OFF-POLICY EVALUATION AND LEARNING FOR EXTERNAL VALIDITY UNDER A COVARIATE SHIFT

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ABSTRACT

We consider the evaluation and training of a new policy for the evaluation data by using the historical data obtained from a different policy. The goal of off-policy evaluation (OPE) is to estimate the expected reward of a new policy over the evaluation data, and that of off-policy learning (OPL) is to find a new policy that maximizes the expected reward over the evaluation data. Although the standard OPE and OPL assume the same distribution of covariate between the historical and evaluation data, there often exists a problem of a covariate shift, i.e., the distribution of the covariate of the historical data is different from that of the evaluation data. In this paper, we derive the efficiency bound of OPE under a covariate shift. Then, we propose doubly robust and efficient estimators for OPE and OPL under a covariate shift by using an estimator of the density ratio between the distributions of the historical and evaluation data. We also discuss other possible estimators and compare their theoretical properties. Finally, we confirm the effectiveness of the proposed estimators through experiments.

1 Introduction

In various applications, such as ad-design selection, personalized medicine, search engines, and recommendation systems, there is a significant interest in evaluating and learning a new policy from historical data (Bevelzimer & Langford, 2009; Li et al., 2010; Athey & Wager, 2017). To accomplish this, we use off-policy evaluation (OPE) and off-policy learning (OPL). The goal of OPE is to evaluate a new policy by estimating the expected reward of the new policy (Dudík et al., 2011; Wang et al., 2017; Narita et al., 2019; Bibaut et al., 2019; Kallus & Uehara, 2019b; Oberst & Sontag, 2019). In contrast, OPL aims to find a new policy that maximizes the expected reward (Zhao et al., 2012; Swaminathan & Joachims, 2015b; Kitagawa & Tetenov, 2018; Zhou et al., 2018; Chen et al., 2019; Chernozhukov et al., 2019).

Even though an OPE algorithm provides an estimator of the expected reward of a new policy, most existing studies presumed that the distribution of covariates is the same between the historical and evaluation data. However, in many real-world applications, the expected reward of a new policy over the distribution of evaluation data is of significant interest, which can be different from the historical data. For example, in the medical literature, it is known that the result of a randomized control trial (RCT) cannot be directly transported because the covariate distribution in a target population is different (Cole & Stuart, 2010). This problem is known as a lack of external validity (a.k.a. transportability) (Pearl & Bareinboim, 2014). These situations where historical and evaluation data follow different distributions are generally known as covariate shifts in machine learning (Shimodaira, 2000; Sugiyama et al., 2008), This situation is illustrated in Figure 1.\

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Contributions: This paper has four main contributions. First, we derive an efficiency bound of OPE under covariate shift (Section 3). Second, in Section 4, we propose estimators constructed by three estimators of nuisance functions, i.e., the density ratio, behavior policy, and conditional average treatment effect. Especially, we employ nonparametric density ratio estimation (Kanamori et al., 2012) to estimate the density ratio. The proposed estimator is an efficient estimator, which can achieve the efficiency bound under mild nonparametric rate conditions of the estimators of nuisance functions. In addition, this estimator is robust to model-misspecification of estimators in the sense that the resulting estimator is consistent if the model of the density ratio and the behavior policy are correct or the conditional average treatment effect is correct. Third, we propose other possible estimators for our problem setting and compared them (Section 5). Fourth, an algorithm of OPL is proposed based on the efficient estimators (Section 6). All proofs are shown in Appendix E.

Related Work: In some studies related to causal inference, the difference between distributions of covariates conditioned on a chosen action is also called a covariate shift (Zhang et al., 2013; Johansson et al., 2016). A covariate shift in this paper refers to the different distributions of covariates between historical and evaluation data. Dahabreh et al. (2019) also considered the treatment effect estimation under a covariate shift. The main differences of this paper from Dahabreh et al. (2019) are in the differences of sampling schemes and parametric assumptions. The difference in sampling schemes is discussed in Section 2. In addition, there are many studies regarding the external validity based on a causal directed acyclic graph (Pearl & Bareinboim, 2011, 2014). This paper focuses on statistical inference and learning instead of a complicated identification strategy.

2 Problem Formulation

In this section, we introduce our problem setting and review existing literatures.

2.1 Data Generating Process with Evaluation Data

Let \( A_i \) be the action taking variable in \( \mathcal{A} \) and \( Y_i \in \mathbb{R} \) be the reward of an individual \( i \in \mathbb{N} \). Let \( X_i \) and \( Z_i \) be the covariate observed by the decision maker when choosing an action, and \( \mathcal{X} \) be the domain of the covariate. Let a policy \( \pi: \mathcal{X} \times \mathcal{A} \to [0, 1] \) be a function of a covariate \( x \) and action \( a \), which can be considered as the probability of taking actions \( a \) given \( x \). In this paper, we have access to historical data and evaluation data. For the historical data, we can observe a set \( \mathcal{D}^{\text{hst}} = \{(X_i, A_i, Y_i)\}_{i=1}^{n^{\text{hst}}} \). For the evaluation data, we can observe a set \( \mathcal{D}^{\text{evl}} = \{Z_i\}_{i=1}^{n^{\text{evl}}} \), where \( n^{\text{hst}} \in \mathbb{N} \) and \( n^{\text{evl}} \in \mathbb{N} \) denote the sample sizes of historical data and evaluation data, respectively. Then, the data generating process is defined as follows:

\[
\mathcal{D}^{\text{hst}} = \{(X_i, A_i, Y_i)\}_{i=1}^{n^{\text{hst}}} \sim p(x)\pi^b(a \mid x)p(y \mid x, a),
\]

\[
\mathcal{D}^{\text{evl}} = \{Z_i\}_{i=1}^{n^{\text{evl}}} \sim q(z), \quad n^{\text{hst}} = \rho n, \quad n^{\text{evl}} = (1 - \rho)n,
\]

Figure 1: OPE under a covariate shift. Covariate, action, reward are denoted by \( X, A, Y \). Evaluation and behavior policies are denoted by \( \pi^e, \pi^b \). Here, \( p(x) \neq q(x) \), and the density ratio \( q(x) / p(x) \) is unknown. The density \( p(y \mid a, x) \) is the same in historical and evaluation data. For the evaluation data, \( A \) and \( Y \) are not observed.
where \( p(x) \) and \( q(x) \) are densities over \( \mathcal{X} \), \( \rho \) is a constant \( \rho \in (0, 1) \), and \( n \in \mathbb{N} \). Here, \( \rho \) can be calculated as \( \rho = \frac{\sum_{i} n_{\text{hst}}(x_i)}{n_{\text{hst}}} \). The policy \( \pi^b(a \mid x) \) of historical data is called a behavior policy. We generally assume \( p(x) \), \( q(x) \) and \( \pi^b(a \mid x) \) to be unknown. In comparison to the usual situation of OPE, the density of historical data, \( p(x) \), can be different from that of the evaluation data, \( q(x) \). This sampling mechanism is called stratified sampling (Imbens & Lancaster, 1996; Wooldridge, 2001).

**Mixture Distribution:** We can consider another data generating process called mixture distribution (Dahabreh et al., 2019). The assumption of mixture distribution includes the assumption that \( \rho \) in the proposed data generating process is a random variable. However, in many practical cases, \( \rho \) is given as a constant value. If we consider a situation where \( \rho \) is fixed, a stratified sampling scheme defined as defined above is more natural.

**Notation:** This paper distinguishes the covariates between the historical and evaluation data as \( X_i \) and \( Z_i \), respectively. Hence, for a function \( \mu : \mathcal{X} \rightarrow \mathbb{R} \), \( \mathbb{E}[\mu(X)] \) and \( \mathbb{E}[\mu(Z)] \) imply taking expectation over historical and evaluation data, respectively. Likewise, the empirical approximation is denoted as \( \mathbb{E}_{n_{\text{hst}}}[\mu(X)] = 1/n_{\text{hst}} \sum_{i} \mu(X_i) \) and \( \mathbb{E}_{n_{\text{evl}}}[\mu(X)] = 1/n_{\text{evl}} \sum_{i} \mu(Z_i) \). Additionally, let \( \|\mu(X, A, Y)\|_2 = \mathbb{E}[\mu^2(X, A, Y)]^{1/2} \) for the function \( \mu \), \( \mathbb{E}_{p(x,a,y)}[\mu(x,a,y)] = \int \mu(x,a,y)p(x,a,y)dx \), the asymptotic MSE of estimator \( \hat{R} \) be \( \text{Asmse}[\hat{R}] = \lim_{n \to \infty} n\mathbb{E}[(\hat{R} - R)^2] \), and \( \mathcal{N}(0, A) \) be a normal distribution with mean 0 and variance \( A \). Besides, we use functions \( r(x) = q(x)p(x) \), \( w(a,x) = \pi^a(a \mid x)/\pi^b(a \mid x) \), and \( f(a) = \mathbb{E}[Y \mid X = x, A = a] \). Let us denote the estimators of \( r(x) \), \( w(a, x) \), and \( f(a, x) \) as \( \hat{r}(x) \), \( \hat{w}(a, x) \), and \( \hat{f}(a, x) \), respectively. Other notations are summarized in Appendix A.

**Assumptions:** We assume overlaps of the distributions of policies and covariates, and corresponding properties for each estimator.

**Assumption 1.** \( 0 \leq r(X) \leq C_1 \), \( 0 \leq w(A, X) \leq C_2 \), \( 0 \leq Y \leq R_{\text{max}} \).

**Assumption 2.** \( 0 \leq \hat{r}(x) \leq C_1 \), \( 0 \leq \hat{w}(a, x) \leq C_2 \), \( 0 \leq \hat{f}(a, x) \leq R_{\text{max}} \).

**Remark 1.** Although we do not explicitly use counterfactual notation (Rubin, 1987), if we assume the usual conditions, our results immediately apply (Appendix B).

### 2.2 Off-Policy Evaluation and Learning

We are interested in estimating the expected reward from any given evaluation policy \( \pi^e(a \mid x) \), which is a pre-specified policy for the evaluation data. Here, we assume a covariate shift, which is a common situation in the literature of external validity. In a covariate shift, while the conditional distribution of \( y \) are the same between historical and evaluation data, the distribution of evaluation data is different from historical data, i.e., the distribution of evaluation data with evaluation policy \( \pi^e \) follows \( q(x)\pi^e(a \mid x)p(y \mid a, x) \). Then, we define the expected reward of evaluation policy over evaluation data as follows:

\[
R(\pi) := \mathbb{E}_{q(x)\pi^e(a\mid x)p(y\mid x,a)}[y].
\]

Then, the first goal is OPE, which estimates \( R(\pi^e) \) using the historical data \( \{X_i, A_i, Y_i\}_{i=1}^{n_{\text{hst}}} \) and evaluation data \( \{Z_i\}_{i=1}^{n_{\text{evl}}} \). The second goal is OPL, which trains a policy that maximizes the expected reward, i.e.,

\[
\pi^* = \arg \max_{\pi(a \mid x) \in \Pi} R(\pi),
\]

where \( \Pi \) is the policy class. In some cases, to construct an estimator \( R(\pi) \), we use the functions \( r(x) \), \( w(a, x) \), and \( f(a, x) \). These functions are called nuisance functions of the parameter of interest, \( R(\pi) \).

### 2.3 Preliminaries

Here, we review the existing works of OPE, OPL, and the density ratio estimation.

**Standard OPE and OPL:** We review three types of standard estimators of \( \mathbb{E}_{p(x)\pi^e(a\mid x)p(y\mid x,a)}[y] \) under the case where \( q(x) = p(x) \) in (1). The first estimator is an inverse probability weighting estimator (IPW) estimator given by \( \mathbb{E}_{n_{\text{evl}}}[w(A, X)Y] \) (Rubin 1987; Hirano et al., 2003; Swaminathan & Joachims, 2015b). Even though this estimator is unbiased when the behavior policy is known, it suffers from high variance. The second estimator is a direct method
where  If we know the behavior policy as in a RCT , we can exactly know 

For OPE under a covariate shift, we propose and analyze an estimator constructed from the following basic form:

\[ \mathbb{E}_{n_{\text{hst}}} [\hat{f}(A, X)] \]  

[Hahn, 1998]. This estimator is known to be weak against model misspecification for \( f(a, x) \). The third estimator is a doubly robust estimator [Robins et al., 1994; Chernozhukov et al., 2018]:

\[ \mathbb{E}_{n_{\text{hst}}} [\hat{w}(A, X) (Y - \hat{f}(A, X)) + \mathbb{E}_{\pi(a|x)} [\hat{f}(a, x) \mid X]]. \] (3)

Under certain conditions, it is known that this estimator achieves the efficiency bound (a.k.a semiparametric lower bound), which is the lower bound of the asymptotic MSE of OPE, among regular \( \sqrt{n} \)-consistent estimators [van der Vaart, 1998, Theorem 25.20]. This efficiency bound is

\[ \mathbb{E}[w^2(A, X) \text{var}[Y \mid A, X]] + \text{var}[\hat{V}(X)], \] (4)

where \( \hat{v}(x) = \mathbb{E}_{\pi(a|x)}[f(a, x) \mid x] \) (Narita et al., 2019). Such estimator is called an efficient estimator. These estimators are also used for OPL [Athey & Wager, 2017; Foster & Syrgkanis, 2019].

Density Ratio Estimation: In this paper, to estimate \( R(\pi) \), we apply an importance weighting using the density ratio between distributions of covariates of historical and evaluation data. For example, if we know \( r(x) \) and \( w(a, x) \), we can construct the following estimator of \( R(\pi^e) \):

\[ \mathbb{E}_{n_{\text{hst}}} [r(X) w(A, X) Y]. \]

If we know the behavior policy as in a RCT, we can exactly know \( w(a, x) \). However, since we do not know the density ratio \( r(x) \) even in a RCT, we have to estimate \( r(x) \) using the covariate data: \( \{X_i\}_{i=1}^{n_{\text{hst}}}, \{Z_i\}_{i=1}^{n_{\text{evl}}} \). To estimate the density ratio \( r(x) \), we use a nonparametric one-step loss based estimator. For example, we can employ Least-Squares Importance Fitting (LSIF), which uses the squared loss to fit the density-ratio function (Kanamori et al., 2012). We show details of the density ratio estimation in Appendix C

3 Efficiency Bound under a Covariate Shift

We discuss the efficiency bound of OPE under a covariate shift following the general literature [Bickel et al., 1998; Tsiatis, 2006]. Efficiency bound is defined for an estimator under some posited models of the data generating process. If this posited model is a parametric model, it is equal to Cramér-Rao lower bound. When this posited model is non or semiparametric model, we can still define a corresponding Cramér-Rao lower bound. In this paper, we modify the standard theory under i.i.d. sampling to the current problem with a stratified sampling scheme. The formal definition is shown in Appendix D.

Here, we show the efficiency bound of OPE under a covariate shift.

Theorem 1. The efficiency bound of \( R(\pi^e) \) under fully nonparametric models, \( T(\pi^e) \), is

\[ \rho^{-1} \mathbb{E}[r^2(X) w^2(A, X) \text{var}[Y \mid A, X]] + (1 - \rho)^{-1} \text{var}[\hat{v}(Z)] \] (5)

where \( \hat{v}(z) = \mathbb{E}_{\pi^e(a|z)}[f(a, z) \mid z] \). The efficiency bound under a nonparametric model with fixed \( p(x) \) and \( \pi^b(a \mid x) \) is the same.

The proof is shown in Appendix D. Here, the knowledge of the density function for the historical data \( p(x) \) and the behavior policy \( \pi^b(a \mid x) \) does not change the efficiency bound. This is an analogous result from a standard situation where the knowledge of \( \pi^b(a \mid x) \) does not change the efficiency bound (4) (Robins et al., 1994; Hahn, 1998).

Comparison of (5) and (4) The efficiency bound under a covariate shift, i.e., (5) is reduced to the bound without a covariate shift (4) as follows. Let us consider the case \( r(x) = 1, \rho = 0.5 \), which means \( p(x) = q(x) \). Then, we can see \( (5) = 2 \times (4) \). The factor 2 originates from the scaling of asymptotic MSE.

4 OPE under a Covariate Shift

For OPE under a covariate shift, we propose and analyze an estimator constructed from the following basic form:

\[ \mathbb{E}_{n_{\text{hst}}} [\hat{r}(X) \hat{w}(A, X) \{Y - \hat{f}(A, X)\}] + \mathbb{E}_{n_{\text{evl}}} [\hat{v}(Z)], \] (6)

where \( \hat{v}(z) = \mathbb{E}_{\pi^e(a|z)}[f(a, z) \mid z] \), and \( \hat{r}(X), \hat{w}(a, x), \) and \( \hat{f}(a, x) \) are nuisance estimators of \( r(x), w(a, x), \) and \( f(a, x) \). As well as the conventional doubly robust estimator (3), the above form is designed to have the double robust
Second, we consider the case where $\hat{K}$ is the average of the $r$ and $\hat{w}(x)$ averages over $w$ and $r$, which are different from $w$ and $r$.

Algorithm 1 Doubly Robust Estimator under a Covariate Shift

**Input:** The evaluation policy $\pi^e$.

- Take a $\Xi$-fold random partition $(I_k)_{k=1}^\Xi$ of observation indices $\{n_{\text{hst}}\} = \{1, \ldots, n_{\text{hst}}\}$ such that the size of each fold $I_k$ is $n_{\text{hst}} = n_{\text{hst}}/\Xi$.
- Take a $\Xi$-fold random partition $(J_k)_{k=1}^\Xi$ of observation indices $\{n_{\text{evl}}\} = \{1, \ldots, n_{\text{evl}}\}$ such that the size of each fold $J_k$ is $n_{\text{evl}} = n_{\text{evl}}/\Xi$.

For each $k \in \Xi = \{1, \ldots, \Xi\}$, define $I_k^c := \{1, \ldots, n_{\text{hst}}\} \setminus I_k$ and $J_k^c := \{1, \ldots, n_{\text{evl}}\} \setminus J_k$.

Define $(\mathcal{S}_k)_{k=1}^\Xi$ with $\mathcal{S}_k = \{(X_i, A_i, Y_i)_{i \in I_k^c}, \{X_j\}_{j \in J_k^c}\}$.

for $k \in \Xi$ do

- Construct an estimator $\hat{w}_k(a, x), \hat{r}_k(x)$, and $\hat{f}_k(a, x)$ using $\mathcal{S}_k$.

end for

Construct an estimator $\hat{R}$ of $R$ by taking the average of $\hat{R}_k$ for $k \in \Xi$, i.e., $\hat{R} = \frac{1}{\Xi} \sum_{k=1}^\Xi \hat{R}_k$.

The formal result is given later in Theorem 3.

We consider estimating $r(x)w(a, x)$ and $f(a, x)$. First, we consider the case where $\hat{r}(x) = r(x)$ and $\hat{w}(a, x) = w(a, x)$, but $\hat{f}(a, x)$ is equal to $f^\dagger(a, x)$ different from $f(a, x)$, i.e., we have correct models for $r(x)$ and $w(a, x)$, but not for $f(a, x)$. Then, (5) is a consistent estimator for $\hat{R}(\pi^e)$ since

\[
\mathbb{E}_{n_{\text{hst}}}[r(X)w(A, X)Y] + \mathbb{E}_{n_{\text{evl}}} [\mathbb{E}_{\pi^e(a|Z)}[f^\dagger(a, Z) | Z] - r(X)w(A, X)f^\dagger(A, X)] \\
\approx \mathbb{E}_{n_{\text{hst}}}[r(X)w(A, X)Y] + 0 \approx R(\pi^e).
\]

Second, we consider the case where $\hat{f}(a, x) = f(a, x)$, but $\hat{r}(x)$ and $\hat{w}(a, x)$ are equal to functions $r^\dagger(x)$ and $w^\dagger(a, x)$, which are different from $r(x)$ and $w(a, x)$, respectively, i.e, we have correct models for $f(a, x)$, but not for $r(x)$ and $w(a, x)$. Then, (6) is a consistent estimator for $\hat{R}(\pi^e)$ since

\[
\mathbb{E}_{n_{\text{hst}}}[r^\dagger(X)w^\dagger(a, x)\{Y - f(a, X)\}] \\
+ \mathbb{E}_{n_{\text{evl}}} [\mathbb{E}_{\pi^e(a|Z)}[f(a, Z) | Z]] \\
\approx \mathbb{E}_{n_{\text{evl}}} [\mathbb{E}_{\pi^e(a|Z)}[f(a, Z) | Z]] + 0 \approx R(\pi^e).
\]

The formal result is given later in Theorem 3.

We consider estimating $r(x), w(a, x)$, and $f(a, x)$.

For example, for $f(a, x)$ and $w(a, x)$, we can apply complex and data-adaptive regression and density estimation methods such as random forests, neural networks, and highly adaptive Lasso (Díaz, 2019). Note that $\hat{w}(a, x)$ is estimated as $\tilde{\pi}^e/\tilde{r}^e$ since $\pi^e$ is known, where $\tilde{\pi}^e$ is an estimator of $\pi^e$. For $r(x)$, we can use the data-adaptive density ratio method in Section 2.3. Although the estimators obtained from such complex estimators approximate the true values well, Chernozhukov et al. (2018) pointed out that such estimators often violate the Donker condition, which is required to obtain the asymptotic distribution of an estimator of interest, such as (5).

4.1 Doubly Robust Estimator under a Covariate Shift

For deriving the asymptotic distribution of an estimator of $\hat{R}(\pi^e)$ using estimators without the Donker condition, we apply cross-fitting (Chernozhukov et al. 2018) based on (6). If the estimator has a doubly robust structure, then the stochastic equivalence term needed for the analysis is controlled without the Donker condition.

The procedure is as follows. First, we separate data $D_{\text{hst}}$ and $D_{\text{evl}}$ into $\Xi$ groups. Next, using samples in each group, we estimate the nuisance functions nonparametrically. Then, we construct an estimator of $\hat{R}(\pi^e)$ using the nuisance estimators. For each group $k \in \{1, 2, \ldots, \Xi\}$, we define an estimator of $R(\pi^e)$ as follows:

\[
\hat{R}_k = \mathbb{E}_{n_{\text{hst}}}[\hat{r}^{(k)}(X)\hat{w}^{(k)}(A, X)\{Y - \hat{f}^{(k)}(A, X)\}] \\
+ \mathbb{E}_{n_{\text{evl}}} [\mathbb{E}_{\pi^e}[\hat{f}^{(k)}(a, Z) | Z]],
\]

where $\mathbb{E}_{n_{\text{hst}}}$ is the sample average over $k$-th partitioned historical data with $n_{\text{hst}}$ samples and $\mathbb{E}_{n_{\text{evl}}}$ is the sample average over $k$-th partitioned evaluation data with $n_{\text{evl}}$ samples. Finally, we construct an estimator of $\hat{R}(\pi^e)$ by taking the average of the $K$ estimators, $\{\hat{R}_k\}$. We call the estimator doubly robust estimator under a covariate shift (DRCS).
and denote it as $\hat{R}_{\text{DRCS}}(\pi^e)$. The whole procedure is given in Algorithm 1. In the following theorem, we show the asymptotic property of this estimator $\hat{R}_{\text{DRCS}}(\pi^e)$.

**Theorem 2 (Efficiency of $\hat{R}_{\text{DRCS}}(\pi^e)$).** For $k \in \{1, \cdots, \Xi\}$, assume there exists $p > 0$, $q > 0$, $p + q \geq 1/2$ such that

\[
\|\hat{r}^{(k)}(X)\hat{w}^{(k)}(A, X) - r(X)w(A, X)\|_2 = o_p(n^{-p}),
\]

\[
\|\hat{f}^{(k)}(A, X) - f(A, X)\|_2 = o_p(n^{-q}).
\]

Then, we have

\[\sqrt{n}(\hat{R}_{\text{DRCS}}(\pi^e) - R(\pi^e)) \xrightarrow{d} \mathcal{N}(0, \Upsilon(\pi^e)),\]

where $\Upsilon(\pi^e)$ is an efficiency bound in Theorem 7.

Importantly, the Donsker condition is not needed for nuisance estimators owing to the cross-fitting and the doubly robust form of the estimator. What we only need are rate conditions. However, the rate conditions are mild since these are nonparametric rates smaller than 1/2. For example, this is satisfied when $p = 1/4$, $q = 1/4$. Under some smoothness conditions, the nonparametric estimator $\hat{f}(a, x)$ is guaranteed to achieve this convergence rate (Wainwright, 2019).

Regarding $r(x)w(a, x)$, we can easily show that if $\hat{\pi}^b(a \mid x)$ and $\hat{w}(a, x)$ similarly satisfy some nonparametric rates, $\hat{r}(x)\hat{w}(a, x)$ satisfies it as well.

**Lemma 1. Assume**

\[
\|\hat{r}(X) - r(X)\|_2 = o_p(n^{-p}),
\]

\[
\|\hat{w}(A, X) - w(A, X)\|_2 = o_p(n^{-p}).
\]

Then,

\[
\|\hat{r}(X)\hat{w}(A, X) - r(X)w(A, X)\|_2 = o_p(n^{-p}).
\]

Next, we formally show double robustness of the estimator, i.e., the estimator is consistent if either $r(x)w(a, x)$ or $f(a, x)$ is correct.

**Theorem 3 (Double robustness).** For $k \in \{1, \cdots, \Xi\}$, assume

\[
\|\hat{f}^{(k)}(A, X) - f^{(k)}(A, X)\|_2 = o_p(1),
\]

\[
\|\hat{r}^{(k)}(X)\hat{w}^{(k)}(A, X) - r^{(k)}(X)r^{\dagger}(A, X)\|_2 = o_p(1).
\]

If $r^1(a, x) = r(x)w(a, x)$ or $q^1(a, x) = q(a, x)$ holds, the estimator $\hat{R}_{\text{DRCS}}(\pi^e)$ is consistent.

**Remark 2 (Asymptotic property scaled by $n^{\text{best}}$).** We consider the scaling by $n^{\text{best}}$ instead of $n$, i.e., $\text{AsmSe}[\hat{R}] = \lim_{n^{\text{best}} \to \infty} n^{\text{best}} \mathbb{E}[(\hat{R} - R)^2]$. Then, by multiplying $p$ by $\Upsilon(\pi^e)$, the asymptotic MSE of $\hat{R}_{\text{DRCS}}(\pi^e)$ is given as

\[
\mathbb{E}[r^2(X)w^2(A, X)\var[Y \mid A, X]] + (1 - \rho)^{-1}\rho\var[v(Z)].
\]

In this case, the asymptotic MSE is

\[
\mathbb{E}[r^2(X)w^2(A, X)\var[Y \mid A, X]].
\]

**4.2 OPE with Known Distribution of Evaluation Data**

As a special case of OPE under a covariate shift, we consider a case where $q(x)$ is known. This case can be observed as a common OPE situation by regarding $p(x)(\pi^e(a \mid x)$ as the behavior policy, the evaluation policy as $q(x)(\pi^e(a \mid x)$, and $(A, X)$ as the action. By applying (4) in Section 2.3, we obtain the following efficiency bound under nonparametric model:

\[
\Upsilon(\pi^e) = \mathbb{E}[r^2(X)w^2(A, X)\var[Y \mid A, X]].
\]

As the estimator $\hat{R}_{\text{DRCS}}(\pi^e)$ in Section 4.1 we construct an estimator with cross-fitting. Instead of (7), we use the following estimator:

\[
\mathbb{E}_{n^{\text{best}}}[r^{(k)}(X)\hat{w}^{(k)}(A, X)|Y - \hat{f}^{(k)}(A, X)] + \mathbb{E}_{q(z)\pi^e(a \mid z)}[(\hat{f}(a, z)]
\]

The algorithm is almost the same as before. To estimate $r(x)$, we can simply use density estimation for $p(x)$ since $q(x)$ is known and the integration in $\mathbb{E}_{q(z)\pi^e(a \mid z)}[\hat{f}(a, z)]$ can be taken exactly since $q(x)$ and $\pi^e(a \mid x)$ are known. Let us denote this estimator as $\hat{R}_{\text{DRCS}}$. We can show that $\hat{R}_{\text{DRCS}}(\pi^e)$ achieves the efficiency bound.
Theorem 4 (Efficiency of $\hat{R}_{DRCS}$). For $k \in \{1, \ldots, \Xi\}$, assume there exists $p > 0$, $q > 0$, $p + q \geq 1/2$ such that
\[
\|\hat{r}^{(k)}(X)\hat{w}^{(k)}(A, X) - r(X)w(A, X)\|_2 = o_p(n^{-p}), \\
\|\hat{f}^{(k)}(A, X) - f(A, X)\|_2 = o_p(n^{-q}).
\]
Then, we have
\[
\sqrt{n} \text{bias}(\hat{R}_{DRCS}(\pi^e)) = R(\pi^e)
\]
This asymptotic variance is equal to the asymptotic variance when $\rho = 0$ as shown in Remark 2 because the case $\rho = 0$ implies that we have infinite data from $q(x)$.

5 Other Candidates of Estimators

We have discussed estimators based on doubly robust estimators in the previous section. Next, we propose other estimators under a covariate shift based on IPW and DM estimators. We analyze each estimator’s property with nuisance estimators obtained from kernel regression (Nadaraya, 1964; Watson, 1964). We show regularity conditions in this section following Newey & Mcfadden (1994) in Appendix E. Note that we can usually obtain results with the same asymptotic MSE under suitable smoothness conditions even if we use nonparametric estimators other than kernel estimators (Chen, 2007).

5.1 IPW Estimators

We consider an IPW estimator under a covariate shift for the cases where we have an oracle of $\pi^b(a \mid x)$ and where we do not have any oracles of nuisance functions.

IPW estimators with oracle $\pi^b(x)$: This is a natural setting in a RCT and A/B testing since we assign actions following a certain probability in these cases. Let us define an IPW estimator under a covariate shift with the true behavior policy $\pi^b(a \mid x)$ (IPWCSB):
\[
\hat{R}_{IPWCSB}(\pi^e) = \mathbb{E}_{n^{evl}} \left[ \frac{\hat{q}(X)\pi^e(A|X)Y}{\hat{p}(X)\pi^e(A|X)} \right].
\]

For example, we can use a kernel density estimator of $q(x)$:
\[
\hat{q}_h(x) = \frac{1}{nh} \sum_{i=1}^{n^{evl}} h^{-d}K\left(\frac{x - x_i}{h}\right),
\]

where $K(\cdot)$ is a kernel function, $h$ is the bandwidth of $K(\cdot)$, and $d$ is a dimension of $x$. The same procedure is applied for the estimation of $p(x)$. When using a kernel estimator, we obtain the following theorem.

Theorem 5 (Informal). When $\hat{q}(x) = \hat{q}_h(x)$, $\hat{p}(x) = \hat{p}_h(x)$ where $\hat{p}_h(x)$ is a kernel estimator based on $D^{n^{evl}}$ as defined in (11). The asymptotic MSE of $\hat{R}_{IPWCSB}(\pi^e)$ is
\[
\rho^{-1} \text{var}[r(X)\{w(A, X)Y - v(X)\}] + (1 - \rho)^{-1} \text{var}[v(Z)].
\]

Fully nonparametric IPW estimators: Let us define an IPW estimator under a covariate shift (IPWCS):
\[
\hat{R}_{IPWCS}(\pi^e) = \mathbb{E}_{n^{evl}} \left[ \frac{\hat{q}(X)\pi^e(A|X)Y}{\hat{p}(X)\pi^e(A|X)} \right].
\]

Under certain conditions in Appendix E this estimator achieves the efficiency bound.

Theorem 6 (Informal). When $\hat{q}(x) = \hat{q}_h(x)$, $\hat{p}(x) = \hat{p}_h(x)$, $\hat{\pi}_h^b(a \mid x) = \pi^b(a \mid x)$, where $\hat{\pi}_h^b(a \mid x)$ is a kernel estimator based on $D^{n^{evl}}$, the asymptotic MSE of $\hat{R}_{IPWCS}(\pi^e)$ is $\Upsilon(\pi^e)$.

5.2 Direct Method Estimator

Let us define a nonparametric DM estimator:
\[
\hat{R}_{DM}(\pi^e) = \mathbb{E}_{n^{evl}} \left[ \mathbb{E}_{\pi^e(a|Z)} f(a, Z) \mid Z \right].
\]

Under certain conditions in Appendix E this estimator achieves the efficiency bound.

Theorem 7 (Informal). When $\hat{f}_h(a, x)$ is a kernel estimator based on $D^{n^{evl}}$, the asymptotic MSE of $\hat{R}_{DM}(\pi^e)$ is $\Upsilon(\pi^e)$.
Table 1: Comparison of estimators. DR means double robustness. Non-Donsker means whether any non-Donsker type complex estimators can be allowed to plug-in with valid theoretical guarantee. All of estimators here do not require any parametric model assumptions.

| Estimator          | Efficiency | Double robustness | Nuisance Functions | Without oracle of $\pi^b(x)$ | Non-Donsker |
|-------------------|------------|------------------|--------------------|-----------------------------|-------------|
| $\hat{R}_{IPWCS}({\pi^c})$ |            |                  | $r$                |                             |             |
| $\hat{R}_{IPWCS}({\pi^c})$ |           |                  | $r, w$             |                             |             |
| $\hat{R}_{DM}({\pi^c})$        |           |                  | $f$                |                             |             |
| $\hat{R}_{DRCS}({\pi^c})$      |           |                  | $r, w, f$          |                             |             |

5.3 Summary of IPWCS, DM and DRCS Estimators

In this section, we summarize the property of the proposed estimators for $R({\pi^c})$. This is also summarized in Table 1.

Order of asymptotic MSEs: The order of the variances of the proposed estimators is given as

$$\text{Asmse}[\hat{R}_{IPWCSB}] \geq \text{Asmse}[\hat{R}_{IPWCS}] = \text{Asmse}[\hat{R}_{DM}] = \text{Asmse}[\hat{R}_{DRCS}].$$

Comparison among IPW estimators: We can observe that the asymptotic MSE of $\hat{R}_{IPWCSB}$ is smaller than that of $\hat{R}_{IPWCS}$. This looks unusual since $\hat{R}_{IPWCSB}$ uses more knowledge. The intuitive reason of this fact is that $\hat{R}_{IPWCS}$ is considered to be using control variate. The same paradox is known in other works of causal inference (Robins et al., 1992; Henmi & Eguchi, 2004). Note that this fact does not imply $\hat{R}_{IPWCS}$ is superior to $\hat{R}_{IPWCSB}$ since more smoothness conditions are required in $\hat{R}_{IPWCS}$, and this can be violated in practice (Robins & Ritov, 1997).

Most practical estimator: It is generally recommended to use $\hat{R}_{DRCS}$ though the asymptotic MSE of $\hat{R}_{IPWCS}$, $\hat{R}_{DM}$ and $\hat{R}_{DRCS}$ are the same. First, the DRCS estimator $\hat{R}_{DRCS}$ allows any non-Donsker type complex estimators with weak convergence rate conditions for the nuisance functions. However, the analyses of $\hat{R}_{IPWCS}$ and $\hat{R}_{DM}$ are specific to the kernel estimators. Even though the kernel estimators can be replaced with any non-Donsker type complex estimators, the rate condition $||\hat{r}(X)\hat{w}(A, X) - r(X)w(A, X)||_2 = o_p(n^{-1/4})$ or $||\hat{f}(A, X) - f(A, X)||_2 = o_p(n^{-1/4})$ cannot guarantee the $\sqrt{n}$-consistency and efficiency of $\hat{R}_{DRCS}$ and $\hat{R}_{IPWCS}$ even if we use cross-fitting. Second, $\hat{R}_{IPWCS}$ and $\hat{R}_{DM}$ do not have double robustnesses. Therefore, $\hat{R}_{DRCS}$ is considered to be more practical.

6 OPL under a Covariate Shift

In this section, we propose an algorithm for OPL based on the doubly robust estimator $\hat{R}_{DRCS}({\pi^c})$ to estimate the optimal policy that maximizes the expected reward over the evaluation data. The optimal policy $\pi^\ast$ is defined as $\pi^\ast = \arg\max_{\pi \in \Pi} R(\pi)$, where recall that $\Pi$ is a policy class. By applying each OPE estimator, we define the following estimators for the optimal policy:

$$\hat{\pi}_{DRCS} = \arg\max_{\pi \in \Pi} \hat{R}_{DRCS}(\pi),$$
$$\hat{\pi}_{DM} = \arg\max_{\pi \in \Pi} \hat{R}_{DM}(\pi),$$
$$\hat{\pi}_{IPWCS} = \arg\max_{\pi \in \Pi} \hat{R}_{IPWCS}(\pi).$$

To obtain a theoretical implication, for simplicity, we assume that $A$ is a finite state space and the policy class $\Pi$ is deterministic. Then, the $\epsilon$-Hamming covering number $N_H(\epsilon, \Pi)$ and its entropy integral are defined as $\kappa(\Pi) = \int_0^\infty \sqrt{\log N_H(\epsilon^2, \Pi)}d\epsilon$ following Zhou et al. (2018). Then, the regret for $\hat{\pi}_{DRCS}$ is obtained as follows.

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In this section, we omit $\pi^c$ from the estimator $\hat{R}(\pi^c)$. 

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8
Theorem 8 (Regret of $\hat{\pi}_{DRCS}$). Assume that for any $0 < \epsilon < 1$, there exists $\omega$ such that $N_H(\epsilon, \Pi) \approx \exp(1/\epsilon)^{\omega}$, $0 < \omega < 0.5$, and

\[
\|\hat{f}^{(k)}(X) - r(X)\|_2 = o_p(n^{-1/4}),
\|1/\hat{\pi}^{(k)}_{b}(A, X) - 1/\pi^b(A, X)\|_2 = o_p(n^{-1/4}),
\|\hat{f}^{(k)}(A, X) - f(A, X)\|_2 = o_p(n^{-1/4}).
\]

Then, by defining $\Upsilon_* = \sup_{\pi \in \Pi} \Upsilon(\pi)$, there exists an integer $N_\delta$ such that with probability at least $1 - 2\delta$, for all $n \geq N_\delta$,

\[
R(\pi^*) - R(\hat{\pi}_{DRCS}) \approx \left(k(\Pi) + \sqrt{\log(1/\delta)}\right) \sqrt{\frac{1}{n}}.
\]

In comparison to the regret results in Swaminathan & Joachims (2015b); Kitagawa & Tetenov (2018), we do not assume that we know the true behavior policy. Because $R_{DRCS}(\pi)$ has the double robustness structure, we can obtain the regret bound under weak nonparametric rate conditions as in Athey & Wager (2017); Foster & Syrgkanis (2019) without assuming the behavior policy is known. In addition, this theorem shows that the variance term is related to attain the low regret. This is achieved by using efficient estimators $R_{DRCS}(\pi)$ for a policy $\pi$.

7 Experiments

In this section, we demonstrate the effectiveness of the proposed estimators using data obtained with bandit feedback. Following Dudík et al. (2011); Farajtabar et al. (2018), we evaluate the proposed estimators using the standard classification datasets from the UCI repository by transforming the classification data into contextual bandit data. From the UCI repository, we use SatImage, Vehicle, and PenDigits datasets.

First, we classify data into historical and evaluation data with probability defined as follows:

\[
p(hist = +1|X_i) = \frac{C_{\text{prob}}}{1 + \exp(-\tau(X_i) + 0.1\epsilon)},
\]

\[
\tau(X_i) = X_{1,i} + X_{2,i} + X_{3,i} + X_{4,i} + X_{5,i},
\]

where $hist = +1$ denotes that the sample $i$ belongs to the historical data, $C_{\text{prob}}$ is a constant, $\epsilon$ is a random variable that follows the standard normal distribution, and $X_{k,i}$ is the $k$-th element of the vector $X_i$. By adjusting $C_{\text{prob}}$, we classify 70% samples as the historical data and 30% samples as the evaluation data. Thus, we generate the historical and evaluation data under a covariate shift. Then, we make a deterministic policy $\pi_d$ by training a logistic regression classifier on the historical data. We construct three behavior policies as mixtures of $\pi^d$ and the uniform random policy $\pi^u$ by changing a mixture parameter $\alpha$, i.e., $\pi^b = \alpha \pi^d + (1 - \alpha) \pi^u$. The candidates of the mixture parameter $\alpha$ are $\{0.7, 0.4, 0.0\}$ as Kallus & Uehara (2019a). In Section 7.1, we show the experimental results of OPE. In Section 7.2, we show the experimental results of OPL. In both sections, the historical $p(x)$ and evaluation distributions $q(x)$ are unknown, and the behavior policy $\pi^b$ is also unknown.

7.1 Experiments of Off-Policy Evaluation

In the experiments of OPE, we use an evaluation policy $\pi^e$ defined as $0.9\pi^d + 0.1\pi^u$. Here, we compare the MSEs of five estimators, DRCS, DM, DM-R, IPWCS, and IPW-R. DRCS is based on the proposed estimator $\hat{R}_{DRCS}$ where we use Ridge regression based on reproducing kernel hilbert space (RKHS) for estimating $f(a, x)$ and $w(a, x)$ and use KuLISF for $r(x)$. For this estimator, we use 2-fold cross-fitting. DM is the direct method estimator $\hat{R}_{DM}(\pi^e)$ with $f(a, x)$ estimated by kernel regression defined in Section 5 DM-R is the same estimator, but we use Ridge regression based on RKHS for $f(a, x)$. IPWCS is the IPW estimator $\hat{R}_{IPWCS}(\pi^e)$ where we use kernel regression defined in Section 5 to estimate $r(x)$ and $w(a, x)$. IPW-R is the same estimator, but we use KuLISF (Kanamori et al., 2012) to estimate $r(x)$. Note that nuisance estimators in DM-R and IPW-R do not satisfy the Donsker condition.

The resulting MSE and the standard deviation (STD) over 20 replications of each experiment are shown in Tables 4, 5 where we highlight in bold the best two estimator in each case. DRCS generally outperforms the other estimators. This shows that the efficiency and double robustness of DRCS translate to good performance. While IPWCS-R shows better performance than DRCS in SatImage dataset, IPWCS-R drops the performance for Vehicle dataset. IPWCS has
Table 2: Off-policy evaluation with SatImage dataset

| Behavior Policy | DRCS    | IPWCS   | DM     | IPWCS-R | DM-R   |
|-----------------|---------|---------|--------|---------|--------|
|                 | MSE std | MSE std | MSE std | MSE std | MSE std |
| 0.7π^d + 0.3π^u | 0.107   | 0.032   | 0.042  | 0.045   | 0.049  |
| 0.4π^d + 0.6π^u | 0.096   | 0.025   | 0.134  | 0.093   | 0.069  |
| 0.0π^d + 1.0π^u | 0.154   | 0.051   | 0.336  | 0.022   | 0.026  |

Table 3: Off-policy evaluation with Vehicle dataset

| Behavior Policy | DRCS    | IPWCS   | DM     | IPWCS-R | DM-R   |
|-----------------|---------|---------|--------|---------|--------|
|                 | MSE std | MSE std | MSE std | MSE std | MSE std |
| 0.7π^d + 0.3π^u | 0.029   | 0.019   | 0.038  | 0.095   | 0.046  |
| 0.4π^d + 0.6π^u | 0.019   | 0.024   | 0.062  | 0.076   | 0.057  |
| 0.0π^d + 1.0π^u | 0.037   | 0.030   | 0.213  | 0.233   | 0.210  |

Table 4: Off-policy learning with SatImage dataset

| Behavior Policy | DRCS    | IPWCS   | DM     |
|-----------------|---------|---------|--------|
|                 | RWD std | RWD std | RWD std |
| 0.7π^d + 0.3π^u | 0.723   | 0.423   | 0.638  |
| 0.4π^d + 0.6π^u | 0.710   | 0.482   | 0.641  |
| 0.0π^d + 1.0π^u | 0.652   | 0.460   | 0.465  |

Table 5: Off-policy learning with Vehicle dataset

| Behavior Policy | DRCS    | IPWCS   | DM     |
|-----------------|---------|---------|--------|
|                 | RWD std | RWD std | RWD std |
| 0.7π^d + 0.3π^u | 0.496   | 0.310   | 0.411  |
| 0.4π^d + 0.6π^u | 0.510   | 0.290   | 0.393  |
| 0.0π^d + 1.0π^u | 0.480   | 0.280   | 0.313  |

7.2 Experiments of Off-Policy Learning

In the experiments of OPL, we compare the performances of three estimators for the optimal policy maximizing expected reward over the evaluation data: \( \hat{\pi}_{\text{DRCS}} \) with \( f(a, x) \) and \( w(a, x) \) estimated by Ridge regression based on RKHS and \( r(x) \) estimated by KuLISF (DRCS), \( \hat{\pi}_{\text{DM}} \) with \( f(a, x) \) estimated by kernel regression defined in Section 5 (DM), and \( \hat{\pi}_{\text{IPWCS}} \) with \( r(x) \) and \( w(a, x) \) estimated by kernel regression defined in Section 5 (IPWCS). For the policy class \( \Pi \), we use a linear-in-parameter model with the Gaussian kernel defined in Appendix G. For DRCS, we use 2-fold cross-fitting and add a regularization term.

We conducted 10 trials for each experiment. The resulting expected reward over the evaluation data (RWD) and the standard deviation (STD) of estimators for OPL are shown in Tables 4 and 5, where we highlight in bold the best estimator in each case. For all cases, the estimator \( \hat{\pi}_{\text{DRCS}} \) outperforms the other estimators. We can find that, when an estimator of OPE shows high performance, a corresponding estimator of OPL also shows high performance. The results show that the statistical efficiency of OPE estimator translates into better regret performance as in Theorem 8.

8 Conclusion and Future Direction

We calculated the efficiency bound for OPE, and proposed OPE and OPL estimators under a covariate shift. Especially, DRCS is doubly robust and achieves the efficiency bound under weak nonparametric rate conditions. As a future work, we will explore the application of our estimators to more complex settings, such as a longitudinal setting.
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A Notations, Terms, and Abbreviations

In this section, we summarize the notations, terms, and abbreviations used in this paper.

Table 6: Summary of notations

| Symbol | Description |
|--------|-------------|
| A, X, Y | Action, covariate, reward |
| $E[\mu(X, A, Y)]$ | $E[p(x) \pi^b(a | x)p(y | a, x)[\mu(x, a, y)]$ |
| $E[\mu(Z)]$ | $E[\mu(z)]$ |
| $\pi^b(a | x)$ | Behavior policy |
| $\pi^e(a | x)$ | Evaluation policy |
| $R(\pi^e)$ | Semi-parametric lower bound of |
| $r(x)$ | Kernel with a bandwidth |
| $w(a, x)$ | Concatenation of |
| $f(a, x)$ | Number of training data |
| $v(x)$ | Train data, evaluation data |
| $A$ | Policy class |
| $A \lesssim B$ | Entropy integral of $A$ w.r.t $\epsilon$-Hamming distance |
| $k(\Pi)$ | Number of training data |
| $n^{\text{hst}}$ | Number of evaluation data |
| $n^{\text{evl}}$ | There exists an absolute constant $C$ s.t. $A \leq CB$ |
| $C_1, C_2, R_{\max}$ | Upper bound of $r(X), w(A, X), Y$ |
| $\rho$ | $n^{\text{hst}}/(n^{\text{hst}} + n^{\text{evl}})$ |
| $D^{\text{hst}}, D^{\text{evl}}$ | Train data, evaluation data |
| $n^{\text{hst}}_1, n^{\text{hst}}_2$ | Split train data |
| $n^{\text{evl}}_1, n^{\text{evl}}_2$ | Split evaluation data |
| $D_i$ | Concatenation of $n^{\text{hst}}_i$ and $n^{\text{evl}}_i$ for $i = 1, 2$ |
| $G^{\text{hst}}$ | $\sqrt{n^{\text{hst}}}(E_{\text{hst}} - E)$ Empirical process based on train data |
| $G^{\text{evl}}$ | $\sqrt{n^{\text{evl}}}(E_{\text{evl}} - E)$ Empirical process based on evaluation data |
| $\Upsilon(\pi^e)$ | Semi-parametric lower bound of $R(\pi^e)$ under nonparametric model |
| $K_h(\cdot)$ | Kernel with a bandwidth $h$ |
| $n^{\text{hst}}_k$ | $k$-th train data |
| $n^{\text{evl}}_k$ | $k$-th evaluation data |

B Identification under Potential Outcome Framework

We explain how to apply our results in the main draft under potential outcome framework, which is a common framework in causal inference literature (Rubin, 1987). In this section, our goal is justifying DM and IPWCS estimators under potential outcome framework.

Let us denote counterfactual variables based on stochastic policies (interventions) as $Y(B)$, where $B$ is a random variable from the conditional density $\pi^e(b | Z)$ and $Z$ is a random variable following the evaluation density $q(z)$. Here, note what we can observe is data:

$$\{X_i, A_i, Y_i\}_{i=1}^{n^{\text{hst}}} \sim p(x)\pi^b(a | x)p(y | a, x), \{Z_j\}_{j=1}^{n^{\text{evl}}} \sim q(z).$$

A detailed review of the stochastic intervention is shown in Muñoz & Van Der Laan (2012); Young et al. (2014).

Then, let us put the following assumptions:

- Consistency: $Y = Y(a)$ if $A = a$ for $\forall a \in A$.
- Unconfoundedness: $A$ and $Y(a)$ are conditionally independent given $X$ for any $a \in A$, $G$ and $Y(a)$ are conditionally independent given $Z$ for any $a \in A$.

\[\text{The reason why we use } B \text{ is to distinguish it from the random variable } A.\]
• Transportability: $E[Y(a) \mid Z = c] = E[Y(a) \mid X = c]$ for any $a \in A, c \in \mathcal{X}$.

Note that transportability is a weaker assumption compared with the assumption in the main draft:

$$p_{\text{train}}(Y(a) \mid c) = p_{\text{test}}(Y(a) \mid c),$$

where $p_{\text{train}}(\cdot \mid \cdot)$ is a condition density of $Y(a)$ given $Z$, $p_{\text{test}}(\cdot \mid \cdot)$ is a condition density of $Y(a)$ given $X$. Following Lemma 1 (Kennedy 2019), we can prove the following lemma.

**Lemma 2** (G-formula). $E[Y(B)] = \int \int E[Y \mid A = a, X = x] \pi^s(a \mid x) q(x) d(a, x)$.

**Proof.**

$$E[Y(B)] = \int \int E[Y(b) \mid B = b, Z = z] \pi^s(b \mid z) q(z) d(b, z)$$

$$= \int \int E[Y(g) \mid Z = z] \pi^s(b \mid z) q(z) d(b, z)$$

$$= \int \int E[Y(g) \mid X = z] \pi^s(b \mid z) q(z) d(b, z)$$

$$= \int \int E[Y(g) \mid A = g, X = z] \pi^s(b \mid z) q(z) d(b, z)$$

$$= \int \int E[Y(a) \mid A = a, X = x] \pi^s(a \mid x) q(x) d(a, x)$$

$$= \int \int E[Y \mid A = a, X = x] \pi^s(a \mid x) q(x) d(a, x).$$

From the first line to the second line, we use a transportability assumption. From the second line to the third line, we use a uncounfedness assumption. From the third line to the fourth line, we use a transportability assumption. From the fourth line to the fifth line, we use a uncounfedness assumption. From the fourth line to the fifth line, the random variables $a, x$ are replaced with $b, z$. From the fifth line to the sixth line, we use a consistency assumption.

Let us note that from this lemma, the DM method can be naturally introduced. \qed

**Theorem 9** (Identification of IPWCS). $E[Y(B)] = E[r(X) w(A, X) Y]$

**Proof.**

$$E[r(X) w(A, X) Y] = E[r(X) w(A, X) E[Y \mid A, X]]$$

$$= \int \int E[Y \mid A = a, X = x] r(x) w(a, x) \pi^v(a \mid x) p(x) d(a, x)$$

$$= \int \int E[Y \mid A = a, X = x] \pi^s(a \mid x) q(x) d(a, x)$$

$$= E[Y(B)].$$

From the third line to the fourth line, we use a Lemma 2. \qed

## C Density Ratio Estimation

Here, we introduce the formulation of LSIF. In LSIF, we estimate the density ratio $r(x) = \frac{q(x)}{p(x)}$ directly. Let $\mathcal{S}$ be the class of non-negative measurable functions $s : \mathcal{X} \to \mathbb{R}^+$. We consider minimizing the following squared error between $s$ and $r$: $\mathbb{E}_{p(x)}[(s(X) - r(x))^2] = \mathbb{E}_{p(x)}[(r(x))^2] - 2\mathbb{E}_{q(z)}[s(z)] + \mathbb{E}_{p(x)}[(s(x))^2].$ \hspace{1cm} (12)

The first term of the last equation does not affect the result of minimization and we can ignore the term, i.e., the density ratio is estimated through the following minimization problem:

$$s^* = \arg\min_{s \in \mathcal{S}} \left[ \frac{1}{2} \mathbb{E}_{p(x)}[(s(x))^2] - \mathbb{E}_{q(z)}[s(z)] \right].$$
where $\mathcal{S}$ is a hypothesis class of the density ratio. As mentioned above, to minimize the empirical version of (12), we use uLSIF [Sugiyama et al., 2012]. Given a hypothesis class $\mathcal{H}$, we obtain $\hat{r}$ by

$$
\hat{r} = \arg \min_{s \in \mathcal{H}} \left[ \frac{1}{2} \mathbb{E}_{n_{\text{hot}}} [(s(X))^2] - \mathbb{E}_{n_{\text{evl}}} [s(Z)] + R(s) \right],
$$

(13)

where $R$ is a regularization term. For a model of uLSIF [Kanamori et al., 2012] proposed using kernel based hypothesis to estimate the density ratio nonparametrically. [Kanamori et al., 2012] called uLSIF with kernel based hypothesis as KuLSIF. [Kanamori et al., 2012] showed that, under some assumptions, the convergence rate of KuLSIF as follows:

$$
\left\| \hat{r}(X) - \left( \frac{\hat{d}(X)}{p(X)} \right) \right\|_2 = \mathcal{O}_{\mathcal{P}} \left( \min (n_{\text{hot}}, n_{\text{evl}})^{\gamma} \right),
$$

(14)

where $0 < \gamma < 2$ is a constant depending on the bracketing entropy of $\mathcal{H}$.

\section{D  Efficiency bound for the stratified sampling mechanism}

In this section, we modify the standard theory, which is derived for a case where samples are i.i.d., to the current problem with a stratified sampling scheme to show Theorem 1. We define the efficiency bound when the data generating process is a stratified sampling with historical data $\{\alpha_i\}^n_{i=1}$ and evaluation data $\{\beta_i\}^n_{i=1}$, where $\alpha_i$ and $\beta_i$ are random variables. Let $H_{n_{\text{hot}}}$ and $G_{n_{\text{evl}}}$ be the distributions of $\{\alpha_i\}^n_{i=1}$ and $\{\beta_i\}^n_{i=1}$. Let us define a set of functions as $\mathcal{M}_n = \{H_{n_{\text{hot}}}, G_{n_{\text{evl}}}; H \in \mathcal{M}, G \in \mathcal{M} \}$. A model $\mathcal{M}^{\text{para}}_n$ is called a regular parametric submodel if the model can be written as $\mathcal{M}^{\text{para}}_n = \{H_{n_{\text{hot}}}, G_{n_{\text{evl}}}; \theta \in \Theta_1, \Theta_2 \}$ and it matches the true distribution at $\theta^*_1$ and $\theta^*_2$, and it has a differentiable density $h_{\theta^*_1, n_{\text{hot}}}(\{a_i\}) = \prod_{i=1}^{n_{\text{hot}}} h(a_i; \theta_1), g_{\theta^*_2, n_{\text{evl}}}(\{b_i\}) = \prod_{i=1}^{n_{\text{evl}}} g(b_i; \theta_2)$. Let $R(H, G) \rightarrow \mathbb{R}$ be a target functional. Then, the Cramér-Rao lower bound of the functional $R$ under the parametric submodel $\mathcal{M}^{\text{para}}_n$ is

$$
\text{CR}(\mathcal{M}^{\text{para}}_n, R) = \nabla_{\theta^*_1} R(H_{\theta^*_1}, G_{\theta^*_2}) \mathbb{E}[\otimes \nabla_{\theta_1} \log h_{\theta^*_1, n_{\text{hot}}}]^{-1} \nabla_{\theta^*_1} R(H_{\theta^*_1}, G_{\theta^*_2}) + \nabla_{\theta^*_2} R(H_{\theta^*_1}, G_{\theta^*_2}) \mathbb{E}[\otimes \nabla_{\theta_2} \log g_{\theta^*_2, n_{\text{evl}}}]^{-1} \nabla_{\theta^*_2} R(H_{\theta^*_1}, G_{\theta^*_2}).
$$

This Cramér-Rao lower bound can be extended when the model is semiparametric. Following [Tsiatis, 2006], the efficiency bound of a target functional $R$ under the model semiparametric model $\mathcal{M}$ is

$$
\lim_{n \rightarrow \infty} \sup_{\mathcal{M}^{\text{para}}_n \subset \mathcal{M}} n \text{CR}(\mathcal{M}^{\text{para}}_n, R).
$$

Using this discussion, we prove Theorem 1.

\textbf{Proof of Theorem 1} We call $\mathcal{M}$ the fully nonparametric model, and denote it with fixed $p(x)$ and $\pi^b(a \mid x)$ as $\mathcal{M}_{\text{fix}}$. We follow the definition of efficiency bound in Section D.

In our setting, we have $\{X_i, A_i, Y_i\}^n_{i=1}$ and $\{Z_i\}^n_{i=1}$. The target functional, that is, the value of the evaluation policy $\pi^e$ defined in (11) is

$$
R(\pi^e) = \int y g(x) \pi^e(x \mid a) p(y \mid a, X, Y) d\mu(a, x, y),
$$

(15)

where $\mu$ is a baseline measure such as Lebesgue or counting measure. Here, the model $\mathcal{M}^{\text{para}}_n$ for a nonparametric model $\mathcal{M}$ is

$$
p(\{x_i\}, \{a_i\}, \{y_i\}^n_{i=1}) = \prod_{i=1}^{n_{\text{hot}}} p(x_i; \theta) \pi^b(a_i \mid x_i) \pi^e(y_i \mid x_i, a_i; \theta),
$$

and

$$
p(\{z_i\}^n_{i=1}) = \prod_{j=1}^{n_{\text{evl}}} q(z_j).
$$

The model $\mathcal{M}^{\text{fix}, \text{para}}_n$ for a nonparametric model $\mathcal{M}_{\text{fix}}$ is

$$
p(\{x_i\}, \{a_i\}, \{y_i\}^n_{i=1}) = \prod_{i=1}^{n_{\text{hot}}} p(x_i) \pi^b(a_i \mid x_i) \pi^e(y_i \mid x_i, a_i; \theta),
$$

and

$$
p(\{z_i\}^n_{i=1}) = \prod_{j=1}^{n_{\text{evl}}} q(z_j).
Then, from the Cauchy Schwartz inequality (Tripathi, 1999), we have the following inequality:

$$E = \frac{1}{\rho} A_1 B_1 A_1^\top + (1 - \rho)^{-1} A_2 B_2^{-1} A_2^\top$$  \hspace{1cm} (16)

is given by

$$A_1 = \mathbb{E}_{x \sim q(x), a \sim \pi^*(a | x), y \sim p(y | a, x)} [y \nabla_{\theta_1} \log p(y | a, x; \theta_1)],$$

$$A_2 = \mathbb{E}_{x \sim q(x), a \sim \pi^*(a | x), y \sim p(y | a, x)} [y \nabla_{\theta_2} \log q(x; \theta_2)],$$

$$B_1 = \mathbb{E}_{x \sim p(x), a \sim \pi^v(a | x), y \sim p(y | a, x)} [\nabla_{\theta_1} \log p(y | a, x; \theta_1)],$$

$$B_2 = \mathbb{E}_{z \sim q(z)} [\nabla_{\theta_2} \log q(z; \theta_2)].$$

Then, from the Cauchy Schwartz inequality (Tripathi, 1999), we have the following inequality:

$$\mathbb{E}[A(Z) B^\top(Z)] \mathbb{E}[B(Z) B^\top(Z)]^{-1} \mathbb{E}[A(Z) B^\top(Z)] \leq \mathbb{E}[A^2(Z)],$$

where $\mathbb{E}[A(Z)] = 0, \mathbb{E}[B(Z)] = 0$. Then, we obtain the following upper bound:

$$A_1^{-1} B_1^{-1} A_1^\top = \mathbb{E}[r(X) w(A, X) Y \nabla_{\theta_1} \log p(Y | A, X; \theta_1)] \mathbb{E}[\nabla_{\theta_1} \log p(Y | A, X; \theta_1)]^{-1}$$

$$\times \mathbb{E}[r(X) w(A, X) Y \nabla_{\theta_1} \log p(Y | A, X; \theta_1)] \mathbb{E}[\nabla_{\theta_1} \log p(Y | A, X; \theta_1)]^{-1}$$

$$\times \mathbb{E}[r(x) w(A, X) \{Y - \mathbb{E}[Y | A, X]\} \nabla_{\theta_1} \log p(Y | A, X; \theta_1)] \mathbb{E}[\nabla_{\theta_1} \log p(Y | A, X; \theta_1)]^{-1}$$

$$\leq \mathbb{E}[r^2(X) w^2(A, X)^2 \{Y - \mathbb{E}[Y | A, X]\}^2] = \mathbb{E}[r^2(X) w^2(A, X)^2] \mathbb{E}[\{Y - \mathbb{E}[Y | A, X]\}^2].$$

In the same way,

$$A_2^{-1} B_2^{-1} A_2^\top = \mathbb{E}[v(Z) \nabla_{\theta_2} \log q(Z; \theta_2)] \mathbb{E}[\nabla_{\theta_2} \log q(Z; \theta_2)]^{-1} \mathbb{E}[v(Z) \nabla_{\theta_2} \log q(Z; \theta_2)]$$

$$\mathbb{E}[\{v(Z) - \mathbb{E}[v(Z)]\} \nabla_{\theta_2} \log q(Z; \theta_2)] \mathbb{E}[\nabla_{\theta_2} \log q(Z; \theta_2)]^{-1} \mathbb{E}[\{v(Z) - \mathbb{E}[v(Z)]\} \nabla_{\theta_2} \log q(Z; \theta_2)]$$

$$\leq \mathbb{E}[\{v(Z) - \mathbb{E}[v(Z)]\}^2] = \text{var}[v(Z)].$$

Therefore,

$$\rho^{-1} A_1^{-1} B_1^{-1} A_1^\top + (1 - \rho)^{-1} A_2 B_2^{-1} A_2^\top$$

$$\leq \rho^{-1} \mathbb{E}[r^2(X) w^2(A, X) \text{var}[Y | A, X]] + (1 - \rho)^{-1} \text{var}[v(Z)].$$

Finally, we have to show there exists a regular parametric model achieving

$$\rho^{-1} \mathbb{E}[r^2(X) w^2(A, X) \text{var}[Y | A, X]] + (1 - \rho)^{-1} \text{var}[v(Z)].$$

This is proved by using (Kallus & Uehara, 2019). The idea is any $L^2$-function is spanned by some basis functions.

**Remark 4** (Results in $\mathcal{M}_{\text{fix}}$). The Cramér-Rao lower bound for regular parametric model under $\mathcal{M}_{\text{fix}}$ is the same since the target function does not include $p(x), \pi^v(a | x)$ as (16). Therefore, the efficiency bound is also the same.

### E Proofs

In this section, we show the proofs of theorems. In the proofs of Theorem 1 and 2, we prove the case where we use a two-fold cross-fitting. The extension of two fold cross-fitting to the general $K$-fold cross-fold is straightforward.
E.1 Required conditions

In order to show Theorems 7–11 we use the following Theorem 10 which shows the convergence rate of kernel regression. Here, we have data \( \{B_i, C_i\}_{i=1}^n \), which are i.i.d. from \( p(b, c) = p(c|b)p(b) \), and \( B_i \) takes a value in \( B \). Then, let us consider a kernel estimation:

\[
n^{-1} \sum_{i=1}^n K_h(B_i - b)C_i,
\]

where \( K_h(b) = h^{-d} K(h/b) \), where \( d \) is a dimension of \( b \). Then, we have the following theorem following Newey & McFadden (1994).

**Theorem 10.** Assume

- the space \( B \) is compact and \( p(b) > 0 \) on \( B \),
- the kernel \( K(u) \) has the bounded derivative of order \( k \), satisfies \( \int K(u)du = 1 \), and has zero moments of order \( \leq m - 1 \) and a nonzero \( m \)-th order moment,
- \( \mathbb{E}[C \mid B = b] \) is continuously differentiable to order \( k \) with bounded derivatives on the opening set in \( B \).
- there is \( v \geq 4 \) such that \( \mathbb{E}[\|C\|^v] \leq \infty \) and \( \mathbb{E}[\|C\|^v \mid B = b]p(b) \) is bounded.

Then, when \( h = h(n) \) and \( h(n) \to 0 \),

\[
\|n^{-1} \sum_{i=1}^n K_h(B_i - b)C_i - \mathbb{E}[C|B]\|_\infty = O_p \left( \frac{\log n^{1/2}}{(nh^{d+2k})^{1/2}} + h^n \right) .
\]

Then, under \( n^{1/2}/\log n \to \infty, \sqrt{nh^{d+2k}} \to \infty, \sqrt{nh^{2m}} \to 0 \), the above \( l_\infty \) risk is \( o_p(n^{-1/2}) \) (Newey & McFadden 1994).

**Additional assumptions:** regarding Theorem 10 we assume the following assumptions when we prove Theorems 11–7

**Theorem 11:** condition when replacing \( B \) with \( X, C \) with \( w(A, X)Y \), condition when replacing \( B \) with \( Z, C \) with 1.

**Theorem 5:** condition when replacing \( B \) with \( X, C \) with \( w(A, X)Y \), condition when replacing \( B \) with \( X, C \) with 1, condition when replacing \( B \) with \( X, C \) with 1.

**Theorem 6:** condition when replacing \( B \) with \( (X, A), C \) with 1, condition when replacing \( B \) with \( (X, A), C \) with \( Y \), condition when replacing \( B \) with \( X, C \) with \( w(A, X)Y \), and condition when replacing \( B \) with \( Z, C \) with 1.

**Theorem 7:** condition when replacing \( B \) with \( (X, A), C \) with \( Y \), condition when replacing \( B \) with \( (X, A), C \) with 1.

E.2 Warming up

As a warm up, first, we prove the asymptotic property of some simple estimator. When \( p(x) \) and \( \pi^h(a \mid x) \) are known, let us define an IPW estimator:

\[
\hat{R}_{IPW1}(\pi^c) = \mathbb{E}_{n \text{ind}} \left[ \frac{\hat{q}(X) \pi^c(A \mid X)Y}{p(X)} \frac{\pi^h(A \mid X)}{\pi^h(A \mid X)} \right] .
\]

**Theorem 11.** When \( \hat{q}(x) = \hat{q}_h(x) \), the asymptotic MSE of \( \hat{R}_{IPW1} \) is

\[
\rho^{-1} \text{var}[r(X)w(A, X)Y] + (1 - \rho)^{-1} \text{var}[v(Z)].
\]

**Proof of Theorem 11** We follow the proof of Newey & McFadden (1994). For the ease of notation, assume \( \rho = k_1/(k_1 + k_2) \). In this case, \( n^{\text{ind}} = k_1 N_o \) and \( n^{\text{env}} = k_2 N_o \), where \( N_o = n/(k_1 + k_2) \). Note that in this asymptotic regime, \( N_o \to \infty \). Therefore, we reindex the sample set as

\[
\{X_i\}_{i=1}^{n^{\text{ind}}} = \{X_{b,i} \mid 1 \leq b \leq k_1, 1 \leq i \leq N_o\},
\]

\[
\{Z_i\}_{i=1}^{n^{\text{ind}}} = \{Z_{c,j} \mid 1 \leq c \leq k_2, 1 \leq j \leq N_o\}.
\]

Here, we only consider the estimator \( \hat{R}_{IPW1}(\pi^c) \) based on based on \( \{X_{b,i}\}_{i=1}^{N_o} \) and \( \{Z_{c,j}\}_{j=1}^{N_o} \), and denote it as \( \hat{R}_{b,c} \).

Then, the final estimator \( \hat{R}_{IPW1}(\pi^c) \) using all set of samples is equal to

\[
\frac{1}{k_1 k_2} \sum_{b=1}^{k_1} \sum_{c=1}^{k_2} \hat{R}_{b,c},
\]

18
since the kernel estimator has a linear property. More specifically, we have

\[
\hat{R}_{1|W1}(\pi^e) = \frac{1}{n_{\text{hst}}} \sum_{i=1}^{n_{\text{hst}}} \left\{ \frac{1}{n_{\text{evl}}} \sum_{j=1}^{n_{\text{evl}}} K_h(Z_j - X_i) \right\} \frac{\pi^e(A_i | X_i) Y_i}{\pi^b(A_i | X_i) p(X_i)} = \frac{1}{n_{\text{hst}}} \sum_{i=1}^{n_{\text{hst}}} \sum_{j=1}^{n_{\text{evl}}} \frac{K_h(Z_j - X_i) \pi^e(A_i | X_i) Y_i}{\pi^b(A_i | X_i) p(X_i)}
\]

\[
= \frac{1}{k_1 k_2} \frac{1}{k_1} \sum_{b=1}^{k_2} \frac{1}{k_2} \sum_{c=1}^{k_2} \left\{ \frac{1}{n_{\text{hst}}} \sum_{i=1}^{n_{\text{hst}}} \sum_{j=1}^{n_{\text{evl}}} K_h(Z_{c,j} - X_{b,i}) \pi^e(A_{b,i} | X_{b,i}) Y_{b,i} \right\} = \frac{1}{k_1 k_2} \sum_{b=1}^{k_2} \sum_{c=1}^{k_2} \hat{R}_{b,c}
\]

First, we analyze \( \hat{R}_{1,1} \).

**Step 1** We prove the following in this step:

\[
\hat{R}_{b,c} = \frac{1}{N_{n_{e}}} \sum_{i=1}^{N_{n_{e}}} r(X_{b,i}) w(X_{b,i}, A_{b,i}) Y_{b,i} + \frac{1}{N_{n_{e}}} \sum_{j=1}^{N_{n_{e}}} v(Z_{c,j}) + o_p(n^{-1/2}).
\]

Especially, we prove the statement for \( \hat{R}_{1,1} \) when \( k_1 = 1, k_2 = 1, n_{\text{hst}} = n_{\text{evl}} = n/2 \). We have

\[
\hat{R}_{1,1} = E_{n_{\text{hst}}} \left[ \frac{\hat{q}(X) \pi^e(A | X) Y}{p(X) \pi^b(A | X)} \right] = \frac{1}{n_{\text{hst}}} \sum_{i=1}^{n_{\text{hst}}} \left\{ \frac{1}{n_{\text{evl}}} \sum_{j=1}^{n_{\text{evl}}} K_h(Z_j - X_i) \right\}
\]

\[
= E_{n_{\text{hst}}} \left[ \frac{q(X) \pi^e(A | X) Y}{p(X) \pi^b(A | X)} \right] + \frac{1}{n_{\text{hst}} n_{\text{evl}}} \sum_{i=1}^{n_{\text{hst}}} \sum_{j=1}^{n_{\text{evl}}} a_{i,j},
\]

where

\[
a_{i,j}((X_i, A_i, Y_i), (Z_j)) = \frac{1}{p(X_j) \pi^b(A_i | X_i)} \{ K_h(Z_j - X_i) - q(X_i) \},
\]

\[
b_{i,j}((X_i, A_i, Y_i, Z_i), (X_j, A_j, Y_j, Z_j)) = 0.5 \{ a_{i,j} + a_{j,i} \}.
\]

Then,

\[
\frac{1}{n_{\text{hst}} n_{\text{evl}}} \sum_{i<j} b_{i,j}(X_i, A_i, Y_i, Z_i, (X_j, A_j, Y_j, Z_j))
\]

\[
= \frac{2}{n_{\text{hst}}} \left\{ \sum_{i=1}^{n_{\text{hst}}} E[b_{i,j} | X_i, A_i, Y_i, Z_i] \right\} + o_p(n^{-1/2})
\]

\[
= \frac{1}{n_{\text{evl}}} \sum_{i=1}^{n_{\text{evl}}} E[a_{i,j} | X_i, A_i, Y_i, Z_i] + \frac{1}{n_{\text{hst}}} \sum_{i=1}^{n_{\text{hst}}} E[a_{i,j} | X_i, A_i, Y_i, Z_i] + o_p(n^{-1/2})
\]

\[
= \frac{1}{n_{\text{evl}}} \sum_{i=1}^{n_{\text{evl}}} \{ v(Z_i) - R(\pi^e) \} + o_p(n^{-1/2}).
\]

From the first line to the second line, we used the U-statistics theory [van der Vaart, 1998, Theorem 12.3]. From the third line to the fourth line, based on Theorem 10 we used

\[
E[a_{j,i} | X_i, A_i, Y_i, Z_i] = o_p(n^{-1/2}) + E[w(A_i, X_i) Y_i | X_i = Z_i] p(X_i) p(X_i)
\]

\[
= o_p(n^{-1/2}) + v(Z_i) - R(\pi^e),
\]

\[
E[a_{i,j} | X_i, A_i, Y_i, Z_i] = o_p(n^{-1/2}) + \frac{1}{p(X_i) \pi^b(A_i | X_i)} \{ q(X_i) - q(X_i) \}
\]

\[
= o_p(n^{-1/2}).
\]
Remark 5.  $\mathbb{E}[h(A_i, X_i, Y_i) \mid X_i = Z_i]$ is an abbreviation of $\{\mathbb{E}[h(A_i, X_i, Y_i) \mid X_i = x] \}_{x = Z_i}$.

Therefore,

$$\hat{R}_{IPWCSB} = \mathbb{E}_n^{\text{hist}} \left[ \frac{q(X) \pi^c(A \mid X)Y}{p(X) \pi^b(A \mid X)} \right] + \mathbb{E}_n^{\text{evl}}[v(Z)] - R(\pi^c) + o_p(n^{-1/2}).$$

Step 2  Based on Step 1, we have

$$\hat{R}_{IPW1} = \frac{1}{k_1k_2} \sum_{b=1}^{k_1} \sum_{c=1}^{k_2} \hat{R}_{b,c}$$

$$= \frac{1}{k_1k_2} \sum_{b=1}^{k_1} \sum_{c=1}^{k_2} \left[ \frac{1}{N_o} \sum_{i=1}^{N_o} r(X_{b,i})w(X_{b,i}, A_{b,i})Y_{b,i} + \frac{1}{N_o} \sum_{j=1}^{N_o} v(Z_{c,j}) \right] - R(\pi^c) + o_p(n^{-1/2})$$

$$= \frac{1}{k_1N_o} \sum_{b=1}^{k_1} \sum_{i=1}^{N_o} r(X_{b,i})w(X_{b,i}, A_{b,i})Y_{b,i} + \frac{1}{k_2N_o} \sum_{c=1}^{k_2} \left[ \frac{1}{N_o} \sum_{j=1}^{N_o} v(Z_{c,j}) \right] - R(\pi^c) + o_p(n^{-1/2})$$

$$= \frac{1}{n_{\text{hist}}} \sum_{i=1}^{n_{\text{hist}}} r(X_i)w(X_i, A_i)Y_i + \frac{1}{n_{\text{evl}}} \sum_{j=1}^{n_{\text{evl}}} v(Z_j) - R(\pi^c) + o_p(n^{-1/2}).$$

Finally, from stratified sampling CLT, the statement is concluded. \qed

E.3 Proof of Theorem \[2\]

Proof. We denote

$$\phi_1(x, a, y; r, w, f) = r(x)w(a, x)\{y - f(a, x)\}, \phi_2(z; f) = v(z).$$

We also denote the union of $n_{\text{hist}}^1$ and $n_{\text{evl}}^1$ as $D_i$ for $i = 1, 2$, and the number of $n_{\text{hist}}^1, n_{\text{hist}}^2, n_{\text{evl}}^1, n_{\text{evl}}^2$ as $n_{11}, n_{12}, n_{21}, n_{22}$. For simplicity, we assume $n_{11} = n_{12}, n_{21} = n_{22}$.

Then, we have

$$\sqrt{n}\left\{ \mathbb{E}_n^{\text{hist}}[\phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)})] + \mathbb{E}_n^{\text{evl}}[\phi_2(Z; \hat{f}^{(1)})] \right\} - R(\pi^c) \right\}$$

$$= \sqrt{n}\left\{ \frac{1}{\sqrt{n_{11}}} \mathbb{G}_n^{\text{hist}}[\phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}) - \phi_1(X, A, Y; r, w, f)] + \frac{1}{\sqrt{n_{12}}} \mathbb{G}_n^{\text{evl}}[\phi_2(Z; \hat{f}^{(1)}) - \phi_2(Z; f)] \right\}$$

$$+ \mathbb{E}[\phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}) \mid \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}] + \mathbb{E}[\phi_2(Z; \hat{f}^{(1)}) \mid \hat{f}^{(1)}]$$

$$- \mathbb{E}[\phi_1(X, A, Y; r, w, f)] - \mathbb{E}[\phi_2(Z; f)] \right\}$$

$$+ \sqrt{n}\left\{ \mathbb{E}_n^{\text{hist}}[\phi_1(X, A, Y; r, w, f)] + \mathbb{E}_n^{\text{evl}}[\phi_2(Z; f)] - R(\pi^c) \right\}. \quad (19)$$

The term (19) is $o_p(1)$ by Step 1. The term Eq. (20) is also $o_p(1)$ by Step 2 as follows.

Step 1: Eq. (19) is $o_p(1)$.

If we can show that for any $\epsilon > 0$,

$$\lim_{n \to \infty} P[|\sqrt{n}\left\{ \frac{1}{\sqrt{n_{11}}} \mathbb{G}_n^{\text{hist}}[\phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}) - \phi_1(X, A, Y; r, w, f)] \right\}$$

$$+ \frac{1}{\sqrt{n_{12}}} \mathbb{G}_n^{\text{evl}}[\phi_2(Z; \hat{f}^{(1)}) - \phi_2(Z; f)]]| > \epsilon | D_2] = 0,$$

then by the bounded convergence theorem, we would have

$$\lim_{n \to \infty} P[|\sqrt{n}\left\{ \frac{1}{\sqrt{n_{11}}} \mathbb{G}_n^{\text{hist}}[\phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}) - \phi_1(X, A, Y; r, w, f)] \right\}$$

$$+ \frac{1}{\sqrt{n_{12}}} \mathbb{G}_n^{\text{evl}}[\phi_2(Z; \hat{f}^{(1)}) - \phi_2(Z; f)]]| > \epsilon] = 0,$$

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yielding the statement.

To show (22), we show that the conditional mean is 0 and the conditional variance is $o_p(1)$. Then, (22) is proved by the Markov inequality following the proof of [Kallus & Uehara, 2019a, Theorem 4). The conditional mean is

$$E[\sqrt{n}(\frac{1}{\sqrt{n_{11}}} G_{n_{11}} \phi_1(X, A, Y; \hat{\rho}(1), \hat{\omega}(1), \hat{f}(1)) - \phi_1(X, A, Y; r, w, f))]$$

$$+ \frac{1}{\sqrt{n_{12}}} G_{n_{12}} \phi_2(Z; \hat{f}(1)) - \phi_2(Z; f))] | D_2]$$

$$\quad = E[\sqrt{n}(\frac{1}{\sqrt{n_{11}}} G_{n_{11}} \phi_1(X, A, Y; \hat{\rho}(1), \hat{\omega}(1), \hat{f}(1)) - \phi_1(X, A, Y; r, w, f))]$$

$$+ \frac{1}{\sqrt{n_{12}}} G_{n_{12}} \phi_2(Z; \hat{f}(1)) - \phi_2(Z; f))] | D_2, \hat{\rho}(1), \hat{\omega}(1), \hat{f}(1)]$$

$$\quad = 0.$$

Here, we used a cross-fitting construction. More specifically, regarding the second term, we have

$$E[\sqrt{n}_1 \phi_2(Z; \hat{f}(1)) - \phi_2(Z; f)] - E[\phi_2(Z; \hat{f}(1)) - \phi_2(Z; f) | D_2, \hat{\rho}(1), \hat{\omega}(1), \hat{f}(1)]$$

$$= E[\phi_2(Z; \hat{f}(1)) - \phi_2(Z; f) | D_2, \hat{\rho}(1), \hat{\omega}(1), \hat{f}(1)] - E[\phi_2(Z; \hat{f}(1)) - \phi_2(Z; f) | \hat{f}(1)]$$

$$= E[\phi_2(Z; \hat{f}(1)) - \phi_2(Z; f) | \hat{f}(1)] - E[\phi_2(Z; \hat{f}(1)) - \phi_2(Z; f) | \hat{f}(1)] = 0.$$

The conditional variance is bounded as

$$\text{var}[\sqrt{n}(\frac{1}{\sqrt{n_{11}}} G_{n_{11}} \phi_1(X, A, Y; \hat{\rho}(1), \hat{\omega}(1), \hat{f}(1)) - \phi_1(X, A, Y; r, w, f))] | D_2]$$

$$+ \frac{1}{\sqrt{n_{12}}} G_{n_{12}} \phi_2(Z; \hat{f}(1)) - \phi_2(Z; f))] | D_2]$$

$$\quad = \frac{n}{n_{11}} \text{var}[\phi_1(X, A, Y; \hat{\rho}(1), \hat{\omega}(1), \hat{f}(1)) - \phi_1(X, A, Y; r, w, f))] | D_2]$$

$$+ \frac{n}{n_{22}} \text{var}[\phi_2(Z; \hat{f}(1)) - \phi_2(Z; f))] | D_2]$$

$$\leq \frac{n}{n_{11}} E[\{(\hat{\rho}(1) X)\hat{\omega}(1) (A, X) (Y - \hat{f}(1) A, X)) - r(X) w(A, X) (Y - f(A, X))|^2 | D_2]$$

$$+ \frac{n}{n_{22}} E[\{(\hat{v}(1) (Z) - v(Z))^2 | D_2] = o_p(1) + o_p(1) = o_p(1).$$

Here, we used

$$\frac{n}{n_{11}} E[\{(\hat{\rho}(1) X)\hat{\omega}(1) (A, X) (Y - \hat{f}(1) A, X)) - r(X) w(A, X) (Y - f(A, X))|^2 | D_2] = o_p(1).$$

and

$$E[\{(\hat{v}(1) (Z) - v(Z))^2 | D_2] = o_p(1).$$

The first equation (23) is proved by

$$E[\{(\hat{\rho}(1) X)\hat{\omega}(1) (Y - \hat{f}(1) A, X)) - r(X) w(A, X) (Y - f(A, X))|^2 | D_2]$$

$$= E[\{(\hat{\rho}(1) X)\hat{\omega}(1) (Y - \hat{f}(1)) - \hat{\rho}(1) X\hat{\omega}(1) (Y - f) + \hat{\rho}(1) X\hat{\omega}(1) (Y - f) - r(X) w(A, X) (Y - f(A, X))|^2 | D_2]$$

$$\leq 2E[\{(\hat{\rho}(1) X)\hat{\omega}(1) (Y - \hat{f}(1)) - \hat{\rho}(1) X\hat{\omega}(1) (Y - f))^2 | D_2] + 2E[\{(\hat{\rho}(1) X\hat{\omega}(1) (Y - f) - r(X) w(A, X) (Y - f))^2 | D_2]$$

$$\leq 2C_1 C_2 |f - \hat{f}(1)|^2 + 2 \times 4 R_{\max}^2 |\hat{\rho}(1) X\hat{\omega}(1) - r w|^2 = o_p(1).$$

Here, we have used a parallelogram law from the second line to the third line. We have use 0 < $\hat{\rho}$ < $C_1$, 0 < $\hat{\omega}$ < $C_2$, $|f| < R_{\max}$ according to the Assumption2 and convergence rate conditions, from the third line to the fourth line.

The second equation (24) is proved by Jensen’s inequality.

**Step 2:** Eq. (20) is $o_p(1)$. 

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We have
\[ |E[\phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}) | \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}] + E[\phi_2(Z; \hat{f}^{(1)}) | \hat{f}] - E[\phi_1(x; r, w, f)] - E[\phi_2(Z; f)]| \]
\[ \leq |E[(r^{(1)}(X)\hat{w}^{(1)}(A, X) - r(X)w(A, X)) \{ -\hat{f}^{(1)}(A, X) + f(A, X) \} | \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}]| \]
\[ + |E[r(x)w(A, X)\{ -\hat{f}(A, X) + f(A, X) \} | \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}] + E[\hat{w}^{(1)}(Z) - v(Z) | \hat{f}^{(1)}]| \]
\[ + |E[\hat{r}^{(1)}(X)\hat{w}^{(1)}(A, X) \{ Y - f(A, X) \} | \hat{r}^{(1)}, \hat{w}^{(1)}]| \]
\[ \leq \| \hat{r}^{(1)}(X)\hat{w}^{(1)}(A, X) - r(X)w(A, X)\|_2 \| \hat{f}^{(1)}(A, X) - f(A, X)\|_2 + 0 + 0 \]
\[ = o_p(n^{-p})o_p(n^{-q}) + 0 + 0 = o_p(n^{-1/2}). \]

Here, we have used Hölder’s inequality:
\[ \|fg\|_1 \leq \|f\|_2\|g\|_2, \]
the relation
\[ E[r(X)w(A, X)\{ -\hat{f}^{(1)}(A, X) + f(A, X) \} | \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}] + E[\hat{w}^{(1)}(Z) - v(Z) | \hat{f}^{(1)}] \]
\[ = E[-r(X)w(A, X)f^{(1)}(A, X) + \hat{w}^{(1)}(z) | \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}] + E[-r(X)w(A, X)f(A, X) + v(Z)] \]
\[ = 0 + 0 = 0, \]
and
\[ E[\hat{r}^{(1)}(X)\hat{w}^{(1)}(A, X) \{ Y - f(A, X) \} | \hat{r}^{(1)}, \hat{w}^{(1)}] = E[\hat{r}^{(1)}(X)\hat{w}^{(1)}(A, X) \{ f(A, X) - f(A, X) \} | \hat{r}^{(1)}, \hat{w}^{(1)}] = 0. \]

**Step 3:** By combining everything, we have
\[ E_{n2} \left[ \phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}) \right] + E_{n2} \left[ \phi_2(Z; \hat{f}^{(1)}) \right] - R(\pi^r) \]
\[ = E_{n2} \left[ \phi_1(X, A, Y; r, w, f) \right] + E_{n2} \left[ \phi_2(Z; f) \right] - R(\pi^r) + o_p(1/\sqrt{n}). \]

Then,
\[ \hat{R}_{\text{DRC5}} = 0.5E_{n2} \left[ \phi_1(X, A, Y; \hat{r}^{(1)}, \hat{w}^{(1)}, \hat{f}^{(1)}) \right] + 0.5E_{n2} \left[ \phi_2(Z; \hat{f}^{(1)}) \right] \]
\[ + 0.5E_{n2} \left[ \phi_1(X, A, Y; \hat{r}^{(2)}, \hat{w}^{(2)}, \hat{f}^{(2)}) \right] + 0.5E_{n2} \left[ \phi_2(Z; \hat{f}^{(2)}) \right] \]
\[ = 0.5E_{n2} \left[ \phi_1(X, A, Y; r, w, f) \right] + 0.5E_{n2} \left[ \phi_2(Z; f) \right] + \]
\[ + 0.5E_{n2} \left[ \phi_1(X, A, Y; r, w, f) \right] + 0.5E_{n2} \left[ \phi_2(Z; f) \right] + o_p(1/\sqrt{n}) \]
\[ = E_{n2} \left[ \phi_1(X, A, Y; r, w, f) \right] + E_{n2} \left[ \phi_2(Z; f) \right] + o_p(1/\sqrt{n}). \]

Finally, by using a stratified sampling CLT [Wooldridge, 2001], the statement is concluded based on Assumption[1].

### E.4 Proof of Lemma[1]

**Proof.** We can bound \( \|\hat{r}(X)\hat{w}(A, X) - r(x)w(A, X)\|_2 = o_p(n^{-p}) \):
\[ \|\hat{r}(X)\hat{w}(A, X) - r(x)w(A, X)\|_2 \leq \|\hat{r}(X)\hat{w}(A, X) - \hat{r}(X)w(A, X)\|_2 \]
\[ + \|\hat{r}(X)w(A, X) - r(X)w(A, X)\|_2 \]
\[ \leq C_1o_p(n^{-p}) + C_2o_p(n^{-p}) = o_p(n^{-p}). \]

Here, we used the assumptions that \( r(X) \) is uniformly bounded by \( C_1 \) and \( w(A, X) \) is uniformly bounded by \( C_2 \). □

### E.5 Proof of Theorem[3]

**Proof.** Let us define \( \phi_1(x, a, y; r, w, f) \) and \( \phi_2(z; f) \):
\[ \phi_1(x, a, y; r, w, f) = r(x)w(a, x)\{ y - f(a, x) \}, \quad \phi_2(z; f) = v(z). \]

We also denote the union of \( n_{i}^{\text{hat}} \) and \( n_{i}^{\text{evl}} \) by \( D_i \) for \( i = 1, 2 \), and the number of \( n_{1}^{\text{hat}}, n_{2}^{\text{hat}}, n_{1}^{\text{evl}}, n_{2}^{\text{evl}} \) by \( n_{11}, n_{21}, n_{12}, n_{22} \). For simplicity, we assume \( n_{11} = n_{12}, n_{21} = n_{22} \).
Then, we have

\[
\{ \mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; \hat{r}(1), \hat{w}(1), \hat{f}(1)) \right] + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; \hat{f}(1)) \right] - R(\pi^c) \} 
\]

\[
= \left\{ \frac{1}{\sqrt{n_{11}}} G_{n_{\text{true}}} \left[ \phi_1(X, A, Y; \hat{r}(1), \hat{w}(1), \hat{f}(1)) - \phi_1(X, A, Y; r^1, w^1, f^1) \right] + \frac{1}{\sqrt{n_{12}}} G_{n_{\text{evl}}} \left[ \phi_2(Z; \hat{f}(1)) - \phi_2(Z; f^1) \right] \right\} + 
\]

\[
+ \left\{ \mathbb{E}[\phi_1(X, A, Y; \hat{r}(1), \hat{w}(1), \hat{f}(1)) | \hat{r}(1), \hat{w}(1), \hat{f}(1)] + \mathbb{E}[\phi_2(Z; \hat{f}(1)) | \hat{f}(1)] 
\]

\[
- \mathbb{E}[\phi_1(X, A, Y; r^1, w^1, f^1)] - \mathbb{E}[\phi_2(Z; f^1)] \right\} 
\]

\[
+ \left\{ \mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; r^1, w^1, f^1) \right] + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; f^1) \right] - R(\pi^c) \right\}. 
\]  


(26)

The term (26) is \( o_p(1/\sqrt{n}) \) by Step 1 in the previous theorem noting that what we have used is \( \|\hat{r}(X)\hat{w}(A, X) - w^1(A, X)r^1(A, X)\| = o_p(1), \|\hat{f}(A, X) - f^1(A, X)\| = o_p(1). \) The term Eq. (27) is also \( o_p(1) \) by Step 1 as we will show soon.

**Step 1:** Eq. (27) is \( o_p(1). \) We have

\[
|\mathbb{E}[\phi_1(X, A, Y; \hat{r}(1), \hat{w}(1), \hat{f}(1)) | \hat{r}(1), \hat{w}(1), \hat{f}(1)] + \mathbb{E}[\phi_2(Z; \hat{f}(1)) | \hat{f}(1)] - \mathbb{E}[\phi_1(x; r, w, f)] - \mathbb{E}[\phi_2(Z; f)]| 
\]

\[
\leq |\mathbb{E}[\{\hat{r}(1)(X)\hat{w}(A, X) - r^1(x)w^1(A, X)\}\{\hat{f}(1)(A, X) + f^1(A, X)\} | \hat{r}(1), \hat{w}(1), \hat{f}(1)] 
\]

\[
+ |\mathbb{E}[r^1(x)w^1(A, X)\{\hat{f}(1)(A, X) + f^1(A, X)\} | \hat{r}(1), \hat{w}(1), \hat{f}(1)] + \mathbb{E}[\hat{r}(1)(Z) - v^1(Z) | \hat{f}(1)]| 
\]

\[
+ |\mathbb{E}[\hat{r}(1)(X)\hat{w}(A, X)(Y - f^1(A, X)) | \hat{r}(1), \hat{w}(1)]. 
\]

Here, if \( f^1(a, x) = f(a, x) \), we have

\[
o_p(1)o_p(1) + o_p(1) + 0 = o_p(1) = o_p(1). 
\]

if \( r^1(x)w^1(a, x) = r(x)w(a, x) \), we have

\[
o_p(1)o_p(1) + 0 + o_p(1) = o_p(1) = o_p(1). 
\]

Therefore, Eq. (27) is \( o_p(1). \)

**Step 2:** By combining together, we have

\[
\mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; \hat{r}(1), \hat{w}(1), \hat{f}(1)) \right] + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; \hat{f}(1)) \right] - R(\pi^c) 
\]

\[
= \mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; r^1, w^1, f^1) \right] + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; f^1) \right] - R(\pi^c) + o_p(1). 
\]

Then,

\[
R_{\text{DRCS}} = 0.5\mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; \hat{r}(1), \hat{w}(1), \hat{f}(1)) + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; \hat{f}(1)) \right] 
\]

\[
+ 0.5\mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; \hat{r}(2), \hat{w}(2), \hat{f}(2)) + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; \hat{f}(2)) \right] \right] 
\]

\[
+ 0.5\mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; r^1, w^1, f^1) \right] + 0.5\mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; f^1) \right] + 
\]

\[
+ 0.5\mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; r^1, w^1, f^1) \right] + 0.5\mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; f^1) \right] + o_p(1) 
\]

\[
= \mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; r^1, w^1, f^1) \right] + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; f^1) \right] + o_p(1). 
\]

Then, the statement is concluded since

\[
\mathbb{E} \left[ \mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; r^1, w^1, f^1) \right] + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; f^1) \right] \right] = R(\pi^c) 
\]

based on the double robust structure and

\[
\mathbb{E}_{n_{\text{true}}} \left[ \phi_1(X, A, Y; r^1, w^1, f^1) \right] + \mathbb{E}_{n_{\text{evl}}} \left[ \phi_2(Z; f^1) \right] = R(\pi^c) + o_p(1) 
\]

from the law of large numbers based on Assumption[1]

### E.6 Proof of Theorem[4]

**Proof.** We can prove similarly as in the proof of Theorem[1] Therefore, we omit the proof.
E.7 Proof of Theorem 5

Proof of Theorem 5 For the ease of notation, we prove the case \( n^{\text{hst}} = n^{\text{evl}} \) noting the kernel estimator is linearized as in Theorem 11 and the generalization is easy. We have

\[
\left| \frac{\hat{p}_h(x)}{p(x)} - \frac{q(x)}{p(x)} - \hat{c}_h(x) \right|_\infty = o_p(n^{-1/2}),
\]

where

\[
\hat{c}_h(x) = \frac{1}{p(x)} \left\{ \frac{\hat{q}_h(x)}{p(x)} - q(x) \right\} - \frac{q(x)}{p(x)} \left\{ \frac{\hat{p}_h(x)}{p(x)} - p(x) \right\}.
\]

This is proved by Theorem 10. Then,

\[
\hat{R}_\text{IPWCSB} = E_{n^{\text{hst}}} \left[ \frac{\hat{q}_h(X) \pi^e(A \mid X)Y}{p_h(X) \pi^b(A \mid X)} \right] = \frac{1}{n^{\text{hst}}} \sum_{i=1}^{n^{\text{hst}}} \frac{\pi^e(A_i \mid X_i)Y_i}{\pi^b(A_i \mid X_i)} \{ r(X_i) + \hat{c}_h(X_i) \} = E_{n^{\text{hst}}} \left[ \frac{q(X) \pi^e(A \mid X)Y}{p(X) \pi^b(A \mid X)} \right] + \frac{1}{n^{\text{hst}}n^{\text{evl}}} \sum_{i=1}^{n^{\text{hst}}} \sum_{j=1}^{n^{\text{evl}}} a_{i,j}
\]

where

\[
a_{i,j}((X_i, A_i, Y_i), (Z_j)) = \frac{1}{p(X_i)} \frac{\pi^e(A_i \mid X_i)Y_i}{\pi^b(A_i \mid X_i)} \{ K_h(Z_j - X_i) - q(X_i) \} - \frac{q(X_i)}{p^2(X_i)} \frac{\pi^e(A_i \mid X_i)Y_i}{\pi^b(A_i \mid X_i)} \{ K_h(X_j - X_i) - p(X_i) \},
\]

and

\[
b_{i,j}((X_i, A_i, Y_i, Z_i), (X_j, A_j, Y_j, Z_j)) = 0.5 \{ a_{i,j} + a_{j,i} \}.
\]

Then,

\[
\frac{2}{n^{\text{hst}}n^{\text{evl}}} \sum_{i < j} b_{i,j}((X_i, A_i, Y_i, Z_i), (X_j, A_j, Y_j, Z_j)) = 2 \frac{1}{n^{\text{hst}}} \left\{ \sum_{i=1}^{n^{\text{hst}}} E[b_{i,j} \mid X_i, A_i, Y_i, Z_i] \right\} + o_p(n^{-1/2})
\]

\[
= \frac{1}{n^{\text{evl}}} \sum_{i=1}^{n^{\text{evl}}} E[a_{i,i} \mid X_i, A_i, Y_i, Z_i] + \frac{1}{n^{\text{hst}}} \sum_{i=1}^{n^{\text{hst}}} E[a_{i,j} \mid X_i, A_i, Y_i, Z_i] + o_p(n^{-1/2})
\]

\[
= \frac{1}{n^{\text{evl}}} \sum_{i=1}^{n^{\text{evl}}} \{ v(Z_i) - r(X_i)v(X_i) \} + o_p(n^{-1/2}).
\]

From the first line to the second line, we have used a U-statistics theory [van der Vaart, 1998, Chapter 12]. From the third line to the fourth line, we have used

\[
E[a_{i,i} \mid Z_i, X_i, A_i, Y_i] = o_p(n^{-1/2}) + \left\{ E \left[ \frac{1}{p(X_i)} \frac{\pi^e(A_i \mid X_i)Y_i}{\pi^b(A_i \mid X_i)} \mid X_i = Z_i \right] - E \left[ \frac{q(X_i)}{p^2(X_i)} \frac{\pi^e(A_i \mid X_i)Y_i}{\pi^b(A_i \mid X_i)} \mid X_i = Z_i \right] \right\} p(X_i)
\]

\[
= o_p(n^{-1/2}) + v(Z_i) - r(X_i)v(X_i),
\]

\[
E[a_{i,j} \mid Z_i, X_i, A_i, Y_i] = o_p(n^{-1/2}).
\]

Therefore,

\[
\hat{R}_\text{IPWCSB} = E_{n^{\text{hst}}} \left[ \frac{q(X)}{p(X)} \left\{ \frac{\pi^e(A \mid X)Y}{\pi^b(A \mid X)} - v(X) \right\} \right] + \frac{1}{n^{\text{evl}}} E[v(Z)] + o_p(n^{-1/2}).
\]

The final statement is concluded by CLT.
E.8 Proof of Theorem 6

Proof. For the ease of the notation, we prove the case \( n_{\text{bst}} = n_{\text{evl}} \) noting the kernel estimator is linearized as in Theorem 11 and the generalization is easy. Here, we concatenate \( X \) and \( A \) as \( D \). We also write \( p(x)\pi^b(A \mid x) \) as \( u(d) \).

\[
\left\| \frac{\hat{q}_h(x)}{u_h(d)} - \frac{q(x)}{u(d)} - \hat{e}_h(d) \right\|_{\infty} = o_p(n^{-1/2}),
\]

where

\[
\hat{e}_h(d) = \frac{1}{u(df)} \left\{ \hat{q}_h(x) - q(x) \right\} - \frac{q(x)}{u(df)} \left\{ \hat{u}_h(d) - u(d) \right\}.
\]

This is proved by Theorem 10. Then,

\[
\hat{R}_{\text{IPWCS}} = E_{n_{\text{bst}}} \left[ \frac{\hat{q}_h(X) \pi^e(A \mid X)Y}{\hat{p}_h(X) \pi^b(A \mid X)} \right]
\]

\[
= \frac{1}{n_{\text{bst}}} \sum_{i=1}^{n_{\text{bst}}} \pi^e(A_i \mid X_i)Y_i \left\{ \frac{q(X_i)}{u(D_i)} + \hat{e}_h(X_i) \right\}
\]

\[
= E_{n_{\text{bst}}} \left[ \frac{q(X) \pi^e(A \mid X)Y}{p(X) \pi^b(A \mid X)} \right] + \frac{1}{n_{\text{bst}} n_{\text{evl}}} \sum_{i=1}^{n_{\text{bst}}} \sum_{j=1}^{n_{\text{evl}}} a_{i,j}
\]

\[
= E_{n_{\text{bst}}} \left[ \frac{q(X) \pi^e(A \mid X)Y}{p(X) \pi^b(A \mid X)} \right] + \frac{2}{n_{\text{bst}} n_{\text{evl}}} \sum_{i<j} b_{i,j},
\]

where

\[
a_{i,j}((X_i, A_i, Y_i), (Z_j)) = \frac{1}{p(X_i)} \frac{\pi^e(A_i \mid X_i)Y_i}{\pi^b(A_i \mid X_i)} \left( K_h(Z_j - X_i) - q(X_i) \right)
\]

\[
- \frac{q(X_i)}{u(D_i)} \pi^e(A_i \mid X_i)Y_i \{ K_h(D_j - D_i) - u(D_i) \},
\]

\[
b_{i,j}((X_i, A_i, Y_i, Z_i), (X_j, A_j, Y_j, Z_j)) = 0.5(a_{i,j} + a_{j,i}).
\]

Then,

\[
\frac{2}{n_{\text{bst}} n_{\text{evl}}} \sum_{i<j} b_{i,j}((X_i, A_i, Y_i, Z_i), (X_j, A_j, Y_j, Z_j))
\]

\[
= \frac{2}{n_{\text{bst}}} \left\{ \sum_{i=1}^{n_{\text{bst}}} E[b_{i,j} \mid X_i, A_i, Y_i, Z_i] \right\} + o_p(n^{-1/2})
\]

\[
= \frac{1}{n_{\text{evl}}} \sum_{i=1}^{n_{\text{evl}}} E[a_{i,i} \mid X_i, A_i, Y_i, Z_i] + \frac{1}{n_{\text{bst}}} \sum_{i=1}^{n_{\text{bst}}} E[a_{i,j} \mid X_i, A_i, Y_i, Z_i] + o_p(n^{-1/2})
\]

\[
= \frac{1}{n_{\text{evl}}} \sum_{i=1}^{n_{\text{evl}}} \{ v(Z_i) - r(X_i)w(X_i, A_i)f(D_i) \} + o_p(n^{-1/2}).
\]

From the first line to the second line, we used the U-statistics theory (van der Vaart 1998, Chapter 12). From the third line to the fourth line, we used

\[
E[a_{i,i} \mid Z_i, X_i, A_i, Y_i]
\]

\[
= o_p(n^{-1/2}) + E \left[ \frac{1}{p(X_i)} w(A_i, X_i)Y_i \mid X_i = Z_i \right] p(X_i) - E \left[ \frac{q(X_i)}{u(D_i)} \pi^e(A_i \mid X_i)Y_i \mid D_i = D_i \right] u(D_i)
\]

\[
= o_p(n^{-1/2}) + v(Z_i) - r(X_i)w(X_i, A_i)f(D_i),
\]

\[
E[a_{i,j} \mid Z_i, X_i, A_i, Y_i] = o_p(n^{-1/2}).
\]

Therefore,

\[
\hat{R}_{\text{IPWCS}} = E_{n_{\text{bst}}} \left[ \frac{q(X) \pi^e(A \mid X)Y}{p(X) \pi^b(A \mid X)} \{ f(A, X) \} \right] + E_{n_{\text{evl}}} [v(Z)] + o_p(n^{-1/2}).
\]

The final statement is concluded by CLT. \qed
E.9 Proof of Theorem 7

Proof. For the ease of the notation, we prove the case \( n^{\text{hst}} = n^{\text{evl}} \) noting the kernel estimator is linearized as in Theorem 11 and generalization is easy. Here, \( \hat{v}_h(a, x) \) is defined as

\[
\hat{v}_h(a, x) = \frac{\hat{p}_h(a, x)}{u_h(a, x)} = \frac{1}{n^{\text{hst}}} \sum_{i=1}^{n^{\text{hst}}} Y_i K_h\{\{X_i, A_i\} - \{x, a\}\}
\]

\[
\hat{u}_h(a, x) = \frac{1}{n^{\text{hst}}} \sum_{i=1}^{n^{\text{hst}}} K_h\{\{X_i, A_i\} - \{x, a\}\}.
\]

We have

\[
\left\| \frac{\hat{p}_h(a, x)}{u_h(a, x)} - \frac{f(a,x)u(a,x)}{u(a,x)} - \hat{e}_h(x, a) \right\| = o_p(n^{-1/2}),
\]

where

\[
\hat{e}_h(x, a) = \frac{1}{u(a,x)} \{ \hat{p}_h(a, x) - f(a, x)u(a, x) \} - \frac{f(a, x)}{u(a, x)} \{ \hat{u}_h(a, x) - u(a, x) \}.
\]

This is proved by Theorem 10. Then, we have

\[
\hat{R}_{\text{DM}} = E_{n^{\text{evl}}} [\hat{v}_h(Z, A)]
\]

\[
= E_{n^{\text{evl}}} [v(Z, A)] + \frac{1}{n^{\text{hst}} n^{\text{evl}}} \sum_{i=1}^{n^{\text{hst}}} \sum_{j=1}^{n^{\text{evl}}} a_{i,j}
\]

\[
= E_{n^{\text{evl}}} [v(Z, A)] + \frac{2}{n^{\text{hst}} n^{\text{evl}}} \sum_{i<j} b_{i,j},
\]

where

\[
a_{i,j}(\{Z_i, A_i\}, \{X_j, A_j, Y_j\}) = \frac{1}{u(Z_i, A_i)} \{ Y_j K_h\{\{X_j, A_j\} - \{Z_i, A_i\}\} - u(Z_i, A_i) f(Z_i, A_i) \} - \frac{f(Z_i, A_i)}{u(Z_i, A_i)} \{ K_h\{\{X_j, A_j\} - \{Z_i, A_i\}\} - u(Z_i, A_i) \},
\]

\[
b_{i,j}(\{X_i, A_i, Y_i, Z_i\}, \{X_j, A_j, Y_j, Z_j\}) = 0.5 \{ a_{i,j} + a_{j,i} \}.
\]

Then,

\[
\frac{2}{n^{\text{hst}} n^{\text{evl}}} \sum_{i<j} b_{i,j}(\{X_i, A_i, Y_i, Z_i\}, \{X_j, A_j, Y_j, Z_j\})
\]

\[
= \frac{2}{n^{\text{hst}}} \left\{ \sum_{i=1}^{n^{\text{hst}}} E[b_{i,j} \mid X_i, A_i, Y_i, Z_i] \right\} + o_p(n^{-1/2})
\]

\[
= \frac{1}{n^{\text{evl}}} \sum_{i=1}^{n^{\text{evl}}} E[a_{j,i} \mid X_i, A_i, Y_i, Z_i] + \frac{1}{n^{\text{hst}}} \sum_{i=1}^{n^{\text{hst}}} E[a_{i,j} \mid X_i, A_i, Y_i, Z_i] + o_p(n^{-1/2})
\]

\[
= \frac{1}{n^{\text{evl}}} \sum_{i=1}^{n^{\text{evl}}} \{ Y_i - f(X_i, A_i) \} r(X_i) w(X_i, A_i) + o_p(n^{-1/2}).
\]

From the first line to the second line, we used a U-statistics theory (van der Vaart, 1998, Chapter 12). From the third line to the fourth line, we used

\[
E[a_{j,i} \mid Z_i, X_i, A_i, Y_i] = o_p(n^{-1/2}) + \left\{ \frac{Y_i}{u(X_i, A_i)} - \frac{f(X_i, A_i)}{u(X_i, A_i)} \right\} q(X_i) q^0(A_i \mid X_i)
\]

\[
= o_p(n^{-1/2}) + Y_i r(X_i) w(A_i, X_i) - r(X_i) f(X_i, A_i) w(A_i, X_i),
\]

\[
E[a_{i,j} \mid Z_i, X_i, A_i, Y_i] = o_p(n^{-1/2}).
\]

This is proved by Theorem 10. Therefore,

\[
\hat{R}_{\text{DM}} = E_{n^{\text{hst}}} [r(X) w(A, X) \{ Y - f(A, X) \}] + E_{n^{\text{evl}}} [v(Z)] + o_p(n^{-1/2}).
\]

The final statement is concluded by CLT. 

□
E.10 Proof of Theorem 8

Proof: We prove the statement following [Zhou et al., 2018]. Though the proof is very similar, for completeness, we sketch the proof the case \( \rho = 0.5 \). Since the estimator is asymptotically linear, the generalization is easy as in Theorem 11.

Define two scores;

\[
\hat{\Gamma}_i = \hat{r}_w(D_i)(X_i, A_i)\{Y_i - f(D_i)(X_i, A_i)\} + [f(a_1, X_i), \cdots, f(a_\alpha, X_i)]^	op,
\]

\[
\Gamma_i = r_w(X_i, A_i)\{Y_i - f(X_i, A_i)\} + [f(a_1, X_i), \cdots, f(a_\alpha, X_i)]^	op,
\]

where \( D_i \) is an indicator which cross-fold estimator is used and \( \alpha \) is a dimension of the action, \( r_w(x) = r(x) / \pi^b(a | x) \). Then, we have \( \hat{R}_{\text{DRCS}}(\pi) = \frac{2}{n} \{ \sum_{i=1}^{n/2} \langle \pi(Z_i), \hat{\Gamma}_i \rangle \} \). Here, we define the estimator with oracle efficient influence function

\[
\hat{R}(\pi) = \frac{2}{n} \sum_{i=1}^{n/2} \langle \pi(Z_i), \Gamma_i \rangle.
\]

In addition, we define

\[
\Delta(\pi_a, \pi_b) = R(\pi_a) - R(\pi_b),
\]

\[
\Delta(\pi_a, \pi_b) = \hat{R}(\pi_a) - \hat{R}(\pi_b).
\]

**Step 1:** First, following [Zhou et al., 2018, Theorem 2], we prove the following. Let \( \hat{\pi} \in \arg \min_{\pi \in \Pi} \hat{R}(\pi) \). Then for any \( \delta > 0 \), with probability at least \( 1 - 2\delta \),

\[
R(\hat{\pi}) - R(\pi^*) \leq O\left( \left\{ k(\Pi) + \sqrt{\log(1/\delta)} \right\} \sqrt{\frac{\Upsilon^*}{n}} \right),
\]

where

\[
\Upsilon^*_s = \sup_{\pi \in \Pi} \mathbb{E}[\langle \Gamma_i, \pi(Z_i) \rangle^2]
\]

\[
= \sup_{\pi \in \Pi} \mathbb{E}[r(X_i)^2 w_\pi^2(X_i, A_i)\{Y_i - f(X_i, A_i)\}^2] + \mathbb{E}[\{v_\pi(Z_i)\}^2],
\]

when \( w_\pi(a, x) = \pi(a, x) / \pi^b(a | x) \), \( v_\pi(x) = \mathbb{E}_{\pi(a|x)}[f(a, x) | x] \).

This is proved as follows. We have

\[
R(\hat{\pi}) - R(\pi^*) \leq \sup_{\pi_a, \pi_b \in \Pi} |\Delta(\pi_a, \pi_b) - \Delta(\pi_a, \pi_b)|.
\]

Then, by using a Chaining argument as Lemma 1 [Zhou et al., 2018], we can bound an expectation of \( \sup_{\pi_a, \pi_b \in \Pi} |\Delta(\pi_a, \pi_b) - \Delta(\pi_a, \pi_b)| \) via Rademacher complexity. Then, as in Lemma 2 [Zhou et al., 2018], the high probability bound is obtained via Talagrand inequality. Then, we have

\[
R(\hat{\pi}) - R(\pi^*) \leq O\left( \left\{ k(\Pi) + \sqrt{\log(1/\delta)} \right\} \sqrt{\frac{\Upsilon^*}{n}} \right),
\]

where

\[
\Upsilon^*_s = \sup_{\pi_a, \pi_b \in \Pi} \mathbb{E}[\langle \Gamma_i, \pi_a(Z_i) - \pi_b(Z_i) \rangle^2].
\]

This concludes the above statement since

\[
\Upsilon^*_s = \sup_{\pi_a, \pi_b \in \Pi} \mathbb{E}[\langle \Gamma_i, \pi_a(Z_i) - \pi_b(Z_i) \rangle^2]
\]

\[
= \sup_{\pi_a, \pi_b \in \Pi} \mathbb{E}[r(X_i)^2 \{w_{\pi_a} - w_{\pi_b}\}^2\{Y_i - f(X_i, A_i)\}^2] + \mathbb{E}[\{v_{\pi_a}(Z_i) - v_{\pi_b}(Z_i)\}^2]
\]

\[
\leq \sup_{\pi \in \Pi} 2\mathbb{E}[r(X_i)^2 w_{\pi}^2(X_i, A_i)\{Y_i - f(X_i, A_i)\}^2] + 2\mathbb{E}[\{v_{\pi}(Z_i)\}^2].
\]
Step 2: Assume $\kappa(\Pi) < \infty$, then
\[
\sup_{\pi_a, \pi_b \in \Pi} |\hat{\Delta}(\pi_a, \pi_b) - \hat{\Delta}(\pi_a, \pi_b)| = o_p(n^{-1/2}).
\]

The proof of this statement is based on the double structure of the influence function and cross-fitting. We omit the proof since it is long, and almost the same as Lemma 3 (Zhou et al., 2018).

Step 3: Finally, based on Theorem 3 (Zhou et al., 2018), we have
\[
R(\hat{\pi}) - R(\pi^*) \leq \sup_{\pi_a, \pi_b \in \Pi} |\hat{\Delta}(\pi_a, \pi_b) - \Delta(\pi_a, \pi_b)| + \sup_{\pi_a, \pi_b \in \Pi} |\hat{\Delta}(\pi_a, \pi_b) - \Delta(\pi_a, \pi_b)|
\leq O_p \left( \left\{ k(\Pi) + \sqrt{\log(1/\delta)} \right\} \sqrt{\frac{\Upsilon_*}{n}} \right).
\]

This means there exists an integer $N_\delta$ such that with probability at least $1 - 2\delta$, for all $n \geq N_\delta$:
\[
R(\hat{\pi}) - R(\pi^*) \leq \frac{k(\Pi) + \sqrt{\log(1/\delta)}}{\sqrt{n}} \sqrt{\frac{\Upsilon_*}{n}}.
\]

Remark 6. In the general case,
\[
\Upsilon_* = \sup_{\pi \in \Pi} R_n^\rho [r(X_i) \omega_\pi^2(X_i, A_i)\{Y_i - f(X_i, A_i)\}^2] + (1 - \rho)^{-1} E\{v_\pi(Z_i)^2\}.
\]

\[\square\]

F Self-Normalized Doubly Robust Estimator with Cross-Fitting

In this section, we define self-normalized versions of estimators $\hat{R}_{DRCS}(\pi^*)$ and $\hat{R}_{IPWCS}(\pi^*)$. Let us define the self-normalized DRCS estimator as follows:
\[
\hat{R}_{DRCS-SN}(\pi^*) = \frac{1}{n^{\text{hst}}} \sum_{i=1}^{n^{\text{hst}}} \frac{1}{\pi^\tau(a_i | X_i)} \frac{1}{n^{\text{hst}}} \sum_{t=1}^{n^{\text{hst}}} \hat{f}(X_i) \hat{w}(a, X_i) \mathbb{1}[A_t = a] \{Y_t - \hat{f}(a, X_t)\}
\]
\[
+ \frac{1}{n^{\text{evi}}} \sum_{i=1}^{n^{\text{evi}}} \sum_{a \in \mathcal{A}} \hat{f}(a, Z_i) \pi^\tau(a | Z_i),
\]

and the self-normalized IPWCS estimator as follows:
\[
\hat{R}_{IPWCS-SN}(\pi^*) = \frac{1}{n^{\text{hst}}} \sum_{i=1}^{n^{\text{hst}}} \frac{1}{\pi^\tau(a_i | X_i)} \frac{1}{n^{\text{hst}}} \sum_{t=1}^{n^{\text{hst}}} \frac{\hat{q}(X_i) \pi^\tau(a_i | X_i) \mathbb{1}[A_t = a] Y_t}{\hat{p}(X_i) \pi^\tau(a_i | X_i)}.
\]

G Algorithm for Off-Policy Learning with Cross-Fitting

In the proposed method of OPL under a covariate shift, we train an evaluation policy by using an estimator $\hat{R}_{DRCS}(\pi^*)$, which is constructed via cross-fitting. In this section, we introduce an algorithm where we use a linear-in-parameter model with kernel functions to approximate a new policy. For $x \in \mathcal{X}$, a linear-in-parameter model is defined as follows:
\[
\pi(a | x; \sigma^2) = \frac{\exp(g(a, x; \sigma^2))}{\sum_{a \in \mathcal{A}} \exp(g(a, x; \sigma^2))},
\]
where $g(a, x; \sigma^2) = \beta_a^T \varphi(x; \sigma^2) + \beta_0, \varphi(x; \sigma^2) = [\varphi_1(x; \sigma^2), \ldots, \varphi_m(x; \sigma^2)]^T$, $\varphi_m(x; \sigma^2)$ is the Gaussian kernel defined as
\[
\varphi_u(x; \sigma^2) = \exp\left( -\frac{\|x-c_u\|^2}{2\sigma^2} \right), 1 \leq u \leq m,
\]
\{c_1, \ldots, c_m\} is $m$ chosen points from $\{X_i\}_{i=1}^{n^{\text{hst}}}, \beta_0 \in \mathbb{R}^m$, and $\beta_0 \in \mathbb{R}$. In optimization, we put a regularization term $\mathcal{R}(\{\beta_0, \beta_{0,a}\})$ and train a new policy as follows:
\[
\hat{\pi}_{DRCS} = \arg\max_{\pi \in \Pi} \hat{R}_{DRCS}(\pi) + \lambda \mathcal{R}(\{\beta_0, \beta_{0,a}\}),
\]
Table 7: Off-policy evaluation with SatImage dataset

| Behavior Policy | DRCS | IPWCS | DM | IPWCS-R | DM-R | DRCS-SN | IPWCS-SN |
|-----------------|------|-------|----|---------|------|---------|---------|
| 0.7πd + 0.3πu  | 0.107| 0.032 | 0.042 | 0.043 | 0.073 | 0.023 | 0.188 |
| 0.4πd + 0.6πu  | 0.096| 0.025 | 0.134 | 0.052 | 0.177 | 0.033 | 0.189 |
| 0.0πd + 1.0πu  | 0.154| 0.051 | 0.336 | 0.079 | 0.372 | 0.050 | 0.358 |

Table 8: Off-policy evaluation with Vehicle dataset

| Behavior Policy | DRCS | IPWCS | DM | IPWCS-R | DM-R | DRCS-SN | IPWCS-SN |
|-----------------|------|-------|----|---------|------|---------|---------|
| 0.7πd + 0.3πu  | 0.029| 0.019 | 0.038 | 0.035 | 0.040 | 0.014 | 0.086 |
| 0.4πd + 0.6πu  | 0.019| 0.024 | 0.095 | 0.062 | 0.089 | 0.019 | 0.086 |
| 0.0πd + 1.0πu  | 0.037| 0.030 | 0.213 | 0.049 | 0.210 | 0.031 | 0.174 |

Table 9: Off-policy evaluation with PenDigits dataset

| Behavior Policy | DRCS | IPWCS | DM | IPWCS-R | DM-R | DRCS-SN | IPWCS-SN |
|-----------------|------|-------|----|---------|------|---------|---------|
| 0.7πd + 0.3πu  | 0.118| 0.020 | 0.083 | 0.035 | 0.052 | 0.045 | 0.089 |
| 0.4πd + 0.6πu  | 0.110| 0.026 | 0.220 | 0.053 | 0.056 | 0.040 | 0.231 |
| 0.0πd + 1.0πu  | 0.314| 0.086 | 0.503 | 0.049 | 0.116 | 0.187 | 0.511 |

Table 10: Off-policy learning with PenDigits dataset

| Behavior Policy | DRCS | IPWCS | DM |
|-----------------|------|-------|----|
| 0.7πd + 0.3πu  | 0.683| 0.030 | 0.241|
| 0.4πd + 0.6πu  | 0.678| 0.039 | 0.252|
| 0.0πd + 1.0πu  | 0.409| 0.067 | 0.204|

where \( \lambda > 0 \). The parameters \( \sigma^2 \) and \( \lambda \) are hyper-parameters selected via cross-validation. Thus, in the proposed method, we use the cross-fitting and cross-validation. We describe the algorithm in Algorithm 2 with \( K \) fold cross-fitting and \( L \) fold cross-validation. In Algorithm 2, we express the objective function with hyper-parameters \( \sigma^2 \) and \( \lambda \) as follows:

\[
\frac{1}{n_{\text{hst}}} \sum_{i=1}^{n_{\text{hst}}} \hat{r}(X_i; \pi(A_i|X_i; \sigma^2)) \left( Y_i - \hat{f}(A_i, X_i) \right) + \frac{1}{n_{\text{evl}}} \sum_{i=1}^{n_{\text{evl}}} \sum_{a \in A} \hat{f}(a, Z_i) \pi(a | Z_i; \sigma^2) + \lambda \mathcal{R}(\{\beta_a, \beta_0,a\}).
\]

H Additional Experimental Results of Section 7.1

In addition to the results shown in Section 7.1, we show the performances of IPWCS and DM estimator with nuisance functions estimated by the kernel Ridge regression, which are referred as IPWCS-R and DM-R, and the self-normalized versions of the proposed estimators, DRCS and IPWCS estimator, which are referred as DRCS-SN and IPWCS-SN, in Table 7-8. We also add the OPE and OPL experiment with PenDigits in Tables 9 and 10.
Algorithm 2 Off-policy learning with $\hat{R}_{\text{DRCS}}(\pi^c)$.

**Input:** A hypothesis class $\Pi$ of $\pi^c$.

**Input:** Candidates of $\sigma^2$, $\{\sigma_1^2, \ldots, \sigma_n^2\}$.

**Input:** Candidates of $\lambda$, $\{\lambda_1, \ldots, \lambda_n\}$.

Take a $K$-fold random partition $(I_k)_{k=1}^K$ of observation indices $[n^\text{hst}] = \{1, \ldots, n^\text{hst}\}$ such that the size of each fold $I_k$ is $n_k^\text{hst} = n^\text{hst}/K$.

Take a $K$-fold random partition $(J_k)_{k=1}^K$ of observation indices $[n^\text{evl}] = \{1, \ldots, n^\text{evl}\}$ such that the size of each fold $J_k$ is $n_k^\text{evl} = n^\text{evl}/K$.

For each $k \in [K] = \{1, \ldots, K\}$, define $I_k^c := \{1, \ldots, n^\text{hst}\} \setminus I_k$ and $J_k^c := \{1, \ldots, n^\text{evl}\} \setminus J_k$.

Define $(\mathcal{S}_k)_{k=1}^K$ with $\mathcal{S}_k = \{(X_i, A_i, Y_i)\}_{i \in I_k^c}$.

For $k \in [K]$ do:

Construct ML estimators $\hat{\pi}^b(a \mid X)$, $\hat{r}_k(x)$, and $\hat{f}_k(a, x)$ using $\mathcal{S}_k$.

end for

Take a $L$-fold random partition $(I_\ell)_{\ell=1}^L$ of observation indices $[n^\text{hst}] = \{1, \ldots, n^\text{hst}\}$ such that the size of each fold $I_\ell$ is $n_\ell^\text{hst} = n^\text{hst}/L$.

Take a $L$-fold random partition $(J_\ell)_{\ell=1}^L$ of observation indices $[n^\text{evl}] = \{1, \ldots, n^\text{evl}\}$ such that the size of each fold $J_\ell$ is $n_\ell^\text{evl} = n^\text{evl}/L$.

For each $\ell \in [L] = \{1, \ldots, L\}$, define $I_\ell^c := \{1, \ldots, n^\text{hst}\} \setminus I_\ell$ and $J_\ell^c := \{1, \ldots, n^\text{evl}\} \setminus J_\ell$.

Define $(\mathcal{S}_\ell)_{\ell=1}^L$ with $\mathcal{S}_\ell = \{(X_i, A_i, Y_i)\}_{i \in I_\ell^c}$.

For $\sigma^2 \in \{\sigma_1^2, \ldots, \sigma_n^2\}$ do:

Define $\text{Score}_{\sigma^2, \lambda} = 0$.

For $\ell \in [L]$ do:

Obtain $\hat{\pi}$ by solving the following optimization problem:

$$
\hat{\pi} = \arg \max_{\pi \in \Pi} \frac{1}{n^\text{hst}} \sum_{i \in I_\ell^c} \hat{r}_{k(i)}(X_i) \pi(A_i \mid X_i; \hat{\sigma}^2) \left( Y_i - \hat{f}_{k(i)}(A_i, X_i) \right) + \frac{1}{n^\text{evl}} \sum_{i \in J_\ell^c} \sum_{a \in \mathcal{A}} \hat{f}_{k(i)}(a, Z_i) \pi(a \mid Z_i; \hat{\sigma}^2)
$$

$$
+ \lambda R(\{\beta_\alpha, \beta_0, a\}),
$$

where $n_\ell \in I_{k(i)}$ and $n_\ell^c \in J_{k(i)}$.

Update the score $\text{Score}_{\sigma^2, \lambda}$ by,

$$
\text{Score}_{\sigma^2, \lambda} = \text{Score}_{\sigma^2, \lambda} + \frac{1}{n^\text{hst}} \sum_{i \in I_\ell^c} \hat{r}_{k(i)}(X_i) \pi(A_i \mid X_i; \hat{\sigma}^2) \left( Y_i - \hat{f}_{k(i)}(A_i, X_i) \right) + \frac{1}{n^\text{evl}} \sum_{i \in J_\ell^c} \sum_{a \in \mathcal{A}} \hat{f}_{k(i)}(a, Z_i) \hat{\pi}(a \mid Z_i; \hat{\sigma}^2).
$$

end for

end for

end for

Obtain $\hat{\pi}$ by solving the following optimization problem:

$$
\hat{\pi} = \arg \max_{\pi \in \Pi} \frac{1}{n^\text{hst}} \sum_{i \in I_\ell^c} \hat{r}_{k(i)}(X_i) \pi(A_i \mid X_i; \hat{\sigma}^2) \left( Y_i - \hat{f}_{k(i)}(A_i, X_i) \right) + \frac{1}{n^\text{evl}} \sum_{i \in J_\ell^c} \sum_{a \in \mathcal{A}} \hat{f}_{k(i)}(a, Z_i) \pi(a \mid Z_i; \hat{\sigma}^2)
$$

$$
+ \lambda R(\{\beta_\alpha, \beta_0, a\}),
$$

where $(\hat{\sigma}^2, \hat{\lambda}) = \arg \max_{(\sigma^2, \lambda) \in \{(\sigma_1^2, \ldots, \sigma_n^2), (\lambda_1, \ldots, \lambda_n)\}} \text{Score}_{\sigma^2, \lambda}$.

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