heterogeneous treatment effects is fundamental in causal inference and provides insights into various fields, including precision medicine, education, online marketing, and offline policy evaluation. Let \( T \) be a treatment, \( Y(t) \) be the potential outcome had a subject received treatment level \( T = t \), and \( X \) be pre-treatment covariates. The treatment effect heterogeneity can be quantified by

\[
\tau(x, t) = E(Y(t) - Y(0) \mid X = x),
\]

where \( t = 0 \) is a reference treatment level. Early works of conditional average treatment effect estimation focus on semiparametric models, including partially linear models (Robinson, 1988) and structural nested models (Robins, 1994). Recent years have witnessed the rapid growth of newly-developed methods with flexible
A prevailing stream of works includes nonparametric meta-learners including S- and X-learners (Künzel et al., 2019) and R-learner (Nie & Wager, 2021), which are model-free and can be implemented via any off-the-shelf regression algorithm. S- and X-learners are tied to approximating the potential outcome surfaces using, e.g., the Bayesian additive regression trees (Hill, 2011), deep learning (Shalit et al., 2017), and the causal random forest (Wager & Athey, 2018). However, they are not directly estimating the treatment effect. On the contrary, the R-learner and its variants (Kennedy, 2020) target the treatment effect estimation. The R-learner capitalizes on the decomposition of the outcome model initially proposed by Robinson (1988) in partially linear models and extends for machine learning-based treatment effect estimation (Nie & Wager, 2021). Notably, if with the two nuisance functions estimated under flexible models, the R-learner maintains the oracle property of the treatment effect estimation as if the nuisance functions were known. Despite these advantages, the current R-learner framework applies only to binary or categorical treatments.

In this article, we extend the R-learner framework to estimate the conditional average treatment effect flexibly with continuous treatment. This extension is nontrivial in both identification and estimation. We first employ the idea of Robinson’s residual (Robinson, 1988) to construct the loss function of the conditional average treatment effect, which is a straightforward generalization of the binary-treatment R-loss considered by Nie & Wager (2021). However, in sharp contrast to the binary-treatment case, we show that directly minimizing the generalized R-loss fails to identify $\tau(x,t)$ but a fairly large class of functions $\tau(x,t) + s(x)$ for any $s(x)$. We resolve the non-identification issue by invoking the idea of Tikhonov regularization (Tikhonov et al., 1995) rooted in the non-linear functional analysis. To the best of the authors’ knowledge, this is the first time that Tikhonov regularization is used to resolve a non-identification problem for a target estimand. Specifically, we modify the generalized R-loss with an $\ell_2$-penalization and propose a novel identification strategy, which we call T-identification, acknowledging the use of Tikhonov regularization. We show that the T-identification is able to identify an intermediary $\tilde{\tau}(x,t) = \tau(x,t) - E\{\tau(X,T) \mid X = x\}$ and ultimately $\tau(x,t)$.

Built upon this new identification strategy, we propose a new $\ell_2$-penalized R-learner framework that allows flexible models and machine learning methods for continuous-treatment conditional average treatment effect and nuisance functions estimation. We elucidate the new R-learning framework using the method of sieves for the conditional average treatment effect and provide a thorough investigation of asymptotic properties. Unlike the classical sieve regression problem, theoretical analysis of the sieve R-learner involves low-rank matrices inherited from the non-identification nature of the generalized R-loss. Our theoretical analysis utilizes the toolkit in the matrix perturbation and matrix spectral analysis theory (Bhatia, 2013). Under standard conditions, we show that whenever the nuisance functions can be approximated under the $o_P(n^{-1/4})$-convergence rate, the convergence rate of our proposed estimator does not rely on the smoothness of the outcome model but relies only on the smoothness of $\tau(x,t)$ and the propensity score, the two intrinsic components in $\tilde{\tau}(x,t)$. Within the sieve approximation framework, we also clarify regularity conditions for point-wise convergence and asymptotic normality of the R-learner, under which we propose a closed-form variance estimator and confidence intervals for inference. Our numerical experiments show the attractive performance of our proposed R-learner in both estimation and inference. An application to MIMIC-III data reveals the heterogeneous treatment effect of oxygen saturation on survival in sepsis patients. All technical regularity conditions and proofs for the main paper are included in the Supplementary Material.
1.1 Setup and notation

Let \( \{Z_i = (X_i, T_i, Y_i)\}_{i=1}^n \) be independent and identically distributed samples from the distribution of \((X, T, Y)\), where \(X = (X^{(1)}, \ldots, X^{(d)})\) is a \(d\)-dimensional vector of covariates. Under Rubin’s causal model framework (Rubin, 1974), \(Y^{(t)}\) is the potential outcome had the unit received treatment level \(T = t \in \mathbb{R}\). The causal estimand is \(\tau(x, t)\) defined in (1.1). Due to the fundamental problem in causal inference that not all potential outcomes can be observed for a particular unit, \(\tau(x, t)\) is not identifiable without further assumptions. We employ common assumptions for continuous treatments (Kennedy et al., 2017).

**Assumption 1** (No unmeasured confounding). We have \(\{Y^{(t)}\}_{t \in \mathbb{T}} \perp X\).

**Assumption 2** (Stable unit and treatment value). When \(T = t \in \mathbb{T}\), we have \(Y = Y^{(t)}\).

**Assumption 3** (Positivity). There exists an \(\varepsilon > 0\) such that the generalized propensity score \(f(T = t \mid X = x) \in (\varepsilon, 1/\varepsilon)\) for any \((x, t) \in \mathbb{X} \times \mathbb{T}\).

We summarize the notation used throughout the paper. For any vector \(v\), \(\|v\|_1\) and \(\|v\|\) denote its \(\ell_1\) and \(\ell_2\) norms. For any random variable \(W \in \mathbb{W}\), \(f(w)\) and \(P(w)\) denote its probability density function and probability measure. For any function \(g(w)\), \(P_n\{g(W)\} = \sum_{i=1}^n g(W_i)/n\) denotes its empirical expectation and \(\|g\|_2 = \left\{ \int_{w \in \mathbb{W}} g^2(w) dw \right\}^{1/2}\). \(\|g\|_{L^p} = \left\{ \int_{w \in \mathbb{W}} g^2(w) dP(w) \right\}^{1/2}\), \(\|g\|_W = \sup_{w \in \mathbb{W}} |g(w)|\) denote its \(L^2\), \(L_p^2\), and \(L^\infty\) norms. \(L_2^p(W)\) represents the function space of all \(g(w)\) with a bounded \(L^2_p\) norm. When \(g(w)\) is a multivariate function, denote \(\|g\|_W = \sup_{w \in \mathbb{W}} |g(w)|\). For any function \(h(w)\) with \(w \in \mathbb{R}^d\), we denote its \(\alpha\)-derivative by \(D^\alpha h(w) = \partial^{\alpha_1 + \cdots + \alpha_d} h(w)/\partial w_1^{\alpha_1} \cdots \partial w_d^{\alpha_d}\), where \(\alpha = (\alpha_1, \ldots, \alpha_d)\) is a vector of positive integers. For asymptotic analysis, we restrict the target functional estimand to the popular \(p\)-smooth Hölder class (Newey, 1997).

\[
\Lambda(p,c,\mathbb{W}) = \left\{ h(w) : \sup_{\|\alpha\|_1 \leq [p]} \sup_{w \in \mathbb{W}} |D^\alpha h(w)| \leq c, \sup_{\|\alpha\|_1 = [p]} \sup_{w_1, w_2 \in \mathbb{W}, w_1 \neq w_2} \frac{|D^\alpha h(w_1) - D^\alpha h(w_2)|}{\|w_1 - w_2\|_2^{-[p]}} \leq c \right\},
\]

(1.2)

where \(c, p > 0\) are fixed, and \(h(w)\) belongs to the class of all \([p]\)-times differentiable functions over \(\mathbb{W}\). We require two nuisance functions, the conditional outcome mean and generalized propensity score,

\[
m(x) = E(Y \mid X = x), \quad \varpi(t \mid x) = f(T = t \mid X = x).
\]

Also denote the full conditional outcome mean model \(\mu(x, t) = E(Y \mid X = x, T = t)\). We hereby define the observation noises,

\[
\varepsilon_i = Y_i - \mu(X_i, T_i), \quad i = 1, \ldots, n,
\]

(1.3)

where \(E(\varepsilon_i \mid X_i, T_i) = 0\), following the definition of \(\mu(x, t)\).

2 Continuous-treatment R-learner

2.1 The generalized R-loss

We first generalize the idea of the Robinson’s residual (Robinson, 1988; Nie & Wager, 2021) to the continuous-treatment scenario. The unconfoundedness and stable unit and treatment value imply,

\[
Y_i^{(T_i)} = \mu(X_i, T_i) + \varepsilon_i = \mu(X_i, 0) + \tau(X_i, T_i) + \varepsilon_i,
\]

(2.1)
where the first equality follows from Assumption 2 and equation (1.3), and the second equality follows from Assumption 1 and the definition of \( \tau(x, t) \). Model (2.1) is nonparametric and free of any structural assumptions. Given \( X_i \), taking the conditional expectation on (2.1) leads to

\[
m(X_i) = E(Y^{(T_i)} \mid X = X_i) = \mu(X_i, 0) + E_{\varpi}\{\tau(X, T) \mid X = X_i\} + E(\epsilon_i \mid X_i)
\]

\[
= \mu(X_i, 0) + E_{\varpi}\{\tau(X, T) \mid X = X_i\},
\]

where the last equality is followed by the law of total expectation such that

\[
E(\epsilon_i \mid X_i) = E\{E(\epsilon_i \mid X_i, T_i) \mid X_i\} = E(0 \mid X_i) = 0.
\]

The notation \( E_{\varpi}\{\tau(X, T) \mid X = X_i\} \) in (2.2) highlights the dependency of the conditional expectation on the generalized propensity score \( \varpi \) as \( E_{\varpi}\{\tau(X, T) \mid X = X_i\} = \int_{t \in T} \tau(x_i, t) \varpi(t \mid X_i) dt \). By subtracting (2.2) from (2.1) on both left- and right-hand sides, we have

\[
Y_i^{(T_i)} - m(X_i) = \tau(X_i, T_i) - E_{\varpi}\{\tau(X, T) \mid X = X_i\} + \epsilon_i.
\]

By treating the left-hand side of (2.3) as the response and the right-hand side except \( \epsilon_i \) as the mean function, we derive the following population loss function,

\[
L_c(h) = E\left[ Y - m(X) - h(X, T) + E_{\varpi}\{h(X, T) \mid X\} \right]^2,
\]

which is minimized at \( h = \tau \). The above derivation is similar to and actually includes that of the binary-treatment R-loss function (Nie & Wager, 2021, Section 2) as a special case, thus we term (2.3) as the generalized R-loss. Under the binary-treatment case, \( \tau(x, t) \) reduces to \( \{\tau(x, 0), \tau(x, 1)\} \), where \( \tau(x, 0) = E(Y^{(0)} - Y^{(0)} \mid X = x) = 0 \) for any \( x \in \mathbb{X} \), and \( \tau(x, 1) \) becomes the conditional average treatment effect of interest. It suffices to estimate \( \tau(x, 1) \) by solving the \( h(\cdot, 1) \) that minimizes (2.4) while imposing an intrinsic shape constraint for \( h(\cdot, 0) \) such that,

\[
h(X, 0) = 0 \quad \text{a.s.}
\]

Furthermore, observing that under (2.5), one has, \( h(X, T) - E_e\{h(X, T) \mid X\} = \sum_{t \in \{0, 1\}} I(T = t) [h(X, t) - e(x) h(X, 1) - (1 - e(x)) h(X, 0)] = (T - e(X)) h(X, 1) \) a.s., where \( I(\cdot) \) is the indicator function and \( e(x) = \Pr(T = 1 \mid X = x) \) is the propensity score for a binary treatment. Thus the R-loss function (2.4) reduces to

\[
L_b(h) = E\left[ Y - m(X) - (T - e(X)) h(X, 1) \right]^2,
\]

introduced in Nie & Wager (2021), which is also minimized at \( h = \tau \).

### 2.2 An identifiability transition of the generalized R-learner

The generalization of the R-loss from the binary treatment to the continuous treatment is natural, which however results in a transition of the identifiability of \( \tau(x, t) \). Suppose we construct \( \hat{\tau}(x, t) \) by directly minimizing the empirical analogy of \( L_c(\cdot) \) following Nie & Wager (2021). Unlike the binary-treatment case, the R-learner for the continuous treatment will have poor estimation performance, due to the non-identifiability of the generalized R-loss. To illustrate, we conduct a simple simulation study. The simulation details are deferred to §S.3. Fig. 1 contrasts the different behaviors of the generalized R-learner in the binary- and continuous-treatment cases. Apparently, the R-learner approximates \( \tau(x, t) \) well for a binary \( T \) (Fig. 1a) and poorly for a continuous \( T \) (Fig. 1c).
Figure 1: Illustration of the identifiability transition of the R-learner from a binary treatment to continuous treatment. Panel (a): when the treatment is binary, the generalized R-learner (the solid blue line) is unbiased of $\tau(x, 1)$ (the dashed red line). When the treatment is continuous, the generalized R-learner (Panel c) is far away from $\tau(x, t)$ (Panel b). The proposed regularized R-learner (Panel d) recovers $\tau(x, t)$. 
We provide a theoretical argument for the success and failure of the identifiability of the generalized R-learner for binary and continuous treatments. We focus on the \( \mathcal{L}^2_P(X,T) \) space and
\[
\mathcal{S} = \{ h \mid h(X,T) = \tau(X,T) + s(X) \text{ a.s., for any } s \in \mathcal{L}^2_P(X) \}.
\] (2.7)

It is easy to check that for any \( h \in \mathcal{S} \),
\[
Y - m(X) - [h(X,T) - E_{\mathcal{P}}\{h(X,T) \mid X\}] = Y - m(X) - [\tau(X,T) - E_{\mathcal{P}}\{\tau(X,T) \mid X\}] \text{ a.s.}
\]

Thus from (2.4), any function \( h \in \mathcal{S} \) is a minimum of our generalized R-loss \( L_c(\cdot) \). Thus, when \( T \) is continuous, directly minimizing the generalized R-loss fails to identify the target estimand \( \tau(x,t) \) as there are infinitely many different solutions. This theoretically justifies the non-identification issue when estimating \( \tau(x,t) \) by minimizing the empirical analogy of \( L_c(\cdot) \) and thus explains the ill-posed problem illustrated in Fig. 1. Part (i) of Proposition 1 below rigorously proves that \( \mathcal{S} \) in fact contains all minima of \( L_c(\cdot) \) in \( \mathcal{L}^2_P(X,T) \). In contrast, minimizing the binary-treatment R-loss (2.6) after imposing the intrinsic shape constraint (2.5) can successfully identify \( \tau(x,t) \) now, because (2.5) narrows the general solution set \( \mathcal{S} \) into
\[
\mathcal{S}^\circ = \{ h \mid h(X,T) = \tau(X,T) \text{ a.s.} \}
\]
with a formal proof relegated to §S.5.4 in the Supplementary Material. Despite the popular use of R-loss (2.6) in literature (Zhao et al., 2017; Nie & Wager, 2021), the corresponding identification problem has not been rigorously addressed. Part (ii) of Proposition 1 fulfills this gap.

**Proposition 1.** Suppose Assumptions 1–2 hold. We have the following identification results.

(i) Suppose \( T \) is a continuous treatment and \( \tau \in \mathcal{L}^2_P(X,T) \). Then \( \mathcal{S} \) is the solution set of the following optimization problem,
\[
\arg \min_{h \in \mathcal{L}^2_P(X,T)} L_c(h).
\] (2.8)

(ii) Suppose \( T \) is a binary treatment and \( \tau(\cdot,1) \in \mathcal{L}^2_P(X) \). Additionally assume the positivity assumption such that \( e(x) \) satisfying \( e(x) \in (e',1-e') \) for some fixed \( e' > 0 \) and for all \( x \in \mathcal{X} \). Then among the set of interested functions, \( \mathcal{L}_b = \{ h \mid h(\cdot,1) \in \mathcal{L}^2_P(X) \text{ and } h(X,0) = 0 \text{ a.s.} \} \), \( \mathcal{S}^\circ \) is the solution set of the following optimization problem,
\[
\arg \min_{h \in \mathcal{L}_b} L_b(h).
\] (2.9)

### 2.3 T-identification

We resolve the non-identification issue for a continuous treatment through a novel identification strategy, termed the **T-identification**, based on the Tikhonov regularization. We consider the population \( \ell_2 \)-penalized \( L_c(\cdot) \),
\[
L_{c,\ell_2}(h \mid \rho) = L_c(h) + \rho \| h \|_{\mathcal{L}^2_P}^2.
\] (2.10)

The penalty term is inspired by Tikhonov regularization (Tikhonov et al., 1995) originally developed in the non-linear functional analysis for solving ill-posed operator equations.

Adding the generalized R-loss with Tikhonov regularization effectively identifies an intermediary
\[
\tilde{\tau}(x,t) = \tau(x,t) - E\{\tau(X,T) \mid X = x\}
\]
and ultimately the target estimand $\tau(x, t)$. First, the new loss $L_{c, \ell_2}(h \mid \rho)$ becomes strictly convex over $\mathcal{L}_2^p(X, T)$ due to the addition of a strictly convex functional $\rho\|h\|_{\mathcal{L}_2^p}^2 = \rho E\{h^2(X, T)\}$. Thus, its minima equal to a unique function $\tau_\rho \in \mathcal{L}_2^p(X, T)$ a.s.. Second, we show that $\tau_\rho$ lies in a $O(\rho^{1/4})$-ball of $\tilde{\tau}$ under the $\mathcal{L}_2^p$ norm, and thus $\tau_\rho \to \tilde{\tau}$ as $\rho \to 0$. Specifically, when $\rho \to 0$, the difference between two loss functions, $L_{c, \ell_2}(h \mid \rho)$ and $L_c(h)$, vanishes. Therefore, $\tau_\rho$ shall approach $L_c(h)$’s solution set $S$ as $\rho \to 0$. On the other hand, among $S$, $\tilde{\tau}$ has the smallest value in terms of $L_{c, \ell_2}(h \mid \rho)$ for any $\rho > 0$. This is because by definition, any function $h$ in $S$ produces the same value of the first term on the right-hand side of (2.10), while $\tilde{\tau}$ can minimize the second term as it has the smallest $\mathcal{L}_2^p$ norm. Therefore, $\tau_\rho$ shall particularly approach $\tilde{\tau}$ in $S$ when $\rho \to 0$ yet $\rho > 0$. Lastly, the identification of $\tau(x, t)$ follows by a simple fact that

$$\tau(x, t) = \tilde{\tau}(x, t) - \tilde{\tau}(x, 0), \quad \text{for any} (x, t) \in X \times T. \quad (2.11)$$

Theorem 1 summarizes the identification result with a formal proof given in §S.5.5.

**Theorem 1.** When Assumptions 1–2 hold and $\tau \in \mathcal{L}_2^2(X, T)$, given $\rho > 0$, the solution set of

$$\arg \min_{h \in \mathcal{L}_2^2(X, T)} L_{c, \ell_2}(h \mid \rho) \quad (2.12)$$

is $S_\rho = \{h \mid h(X, T) = \tau_\rho(X, T) \text{ a.s.}\}$ where $\tau_\rho \in \mathcal{L}_2^p(X, T)$ is a unique function. When $\rho \to 0$, one has $\tau_\rho \to \tilde{\tau}$ under the $\mathcal{L}_2^p$ norm. Finally, $\tau(x, t)$ can be identified by $\tilde{\tau}(x, t)$ through (2.11).

Our two-step T-identification strategy for $\tau(x, t)$ differs fundamentally from the classic, direct expectation-based identification strategies but relies on a sequence of functionals indexed by $\rho$. It also generates an important implication of the bias-variance tradeoff in finite samples. Under the finite-sample scenario, if one develops the generalized R-learner by minimizing the empirical analogy of $L_{c, \ell_2}(h \mid \rho)$, an excessively small $\rho$ will introduce large estimation variance. Intuitively, a small $\rho$ will result in a weak $\ell_2$-penalization. Then with finite samples, such weak $\ell_2$-penalization can not make the minimization of the empirical analogy of $L_{c, \ell_2}(h \mid \rho)$ significantly different from naively minimizing the empirical analogy of $L_c(h)$, which is ill-posed as shown in §2.2. On the other hand, a large $\rho$ will bring an extreme bias, because $\tau_\rho$ in Theorem 1 may not approximate $\tilde{\tau}$ well with large $\rho$. Such phenomenon will later be revealed by Theorem 2, where both extremely small or large $\rho$ can result in large terms in the convergence rate of our proposed estimator.

**Remark 1.** The $\ell_2$-penalization has been used in classic statistical methods, including linear and logistic ridge regression (Hoerl & Kennard, 1970), penalized spline regression (O’Sullivan, 1986), kernel ridge regression (Aiernan et al., 1964), among others. The previous works use the $\ell_2$ penalty to regularize the estimation complexity, resulting in stable and theoretically guaranteed estimators. However, those works require that the target estimand is at least a locally unique minimum of the corresponding loss function at the population level. To the best of the authors’ knowledge, this paper distinguishes itself from the previous works as we use $\ell_2$-penalization, for the first time, to resolve a population-level non-identification problem, where the original loss function has infinitely many minima but also regularize the complexity of the proposed estimator (§2.4).

**2.4 $\ell_2$-penalized R-learner**

Given the T-identification strategy, we formally propose the $\ell_2$-penalized R-learner in Algorithm 1 using cross fitting (Chernozhukov et al., 2018, Definition 3.1). Algorithm 1 includes a general algorithm and a
specific illustration with sieve approximation. The latter will be discussed in details in §3. Continuing with the numerical experiment in §2.2, we demonstrate the effectiveness of the proposed penalized R-learner (Fig. 1d), which well approximate the true τ(x, t).

**Remark 2.** The newly proposed R-learner inherits many practical and theoretical advantages from the original R-learner (Nie & Wager, 2021). Practically, minimizing the empirical analogy of $L_c, \ell_2$ separates the process of estimating the nuisance functions and that of estimating the target estimand. In addition, loss-minimization methods, e.g., the penalized nonparametric regression, deep neural networks, and boosting can be flexibly used to minimize (2.13). Theoretically, as we will show later, similar to the original R-learner, our proposed R-learner is robust to slow convergence rates of the nuisance estimators.

**Remark 3.** A variant of cross fitting (Chernozhukov et al., 2018, Definition 3.2) can be similarly adapted in Algorithm 1. Specifically, in Step 3, we can obtain $J$ different estimators of $\hat{\tau}(x, t)$ by minimizing the empirical loss within each sub-sample set and obtain the final $\hat{\tau}(x, t)$ by averaging the $J$ estimators. Although the resulting estimators can differ slightly, their asymptotic properties remain the same (Chernozhukov et al., 2018, Remark 3.1).

### 3 Sieve approximation and theoretical properties

We elucidate the proposed R-learner with the method of sieves. The sieve approximation (Geman & Hwang, 1982) has been broadly studied and applied for nonparametric estimation due to its good interpretability and theoretical properties (e.g., Chen, 2007). In particular, we consider a triangular array expansion of $h(x, t)$,

$$h(x, t) = \phi^T \left[ \Psi_1(x, t), \cdots, \Psi_K(x, t) \right]^T = \phi^T \Psi(x, t),$$

where $\phi$ is an $J \times K$ matrix, $\Psi$ is an $n \times K$ matrix, and $\Psi_k$ is a $n \times 1$ vector.

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**Algorithm 1:** General $\ell_2$-penalized R-learner and an illustration with sieve approximation in §3

1. **Step 1.** Split $\{Z_i\}_{i=1}^n$ into $J$ mutually exclusive ($J > 1$), and equally sized or nearly equally sized sub-sample sets $S_1, \ldots, S_J$, such that $\cup_{j=1}^J S_j = \{Z_i\}_{i=1}^n$; let $i$th sample belongs to $j_i$th subset.
2. **Step 2.** For each $j \in [J]$, train the nuisance function estimator $\{\hat{m}^{(-j)}(x), \hat{\phi}^{(-j)}(t \mid x)\}$ with all data except $S_j$ via any generic and fine-tuned machine learning method.
3. **Step 2* (Sieve approximation).** For each $j \in [J]$, obtain $\{\hat{m}^{(-j)}(x), \hat{\Gamma}^{(-j)}(x)\}$ with all data except $S_j$ by the method of sieves; see Remark 4 for two options of $\hat{\Gamma}^{(-j)}(x)$.
4. **Step 3.** Choosing $\rho > 0$, estimate $\hat{\tau}(x, t)$ by

$$\hat{\tau}(x, t) = \arg\min_{h(\cdot, \cdot)} \hat{L}_{c, \ell_2} \{h(\cdot, \cdot) \mid \rho\}$$

$$= \arg\min_{h(\cdot, \cdot)} \frac{1}{n} \sum_{i=1}^n \left[ Y_i - \hat{m}^{(-j_i)}(X_i) - h(X_i, T_i) + E_{\hat{\phi}^{(-j_i)}} \{h(X_i, T) \mid X_i\} \right]^2 + \rho P_n \{h^2(X, T)\}. \tag{2.13}$$

5. **Step 3* (Sieve approximation).** Obtain $\hat{\phi}$ from (3.1) with $\rho > 0$, and obtain

$$\hat{\tau}(x, t) = \hat{\phi}^T \Psi(x, t);$$

6. **Step 4.** Output $\hat{\tau}(x, t) = \hat{\tau}(x, t) - \hat{\tau}(x, t = 0)$. 

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**Remark 1.** The proposed $\ell_2$-penalized R-learner inherits many practical and theoretical advantages from the original R-learner (Nie & Wager, 2021). Practically, minimizing the empirical analogy of $L_c, \ell_2$ separates the process of estimating the nuisance functions and that of estimating the target estimand. In addition, loss-minimization methods, e.g., the penalized nonparametric regression, deep neural networks, and boosting can be flexibly used to minimize (2.13). Theoretically, as we will show later, similar to the original R-learner, our proposed R-learner is robust to slow convergence rates of the nuisance estimators.
Remark 4. We discuss two options for obtaining \( \hat{\Gamma}(x) \) for any \( j \in [J] \).

(i) \( \hat{\Gamma}(x) = E_{\tilde{\psi}(x)} \{ \Psi(X, T) \mid X = x \} \), where \( \tilde{\psi}(x) \) is the generalized propensity score estimator over \( \{ Z_i \}_{i=1}^n \setminus S_j \). One-dimensional numerical integration can be implemented to approximate the conditional expectation.

(ii) \( \hat{\Gamma}(x) \) consists of coordinate-wise nonparametric regressions. For simplicity, we consider \( \Psi(x, t) \) as the tensor-product of B-splines (§S.5.2). First, observing that \( \Gamma(x) = E \{ \psi(T) \mid X = x \} \otimes \Psi(x) \), where \( \Psi(x) \) denotes \( \psi(x(1)) \otimes \cdots \otimes \psi(x(d)) \), we can estimate \( \hat{\Gamma}(x) \) by \( \hat{\Gamma}(x) = \hat{E}^j(\{ \psi(T) \mid X = x \}) \otimes \Psi(x) \), where \( \hat{E}^j(\{ \psi(T) \mid X = x \}) \) is obtained by multivariate regression over the covariates-response pairs \( \{ X_i, \psi(T_i) \} \) fitted with all data except \( S_j \). Suppose \( \psi(t) \in \mathbb{R}^{k_T} \) is a \( k_T \)-dimensional B-spline basis for the treatment variable, and let \( 1_{k_T} = (1, \ldots, 1)^T \in \mathbb{R}^{k_T} \). Inspired by the sum invariance property of B-splines (Lemma 1) such that \( 1_{k_T}^T E \{ \psi(T) \mid X = x \} = E \{ 1_{k_T} \psi(T) \mid X = x \} = E(\sqrt{k_T} \mid X = x) = \sqrt{k_T} \) for any \( x \in \mathbb{R} \), we further impose a shape constraint for \( \hat{E} \{ \psi(T) \mid X = x \} \),

\[
1_{k_T}^T \hat{E}^j(\{ \psi(T) \mid X = x \}) = \sqrt{k_T}, \quad \text{for any } x \in \mathbb{R}, j \in [J].
\]

A simple strategy can be used to satisfy the above shape constraint. First obtain \( \hat{E}^j(\{ \psi(T) \mid X = x \}) \) by coordinate-wise regression when \( j \in [k_T - 1] \), and then obtain

\[
\hat{E}^{(k_T)}(\{ \psi(T) \mid X = x \}) = \sqrt{k_T} - \sum_{j=1}^{k_T-1} \hat{E}^j(\{ \psi(T) \mid X = x \}).
\]

The above approaches apply similarly to other types of basis functions. Conditional density estimation in method (i) is often difficult, especially when \( X \) is high dimensional. In these cases, method (ii) provides a flexible alternative, which replaces conditional density estimation with a series of regressions.

3.1 Asymptotic properties

For theoretical analysis, we choose \( \Psi(x, t) \) as the tensor-product of B-splines (e.g., Chen & Christensen, 2015). We provide technicality including the theoretical properties of the B-spline basis in §S.5.2 and regularity conditions in §S.5.1.
Algorithm 2: Cont’d Algorithm 1: Variance estimator of \(\tilde{\tau}(x_0, t_0)\)

| Step 1. Obtain top-\((K - K/k)\) singular value decomposition \(\tilde{U} \Sigma \tilde{U}^T\) of \(\hat{G}_n = \tilde{R}_n + \rho \tilde{Q}_n\); |
| Step 2. Set \(\hat{A}_n = \tilde{U} \mathbb{S}^{-1} \tilde{U}^T\); |
| Step 3. For each \(j \in \mathcal{J}\), obtain \(\hat{\mu}^{-j}(x, t)\) with all data except \(S_j\), via flexible machine learning methods. Then obtain |
\[
\hat{B}_n^{(j)} = \frac{1}{|S_j|} \sum_{Z_i \in S_j} \{ Y_i - \hat{\mu}^{(j)}(X_i, T_i)\}^2 \{ \Psi(X_i, T_i) - \hat{\Gamma}^{(j)}(X_i)\} \{ \Psi(X_i, T_i) - \hat{\Gamma}^{(j)}(X_i)\}^T;
\]
| Step 4. Set \(\hat{B}_n = \mathcal{J}^{-1} \sum_{j=1}^J \hat{B}_n^{(j)}\); |
| Step 5. Output \(\hat{\sigma}^2 = \{ \Psi(x_0, t_0) - \Psi(x_0, 0)\}^T \hat{A}_n \hat{B}_n \hat{A}_n \{ \Psi(x_0, t_0) - \Psi(x_0, 0)\}\). |

Classic nonparametric sieve regression (Newey, 1997) often assumes a full-rank gram matrix \(Q_n = E\{\Psi(X, T)\Psi^T(X, T)\}\) where the dimension of \(\Psi\) depends on \(n\). In stark contrast, theoretical analysis of the proposed R-learner involves a low-rank gram matrix,

\[
R_n = E\left[\{\Psi(X, T) - \Gamma(X)\} \{\Psi(X, T) - \Gamma(X)\}^T\right] = (U \quad U_\perp) \begin{pmatrix} \Sigma & 0 \\ 0 & U_\perp^T \end{pmatrix}, \quad (3.4)
\]

where the right-hand side of (3.4) is the singular value decomposition of \(R_n\), with \(\text{rank}(R_n) = \zeta \leq \zeta = \text{diag}\{\sigma_1, \ldots, \sigma_\zeta\}\) such that and \(\sigma_1 \geq \cdots \geq \sigma_\zeta > 0\). Each entry of \(R_n\) is the probability limit of the corresponding entry of \(R_n\) in (3.1). Intuitively, the low rank of \(R_n\) is tied to the non-identification issue of the generalized R-loss in \(\S 2.3\) when setting \(\rho = 0\). In this case, \(\hat{\phi}\) is asymptotically unsolvable, or equivalently \(\hat{R}_n\) in (3.1) is asymptotically non-invertible; i.e., \(\hat{R}_n\) is low-rank. We denote \(\sigma_\zeta \leq \beta_n > 0\), which plays an essential quantity in our theoretical results. See Lemma 4 for detailed spectral properties of \(R_n\). To address the effect of nuisance function estimation, we consider the following concentration conditions for \(\hat{m}(x)\) and \(\hat{\Gamma}(x)\) with \(r_m, r_\gamma, r'_\gamma \asymp 1\),

\[
\left\| \hat{m} - m \right\|_{L^2_p} = o_P(r_m),
\]

\[
\left\| \hat{\Gamma} - \Gamma \right\|_{\mathcal{H}/\sqrt{K}} = o_P(r'_\gamma),
\]

\[
\left\| \int_{x \in \mathbb{X}} \{ \hat{\Gamma}(x) - \Gamma(x)\} \{ \hat{\Gamma}(x) - \Gamma(x)\}^T d\mathcal{P}(x) \right\|_{L^2}^{1/2} = o_P(r_\gamma). \quad (3.7)
\]

The convergence rate condition of \(\hat{m}(x)\) is commonly assumed; see, e.g., Kennedy et al. (2017). The following proposition further implies that, if we obtain \(\hat{\Gamma}(x)\) through \(\hat{\phi}(t \mid x)\) by method (i) in Remark 4, the convergence rates in (3.6) and (3.7) are simultaneously attained as long as \(\hat{\phi}(t \mid x)\) satisfies a certain \(L^2\)-convergence rate uniformly for all \(x \in \mathbb{X}\).

Proposition 2. Suppose regularity conditions 4 and 7 hold, and \(\hat{\Gamma}(x) = E_{\hat{\phi}}\{\Psi(X, T) \mid X = x\}\). When \(\hat{\phi}(t \mid x)\) satisfies \(\sup_{x \in \mathbb{X}} \left\| \hat{\phi}(\cdot \mid x) - \phi(\cdot \mid x) \right\|_{L^2} = o_P(r_{\phi})\). Then (3.6) and (3.7) hold with \(r'_\gamma = r_\gamma = r_\phi\).

Theorem 2 summarizes the asymptotic results for the R-learner \(\hat{\tau}(x, t)\) obtained by Algorithm 1.

Theorem 2. Suppose Assumptions 1–3 and regularity conditions in \(\S S.5.1\) hold, and \(\hat{m}(x), \hat{\Gamma}(x)\) satisfy (3.5)–(3.7). Suppose further the conditions hold: (i) \(r_\gamma^2 \asymp \sqrt{K \log n/n}\); (ii) \(\sqrt{K \log n/n} \prec \beta_n\); (iii)
\( \rho < \sqrt{K \log n/n} \); (iv) \( \hat{\tau}(x, t) \in \Lambda(p, c, X \times T) \) for some \( p, c > 0 \); and (v) \( \hat{\Gamma}(x) \) is trained via either one of the methods in Remark 4. Then for any \((x_0, t_0) \in X \times T\), we have the general upper bound,

\[
|\hat{\tau}(x_0, t_0) - \tau(x_0, t_0)| \leq r(n, K, \beta_n, \rho, r_m, r_\gamma, r_\gamma') ,
\]

as \( n \to \infty \). An explicit form of \( r(n, K, \beta_n, \rho, r_m, r_\gamma, r_\gamma') \) is given in (S.5.104) in the Supplementary Material. Specifically, when \( \beta_n \asymp 1, p > d + 1 \), and \( r_m, r_\gamma, r_\gamma' \preceq n^{-1/4} \), we have

- (Consistency). When choosing \( K \asymp n^{(d+1)/(2p)} \) and \( \rho \asymp n^{-1/2} \), the rate in (3.8) can be minimized by

\[
\left| \hat{\tau}(x_0, t_0) - \tau(x_0, t_0) \right| = O_P(n^{-1/2+(d+1)/(4p)});
\]

- (Limiting distribution). Suppose further the \((2 + c_0)\)-order moment condition,

\[
\sup_{(x,t) \in X \times T} E \{|Y - E(Y | X, T)|^{2+c_0} | X = x, T = t \} < +\infty,
\]

holds for some fixed \( c_0 > 0 \). When choosing \( K \asymp n^{\epsilon_{clt} + (d+1)/(2p)} \) for any \( \epsilon_{clt} \in (0, 1/2 - (d+1)/(2p)) \) and \( \rho \asymp n^{-1/2} \), we have

\[
\sqrt{n} \hat{\sigma}^{-1} \{ \hat{\tau}(x_0, t_0) - \tau(x_0, t_0) \} \sim \mathcal{N}(0, 1),
\]

where \( \hat{\sigma} \) is defined in (S.5.110) in the Supplementary Material.

- (Confidence interval). Let \( \hat{\sigma} \) be obtained by Algorithm 2 with \( \hat{\mu}(x, t) \) satisfying \( ||\hat{\mu} - \mu||_{X \times T} = o_P(1) \). Then we have

\[
\sqrt{n} \hat{\sigma}^{-1} \{ \hat{\tau}(x_0, t_0) - \tau(x_0, t_0) \} \sim \mathcal{N}(0, 1).
\]

In Theorem 2, we first state the upper bound of the \( \ell_2 \)-penalized R-learner with sieve approximation. Condition (i) holds whenever \( r_\gamma \preceq n^{-1/4} \). Conditions (ii) and (iii) hold when \( \beta_n \) and \( \rho \) decay slowly with \( n \). Condition (iv) specifies the smoothness of \( \hat{\tau}(x, t) \). Recall that \( \hat{\tau}(x, t) = \tau(x, t) - E\{\tau(X, T) | X = x\} \). A sufficient condition for condition (iv) to hold is that both \( \tau \) and \( \tau_{\infty} \) are in \( \Lambda(p, c, X \times T) \). Therefore, our theoretical results do not rely on the smoothness of the outcome model. Condition (v) covers the two training strategies of \( \hat{\Gamma}(\cdot) \) introduced in Remark 4.

The general upper bound \( r(n, K, \beta_n, \rho, r_m, r_\gamma, r_\gamma') \) has a complicate form, thus we defer its explicit form to the Supplementary Material. To ease the exposition, we consider a simple but reasonable condition such that \( \beta_n \asymp 1, p > d + 1 \), and \( r_m, r_\gamma, r_\gamma' \preceq n^{-1/4} \) to elucidate results in (3.9), (3.11), and (3.12). The asymptotic behavior of \( \beta_n \) relies on the joint design of \((X, T)\). One sufficient condition for \( \beta_n \asymp 1 \) to hold is that \( T \) follows complete randomization (Neyman, 1923/1990); see Lemma 4 (iii). The relationship \( p > d + 1 \) means that \( \hat{\tau}(x, t) \) is smooth enough with respect to its dimension. A similar condition is also considered in the theoretical analysis of other sieve-type estimators; see e.g., Shi et al. (2022+). We emphasize that assumptions like \( \beta_n \asymp 1 \) and \( p > d + 1 \) are made mainly for succinct conditions and results. With more careful bookkeeping, the consistency result remains valid, yet with a more complicated form of the convergence rate, when \( p \) is slightly smaller than \( d + 1 \), and the limiting distribution results still hold when \( \beta_n \) is slowly decaying. Finally, the nuisance functions are estimated with the \( o_P(n^{-1/4}) \) rate, which are relaxed from the \( O_P(n^{-1/2}) \) rate, demonstrating the robustness of our proposed estimator to slower rates of convergence of nuisance function estimators. Similar conditions are assumed in Nie & Wager (2021); Yadlowsky et al. (2018), among others.
Our consistency result (3.9) is attained after choosing $K$ and $\rho$ to balance the bias-variance tradeoff. If a higher-order moment condition (3.10) holds, we further have the limiting distribution result (3.11), as long as we slightly increase $K$ resulting in an undersmoothing estimator. Similar conditions appear when studying the limiting distribution of the classic nonparametric sieve regression (Newey, 1997). Finally, we propose a closed-form variance estimator $\hat{\sigma}^2$ of $\hat{\tau}(x_0, t_0)$ in Algorithm 2, for any given $(x_0, t_0) \in \mathbb{X} \times \mathbb{T}$. The variance estimator requires an additional consistent estimator for $\mu(x, t)$ under $L^\infty$ norm. Such condition is common (e.g., Kennedy et al., 2017). Then we construct a $(1 - c)$ confidence interval as

$$
\left( \hat{\tau}(x_0, t_0) - z_{c/2} \frac{\hat{\sigma}}{\sqrt{n}}, \hat{\tau}(x_0, t_0) + z_{c/2} \frac{\hat{\sigma}}{\sqrt{n}} \right).
$$

(3.13)

We use $z_c$ to represent the $(1 - c)$-quantile of the standard normal distribution for any $c \in (0, 1)$.

**Remark 5** (Tuning parameter selection). Theorem 2 indicates that, to attain the best theoretical performance of our proposed method, one needs to carefully select the tuning parameters $K$ and $\rho$ and thereby balance the bias-variance tradeoff. The R-learner with sieve approximation permits a closed-form solution (3.1). It allows a fast generalized cross validation-based algorithm for selecting $K$ and $\rho$; see §S.1. For inference, as illustrated in Theorem 2, one could slightly increase the optimal $K$ selected by generalized cross validation before constructing the confidence interval (3.13); the effectiveness of such strategy is further demonstrated by numerical experiments in §4.

## 4 Numerical experiment

We run simulations to evaluate the finite-sample performance of our proposed methods. With sample size $n$, we generate random samples $\{Z_i\}_{i=1}^n$, where $Z$ takes the form of $Z = \{X = (X^{(1)}, X^{(2)}), T, Y\}$. The generating process of $Z$ is as follows:

- Generate $X^{(1)} \sim \text{Bernoulli}(0.5)$ and $X^{(2)} \sim \text{Uniform}(0, 1)$.
- Generate $T$ from one of the following generalized propensity score distributions:
  - (Complete randomized experiment). Uniform(0, 1);
  - (Beta distribution). $\text{Beta}(\lambda_X, 1 - \lambda_X)$, where we set $\text{logit}(\lambda_X) = (1, X^{(1)}, X^{(2)})\eta$ with $\eta = (0.8, 0.2, -0.8)^T$. Such distribution has been considered by Kennedy et al. (2017, Section 4).
- Generate $Y = \mu(X, 0) + \tau(X, T) + \mathcal{N}(0, 0.3^2)$, where we set $\mu(X, 0) = X^{(1)}X^{(2)} + \sin(2X^{(2)}) + (X^{(2)})^2$, and
  $$
  \tau(X, T) = \begin{cases} 
  I(r_{0.5} \leq 0.5)v(r_{0.5}) & X^{(1)} = 1 \\
  I(r_{0.5} \leq 0.5)v(r_{0.5}) + I(r_{0.8} \leq 0.5)v(r_{0.8})/2 & X^{(1)} = 0,
  \end{cases}
  $$

  where $r_a$ is the Euclidean distance between $(X^{(2)}, T)$ and $(a, a)$, and $v(r) = \sin(2\pi r + \pi/2) + 1$ and $I(\cdot)$ is the indicator function.

To fit data, we first stratify the simulated data by $X^{(1)}$. We then fit each stratum by the $\ell_2$-penalized R-learner with sieve approximation stated in Algorithm 1, where $\Psi(x^{(2)}, t) = \psi(t) \otimes \psi(x^{(2)})$ and $\mathcal{J} = 6$; here $x^{(2)}$ corresponds $X^{(2)}$. Both $\psi(t)$ and $\psi(x^{(2)})$ are B-spline functions with a quadratic degree and equally
spaced knots over $[0, 1]$. We select the optimal basis numbers $k_{T, \text{opt}}$ and $k_{X, \text{opt}}$ for $\psi(t)$ and $\psi(x^{(2)})$ and regularization parameter $\rho_{\text{opt}}$ by the generalized cross validation-based algorithm in \S S.1, among a candidate pool $\mathcal{L} = \{(k_{X, \text{opt}}, k_T, \rho) \mid 4 \leq k_{X, \text{opt}}, k_T \leq 6, \rho = 0.005, 0.01, \ldots, 0.5\}$. We choose basis numbers for our proposed R-learner under two scenarios:

(A) The dimensions of $\psi(t)$ and $\psi(x^{(2)})$ are $k_{T, \text{opt}}$ and $k_{X, \text{opt}}$.

(B) The dimensions of $\psi(t)$ and $\psi(x^{(2)})$ are $k_{T, \text{opt}} + 1$ and $k_{X, \text{opt}} + 1$.

The nuisance functions are estimated via one of the following two strategies.

(i). Estimate $\tilde{m}^{(j)}(x^{(2)})$ via SUPERLEARNER, combining adaptive polynomial splines, adaptive regression splines, single-layer neural networks, linear regression, and recursive partitioning-based regression trees. Estimate $\hat{\Gamma}^{(j)}(x^{(2)})$ through method (i) in Remark 4. When $T$ is generated from the complete randomized experiment, $\pi(t \mid x^{(2)})$ is assumed to be known as 1 over $[0, 1]^2$. When $T$ is generated from the Beta distribution, we estimate $\hat{\pi}^{(j)}(t \mid x^{(2)})$ by estimating the parameters $\eta$ of mean function $\lambda_X$ through logistic regression following Kennedy et al. (2017).

(ii). Estimate $\tilde{m}^{(j)}(x^{(2)})$ in the same way as strategy (i). Estimate $\hat{\Gamma}^{(j)}(x^{(2)})$ through method (ii) in Remark 4, where the coordinate-wise regressions are conducted by the same SUPERLEARNER algorithm as for $\hat{m}^{(j)}(x^{(2)})$.

We test the performance of our proposed R-learners at six different points of $(x^{(1)}, x^{(2)}, t)$, namely, $(0, 0.25, 0.25), (0, 0.5, 0.5), (0, 0.75, 0.75), (1, 0.25, 0.25), (1, 0.25, 0.75), (1, 0.5, 0.25)$; we term these points pt1–pt6 for brevity. In each round of the simulation, we report the point-wise difference between the estimated $\tau(x, t)$ and the true $\tau(x, t)$ as the estimation error. We further construct 90% confidence interval (3.13) for each tested point, and check if it covers the truth; here $\hat{\sigma}$ is estimated following Algorithm 2 and $\hat{\mu}^{(j)}(x^{(2)}, t)$ is trained by same SUPERLEARNER algorithm as for $\hat{m}^{(j)}(x^{(2)})$. For comparison, we additionally report estimation errors of generalized S-learner and X-learners (Künzel et al., 2019), which are introduced in details in \S S.2. In our simulations, all regressions in S- and X-learners are performed by SUPERLEARNER similar to $\hat{m}^{(j)}(x^{(2)})$, yet additionally combining with random forest, XGboost, and Bayesian Additive Regression Trees.

We run 500 Monte Carlo simulations under each setting. Simulation results when $n = 2000$ and $T$ is generated under the complete randomized trial, are presented in Fig. 2. The top panel of Fig. 2 shows the superior performances of our proposed method in terms of small estimation errors over all simulation settings and tested points. Both Strategies (i) and (ii) for nuisance function training produce valid results. The bottom panel of Fig. 2 shows that when conducting proposed methods under Scenario (B), the empirical coverage rates are close to 90% for all points, meanwhile the estimation variance is slightly larger. Such observations verify the theoretical claims in Remark 5, and show the effectiveness of our proposed confidence interval after undersmoothing. Additional results with $T$ generated under the Beta distribution and/or $n = 4000$, are contained in \S S.4 with similar conclusions.

5 Real data application

We assess the heterogeneous causal effect of Oxygen saturation, a.k.a., SpO2 on a patient’s survival rate by analyzing the MIMIC-III clinical database (Johnson et al., 2016). The dataset contains 11698 female individuals and 9256 male individuals. In MIMIC-III, medical information of patients in intensive care units of the Beth Israel Deaconess Medical Center between 2001 and 2012, is recorded and followed up for the
Figure 2: Simulation results under the setting when \( n = 2000 \) and \( T \) is generated from the uniform distribution based on 500 Monte Carlo simulated datasets. Different colors represent simulation results of different methods. The top penal shows the box-plots of pointwise errors for all comparative estimators, and the bottom panel shows the empirical coverage rates for the proposed estimators excluding S- and X-learners for which confidence intervals are not available. Different methods are labeled in different colors and/or shapes: S-learner (Green), X-learner (purple), proposed R-learner with the nuisance function estimated by Strategy (i) (light blue/triangle) or (ii) (light red/triangle) under Scenario (A) and with the nuisance function estimated by Strategy (i) (dark blue/star) or (ii) (dark red/star) under Scenario (B).

Figure 3: Left penal represents the estimation of \( \tau(x, t) \) as a function of \( t \), where \( t \) is the SpO2 level, for male patients, where red line represents age = 65 and blue line represents age = 80; all other covariates are set on the median levels. Red and blue bands are the corresponding 90% confidence intervals. Similarly, right penal represents the estimation of \( \tau(x, t) \) for female patients.
mortality. Recent retrospective study reveals that the patients with SpO2s maintained at [94%, 98%], are associated with decreased hospital mortality (van den Boom et al., 2020). Tan et al. (2021) provide causal evidence of this clinical discovery by estimating the heterogeneous effects of a binary treatment defined as the indicator of whether or not a patient’s SpO2 is within [94%, 98%]. We take SpO2 as the continuous treatment variable \( T \), and estimate its heterogeneous effect on the mortality outcome by our proposed sieve-type R-learner; the outcome \( Y \) is 0 if a patient died due to sepsis and 1 otherwise. We thereby provide a more nuanced causal analysis than the previous works. The individual-level covariates \( X \) include gender, age, weight, and Sequential Organ Failure Assessment score. We take SpO2 = 94% as control-level treatment, which is around the 0.05 quantile among all samples.

We implement our proposed method similar to §4, where we choose the optimal basis number under Scenario (A) and train nuisance functions through Strategy (ii). All continuous variables are normalized by first standardization and then mapping them through the standard normal cumulative distribution function. The estimated \( \tau(x, t) \) along with the confidence bands are presented in Fig. 3, where we vary the treatment SpO2 from \( t = 94\% \) to \( t = 100\% \) and consider individual levels crossing different genders and ages, meanwhile setting other covariates at the median levels. We consider two age values: 65 and 90, which are roughly the 0.5- and 0.8-quantiles among all samples, respectively. The U-shapes of the treatment effect curves indicate that the causal effects of SpO2 are not necessarily “the higher, the better,” and the optimal SpO2 percentages of different curves lie in [94%, 98%]. These results comply with the previous findings (van den Boom et al., 2020; Tan et al., 2021). We further find that keeping other covariates unchanged, the optimal SpO2 becomes larger when age increases. In addition, the increase of SpO2 from 98% to 100% is more harmful to older individuals’ survival probability. These findings shed new insights into optimal treatment strategies for patients with sepsis.

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Supplementary material for “Towards R-learner of conditional average treatment effects with a continuous treatment: T-identification, estimation, and inference”

S.1 Generalized cross validation-based tuning parameter selection

Parameters $K$ and $\rho$ for our sieve-type $\ell_2$-penalized R-learner (Algorithm 1) control the bias-variance tradeoff. An essential problem in practice is how to select the optimal $K$ and $\rho$ based on samples and minimize the finite-sample error. For sieve-type estimators, many data-driven methods have been considered to select the optimal number of basis functions, including AIC, BIC, cross validation, Lepski’s method, Mallows criterion. We refer interested readers to Ichimura & Todd (2007); Hansen (2014) for reviews.

In this section, we adapt the generalized cross validation (Golub et al., 1979) as the parameter selection method for our sieve-type $\ell_2$-penalized R-learner. The generalized cross validation is known to be efficient and valid in many model selection problems. In comparison to ad-hoc cross validation methods that have been popularly studied for sieve-type estimators (Belloni et al., 2015, 2019), the generalized cross validation is preferable under our framework as it permits a closed-form solution and avoids introducing additional computational complexity.

For given samples $\{Z_i\}_{i=1}^n$, we first set the candidate pool for relative parameters $K$ and $\rho$

$$\mathcal{L} = \{(K, \rho) \mid K = K_1, \ldots, K_{n_1}, \rho = \rho_1, \ldots, \rho_{n_2}\}.$$  

Following the convention and without loss of generality, we assume that for each $K = K_a$ with $a \in [n_1]$, the corresponding basis function $\Psi(x, t)$ is determined. We then select the optimal $(K, \rho)$ from $\mathcal{L}$ by the generalized cross validation. Recalling that in Algorithm 1, we split the full data into $J$ folds $S_1, \ldots, S_J$ with sample sizes $n_1, \ldots, n_J$, respectively. Without loss of generality, we assume $S_j = \{Z_{1+\sum_{i=1}^{j-1} n_i}, \ldots, Z_{\sum_{i=1}^j n_i}\}$ for each $j = 1, \ldots, J$.

Given specific $(K, \rho) = (K_a, \rho_b) \in \mathcal{L}$, we define the following quantities:

$$Y = (Y_1, \ldots, Y_n)^T,$$

$$\hat{m} = \{\hat{m}^{(1)}(X_1), \ldots, \hat{m}^{(J)}(X_n)\}^T,$$

$$\Lambda = \{\Psi(X_1, T_1) - \hat{\Gamma}^{(1)}(X_1), \ldots, \Psi(X_n, T_n) - \hat{\Gamma}^{(J)}(X_n)\},$$

$$\hat{\tau} = \{\hat{\phi}^T\Psi(X_1, T_1) - \hat{\phi}^T\hat{\Gamma}^{(1)}(X_1), \ldots, \hat{\phi}^T\Psi(X_n, T_n) - \hat{\phi}^T\hat{\Gamma}^{(J)}(X_n)\}^T,$$

for all $j \in [J]$. Based on Algorithm 1, we then write

$$\hat{\tau} = n^{-1}\Lambda^T \hat{G}_n^{-1} \Lambda(Y - \hat{m}),$$

(S.1.1)

where $\hat{S}_{(K_a, \rho_b)}$ is the so-called smoothing matrix of the generalized cross-validation for a particular parameter group $(K_a, \rho_b)$; see, e.g., Wasserman (2006, Section 5.3). Following Wasserman (2006), the corresponding empirical error criterion for the generalized cross-validation is

$$\text{Error}(K_a, \rho_b) = \frac{1}{n} \sum_{i=1}^n \left[ \frac{Y_i - \hat{m}^{(1)}(X_i) - \{\hat{\phi}^T\Psi(X_i, T_i) - \hat{\phi}^T\hat{\Gamma}^{(1)}(X_i)\}}{1 - \text{tr}\{\hat{S}_{(K_a, \rho_b)}\}/n} \right]^2,$$

(S.1.2)
Algorithm S1: Generalized S-learner and X-learner for continuous treatments

**Step 1.** Obtain $\hat{\mu}(x, t) = \hat{E}(Y \mid X = x, T = t)$ over all $\{Z_i\}_{i=1}^n$ via a flexible machine learning algorithm;

**Step 2.** S- and X-learners proceed as follows.

- (S-learner). Obtain $\hat{\tau}_{SL}(x, t) = \hat{\mu}(Y \mid X = x, T = t) - \hat{\mu}(Y \mid X = x, T = 0)$;
- (X-learner). Construct pseudo-individual treatment effect $D_i = Y_i - \hat{\mu}(X_i, 0)$, based on which fit $\hat{\tau}_{XL}(x, t) = \hat{E}(D \mid X = x, T = t)$, via a flexible machine learning algorithm.

where $j_i$ is the splitting fold of $i$th sample. Finally, we choose the optimal $(K, \rho)$ among $\mathcal{L}$ that minimizes (S.1.2).

### S.2 Generalized S- and X-learners

Künzel et al. (2019) described two meta-learners for conditional average treatment effect estimation under the binary-treatment scenario; namely, the S- and X-learners. Algorithm S1 extends S- and X-learners to the continuous-treatment case.

### S.3 Simulation details for Fig. 1

We simulate two data examples with one binary-treatment setting and one continuous-treatment setting, respectively. In both examples, the sample size is $n = 1000$.

- (A binary-treatment setting) Generate a single covariate $X_i \sim \text{Uniform}(0, 1)$, a binary treatment $T_i \sim \text{Bernoulli}(0.5)$, and $Y_i = \sin(2X_i) + X_i^2 + \tau(X_i, T_i) + \varepsilon_i$ with $\tau(X_i, 0) = 0, \tau(X_i, 1) = \tau(X_i) = \sin(2\pi r_i + \pi/2) + 1, r_i = |X_i - 0.5|$, and $\varepsilon_i \mid X_i, T_i \sim \mathcal{N}(0, 0.3^2)$.

- (A continuous-treatment setting) Generate a single covariate $X_i \sim \text{Uniform}(0, 1)$, a continuous treatment $T_i \sim \text{Uniform}(0, 1)$, and $Y_i = \sin(2X_i) + X_i^2 + \tau(X_i, T_i) + \varepsilon_i$ with $\tau(X_i, T_i) = I(r'_{i} \leq 0.5)\{\sin(2\pi r'_{i} + \pi/2) + 1\}, r'_{i}$ the Euclidian distance between $(X_i, T_i)$ and $(0.5, 0.5)$, and $\varepsilon_i \mid X_i, T_i \sim \mathcal{N}(0, 0.3^2)$. Here $I(\cdot)$ is the indicator function.

Both settings can be seen as completely randomized experiments. For the binary-treatment setting, we approximate $\tau(x, t = 1) = \tau(x)$, with a 5-dimensional B-spline basis $\psi(x)$ such that $\tau(x) \approx \phi^T \psi(x)$. The $\psi(\cdot)$ has equally-spaced knots over $[0, 1]$; see §S.5.2 for more details of B-splines. We construct the empirical analogy of the binary-treatment R-loss $L_b(h)$ in (2.6), with $h(x) = \phi^T \psi(x)$ and the true nuisance functions. We then estimate $\hat{\tau}(x) = \hat{\phi}^T \hat{\psi}(x)$ as the minimum of this empirical R-loss.

For the continuous-treatment setting, we use a 25-dimensional tensor-productive B-spline function $\Psi(x, t)$ to approximate $\tau(x, t)$, where $\Psi(x, t) = \psi(t) \otimes \psi(x)$ and $\psi(\cdot)$ is defined in the same way as before. Specifically, the empirical analogy of our generalized R-loss $L_c(h)$ in (2.4) is constructed with $h(x, t) = \phi^T \Psi(x, t)$.
Figure S1: When the treatment is continuous, the generalized S-learner (Panel a) and the generalized X-learner (Panel b) roughly captures $\tau(x,t)$ (Fig. 1b). However, their performances are not as good as the proposed R-learner (Fig. 1d).

and the true nuisance functions. The simple generalized R-learner $\hat{\tau}_{\text{naive}}(x,t) = \hat{\phi}_c^T \Psi(x,t)$ is the minimum of this empirical generalized R-loss.

We also apply our proposed estimator in Algorithm 1 with sieve approximation on the data generated under the continuous-treatment setting. For simplicity, we do not impose sample splitting, i.e., set $J = 1$. We use the same B-spline basis functions $\Psi(x,t)$ as the simple generalized R-learner $\hat{\tau}_{\text{naive}}(x,t)$. Nuisance functions are trained via strategy (i) based on the SUPERLEARNER, which is considered in the simulation study in §4. The $\rho$ is set to be 0.05.

Finally, we assess the generalized S- and X-learners defined in Algorithm S1. All regression procedures in Algorithm S1 are carried out using SUPERLEARNER (Van der Laan et al., 2007), which combines random forest, XGboost, Bayesian Additive Regression Trees, adaptive polynomial splines, adaptive regression splines, single-layer neural networks, linear regression, and recursive partitioning-based regression trees. We show the results of $\hat{\tau}_SL(x,t)$ and $\hat{\tau}_XL(x,t)$ in Figure S1. Comparing Figure 1 and Figure S1, the proposed R-learner $\hat{\tau}(x,t)$ is the best among all comparative approaches.

S.4 Additional simulation results for §4

We include the additional simulation results in Figure S2. Across all different settings, our proposed estimators present superior performance with small estimation errors, and the empirical coverage rates are closed to the nominal level 90% after undersmoothing. With larger $n$, our proposed estimators have smaller estimation variances, which is consistent with our theoretical results for consistency.

S.5 Proofs of propositions and theorems

Before delving into the main proofs, we first simplify the setting for theoretical analysis, define some shorthand notation, and state some regularization conditions in §S.5.1. We briefly review some technical details of B-spline functions in §S.5.2. We list useful lemmas in §S.5.3 and give the proofs for our main propositions and theorems in the remaining of the section.
Figure S2: From top to bottom, different subfigures report simulation results under different settings. In each subfigure, different colors represent simulation results of different methods. The top penal shows the box-plots of pointwise errors for all comparative estimators, and the bottom panel shows the empirical coverage rates for the proposed estimators excluding S- and X-learners for which confidence intervals are not available. Different methods are labeled in different colors and/or shapes: S-learner (Green), X-learner (purple), proposed R-learner with the nuisance function estimated by Strategy (i) (light blue/triangle) or (ii) (light red/triangle) under Scenario (A) and with the nuisance function estimated by Strategy (i) (dark blue/star) or (ii) (dark red/star) under Scenario (B).
S.5.1 Preliminaries

Simplification of the sample-splitting procedure: Recall \( \hat{\phi} \) and \( \hat{\sigma} \) are constructed based on the double machine learning framework, with \( K \)-fold sample splitting. During the proof, we consider a simple 2-fold training scenario such that, \( \hat{\phi} \) and \( \hat{\sigma} \) are fit based on \( n \) i.i.d. samples, while the nuisance functions \( \hat{\Gamma} \), \( \hat{m} \) and \( \hat{\mu} \) are all trained via another independent \( n \) i.i.d. samples. In the sense of the asymptotic theoretical analysis considered in this paper, such simplification does not lose generality, and it has been popularly employed by the splitting-based estimators (Nie & Wager, 2021; Kennedy, 2020; Kennedy et al., 2020).

Notation: For simplicity, we occasionally omit some function arguments during the proof. For any function of random variable \( h(W) \), we may use \( h \) to represent it. Similarly, we denote \( h(W_i) \) by \( h_i \). For random variable \( W \), we denote \( P\{f(W)\} = \int_{w \in \mathcal{W}} f(w)d\mathcal{P}(w) \) as the expectation for \( W \) treating \( f \) as a fixed function or matrix. Thus if \( f \) is sample-based, \( P\{f(W)\} \) is a random variable or random matrix. The constants in the form of \( C, C_1, C_2, \ldots \) can change the meanings in different proofs. We also write “wpa1” as a short notation of “with probability approaching 1”. For two matrices \( A \) and \( B \), we write \( A \succeq B \), if \( A - B \) is positive definite. We use \( \|A\|_2 \) to represent the spectral norm of \( A \).

We now introduce some basic matrix notation involved in our main proof,

\[
Q_n = E\{\Psi(X, T)\Psi^T(X, T)\},
\]
\[
R_n = E[\{\Psi(X, T) - \Gamma(X)\}\{\Psi(X, T) - \Gamma(X)\}^T],
\]
\[
G_n = R_n + \rho Q_n.
\]

It is easy to see both \( R_n \) and \( G_n \) are positive semi-definite matrices. Let the singular value decompositions of \( R_n \) and \( G_n \) be

\[
R_n = (U \quad U_\perp) \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} \begin{pmatrix} U^T \\ U_\perp^T \end{pmatrix},
\]
\[
G_n = (\hat{U} \quad \hat{U}_\perp) \begin{pmatrix} \hat{\Sigma} \\ \hat{\Sigma}_\perp \end{pmatrix} \begin{pmatrix} \hat{U}^T \\ \hat{U}_\perp^T \end{pmatrix},
\]

where \( \Sigma = \text{diag}(\sigma_1, \ldots, \sigma_\zeta) \) such that \( \zeta = \text{rank}(R_n) \) and \( \sigma_1 \geq \cdots \geq \sigma_\zeta \); \( \hat{\Sigma} = \text{diag}(\hat{\sigma}_1, \ldots, \hat{\sigma}_\zeta) \), \( \hat{\Sigma}_\perp = \text{diag}(\hat{\sigma}_{\zeta+1}, \ldots, \hat{\sigma}_K) \) and \( \hat{\sigma}_1 \geq \cdots \geq \hat{\sigma}_K \). Similarly, we write the empirical versions of \( Q_n \) and \( R_n \) as,

\[
\hat{Q}_n = P_n\{\Psi(X, T)\Psi^T(X, T)\},
\]
\[
\hat{R}_n = P_n[\{\Psi(X, T) - \hat{\Gamma}(X)\}\{\Psi(X, T) - \hat{\Gamma}(X)\}^T]
\]

Recalling the definition of \( \hat{G}_n \), we then have \( \hat{G}_n = \hat{R}_n + \rho \hat{Q}_n \). We also define,

\[
\tilde{G}_n = P[\{\Psi(X, T) - \hat{\Gamma}(X)\}\{\Psi(X, T) - \hat{\Gamma}(X)\}^T] + \rho Q_n
\]
\[
\tilde{R}_n = P[\{\Psi(X, T) - \hat{\Gamma}(X)\}\{\Psi(X, T) - \hat{\Gamma}(X)\}^T].
\]

Finally, we write the SVD form of \( \hat{G}_n \),

\[
\hat{G}_n = (\hat{U} \quad \hat{U}_\perp) \begin{pmatrix} \hat{\Sigma} \\ \hat{\Sigma}_\perp \end{pmatrix} \begin{pmatrix} \hat{U}^T \\ \hat{U}_\perp^T \end{pmatrix},
\]

where \( \hat{\Sigma} = \text{diag}(\hat{\sigma}_1, \ldots, \hat{\sigma}_\zeta) \), \( \hat{\Sigma}_\perp = \text{diag}(\hat{\sigma}_{\zeta+1}, \ldots, \hat{\sigma}_K) \), and \( \hat{\sigma}_1 \geq \cdots \geq \hat{\sigma}_K \).
**True coefficient vector** \( \phi^* \): For our theoretical analysis, we need \( \hat{\phi} \) converging to some target vector. We choose the least squares approximation coefficients of \( \tilde{\tau}(X,T) \) as this target vector. In particular, consider the population-level least squares approximation,

\[
\phi^* = \arg \min_{\phi \in \mathbb{R}^K} E \left[ \{ \tilde{\tau}(X,T) - \phi^T \Psi(X,T) \}^2 \right].
\]

With simple algebra, one has

\[
\phi^* = Q_n^{-1} E \left[ \tilde{\tau}(X,T) \Psi(X,T) \right]. \tag{S.5.2}
\]

For the tensor product of B-spline basis, Huang et al. (2003); Belloni et al. (2015) have shown the \( \mathcal{L}^\infty \) norm approximation power of least-square approximation \( (\phi^*)^T \Psi(X,T) \), when \( \tilde{\tau}(X,T) \) is in the \( p \)-smooth Hölder class. The following proposition is a direct application of Huang et al. (2003); Belloni et al. (2015)'s general results; see, e.g., the Appendix of Huang et al. (2003), and Belloni et al. (2015, Proposition 3.1 & Example 3.8).

**Proposition 3.** Suppose \( \tilde{\tau} \in \Lambda(p,c,\mathbb{X} \times \mathbb{T}) \) for some \( p, c > 0 \), and Assumptions 4, 7 hold. We have \( \| \tilde{\tau} - (\phi^*)^T \Psi \|_{\mathbb{X} \times \mathbb{T}} \lesssim K^{-p/(d+1)}. \)

**Regularization conditions:** We summarize the regularity conditions for our asymptotic results as follows.

**Assumption 4.** Assume the basis \( \Psi(x,t) \in \mathbb{R}^K \) takes the tensor-product form,

\[
\Psi(x,t) = \psi(t) \otimes \psi(x^{(1)}) \otimes \cdots \otimes \psi(x^{(d)}).
\]

Here \( \psi(\cdot) = [\psi^{(1)}(\cdot), \ldots, \psi^{(k)}(\cdot)]^T \in \mathbb{R}^k \) is a vector of the B-spline functions for a single variable over \([0,1]\); thus \( K = k^{d+1} \). The splines in \( \psi(\cdot) \) are of degree \( r \geq \lceil p \rceil \). The generation intervals (see §S.5.2) of \( \psi(\cdot) \) are \( I_1 = [0,s_1), I_2 = [s_1,s_2), \ldots, I_m = [s_m,1] \) with \( 0 \leq s_1 \leq \cdots \leq s_m \leq 1, m \geq 2 \) and \( k = r + m \). Finally, we assume there exists a \( \kappa > 0 \) not dependent on \( n \), such that for any \( n \in \mathbb{Z}^+ \),

\[
\frac{\max_{0 \leq m_0 \leq m}(s_{m_0+1} - s_{m_0})}{\min_{0 \leq m_0 \leq m}(s_{m_0+1} - s_{m_0})} \leq \kappa. \tag{S.5.3}
\]

**Assumption 5.** \( \mathbb{X} \times \mathbb{T} \subseteq \mathbb{R}^{d+1} \) is compact. Without loss of generality and for simplicity, we let \( \mathbb{X} = [0,1]^d \) and \( \mathbb{T} = [0,1] \).

**Assumption 6.** For some \( 0 < a_1 \leq a_2 < 1 \), one has \( n^{a_1} \lesssim K \lesssim n^{a_2} \).

**Assumption 7.** There exists some fixed constants \( 0 < c_f < C_f < +\infty \), such that \( c_f \leq \inf_{x \in \mathbb{X}} f(x) \leq \sup_{x \in \mathbb{X}} f(x) \leq C_f \).

**Assumption 8.** (i) \( 0 < \inf_{(x,t) \in \mathbb{X} \times \mathbb{T}} \text{Var}(Y \mid X = x, T = t) \leq \sup_{(x,t) \in \mathbb{X} \times \mathbb{T}} \text{Var}(Y \mid X = x, T = t) < +\infty \); (ii) \( \sup_{x \in \mathbb{X}} \text{Var}(Y \mid X = x) < +\infty \); (iii) \( \sup_{x \in \mathbb{X}} |E(Y \mid X = x)| < +\infty \).

**Assumption 9.** (i) \( \| \hat{\mu} - m \|_{\mathbb{X}} = o_P(1) \); (ii) \( \| \hat{\Gamma}^T \phi^* - \Gamma^T \phi^* \|_{\mathbb{X}} = o_P(1) \).
For the ease of exposition, we use the same univariate B-spline function $\psi(\cdot)$ for all variables $X^{(1)}, \ldots, X^{(d)}$ and $T$ in Assumption 4. We note the theoretical results remain the same when dimension $k$ and $I_1, \ldots, I_m$ vary for each variable, as long as the dimensions of all univariate B-splines are on the same asymptotic order and their mesh ratios given in (S.5.3) are bounded by an uniform constant $\kappa > 0$. Overall the Assumption 4 is mild; see, e.g., Douglas et al. (1975); Huang et al. (2003). Assumption 5 is a common assumption for the sieve-type estimator (Newey, 1997; Huang et al., 2003; Belloni et al., 2015; Shi et al., 2022+). Assumption 6 mildly controls the growing speed of the basis number, so that we can approximate $\tau(X, T)$ nonparametrically. Assumption 7 is a standard condition for sieve method (Huang et al., 2003; Chen & Christensen, 2015). Assumption 8 contains some weak moment conditions; Similar assumptions are often employed in sieve estimation and causal inference literature (Chen & Christensen, 2015; Cui et al., 2020). Assumption 9 states that the nuisance functions $\hat{\psi}(t \mid x)$ and $\hat{\tau}^T(x)\phi^*$ are both uniformly consistent estimators for their true counterparts. Assumption 9 (i) has previously been considered by Kennedy et al. (2017) for the doubly robust average treatment effect estimation with continuous treatments. Moreover, one sufficient condition that makes Assumption 9 (ii) hold is that $\hat{\Gamma}(\cdot)$ is estimated by the generalized propensity score $\hat{\psi}(t \mid x)$, and $\hat{\psi}(t \mid x)$ satisfies a similar uniform consistency as $\hat{m}(x)$,

$$\|\hat{\psi} - \psi\|_{\mathbb{X} \times \mathbb{T}} = o_P(1).$$  

(S.5.4)

Condition (S.5.4) has previously been considered by Kennedy et al. (2017) as a regularization condition. Proposition 4 formalizes the justification that Condition (S.5.4) is a sufficient condition for Assumption 9 (ii).

**Proposition 4.** Suppose $\hat{\tau} \in \Lambda(p, c, \mathbb{X} \times \mathbb{T})$ for some $p, c > 0$, and Assumptions 4, 5, 7 hold. When $\hat{\Gamma}(x) = E_{\hat{\phi}}\{\Psi(X, T) \mid X = x\}$, then we have Assumption 9 (ii) holds, whenever (S.5.4) holds.

**Proof of Proposition 4.** By Proposition 3, we have $\|\hat{\tau} - \{\phi^*\}^T\Psi\|_{\mathbb{X} \times \mathbb{T}} \lesssim 1$. Also, $\|\hat{\tau}\|_{\mathbb{X} \times \mathbb{T}} \leq C$ for some $C > 0$ due to $\hat{\tau} \in \Lambda(p, c, \mathbb{X} \times \mathbb{T})$. We thus have

$$\|\{\phi^*\}^T\Psi\|_{\mathbb{X} \times \mathbb{T}} \leq \|\hat{\tau} - \{\phi^*\}^T\Psi\|_{\mathbb{X} \times \mathbb{T}} + \|\hat{\tau}\|_{\mathbb{X} \times \mathbb{T}} \lesssim 1. \quad (S.5.5)$$

On the other hand, we note that

$$\hat{\Gamma}^T(x)\phi^* - \Gamma^T(x)\phi^* = E_{\hat{\phi}}\{\Psi^T(X, T)\phi^* \mid X = x\} - E_{\phi^*}\{\Psi^T(X, T)\phi^* \mid X = x\}$$

$$= \int_{\mathbb{T}} \Psi^T(x, t)\phi^*\left\{\hat{\psi}(t \mid x) - \psi(t \mid x)\right\} dt.$$  

Thus we have

$$\|\hat{\Gamma}^T\phi^* - \Gamma^T\phi^*\|_\mathbb{X} = \sup_{x \in \mathbb{X}} \int_{\mathbb{T}} \Psi^T(x, t)\phi^*\left\{\hat{\psi}(t \mid x) - \psi(t \mid x)\right\} dt$$

$$\leq \|\hat{\psi} - \psi\|_{\mathbb{X} \times \mathbb{T}} \cdot \sup_{x \in \mathbb{X}} \int_{\mathbb{T}} \Psi^T(x, t)\phi^* \cdot \Psi \mid_{\mathbb{X} \times \mathbb{T}} dt$$

$$\leq \|\hat{\psi} - \psi\|_{\mathbb{X} \times \mathbb{T}} \cdot \int_{\mathbb{T}} \{\phi^*\}^T\Psi \|_{\mathbb{X} \times \mathbb{T}} dt$$

$$\lesssim o_P(1),$$

by (S.5.5), whenever (S.5.4) holds and $\mathbb{T}$ is compact. This completes the proof. \qed
S.5.2 Brief review of the B-spline functions

We give some precise descriptions of how to construct $\psi(x,t)$ and the corresponding theoretical properties. We construct $\psi(w) = [\psi^{(1)}(w), \ldots, \psi^{(k)}(w)]^T$ for $w \in [0, 1]$. Define

$$N_j^{(1)}(w) = I(w \in I_j) \quad j = 1, \ldots, m.$$  

For $r \geq 2$ and $j = -(r-1), \ldots, m$, define

$$N_j^{(r)}(w) = \frac{w - s_j}{s_{j+r-1} - s_j} N_j^{(r-1)}(w) + \frac{s_{j+r} - w}{s_{j+r} - s_{j+1}} N_j^{(r-1)}(w), \quad (S.5.6)$$

where $s_{-(r-1)} = \cdots = s_{-1} = 0$, $s_{m+1} = \cdots = s_{m+r} = 1$, and take $1/0 = 0$ as the convention. We thus have the relationship $k = r + m$. We define $\psi(w)$ by normalizing $N_j^{(r)}(w)$ as,

$$\psi(w) = \left[\psi^{(1)}(w), \ldots, \psi^{(k)}(w)\right]^T = \sqrt{k} \cdot \left[ N_j^{(r)}(w), \ldots, N_j^{(r)}(w) \right]^T. \quad (S.5.7)$$

This constitutes the univariate B-spline function. Finally, we form the multivariate B-spline functions $\Psi(x,t)$ by the tensor product of $\psi(t), \psi(x^{(1)}), \ldots, \psi(x^{(d)})$ as

$$\Psi(x,t) = \psi(t) \otimes \psi(x^{(1)}) \otimes \cdots \otimes \psi(x^{(d)});$$

here $x^{(1)}, \ldots, x^{(d)}$ correspond to the coordinate-wise random variables $X^{(1)}, \ldots, X^{(d)}$ of $X$.

The following lemmas state some standard results for the B-spline functions, which will be useful in our theoretical analysis. In particular, letting $1_k = (1, \ldots, 1)^T \in \mathbb{R}^k$, Lemma 1 shows that $1_k^T \psi(w)$ will be a fixed constant for any $w \in [0, 1]$. Lemma 2 provides explicit properties of $N_j^{(r)}(w)$. Lemma 3 states asymptotic properties of $\Psi(x,t)$.

**Lemma 1.** Given any fixed $r \in \mathbb{Z}^+$, for the $\{N_j^{(r)}(w)\}^m_{j=1}$ defined in $(S.5.6)$, we have

$$\sum_{j=-(r-1)}^m N_j^{(r)}(w) \equiv 1$$

for any $w \in [0, 1]$. Furthermore, for any $w \in [0, 1]$, $1_k^T \psi(w) \equiv \sqrt{k}$.

**Proof of Lemma 1.** When $r = 1$, we have

$$\sum_{j=1}^m N_j^{(1)}(w) = \sum_{j=1}^m I(w \in I_j) = I(w \in [0, 1]) \equiv 1.$$
When \( r \geq 2 \), by (S.5.6), one has

\[
\sum_{j=-(r-1)}^{m} N_j^{(r)}(w) = \frac{w-s_{-(r-1)}}{s_0-s_{-(r-1)}} N_{-(r-1)}^{(r-1)}(w) + \left\{ \sum_{j=-(r-1)}^{m-1} \frac{s_{j+r}-w}{s_{j+r}-s_j} N_j^{(r-1)}(w) \right\} + \frac{w-s_{j+r}}{s_{j+r}-s_j} N_{j+1}^{(r-1)}(w) \]

\[
= \sum_{j=-(r-1)}^{m} \frac{s_{j+r}-w}{s_{j+r}-s_j} N_j^{(r-1)}(w) \]

where the first equality follows by \( s_0-s_{-(r-1)} = s_{m+1}-s_{m+1} = 0 \) and \( 1/0 = 0 \). Thus we have \( \sum_{j=-(r-1)}^{m} N_j^{(2)}(w) = \sum_{j=-(r-1)}^{m} N_j^{(1)}(w) = 1 \) for any \( w \in [0,1] \). Finally, by (S.5.8) and mathematical induction, one has \( \sum_{j=-(r-1)}^{m} N_j^{(r)}(w) \equiv 1 \) for all \( w \in [0,1] \) and \( r \geq 2 \). By (S.5.7), we conclude that for any \( w \in [0,1] \),

\[
(1,\ldots,1) \cdot \psi(w) = \sqrt{k} \sum_{j=-(r-1)}^{m} N_j^{(r)}(w) = \sqrt{k},
\]

which completes the proof.

**Lemma 2.** Given any fixed \( r \in \mathbb{Z}^+ \), for the \( \{N_j^{(r)}(w)\}_{j=1}^{m} \) defined in (S.5.6), we have

(i)* For any given \( j = -(r-1), \ldots, m \), we have \( N_j^{(r)}(w) = 0 \) for all \( w \not\in [s_j, s_{j+r}] \).

(ii)* For any given \( j = -(r-1), \ldots, m \), we have \( N_j^{(r)}(w) > 0 \) for all \( w \in (s_j, s_{j+r}) \).

(iii)* For any given \( \ell = 0, \ldots, m \), when \( w \in [s_{\ell}, s_{\ell+1}) \), we have

\[
\sum_{j=-(r-1)}^{m} \tilde{\beta}_j N_j^{(r)}(w) = \sum_{j=-(r-1)+\ell}^{\ell} \tilde{\beta}_j N_j^{(r)}(w),
\]

for any \( (\tilde{\beta}_{-(r-1)}, \ldots, \tilde{\beta}_m)^T \in \mathbb{R}^{m+r} \).

(iv)* Under Assumption 4, we have \( \sup_{j=-(r-1), \ldots, m \atop w \in [0,1]} |N_j^{(r)}(w)| = O(1) \) when \( m \to +\infty \).

By (S.5.7), we then have that \( \psi(w) \) satisfies the corresponding properties:

(i) For any given \( \tilde{k} = 1, \ldots, k \), we have \( \psi^{(\tilde{k})}(w) = 0 \) for all \( w \not\in [s_{\tilde{k}-r}, s_{\tilde{k}}] \).

(ii) For any given \( \tilde{k} = 1, \ldots, k \), we have \( \psi^{(\tilde{k})}(w) > 0 \) for all \( w \in (s_{\tilde{k}-r}, s_{\tilde{k}}) \).
(iii) For any given \( \ell = 0, \ldots, m \), when \( w \in [s_{\ell}, s_{\ell+1}) \), we have
\[
\sum_{k=1}^{k} \beta_k \psi_k (w) = \sum_{k=\ell+1}^{\ell+r} \beta_k \psi_k (w),
\]
for any \((\beta_1, \ldots, \beta_r)^T \in \mathbb{R}^k\).

(iv) Under Assumption 4, we have \( \sup_{k=1, \ldots, k} |\psi_k (w)| = O(\sqrt{k}) \) when \( m \to +\infty \).

Proof of Lemma 2. The results in (i)–(iv) follow from (i)–(iv) by recalling (S.5.7) and the relationship \( j = k - r \). So it suffices to show (i)–(iv)∗. The results in (i)∗, (ii)∗ and (iii)∗ are adapted from (1.6), (1.7) and (1.36) in Kunoth et al. (2018), respectively, with their \( B_{j+r, r-1, \xi} (w) \) being our notation \( N_j^{(r)} (w) \) and \( \xi = (s_{-(r-1)}, \ldots, s_{m+r}) \). For the B-spline functions with regularization conditions assumed in Assumption 4, the (iv) and (iv)∗ are standard results; see, e.g., Newey (1997); Belloni et al. (2015). □

Lemma 3. Suppose \( \Psi (x, t) \) satisfies Assumption 4. When \( n \to +\infty \), we have

(i) (Uniform boundedness): \( \|\Psi\|_{X \times T} \lesssim \sqrt{K} \).

(ii) (Bounded spectrums): Let \( J_{X,T} = \int_{X \times T} \Psi (x, t) \Psi^T (x, t) dx dt \). One has \( \lambda_{\min} (J_{X,T}) \) and \( \lambda_{\max} (J_{X,T}) \) are bounded away from both 0 and \( +\infty \). Similar upper and lower bounds also hold for \( J_T = \int_T \psi (t) \psi^T (t) dt \).

(iii) (Belonging to \( L^2_p (X, T) \) space): \( \phi^T \Psi \) is in \( L^2_p (X, T) \) for any given \( n \) and \( \phi \in \mathbb{R}^K \).

Proof of Lemma 3. These are standard results for B-splines under Assumption 4; see, e.g., Belloni et al. (2015); Chen & Christensen (2015). □

### S.5.3 Technical lemmas

In this section, we present all the technical lemmas for the proofs of our main propositions and theorems.

**Lemma 4.** Suppose Assumptions 3, 4, 5 and 7 hold. Let \( \text{span}(U_\perp) \) be the linear subspace in \( \mathbb{R}^K \) which is spanned by the column vectors in \( U_\perp \), and \( \text{span}(U) \) is defined correspondingly. We have the following spectral properties of \( R_n \).

(i) We have \( \text{span}(U_\perp) = \{u \mid u^T \Psi (x, t) \text{ is free of } t\} \). Specifically, if \( u \in \text{span}(U_\perp) \), we have \( u^T \Psi (x, t) = u^T \Gamma (x) \) for any \( (x, t) \in \mathbb{K} \times \mathbb{T} \).

(ii) Let \( f_j = (1, 0^T_{j-1}, -1, 0^T_{k-j-1})^T \in \mathbb{R}^k \) for \( j = 1, \ldots, k - 1, \) and \( F = [f_1, \ldots, f_{k-1}] \). The \( \text{span}(U) \) and \( \text{span}(U_\perp) \) can be represented as follows:

(a) \( \text{span}(U) = \text{span}\{v_T \otimes v\} \) where (i) \( v_T = \hat{\beta}^T F \); (ii) \( \hat{\beta} \) and \( v \) can be any vectors in \( \mathbb{R}^{k-1} \) and \( \mathbb{R}^{K/k} \), respectively. Here \( \text{span}\{v_T \otimes v\} \) represents the linear subspace spanned by all vectors taking the form of \( v_T \otimes v \).

(b) \( \text{span}(U_\perp) = \{1_k \otimes v \mid v \text{ can be any vector in } \mathbb{R}^{K/k}\} \).

With the dimensions of \( \text{span}(U) \) and \( \text{span}(U_\perp) \) being specified, we can further conclude that \( \zeta = K - K/k \).
(iii) When \(\varpi(t \mid x)\) is free of \(x\), i.e., \(T\) is completely random, one has

\[
\sigma_{\zeta} = \sigma_{K - K/k} \gtrsim 1.
\]

(iv) Suppose \(\hat{\Gamma}(x)\) is trained via the methods according to Remark 4. We have \(U_\perp \{\Gamma(x) - \hat{\Gamma}(x)\} = 0\) for any \(x \in \mathbb{X}\).

**Proof of Lemma 4.** We prove the four parts of Lemma 4 in order.

**Proof of Lemma 4 (i)** By the basic property of singular value decomposition, we have \(u \in \text{span}(U_\perp)\) if and only if \(u^T R_n u = 0\). Then, if \(u \in \text{span}(U_\perp)\), one has,

\[
E\left[\left\{ u^T \Psi(X, T) - E[u^T \Psi(X, T) \mid X]\right\}^2 \right] = u^T R_n u = 0,
\]

which is equivalent to that

\[
u^T \Psi(X, T) = E\{u^T \Psi(X, T) \mid X\}\]

a.s.. This implies that,

\[
u^T \Psi(x, t) = E\{u^T \Psi(X, T) \mid X = x\}
\]

holds almost everywhere on the Lebesgue measure over \([0, 1]^{d+1}\), since \(f(x, t) = f(x)f(x \mid t)\) is an upper and lower bounded density function over \(\mathbb{X} \times \mathbb{T} = [0, 1]^{d+1}\), under Assumptions 3, 5 and 7. By the continuity of the B-spline function (§S.5.2), we further have that

\[
u^T \Psi(x, t) = E\{u^T \Psi(X, T) \mid X = x\}
\]

holds for any \((x, t) \in [0, 1]^{d+1}\). In addition, since \(E\{u^T \Psi(X, T) \mid X = x\}\) does not contain \(t\), we conclude from (S.5.10) that \(u^T \Psi(x, t)\) now is a function dependent only on \(x\), over \((x, t) \in [0, 1]^{d+1}\).

On the other hand, suppose \(u\) satisfies that \(u^T \Psi(x, t)\) is a function only of \(x\) over \([0, 1]^{d+1}\). We then have, \(E\{u^T \Psi(X, T) \mid X = x\} = u^T \Psi(x, t)\) and thus

\[
E\left[\left\{ u^T \Psi(X, T) - E[u^T \Psi(X, T) \mid X]\right\}^2 \right] = 0,
\]

which implies \(u^T R_n u = 0\) and thus \(u \in \text{span}(U_\perp)\). Summarizing the two sides of the equivalence shown above, the result (i) is hence proved.

**Proof of Lemma 4 (ii)** Let \(S_{U_\perp} = \{1_k \otimes v \mid v\) can be any vector in \(\mathbb{R}^{K/k}\}\} and \(S_U = \text{span}\{v_T \otimes v\}\) where (i) \(v_T = \beta^T F\); (ii) \(\beta\) and \(v\) can be any vectors in \(\mathbb{R}^{K-1}\) and \(\mathbb{R}^{K/k}\), respectively. It is easy to verify \(S_{U_\perp}\) and \(S_U\) are both linear subspaces in \(\mathbb{R}^K\). Specifically, let \(1_k \otimes v_1\) and \(1_k \otimes v_2\) be two arbitrary vectors in \(S_{U_\perp}\). We note their linear combination takes the form of

\[
c_1(1_k \otimes v_1) + c_2(1_k \otimes v_2) = 1_k \otimes (c_1v_1 + c_2v_2),
\]

which is also in \(S_{U_\perp}\). Similar arguments hold for \(S_U\) as well. In addition, by checking the definition, one can also see that \(\{f_{j_1} \otimes e_{j_2}, j_1 = 1, \ldots, K - 1, j_2 = 1, \ldots, K/k\}\) and \(\{1_k \otimes e_{j_2}, j_2 = 1, \ldots, K/k\}\) form basis of \(S_U\) and \(S_{U_\perp}\), respectively. Here \(\{e_{j_2}\}_{j_2=1}^{K/k}\) are the standard basis of \(\mathbb{R}^{K/k}\). Therefore, \(\dim(S_U) = K - K/k\), \(\dim(S_{U_\perp}) = K/k\), and \(\dim(S_U) + \dim(S_{U_\perp}) = K\); here \(\dim(\cdot)\) is the dimension of the corresponding linear subspace.
We first show $S_{U_\perp} = \text{span}(U_\perp)$. Denote $\Psi(x) = \psi(x^{(1)}) \otimes \cdots \otimes \psi(x^{(d)})$. By Lemma 1 and the basic property of Kronecker product multiplication (e.g., Horn & Johnson, 1991), we observe for any $v \in \mathbb{R}^{K/k}$,

$$
\{1_k \otimes v\}^T \Psi(x, t) = \{1_k \otimes v\}^T \{\psi(t) \otimes \Psi(x)\} = 1_k^T \psi(t) \cdot v^T \Psi(x) = \sqrt{K} v^T \Psi(x),
$$

which is free of $t$, thus $1_k \otimes v \in \text{span}(U_\perp)$ and

$$
S_{U_\perp} \subseteq \text{span}(U_\perp).
$$

Since both $S_{U_\perp}$ and $\text{span}(U_\perp)$ are linear subspaces, to show $S_{U_\perp} = \text{span}(U_\perp)$, it is left to show

$$
\text{dim}(S_{U_\perp}) = K/k \geq \text{dim}\{\text{span}(U_\perp)\}. \quad (S.5.11)
$$

Now for any $f_{j_1} \otimes e_{j_2}$ as one basis function of $S_U$, we have for $j_1 = 1, \ldots, k - 1$,

$$
\{f_{j_1} \otimes e_{j_2}\}^T \Psi(x, t) = \{\psi^{(1)}(t) - \psi^{(j_1 + 1)}(t)\} \cdot e_{j_2}^T \Psi(x). \quad (S.5.12)
$$

The above function depends on $t$ and thus is not in $\text{span}(U_\perp)$ by the result in (i). This is because by Lemma 2, $\psi^{(1)}(t) = 0$ when $t \in (s_{j_1}, s_{j_1 + 1})$, while $\psi^{(1)}(t) > 0$ when $t \in (s_{j_1}, s_{j_1 + 1})$, and thus

$$
\psi^{(1)}(t) - \psi^{(j_1 + 1)}(t) < 0
$$

when $t \in (s_{j_1}, s_{j_1 + 1})$. On the other hand, if $j_1 < k - 1$, we have

$$
\psi^{(1)}(t) = \psi^{(j_1 + 1)}(t) = 0
$$

when $t \in (s_{j_1 + 1}, 1)$. If $j_1 = k - 1$, we have $\psi^{(1)}(t) = \psi^{(j_1 + 1)}(t) = 0$ when $t \in (s_1, s_m)$; note here $m \geq 2$ and $s_m \geq s_1$ under Assumption 4. Therefore for any $j_1 = 1, \ldots, k - 1$, there exists some $a, b \in [0, 1]$ such that $\psi^{(1)}(t = a) - \psi^{(j_1 + 1)}(t = a) < 0$ while $\psi^{(1)}(t = b) - \psi^{(j_1 + 1)}(t = b) = 0$, which directly implies from (S.5.12) that $\{f_{j_1} \otimes e_{j_2}\}^T \Psi(x, t)$ is a function that can change with $T$, for any given basis function $f_{j_1} \otimes e_{j_2}$ of $S_U$. By results in (i), we know all $K - K/k$ linearly independent vectors in $\{f_{j_1} \otimes e_{j_2} \mid j_1 = 1, \ldots, k - 1, j_2 = 1, \ldots, K/k\}$ are not in $\text{span}(U_\perp)$. By the basic property of the linear space, we conclude $\text{dim}\{\text{span}(U_\perp)\} \leq K - (K - K/k) = \text{dim}(S_{U_\perp})$, which verifies (S.5.11) and thus shows

$$
S_{U_\perp} = \text{span}(U_\perp)
$$

Finally, observing that for any basis function $f_{j_1} \otimes e_{j_2}$ of $S_U$ and any vector $1_k \otimes v \in S_{U_\perp} = \text{span}(U_\perp)$, we have

$$
(f_{j_1} \otimes e_{j_2})^T \cdot 1_k \otimes v = (f_{j_1}^T \cdot 1_k) \cdot (e_{j_2}^T \cdot v) = 0,
$$

as $f_{j_1} \cdot 1_k = 1 - 1 = 0$ by definition. We thus have

$$
S_U \perp \text{span}(U_\perp) \quad (S.5.13)
$$

and $S_U \oplus \text{span}(U_\perp) = \mathbb{R}^K$, since $\text{dim}(S_U) + \text{dim}\{\text{span}(U_\perp)\} = K - K/k + K/k = K$; here $\oplus$ denotes the direct sum of two linear spaces. With same argument, we can also show that

$$
\text{span}(U) \perp \text{span}(U_\perp) \quad (S.5.14)
$$
We first present the general Weyl’s inequality of matrix eigenvalue perturbation. By the result in (i), we have (S.5.19) in what follows. For simplicity, we denote such that (S.5.14), we conclude that, Proposition 5 (General Weyl’s inequality) which will be frequently used in the paper. The proof can be found in (Horn & Johnson, 1991, Theorem 3.3.16)

\[ \sigma_{i+j-1}(\hat{R}) - \sigma_i(\mathcal{R}) \leq \sigma_j(\mathcal{E}). \]  

(S.5.15) Specifically, for any \( i \leq \min\{d_1, d_2\} \),

\[ |\sigma_i(\hat{R}) - \sigma_i(\mathcal{R})| \leq \|\mathcal{E}\|_2. \]  

(S.5.16)

We now get into our main proof. Note by the law of total expectation, we have

\[ \Gamma \Gamma^T = \mathcal{E} \]

\[ Q_n = R_n + E(\Gamma^T); \]

see (S.5.19) in what follows. For simplicity, we denote \( \gamma = E\{\psi(T) \mid X = x\} \). Note \( \gamma \) is free of \( x \) as \( \varpi(t \mid x) \) is free of \( x \). We thus also write \( \varpi(t \mid x) = \varpi(t) \) for abbreviation. By the basic property of Kronecker product (Schacke, 2004), we then have

\[ E(\Gamma^T) = E\left[ E\{\psi(T) \mid X\} \otimes \Psi(X) \right]\left[ E\{\psi(T) \mid X\} \otimes \Psi(X) \right]^T \]

\[ = E\left\{ \gamma\gamma^T \otimes \Psi(X)\Psi^T(X) \right\} \]

\[ = \gamma\gamma^T \otimes E\{\Psi(X)\Psi^T(X)\}. \]  

(S.5.17)

Since \( \gamma\gamma^T \) is a rank-one matrix, by e.g. Horn & Johnson (1991, Theorem 4.2.12) and (S.5.17), we have

\[ \operatorname{rank}\{E(\Gamma^T)\} \leq 1 \cdot \operatorname{rank}\left\{ E\{\Psi(X)\Psi^T(X)\} \right\} \]

\[ \leq K/k, \]

which implies \( \sigma_{K/k+1}\{E(\Gamma^T)\} = 0 \). Taking \( \hat{\mathcal{R}} = Q_n, \mathcal{R} = R_n, \mathcal{E} = E(\Gamma^T), j = K/k + 1, \) and \( i = K - K/k \) in Proposition 5, we have that,

\[ \sigma_{K-K/k}(R_n) \geq \sigma_K(Q_n) - \sigma_{K/k+1}\{E(\Gamma^T)\} \]

\[ = \sigma_K(Q_n) \]

\[ \gtrsim 1, \]

where the last inequality is because the smallest singular value of \( Q_n \) is bounded away from 0; see Lemma 5.

Proof of Lemma 4 (iv) By the result in (i), we have \( U_\perp \Psi(x, t) \) is free of \( t \). We then have

\[ U_\perp \left\{ \Gamma(x) - \hat{\Gamma}(x) \right\} = E\{U_\perp \Psi(X, T) \mid X = x\} - E_{\mathcal{E}}\{U_\perp \Psi(X, T) \mid X = x\} \]

\[ = U_\perp \Psi(x, t) - U_\perp \Psi(x, t) \]

\[ = 0. \]

\[ \square \]
Lemma 5. Assumptions 3, 4, 7 hold. When \( n \to +\infty \), we have following bounds.

(i) The eigenvalues of \( Q_n \) are bounded away from 0 and \( +\infty \), and \( \|R_n\|_2, \|E(\Gamma^{T})\|_2, \|E\{\psi(T) \mid X\} E\{\psi^{T}(T) \mid X\}\|_2 \lesssim 1 \).

(ii) If \( \tau \in \Lambda(p, c, X \times T) \) for some \( p, c > 0 \), we have \( \|\phi^{*}\| \lesssim 1 \).

Proof of Lemma 5. We prove the two parts of Lemma 5 in order.

Proof of Lemma 5 (i) First we note that by the forms of \( Q_n, R_n, E(\Gamma^{T}) \), and \( E\{\psi(T) \mid X\} E\{\psi^{T}(T) \mid X\} \), it is clear to see they are all symmetric and positive semi-definitive.

Let \( v \in \mathbb{R}^{K} \) be any vector with \( \|v\| = 1 \). One has

\[
\lambda_{\max}(Q_n) = \sup_{\|v\| = 1} |v^{T}E[\Psi(T, X)\Psi(T, X)^{T}]v|
\]

\[
= \sup_{\|v\| = 1} \int_{X \times T} \{v^{T}\Psi(x, t)\}^{2}f(t \mid x)f(x)dxdt
\]

\[
\leq C_{f}/\epsilon \cdot \sup_{\|v\| = 1} \int_{X \times T} \{v^{T}\Psi(x, t)\}^{2}dxdt \quad \text{(Assumptions 4 and 7)}
\]

\[
\lesssim 1,
\]

where the last inequality follows by Lemma 3. Similarly, we have \( \lambda_{\min}(Q_n) \geq c_{f}/\epsilon \cdot \inf_{\|v\| = 1} \int_{X \times T} \{v^{T}\Psi(x, t)\}^{2}dxdt \gtrsim 1 \) also by Lemma 3 and the corresponding assumptions.

By the property of spectral norm (e.g., Golub & Van Loan, 2013), one has

\[
\|E(\Gamma^{T})\|_2 = \sup_{\|u\| = 1} |u^{T}E(\Gamma^{T})u|
\]

\[
= \sup_{\|u\| = 1} \left|E\left[E\{u^{T}\Psi(X, T) \mid X\}^{2}\right]\right|
\]

\[
\leq \sup_{\|u\| = 1} \left|E\left[E\{u^{T}\Psi(X, T)^2 \mid X\}\right]\right|
\]

\[
= \sup_{\|u\| = 1} \left|E\{\{u^{T}\Psi(X, T)\}^{2}\}\right|
\]

\[
= \|Q_n\|_2 \lesssim 1,
\]

where the first inequality follows by Cauchy-Schwarz inequality and the last inequality follows by (S.5.18). The \( \|E\{\psi(T) \mid X\} E\{\psi^{T}(T) \mid X\}\|_2 \) can be bounded by similar arguments. This is because \( \|E(\Gamma^{T})\|_2 \) is actually the same type of matrix as \( E(\Gamma^{T}) \), which only replaces the \( \Gamma(x) = E\{\Psi(X, T) \mid X = x\} \) with \( E\{\psi(T) \mid X = x\} \). Finally, rewrite \( R_n \) as

\[
R_n = E\{(\Psi - \Gamma)(\Psi - \Gamma)^{T}\}
\]

\[
= Q_n - E\{\Psi(X, T)\Gamma^{T}(X)\} - E\{\Gamma(X)\Psi^{T}(X, T)\} + E[\Gamma^{T}]
\]

\[
= Q_n - E[\Gamma^{T}],
\]

where the last equality follows by \( E\{\Psi(X, T)\Gamma^{T}(X)\} = E\{E\{\Psi(X, T) \mid X\}\Gamma^{T}(X)\} = E(\Gamma^{T}) \). due to the law of total expectation, and similarly \( E\{\Gamma(X)\Psi^{T}(X, T)\} = E(\Gamma^{T}) \). Summarizing the above upper bounds, one has \( \|R_n\|_2 \leq \|Q_n\|_2 + \|E(\Gamma^{T})\|_2 \lesssim 1 \).
Proof of Lemma 5 (ii) Recalling (S.5.2), if $\tilde{\tau} \in \Lambda(p, c, X \times T)$ for some $p, c > 0$, we have $\|\tilde{\tau}\|_{X \times T} \preceq 1$ and thus

$$\|\phi^*\| \leq \left\| Q_n^{-1} \right\|_2 E[\tilde{\tau}(X, T) \Psi(X, T)]$$

$$= \left\| Q_n^{-1} \right\|_2 \sup_{\|u\|=1} E[\tilde{\tau}(X, T)u^T \Psi(X, T)]$$

$$\leq \|\tilde{\tau}\|_{X \times T} \left\| Q_n^{-1} \right\|_2 \sup_{\|u\|=1} \sqrt{E[u^T \Psi(X, T)]^2}$$

$$\preceq 1,$$

where the second inequality follows by Cauchy-Schwarz inequality, and the last inequality follows from the lower and upper bound of $Q_n$’s eigenvalues. 

Lemma 6. Suppose Assumptions 4 and 8 hold. We have $\|m(x)\|_X, \|\hat{m}(x)\|_X, \|\hat{\Gamma}(x)\|_X/\sqrt{K}, \|\Gamma(x)\|_X/\sqrt{K}$ are all bounded away from $+\infty$ when $n$ grows, wpa1.

Proof of Lemma 6. By Assumption 8, we have $\|m\|_X = \sup_{x \in X} |E(Y \mid X = x)| \preceq 1$ as $n \to +\infty$. By Lemma 3 and the fact $\|\cdot\|$ in convex,

$$\|\Gamma\|_X = \sup_{x \in X} \left\| E\{\Psi(X, T) \mid X = x\} \right\|$$

$$\leq \sup_{x \in X} E\left\{ \left\| \Psi(X, T) \right\| \mid X = x \right\}$$

$$\leq \sup_{(x, t) \in X \times T} \left\| \Psi(x, t) \right\|$$

$$\preceq \sqrt{K}.$$

Finally, recalling (3.5) and (3.6), by the triangle inequality we have

$$\|\hat{m}\|_X \leq \|m\|_X + \|\hat{m} - m\|_X \preceq 1 + o_P(1),$$

which implies $\|\hat{m}\|_X \preceq 1$, wpa1. Similar argument also yields $\|\hat{\Gamma}\|_X/\sqrt{K} \preceq 1$ wpa1.

Lemma 7. Suppose Assumptions 3, 4, 7 hold, and also (3.6) holds. When $n \to +\infty$, we have $\|\bar{G}_n - G_n\|_2 = o_P(r_n^2)$, and $\|R_n\|_2 \preceq 1$ wpa1.

Proof of Lemma 7. First we decompose,

$$\bar{G}_n - G_n = P\{(\hat{\Gamma} - \Psi)(\hat{\Gamma} - \Psi)^T\} + \rho Q_n - E\{(\Gamma - \Psi)(\Gamma - \Psi)^T\} - \rho Q_n$$

$$= \bar{R}_n - R_n$$

$$= P\{(\hat{\Gamma} - \Psi)(\hat{\Gamma} - \Psi)^T\} - P\{(\Gamma - \Psi)(\Gamma - \Psi)^T\}$$

$$= P\{(\hat{\Gamma} - \Gamma)(\hat{\Gamma} - \Gamma)^T\} + P\{(\hat{\Gamma} - \Gamma)(\Gamma - \Psi)^T\} + P\{(\Gamma - \Psi)(\hat{\Gamma} - \Gamma)^T\}$$

$$+ E\{(\Gamma - \Psi)(\Gamma - \Psi)^T\} - E\{(\Gamma - \Psi)(\Gamma - \Psi)^T\}$$

$$= P\{(\hat{\Gamma} - \Gamma)(\hat{\Gamma} - \Gamma)^T\}. (S.5.20)$$
Note here $P\{ (\hat{\Gamma} - \Gamma)(\Gamma - \Psi)^T \} = P\{ (\Gamma - \Psi)(\hat{\Gamma} - \Gamma)^T \} = 0$ as

$$
P[\{\hat{\Gamma}(X) - \Gamma(X)\} (\Gamma(X) - \Psi(X,T))^T]
= P[\{\hat{\Gamma}(X) - \Gamma(X)\} \cdot E[\{\Gamma(X) - \Psi(X,T)\}^T | X]]
= P[\{\hat{\Gamma}(X) - \Gamma(X)\} (\Gamma(X) - \Gamma(X))^T]
= 0,
$$

where the first equality follows by the law of total expectation. Thus $\|\hat{G}_n - G_n\|^2 = \|P\{ (\hat{\Gamma} - \Gamma)(\hat{\Gamma} - \Gamma)^T \}\|^2 = o_P(r_n^2)$ follows from (3.6). In addition, by Lemma 5 and (S.5.20), one has $\|\hat{R}_n\|_2 \leq \|R_n\|_2 + \|\hat{G}_n - G_n\|^2 \leq 1 + o_P(1) \leq 1$ wpa1 since $r_n \leq 0$.

**Lemma 8.** Suppose the general settings of Theorem 2 hold. We have

(i) $\|\hat{Q}_n - Q_n\|_2 = O_P(\sqrt{n \log n / n})$, $\|\hat{G}_n - G_n\|_2 = O_P(\sqrt{n \log n / n})$, and we also have $\|\hat{Q}_n\|_2 \leq 1$ and $\|P_n(\Gamma^T)\|_2 \leq 1$ wpa1;

(ii) $\|\hat{G}_n - G_n\|_2 = O_P(\rho^{-2} \sqrt{n \log n / n})$;

(iii) $\|\Sigma^{-1}\|_2 \geq \beta_n^{-1}$, $\|\Sigma_{-1/2}^{-1}\|_2 \geq \rho^{-1}$, $\|\hat{U}_{1/2}^{{1/T}}\|_2 \geq \rho \beta_n^{-1}$, $\sigma_{\text{min}}(U^T U) \to 1$;

(iv) $\|\Sigma_{-1/2}^{-1}\|_2 \geq \beta_n^{-1}$, $\|\Sigma_{-1/2}^{-1}\|_2 \geq \beta_n^{-1}$, $\|\Sigma_{-1/2}^{-1}\|_2 \geq \rho^{-1}$, wpa1, and $\|\hat{U}_{1/2}^{{1/T}}\|_2 = O_P(\beta_n^{-1} \sqrt{n \log n / n})$.

(v) Recall $\hat{A}_n, \hat{B}_n$ in Algorithm 2, and let $A_n = \hat{U}\Sigma^{-1/2}U^T$, $B_n = E[\{\Psi(X,T) - \Gamma(X)\} \{\Psi(X,T) - \Gamma(X)\}^T \{Y - \mu(X,T)\}]$ be their population counterparts. Further assuming the conditions in the confidence interval part of Theorem 2 hold, we have $\|\hat{A}_n\|_2, \|\hat{B}_n\|_2, \|A_n\|_2, \|B_n\|_2$ are all constantlybounded wpa1. In addition, we have,

$$
\|\hat{A}_n - A_n\|_2 = o_P(1), \quad \|\hat{B}_n - B_n\|_2 = o_P(1).
$$

**Proof of Lemma 8.** During the proofs, we will frequently use several classic matrix concentration and perturbation results. For the completeness, we first present these results and then get into the main proof.

**Proposition 6** (Rudelson’s matrix LLN (Rudelson, 1999)). Let $R_1, \ldots, R_n \in \mathbb{R}^{d \times d}$ be i.i.d. random matrices with $d \geq 2$. Suppose $R = E(R_i)$ and $\|R_i\|_2 \leq C$ a.s., for any $i \in [n]$, then

$$
E\|P_n(R) - R^*\|_2 \leq C \frac{\log d}{n} + \sqrt{\frac{C\|R\|_2 \log d}{n}}.
$$

**Proposition 7** (Weyl’s inequality (Weyl, 1912)). Let $\hat{\mathcal{R}}$ and $\mathcal{R}$ be $d \times d$ symmetric matrices. We have for any $i \in [d]$,

$$
\lambda_i(\mathcal{R}) + \lambda_d(\hat{\mathcal{R}} - \mathcal{R}) \leq \lambda_i(\hat{\mathcal{R}}) \leq \lambda_i(\mathcal{R}) + \lambda_1(\hat{\mathcal{R}} - \mathcal{R}).
$$

Therefore, if $\hat{\mathcal{R}} - \mathcal{R}$ is positive semi-definite or $\hat{\mathcal{R}} \succeq \mathcal{R}$, one has $\lambda_i(\hat{\mathcal{R}}) \leq \lambda_i(\mathcal{R})$ for any $i \in [n]$.

**Proposition 8** (Davis-Kahan theorem (Davis & Kahan, 1970)). Let symmetric matrix $\hat{\mathcal{R}} \in \mathbb{R}^{d \times d}$ be the perturbed version of a symmetric matrix $\mathcal{R} \in \mathbb{R}^{d \times d}$ such that

$$
\hat{\mathcal{R}} = \mathcal{R} + \mathcal{E}.
$$
Define their singular value decompositions

\[ \hat{\mathbf{R}} = \hat{\mathbf{U}} \hat{\mathbf{S}} \hat{\mathbf{U}}^T + \hat{\mathbf{U}}_\perp \hat{\mathbf{S}}_\perp \hat{\mathbf{U}}_\perp^T, \]

\[ \mathbf{R} = \mathbf{U} \mathbf{S} \mathbf{U}^T + \mathbf{U}_\perp \mathbf{S}_\perp \mathbf{U}_\perp^T, \]

where \( \hat{\mathbf{U}} \) and \( \hat{\mathbf{S}} \) correspond to the top-\( r \) singular vectors and top-\( r \) singular values of \( \hat{\mathbf{R}} \), respectively; similar notation also holds for \( \mathbf{R} \). We then have

\[ \|\hat{\mathbf{U}}_\perp^T \mathbf{U}\|_2 \leq \|\hat{\mathbf{U}}^T \mathbf{E}\|_2 \sigma_r(\hat{\mathbf{R}}) - \sigma_{r+1}(\mathbf{R}). \]

**Proof of Lemma 8 (i)** By definition one has

\[ \hat{G}_n - \bar{G}_n = \left[ P_n \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} - P \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} \right] + \rho(\hat{Q}_n - Q_n) \quad (S.5.21) \]

Recalling that by Lemma 6 and Lemma 7, we have wpa1,

\[ \|\Psi - \hat{\Gamma}\|_{\mathbb{X} \times T}^2 \leq (\|\Psi\|_{\mathbb{X} \times T} + \|\hat{\Gamma}\|_{\mathbb{X} \times T})^2 \]

\[ \lesssim K, \]

and

\[ \| P \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} \|_2 \lesssim 1. \quad (S.5.22) \]

Now we first condition on given \( \hat{\Gamma}(\cdot) \) which satisfies \( (S.5.22) \) as \( n \to +\infty \). Since \( \hat{\Gamma}(\cdot) \) is trained separately, one has \( \{ (\Psi_i - \hat{\Gamma}_i)(\Psi_i - \hat{\Gamma}_i)^T \}_{i=1}^n \) are i.i.d. now random matrices and

\[ P \left[ (\Psi_i - \hat{\Gamma}_i)(\Psi_i - \hat{\Gamma}_i)^T - P \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} \right] = 0. \]

By \( (S.5.22) \), we also have

\[ \| (\Psi_i - \hat{\Gamma}_i)(\Psi_i - \hat{\Gamma}_i)^T \|_2 \leq \sup_{x \in \mathbb{X}} \|\Psi(x) - \hat{\Gamma}(x)\|^2 \]

\[ = \|\Psi - \hat{\Gamma}\|_{\mathbb{X} \times T}^2 \lesssim K. \]

By taking \( \mathbf{R}_i = (\Psi_i - \hat{\Gamma}_i)(\Psi_i - \hat{\Gamma}_i)^T \) in Proposition 6 and given \( \hat{\Gamma}(\cdot) \), one has

\[ \| P_n \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} - P \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} \|_2 \lesssim \frac{K \log K}{n} + \sqrt{\frac{K \log K}{n}} \]

\[ \lesssim \sqrt{\frac{K \log n}{n}}, \quad (S.5.23) \]

as \( (K \log K)/n \to 0 \) under Assumption 6. Since the conditioned event \( (S.5.22) \) happens wpa1, we can directly uncondition it and \( (S.5.23) \) implies

\[ \| P_n \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} - P \left\{ (\Psi - \hat{\Gamma})(\Psi - \hat{\Gamma})^T \right\} \|_2 = O_P \left( \sqrt{\frac{K \log n}{n}} \right), \]

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Similarly, we can show
\[ \| \hat{Q}_n - Q_n \|_2 = O_P(\sqrt{K \log n/n}) . \]
Note this also implies \( \| \hat{Q}_n - Q_n \|_2 \to 0 \) wpa1, since \( \sqrt{K \log n/n} \) vanishes under Assumption 6. Thus we further have \( \| \hat{Q}_n \|_2 \leq \| Q_n \|_2 + \| \hat{Q}_n - Q_n \|_2 \leq \| Q_n \|_2 \lesssim 1 \), wpa1, by Lemma 5. Similarly, we can also show \( \| P_n(TT^T) \|_2 \lesssim 1 \).

In summary, by (S.5.21) and the bounds derived above, one has
\[ \min_n \| G_n - \hat{G}_n \|_2 \leq \| G_n - \hat{G}_n \|_2 + \| \hat{G}_n - G_n \|_2 = O_P(\sqrt{K \log n/n}) , \]
follows from Lemma 7, whenever \( n^2 \lesssim \sqrt{K \log n/n} \).

**Proof of Lemma 8 (ii)** We first show \( \hat{G}_n \) is invertible wpa1. By definition, we write
\[ \hat{G}_n = P_n \{(\hat{\Psi} - \hat{\Gamma})(\hat{\Psi} - \hat{\Gamma})^T\} + \rho \hat{Q}_n \geq \rho \hat{Q}_n , \]
as both \( P_n \{(\hat{\Psi} - \hat{\Gamma})(\hat{\Psi} - \hat{\Gamma})^T\} \) and \( \hat{Q}_n \) are positive semi-definite matrices. Then (S.5.25) and Proposition 7 imply that
\[ \lambda_{\min}(\hat{G}_n) \geq \lambda_{\min}(\rho \hat{Q}_n) = \rho \lambda_{\min}(\hat{Q}_n) . \]
Recall \( \| \hat{Q}_n - Q_n \|_2 \to 0 \) wpa1. By (S.5.16) in Proposition 5 with \( \bar{R} = \hat{Q}_n \) and \( R = Q_n \), one has \( \lambda_{\min}(\hat{Q}_n) \geq \lambda_{\min}(Q_n) - \| \hat{Q}_n - Q_n \|_2 \lesssim 1 \) wpa1. Thus by \( \lambda_{\min}(\hat{Q}_n) \gtrsim 1 \) and (S.5.26) we conclude that,
\[ \lambda_{\min}(\hat{G}_n) \gtrsim \rho , \]
wpa1, thus \( \hat{G}_n \) is invertible wpa1. On the other hand, recalling (S.5.1), one has \( \lambda_{\min}(G_n) \geq \rho \lambda_{\min}(Q_n) \gtrsim \rho \) by Lemma 3. Now wpa1, we can decompose,
\[ \hat{G}_n^{-1} - G_n^{-1} = G_n^{-1}(G_n - \hat{G}_n)\hat{G}_n^{-1} , \]
which combining with (S.5.27) implies, wpa1,
\[ \| \hat{G}_n^{-1} - G_n^{-1} \|_2 \leq \| G_n^{-1} \|_2 \| G_n - \hat{G}_n \|_2 \| \hat{G}_n^{-1} \|_2 \]
\[ = \lambda_{\min}(\hat{G}_n)^{-1} \lambda_{\min}(G_n)^{-1} \| G_n - \hat{G}_n \|_2 \]
\[ \gtrsim \rho^{-2} \| \hat{G}_n - G_n \|_2 . \]
Finally by (S.5.24) and (S.5.29), we conclude \( \| \hat{G}_n^{-1} - G_n^{-1} \|_2 = O_P(\rho^{-2} \sqrt{K \log n/n}) \).

**Proof of Lemma 8 (iii)** Recall \( G_n = R_n + \rho Q_n \). By definition, it is easy to see both \( R_n \) and \( \rho Q_n \) are positive semi-definite matrices. Thus we have \( G_n \succeq R_n \), and by Proposition 7,
\[ \sigma_\zeta(G_n) \geq \sigma_\zeta(R_n) = \beta_n , \]
(S.5.30)
which implies that,
\[
\|\tilde{\Sigma}^{-1}\|_2 = \sigma^{-1}_\zeta(G_n) \leq \beta_n^{-1}.
\]  
(S.5.31)

On the other hand, since \(G_n \succeq \rho Q_n\), we have
\[
\sigma_{\min}(G_n) \geq \rho \sigma_{\min}(Q_n) \gtrsim \rho,
\]  
(S.5.32)

also by Lemma 5. Therefore, \(G_n\) is invertible and \(\|\tilde{\Sigma}^{-1}\|_2 = \sigma^{-1}_{\min}(G_n) \gtrsim \rho^{-1}\). Finally, by taking \(\hat{\mathcal{R}} = G_n\), \(\mathcal{R}_n = R_n\), and \(\mathcal{E} = \rho Q_n\) in Proposition 8, we have
\[
\|\hat{U}_\perp^T U\|_2 \leq \frac{\rho \|Q_n\|}{\sigma_\zeta(G_n) - \sigma_{\zeta+1}(R_n)} \lesssim \rho \beta_n^{-1},
\]  
(S.5.33)
recalling that \(\|Q_n\| \lesssim 1\), \(\sigma_\zeta(G_n) \gtrsim \beta_n\), and \(\sigma_{\zeta+1}(R_n) = 0\) due to Lemma 4 and the fact that \(R_n\) is rank-\(\zeta\).

Finally Cai & Zhang (2018, Lemma 1) implies
\[
\sigma_{\min}^2(\tilde{U}_\perp^T U) = 1 - \|\tilde{\Sigma}^{-1}\|_2.
\]  
(S.5.34)

Under the settings of Theorem 2, one has \(\rho < \sqrt{K \log n/n} < \beta_n\). Then by \(\rho < \beta_n\) and (S.5.33)-(S.5.34), we have \(\sigma_{\min}^2(\hat{U}_\perp^T U) \to 1\) as \(n \to +\infty\).

Proof of Lemma 8 (iv) Recalling definition (3.4), one has \(\|\Sigma^{-1}\|_2 = \sigma^{-1}_\zeta = \beta_n^{-1}\). By taking \(\hat{\mathcal{R}} = \hat{G}_n\) and \(\mathcal{R} = G_n\) in Proposition 5, one has
\[
|\hat{\sigma}_\zeta - \sigma_\zeta(G_n)| \leq \|\hat{G}_n - G_n\|_2 = O_P(\sqrt{\log n/n}).
\]  
(S.5.35)

On the other hand, recalling (S.5.30) and (S.5.32), we have
\[
\sigma_\zeta(G_n) \gtrsim \beta_n + \rho,
\]
which combining with (S.5.35), implies
\[
\hat{\sigma}_\zeta \asymp \beta_n + \rho,
\]
wpa1, under the assumed condition \(\beta_n + \rho > \sqrt{K \log n/n}\). This implies
\[
\|\hat{\Sigma}^{-1}\|_2 = \hat{\sigma}_\zeta^{-1} \lesssim (\beta_n + \rho)^{-1}
\]  
(S.5.36)
wpa1. By (S.5.27), we have \(\|\hat{\Sigma}^{-1}_\perp\|_2 = \lambda_{\min}^{-1}(\hat{G}_n) \lesssim \rho^{-1}\) wpa1.

By taking \(\mathcal{R} = \hat{G}_n\) and \(\mathcal{R} = R_n\) in Proposition 8, we have
\[
\|\hat{U}^T U\|_2 \leq \frac{\|\hat{G}_n - R_n\|_2}{\lambda_\zeta(\hat{G}_n) - \lambda_{\zeta+1}(R_n)} \leq \frac{\|\hat{G}_n - G_n\|_2 + \rho \|Q_n\|_2}{\hat{\sigma}_\zeta} = O_P\{(\beta_n + \rho)^{-1}(\sqrt{K \log n/n} + \rho)\},
\]
recalling that \( \bar{\sigma}_\zeta \asymp \beta_n + \rho, \| Q_n \|_2 \asymp 1 \), and \( \| \hat{G}_n - G_n \|_2 = O_P(\sqrt{K \log n/n}) \). The final results follow, after taking the assumed condition \( \rho < \sqrt{K \log n/n} < \beta_n \) into account.

**Proof of Lemma 8 (v)** First when \( \beta_n \asymp 1 \), clearly we have

\[
\| A_n \|_2 \leq \| \hat{U} \|_2^2 \| \Sigma^{-1} \|_2 \asymp \beta_n^{-1} \asymp 1, \tag{S.5.37}
\]

by (S.5.31). On the other hand, we have

\[
\hat{A}_n - A_n = (\hat{U} \hat{\Sigma} \hat{U}^t)^{-1} - (\hat{\Sigma} \hat{U}^t)^{-1}
 = (\hat{U} \hat{\Sigma} \hat{U}^t)^{-1}(\hat{\Sigma} \hat{U}^t - \hat{\Sigma} \hat{U}^t)(\hat{U} \hat{\Sigma} \hat{U}^t)^{-1},
\]

and thus

\[
\| \hat{A}_n - A_n \|_2 \leq \| \Sigma^{-1} \|_2 \| \Sigma^{-1} \|_2 \| \hat{U} \hat{\Sigma} \hat{U}^t - \hat{\Sigma} \hat{U}^t \|_2
 \asymp \| \hat{U} \hat{\Sigma} \hat{U}^t - \hat{\Sigma} \hat{U}^t \|_2,
\]

by (S.5.31) and (S.5.36). In addition, one has

\[
\| \hat{U} \hat{\Sigma} \hat{U}^t - \hat{\Sigma} \hat{U}^t \|_2 \leq 2\| \hat{G}_n - G_n + \tilde{U}_\perp \tilde{\Sigma}_\perp \tilde{U}_\perp^t \|_2
 \leq 2\| \hat{G}_n - G_n \|_2 + 2\| \tilde{U}_\perp \tilde{\Sigma}_\perp \tilde{U}_\perp^t \|_2
 = O_P(\sqrt{K \log n/n + \rho})
 = o_P(1), \tag{S.5.38}
\]

where the last two equalities are by the previous derived bounds, and the conditions that \( K \asymp n^{a_2} \) and \( \rho \to 0 \) for some \( a_2 < 1 \). The first inequality of (S.5.38) follows by that \( \hat{G}_n \) can be seen as a perturbed version of \( \hat{U} \hat{\Sigma} \hat{U}^t \) such that

\[
\hat{G}_n = \hat{U} \hat{\Sigma} \hat{U}^t + (\hat{G}_n - G_n + \tilde{U}_\perp \tilde{\Sigma}_\perp \tilde{U}_\perp^t).
\]

Thus as the best rank-\( \zeta \) approximation of \( \hat{G}_n \), the \( \hat{U} \hat{\Sigma} \hat{U}^t \) satisfies the first inequality of (S.5.38) by Eckart–Young–Mirsky theorem (Eckart & Young, 1936) such that,

\[
\| \hat{G}_n - \hat{U} \hat{\Sigma} \hat{U}^t \|_2 \leq \| \hat{G}_n - \hat{U} \hat{\Sigma} \hat{U}^t \|_2
 = \| \hat{G}_n - G_n + \tilde{U}_\perp \tilde{\Sigma}_\perp \tilde{U}_\perp^t \|_2,
\]

and thus \( \| \hat{U} \hat{\Sigma} \hat{U}^t - \hat{\Sigma} \hat{U}^t \|_2 \leq \| \hat{U} \hat{\Sigma} \hat{U}^t - \hat{G}_n \|_2 + \| \hat{G}_n - \hat{U} \hat{\Sigma} \hat{U}^t \|_2 \leq 2\| \hat{G}_n - G_n + \tilde{U}_\perp \tilde{\Sigma}_\perp \tilde{U}_\perp^t \|_2 \).

Summarizing the results above we have

\[
\| \hat{A}_n - A_n \|_2 = o_P(1),
\]

and thus by (S.5.37), \( \| \hat{A}_n \|_2 \leq \| A_n \|_2 + \| \hat{A}_n - A_n \|_2 \asymp 1 \) wpa1.

We note \( \| \mu \|_{X \times T} < +\infty \) under Assumption 8 (iii). By the new condition that

\[
\| \mu - \hat{\mu} \|_{X \times T} = O_P(1), \tag{S.5.39}
\]

we have wpa1,

\[
\| \mu \|_{X \times T} \leq \| \mu \|_{X \times T} + \| \mu - \hat{\mu} \|_{X \times T}
 \asymp 1. \tag{S.5.40}
\]

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Similar to (S.5.22) and (S.5.23), we show the convergence of \( \hat{B}_n \) by matrix concentration. It is easy to see \( P(\hat{B}_n) = B_n \), with \( \hat{B}(X) \) trained separately. Based on Assumption 8, Lemma 7 and (S.5.39), we have, wpa1,

\[
\|B_n\|_2 = \sup_{\|\ell\|=1} P \left[ \{Y - \hat{\mu}(X, T)\}^2 \left\{ \ell^T \{\Psi(X, T) - \hat{\Gamma}(X)\} \right\}^2 \right] \\
\leq \sup_{\|\ell\|=1} P \left[ \left\{ 2(Y - \mu(X, T))^2 + 2(\mu(X, T) - \hat{\mu}(X, T))^2 \right\} \left\{ \ell^T \{\Psi(X, T) - \hat{\Gamma}(X)\} \right\}^2 \right] \\
= \sup_{\|\ell\|=1} P \left[ \left\{ 2\text{Var}(Y | X, T) + 2(\mu(X, T) - \hat{\mu}(X, T))^2 \right\} \left\{ \ell^T \{\Psi(X, T) - \hat{\Gamma}(X)\} \right\}^2 \right] \\
\leq \left\{ \sup_{(x,t) \in \mathcal{X} \times \mathcal{T}} 2\text{Var}(Y | X = x, T = t) + 2\|\hat{\mu} - \mu\|_{\mathcal{X} \times \mathcal{T}} \right\} \sup_{\|\ell\|=1} P \left[ \left\{ \ell^T \{\Psi(X, T) - \hat{\Gamma}(X)\} \right\}^2 \right] \\
\leq \sup_{\|\ell\|=1} P \left[ \left\{ \ell^T \{\Psi(X, T) - \hat{\Gamma}(X)\} \right\}^2 \right] \\
= \|P\{\Psi - \hat{\Gamma}(\Psi - \hat{\Gamma})^T\}\|_2 \\
\leq 1,
\]

where the last inequality follows by (S.5.22). By Proposition 6, one has

\[
\|\hat{B}_n - B_n\|_2 = O_P\left(\sqrt{\frac{K \log n}{n}}\right) = o_P(1).
\]

In addition, we have

\[
\hat{B}_n - B_n = P \left[ \left\{ Y - \hat{\mu}(X, T) \right\}^2 \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\} \right] + P \left[ \left\{ Y - \hat{\mu}(X, T) \right\} \left\{ \Psi(X, T) - \Gamma(X) \right\} \right] + P \left[ \left\{ Y - \mu(X, T) \right\} \left\{ \Gamma(X) - \hat{\Gamma}(X) \right\} \right] \\
= \Delta_{B,1} + \Delta_{B,2} + \Delta_{B,3}.
\]

We bound the spectral norms of three terms on the right-hand side of above display, respectively. We have

\[
\Delta_{B,1} = P \left[ \left\{ 2Y - \hat{\mu}(X, T) - \mu(X, T) \right\} \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\} \right],
\]

Under our simplified two-fold training setting such that one fold trains nuisance functions and one fold trains the proposed estimator and \( \hat{\sigma} \), we can write \( \hat{B}_n \) as

\[
\hat{B}_n = \frac{1}{n} \sum_{i=1}^{n} \{Y_i - \hat{\mu}(X_i, T_i)\}^2 \{\Psi(X_i, T_i) - \hat{\Gamma}(X_i)\} \{\Psi(X_i, T_i) - \hat{\Gamma}(X_i)\}^T.
\]

We also define

\[
\bar{B}_n = P \left[ \{Y - \hat{\mu}(X, T)\}^2 \{\Psi(X, T) - \hat{\Gamma}(X)\} \right] \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\}^T.
\]
and thus \( wpa1, \)
\[
\|\Delta_{B,1}\|_2
\leq \sup_{\|\ell\|_1} \left[ \left\{ 2Y - \hat{\mu}(X, T) - \mu(X, T) \right\} \left\{ \mu(X, T) - \hat{\mu}(X, T) \right\} \right] \|\ell\|_1 \|\Psi(X, T) - \hat{\Gamma}(X)\|^2
\]
\[
= o_P(1),
\]
where the last inequality follows by the moment conditions in Assumption 8, (S.5.40), \( \|\mu - \hat{\mu}\|_{x \times T} = o_P(1), \) and (S.5.22). With similar arguments, we can further show
\[
\|\Delta_{B,2}\|_2 = \sup_{\|\ell\|_1} \left[ \left\{ Y - \mu(X, T) \right\} \left\{ \ell^T \{ \Psi(X, T) - \Gamma(X) \} \right\} \right] \|\ell\|_1 \|\Psi(X, T) - \hat{\Gamma}(X)\|^2
\]
\[
\leq \sup_{\|\ell\|_1} \left[ \left\{ Y - \mu(X, T) \right\} \left\{ \ell^T \{ \Psi(X, T) - \Gamma(X) \} \right\} \right] \|\ell\|_1 \|\Gamma(X) - \hat{\Gamma}(X)\|^2
\]
\[
\leq \sup_{(x,t) \in X \times T} \text{Var}(Y | X = x, T = t) \sup_{\|\ell\|_1} \left[ \left\{ \ell^T \{ \Psi(X, T) - \Gamma(X) \} \right\} \right] \|\ell\|_1 \|\Gamma(X) - \hat{\Gamma}(X)\|^2
\]
\[
= o_P(1),
\]
where the second inequality follows by Cauchy–Schwarz inequality, and the last equality follows by (3.7). Similarly, we can also show \( \|\Delta_{B,3}\|_2 = o_P(1) \) and \( \|\hat{B}_n\|_2 \leq 1. \) Summarizing all results above, we conclude wp1,
\[
\|\hat{B}_n - B_n\|_2 \leq \|\hat{B}_n - \hat{B}_n\|_2 + \|\Delta_{B,1}\|_2 + \|\Delta_{B,2}\|_2 + \|\Delta_{B,3}\|_2
\]
\[
= o_P(1),
\]
and furthermore \( \|\hat{B}_n\|_2 \leq \|B_n\|_2 + \|\hat{B}_n - B_n\|_2 \leq 1 \) wp1.

**Lemma 9.** Suppose the general settings of Theorem 2 hold. Define \( \Delta_{1,1} \sim \Delta_{1,5} \) in (S.5.89) through (S.5.90).

(i) Suppose \( \ell_n \in \mathbb{R}^K \) is a vector that can depend on \( \{(X_i, T_i)\}^n_{i=1} \) when \( n \) grows, and \( \|\ell_n\| = 1 \) for any \( n > 0. \) We have \( \|\Delta_{1,1}\| = O_P(\sqrt{K/n}) \) and \( \|\ell_n \Delta_{1,1}\| = O_P(1/\sqrt{n}); \)

(ii) Suppose \( \ell_n \in \mathbb{R}^K \) is a vector that depends only on \( n, \) and \( \|\ell_n\| = 1 \) for any \( n > 0. \) We have \( \|\Delta_{1,2}\| = O_P(K^{-p/(d+1)}) \) and \( \|\ell_n \Delta_{1,2}\| = O_P(K^{-p/(d+1)}); \)

(iii) Suppose \( \ell_n \in \mathbb{R}^K \) is a vector that depends only on \( n, \) and \( \|\ell_n\| = 1 \) for any \( n > 0. \) We have \( \|\Delta_{1,3}\| = O_P(r^\gamma \sqrt{K/n}) \) and \( \|\ell_n \Delta_{1,3}\| = O_P(r^\gamma /\sqrt{n}); \)

(iv) Suppose \( \ell_n \in \mathbb{R}^K \) is a vector that depends only on \( n, \) and \( \|\ell_n\| = 1 \) for any \( n > 0. \) We have \( \|\Delta_{1,4}\| = O_P(r_m \sqrt{K/n} + r^\gamma \sqrt{K/n}) \) and \( \|\ell_n \Delta_{1,4}\| = O_P(1/\sqrt{n}); \)

(v) Suppose \( \ell_n \in \mathbb{R}^K \) is a vector that depends only on \( n, \) and \( \|\ell_n\| = 1 \) for any \( n > 0. \) We have \( \|\Delta_{1,5}\| = o_P(r_m r^2 + r^\gamma r_m \sqrt{K/n} + r^\gamma r_m \sqrt{K/n}) \) and \( \|\ell_n \Delta_{1,5}\| = o_P(r^\gamma /\sqrt{n} + r_m r^\gamma + r^\gamma); \)
Proof of Lemma 9. We first present the following concentration result which will be repeatedly used during the proof. This proposition can be simply proved by high-order Markov inequality.

**Proposition 9.** Given $n$, let $v_1, \ldots, v_n$ are i.i.d. copies of random vector $v \in \mathbb{R}^d$. Suppose $E(\|v\|^2) \leq A_n$, where $A_n > 0$ is allowed to diverge. We have for any $J > 0$,

$$\text{pr}\{\|P_n(v) - E(v)\| > J \sqrt{d/n}\} \leq \frac{4A_n J^2}{J^2d}.$$

**Proof of Proposition 9.** By the second-order Markov’s inequality, we have for any $J > 0$,

$$\text{pr}\{\|P_n(v) - E(v)\| > J \sqrt{d/n}\} \leq \frac{n J^2 d E\{\|P_n(v) - E(v)\|^2\}}{J^2d}.$$

Now we bound $E\{\|P_n(v) - E(v)\|^2\}$. We can write

$$E\{\|P_n(v) - E(v)\|^2\} = E\left[\left\|\frac{1}{n} \sum_{i=1}^{n} \{v_i - E(v)\}\right\|^2\right]$$

$$= \frac{1}{n^2} E\left[\left\|\sum_{i=1}^{n} \{v_i - E(v)\}\right\|^2\right]$$

$$= \frac{1}{n} E\left\{\|v_i - E(v)\|^2\right\}$$

$$\leq \frac{2}{n} E(\|v\|^2) + \|E(v)\|^2$$

$$\leq \frac{4}{n} E(\|v\|^2)$$

$$\leq \frac{4A_n}{n}.$$

The third equality in the above display follows because

$$\frac{1}{n^2} E\left[\left\|\sum_{i=1}^{n} \{v_i - E(v)\}\right\|^2\right] = \sum_{k=1}^{d} \frac{1}{n^2} E\left[\sum_{i=1}^{n} \{v_i^{(k)} - E(v^{(k)})\}\right]^2$$

$$= \sum_{k=1}^{d} \frac{1}{n^2} \text{Var} \left(\sum_{i=1}^{n} v_i^{(k)}\right)$$

$$= \sum_{k=1}^{d} \frac{1}{n} \text{Var} (v^{(k)})$$

$$= \frac{1}{n} E\{\|v_i - E(v)\|^2\},$$

where we define $v_i^{(k)}, v^{(k)}$ as the $k$th coordinates of $v_i, v$, respectively; the second equality follows by $E(\sum_{i=1}^{n} v_i^{(k)}) = nE(v^{(k)})$; the third equality follows by $v_1^{(k)}, \ldots, v_n^{(k)}$ are independent and identically distributed. Combining (S.5.41) and (S.5.42) yields the desired result. □

Given $n$ samples, during the following proof we will frequently condition on the following event $E_n$: the nuisance functions $(\hat{m}, \hat{\Gamma})$ are already obtained from the separate data set for nuisance function training (see §S.5.1), and $(\hat{m}, \hat{\Gamma})$ satisfies the following conditions:
• $\|\hat{m}\|_X$ and $\|\hat{\Gamma}\|_X/\sqrt{K}$ are bounded by some fixed constant $C > 0$;

• All of the following quantities: (i) $r^{-1}_J \|\hat{\Gamma} - \Gamma\|_X/\sqrt{K}$; (ii) $r^{-1}_m \|\hat{m} - m\|_{\mathcal{E}_K}$; (iii) $r^{-1}_\gamma \mathbb{P}\{\hat{\Gamma}(X) - \Gamma(X)\} \{\hat{\Gamma}(X) - \Gamma(X)\}^2 \leq 1/2$; (iv) $\|\hat{m} - m\|_X$; (v) $\|\hat{\Gamma}^T \phi^* - \Gamma^T \phi^*\|_X$ are bounded by $\epsilon_n$, where $\epsilon_n$ is a sequence vanishing to zero, when $n \to +\infty$.

By Lemma 6, Assumption 9, and rates (3.5)–(3.6), we can choose some fixed $C_1 > 0$ and a deterministic positive sequence $\epsilon_n \to 0$, such that $\mathcal{E}_n$ happens wp.a1 when $n \to +\infty$. For simplicity, during the following proof, we use $\operatorname{pr}_n(\cdot)$ to represent the probability that condition on $\mathcal{E}_n$. Note that since nuisance functions are trained separately from the samples involved in this proof, the expectation in this proof conditional on obtained nuisance functions can be simply represented by $\mathbb{P}(\cdot)$.

Now we prove (i)–(iv) sequentially.

Proof of Lemma 9 (i) For simplicity, let $m_{i,1} = \{Y_i - \mu(T_i, X_i)\} \{\psi(T_i, X_i) - \Gamma(X_i)\}$. Thus $\Delta_{1,1} = P_n(m_{i,1})$. We have

$$E(m_{i,1}) = E \left[ \{Y - \mu(X, T)\} \{\psi(X, T) - \Gamma(X)\} \right]$$
$$= E \left[ E \left( Y \mid X, T \right) - \mu(X, T) \right] \{\psi(X, T) - \Gamma(X)\}$$
$$= 0,$$

where the second equality follows by the law of total expectation. On the other hand,

$$E(\|m_{i,1}\|^2) = E \left[ \{Y - \mu(X, T)\}^2 \|\psi(X, T) - \Gamma(X)\|^2 \right]$$
$$= E \left\{ \operatorname{Var}(Y \mid X, T) \|\psi(X, T) - \Gamma(X)\|^2 \right\}$$
$$\leq \sup_{(x,t) \in X \times T} \operatorname{Var}(Y \mid X = x, T = t) \cdot E \left\{ \|\psi(X, T) - \Gamma(X)\|^2 \right\}.$$

Under Assumption 8, one has $\sup_{(x,t) \in X \times T} \operatorname{Var}(Y \mid X = x, T = t) \lesssim 1$. On the other hand,

$$E \left\{ \|\psi(X, T) - \Gamma(X)\|^2 \right\} \leq 2 \|\psi\|^2_{X \times T} + 2 \|\Gamma\|^2_X \lesssim K$$

by Lemma 6. Thus $E(\|m_{i,1}\|^2) \lesssim K$. Let $v_i = m_{i,1}$ in Claim 9. With results above, we have for any fixed $J = J_0 > 0$

$$\operatorname{pr}(\|\Delta_{1,1}\| > J_0 \sqrt{K/n}) = \operatorname{pr}(\|P_n(m_{i,1})\| > J_0 \sqrt{K/n})$$
$$\leq \frac{C_1 K}{J_0^2 K} = \frac{C_1}{J_0^2}$$

where $C_1$ is some fixed constant independent with $n$ and $J_0$. Therefore, when $J_0$ is sufficiently large, the right-hand side of the above display can by arbitrarily small, and thus $\|\Delta_{1,1}\| = O_P(\sqrt{K/n})$.

Now we bound $|\ell_n^T \Delta_{1,1}|$. We first condition on $\{(X_i, T_i)\}_{i=1}^n$. We note that given $\{(X_i, T_i)\}_{i=1}^n$, $\{\ell_n^T m_{i,1}\}_{i=1}^n$ are independent random variables since $\{Y_i\}_{i=1}^n$ are independent and $\ell_n$ depends only on $n$ and $\{(X_i, T_i)\}_{i=1}^n$.

Furthermore, they are mean-zero,

$$E[\ell_n^T m_{i,1} \mid \{(X_i, T_i)\}_{i=1}^n] = E[\ell_n^T m_{i,1} \mid X_i, T_i]\]$$
$$= \{E(Y \mid X_i, T_i) - \mu(X_i, T_i)\} \{\ell_n^T \psi(X_i, T_i) - \ell_n^T \Gamma(X_i)\}$$
$$= 0.$$
Here we use $\tilde{\ell}_n$ to denote $\ell_n$ given specific $\{(X_i, T_i)\}_{i=1}^n$. Then the conditional variance for each $\ell^T_n m_{i,n}$ is

$$
\text{Var}[\ell^T_n m_{i,n} | \{(X_i, T_i)\}_{i=1}^n] = E\left\{ (\tilde{\ell}^T_n m_{i,n})^2 | X_i, T_i \right\}
$$

$$
= E\left\{ (Y_i - \mu(T_i, X_i))^2 \left( \tilde{\ell}_n \Psi(T_i, X_i) - \tilde{\ell}_n \Gamma(X_i) \right)^2 | X_i, T_i \right\}
$$

$$
\leq \text{Var}(Y | X_i, T_i) \cdot \left( \tilde{\ell}^T_n \Psi(T_i, X_i) - \tilde{\ell}^T_n \Gamma(X_i) \right)^2
$$

$$
\leq \left[ 2\left( \tilde{\ell}^T_n \Psi(T_i, X_i) \right)^2 + 2\left( \tilde{\ell}^T_n \Gamma(X_i) \right)^2 \right] \sup_{(x,t) \in \mathcal{X} \times \mathcal{T}} \text{Var}(Y | X = x, T = t)
$$

$$
\leq C_2 \left[ \left( \tilde{\ell}^T_n \Psi(T_i, X_i) \right)^2 + \left( \tilde{\ell}^T_n \Gamma(X_i) \right)^2 \right] \quad \text{(Assumption 8)}
$$

for some fixed $C_2$ independent of $n$ and $\{(X_i, T_i)\}_{i=1}^n$. Therefore, given $\{(X_i, T_i)\}_{i=1}^n$, we have that $P_n(\ell^T_n m_{i,n})$ is mean zero and has variance,

$$
\text{Var}[P_n(\ell^T_n m_{i,n}) | \{(X_i, T_i)\}_{i=1}^n] = \text{Var}\left[ \frac{1}{n} \sum_{i=1}^n \ell^T_n m_{i,n} | \{(X_i, T_i)\}_{i=1}^n \right]
$$

$$
= \frac{1}{n^2} \sum_{i=1}^n \text{Var}[\ell^T_n m_{i,n} | \{(X_i, T_i)\}_{i=1}^n]
$$

$$
\leq \frac{C_2}{n} \cdot \frac{1}{n} \sum_{i=1}^n \left[ \left( \tilde{\ell}^T_n \Psi(T_i, X_i) \right)^2 + \left( \tilde{\ell}^T_n \Gamma(X_i) \right)^2 \right].
$$

By Chebyshev’s inequality, given any $\{(X_i, T_i)\}_{i=1}^n$,

$$
|P_n(\ell^T_n m_{i,n})| = O_P \left[ n^{-1/2} \sqrt{\frac{1}{n} \sum_{i=1}^n \left[ \left( \tilde{\ell}^T_n \Psi(T_i, X_i) \right)^2 + \left( \tilde{\ell}^T_n \Gamma(X_i) \right)^2 \right]} \right] \quad \text{(S.5.44)}
$$

Now we do not condition on specific $\{(X_i, T_i)\}_{i=1}^n$, and consider the following positive random variable, which has a constant upper bound wp1,

$$
\xi_1 = \sqrt{\frac{1}{n} \sum_{i=1}^n \left[ \left( \tilde{\ell}^T_n \Psi(T_i, X_i) \right)^2 + \left( \tilde{\ell}^T_n \Gamma(X_i) \right)^2 \right]}
$$

$$
= \sqrt{P_n \left[ \left( \ell^T_n \Psi(T, X) \right)^2 \right] + P_n \left[ \left( \ell^T_n \Gamma(X) \right)^2 \right]}
$$

$$
\leq \sup_{\|\ell\|=1} P_n \left[ \left( \ell^T \Psi(T, X) \right)^2 \right] + \sup_{\|\ell\|=1} P_n \left[ \left( \ell^T \Gamma(X) \right)^2 \right]
$$

$$
= \sqrt{\|Q_n\|_2 + \|P_n(\Gamma^T)\|_2}
$$

$$
\lesssim 1,
$$

where the last equality follows by Lemma 8. Combining (S.5.44) and (S.5.45), we directly uncondition the given $\{(X_i, T_i)\}_{i=1}^n$, and conclude $|P_n(\ell^T_n m_{i,n})| = O_P(1/\sqrt{n})$. 

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Proof of Lemma 9 (ii) First, by definition, we observe
\[
\tau(X, T) - E\{\tau(X, T) \mid X\} - \{\Psi(X, T) - \Gamma(X)\}^T \phi^*
\]
\[
= \tau(X, T) - E\{\tau(X, T) \mid X\} - \{\Psi(X, T) - \Gamma(X)\}^T \phi^*
\]
\[
= \tilde\tau(X, T) - E\{\tilde\tau(X, T) \mid X\} - \{\Psi(X, T) - \Gamma(X)\}^T \phi^*.
\]
We now let
\[
m_{i,2} = \left[\tilde\tau(X_i, T_i) - E\{\tilde\tau(X, T) \mid X_i\} - \{\Psi(X_i, T_i) - \Gamma(X_i)\}^T \phi^*\right] \{\Psi(X_i, T_i) - \Gamma(X_i)\}
\]
\[
= \left[\tau(X_i, T_i) - E\{\tau(X, T) \mid X_i\} - \{\Psi(X_i, T_i) - \Gamma(X_i)\}^T \phi^*\right] \{\Psi(X_i, T_i) - \Gamma(X_i)\};
\]
thus \(\Delta_{1,2} = P_n(m_{i,2})\). We then have
\[
E(m_{i,2}) = E\left[\left[\tilde\tau(X, T) - E\{\tilde\tau(X, T) \mid X\} - \{\Psi(X, T) - \Gamma(X)\}^T \phi^*\right] \Psi(X, T)\right]
\]
\[
- E\left[\left[\tilde\tau(X, T) - E\{\tilde\tau(X, T) \mid X\} - \{\Psi(X, T) - \Gamma(X)\}^T \phi^*\right] \Gamma(X)\right]
\]
\[
= E\left[\left[\tilde\tau(X, T) - E\{\tilde\tau(X, T) \mid X\} - \{\Psi(X, T) - \Gamma(X)\}^T \phi^*\right] \Psi(X, T)\right]
\]
\[
- E\left[\left[\tilde\tau(X, T) - E\{\tilde\tau(X, T) \mid X\} - \{\Psi(X, T) - \Gamma(X)\}^T \phi^*\right] \mid X\right] \Gamma(X)
\]
\[
= E\left[E\{\Gamma^T(X)\phi^* - \tilde\tau(X, T) \mid X\} \Psi(X, T)\right].
\]
by the law of total expectation. Therefore, by Lemma 5 and Proposition 3, we have
\[
\|E(\Delta_{1,2})\| = \|E(m_{i,2})\|
\]
\[
= \sup_{\|\ell\|_1 = 1} \left|E\left[E\{\Gamma^T(X)\phi^* - \tilde\tau(X, T) \mid X\} \ell^T \Psi(X, T)\right]\right|
\]
\[
\leq \sqrt{E\left[E\{\Gamma^T(X)\phi^* - \tilde\tau(X, T) \mid X\}\right]^2} \sup_{\|\ell\|_1 = 1} \sqrt{E\left[\ell^T \Psi(X, T)\right]^2} \quad \text{(Cauchy–Schwarz inequality)}
\]
\[
= \sqrt{E\left[E\{\Psi^T(X, T)\phi^* - \tilde\tau(X, T) \mid X\}\right]^2} \|Q_n\|^{1/2}_2
\]
\[
\leq \sup_{x \in X} \left|E\left[E\{\Psi^T(X, T)\phi^* - \tilde\tau(X, T) \mid X = x\}\right]\|Q_n\|^{1/2}_2
\]
\[
\leq \|\tilde\tau - \{\phi^*\}^T \Psi\|_{X \times T} \|Q_n\|^{1/2}_2
\]
\[
= O(K^{-n/(d+1)}).
\]
Recalling $\Psi_n^r(T_i, X_i)\phi^*$ is a sieve approximation to $\tilde{\tau}(T_i, X_i)$, we then have

$$E\left(\|m_{i,2}\|^2\right)$$

\[
\leq \sup_{(x,t)\in\mathbb{X} \times T} \left| \tilde{\tau}(X = x, T = t) - E\{\tilde{\tau}(X, T) \mid X = x\} - \{\Psi(X = x, T = t) - \Gamma(X = x)\}^T \phi^* \right|^2
\]

\[
\cdot E\left(\|\Psi(X, T) - \Gamma(X)\|^2\right)
\]

\[
\leq 2\|\tilde{\tau} - \Psi_n^r \phi^*\|_{\mathbb{X} \times T}^2 + \sup_{x \in \mathbb{X}} 2E\{\tilde{\tau}(X, T) - \Psi_n^r (X, T) \phi^* \mid X = x\}^2 \cdot \left(2\|\Psi\|^2_{\mathbb{X} \times T} + 2\|\Gamma\|^2_{\mathbb{X}}\right)
\]

\[
\leq \left(4\|\tilde{\tau} - \Psi_n^r \phi^*\|_{\mathbb{X} \times T}^2\right) \left(2\|\Psi\|^2_{\mathbb{X} \times T} + 2\|\Gamma\|^2_{\mathbb{X}}\right)
\]

\[
= O(K^{-2p/(d+1)}), \quad \text{(S.5.48)}
\]

by Lemma 3, Proposition 3 and Lemma 6. By taking $v_i = m_{i,2}$, $A_n = C_3K^{1-2p/(d+1)}$, $d = K$, and $J = C_3K^{-p/(d+1)}$ in Claim 9, then for any $c > 0$, there exists large enough yet fixed $C_3 > 0$ such that

$$\text{pr}\left\{\|\Delta_{1,2} - E(\Delta_{1,2})\| > C_3K^{-p/(d+1)}\sqrt{K/n}\right\} \leq c.$$ 

Therefore $\|\Delta_{1,2} - E(\Delta_{1,2})\| = O_P(K^{-p/(d+1)}\sqrt{K/n}) = o_P(K^{-p/(d+1)})$. Then by (S.5.47), one has

$$\|\Delta_{1,2}\| \leq \|\Delta_{1,2} - E(\Delta_{1,2})\| + \|E(\Delta_{1,2})\| = O_P(K^{-p/(d+1)})$$

When $\ell_n$ depends only on $n$ and $\|\ell_n\| = 1$, then similar to (S.5.47), we have

$$\left|E(\ell_n^r m_{i,2})\right| = \left|E\left[ E\{\Gamma^T(X)\phi^* - \tilde{\tau}(X, T) \mid X\} \ell_n^r \Psi(X, T) \right]\right|$$

\[
= O(K^{-p/(d+1)}). \quad \text{(S.5.49)}
\]

Also, similar to (S.5.48) and by Lemma 5, we have

$$E(\ell_n^r m_{i,2})^2$$

\[
\leq \sup_{(x,t)\in\mathbb{X} \times T} \left| \tilde{\tau}(x, t) - E\{\tilde{\tau}(X, T) \mid X = x\} - \{\Psi(x, t) - \Gamma(x)\}^T \phi^* \right|^2
\]

\[
\cdot E\left[\ell_n^r \left\{\Psi(X, T) - \Gamma(X)\right\}\right]^2
\]

\[
\leq \left(4\|\tilde{\tau} - \Psi_n^r \phi^*\|_{\mathbb{X} \times T}^2\right) \left(\|Q_n\|_2 + \|E(\Gamma^T)\|_2\right)
\]

\[
= O(K^{-2p/(d+1)}).
\]

Take $v_i = \ell_n^r m_{i,2}$, $d = 1$, $A_n = C_4K^{-2p/(d+1)}$, $J = 2\sqrt{C_4}K^{-p/(d+1)}/c$ in Proposition 9. We then have for any fixed $c > 0$ and sufficiently large $C_4 > 0$,

$$\text{pr}\left\{\left|P_n(\ell_n^r m_{i,2}) - E(\ell_n^r m_{i,2})\right| > 2\sqrt{C_4}/cK^{-p/(d+1)}n^{-1/2}\right\} \leq c,$$
We now condition on \( \ell_n \Delta_{1,2} \), which combining with (S.5.49) implies that \( |\ell_n \Delta_{1,2}| = |P_n(\ell_n m_{i,2})| \leq |P_n(\ell_n m_{i,2}) - E(\ell_n m_{i,2})| + |E(\ell_n m_{i,2})| = O_P(K^{-p/(d+1)}n^{-1/2}) + O_P(K^{-p/(d+1)}) = O_P(K^{-p/(d+1)}). \)

Proof of Lemma 9 (iii) We now condition on \( \mathcal{E}_n \) with well-conditioned \((\hat{m}, \hat{\Gamma})\). We let \( m_{i,3} = [Y_i - m(X_i) - \{\Psi(T_i, X_i) - \Gamma(X_i)\}^T \phi^*] \{\Gamma(X_i) - \hat{\Gamma}(X_i)\} \) and thus \( \Delta_{1,3} = P_n(m_{i,3}) \). Recall the nuisance functions and proposed estimators are trained independently. The conditional expectations then can be bounded as follows

\[
P(m_{i,3}) = P \left[ Y - m(X) - \{\Psi(X, T) - \Gamma(X)\}^T \phi^* \right] \{\Gamma(X) - \hat{\Gamma}(X)\} \]

where the last equality follows by \( E(Y \mid X) = m(X) \) and \( E\{\Psi^T(X,T)\phi^* \mid X\} = \Gamma^T(X)\phi^* \); thus \( E(\Delta_{1,3}) = 0 \). We also have

\[
P(\|m_{i,3}\|^2)
= P \left[ Y - m(X) - \{\Psi(X, T) - \Gamma(X)\}^T \phi^* \right] \|\Gamma(X) - \hat{\Gamma}(X)\|^2
\leq P \left[ Y - m(X) - \{\Psi(X, T) - \Gamma(X)\}^T \phi^* \right]^2 \|\Gamma - \hat{\Gamma}\|_X^2
= O(1) \cdot O(Kr_\gamma^2 e_n)
= O(Kr_\gamma^2 e_n),
\]

where the inequality follows by

\[
P \left[ Y - m(X) - \{\Psi(X, T) - \Gamma(X)\}^T \phi^* \right]^2 \leq 2E \left[ Y - m(X) \right]^2 + 2E \left[ (\{\Psi(X, T) - \Gamma(X)\}^T \phi^*)^2 \right]
= 2E \left[ \text{Var}(Y \mid X) \right] + 2(\phi^*)^T R_n \phi^*
\leq 2E \left[ \text{Var}(Y \mid X) \right] + 2\|\phi^*\|^2 \|R_n\|_2
= O(1), \quad \text{(Assumptions 8 and Lemma 5)}
\]

and last two equalities are by the event defined in \( \mathcal{E}_n \). Let \( v_i = m_{i,3}, d = K, A_n = C_5 Kr_\gamma^2 e_n, \) and \( J = c_5 r_\gamma^2 \) in Proposition 9. We have when \( n \to +\infty, \)

\[
\text{pr}_n \left( \|\Delta_{1,3}\| > c_5 r_\gamma^2 \sqrt{K/n} \right) \leq \frac{4C_5 Kr_\gamma^2 e_n}{c_5^2 r_\gamma^2 K}
= 4C_5 e_n / c_5^2
\to 0,
\]

for some sufficiently large yet fixed \( C_5 > 0 \) and any fixed \( c_5 > 0 \). We thus have, conditional on \( \mathcal{E}_n, \|\Delta_{1,3}\| = o_P(r_\gamma^2 \sqrt{K/n}). \) Recall \( \mathcal{E}_n \) is a event happens wpa1. We thus can directly uncondition \( \mathcal{E}_n \) and have
\[ \| \Delta_{1.3} \| = o_P(r'_n \sqrt{K/n}). \] To be more specific, for any fixed \( C_6 > 0 \), we have

\[
\begin{align*}
\Pr \left( \| \Delta_{1.3} \| > c_5 r'_n \sqrt{K/n} \right) \\
= \Pr \left( \left\{ \| \Delta_{1.3} \| > c_5 r'_n \sqrt{K/n} \right\} \cap \mathcal{E}_n \right) + \Pr \left( \left\{ \| \Delta_{1.3} \| > c_5 r'_n \sqrt{K/n} \right\} \cap \mathcal{E}_n^c \right) \\
\leq \Pr \left( \left\{ \| \Delta_{1.3} \| > c_5 r'_n \sqrt{K/n} \right\} \cap \mathcal{E}_n \right) + \Pr(\mathcal{E}_n^c) \\
= \Pr_n \left( \| \Delta_{1.3} \| > c_5 r'_n \sqrt{K/n} \right) \cdot \Pr(\mathcal{E}_n) + \Pr(\mathcal{E}_n^c) \\
\to 0,
\end{align*}
\]

by \( \Pr(\mathcal{E}_n^c) \to 0, \Pr(\mathcal{E}_n) \leq 1 \), and (S.5.53).

Now we bound \( |\ell_n^2 \Delta_{1.3}| \). Similar to (S.5.50), we have \( P(\ell_n^{2i} m_{i,3}) = 0 \). Similar to (S.5.51), we have

\[
\begin{align*}
P(\ell_n^{2i} m_{i,3})^2 \\
= P \left[ (Y - m(X)) - \{\Psi(X, T) - \Gamma(X)\}^T \phi^* \right] \left[ \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\} \right]^2 \\
\leq 3P \left[ (Y - m(X))^2 \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\}^2 \right] \\
+ 3P \left[ \{\Psi(X, T) - \Gamma(X)\}^T \phi^* - [\tilde{\tau}(X, T) - E\{\tilde{\tau}(X, T) \mid X\}] \right] \left[ \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\}^2 \right] \\
+ 3P \left[ \tilde{\tau}(X, T) - E\{\tilde{\tau}(X, T) \mid X\} \right] \left[ \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\}^2 \right]
\end{align*}
\]

by the triangle inequality. The first term in (S.5.55) can be bounded by the law of total expectation,

\[
\begin{align*}
P \left[ (Y - m(X))^2 \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\} \right]^2 \\
= P \left[ \text{Var}(Y \mid X) \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\} \right]^2 \\
\leq \sup_{x \in \mathcal{X}} \text{Var}(Y \mid X = x) \cdot P \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\} \right]^2 \\
\leq P \ell_n^2 \{\Gamma(X) - \hat{\Gamma}(X)\} \right]^2
\end{align*}
\]

(S.5.56)

where the second inequality follows by Assumption 8 and \( \mathcal{E}_n \). For the second term on the right-hand side of (S.5.55), we first note

\[
\sup_{(x, t) \in \mathcal{X} \times \mathcal{T}} \left| \tilde{\tau}(x, t) - E\{\tilde{\tau}(X, T) \mid X = x\} - \{\Psi(x, t) - \Gamma(x)\}^T \phi^* \right| \right|^2 \\
= O(K^{-2p/(d+1)}),
\]

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by Proposition 3 similar to (S.5.48). Then we have
\[
P\left[\left[(\Psi(X, T) - \Gamma(X))^T \phi^* - [\hat{\tau}(X, T) - E\{\hat{\tau}(X, T) \mid X\}]^T \epsilon_n^T \{\Gamma(X) - \hat{\Gamma}(X)\}\right]^2\right]
\leq \sup_{(x, t) \in \mathbb{X} \times T} \left[|\hat{\tau}(x, t) - E\{\hat{\tau}(X, T) \mid x\} - \{\Psi(x, t) - \Gamma(x)\}^T \phi^*|^2\right] \cdot P\left[\|\epsilon_n^T \{\Gamma(X) - \hat{\Gamma}(X)\}\|^2\right]
= O(K^{-2p/(d+1)} r^2 \gamma^2 e^2_n).
\]
For the third term on the right-hand side of (S.5.55), we note \(\|\hat{\tau}\|_{\mathbb{X} \times T} \lesssim 1\) as \(\hat{\tau}\) is in the Hölder class, and thus \(\|E(\hat{\tau} \mid \cdot)\|_{\mathbb{X}} \leq \sup_{x \in \mathbb{X}} E(\|\hat{\tau}\|_{\mathbb{X} \times T} \mid X = x) = \|\hat{\tau}\|_{\mathbb{X} \times T} \lesssim 1\). Then we have
\[
P\left[\|\hat{\tau}(X, T) - E\{\hat{\tau}(X, T) \mid X\}\|^2 \cdot P\left[\epsilon_n^T \{\Gamma(X) - \hat{\Gamma}(X)\}\right]^2\right]
\leq \left[2 \|\hat{\tau}\|^2_{\mathbb{X} \times T} + 2\|E\{\hat{\tau}(X, T) \mid X = \cdot\}\|^2\right] \cdot P\left[\epsilon_n^T \{\Gamma(X) - \hat{\Gamma}(X)\}\right]^2
\approx P\left[\epsilon_n^T \{\Gamma(X) - \hat{\Gamma}(X)\}\right]^2
= O(r^2 \gamma^2 e^2_n),
\]
similar to (S.5.56). In summary, we have
\[
P(\ell_n^T m_{i, 3})^2 = O(r^2 \gamma e^2_n).
\]
By taking \(v_i = \ell_n^T m_{i, 3}, \; d = 1, A_n = C_6 r^2 \gamma^2 e^2_n, \; J = c_6 r^{-1}\) in Proposition 9, we have
\[
\frac{\text{pr}_n\left(|\ell_n^T \Delta_{1, 3}| > c_6 r^{-1} \sqrt{n}\right)}{r^2 \gamma^2 e^2_n} \leq 4C_6 r^2 \gamma^2 e^2_n/c_6^2 \to 0.
\]
Thus similar to (S.5.54), we can directly uncondition \(E_n\) and conclude \(|\ell_n^T \Delta_{1, 3}| = o_P(r^{-1} \sqrt{n})\).

**Proof of Lemma 9 (iv)** We still condition on \(E_n\). We let \(m_{i, 4} = [m(X_i) - \hat{m}(X_i) - \{\Gamma(X_i) - \hat{\Gamma}(X_i)\}^T \phi^*] \{\Psi(X_i, T_i) - \Gamma(X_i)\}\), thus \(\Delta_{1, 4} = P_n(m_{i, 4})\). By the law of total expectation we have,
\[
P[m_{i, 4}]
= P\left[\{m(X) - \hat{m}(X) - \{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*\} \{\Psi(X, T) - \Gamma(X)\}\right]
= P\left[\{m(X) - \hat{m}(X) - \{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*\} P\{\Psi(X, T) - \Gamma(X) \mid X\}\right]
= 0.
\]
By the triangle inequality, we have
\[
P[|m_{i, 4}|^2]
\leq 2P\left[|m(X) - \hat{m}(X)|^2\|\Psi(X, T) - \Gamma(X)\|^2\right] + 2P\left[|\{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*|^2\|\Psi(X, T) - \Gamma(X)\|^2\right]
\leq 2\|\Psi - \Gamma\|^2_{\mathbb{X} \times T} \left[2\|m(X) - \hat{m}(X)\|^2 + \|\phi^*\|^2 P\left[\|\Gamma(X) - \hat{\Gamma}(X)\|^2 (\phi^*/\|\phi^*\|)^2\right]\right]
\leq 2\|\Psi - \Gamma\|^2_{\mathbb{X} \times T} \left\{2\|\hat{m} - m\|^2_{\ell^2_{\mathbb{X} \times T}} + \|\phi^*\|^2 P\left[\|\hat{\Gamma}(X) - \Gamma(X)\|^2 (\Gamma(X) - \hat{\Gamma}(X))^T\|_2\right]\right\}
= O(K r^2 \gamma^2 e^2_n + K r^2 \gamma^2 e^2_n),
\]
where the last equality follows by \( \mathcal{E}_n \). By taking \( v_i = \ell_n^T m_{i,4} \), \( d = K \), \( A_n = C_7(Kr_m^2e_n^2 + Kr_r^2e_n^2) \), \( J = c_7r_m + c_7r_\gamma \) in Proposition 9, for some sufficiently large yet fixed \( C_7 > 0 \) and any given \( c_7 > 0 \),

\[
\Pr_n \left\{ \| \Delta_{1,4} \| > c_7(r_m + r_\gamma)\sqrt{K/n} \right\} \\
\leq \frac{4C_7(Kr_m^2e_n^2 + Kr_r^2e_n^2)}{c_7^2(r_m + r_\gamma)^2K} \\
\lesssim c_7^2 \\
\rightarrow 0.
\]

which implies \( \| \Delta_{1,4} \| = o_P(r_m\sqrt{K/n} + r_\gamma\sqrt{K/n}) \) by directly unconditioning \( \mathcal{E}_n \), similar to (S.5.54).

On the other hand, similar to (S.5.57) one has \( P(\ell_n^T m_{i,4}) = 0 \). Also we have

\[
P(\ell_n^T m_{i,4})
= P\left[ \left( m(X) - \hat{m}(X) - \{ \Gamma(X) - \hat{\Gamma}(X) \}^T \phi^* \right)^T \left( \ell_n^T \Psi(X, T) - \ell_n^T \Gamma(X) \right) \right] \\
\leq 2 \left\| m - \hat{m} \right\|_2 + \left\| \{ \Gamma - \hat{\Gamma} \}^T \phi^* \right\|_2 \cdot P\left[ \ell_n^T \Psi(X, T) - \ell_n^T \Gamma(X) \right]^2 \\
\leq 4e_n^2 \| R_n \|_2 \\
= O(e_n^2),
\]

where the second inequality is due to \( \mathcal{E}_n \), and the last equality follows by Lemma 5 such that \( \| R_n \|_2 \lesssim 1 \). By taking \( v_i = \ell_n^T m_{i,4} \), \( d = 1 \), \( A_n = C_8e_n^2 \), and \( J = c_8 \) for some sufficiently large yet fixed \( C_8 > 0 \) and any given \( c_8 > 0 \), we then have

\[
\Pr_n \left( | \ell_n^T \Delta_{1,4} | > c_8 / \sqrt{n} \right) \leq \frac{4C_8e_n^2}{c_8^2} \rightarrow 0,
\]

which, after unconditioning \( \mathcal{E}_n \) similar to (S.5.54), we have \( | \ell_n^T \Delta_{1,4} | = o_P(1 / \sqrt{n}) \).

**Proof of Lemma 9 (v)** We still condition on \( \mathcal{E}_n \). Let \( m_{i,5} = [ m(X_i) - \hat{m}(X_i) - \{ \Gamma(X_i) - \hat{\Gamma}(X_i) \}^T \phi^* \} \{ \Gamma(X_i) - \hat{\Gamma}(X_i) \} \cdot X_i \). 
\( \hat{\Gamma}(X_i) \), and thus \( \Delta_{1,5} = P_n(m_{i,5}) \). First we have

\[
\|P(m_{i,5})\| = \sup_{\|\ell\|=1} \left| P \left[ (m(X) - \hat{m}(X) - \{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^* \right) \{\ell^T \Gamma(X) - \ell^T \hat{\Gamma}(X) \} \right] \\
\leq \sup_{\|\ell\|=1} \left| P \left[ \{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*/\|\phi^*\| \right) \{\ell^T \Gamma(X) - \ell^T \hat{\Gamma}(X) \} \right] \\
+ \|\phi^*\| \sup_{\|\ell\|=1} \left| P \left[ \{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*/\|\phi^*\| \right) \{\ell^T \Gamma(X) - \ell^T \hat{\Gamma}(X) \} \right] \\
\leq \|\hat{m} - m\|_{L_p^2} \|P[\{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*/\|\phi^*\| \right) \{\ell^T \Gamma(X) - \ell^T \hat{\Gamma}(X) \} \right] \|_2 \}
\]

where the second inequality follows by Cauchy–Schwarz inequality; the last equality follows by \( E_n \) and Proposition 3 such that \( \|\phi^*\| \lesssim 1 \). On the other hand,

\[
P(\|m_{i,5}\|^2) \\
\leq 2P \left[ \|m(X) - \hat{m}(X)\|^2 \|\Gamma(X) - \hat{\Gamma}(X)\|^2 \right] + 2P \left[ \|\{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*/\|\phi^*\| \right) \|\Gamma(X) - \hat{\Gamma}(X)\|^2 \right] \\
\leq 2\|\Gamma - \hat{\Gamma}\|_2^2 \cdot \left[ \|m - \hat{m}\|_{L_p^2}^2 + \|\phi^*\|^2 \right] \|P[\{\hat{\Gamma}_n(X) - \hat{\Gamma}_n(X)\} \{\Gamma(X) - \hat{\Gamma}(X)\}^T \right] \|_2 \}
\]

Then by taking \( v_i = m_{i,5}, d = K, A_n = C_9 e_n^4 K r_{\gamma}^2 r_m^2 + C_9 e_n^4 K r_{\gamma}^2 r_m^2 \) and \( J = c_9 (r_{\gamma}^2 r_m + r_{\gamma}^2 r_r) \) in Proposition 9, we have, for any fixed \( c_0 > 0 \) and some sufficiently large yet fixed \( C_9 > 0 \),

\[
\pr_n \left\{ \|\Delta_{1,5} - P(m_{i,5})\| > c_9 (r_{\gamma}^2 r_m + r_{\gamma}^2 r_r) \sqrt{K/n} \right\} \leq \frac{4C_9 e_n^4 K r_{\gamma}^2 r_m^2 + 4C_9 e_n^4 K r_{\gamma}^2 r_m^2}{c_0^2 (r_{\gamma}^2 r_m + r_{\gamma}^2 r_r)^2 K} \\
\lesssim e_n^4 \to 0.
\]

Thus under \( E_n \), we have

\[
\|\Delta_{1,5}\| \leq \|P(m_{i,5})\| + \|\Delta_{1,5} - P(m_{i,5})\| \\
= o_P (r_m r_{\gamma} + r_{\gamma}^2 + r_{\gamma}^2 r_m \sqrt{K/n} + r_{\gamma}^2 r_{\gamma} \sqrt{K/n}).
\]

Similar to (S.5.54), we can uncondition \( E_n \), and the same bound of \( \|\Delta_{1,5}\| \) still holds.
On the other hand, by (S.5.58) we further have

\[
|P(\ell_n^T m_{i,5})| \leq \sup_{\|P\|=1} |P(\ell^T m_{i,5})| \\
= \|P(m_{i,5})\| \\
= O(e_n^2r_mr_\gamma + e_n^2r_\gamma^2) \\
= o(r_mr_\gamma + r_\gamma^2).
\]

In addition, under \( E_n \), we have

\[
P(\ell_n^T m_{i,5})^2 = P\left[|m(X) - \hat{m}(X) - \{\Gamma(X) - \hat{\Gamma}(X)\}^T \phi^*|^2|\ell_n^T \Gamma(X) - \ell_n^T \hat{\Gamma}(X)\}^2\right] \\
\leq 2\left\{\|m - \hat{m}\|_2^2 + \|\Gamma - \hat{\Gamma}\|_2^2\right\} \cdot P\left\{\|\ell_n^T \Gamma(X) - \ell_n^T \hat{\Gamma}(X)\|_2^2\right\} \\
\leq e_n^2\|\Gamma - \hat{\Gamma}\|_2^2 \cdot P\left\{\|\ell_n^T \Gamma(X) - \ell_n^T \hat{\Gamma}(X)\|_2^2\right\} \\
= O(e_n^2r_\gamma^2).
\]

Then by taking \( v = \ell_n^T m_{i,5}, d = 1, A_n = C_{10}e_n^2r_\gamma^2 \), and \( J = c_{10} \) in Proposition 9, we have, for any fixed \( c_{10} > 0 \) and some sufficiently large yet fixed \( C_{10} > 0 \),

\[
\text{pr}_n\left\{|\ell_n^T \Delta_{1,5} - P(\ell_n^T m_{i,5})| > c_{10}r_\gamma/\sqrt{n}\right\} \leq \frac{4C_{10}e_n^2r_\gamma^2}{c_{10}^2r_\gamma^2} \to 0.
\]

Thus under \( E_n \), \(|\ell_n^T \Delta_{1,5}| \leq |\ell_n^T \Delta_{1,5} - P(\ell_n^T m_{i,5})| + |P(\ell_n^T m_{i,5})| = o_P(r_\gamma/\sqrt{n} + r_mr_\gamma + r_\gamma^2) \). Similar to (S.5.54), we can then uncondition \( E_n \), and the same bound of \(|\ell_n^T \Delta_{1,5}| \) still holds. \( \square \)

### S.5.4 Proof of Proposition 1

**Proof of Proposition 1 (i)** We first consider a more general minimization problem,

\[
q = \arg\min_{h \in \mathcal{L}_b^c(Y \mid X)} E\left\{Y - m(X) - h(X, T)\right\}^2 \\
= \arg\min_{h \in \mathcal{L}_b^c(Y \mid X)} E\left\{Y - E(Y \mid X) - h(X, T)\right\}^2.
\]

(T5.59)

Treat \( Y - E(Y \mid X) \) as a random variable. Then based on the least-square form of (S.5.59), we know (S.5.59) is minimized, if and only if \( q(X, T) \) is the conditional mean of \( Y - E(Y \mid X) \) given \( X \) and \( T \) a.s., or equivalently,

\[
q(X, T) = E\{Y - E(Y \mid X) \mid X, T\} \text{ a.s.}
\]

(S.5.60)

We show the above statement by contradiction. Suppose \( q(X, T) \) is not a.s. \( E\{Y - E(Y \mid X) \mid X, T\} \). Then we have

\[
q(X, T) = E\{Y - E(Y \mid X) \mid X, T\} + u(X, T) \text{ a.s.,}
\]

(S.5.61)
for some \( u(X, T) \neq 0 \) with probability larger than 0. We then have

\[
E\left\{ Y - E(Y \mid X) - q(X, T) \right\}^2
\]

\[
= E\left[ Y - E(Y \mid X) - E\{Y - E(Y \mid X) \mid X, T\} - u(X, T) \right]^2
\]

\[
= E\left[ Y - E(Y \mid X) - E\{Y - E(Y \mid X) \mid X, T\} \right]^2
\]

\[
- 2E\left[ Y - E(Y \mid X) - E\{Y - E(Y \mid X) \mid X, T\} \right]u(X, T) + E\{u^2(X, T)\}
\]

\[
= E\left[ Y - E(Y \mid X) - E\{Y - E(Y \mid X) \mid X, T\} \right]^2 + E\{u^2(X, T)\}
\]

\[
> E\left[ Y - E(Y \mid X) - E\{Y - E(Y \mid X) \mid X, T\} \right]^2,
\]

where by the law of total expectation,

\[
E\left[ Y - E(Y \mid X) - E\{Y - E(Y \mid X) \mid X, T\} \right]u(X, T)
\]

\[
= E\left[ E\left[ Y - E(Y \mid X) - E\{Y - E(Y \mid X) \mid X, T\} \right] \mid X, T \right]u(X, T)
\]

\[
= E\{0 \cdot u(X, T)\}
\]

\[= 0.\]

Thus (S.5.62) implies that \( q(X, T) \) satisfies (S.5.59) if and only if (S.5.60) holds. We then have

\[
q(X, T) = E\{Y - E(Y \mid X) \mid X, T\}
\]

\[
= E(Y \mid X, T) - E(Y \mid X)
\]

\[
= E(Y \mid X, T) - E\{E(Y \mid X, T) \mid X\}
\]

\[
= \tau(X, T) - E\{\tau(X, T) \mid X\}, \text{ a.s.}
\]

The last equality follows by \( \tau(X, T) = E(Y \mid X, T) - E(Y \mid X, T = 0) \) under Assumptions 1 and 2. Since \( \tau \in L_p^2(X, T) \), it is easy to verify that \( q \) is also in \( L_p^2(X, T) \) based on (S.5.63) and the Cauchy-Schwarz inequality,

\[
E[\tau(X, T) - E\{\tau(X, T) \mid X\}]^2 \leq 2E[\tau^2(X, T)] + 2E[E\{\tau(X, T) \mid X\}]^2
\]

\[
\leq 2E[\tau^2(X, T)] + 2E[E\{\tau^2(X, T) \mid X\}]
\]

\[
= 4E[\tau^2(X, T)]
\]

\[< +\infty.\]

Comparing (S.5.59) and (2.8), if \( h \in L_p^2(X, T) \) is a minimum of \( L_c(h), h(X, T) - E\{h(X, T) \mid X\} \) must minimize the general problem in (S.5.59), i.e.,

\[
h(X, T) - E\{h(X, T) \mid X\} = q(X, T)
\]

\[
= \tau(X, T) - E\{\tau(X, T) \mid X\}, \text{ a.s.}
\]

which is equivalent to

\[
h(X, T) = \tau(X, T) + E\{h(X, T) \mid X\} - E\{\tau(X, T) \mid X\} \text{ a.s.} \quad (S.5.64)
\]
by (S.5.63). Thus any $h \in \mathcal{L}^2_p(X, T)$ minimizing (2.8) must satisfy

$$h(X, T) = \tau(X, T) + s(X) \text{ a.s.,}$$

for some $s \in \mathcal{L}^2_p(X)$ such that $s(x) = E\{h(X, T) \mid X = x\} - E\{\tau(X, T) \mid X = x\}$.

On the other hand, for arbitrary $s \in \mathcal{L}^2_p(X)$, if $h(X, T) = \tau(X, T) + s(X)$ a.s, $h$ must satisfy

$$h(X, T) - E\{h(X, T) \mid X\} = \tau(X, T) - E\{\tau(X, T) \mid X\} = q(X, T), \text{ a.s.,}$$

recalling $q$ is the solution of the general minimization problem (S.5.59). It is also easy to see that $h \in \mathcal{L}^2_p(X, T)$ as both $s$ and $\tau$ have bounded $\mathcal{L}^2_p$ norms. Therefore, $h$ is a minimum of $L_c(h)$.

Summarizing the above results, we conclude that the solution set in $\mathcal{L}^2_p(X, T)$ that minimizes $L_c(h)$ is exactly $\mathcal{S} = \{h \mid h(X, T) = \tau(X, T) + s(X) \text{ a.s.}, \text{for any } s(x) \in \mathcal{L}^2_p(X)\}$.

**Formal proof of Proposition 1 (ii)** Before heading to the formal proof of Proposition 1 (ii), we first give an explanation about how (2.5) narrows $\mathcal{S}$ to $\mathcal{S}^2$. This explanation also gives some intuitions for the formal proof.

Notice that any other solution $h$ in $\mathcal{S}$ but not in $\mathcal{S}^2$, satisfies that $h(X, T) = \tau(X, T) + s(X)$ a.s., with some $s(X)$ that is not a.s. zero, i.e., $\text{pr}\{\Omega = \{X \text{ satisfies } s(X) \neq 0\}\} > 0$. Therefore, under the positivity assumption such that $\text{pr}(T = 0 \mid X = x) > \epsilon'$ for some fixed $\epsilon' > 0$ and any $x \in \mathbb{X}$, we have

$$\text{pr}\{h(X, 0) = \tau(X, 0) + s(X) = s(X) \neq 0\} \geq \text{pr}\{(T = 0) \cap \Omega\} = \text{pr}(T = 0 \mid \Omega)\text{pr}(\Omega) \geq \epsilon' \cdot \text{pr}(\Omega) > 0,$$

(S.5.65)

which is in conflict with (2.5) such that $h(X, 0) = 0$ with probability 1.

**Formal proof of Proposition 1 (ii)** Write the optimization problem (2.9) for the binary treatment as

$$\arg \min_{h \in \{h \mid h(\cdot, 1) \in \mathcal{L}^2_p(X) \text{ and } h(X, 0) = 0 \text{ a.s.}\}} E[Y - m(X) - \{T - e(X)\}h(X, 1)]^2.$$  

(S.5.66)

Since the objective function above only involves $h(\cdot, 1)$, we consider a simplified problem

$$\arg \min_{h' \in \mathcal{L}^2_p(X)} E[Y - m(X) - \{T - e(X)\}h'(X)]^2.$$  

(S.5.67)

Let $\mathcal{S}'$ be the solution set of (S.5.67), and let $\tilde{\mathcal{S}}^2$ be the solution set of (2.9) and thus is also the solution set of (S.5.66). In the following, we show

$$\tilde{\mathcal{S}}^2 = \{h \mid h(X, T) = \tau(X, T) \text{ a.s.}\} = \mathcal{S}^2$$

(S.5.68)

and thus finish the proof.

Comparing (S.5.66) and (S.5.67), we have that any $h$ being a solution of (S.5.66) must satisfy

$$h(X, 1) = h'(X) \text{ a.s..}$$

On the other hand, by the constraint of (S.5.66), we also have $h(X, 0) = 0$ a.s., when $h \in \tilde{\mathcal{S}}^2$. Therefore we have

$$\tilde{\mathcal{S}}^2 \subseteq \mathcal{S}^2 = \{h \mid h(X, 1) = h'(X) \text{ a.s. for any } h' \in \mathcal{S}', \text{ and } h(X, 0) = 0 \text{ a.s.}\}. $$

(S.5.69)
It is also easy to check that if \( h \in S^2 \), \( h(\cdot, 1) \) must minimize the objective function in \((S.5.66)\). Meanwhile, if \( h \in S'^2 \), we also have \( h(\cdot, 1) \in L^2_T(X) \) as \( h' \in L^2_T(X) \) and \( h(X, 0) = 0 \) a.s., thus \( h \) satisfies all the constraints and is a solution of \((S.5.66)\). So \( S'^2 \subseteq \hat{S}^2 \), and by \((S.5.69)\), we have
\[
\hat{S}^2 = S'^2 = \{ h \mid h(X, 1) = h'(X) \text{ a.s. for any } h' \in S', \text{ and } h(X, 0) = 0 \text{ a.s.} \}.
\]

For simplicity, we denote \( \tau(x) = \tau(x, 1) \). Therefore, we have \( \tau(\cdot) \in L^2_T(X) \) as \( \tau(\cdot, 1) \in L^2_T(X) \). We first prove that,
\[
S' = \{ h' \mid h'(X) = \tau(X) \text{ a.s.} \}.
\]

Any \( h' \in L^2_T(X) \) can be written as \( h'(x) = \tau(x) + s'(x) \), where \( s'(x) = \tau(x) - h'(x) \in L^2_T(X) \) since both \( h'(x) \) and \( \tau(x) \) are in \( L^2_T(X) \). Then solving \((S.5.67)\) is equivalent to solving
\[
\arg \min_{s' \in L^2_T(X)} E\left[ Y - m(X) - \{ T - e(X) \} \{ s'(X) + \tau(X) \} \right]^2.
\]

The above square loss function can be decomposed into
\[
E\left[ Y - m(X) - \{ T - e(X) \} \{ s'(X) + \tau(X) \} \right]^2
= E\left[ \left( Y - m(X) - \{ T - e(X) \} \tau(X) \right) - \{ T - e(X) \} s'(X) \right]^2
= E\left[ Y - m(X) - \{ T - e(X) \} \tau(X) \right]^2
- 2E\left[ \left( Y - m(X) - \{ T - e(X) \} \tau(X) \right) \{ T - e(X) \} s'(X) \right]
+ E\left[ \{ T - e(X) \} s'(X) \right]^2.
\]

For the second term on the right-hand side of \((S.5.73)\),
\[
E\left[ \left( Y - m(X) - \{ T - e(X) \} \tau(X) \right) \{ T - e(X) \} s'(X) \right]
= E\left[ E\left[ Y - m(X) - \{ T - e(X) \} \tau(X) \mid X, T \right] \{ T - e(X) \} s'(X) \right]
= E\left[ 0 \cdot \{ T - e(X) \} s'(X) \right]
= 0,
\]
where the first equality follows by the law of total expectation, and the second inequality follows by
\[
E\left[ Y - m(X) - \{ T - e(X) \} \tau(X) \mid X, T \right]
= \mu(X, T) - m(X) - \{ T - e(X) \} \tau(X)
= E(Y \mid X, T) - E(Y \mid X) - \{ T - \text{pr}(T = 1 \mid X) \} \left\{ E(Y \mid X, T = 1) - E(Y \mid X, T = 0) \right\}
= E(Y \mid X, T) - \{ \text{pr}(T = 1 \mid X) E(Y \mid X, T = 1) + \text{pr}(T = 0 \mid X) E(Y \mid X, T = 0) \}
- \{ T - \text{pr}(T = 1 \mid X) \} \left\{ E(Y \mid X, T = 1) - E(Y \mid X, T = 0) \right\}
= TE(Y \mid X, T = 1) + (1 - T)E(Y \mid X, T = 0)
- \text{pr}(T = 1 \mid X) E(Y \mid X, T = 1) - (1 - \text{pr}(T = 1 \mid X)) E(Y \mid X, T = 0)
- \{ T - \text{pr}(T = 1 \mid X) \} \left\{ E(Y \mid X, T = 1) - E(Y \mid X, T = 0) \right\}
= TE(Y \mid X, T = 1) - TE(Y \mid X, T = 0)
- \text{pr}(T = 1 \mid X) E(Y \mid X, T = 1) + \text{pr}(T = 1 \mid X) E(Y \mid X, T = 0)
- \{ T - \text{pr}(T = 1 \mid X) \} \left\{ E(Y \mid X, T = 1) - E(Y \mid X, T = 0) \right\}
= 0,
\]

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For the third term on the right-hand side of (S.5.73), if \( s(X) \) is not 0 a.s.,

\[
E\left[\{T - e(X)\}^2 \{s'(X)\}^2\right] \\
= E\left[E\left[\{T - e(X)\}^2 \ | \ X\right] \{s'(X)\}^2\right] \\
> (\epsilon')^3 E\{s'(X)\}^2 \\
> 0,
\]

where the first equality follows by the law of total expectation, the first inequality follows by that \( h \) only if \( s'(X) \) is solved if and only if \( (S.5.72) \) is solved if and only if \( e(x) \in (\epsilon', 1 - \epsilon') \), and the last inequality is because \( E\{s'(X)\}^2 > 0 \) when \( s'(X) \) is not 0 a.s..

Summarizing the above results, when \( s'(X) \) is not 0 a.s., we have

\[
E\left[Y - m(X) - \{T - e(X)\} \{s'(X) + \tau(X)\}\right]^2 \\
= E\left[Y - m(X) - \{T - e(X)\}\tau(X)\right]^2 \\
+ E\left[\{T - e(X)\} s'(X)\right]^2 \\
> E\left[Y - m(X) - \{T - e(X)\}\tau(X)\right]^2.
\]

That is, \( (S.5.72) \) is solved if and only if \( s'(X) = 0 \) a.s., which is equivalent to that \( (S.5.67) \) is solved if and only if \( h'(x) \) satisfies that \( h'(X) = \tau(X) \) a.s.. Thus \( (S.5.71) \) is verified as desired. Combining \( (S.5.70) \) and \( (S.5.71) \), we have

\[ \hat{S}^2 = \{h \mid h(X, 1) = \tau(X, 1) \text{ a.s.}, \text{ and } h(X, 0) = 0 \text{ a.s.}\}. \]

Now we aim at showing that, under the positivity assumption,

\[
\{h \mid h(X, 1) = \tau(X, 1) \text{ a.s.}, \text{ and } h(X, 0) = 0 \text{ a.s.}\} = \{h \mid h(X, T) = \tau(X, T) \text{ a.s.}\}, \quad (S.5.74)
\]

and thus show \( (S.5.68) \) and finish the proof. First suppose \( h \in \{h \mid h(X, 1) = \tau(X, 1) \text{ a.s.}, \text{ and } h(X, 0) = 0 \text{ a.s.}\} \). Then we have two subsets of \( \mathbb{X} \), \( \mathcal{X}_1, \mathcal{X}_2 \subseteq \mathbb{X} \) such that \( h(x, 1) = \tau(x, 1) \) when \( x \in \mathcal{X}_1 \), \( h(x, 0) = 0 \) when \( x \in \mathcal{X}_0 \), and \( \text{pr}(X \in \mathcal{X}_1) = \text{pr}(X \in \mathcal{X}_2) = 1 \). Thus we have when \( (x, t) \in \mathcal{X}_1 \cap \mathcal{X}_2 \times \{0, 1\} \),

\[
h(x, t) = \tau(x, t).
\]

On the other hand, since \( \text{pr}\{(X, T) \in \mathcal{X}_1 \cap \mathcal{X}_2 \times \{0, 1\}\} = \text{pr}(X \in \mathcal{X}_1 \cap \mathcal{X}_2) = 1 \), we have \( h(X, T) = \tau(X, T) \) a.s., which implies

\[
\{h \mid h(X, 1) = \tau(X, 1) \text{ a.s.}, \text{ and } h(X, 0) = 0 \text{ a.s.}\} \subseteq \{h \mid h(X, T) = \tau(X, T) \text{ a.s.}\}.
\]

Second, suppose \( h \in \{h \mid h(X, T) = \tau(X, T) \text{ a.s.}\} \). Then there exists some \( \Omega_1 \in \mathbb{X} \times \mathbb{T} \) such that \( \text{pr}\{(X, T) \in \Omega_1\} = 1 \), and when \( (x, t) \in \Omega_1 \) one has \( h(x, t) = \tau(x, t) \) and \( h(x, t) = \tau(x, t) \) otherwise. We now define two marginal sets,

\[
\mathcal{X}_3^{(0)} = \{x \mid (x, 0) \in \Omega_1\}, \text{ and } \mathcal{X}_3^{(1)} = \{x \mid (x, 1) \in \Omega_1\}.
\]
Now we prove \( \Pr(X \in \mathcal{A}_3^{(0)}) = \Pr(X \in \mathcal{A}_3^{(1)}) = 1 \) by contradiction. Assume \( \Pr(X \in \mathcal{A}_3^{(0)}) < 1 \). We have

\[
\begin{align*}
\Pr[(X, T) \in (\mathbb{X} \setminus \mathcal{A}_3^{(0)}) \times \{0\}] &= \Pr(X \in \mathbb{X} \setminus \mathcal{A}_3^{(0)}) \Pr(T = 0 \mid \text{given } X \in \mathbb{X} \setminus \mathcal{A}_3^{(0)}) \\
&\geq \{1 - \Pr(X \in \mathcal{A}_3^{(0)})\} \cdot \epsilon' \\
&> 0.
\end{align*}
\]

By definition, we know \( (\mathbb{X} \setminus \mathcal{A}_3^{(0)}) \times \{0\} \cap \Omega_1 = \emptyset \). Thus (S.5.76) implies that with probability larger than 0, we have \((X, T) \in (\mathbb{X} \times \mathbb{T}) \setminus \Omega_1\), which is in conflict with \( \Pr\{(X, T) \in \Omega_1\} = 1 \). So we conclude \( \Pr(X \in \mathcal{A}_3^{(0)}) = 1 \). Recall that when \( x \in \mathcal{A}_3^{(0)} \), we have \((x, 0) \in \Omega_1\) and thus \( h(x, 0) = \tau(x, 0) = 0 \). We then have

\[h(X, 0) = 0 \text{ a.s.}\]

With the same argument, we can show \( \Pr(X \in \mathcal{A}_3^{(1)}) = 1 \) and thus \( h(X, 1) = \tau(X, 1) \text{ a.s.} \). So we have \( h \in \{h \mid h(X, 1) = \tau(X, 1) \text{ a.s.}, \text{ and } h(X, 0) = 0 \text{ a.s.}\} \) and thus

\[\{h \mid h(X, T) = \tau(X, T) \text{ a.s.}\} \subseteq \{h \mid h(X, 1) = \tau(X, 1) \text{ a.s.}, \text{ and } h(X, 0) = 0 \text{ a.s.}\}.\]

Combining (S.5.75) and (S.5.77), we thus show (S.5.74) and (S.5.68) and thereby complete the proof. \( \square \)

### S.5.5 Proof of Theorem 1

With a basic decomposition, one has

\[
\begin{align*}
L_c(h) &= E[\tau(X, T) - E{\tau(X, T) \mid X} - h(X, T) - E{h(X, T) \mid X}]^2 \\
&\quad + E[Y - m(X) - \tau(X, T) - E{\tau(X, T) \mid X}]^2 \\
&\quad + 2E\left[(\tau(X, T) - E{\tau(X, T) \mid X} - h(X, T) - E{h(X, T) \mid X})\right]\left[Y - m(X) - \tau(X, T) - E{\tau(X, T) \mid X}\right].
\end{align*}
\]

Under Assumptions 1 and 2 and by the law of total expectation, one has

\[
\begin{align*}
E\{Y - m(X) \mid X, T\} &= E(Y \mid X, T) - E(Y \mid X, T = 0) - E(Y \mid X) - E(Y \mid X, T = 0) \\
&= \tau(X, T) - \{E\{E(Y \mid X, T) \mid X\} - E(Y \mid X, T = 0)\} \\
&= \tau(X, T) - E\{E(Y \mid X, T) - E(Y \mid X, T = 0) \mid X\} \\
&= \tau(X, T) - E\{\tau(X, T) \mid X\},
\end{align*}
\]

and therefore,

\[
\begin{align*}
E\left[(\tau(X, T) - E{\tau(X, T) \mid X} - h(X, T) - E{h(X, T) \mid X})\right]\left[Y - m(X) - \tau(X, T) - E{\tau(X, T) \mid X}\right]
&= E\left[(\tau(X, T) - E{\tau(X, T) \mid X} - h(X, T) - E{h(X, T) \mid X})\right] \\
&\cdot E\left[Y - m(X) - \tau(X, T) - E{\tau(X, T) \mid X} \mid X, T\right] \\
&= E\left[(\tau(X, T) - E{\tau(X, T) \mid X} - h(X, T) - E{h(X, T) \mid X})\right] \\
&\cdot \left[E\{Y - m(X) \mid X, T\} - \tau(X, T) - E{\tau(X, T) \mid X}\right]
&= 0.
\end{align*}
\]

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Combining (S.5.78) with the above display, one has
\[
L_c(h) = E\left[\tau(X, T) - E\{\tau(X, T) \mid X\} - [h(X, T) - E\{h(X, T) \mid X\}]^2 + E[Y - m(X) - [\tau(X, T) - E\{\tau(X, T) \mid X\}]^2 \right].
\]
For simplicity, we define an operator \( \Pi(\cdot) \) for any \( h \in \mathcal{L}_p^2(X, T) \) such that
\[
\Pi(h)(x, t) = h(x, t) - E\{h(X, T) \mid X = x\}.
\]
Therefore, we have,
\[
L_{c,\ell_2}(h \mid \rho) = L_c(h) + \rho\|h\|^2_{\mathcal{L}_p^2} = E\left[\tau(X, T) - E\{\tau(X, T) \mid X\} - [h(X, T) - E\{h(X, T) \mid X\}]^2 + E[Y - m(X) - [\tau(X, T) - E\{\tau(X, T) \mid X\}]^2 + \rho\|h\|^2_{\mathcal{L}_p^2} \right].
\]
which implies that \( \arg\min_{h \in \mathcal{L}_p^2(X, T)} L_{c,\ell_2}(h \mid \rho) \) is equivalent to
\[
\arg\min_{h \in \mathcal{L}_p^2(X, T)} E\left[\Pi(h)(X, T) - [\tau(X, T) - E\{\tau(X, T) \mid X\}]^2 + \rho\|h\|^2_{\mathcal{L}_p^2} \right] = \arg\min_{h \in \mathcal{L}_p^2(X, T)} \mathcal{F}(h),
\]
where we define \( \mathcal{F}(h) = E\left[\Pi(h)(X, T) - \tau(X, T)\right]^2 + \rho E\left\{h(X, T)\right\}^2 \) and \( \tau(x, t) = \tau(x, t) - E\{\tau(X, T) \mid X = x\} \).

Next, we prove \( L_{c,\ell_2}(h \mid \rho) \) has a unique minimum among \( \mathcal{L}_p^2(X, T) \). By above derivations, we only need to show the minimum of (S.5.79) is unique. An argument similar to the proof of Lemma 1.1 in Tikhonov et al. (1995) can shows that \( \mathcal{F}(h) \) has a unique solution. In particular, we first show \( \Pi(\cdot) \) is a self-adjoint operator; see, e.g., Rudin (1991, §12.11) for the definition of a self-adjoint operator. For any \( h_1, h_2 \in \mathcal{L}_p^2(X, T) \), we have
\[
\langle \Pi(h_1), h_2 \rangle_{\mathcal{L}_p^2(X, T)} = E\left[\Pi(h_1)(X, T)h_2(X, T)\right] = E\left[\left[h_1(X, T) - E\{h_1(X, T) \mid X\}\right]h_2(X, T)\right] = E\left[h_1(X, T)h_2(X, T)\right] - E\left[E\{h_1(X, T) \mid X\}h_2(X, T)\right] = E\left[h_1(X, T)h_2(X, T)\right] - E\left[E\{h_1(X, T) \mid X\}E\{h_2(X, T) \mid X\}\right],
\]
where \( \langle \cdot, \cdot \rangle_{\mathcal{L}_p^2(X, T)} \) denotes the inner product of the Hilbert space \( \mathcal{L}_p^2(X, T) \), and the last equality follows by the law of total expectation. By symmetry, we can also show
\[
\langle h_1, \Pi(h_2) \rangle_{\mathcal{L}_p^2(X, T)} = E\left[h_1(X, T)h_2(X, T)\right] - E\left[E\{h_1(X, T) \mid X\}E\{h_2(X, T) \mid X\}\right] = \langle \Pi(h_1), h_2 \rangle_{\mathcal{L}_p^2(X, T)}.
\]
which by definition (e.g., Rudin, 1991, §12.11), implies that $\Pi(\cdot)$ is a self-adjoint operator from $L^2_P(X, T)$ to $L^2_P(X, T)$, i.e. the adjoint operator of $\Pi(\cdot)$ is still $\Pi(\cdot)$. Then, similar to the proof of Lemma 1.1 in Tikhonov et al. (1995), we can denote the second-order Fréchet derivative of $F(h)$ by $D^2F(h)$ and have that

$$D^2F(h) = 2\Pi\{\Pi(h)\} + 2\rho h$$

$$= 2\Pi(h) + 2\rho h$$

$$= 2h - 2E\{h(X, T) \mid X = \cdot\} + 2\rho h,$$

where the second equality follows by the law of expectation, the first inequality follows by Cauchy-Schwarz inequality. (S.5.80) implies that $F(h)$ is a strictly convex functional, and thus $F(h)$ has a unique minimum among $L^2_P(X, T)$; see, e.g., Zeidler (2013). Thus (2.12) has a unique solution, namely, $\tau_\rho$ in $L^2_P(X, T)$.

Now, we show that when $\rho \to 0$, one has $\|\tau_\rho - \tilde{\tau}\|_{L^2_P} \to 0$. Note $\tilde{\tau} \in L^2_P(X, T)$ as both $\tau$ and $E\{\tau(X,T) \mid X = \cdot\}$ have bounded $L^2_P$ norms. In particular, $\tilde{\tau} \in L^2_P(X, T)$ by definition and,

$$E\{E\{\tau(X,T) \mid X\}^2\} \leq E\{E\{\tau^2(X,T) \mid X\}\}$$

$$= E\{\tau^2(X,T)\}$$

$$< +\infty,$$

by Cauchy-Schwarz inequality. Since $\tau_\rho(X, T)$ minimizes $F(h)$, we have

$$\|\Pi(\tau_\rho) - [\tau(x, t) - E\{\tau(X,T) \mid X = \cdot\}]\|_{L^2_P}^2 + \rho\|\tau_\rho\|_{L^2_P}^2$$

$$\leq \|\Pi(\tilde{\tau}) - [\tau(x, t) - E\{\tau(X,T) \mid X = \cdot\}]\|_{L^2_P}^2 + \rho\|\tilde{\tau}\|_{L^2_P}^2$$

(S.5.81)

by noticing that $\Pi(\tilde{\tau})(x, t) = \tau(x, t) - E\{\tau(X,T) \mid X = x\} - [E\{\tau(X,T) \mid X = x\} - E\{\tau(X, T) \mid X = x\}] = \tau(x, t) - E\{\tau(X,T) \mid X = x\}$. Because $\|\Pi(\tilde{\tau}) - [\tau(x, t) - E\{\tau(X,T) \mid X = \cdot\}]\|_{L^2_P}^2 > 0$, we have

$$\rho\|\tau_\rho\|_{L^2_P}^2 \leq \rho\|\tilde{\tau}\|_{L^2_P}^2,$$

which is equivalent to

$$E\{\tau_\rho(X, T)^2\}$$

$$\leq E\{\tilde{\tau}(X, T)^2\} + E\{\tilde{\tau}(X, T) - \tau_\rho(X, T)^2\} + 2E\{\tilde{\tau}(X, T) - \tau_\rho(X, T)\}\tau_\rho(X, T)$$

$$= E\{\tau_\rho(X, T)^2\} + E\{\tilde{\tau}(X, T) - \tau_\rho(X, T)^2\} + 2E\{\tilde{\tau}(X, T) - \tau_\rho(X, T)\}\{\tau_\rho(X, T) - \tilde{\tau}(X, T) + \tilde{\tau}(X, T)\}$$

$$= E\{\tilde{\tau}(X, T)^2\} - E\{\tilde{\tau}(X, T) - \tau_\rho(X, T)^2\} + 2E\{\tilde{\tau}(X, T) - \tau_\rho(X, T)\}\tilde{\tau}(X, T).$$
With simple algebra, we then deduce

\[
E\{\tilde{\tau}(X,T) - \tau_\rho(X,T)\}^2 \leq 2E\left[\{\tilde{\tau}(X,T) - \tau_\rho(X,T)\}\tilde{\tau}(X,T)\right] \\
= 2E\left[\tilde{\tau}(X,T) - \tau_\rho(X,T) + E\{\tau_\rho(X,T) \mid X\}\tilde{\tau}(X,T)\right] \\
\leq 2\|\tilde{\tau}\|_{L^2_p}[E[\tilde{\tau}(X,T) - \tau_\rho(X,T) + E\{\tau_\rho(X,T) \mid X\}]^2]^{1/2} \quad \text{(S.5.82)} \\
= 2\|\tilde{\tau}\|_{L^2_p}\|\Pi(\tau_\rho) - [\tau(x,t) - E\{\tau(X,T) \mid X = \cdot\}]\|_{L^2_p},
\]

where the first equality follows by the law of total expectation such that

\[
E[\{\tau_\rho(X,T) \mid X\}\tilde{\tau}(X,T)] = E\left[\tau_\rho(X,T) \mid X\right]E[\tilde{\tau}(X,T) - E\{\tau(X,T) \mid X\} \mid X] = 0,
\]

and the second inequality follows by Cauchy-Schwarz inequality. Finally, by \(\|\tilde{\tau}\|_{L^2_p} \leq 1\) as we alluded earlier and \(S.5.81\), we conclude

\[
\|\Pi(\tau_\rho) - [\tau(x,t) - E\{\tau(X,T) \mid X = \cdot\}]\|^2_{L^2_p} \leq \rho\|\tilde{\tau}\|^2_{L^2_p} = O(\rho).
\]

Combining with \(S.5.82\) yields

\[
\|\tau_\rho - \tilde{\tau}\|_{L^2_p} = O(\rho^{1/4}) = o(1),
\]

when \(\rho \to 0\), and thus \(\tau_\rho \to \tilde{\tau}\) under the \(L^2_p\) norm.

Finally we show (2.11). Under Assumptions 1 and 2, one has \(\tau(x,t) = E(Y \mid X = x, T = t) - E(Y \mid X = x, T = 0)\) and thus,

\[
\tilde{\tau}(x,t) = E(Y \mid X = x, T = t) - E(Y \mid X = x, T = 0) \\
- E\{E(Y \mid X = x, T) - E(Y \mid X = x, T = 0) \mid X = x\} \\
= E(Y \mid X = x, T = t) - E(Y \mid X = x).
\]

Then we have

\[
\tilde{\tau}(x,t) - \tilde{\tau}(x,0) \\
= E(Y \mid X = x, T = t) - E(Y \mid X = x) - E(Y \mid X = x, T = 0) + E(Y \mid X = x) \\
= E(Y \mid X = x, T = t) - E(Y \mid X = x, T = 0) \\
= \tau(x,t).
\]

\[\square\]

**S.5.6 Proof of Proposition 2**

First we note that when estimating \(\hat{\Gamma}(x)\) through \(\hat{\Gamma}(x) = E_{\Theta}\{\Psi(X,T) \mid X = x\}\), we have

\[
\hat{\Gamma}(x) = E_{\Theta}\{\psi(T) \otimes \Psi(X) \mid X = x\} \\
= E_{\Theta}\{\psi(T) \mid X = x\} \otimes \Psi(x),
\]
where we denote $\Psi(x) = \psi(x^{(1)}) \otimes \cdots \otimes \psi(x^{(d)})$. Correspondingly, $\Gamma(x) = E_{\omega} \{ \psi(T) \mid X = x \} \otimes \Psi(x)$ and thus
\[
\hat{\Gamma}(x) - \Gamma(x) = [E_{\omega} \{ \psi(T) \mid X = x \} - E_{\omega} \{ \psi(T) \mid X = x \}] \otimes \Psi(x)
\]
\[
= \left[ \int_{T} \psi(t) \{ \hat{\omega}(t \mid x) - \omega(t \mid x) \} dt \right] \otimes \Psi(x)
\]
\[
= \int_{T} [\psi(t) \otimes \Psi(x)] \{ \hat{\omega}(t \mid x) - \omega(t \mid x) \} dt
\]
\[
= \int_{T} \Psi(x,t) \{ \hat{\omega}(t \mid x) - \omega(t \mid x) \} dt.
\]
On the other hand,
\[
\sup_{x \in \mathcal{X}} \int_{T} \{ \hat{\omega}(t \mid x) - \omega(t \mid x) \}^2 dt = \sup_{x \in \mathcal{X}} \| \hat{\omega}(\cdot \mid x) - \omega(\cdot \mid x) \|_{L^2}^2
\]
\[
= o_P(r_\omega^2).
\]
First we have,
\[
\| P[\{ \hat{\Gamma}(X) - \Gamma(X) \} \{ \hat{\Gamma}(X) - \Gamma(X) \}^T] \|_2
\]
\[
= \sup_{\| \ell \| = 1} P[\ell^T (\hat{\Gamma}(X) - \Gamma(X))]^2
\]
\[
= \sup_{\| \ell \| = 1} P\left[ \int_{T} \ell^T \Psi(X,t) \{ \hat{\omega}(t \mid X) - \omega(t \mid X) \} dt \right]^2
\]
\[
\leq \sup_{\| \ell \| = 1} P\left[ \int_{T} \{ \ell^T \Psi(X,t) \}^2 dt \int_{T} \{ \hat{\omega}(t \mid X) - \omega(t \mid X) \}^2 dt \right]
\]
\[
\leq \sup_{x \in \mathcal{X}} \| \hat{\omega}(\cdot \mid x) - \omega(\cdot \mid x) \|_{L^2}^2 \cdot \sup_{\| \ell \| = 1} P\left[ \int_{T} \{ \ell^T \Psi(x,t) \}^2 dt \right]
\]
\[
\leq \sup_{x \in \mathcal{X}} \| \hat{\omega}(\cdot \mid x) - \omega(\cdot \mid x) \|_{L^2}^2 \cdot \sup_{\| \ell \| = 1} \left[ \int_{\mathcal{X} \times T} \{ \ell^T \Psi(x,t) \}^2 dx dt \right] \cdot C_f \quad (Assumption \ 7)
\]
\[
\leq \sup_{x \in \mathcal{X}} \| \hat{\omega}(\cdot \mid x) - \omega(\cdot \mid x) \|_{L^2}^2 \quad (Lemma \ 3)
\]
\[
= o_P(r_\omega^2),
\]
which directly yields $\| P[\{ \hat{\Gamma}(X) - \Gamma(X) \} \{ \hat{\Gamma}(X) - \Gamma(X) \}^T] \|_2^{1/2} = o_P(r_\omega)$. Second, by the property of Kronecker product (Schacke, 2004), we have
\[
\| \hat{\Gamma} - \Gamma \|_X^2 = \sup_{x \in \mathcal{X}} \left\| \int_{T} \Psi(x,t) \{ \hat{\omega}(t \mid x) - \omega(t \mid x) \} dt \right\|^2
\]
\[
\leq \| \Psi \|_{\mathcal{X} \times T}^2 \cdot \sup_{x \in \mathcal{X}} \left[ \int_{T} \{ \hat{\omega}(t \mid x) - \omega(t \mid x) \}^2 dt \right]
\]
\[
= o_P(Kr_\omega^2),
\]
where the last equality is because that by Lemma 3, we have $\| \Psi \|_{\mathcal{X} \times T}^2 \sim K$. We thus show $\| \hat{\Gamma} - \Gamma \|_X / \sqrt{K} = o_P(r_\omega)$. \hfill \square
S.5.7 Proof of Theorem 2

For fixed \((x_0, t_0) \in X \times T\), we decompose

\[
|\tilde{\tau}(x_0, t_0) - \tau(x_0, t_0)| = \left| \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}^T (\hat{\phi} - \phi^*) + \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}^T \phi^* - \tau(x_0, t_0) \right| \\
\leq \left| \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}^T (\hat{\phi} - \phi^*) \right| + \left| \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}^T \phi^* - \tau(x_0, t_0) \right| \tag{S.5.83} \\
= T_1 + T_2.
\]

The second term is the bias term, which can be bounded by Proposition 3. In particular, recalling Theorem 1 that \(\tau(x_0, t_0) = \tilde{\tau}(x_0, t_0) - \tilde{\tau}(x_0, 0)\), we have

\[
T_2 \leq \left| \Psi^T(x_0, t_0)\phi^* - \tilde{\tau}(x_0, t_0) \right| + \left| \Psi^T(x_0, 0)\phi^* - \tilde{\tau}(x_0, 0) \right| \\
\leq 2\| (\phi^*)^T \Psi - \tilde{\tau} \|_{X \times T} \tag{S.5.84} \\
\lesssim K^{-p/(d+1)}
\]

by Proposition 3.

Next we bound the term \(T_1\). Since \(UU^T + U^\perp U^\perp_T = I\), we observe that

\[
T_1 = \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}^T (\hat{\phi} - \phi^*) \\
= \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}^T (UU^T + U^\perp U^\perp_T)(\hat{\phi} - \phi^*) \\
= \left\{ \Psi^T(x_0, t_0)U - \Psi^T(x_0, 0)U \right\} U^T (\hat{\phi} - \phi^*) + \left\{ \Psi^T(x_0, t_0)U - \Psi^T(x_0, 0)U \right\} U^\perp (\hat{\phi} - \phi^*) \\
= \left\{ \Psi^T(x_0, t_0)U - \Psi^T(x_0, 0)U \right\} U^T (\hat{\phi} - \phi^*) \\
= v_n^T U^T (\hat{\phi} - \phi^*), \tag{S.5.85}
\]

where we denote \(v_n = U^T \Psi(x_0, t_0) - U^T \Psi(x_0, 0)\) for simplicity, and thus

\[
\|v_n\| \leq \|U\|_2 \left\{ \|\Psi(x_0, t_0)\| + \|\Psi(x_0, 0)\| \right\} \lesssim \sqrt{K}, \tag{S.5.86}
\]

by Lemma 3. The second equality of (S.5.85) is because that by Lemma 4, \(\Psi^T(x, t)U^\perp\) are functions free of \(t\) and thus \(\Psi^T(x, t)U^\perp\) is the same for all \(t \in T\), which implies that

\[
\Psi^T(x_0, t_0)U^\perp = \Psi^T(x_0, 0)U^\perp - \Psi^T(x_0, 0)U^\perp = 0.
\]

Now we focus on bounding \(|v_n^T U^T (\hat{\phi} - \phi^*)|\). Recall the form of \(\hat{\phi}\) in (3.1) and the simplifying setting of training nuisance functions by a single separate dataset (S.5.1). We then have

\[
T_1 = v_n^T U^T (\hat{\phi} - \phi^*) \\
= v_n^T U^T \hat{G}_n^{-1} \left[ P_n \left\{ Y - \hat{m}(X) \right\} \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\} \right] - \hat{G}_n \phi^* \\
= v_n^T U^T \hat{G}_n^{-1} \left[ P_n \left\{ Y - \hat{m}(X) - \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\}^T \phi^* \right\} \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\} \right] \tag{S.5.87} \\
+ v_n^T U^T \hat{G}_n^{-1} (\rho \hat{Q}_n \phi^* ) \\
= v_n^T U^T \hat{G}_n^{-1} \Delta_1 + v_n^T U^T \hat{G}_n^{-1} \Delta_2.
\]
In the following, we bound $|v_n^T U^T \hat{G}_n^{-1} \Delta_1|$ and $|v_n^T U^T \hat{G}_n^{-1} \Delta_2|$, respectively. By Lemma 8, we know wp1, $\hat{G}_n$ and $G_n$ are full-rank and their inverse have the singular value decomposition,

$$
\hat{G}_n^{-1} = (\hat{U} \hat{U}_\perp) \left( \hat{\Sigma}^{-1} \hat{\Sigma}_\perp \right) \left( \hat{U}^T \hat{U}_\perp \right),
$$

(S.5.88)

$$
G_n^{-1} = (U \ U_\perp) \left( \Sigma^{-1} \Sigma_\perp \right) \left( U^T \ U_\perp \right).
$$

Bound of $|v_n^T U^T \hat{G}_n^{-1} \Delta_1|$. We first bound $|v_n^T U^T \hat{G}_n^{-1} \Delta_1|$. With straightforward algebra, we further write the following decomposition of $\Delta_1$,

$$
\Delta_1 = P_n \left[ (Y - m(X)) - \tau(X, T) + E[\tau(X, T) \mid X] \right] \{ \Psi(X, T) - \Gamma(X) \}
+ P_n \left[ \tau(X, T) - E[\tau(X, T) \mid X] \right] \{ \Psi(X, T) - \Gamma(X) \}^T \{ \Psi(X, T) - \Gamma(X) \}
+ P_n \left[ (Y - m(X)) - \{ \Psi(X, T) - \Gamma(X) \}^T \phi \right] \{ \Gamma(X) - \hat{\Gamma}(X) \}
+ P_n \left[ (m(X) - \hat{m}(X)) - \{ \Gamma(X) - \hat{\Gamma}(X) \}^T \phi \right] \{ \Psi(X, T) - \Gamma(X) \}
+ P_n \left[ (m(X) - \hat{m}(X)) - \{ \Gamma(X) - \hat{\Gamma}(X) \}^T \phi \right] \{ \Gamma(X) - \hat{\Gamma}(X) \}
= \Delta_{1,1} + \Delta_{1,2} + \Delta_{1,3} + \Delta_{1,4} + \Delta_{1,5},
$$

(S.5.89)

which further yields the decomposition,

$$
v_n^T U^T \hat{G}_n^{-1} \Delta_1 = \sum_{j=1}^{5} v_n^T U^T \hat{G}_n^{-1} \Delta_{1,j}.
$$

We bound $|v_n^T U^T \hat{G}_n^{-1} \Delta_1|$ by deriving the bounds of $|v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1}|$ through $|v_n^T U^T \hat{G}_n^{-1} \Delta_{1,5}|$.

- **Bounding $|v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1}|$**: Recall $\mu(x, t) = E(Y \mid X = x, T = t)$. We first note $\Delta_{1,1}$ can be further simplified to,

$$
\Delta_{1,1} = P_n \left[ \{ Y - \mu(X, T) \} \{ \Psi(X, T) - \Gamma(X) \} \right],
$$

as, by definition for any $i = 1, \ldots, n$,

$$
\begin{align*}
Y_i - m(X_i) - \tau(T_i, X_i) + E[\tau(X, T) \mid X = X_i] \\
= Y_i - E(Y \mid X_i) - \mu(X_i, T_i) + \mu(X_i, 0) + E[\mu(X, T) - \mu(X, 0) \mid X = X_i] \\
= Y_i - E(Y \mid X_i) - \mu(X_i, T_i) + \mu(X_i, 0) + E(Y \mid X_i) - \mu(X_i, 0) \\
= Y_i - \mu(X_i, T_i).
\end{align*}
$$

Again by $(U \ U_\perp) (U \ U_\perp)^T = I$, we have

$$
\Delta_{1,1} = (U \ U_\perp) \left( U^T \right) \Delta_{1,1} = UU^T \Delta_{1,1},
$$

(S.5.91)
because,

\[ U_1^T \Delta_{1,1} = P_n \left[ (Y - m(X) - \{ \Psi(X, T) - \Gamma(X) \}^T \phi^* \right] \cdot \left\{ U_1^T \Psi(X, T) - U_1^T \Gamma(X) \right\} \]
\[ = P_n \left[ (Y - m(X) - \{ \Psi(X, T) - \Gamma(X) \}^T \phi^* \right] \cdot 0 \]  
\[ = 0. \]  

(S.5.92)

The second equality above is due to that, by Lemma 4, \( U_1^T \Psi(X, T) \) is a vector of functions free of \( T \) and thus,

\[ U_1^T \Gamma(x) = E[U_1^T \Psi(X, T) \mid X = x] = U_1^T \Psi(x, t), \]  

(S.5.93)

for any \((x, t) \in X \times T\). Summarizing the results above, we have wpa1,

\[
v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1} \\
= v_n^T U^T G_n^{-1} \Delta_{1,1} + v_n^T U^T (\hat{G}_n^{-1} - G_n^{-1}) \Delta_{1,1} \\
= v_n^T U^T G_n^{-1} \Delta_{1,1} + v_n^T U^T G_n^{-1}(G_n - \hat{G}_n) \hat{G}_n^{-1} \Delta_{1,1} \\
= v_n^T U^T \hat{G}_n^{-1} U U^T \Delta_{1,1} + v_n^T U^T G_n^{-1}(G_n - \hat{G}_n) \hat{G}_n^{-1} \Delta_{1,1} \\
= v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1} + v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1} \\
= \sum_{m=1}^{6} \ell_{m,n}^T \Delta_{1,1}, \]  

(S.5.94)

where the third equality follows by (S.5.91); the fourth equality follows by (S.5.88); and we define

\[
\ell_{1,n} = (v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1})^T, \\
\ell_{2,n} = (v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1})^T, \\
\ell_{3,n} = \left( v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1} \right)^T, \\
\ell_{4,n} = \left( v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1} \right)^T, \\
\ell_{5,n} = \left( v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1} \right)^T, \\
\ell_{6,n} = \left( v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1} \right)^T. 
\]

We note \( \ell_{1,n} \) and \( \ell_{2,n} \) depend only on \( n \), and \( \ell_{3,n} - \ell_{6,n} \) depend on both \( n \) and \( (X_1, T_1), \ldots, (X_n, T_n) \) since the \( \hat{G}_n \) is involved. For each \( m = 1, \ldots, 6 \), by taking \( \ell_n = \ell_{m,n} / \| \ell_{m,n} \| \) in Lemma 9 (i), we have

\[
|\ell_{m,n}^T \Delta_{1,1}| = O_P(\| \ell_{m,n} \| / \sqrt{n}). \]  

(S.5.95)
We now bound \( \|\ell_{m,n}\| \) for each \( m = 1, \ldots, 6 \) as \( n \to +\infty \), by Lemma 8,

\[
|v_n^T U^T \hat{G}_n^{-1} \Delta_{1,1}| = \mathcal{O}_P \left( \|v_n\| n^{-1/2} \beta_n^{-1} \left( 1 + \rho \beta_n^{-1} + \beta_n^{-1} \sqrt{K \log n/n} \right) \right)
\]
\[
= \mathcal{O}_P \left( \|v_n\| n^{-1/2} \beta_n^{-1} \left( 1 + \rho \beta_n^{-1} K \log n/n \right) \right),
\]

since \( \beta_n > \sqrt{K \log n/n} \rho > \beta_n \) implies that \( 1 > \rho \beta_n^{-1} \) and \( \beta_n^{-1} \rho^{-1} K \log n/n > \beta_n^{-1} \sqrt{K \log n/n} \).

- **Bounding \( v_n^T U^T \hat{G}_n^{-1} \Delta_{1,2} \):** With the same derivations as (S.5.91)–(S.5.93), we have \( \Delta_{1,2} = UU^T \Delta_{1,2} \), and thus similar to (S.5.94),

\[
v_n^T U^T \hat{G}_n^{-1} \Delta_{1,2} = \sum_{m=1}^{6} \ell_{m,n}^T \Delta_{1,2}.
\]

For \( m = 1, 2 \), we can apply Lemma 9 (ii) and bound

\[
|\ell_{m,n}^T \Delta_{1,2}| = \|\ell_{m,n}\| \|\ell_{m,n}^T / \|\ell_{m,n}\|\| \cdot \Delta_{1,2}| = \mathcal{O}_P(\|\ell_{m,n}\| K^{-p/(d+1)}),
\]

since \( \ell_{1,n}/\|\ell_{1,n}\| \) and \( \ell_{2,n}/\|\ell_{2,n}\| \) depend only on \( n \). For \( m = 3, \ldots, 6 \), we have

\[
|\ell_{m,n}^T \Delta_{1,2}| \leq \|\ell_{m,n}\| \|\Delta_{1,2}\| = \mathcal{O}_P(\|\ell_{m,n}\| K^{-p/(d+1)}).
\]

Combining the above results with (S.5.95), we conclude

\[
v_n^T U^T \hat{G}_n^{-1} \Delta_{1,2} = \mathcal{O}_P \left( \|v_n\| \beta_n^{-1} n^{-1/2} K^{-p/(d+1)} \left( 1 + \beta_n^{-1} \rho^{-1} K \log n/n \right) \right).
\]

- **Bounding \( v_n^T U^T \hat{G}_n^{-1} \Delta_{1,3} \):** By Lemma 4 (iv), we have \( U_T^T \{\Gamma(x) - \hat{\Gamma}(x)\} = 0 \) for any \( x \in \mathcal{X} \), which implies

\[
U_T^T \Delta_{1,3} = P_n \left[ \{Y - m(X) - \{\Psi(X, T) - \Gamma(X)\}^T \phi^* \} \{U_T^T \Gamma(X) - U_T^T \hat{\Gamma}(X)\} \right] = 0.
\]

Then with similar derivations as (S.5.91)–(S.5.93), we have \( \Delta_{1,3} = UU^T \Delta_{1,3} \). And thus similar to (S.5.94),

\[
v_n^T U^T \hat{G}_n^{-1} \Delta_{1,3} = \sum_{m=1}^{6} \ell_{m,n}^T \Delta_{1,3}.
\]
For $m = 1, 2$, we can apply Lemma 9 (iii) and bound

$$|\ell_{m,n}^T \Delta_{1,3}| = \|\ell_{m,n}|| (\ell_{m,n}/||\ell_{m,n}||)^T \Delta_{1,3}| = o_P(||\ell_{m,n}||r_\gamma/\sqrt{n}),$$

since $\ell_{1,n}/||\ell_{1,n}||$ and $\ell_{2,n}/||\ell_{2,n}||$ depend only on $n$. For $m = 3, \ldots, 6$, we have

$$|\ell_{m,n}^T \Delta_{1,3}| \leq \|\ell_{m,n}||\Delta_{1,3}| = o_P(||\ell_{m,n}||r_\gamma^*/\sqrt{Kn})\).$$

Combining the above results with (S.5.95), we conclude

$$|v_n^T U^T \hat{G}^{-1}_n \Delta_{1,3}| = o_P\left(\|v_n\|\beta_n^{-1}n^{-1/2}r_\gamma\right) + o_P\left(\|v_n\|\beta_n^{-2}(\log n)K^{3/2}n^{-3/2}r_\gamma\rho^{-1}\right).$$

• **Bounding $|v_n^T U^T \hat{G}^{-1}_n \Delta_{1,4}|$:** With the same derivations as (S.5.91)–(S.5.94), we have

$$v_n^T U^T \hat{G}^{-1}_n \Delta_{1,4} = \sum_{m=1}^{6} \ell_{m,n}^T \Delta_{1,4}.\)$$

For $m = 1, 2$, we can apply Lemma 9 (iv) and bound

$$|\ell_{m,n}^T \Delta_{1,4}| = \|\ell_{m,n}|| (\ell_{m,n}/||\ell_{m,n}||)^T \Delta_{1,4}| = o_P(||\ell_{m,n}||/\sqrt{n}),$$

since $\ell_{1,n}/||\ell_{1,n}||$ and $\ell_{2,n}/||\ell_{2,n}||$ depend only on $n$. For $m = 3, \ldots, 6$, we have

$$|\ell_{m,n}^T \Delta_{1,4}| \leq \|\ell_{m,n}||\Delta_{1,4}| = o_P(r_m||\ell_{m,n}||\sqrt{Kn} + r_\gamma||\ell_{m,n}||\sqrt{Kn}).$$

Combining the above results with (S.5.95), we conclude

$$|v_n^T U^T \hat{G}^{-1}_n \Delta_{1,4}| = o_P\left(\|v_n\|n^{-1/2}\beta_n^{-1}\right) + o_P\left(\|v_n\|\beta_n^{-2}(\log n)K^{3/2}n^{-3/2}\rho^{-1}(r_m + r_\gamma)\right).$$

• **Bounding $|v_n^T U^T \hat{G}^{-1}_n \Delta_{1,5}|$:** Similar to (S.5.97), we have $U^T \Delta_{1,5} = 0$ and thus with the same derivations as (S.5.91)–(S.5.94), we have

$$v_n^T U^T \hat{G}^{-1}_n \Delta_{1,5} = \sum_{m=1}^{6} \ell_{m,n}^T \Delta_{1,5}.\)$$

For $m = 1, 2$, we can apply Lemma 9 (v) and bound

$$|\ell_{m,n}^T \Delta_{1,5}| = \|\ell_{m,n}|| (\ell_{m,n}/||\ell_{m,n}||)^T \Delta_{1,5}| = o_P(r_\gamma||\ell_{m,n}||/\sqrt{n} + ||\ell_{m,n}||r_\gamma + ||\ell_{m,n}||r_\gamma^2),$$

since $\ell_{1,n}/||\ell_{1,n}||$ and $\ell_{2,n}/||\ell_{2,n}||$ depend only on $n$. For $m = 3, \ldots, 6$, we have

$$|\ell_{m,n}^T \Delta_{1,5}| \leq \|\ell_{m,n}||\Delta_{1,5}| = o_P(||\ell_{m,n}||r_\gamma + ||\ell_{m,n}||r_\gamma^2 + ||\ell_{m,n}||r_\gamma r_m \sqrt{Kn} + ||\ell_{m,n}||r_\gamma^2 r_m \sqrt{Kn}).$$

Combining the above results with (S.5.95), we conclude

$$|v_n^T U^T \hat{G}^{-1}_n \Delta_{1,5}| \leq o_P\left(\|v_n\|\beta_n^{-1}(r_\gamma/\sqrt{n} + r_\gamma + r_\gamma^2)\right) + o_P\left(\|v_n\|\beta_n^{-2}(\log n)Kn^{-1}\rho^{-1}(r_m r_\gamma + r_\gamma^2 + r_\gamma r_m \sqrt{Kn} + r_\gamma^2 r_m \sqrt{Kn})\right).$$

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After summarizing all bounds above and dropping some negligible terms, we conclude
\[ |v_n^T U^T \hat{G}_n^{-1} \Delta_1| = O_P \left\{ \|v_n\| \beta_n^{-1} (n^{-1/2} + K^{-p/(d+1)}) (1 + \beta_n^{-1} \rho^{-1} K \log n/n) \right\} \]
\[ + o_P \left\{ \|v_n\| \beta_n^{-2} (\log n) K^{3/2} n^{-3/2} \rho^{-1} (r'_\gamma + r_m + r_\gamma) \right\} \]
\[ + o_P \left\{ \|v_n\| \beta_n^{-1} \left( r_\gamma / \sqrt{n} + r_m r_\gamma + r_\gamma^2 \right) \right\} \]
\[ + o_P \left\{ \|v_n\| \beta_n^{-2} \rho^{-1} \left( r_m r_\gamma + r_\gamma^2 + r'_\gamma r_m \sqrt{K/n} + r'_\gamma r_\gamma \sqrt{K/n} \right) \right\} \]
\[ = O_P \left\{ \|v_n\| \beta_n^{-1} (n^{-1/2} + K^{-p/(d+1)}) (1 + \beta_n^{-1} \rho^{-1} K \log n/n) \right\} \]
\[ + o_P \left\{ \|v_n\| \beta_n^{-2} (\log n) K^{3/2} n^{-3/2} \rho^{-1} (r'_\gamma + r_m + r_\gamma) \right\} \]
\[ + o_P \left\{ \|v_n\| \beta_n^{-1} \left( r_\gamma / \sqrt{n} + r_m r_\gamma + r_\gamma^2 \right) \right\}, \]

because \( \sqrt{K/n} < 1 \) and \( r_\gamma r_m r_\gamma^2 + r'_\gamma r_m \sqrt{K/n} + r'_\gamma r_\gamma \sqrt{K/n} \lesssim r'_\gamma + r_m + r_\gamma, \) due to Assumption 6 and \( r_m, r_\gamma, r'_\gamma \lesssim 1. \)

**Bound of \( |v_n^T U^T \hat{G}_n^{-1} \Delta_2|**

We decompose
\[ |v_n^T U^T \hat{G}_n^{-1} \Delta_2| = \rho |v_n^T U^T \hat{G}_n^{-1} \hat{Q}_n \phi^*| \]
\[ \leq \rho |v_n^T U^T \hat{G}_n^{-1} (\hat{Q}_n - Q_n) \phi^*| + \rho |v_n^T U^T \hat{G}_n^{-1} Q_n \phi^*|. \]  \( \text{(S.5.99)} \)

For the first term on the right-hand side, we have
\[ \rho v_n^T U^T \hat{G}_n^{-1} (\hat{Q}_n - Q_n) \phi^* = \rho v_n^T U^T \hat{U} \hat{\Sigma}^{-1} \hat{U}^T (\hat{Q}_n - Q_n) \phi^* + \rho v_n^T U^T \hat{U} \hat{\Sigma}^{-1} \hat{U}^T (\hat{Q}_n - Q_n) \phi^*. \]

Then by Lemmas 5 and 8, we have,
\[ |\rho v_n^T U^T \hat{U} \hat{\Sigma}^{-1} \hat{U}^T (\hat{Q}_n - Q_n) \phi^*| \leq \rho \|v_n\| \|U^T \hat{U}\|_2 \|\hat{\Sigma}^{-1}\|_2 \|\hat{U}^T\|_2 \|\hat{Q}_n - Q_n\|_2 \|\phi^*\|_2 \]
\[ = O_P (\|v_n\| \rho \sqrt{K \log n/n \beta_n^{-1}}), \]  \( \text{(S.5.100)} \)

and
\[ |\rho v_n^T U^T \hat{U} \hat{\Sigma}^{-1} \hat{U}^T (\hat{Q}_n - Q_n) \phi^*| \leq \rho \|v_n\| \|U^T \hat{U}\|_2 \|\hat{\Sigma}^{-1}\|_2 \|\hat{U}^T\|_2 \|\hat{Q}_n - Q_n\|_2 \|\phi^*\|_2 \]
\[ = O_P (\|v_n\| (\log n) K^{-1} n \beta_n^{-1}), \]  \( \text{(S.5.101)} \)

which together yield
\[ |\rho v_n^T U^T \hat{G}_n^{-1} (\hat{Q}_n - Q_n) \phi^*| = O_P (\|v_n\| \sqrt{\log n \rho K^{1/2} n^{-1/2} \beta_n^{-1}} + \|v_n\| (\log n) K^{-1} n \beta_n^{-1}). \]  \( \text{(S.5.102)} \)

For the second term on the right-hand side of \( \text{(S.5.99)} \), we have by \( \text{(S.5.2)} \),
\[ Q_n \phi^* = E \{ \Psi(X, T) \tilde{\tau}(X, T) \}. \]

Since \( U^T \Psi(X, T) \) is a function only of \( X \), by the law of total expectation,
\[ U^T Q_n \phi^* = E \{ U^T \Psi(X, T) \tilde{\tau}(X, T) \} \]
\[ = E [U^T \Psi(X, T) E \{ \tilde{\tau}(X, T) \mid X \}] \]
\[ = 0, \]
as $E\{\hat{\tau}(X, T) \mid X = x\} = E\{\tau - E(\tau \mid X) \mid X = x\} = E(\tau \mid X = x) - E(\tau \mid X = x) = 0$. Thus we have

$$Q_n\phi^* = UU^TQ_n\phi^* + U_1U_1^TQ_n\phi^* = UU^TQ_n\phi^*.$$  

We then have

$$\rho v_n^\top UU^\top \hat{G}_n^{-1}Q_n\phi^* = \rho v_n^\top UU^\top \hat{G}_n^{-1}UU^TQ_n\phi^* = \rho v_n^\top UU^\top \hat{G}_n^{-1}UU^TQ_n\phi^* + \rho v_n^\top UU^\top \hat{G}_n^{-1}U_1U_1^TUU^TQ_n\phi^*.$$  

Similar to (S.5.100) and (S.5.101), we have

$$\|v_n^\top UU^\top \hat{G}_n^{-1}U_1U_1^TUU^TQ_n\phi^*\| = O_P\{\rho\|v_n\|\beta_n^{-1} + \|v_n\|(log n)K^{-1}\beta_n^{-2}\},$$

which yields $|v_n^\top UU^\top \hat{G}_n^{-1}Q_n\phi^*| = O_P\{\rho\|v_n\|\beta_n^{-1} + \|v_n\|(log n)K^{-1}\beta_n^{-2}\}$. This combining with (S.5.102) results that

$$\|v_n^\top UU^\top \hat{G}_n^{-1}\Delta_2\| = O_P\left\{\left\|v_n\right\|\sqrt{\log n}\rho K^{-p/(d+1)}(1 + \beta_n^{-1}\rho^{-1}K\log n/n) + \|v_n\|\beta_n^{-1}\rho + \|v_n\|\beta_n^{-2}(log n)K^{-1}\beta_n^{-2}\right\}$$

noting here we use the fact $\sqrt{\log n}\rho K^{-p/(d+1)}(1 + \beta_n^{-1}\rho^{-1}K\log n/n) < \rho\sqrt{K}\beta_n^{-1}$ under Assumption 6.

[Summary of convergence rates] We now prove the convergence rate results in Theorem 2. Combining (S.5.83), (S.5.84), (S.5.87), (S.5.98), and (S.5.103), we finally have

$$\|\hat{\tau}(x_0, t_0) - \tau(x_0, t_0)\| \leq r(n, K, \beta_n, \rho, r_m, r_\gamma, r'_\gamma)$$

$$= O_P\left\{\left\|v_n\right\|\beta_n^{-1}(n^{-1/2} + K^{-p/(d+1)}(1 + \beta_n^{-1}\rho^{-1}K\log n/n) + \|v_n\|\beta_n^{-1}\rho + \|v_n\|\beta_n^{-2}(log n)K^{-1}\beta_n^{-2}\right\}$$

$$+ o_P\left\{\left\|v_n\right\|\left(\beta_n^{-1}(r_\gamma/\sqrt{n} + r_mr_\gamma + r'_\gamma) + \|v_n\|\beta_n^{-2}(log n)K^{-3/2}n^{-3/2}(r'_\gamma + r_m + r_\gamma)\right)\right\}.$$  

(S.5.104)

Here $\|v_n\| \leq \|U\|_2\|\Psi(x_0, t_0) - \Psi(x_0, 0)\| = \|\Psi(x_0, t_0) - \Psi(x_0, 0)\|$ depends on $x_0$ and $t_0$, and it has a general bound (S.5.86).

When $\beta_n \asymp 1$, $r_m, r_\gamma, r'_\gamma \asymp n^{-1/4}$, and $p > d + 1$, the above bound can be simplified to

$$\|\hat{\tau}(x_0, t_0) - \tau(x_0, t_0)\|$$

$$= O_P\left\{\left\|v_n\right\|(n^{-1/2} + K^{-p/(d+1)}(1 + \rho^{-1}K\log n/n) + \|v_n\|\rho + \|v_n\|(log n)K^{-1}\right\}$$

$$+ o_P\left\{\left\|v_n\right\|\left(\rho^{-1}K^{3/2}n^{-7/4}\right)\right\}$$

$$= O_P\left\{\sqrt{K/n} + K^{1/2-p/(d+1)}\right\}$$

$$+ o_P\left\{(\sqrt{K/n} + K^{1/2-p/(d+1)}(\rho^{-1}K\log n/n) + \rho K^{1/2} + (log n)K^{3/2}n^{-1}\right\}$$

$$+ o_P\left\{(log n)\rho^{-1}K^2n^{-7/4}\right\},$$  

(S.5.105)
In this part, we show the central limiting theorem (CLT) result for our proposed estimator. In the following, we balance the rate of (S.5.105) by selecting $K \asymp n^{(d+1)/2p}$, and then
\[
\sqrt{K/n} + K^{1/2-p/(d+1)} \asymp n^{-1/2+(d+1)/(4p)}.
\]
Now we show the second term in (S.5.105) is negligible. When $\rho \asymp n^{-(d+1)/(2p)} \log n$, we have
\[
\rho^{-1} K \log n/n \asymp n^{1-(d+1)/(2p)} \cdot n^{(d+1)/(2p)} \cdot n^{-1} = 1.
\]
This implies $(\sqrt{K/n} + K^{1/2-p/(d+1)}) (\rho^{-1} K \log n/n) \ll (\sqrt{K/n} + K^{1/2-p/(d+1)})$, which is negligible compared with the rate of the first term in (S.5.105). On the other hand, since $\rho \asymp n^{-1/2}$, we have
\[
\rho K^{1/2} \asymp \sqrt{K/n},
\]
which implies that $\rho K^{1/2}$ is also negligible compared with the first term in (S.5.105). We also have
\[
(\log n) K^{3/2} n^{-1} \asymp (\log n) n^{-1+(d+1)/(2p)} = (\log n) \left( n^{-1/2+(d+1)/(4p)} \right)^2 < n^{(d+1)/(2p)} \cdot n^{-1} \asymp \sqrt{K/n} + K^{1/2-p/(d+1)},
\]
where the inequality is because that $n^{-1/2+(d+1)/(4p)}$ is polynomially decaying when $p > d+1$. Summarizing the results above, we conclude
\[
(\sqrt{K/n} + K^{1/2-p/(d+1)}) (\rho^{-1} K \log n/n) + \rho K^{1/2} + (\log n) K^{3/2} n^{-1} \ll \sqrt{K/n} + K^{1/2-p/(d+1)},
\]
and thus the second term in (S.5.105) is negligible. Finally
\[
(\log n) \rho^{-1} K^2 n^{-7/4} \ll n^{-1-(d+1)/2p} \cdot n^{(d+1)/p} \cdot n^{-7/4} = n^{-1/2+(d+1)/4p} \cdot n^{-1/4+(d+1)/4p} < n^{-1/2+(d+1)/4p},
\]
since $-1/4+(d+1)/(4p) < 0$ due to $d+1 < p$. Thus the third term in (S.5.105) is also negligible compared with the first term in (S.5.105). In summary, the first term in (S.5.105) is optimized as $O_P(n^{-1/2+(d+1)/(4p)})$ when $K \asymp n^{(d+1)/(2p)}$. Moreover, when selecting $n^{-1+(d+1)/(2p)} \log n \ll \rho \lessapprox n^{-1/2}$, other terms than the first term in (S.5.105) are negligible, and thus the whole rate is minimized to $O_P(n^{-1/2+(d+1)/(4p)})$.

[Central limiting distribution] In this part, we show the central limiting theorem (CLT) result for our proposed estimator. In the previous parts, if carefully tracking the derivations, we can show by (S.5.105) that
\[
|\hat{\tau}(x_0, t_0) - \tau(x_0, t_0)| = v_n^T U^T \hat{\Sigma}^{-1} \hat{U}^T U^T \Delta_{1,1} + R_n,
\]
where
\[
R_n = O_P \left\{ \|v_n\| K^{-p/(d+1)} (1 + \rho^{-1} K \log n/n) + \|v_n\| \rho + \|v_n\| (\log n) K n^{-1} \right\} + o_P \left\{ \|v_n\| (\log n) \rho^{-1} K^{3/2} n^{-7/4} \right\}.
\]
This is because only the term \( v_n^T \tilde{U} \tilde{v} \Sigma^{-1} \tilde{U}^T U U^T \Delta_{1,1} \) in (S.5.94) produces the rate term \( O_P\{\|v_n\|n^{-1/2}\} \), on the right-hand side of the second equality in (S.5.105). In the following, we will first show the limiting distribution of the first term \( v_n^T \tilde{U} \tilde{v} \Sigma^{-1} \tilde{U}^T U U^T \Delta_{1,1} \) on the right-hand side of (S.5.107). We then show that the second term in (S.5.107) is negligible. Finally, we will show the consistency of the our asymptotic variance estimator, which helps us to construct the confidence interval.

First we have

\[
\sqrt{n} \tilde{\sigma}^{-1} v_n^T \tilde{U} \tilde{v} \Sigma^{-1} \tilde{U}^T U U^T \Delta_{1,1} = \sqrt{n} \tilde{\sigma}^{-1} P_n \left[ \kappa_n(X,T) \left[ Y - m(X) - \tau(X,T) + E\{\tau(X,T) \mid X\} \right] \right] = \sum_{i=1}^{n} \xi_n(x_i, t_i, y_i),
\]

where we define

\[
\tilde{\sigma} = \sqrt{E[\kappa_n^2(X,T) \{ Y - \mu(X,T) \}^2]}
\]

\[
\kappa_n(x,t) = v_n^T \tilde{U} \tilde{v} \Sigma^{-1} \tilde{U}^T \{ \Psi(x,t) - \Gamma(x) \}
\]

\[
\xi_n(x, t, y) = \frac{1}{\sqrt{n} \tilde{\sigma}^2} \kappa_n(x, t) \left[ y - m(x) - \tau(x,t) + E\{\tau(X,T) \mid X = x\} \right] = \frac{1}{\sqrt{n} \tilde{\sigma}^2} \kappa_n(x, t) \left[ y - E(Y \mid X = x) - \mu(x,t) + \mu(x,0) + E\{\mu(X,T) \mid X = x\} - E\{\mu(X,0) \mid X = x\} \right] = \frac{1}{\sqrt{n} \tilde{\sigma}^2} \kappa_n(x, t) \left[ y - E(Y \mid X = x) - \mu(x,t) + \mu(x,0) + E(Y \mid X = x) - \mu(x,0) \right] = \frac{1}{\sqrt{n} \tilde{\sigma}^2} \kappa_n(x, t) \left\{ y - \mu(x, t) \right\},
\]

recalling that \( \mu(x, t) = E(Y \mid X = x, T = t) \). We now verify (S.5.109) satisfies the Lindberg’s condition for the CLT. We emphasize \( v_n^T \tilde{U} \tilde{v} \Sigma^{-1} \tilde{U}^T U U^T \) is a deterministic vector independent of samples. Therefore, \( \xi_n(x_i, t_i, y_i) \) with \( i = 1, \ldots, n \), are i.i.d. samples with

\[
E\{\xi_n(X,T,Y)\} = \frac{1}{\sqrt{n} \tilde{\sigma}^2} E \left[ E[\kappa_n(X,T) \{ Y - \mu(X,T) \} \mid X,T] \right] = \frac{1}{\sqrt{n} \tilde{\sigma}^2} E \left[ \kappa_n(X,T) E[ Y - \mu(X,T) \mid X,T] \right] = 0.
\]  

Therefore we have

\[
\text{Var}\left\{ \sum_{i=1}^{n} \xi_n(x_i, t_i, y_i) \right\} = \frac{1}{\tilde{\sigma}^2} \text{Var}\left[ \kappa_n(X,T) \{ Y - \mu(X,T) \} \right] = 1.
\]

Next we derive the lower bound of \( \tilde{\sigma} \). By definition, we have

\[
\tilde{\sigma}^2 = v_n^T \tilde{U} \tilde{v} \Sigma^{-1} \tilde{U}^T U U^T E \left[ \{ \Psi(X,T) - \Gamma(X) \} \{ \Psi(X,T) - \Gamma(X) \}^T \{ Y - \mu(X,T) \}^2 \right] U U^T \tilde{U} \Sigma^{-1} \tilde{U}^T u_n.
\]  

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Observe that by the law of total expectation,

\[
E\left[ \{ \Psi(X, T) - \Gamma(X) \} \{ \Psi(X, T) - \Gamma(X) \}^T \{ Y - \mu(X, T) \}^2 \right] = E\left[ \{ \Psi(X, T) - \Gamma(X) \} \{ \Psi(X, T) - \Gamma(X) \}^T \text{Var}(Y \mid X, T) \right] \geq c_1 E \left[ \{ \Psi(X, T) - \Gamma(X) \} \{ \Psi(X, T) - \Gamma(X) \} \right] = c_1 R_n, \tag{S.5.114}
\]

since \text{Var}(Y \mid X, T) is uniformly lower bounded by some fixed \(c_1 > 0\) under Assumption 8. Combining (S.5.113) and (S.5.114), we have

\[
\hat{\sigma}^2 \geq c_1 v_n^T U^T \tilde{\Sigma}^{-1} U^T U \tilde{\Sigma}^{-1} U^T U v_n = c_1 v_n^T M_{clt} v_n, \tag{S.5.115}
\]

where \(M_{clt} = U^T \tilde{\Sigma}^{-1} U^T U \Sigma U^T U \) is a \(\zeta \times \zeta\) matrix. Its smallest singular value can be bounded by Lemma 8,

\[
\sigma_{\min}(M_{clt}) \geq \sigma_{\min}(U^T \tilde{\Sigma}) \sigma_{\min}(\tilde{\Sigma}^{-1}) \sigma_{\min}(U^T U) \sigma_{\min}(\tilde{\Sigma}^{-1}) \sigma_{\min}(U^T U) \sigma_{\min}(\tilde{\Sigma}^{-1}) \sigma_{\min}(U^T U) \geq \ldots \geq \sigma_{\min}(U^T \tilde{\Sigma}) \sigma_{\min}(\tilde{\Sigma}^{-1}) \sigma_{\min}(U^T U) \sigma_{\min}(\tilde{\Sigma}^{-1}) \sigma_{\min}(U^T U) \sigma_{\min}(\tilde{\Sigma}^{-1}) \sigma_{\min}(U^T U) \geq 1. \tag{S.5.116}
\]

In (S.5.116), we treat \(M_{clt}\) as the multiplication of \(n\) \(\zeta \times \zeta\) matrices \(U^T \tilde{\Sigma}, \tilde{\Sigma}^{-1}, \ldots, U^T U\), where each of them is full-rank with smallest singular values bounded away from 0; see Lemma 8 and note \(U^T U = I_{\zeta}\). Then the first three inequalities in (S.5.116) follow by repeatedly using the fact that

\[
\sigma_{\min}(AB) \geq \sigma_{\min}(A) \sigma_{\min}(B),
\]

for two full-rank and square matrices \(A\) and \(B\); see, e.g., Bhatia (2013, Problem III.6.14). Combining (S.5.115) and (S.5.116), we conclude that

\[
\hat{\sigma}^2 \geq \|v_n\|^2 \cdot c_1 (v_n/\|v_n\|)^T M_{clt} (v_n/\|v_n\|) \geq \|v_n\|^2 \sigma_{\min}(M_{clt}) \geq \|v_n\|^2. \tag{S.5.117}
\]

We thus derive the lower bound \(\hat{\sigma} \gtrsim \|v_n\|^2\). On the other hand, we aim at deriving

\[
\sum_{i=1}^{n} E \left[ \xi_n(X_i, T_i, Y_i) \right] = E \left[ \xi_n(X, Y) \right] = 0 \tag{S.5.118}
\]

to verify the Lindberg’s condition. By Hölder’s inequality for fixed \(c_0 > 0\) and any \(\delta > 0\),

\[
E \left[ \xi_n(X, Y) \right]^2 1 \{ |\xi_n(X, Y)| > \delta \} \leq \left[ E \left[ |\xi_n(X, Y)|^{2(2+c_0)/2} \right] \right]^{2(2+c_0)} \left[ E \left[ 1 \{ |\xi_n(X, Y)| > \delta \} \right] \right]^{1-2/(2+c_0)}, \tag{S.5.119}
\]

\[
= \left[ E \left[ |\xi_n(X, Y)|^{2+c_0} \right] \right]^{2/(2+c_0)} \left[ \text{Pr} \left[ |\xi_n(X, Y)| > \delta \right] \right]^{1-2/(2+c_0)}.
\]

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For the first factor on the right-hand side of (S.5.119), we have

\[
E \left\{ \left| \xi_n(X, T, Y) \right|^{2+c_0} \right\}
= n^{-(2+c_0)/2} \sigma^{-(2+c_0)} E \left[ \kappa_1^2(X, T) \left| Y - \mu(X, T) \right|^{2+c_0} \right]
\leq n^{-(2+c_0)/2} \sigma^{-(2+c_0)} \cdot \sup_{(x, t) \in X \times T} \kappa_n(x, t)^{c_0} \cdot E \left[ \kappa_n^2(X, T) \left| Y - \mu(X, T) \right|^{2+c_0} \right]
\lesssim n^{-(2+c_0)/2} K^{c_0}/2,
\]

where the last inequality follows by \( \tilde{\sigma} \lesssim \|v_n\| \) and the following bounds.

- By Lemmas 3 and 6, we have

\[
\sup_{(x, t) \in X \times T} \kappa_n(x, t) \leq \sup_{(x, t) \in X \times T} v_n^T U^T \tilde{U} \tilde{\Sigma}^{-1} \tilde{U}^T U^T \{ \Psi(x, t) - \Gamma(x) \} \leq \|v_n\| \|U\|_2 \|\tilde{U}\|_2 \|\tilde{\Sigma}^{-1}\|_2 \|U\|_2 \|\Psi\|_X + \|\Gamma\|_X
\lesssim \sqrt{K} \|v_n\|.
\]

- Similar to (S.5.113), we have

\[
E \left\{ \kappa_n^2(X, T) \left| Y - \mu(X, T) \right|^{2+c_0} \right\}
= v_n^T U^T \tilde{U} \tilde{\Sigma}^{-1} \tilde{U}^T U^T \{ \Psi(X, T) - \Gamma(X) \} \{ \Psi(X, T) - \Gamma(X) \}^T \{ \Psi(X, T) - \Gamma(X) \}^2 \|X, T\|_2 \|X, T\|_2 \|\Psi\|_X + \|\Gamma\|_X
\lesssim \sqrt{K} \|v_n\|^2,
\]

where the second equality follows by the law of total expectation, the first inequality follows by (3.10), and the last inequality is similar to (S.5.121).

We note the bound (S.5.120) actually holds for not only \( c_0 \) but also all \( c \in [0, c_0] \) with similar arguments. Thus when \( c = 0 \), one has \( E|\xi_n(X, T, Y)|^2 \lesssim n^{-1} \). Then for the second factor on the right-hand side of (S.5.119), by Chebyshev’s inequality,

\[
\Pr \left\{ |\xi_n(X, T, Y)| > \delta \right\} \leq \frac{E|\xi_n(X, T, Y)|^2}{\delta^2} \lesssim n^{-1},
\]

with fixed \( \delta > 0 \). Combining (S.5.119), (S.5.120), and (S.5.122), we conclude

\[
\sum_{i=1}^n E \left[ |\xi_n(X, T, Y)|^2 1 \{ |\xi_n(X, T, Y)| > \delta \} \right] \lesssim n \cdot (n)^{-1} \cdot K^{c_0/(2+c_0)} \cdot n^{-1+2/(2+c_0)}
= (K/n)^{c_0/(2+c_0)} \to 0,
\]

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under Assumption 6. Thus (S.5.118) is verified. By (S.5.111), (S.5.112), and (S.5.123), the conditions of the Lindeberg-Feller CLT are verified. Thus we have

\[ \sqrt{n} \hat{\sigma}^{-1} v_n^T \tilde{U} \tilde{U}^{-1} \tilde{U}^T \Delta_{1,1} \sim \mathcal{N}(0, 1). \]  

(S.5.124)

By (S.5.108) and (S.5.117), \( K \sim n^{\epsilon_{clt} + (d + 1)/2p} \) with \( \epsilon_{clt} < 1/2 - (d + 1)/(ep) \) and \( \rho \asymp n^{-1} \), we have

\[ \sqrt{n} \hat{\sigma}^{-1} R_n \]
\[ = O_P \{ \sqrt{n} K^{-p/(d+1)} (1 + \rho^{-1} K \log n/n) + \rho \sqrt{n} + (\log n) Kn^{-1/2} \}
\]
\[ + o_P \{ (\log n) \rho^{-1} K^{3/2} n^{-5/4} \} \]
\[ = O_P(1), \]  

(S.5.125)

with similar rate comparison arguments as (S.5.105)–(S.5.106). For example, the rate term \( \rho^{-1} K \log n/n = (\log n) n^{-1/2 + (d+1)/(2p) + \epsilon_{clt}} \to 0 \) as \( \epsilon_{clt} < 1/2 - (d + 1)/(2p) \). Other terms can be bounded similarly. Finally combining (S.5.107), (S.5.124), (S.5.125), and applying the Slutsky’s theorem leads to (3.11).

Confidence interval

We finally prove the confidence interval part of Theorem 2. First we simplify \( \sigma_n^2 \). From (S.5.85), we have

\[ v_n^T U = \Psi^T(x_0, t_0) - \Psi^T(x_0, 0). \]  

(S.5.126)

On the other hand, by Lemma 4 (i), we have \( U_\perp^T \{ \Psi(x, t) - \Gamma(x) \} = 0 \) and thus

\[ E \left[ \left\{ \Psi(X, T) - \Gamma(X) \right\} \left\{ \Psi(X, T) - \Gamma(X) \right\}^T \left\{ Y - \mu(X, T) \right\}^2 \right] \]
\[ = U U^T E \left[ \left\{ \Psi(X, T) - \Gamma(X) \right\} \left\{ \Psi(X, T) - \Gamma(X) \right\}^T \left\{ Y - \mu(X, T) \right\}^2 \right] U U^T \]
\[ + U_\perp U_\perp^T E \left[ \left\{ \Psi(X, T) - \Gamma(X) \right\} \left\{ \Psi(X, T) - \Gamma(X) \right\}^T \left\{ Y - \mu(X, T) \right\}^2 \right] U_\perp U_\perp^T \]
\[ = U U^T E \left[ \left\{ \Psi(X, T) - \Gamma(X) \right\} \left\{ \Psi(X, T) - \Gamma(X) \right\}^T \left\{ Y - \mu(X, T) \right\}^2 \right] U U^T \]
\[ + U_\perp E \left[ \underbrace{U_\perp^T \{ \Psi(X, T) - \Gamma(X) \} \{ \Psi(X, T) - \Gamma(X) \}^T}_{=0} \underbrace{U_\perp \{ Y - \mu(X, T) \}^2}_{=0} \right] U_\perp^T \]
\[ = U U^T E \left[ \left\{ \Psi(X, T) - \Gamma(X) \right\} \left\{ \Psi(X, T) - \Gamma(X) \right\}^T \left\{ Y - \mu(X, T) \right\}^2 \right] U U^T. \]

By (S.5.113), (S.5.126), and (S.5.127), \( \hat{\sigma} \) can be simplified to

\[ \hat{\sigma}^2 = \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}^T A_n B_n A_n \left\{ \Psi(x_0, t_0) - \Psi(x_0, 0) \right\}, \]

where \( A_n = \tilde{U} \tilde{\Sigma}^{-1} \tilde{U}^T \) and \( B_n = E \left[ \left\{ \Psi(X, T) - \Gamma(X) \right\} \left\{ \Psi(X, T) - \Gamma(X) \right\}^T \left\{ Y - \mu(X, T) \right\}^2 \right] \). Recall that in Algorithm 2, our variance estimator is

\[ \hat{\sigma}^2 = \tilde{v}_n^T \hat{A}_n \tilde{B}_n \hat{A}_n \tilde{v}_n, \]

where we define,

\[ \hat{A}_n = \tilde{U} \tilde{\Sigma}^{-1} \tilde{U}^T, \]
\[ \tilde{B}_n = P_n \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\} \left\{ \Psi(X, T) - \hat{\Gamma}(X) \right\}^T \left\{ Y - \hat{\mu}(X, T) \right\}^2 \]
\[ \tilde{v}_n = \Psi(x_0, t_0) - \Psi(x_0, 0). \]
We then decompose
\[
\hat{\sigma}^2 - \sigma^2 = \tilde{v}_n^T \hat{A}_n \hat{B}_n \hat{A}_n \tilde{v}_n - \tilde{v}_n^T A_n B_n A_n \tilde{v}_n \\
= \tilde{v}_n^T (\hat{A}_n - A_n) \hat{B}_n \hat{A}_n \tilde{v}_n + \tilde{v}_n^T A_n (\hat{B}_n - B_n) \hat{A}_n \tilde{v}_n + \tilde{v}_n^T A_n B_n (\hat{A}_n - A_n) \tilde{v}_n.
\]

By Lemma 8 (v), we have the spectral norms of \( \hat{A}_n, A_n, \hat{B}_n, B_n \) are constantly bounded, while \( \| \hat{A}_n - A_n \|_2, \| \hat{B}_n - B_n \|_2 \to 0 \) wpa1. We thus have wpa1,
\[
|\hat{\sigma}^2 - \sigma^2| = \| v_n \|_2^2, \tag{S.5.128}
\]
where the second and third equalities can be derived similar to (S.5.85). With (S.5.117) and (S.5.128), we have wpa1,
\[
\frac{\hat{\sigma}^2}{\sigma^2} = 1 + \frac{\sigma^2 - \hat{\sigma}^2}{\sigma^2} \to 1,
\]
and thus \( \hat{\sigma}^{-1} \sigma \to 1 \) wpa1. Then by (3.11) and Slutsky’s theorem, we finally have
\[
\sqrt{n} \hat{\sigma}^{-1} \{ \hat{\tau}(x_0, t_0) - \tau(x_0, t_0) \} = \hat{\sigma}^{-1} \hat{\sigma} \cdot \sqrt{n} \hat{\sigma}^{-1} \{ \hat{\tau}(x_0, t_0) - \tau(x_0, t_0) \} \\
\sim N(0, 1).
\]
□