Conditional and transductive inference
about populations with fixed attributes

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May 30, 2022

Abstract

It has been argued that parameters that characterize sub-populations can be more relevant than super-population parameters. For example, a video subscription service might be interested in estimating the satisfaction of its current customers, as opposed to estimating that of a hypothetical infinite super-population. In this case, the customers might be viewed as fixed, while the satisfaction measurements might be random due to measurement noise and temporal variation. More generally, inference for populations with fixed attributes can be modeled as inferring parameters of conditional distributions given these attributes. Since the data for such sub-population are drawn from a conditional distribution, it is desirable that confidence intervals have conditional coverage guarantees, as opposed to marginal coverage guarantees.

We provide a framework for statistical inference on parameters of sub-populations with fixed attributes. We construct confidence intervals that attain asymptotic validity given the attributes. In addition, we develop a set of tools to infer the parameters of new populations with partially observed attributes under covariate shift; the confidence intervals also attain asymptotic conditional validity under mild conditions. The validity and applicability of the proposed methods are demonstrated on simulated and real-world data.

1 Introduction

While traditional statistical inference often focuses on parameters that characterize super-populations, there has been a surge of interest in estimation or inference for specific targets. For instance, instead of inferring average treatment effects (ATE) for a super-population, estimation of conditional average treatment effects (CATE) helps understand heterogeneous reactions based on relevant attributes \[5, 44, 30\], and predictive inference quantifies variability in individual’s response \[43, 36, 31\]. However, estimation of the CATE function can be noisy, and prediction intervals that are valid for the unit at hand (i.e., conditional on observed individual attributes) might not be available \[21\].

The setting of this paper is situated in-between super-population and unit-specific inference. We aim to infer parameters of a finite population with some fixed (or observed) attributes; such population can be viewed as drawn from the conditional distribution given these attributes. The inferential target is thus a functional of the conditional distribution, termed conditional parameter. It has been argued in \[2\] that sometimes conditional parameters are more relevant than super-population parameters.

Let us start with two scenarios where conditional parameters might be of interest; these motivating examples will be kept throughout the paper. Imagine a video streaming platform is interested in the satisfaction of some subscribers after releasing a new feature. The platform has collected some attributes such as age, country of residence, etc., on these customers. One can model the customers’ attributes as independently and identically distributed (i.i.d.) draws from a super-population. However, if the company is interested in the satisfaction of the current customer base, these attributes are fixed at the observed values and the randomness in the satisfaction measurements is only due to measurement error and day-to-day variation. Formally, one can view the attributes as fixed, or conditioned, on the observed values, and the satisfaction

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measurements as drawn from the conditional distribution given these attributes. Thus, the task is to infer parameters of the conditional distribution. We call such parameters \textit{conditional parameters} and refer to this setting as inference \textit{for the population at hand}. This is distinct from super-population inference: the latter would infer the overall satisfaction of an (imaginary) infinite customer base, which might be irrelevant for decision-making.

Taking a step further, consider a scenario where the same company is interested in rolling out the feature to a different set of subscribers after collecting the first batch of data, and some attributes of the new set of customers are known. Again, instead of inferring the parameter of an infinite customer base, the satisfaction of this specific group of new subscribers might be more relevant. We model the attributes as i.i.d. draws from a new super-population. However, for the purpose of inference, the attributes are again viewed as fixed, and the satisfaction of the new subscribers can be viewed as drawn from a conditional distribution given the observed attributes. The task is then to transfer the knowledge to the new population, or equivalently, to infer parameters of the new conditional distribution. In the following, we will call this setting \textit{transductive inference}.

In addition, inference for conditional parameters can be more reliable than super-population inference in some situations—it is valid conditional on the attributes, and thus relevant to the particular population of interest. This is further discussed in the following example.

\textbf{Example 1.1} (Conditional versus marginal inference). In this example, we discuss that inference for conditional parameters can be more reliable than inference for super-population parameters. Continuing the example of companies estimating customer satisfaction, suppose there are \( N = 1000 \) companies \( j = 1, \ldots, N \), each having \( n = 10000 \) fixed customers with attributes \( Z_{ij} \sim \mathcal{N}(0,1) \). Each company conducts a survey of customer satisfaction. We assume that the observations are

\[ Y_{ij} = f_j(Z_{ij}) + \epsilon_{ij}, \]

where \( \epsilon_{ij} \) is the measurement noise, and \( f_j(z) \) is the average satisfaction of a customer with attributes \( Z = z \), which can vary with \( j \). We also assume \( f_j(Z_{ij}) \) and \( \epsilon_{ij} \) have finite second moments. In our simulation, the attributes \( Z_{ij} \) are fixed at their observed values, while the measurement noise \( \epsilon_{ij} \) are repeatedly drawn.

Let us first consider super-population inference. Each company can construct marginally valid 95\% confidence intervals for the super-population parameter \( \mathbb{E}[f_j(Z)] \) via

\[ \frac{1}{n} \sum_{i=1}^n Y_{ij} \pm 1.96 \frac{\text{sd}(Y_{ij})}{\sqrt{n}}. \]

We show the histogram of coverage across companies in the left-hand side of Figure 1 where we observe undercoverage for some companies. Indeed, 26\% of companies have coverage below .95, and the average coverage among these companies is only .85. Furthermore, if these companies would repeat similar surveys many times, their confidence intervals would consistently suffer from undercoverage. On the other hand, the confidence intervals of some other companies will consistently overcover, if similar studies are repeated many times.

Mathematically, the issue is that for each company \( j \), the customers \( \{Z_{ij}\}_{i=1}^n \) are fixed and only the measurement noise \( \{\epsilon_{ij}\}_{i=1}^n \) are drawn repeatedly. Super-population inference that accounts for the randomness of both \( Z_{ij} \) and \( \epsilon_{ij} \) is marginally valid (the coverage is .95 averaged over all companies). In this situation, however, it would be more desirable to have coverage close to .95 for all companies, which corresponds to .95 coverage conditional on \( \{Z_{ij}\}_{i=1}^n \) for each \( j \).

As discussed above, the data scientist might find conditional parameters more relevant. One can conduct inference for the conditional parameter \( \frac{1}{n} \sum_{i=1}^n f_j(Z_{ij}) \), the average satisfaction of the fixed customers of company \( j \). 95\% confidence intervals can be constructed via

\[ \frac{1}{n} \sum_{i=1}^n Y_{ij} \pm 1.96 \frac{\text{sd}(\epsilon_{ij})}{\sqrt{n}}. \]

Note that the width of these confidence intervals is shorter than the width of confidence intervals for the super-population parameter. Here we assume the variance of \( \epsilon_{ij} \) is known; the asymptotic behavior of these confidence intervals remains the same when \( \text{sd}(\epsilon_{ij}) \) is replaced by a consistent estimator, which is available under mild conditions.

The histogram of coverage of these confidence intervals are shown on the right-hand side of Figure 1 where we observe coverage consistently close to .95 for all companies. By switching to conditional parameters, the confidence intervals are more reliable for customers in each company; at the same time, the inference is more reliable for any specific company.

In this paper, we study the estimation and inference of a population with some fixed attributes. The inferential target is a functional of conditional distributions, i.e., a \textit{conditional parameter}. Our contributions are two-fold: in the first setup that is close to that of \([2, 9, 8]\), we provide conditionally valid inference for a large class of estimands, that means, inference that is valid \textit{given} the observed attributes, instead of marginalizing over new draws. This generalizes the observation in Example [1.1] that conditional parameters...
coverage of superpopulation parameter

Coverage across companies

Frequency

0.75 0.80 0.85 0.90 0.95 1.00

0 50 100 150 200

Coverage of conditional parameter

Coverage across companies

Frequency

0.75 0.80 0.85 0.90 0.95 1.00

0 200 600 1000

Figure 1: Left: coverage of super-population confidence intervals across companies (37 companies with coverage < .75 are not shown in the histogram). Right: coverage of the conditional confidence intervals across companies. In both cases, the marginal coverage is .95. Details about the simulation setup can be found in Example 1.1.

The rest of the paper is organized as follows. In Section 2 we introduce the notion of conditional parameter as the estimand; we then formalize the two types of problems we study, with an overview of the conditional inference guarantees we are to provide, followed by a review of related literature. Section 3 presents the main results of this paper; in Section 3.1 we provide conditional inference for the population at hand; in Section 3.2 we develop conditionally valid transductive inference on a partially observed new dataset under known covariate shift; in Section 3.3 we study the same transductive inference setting with unknown covariate shift. In Sections 4 and 5 we apply the proposed methods to simulated and real-world data, showing reliable empirical performance.

2 Inferential targets

2.1 Conditional parameters

In this section, we introduce the conditional parameter as our inferential target, which characterizes a conditional distribution. It generalizes the conventional setting where a parameter characterizes a fixed super-population. Conditional parameters have been considered in [2, 9], and are closely related to several well-studied problems; we elaborate on the connections and distinctions in Section 2.3.

Let us start with a recap on classical settings [42, 41]. Given a super-population \( P \), an unknown parameter \( \theta_0 \in \Theta \subset \mathbb{R}^p \) is defined as a solution to

\[
\mathbb{E}[s(D, \theta)] = 0
\]

(2.1)

for some score function \( s : \mathbb{D} \times \Theta \rightarrow \mathbb{R}^p \), where \( \mathbb{E} \) denotes the expectation under \( P \). Here and in the following, we adopt the common assumption in the literature [42] that the solution to equation (2.1) is unique. Therefore, \( \theta_0 \) is a deterministic quantity that characterizes the super-population \( P \); inference of \( \theta_0 \) is often based on i.i.d. data \( \{D_i\}_{i=1}^n \) from \( P \).
In situations where some attributes are fixed, as inferential target we consider a functional of the conditional distribution from which the population of interest is drawn. Concretely, following [20][8], we suppose $(D_1, Z_1), \ldots, (D_n, Z_n)$ are i.i.d. from an unknown distribution $P$, where $D_i \in \mathcal{D}$ are observations, and $Z_i \in \mathcal{Z}$ are the (observed) attributes we condition on. Given the attributes $Z_n = (Z_1, \ldots, Z_n)$, the observations $D_n = (D_1, \ldots, D_n)$ are from $P[\cdot | Z_n]$, the conditional distribution given $Z_n$. We define the $Z_n$-conditional parameter $\theta_n^{\text{cond}} = \theta_n^{\text{cond}}(Z_n)$ as the solution to

$$
\sum_{i=1}^{n} E[s(D_i, \theta) | Z_i] = 0,
$$

(2.2)

which is assumed to be unique. Note that $\theta_n^{\text{cond}}$ depends on the observed $Z_1, \ldots, Z_n$, hence from a marginal perspective it is random and varies with the sample size. The conditional parameter $\theta_n^{\text{cond}}$ characterizes the distribution of $(D_1, \ldots, D_n)$ given that $(Z_1, \ldots, Z_n)$ are fixed at their observed values, as opposed to $\theta_0$ that characterizes the super-population. We also remark that conditional parameter can be seen as a generalization of the super-population parameter in the sense that $\theta_0 = \theta_n^{\text{cond}}(\emptyset)$.

**Example 2.1** (Customer satisfaction). In our motivating example of estimating customer satisfaction, we let $Z$ be the attributes, $Y \in \mathbb{R}$ be the satisfaction, and assume the data scientist observes i.i.d. data $(D_i, Z_i)_{i=1}^n$ where $D = (Y, Z)$ from $P$. The super-population parameter is $\theta_0 = E[D_i]$, which is the solution to equation (2.1) where $s(D, \theta) = D - \theta$. Correspondingly, the conditional parameter is $\theta_n^{\text{cond}} = \frac{1}{n} \sum_{i=1}^{n} E[D_i | Z_i]$, which is the average of conditional means among the $n$ subscribers, averaged over measurement error.

Conditional parameters generalize several well-studied settings such as fixed-X regression and finite-population causal effects, where some attributes are fixed and the inference is closely related to the populations at hand. In the following, we show such connection and illustrate how conditional parameters might differ from unconditional parameters.

**Example 2.2** (Linear regression under model misspecification). For linear regression with model misspecification [9], conditional parameters are defined by conditional least-squares. Assume that data $D = (X, Y)$ consists of a target response $Y$ and predictors $X \in \mathbb{R}^p$. We consider the ordinary least square (OLS) parameter, where $\theta_0 = \text{argmin}_b E[(Y - X^T b)^2]$ is the least-squares projection of $Y$ on $X$, and the estimating function is $s(D, \theta) = 2X(Y - X^T \theta)$. The conditional parameter is the solution to (2.2), i.e.,

$$
\theta_n^{\text{cond}} = \text{argmin}_b \sum_{i=1}^{n} E[(Y_i - X_i^T b)^2 | Z_i].
$$

Thus, $\theta_n^{\text{cond}}$ is the least-square projection of $Y$ on $X$ when the observations are sampled from the conditional distribution given $(Z_1, \ldots, Z_n)$. If $Z_i = X_i$, the parameter $\theta_n^{\text{cond}}$ can be viewed as the regression coefficient for a set of subjects with fixed regressors, averaging over measurement noise. In model-based statistical inference, if $Z_i = X_i$ and $Y_i = X_i^T \theta_0 + \epsilon_i$ for $\epsilon_i$ independent of $X_i$, i.e., well-specified model, the conditional parameters are identical to the super-population parameter. In practice, however, this will usually not hold; therefore, the conditional parameter might vary with different realizations of $X_i$. More generally, $Z$ might also be a variable that is not included in the set of predictors; for example, one might be interested in the relationship between input covariates and emissions for a specific set of industrial plants. If $Z$ is correlated with both the predictors and the residuals, conditioning on the variable can change the parameters.

**Example 2.3** (Finite-sample causal inference). Finite-sample treatment effects are a common target of causal inference [28]. In the social sciences, for example, it is expected that individuals react differently to treatments. In this case, conditional inference can be used to understand how a specific population reacts to the treatment. Consider random variables $(T, X, Y(1), Y(0))$ sampled from a super-population $P$, where $T \in \{0, 1\}$ is the treatment indicator, $X$ is the covariates, $Y(1)$ is the potential outcome if the treatment is received ($T = 1$), and $Y(0)$ is that under no treatment ($T = 0$). Under SUTVA and consistency [28], for each unit we observe $D = (T, X, Y)$, where $Y = T Y(1) + (1 - T) Y(0)$. The (super-population) average treatment effect $\theta_0 = E[Y(1) - Y(0)]$ is the solution to equation (2.1), where

$$
s(D, \theta) = Y(1) - Y(0) - \theta.
$$
There are many choices of conditioning variables $Z$. The finite-population perspective is equivalent to conditioning on the (unobserved) potential outcomes $Z_i = (Y_i(1), Y_i(0))$, in which case the conditional parameter
\[
\theta_n^{\text{cond}} = \frac{1}{n} \sum_{i=1}^{n} (Y_i(1) - Y_i(0)),
\]
characterizes the population where potential outcomes of the subjects are fixed. This is commonly the target in finite-sample causal inference [39, 25, 22, 37, 28]. By conditioning on potential outcomes, we only account for the randomness in treatment assignment. In some cases, it can be more meaningful to condition on covariates and average over measurement noise, leading to $\theta_n^{\text{cond}} = \frac{1}{n} \sum_{i=1}^{n} E[Y_i(1) - Y_i(0) \mid X_i] = \frac{1}{n} \sum_{i=1}^{n} \tau(X_i)$ for the population characterized by $\{X_i\}_{i=1}^{n}$. Here $\tau(x) = E[Y(1) - Y(0) \mid X=x]$ is often called conditional treatment effect function and indicates treatment effect heterogeneity on the covariate level. Finally, conditioning on the empty set, we obtain $\theta_0$ that represents the super-population the units are sampled from.

### 2.2 Conditional inference

Conditional parameters can be defined for the data at hand, or a new population with some observed attributes. As discussed in Example 1.1, it might be desirable to have conditionally valid inference for the customers at hand, instead of marginal validity. We take a moment here to formalize these two settings and the conditional inference guarantees we are to provide.

**Conditional inference for the population at hand.** As discussed earlier, the video streaming platform might be interested in the satisfaction of the current customer base, averaging over measurement error and temporal variation. We will first consider the setting where the company has satisfaction measurements on the current customers at hand, instead of marginal validity. We take a moment here to formalize these two settings and the conditional inference guarantees we are to provide.

We observe i.i.d. data $\{(D_i, Z_i)\}_{i=1}^{n}$ from a super-population $P$, where $Z_n = \{Z_i\}_{i=1}^{n}$ is the conditioning set (e.g., the attributes of the customers), and $D_n = \{D_i\}_{i=1}^{n}$ are the observations (e.g., the observed satisfaction). The conditional parameter $\theta_n^{\text{cond}} = \theta_n^{\text{cond}}(Z_n)$ defined in (2.2) characterizes the current customers—it provides a more precise characterization than the super-population quantity; the latter instead characterizes the overall satisfaction of an hypothetical infinite customer base. In Section 3.1, we construct a confidence interval $\tilde{C}(D_n, Z_n)$ obeying
\[
P(\theta_n^{\text{cond}} \in \tilde{C}(D_n, Z_n) \mid Z_n) \rightarrow 1 - \alpha \tag{2.3}
\]
in probability as $n \to \infty$. Put another way, our inference on $\theta_n^{\text{cond}}$ is asymptotically valid conditional on any realized attributes. In our motivating example, the conditional guarantee (2.3) means the validity given the current customers; it is in contrast to marginal guarantees where the coverage is valid marginalized over many draws of customers.

**Transductive inference for new population.** The video streaming platform might also be interested in estimating the satisfaction of a subgroup (dubbed target units) of its customer base, based on satisfaction measurements of another subgroup of its customer base (dubbed source units). In the following, we will formalize this problem.

We denote the target data as $\{(D_j^{\text{new}}, Z_j)\}_{j=1}^{m}$ from a super-population $Q$, where $Z^{\text{new}}_m = \{Z^{\text{new}}_j\}_{j=1}^{m}$ are the new attributes we condition on, and $D^{\text{new}}_m = \{D^{\text{new}}_j\}_{j=1}^{m}$ are the unobserved data (e.g., the satisfaction measurements of the target units). The source units $\{(D_j, Z_j)\}_{j=1}^{n}$ are i.i.d. from a super-population $P$ (e.g., the satisfaction measurements of the source units). The quantity of interest is $\theta_m^{\text{cond,new}} = \theta_m^{\text{cond}}(Z^{\text{new}}_m)$ as a functional of the conditional distribution of $D^{\text{new}}_m$ given $Z^{\text{new}}_m$. In Sections 3.2 and 3.3, we construct a confidence interval $\tilde{C}(D_n, Z_n, Z^{\text{new}}_m)$ that obeys
\[
P(\theta_m^{\text{cond,new}} \in \tilde{C}(D_n, Z_n, Z^{\text{new}}_m) \mid Z^{\text{new}}_m) \rightarrow 1 - \alpha
\]
in probability as $m, n \to \infty$. In particular, we allow $Q$ to admit a covariate shift $w(z) = \frac{dQ}{dP}(d, z)$ from the fully observed data; here the conditional distribution of $D$ given $Z$ is assumed to be invariant, which is necessary.
to ensure that the parameter $\theta_{\text{cond, new}}^m$ is identifiable. The covariate shift $w$ is potentially unknown and may be estimated from data, in which case our procedure allows the estimation to have lower-than-parametric convergence rates.

2.3 Related work

Several strands of literature have touched conditional estimation or inference of a similar estimand as ours, usually with different guarantees or motivations from ours.

**Conditional parameter with random covariates.** There are several works that study the same estimand as ours under similar assumptions yet with different guarantees. For example, [2] quantify the asymptotic deviation of estimators from conditional parameters for maximum likelihood and method of moment estimators; [9, 8] argue that models should be seen as approximations. The authors define conditional parameters and derive marginally valid asymptotics for the deviation of the estimator from the conditional parameter; their approaches argue to treat the covariates as random and focuses on marginal inference. Here, we study a similar setting; however, we substantially generalize their framework by providing conditionally valid inference and studying transductive inference on new populations.

**Finite-sample causal inference.** In the literature of finite-sample causal inference [39, 25, 22, 37, 28], it is common to condition on potential outcomes and derive bounds for the asymptotic variance of estimators of causal effects. Inference conditionally on potential outcomes is similar to our goal; however, an additional difficulty is that potential outcomes are unobserved, while we assume that the attributes $Z_i$ are observed. In addition, finite-sample causal inference usually does not rely on super-population assumptions, which are necessary in our setting to characterize the behavior of the fixed attributes. Furthermore, in this literature, conditional inference results are usually derived on a case-by-case basis, while we study a general class of estimators.

**Fixed-design regression.** In the special case of OLS coefficients, our framework bears similarity to fixed-design linear regression. For example, [29] investigate linear regression in settings where all regressors are fixed. [1] derive central limit theorems for the deviation of regression estimators from finite-sample parameters in the case where some regressors are fixed. Compared to our setting, the authors do not assume that the data is sampled from a super-population; however, they make a linear model on the outcomes, which can be restrictive. Similarly, [4] derive conditionally valid confidence intervals for linear moment models. Our setting is more general in the sense that we discuss conditional inference on general estimands, while more restrictive in that we assume that the attributes is drawn from a super-population and then conditioned on.

**Distribution shift and missing data.** Our transductive inference procedures are connected to a vast literature of inference under covariate shift. In a general spirit, our procedure in Section 3.3 is similar to that of AIPW estimators [35]. More recent works of [38] and [32] are also related, both of which study inference with estimated covariate shift and provide doubly-robust property similar to our Section 3.3. In contrast, we provide conditional validity for conditional parameters instead of marginal validity for super-population quantities, leading to different variances. Moreover, our framework works for estimands beyond moment equations and linear regression settings.

**Classical conditional inference.** A classical line of work [20, 14] tackles inference problems in a conditional fashion by conditioning on ancillary statistics or estimators of nuisance parameters (see e.g., a review in [10]), stemming from the ideas of Fisher [18, 19]. One strand uses conditional inference to reduce the effect of nuisance parameters, including [14]. Our framework directly conditions on some attributes of the data instead of summary statistics, which leads to a different parameter, different interpretation and different inferential guarantees than the traditional ones. Another strand under the name of conditional inference uses conditioning to induce relevance of probabilistic analysis to the data at hand, including permutation tests [20, 17, 16] and methods in testing categorical data [3], where inference relies on the conditional distribution of test statistic given the observations. Our framework also works by conditioning on some attributes,
Proposition 3.1

Asymptotic linearity of conditional parameters for super-population, whose proof is deferred to Appendix B.1.

Recall the motivating example where the video streaming platform is interested in learning a parameter that is specific to the current customers. In this part, we construct confidence interval for the conditional parameter with conditional validity. Our results imply that inference for super-population quantities might be overly conservative, since it unnecessarily takes into account the variation in the attributes.

3 Conditional Inference

3.1 Conditional inference for the population at hand

Recall the motivating example where the video streaming platform is interested in learning a parameter that is specific to the current customers. In this part, we construct confidence interval for the conditional parameter with conditional validity. Our results imply that inference for super-population quantities might be overly conservative, since it unnecessarily takes into account the variation in the attributes.

As introduced in Section 2.2, we assume access to i.i.d. data \( \{(D_i, Z_i)\}_{i=1}^n \) from a super-population \( \mathbb{P} \). The conditional parameter is defined in equation (2.2). For simplicity of illustration, we present our theoretical results for parametric and semi-parametric estimators.

Assume we are given an asymptotically linear estimator \( \hat{\theta}_n = \hat{\theta}_n(D_n) \in \mathbb{R} \), i.e.,

\[
\sqrt{n}(\hat{\theta}_n - \theta_0) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \phi(D_i) + o_P(1),
\]

for some \( \phi \in L_2(\mathbb{P}) \) with mean zero. Many parametric and semi-parametric estimators are asymptotically linear in standard asymptotic settings, see for example [42] or [11]. Under regularity conditions [9], conditional parameters (2.2) are asymptotically linear with expansion

\[
\sqrt{n}(\theta_n^{\text{cond}} - \theta_0) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \mathbb{E}[\phi(D_i) \mid Z_i] + o_P(1).
\]

We establish sufficient conditions for equations (3.1) and (3.2) to hold when \( (D_i, Z_i) \) are i.i.d. from some super-population, whose proof is deferred to Appendix B.1.

**Proposition 3.1** (Asymptotic linearity of conditional parameters). Suppose the following conditions hold:

(i) \( \hat{\theta}_n \) is the unique solution to \( \sum_{i=1}^n s(D_i, \theta) = 0 \), \( \theta_0 \) is the unique solution to (2.1) and \( \theta_n^{\text{cond}} \) is the unique solution to (2.2). (ii) The parameter space \( \Theta \) is compact. (iii) In a small neighborhood of \( \theta_0 \), \( s(D, \theta) \) and \( t(Z, \theta) = \mathbb{E}[s(D, \theta) \mid Z] \) are twice differentiable in \( \theta \), with \( s(D, \theta) = \nabla_\theta s(D, \theta) \in \mathbb{R}^{p \times p} \) the derivative matrix of \( s(D, \theta) \) at \( \theta \) and \( \hat{s}(D, \theta) = \nabla_\theta \hat{s}(D, \theta) \) the derivative tensor of \( \hat{s}(D, \theta) \) at \( \theta \). Additionally, \( \hat{t}(Z, \theta) = \nabla_\theta \hat{t}(Z, \theta) = \mathbb{E}[\hat{s}(D, \theta) \mid Z] \) and \( \hat{t}(Z, \theta) = \nabla_\theta \hat{t}(Z, \theta) = \mathbb{E}[\hat{s}(D, \theta) \mid Z] \). (iv) For each \( j, k \), \( \|s_{jk}(D, \theta)\| = \|\nabla_\theta s(D, \theta)/\partial \theta_j \partial \theta_k\| \leq g(D) \) for some \( g \) with \( \mathbb{E}[\|g(D)\|] < \infty \). Also, the matrix \( \mathbb{E}[s(D, \theta_0)] \) is assumed to be non-singular. Then equations (3.1) and (3.2) hold with influence function

\[
\phi(D) = -(\mathbb{E}[s(D, \theta_0)])^{-1} s(D, \theta_0),
\]

where all the expectations are induced by the joint distribution of \( (D, Z) \).

The conditions in Proposition 3.1 resemble the well-established results for Z-estimators [42], and has been informally stated in [9]. We impose the linear expansion as the following assumption for convenience.

**Assumption 3.2.** \( \hat{\theta}_n \) and \( \theta_n^{\text{cond}} \) satisfy equations (3.1) and (3.2), respectively.
Assumption 3.3. The influence function φ(·) defined in (3.3) satisfies E[φ(D)^2] < ∞.

We construct conditionally valid confidence intervals for conditional parameters as follows.

Theorem 3.4 (Asymptotic validity of conditional confidence intervals). Suppose Assumptions 3.2 and 3.3 hold. If an estimator \( \hat{\sigma} \) converges in probability to \( \sigma > 0 \), where

\[
\sigma^2 = E\left[ \left( \phi(D) - E[\phi(D) \mid Z] \right)^2 \right], \tag{3.4}
\]

then for any \( \alpha \in (0, 1) \), it holds that the conditional coverage

\[
P\left( \theta^\text{cond} \in \left[ \hat{\theta}_n - z_{1-\alpha/2}/\sqrt{n}, \hat{\theta}_n + z_{1-\alpha/2}/\sqrt{n} \right] \mid Z\right),
\]

as a random variable measurable with respect to \( Z_n = \{Z_i\}_{i=1}^n \), converges in probability to \( 1 - \alpha \) as \( n \to \infty \), where \( z_{1-\alpha/2} \) is the \( (1 - \alpha/2) \) quantile of standard Gaussian distribution.

The proof of Theorem 3.4 is deferred to Appendix B.4. The asymptotic conditional validity relies on the convergence of the conditional distribution of \( \sqrt{n}(\theta_n - \theta^\text{cond}) \), derived from a conditional central limit theorem \([15, 24]\); we include Lemma D.1 in the Appendix for completeness.

Many results in the literature are close to Theorem 3.4. Super-population inference with Z-estimators relies on CLT as well, often with a larger variance of the form \( \sigma^2 = \text{Var}(\phi(D)) \). However, these results all provide marginal coverage guarantees. As discussed in Example 1.1, marginal coverage guarantees are insufficient for reliable inference in some cases.

Remark 3.5. In super-population inference, a similar protocol is carried out with an estimator of the (unconditional) asymptotic variance, usually of the form \( \sigma^2_0 := \text{Var}(\phi(D)) \). The asymptotic variance (3.4) we utilize here is always no greater than \( \sigma^2_0 \), as \( \sigma^2 = \text{Var}(\phi(D)) - \text{Var}(E[\phi(D) \mid Z]) \leq \text{Var}(\phi(D)) \). Take the least-square parameter as an example. The linear expansion (3.1) and (3.2) hold with \( \phi(D) = (E[X X^\top])^{-1} X (Y - X^\top \theta_0) \) in \( \mathbb{R}^d \). Consider the first entry of \( \theta_0 \) as the target. If the linear model \( Y = X^\top \theta_0 + \epsilon \) is well-specified, i.e., \( E[\epsilon \mid X] = 0 \) almost surely, we have \( \sigma^2 = \sigma^2_0 \) when \( Z \) is contained in \( X \). With a mis-specified linear model, \( \theta_0 \) can be viewed as the least-square projection of \( Y \) onto \( X \) \([2, 9, 8]\). If \( E[\epsilon \mid Z] \) is not almost surely zero, our confidence interval is shorter than that for super-population inference.

It remains to construct a consistent estimator \( \hat{\sigma}^2 \) for the asymptotic variance (3.4). In Section 3.4 we describe a detailed estimation procedure (c.f. Algorithm 3) with consistency guarantees, relying on the explicit formula (3.3) and nonparametric estimation of \( \varphi(Z) = E[\phi(D) \mid Z] \). \[2\] propose a matching-based algorithm to estimate the same asymptotic variance, whose proof relies on assuming compactness of \( Z \) and smoothness of \( \varphi(\cdot) \). In contrast, we prove that our variance estimator is consistent under the consistency of generic nonparametric regression, which avoids the compactness assumption and overcomes the difficulty of exact matching in practice.

3.2 Transductive inference with known covariate shift

As discussed in the motivating example, after collecting a first batch of data on some subscribers, the video streaming company might be interested in estimating the satisfaction of a different set of subscribers that were not part of the original survey. To this end, one can use the data from the first survey and the covariates of the new population to infer the satisfaction of the new population. In this section, we show that conditionally-valid inference on the new conditional parameter is possible under known covariate shift. The more challenging case of unknown covariate shift is discussed in Section 3.3.

We assume that \( \{(D_j^\text{new}, Z_j^\text{new})\}_{j=1}^m \overset{\text{i.i.d.}}{\sim} Q \) and \( \{D_i, Z_i\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} P \). Here, the data scientist observes \( \{D_i, Z_i\}_{i=1}^n \) and \( \{Z_j^\text{new}\}_{j=1}^m \), but not \( \{D_j^\text{new}\}_{j=1}^m \). In this section, we assume the two distributions \( P \) and \( Q \) are related by a known covariate shift \( w(z) = \frac{dP}{dQ}(d, z) \). The invariance of the conditional distribution of \( D \) given \( Z \) across the two datasets is necessary to ensure that the transductive inference based on \( \{Z_j^\text{new}\}_{j=1}^m \) is possible. We denote the new super population parameter as \( \theta_0^\text{new} \), which is the unique solution to

\[
E[w(Z)s(D, \theta)] = E_Q[s(D^\text{new}, \theta)] = 0, \tag{3.5}
\]
where the first expectation is over $(D, Z) \sim P$ and the second expectation is over $D^{new} \sim Q$. The new conditional parameter is denoted as $\theta^{cond,new}_m$, which is the solution to

$$\sum_{j=1}^{m} E[s(D_j^{new}, \theta) \mid Z_j^{new}] = 0, \tag{3.6}$$

where the conditional expectation is induced by $Q$. This setting includes the special case where the two populations are drawn from the same super-population.

A reasonable starting point is to estimate the parameter by a re-weighted $Z$-estimator $\hat{\theta}^{new}_n$, which is a unique solution to

$$\sum_{i=1}^{n} w(Z_i)s(D_i, \theta) = 0. \tag{3.7}$$

As we shall see in the linear expansion, $\hat{\theta}^{new}_n$ is conditionally biased for $\theta^{cond,new}_m$ (conditional on $Z^{new}$); we are to use a correction term to remove the conditional bias.

For convenience, we impose the linear expansion of $\hat{\theta}^{new}_n$ and $\theta^{cond,new}_m$ as an assumption. It is justified in Proposition A.1 in Appendix A.1 under mild regularity conditions that are similar to the conditions in Proposition 3.1.

**Assumption 3.6.** $\hat{\theta}^{trans}_n$ and $\theta^{cond,new}_m$ admit the asymptotic linear expansion

$$\sqrt{n}(\hat{\theta}^{trans}_n - \theta^{new}_0) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D_i)w(Z_i) + o_P(1), \tag{3.8}$$

$$\sqrt{m}(\theta^{cond,new}_m - \theta^{new}_0) = \frac{1}{\sqrt{m}} \sum_{j=1}^{m} E[\psi(D_j^{new}) \mid Z_j^{new}] + o_P(1), \tag{3.9}$$

as $m, n \to \infty$, where $\psi(d) = -\left(\mathbb{E}_Q[s(D^{new}, \theta^{new}_0)]\right)^{-1}s(d, \theta^{new}_0)$.

Under this expansion, the estimator $\hat{\theta}^{trans}_n$ has considerable bias: ignoring lower order terms, under Assumption 3.6 $\hat{\theta}^{trans}_n - \theta^{cond,new}_m$ is equal to

$$\frac{1}{n} \sum_{i=1}^{n} \psi(D_i)w(Z_i) \quad \text{mean zero under } \mathbb{P}(\cdot \mid Z^{new}_m)$$

$$- \frac{1}{m} \sum_{j=1}^{m} E[\psi(D_j^{new}) \mid Z_j^{new}] \quad \text{nonzero mean under } \mathbb{P}(\cdot \mid Z^{new}_m).$$

To mitigate this issue, we add a correction term to the estimator. We first split the index set $I = \{1, \ldots, n\}$ of $\{(D_i, Z_i)\}_{i=1}^{n}$ into equally-sized halves $I_1$ and $I_2$. Then for $k = 1, 2$, we obtain estimator $\hat{\eta}^{I_k}(\cdot)$ for $\eta(\cdot) = E[\psi(D_j^{new}) \mid Z_j^{new} = \cdot]$, using only the data in $I_k$. We then define the estimator

$$\hat{\theta}^{trans}_{m,n} = \hat{\theta}^{trans}_n - \tilde{c}^{trans}, \tag{3.10}$$

with the following correction term:

$$\tilde{c}^{trans} := \frac{1}{2|I_1|} \sum_{i \in I_1} \hat{\eta}^{I_1}(Z_i)w(Z_i) + \frac{1}{2|I_2|} \sum_{i \in I_2} \hat{\eta}^{I_2}(Z_i)w(Z_i) - \frac{1}{2m} \sum_{k=1}^{2} \sum_{j=1}^{m} \hat{\eta}^{I_k}(Z_j^{new}).$$

We construct a confidence interval centered around $\hat{\theta}^{trans}_{m,n}$ in Theorem 3.8. We assume the $L_2(Q)$ consistency of $\hat{\eta}^{I_k}$; note that we do not impose any assumptions on convergence rates of $\hat{\eta}^{I_k}$.\footnote{To be specific, $\hat{\eta}^{I_k}$ is the output of Algorithm 3 (c.f. Section 3.4 for details) with inputs $w$ and $I_k$. With known $w(\cdot)$, the algorithm does not need the new attributes as input.}
Assumption 3.7. \( \|\hat{\eta}^{T_k}(\cdot) - \eta(\cdot)\|_{L_2(P)} \) and \( \|\hat{\eta}^{T_k}(\cdot) - \eta(\cdot)\|_{L_2(Q)} \) converges in probability to zero for \( k = 1, 2 \).

Theorem 3.8. Suppose Assumptions 3.6 and 3.7 hold, and \( m \geq \epsilon n \) for some constant \( \epsilon > 0 \). If an estimator \( \sigma_{\text{shift}} \) converges in probability to \( \sigma_{\text{shift}}>0 \), where

\[
\sigma_{\text{shift}}^2 = \text{Var} \left\{ w(Z_i) (\psi(D_i) - \eta(Z_i)) \right\},
\]

(3.11)

and the variance is induced by \( (D_i, Z_i) \sim \mathbb{P} \), then the random variable

\[
\mathbb{P}\left( \hat{\sigma}_{\text{shift}}^{\text{trans}} \in \left[ \frac{d_{\text{trans}}}{m,n} - \sigma_{\text{shift}} \cdot z_1 - z_2/\sqrt{n}, \frac{d_{\text{trans}}}{m,n} + \sigma_{\text{shift}} \cdot z_1 - z_2/\sqrt{n} \right] \right| Z_n^{\text{new}}
\]

converges in probability to \( 1 - \alpha \) as \( n \to \infty \), where \( \hat{\sigma}_{\text{shift}}^{\text{trans}} \) is defined in equation (3.10).

It may come as a surprise to the reader that the asymptotic variance does not depend on \( m \); this is due to the fact that bias correction is statistically an easy task in this setting. We defer the detailed proof of Theorem 3.8 to Appendix B.5.

It thus remains to construct a consistent estimator for \( \sigma_{\text{shift}}^2 \) (c.f. (3.11)) as well as an \( L_2 \)-consistent estimator for \( \eta(\cdot) \). In Section 3.4, we include a detailed estimation procedure for \( \sigma_{\text{shift}}^2 \) (c.f. Algorithm 5). The construction of \( \hat{\eta}^{T_k} \) is new to the literature; we discuss a detailed procedure (c.f. Algorithm 5) in Section 3.4 with theoretical analysis.

3.3 Transductive inference with estimated covariate shift

In this section, we discuss the case where the covariate shift \( w(z) \) between target distribution \( Q \) and the training distribution \( P \) is unknown and needs to be estimated. We develop an estimator based on which the inference procedure allows for slower-than-parametric estimation error.

The general idea is to replace \( w(\cdot) \) with an estimate to construct \( \hat{\theta}^{\text{trans}}_{m,n} \) in (3.10), where we employ cross-fitting \( \{1, \ldots, n\} \) to decouple the estimation of \( w(\cdot) \) and other quantities. The index set \( I = \{1, \ldots, n\} \) of the original dataset \( \{(D_i, Z_i)\}_{i=1}^n \) is randomly split into three equally-sized folds, denoted as \( I_1, I_2 \) and \( I_3 \). The index set \( I^{\text{new}} = \{1, \ldots, m\} \) of the new dataset \( Z_n^{\text{new}} = \{Z_i^{\text{new}}\}_{i=1}^m \) is randomly split into three equally-sized folds \( I_1^{\text{new}}, I_2^{\text{new}} \) and \( I_3^{\text{new}} \). We then carry out a three-fold estimation—for each \( \ell = 1, 2, 3 \), we first use \( I_\ell \) and \( I_\ell^{\text{new}} \) to obtain an estimator \( \hat{\theta}_n^{\ell}(\cdot) \) of the covariate shift \( \hat{\eta}^{T_k} \). Then we use all remaining data to obtain \( \hat{\theta}_{n,(\ell)} \), which is a unique solution to

\[
\sum_{i \in I_\ell} \hat{\theta}_n^{\ell}(Z_i) s(D_i, \theta) = 0.
\]

(3.12)

Next, for each \( k \neq \ell \), we obtain an estimator \( \hat{\eta}^{T_k}(\cdot) \) for \( \eta(\cdot) \) using only \( I_k \) and \( I_k^{\text{new}} \). We define the \( \ell \)-th correction term as

\[
\hat{c}(\ell) = \sum_{k \neq \ell} \frac{3}{2n} \sum_{i \in I_\ell \cup I_k} \hat{\theta}_n^{\ell}(Z_i) \hat{\eta}^{T_k}(Z_i) - \sum_{k \neq \ell} \frac{3}{2m} \sum_{j \in I_\ell^{\text{new}} \cup I_k^{\text{new}}} \hat{\eta}^{T_k}(Z_j^{\text{new}}).
\]

Finally, we define the transductive estimator as

\[
\hat{\theta}^{\text{trans,shift}}_{m,n} = \frac{1}{3} \sum_{\ell=1}^3 \left( \hat{\theta}^{\text{new},(\ell)}_n - \hat{c}(\ell) \right).
\]

(3.13)

Without loss of generality, we assume \( n_0 = n/3, m_0 = m/3 \) are integers, so that the split folds are of exactly the same size; otherwise the induced bias is of a negligible order \( O(1/m + 1/n) \).

We assume consistency of \( \hat{\theta}_n \) as follows.

Assumption 3.9. For \( \ell = 1, 2, 3 \), \( \sup_{z} |\hat{\theta}_n(z) - \psi(z)| \to 0 \) in probability as \( n \to \infty \).

\(^2\)We give an example in Algorithm 1 for estimating \( w(\cdot) \).

\(^3\)To be specific, \( \hat{\eta}^{T_k}(\cdot) \) is the output \( \eta(s, \omega, I_k, \hat{I}_k^{\text{new}})(\cdot) \) from Algorithm 5 that only depends on \( I_k \) and \( I_k^{\text{new}} \).
For convenience, we impose the linear expansion of $\hat{\theta}_n^{\text{new},(\ell)}$ as the following assumption. It holds under Assumption 3.9 and regularity conditions similar to previous cases; the detailed justification is in Proposition A.2 in Appendix A.1.

**Assumption 3.10.** For $\ell = 1, 2, 3$, $\hat{\theta}_n^{\text{new},(\ell)}$ is unique solution to (3.12) and admits linear expansion

$$\sqrt{2n/3}(\hat{\theta}_n^{\text{new},(\ell)} - \theta_0^{\text{new}}) = \frac{1}{\sqrt{2n/3}} \sum_{i \notin \mathcal{I}_x} \hat{w}_t(Z_i)\psi(D_i) + op(1). \tag{3.14}$$

In the linear expansion (3.14), $\sqrt{2n/3}$ is due to sample splitting where $\hat{\theta}_n^{\text{new},(\ell)}$ only uses a fold of cardinality $2n/3$; we still obtain $\sqrt{n}$ order for inference by reusing all folds.

We will elaborate on detailed conditions for it to hold in the analysis of our estimation procedures, see Proposition 3.17 of Section 3.5.

**Assumption 3.11.** $\|w(\cdot)[\hat{\eta}_t^{\text{shift}}(\cdot) - \eta(\cdot)]\|_{L_2(\mathbb{P})} \to 0$ in probability, $\mathbb{E}_\mathcal{D} |w(Z_i)^4\psi(D_i)^4| < \infty$ and $\|\hat{w}_t(\cdot) - w(\cdot)\|_{L_2(\mathbb{P})}, \|\hat{\eta}_t(\cdot) - \eta(\cdot)\|_{L_2(\mathbb{P})} = op(1/\sqrt{n})$ for $k = 1, 2$ and $\ell = 1, 2, 3$.

The following theorem proved in Appendix B.6 provides inference that is robust to estimation error—we obtain $n^{-1/2}$-rate inference with the same asymptotic variance as the case of known covariate shift, as long as the product of the errors is not grater than $O(n^{-1/2})$.

**Theorem 3.12.** Suppose Assumptions 3.9, 3.10 and 3.11 hold, and $m \geq cn$ for some fixed $c > 0$. If an estimator $\hat{\sigma}_\text{shift} \rightarrow \sigma_\text{shift}$ in probability for the variance $\sigma_\text{shift}^2$ defined in (3.11), then

$$\mathbb{P} \left( \theta_m^{\text{new},\text{cond}} \in \left[ \hat{\theta}_m^{\text{trans},\text{shift}} - \hat{\sigma}_\text{shift} \cdot z_{1-\alpha/2}/\sqrt{n}, \hat{\theta}_m^{\text{trans},\text{shift}} + \hat{\sigma}_\text{shift} \cdot z_{1-\alpha/2}/\sqrt{n} \right] \mid Z^{\text{new}} \right),$$

as a random variable measurable with respect to $\{Z_j^{\text{new}}\}_{j=1}^m$, converges in probability to $1 - \alpha$ as $n \to \infty$, where $\hat{\theta}_m^{\text{trans},\text{shift}}$ is defined in equation (3.13).

As before, a noteworthy feature of this result is that asymptotically the variance does not depend on $m$.

The inference procedure in Theorem 3.12 relies on the construction of $\hat{\sigma}_\text{shift}$, $\hat{w}_t(\cdot)$ and $\hat{\eta}_t(\cdot)$. In Section 3.4 we provide a stand-alone procedure to obtain $\hat{\eta}_t(\cdot)$ with a single fold $\mathcal{I}_k$ (c.f. Algorithm 5) and a detailed procedure to estimate $\sigma_\text{shift}^2$ (c.f. Algorithm 6).

### 3.4 Algorithms

In this section, we describe concrete algorithms for estimating $\varphi(\cdot)$, $\eta(\cdot)$, $\sigma^2$ and $\sigma_\text{shift}^2$. Corresponding theory can be found in Section 3.5. Similar to previous sections, the estimation of variances is discussed for the one-dimensional case, while the arguments naturally carry over to the estimation of covariance matrix for multi-dimensional influence functions. Other quantities like conditional mean functions are discussed in the general multivariate case.

Note that the influence functions $\phi(\cdot)$, $\psi(\cdot)$ and their corresponding conditional mean functions $\varphi(\cdot)$, $\eta(\cdot)$ all admit the generic form

$$f(d) = M(s, w, \theta)s(d, \theta), \quad g(z) = M(s, w, \theta)\mathbb{E}[s(D_i, \theta) \mid Z_i = z]$$

for some weight function $w(\cdot)$, $\theta \in \mathbb{R}^p$, score function $s : \mathbb{D} \times \Theta \rightarrow \mathbb{R}^p$ and

$$M(s, w, \theta) = -\left(\mathbb{E}[w(Z_i)s(D_i, \theta)]\right)^{-1} \in \mathbb{R}^{p \times p}, \quad (D_i, Z_i) \sim \mathbb{P}. \tag{3.15}$$

The general recipe is to estimate $M(s, w, \theta)$ and $\mathbb{E}[s(D_i, \theta) \mid Z_i = z]$ separately with plug-in nuisance components. We build our procedures upon the following two meta algorithms.
Algorithm 1 Meta Algorithm: Estimation of $\mathbb{E}[h(D) | Z = \cdot]$

**Input**: Function $h(\cdot) : \mathcal{D} \to \mathbb{R}^p$, dataset $\{(D_i, Z_i)\}_{i \in \mathcal{I}}$ independent of $h(\cdot)$.

**Output**: function $\mathcal{G}(h, \mathcal{I})(\cdot) : \mathcal{Z} \to \mathbb{R}^p$.

Algorithm 2 Meta Algorithm: Matrix Estimation.

**Input**: Score function $s : \mathcal{D} \times \Theta \to \mathbb{R}^p$, weight function $w : \mathbb{Z} \to \mathbb{R}$, $\theta \in \Theta$, data $\{(Z_i, D_i)\}_{i \in \mathcal{I}}$.

**Output**: Matrix $\hat{M}(s, w, \theta, \mathcal{I}) = (\frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{Z}} w(Z_i) s(D_i, \theta))^{-1} \in \mathbb{R}^{p \times p}$.

**Estimation for conditional inference in Section 3.1**: Recall that in Theorem 3.4 the only quantity needed for constructing confidence intervals (besides $\theta$) is a consistent estimator $\hat{\sigma}^2$ for $\sigma^2 = \text{Var}((\phi(D) - \varphi(Z)))$. The estimation with data $\{(D_i, Z_i)\}_{i \in \mathcal{I}}$ is detailed in Algorithm 3. Roughly speaking, we first obtain estimators for $\phi(D_i)$, $i \in \mathcal{I}_2$; then we estimate $\varphi(\cdot) = \mathbb{E}[\phi | Z = \cdot]$ only using data in one fold $\mathcal{I}_1$ and apply to another independent fold $\mathcal{I}_2$, which are finally used to estimate $\sigma^2$. The sub-routine of estimating $\varphi(\cdot)$ is detailed in Algorithm 7 of Appendix A.2.

**Estimation for transductive inference in Sections 3.2 and 3.3**: The transductive inference part requires a consistent estimator for $\sigma^2_{\text{shift}}$ defined in equation (3.11), and an estimator for $\eta(\cdot)$ only using one fold $\mathcal{I}_k$. For preparation, we describe in Algorithm 4 a generic method to estimate the covariate shift $w(\cdot)$ when it is unknown. It is not the only choice; there have been a rich literature on estimating density ratios, see, e.g., [10] for a comprehensive review.

In Algorithm 5, we describe in details estimation of $\eta(\cdot)$ using any fold $\mathcal{I}$ and $\mathcal{I}^\text{new}$. Note that when $w(\cdot)$ is known, it is directly used to construct $\hat{\theta}_{m,n}^{\text{trans}}$ for Theorem 3.8 so that $\mathcal{I}^\text{new}$ is in fact not used. Otherwise, we set aside a part of $\mathcal{I}$ to estimate it and construct $\hat{\theta}_{m,n}^{\text{trans,shift}}$ in Theorem 3.12.

The estimation of $\sigma^2_{\text{shift}} = \text{Var}(w(Z)(\phi(D) - \varphi(Z)))$ is described in Algorithm 6. After sample splitting, we first estimate $\psi(D_i)$ for $i \in \mathcal{I}_3$; then we use only $\mathcal{I}_1, \mathcal{I}_2$ to estimate $\eta(\cdot)$ and apply to estimate $\eta(Z_i)$, $i \in \mathcal{I}_3$, which are used to estimate $\sigma^2_{\text{shift}}$.

**3.5 Estimation guarantees**

In this section, we provide estimation guarantees for algorithms in Section 3.4 with explicit and detailed conditions. The conditions are stated for parameters in $\mathbb{R}^p$.

We begin with generic assumptions on the meta Algorithms 1 and 2. For any function $f(\cdot)$, we let $\mathcal{G}(f)(z) = \mathbb{E}[f(D) | Z = z]$ be the conditional mean function, viewing $f$ as fixed; also, recall that $\mathcal{G}(f, \mathcal{I})$ is the output of Algorithm 1 using data $\mathcal{I}$. Also, recall that $\hat{M}(s, w, \theta, \mathcal{I})$ is the output of Algorithm 2 using data $\mathcal{I}$ and $M(s, w, \theta)$ in (3.3.5) is its estimation target.

**Assumption 3.13.** For any fixed input function $f$ and dataset $\mathcal{I}$, the output of Algorithm 7 satisfies that $\|\mathcal{G}(f, \mathcal{I})(\cdot) - \mathcal{G}(f)(\cdot)\|_{L_2(\mathcal{P})} = O_p(\mathcal{R}_r(\mathcal{I}))$ for some rate function $\mathcal{R}_r(\cdot) : \mathbb{N} \to \mathbb{R}^+$.

Algorithm 3 Estimate $\sigma^2$.

**Input**: Dataset $\{(D_i, Z_i)\}_{i \in \mathcal{I}}$, score function $s : \mathcal{D} \times \Theta \to \mathbb{R}^p$.

1. Split indices $\mathcal{I}$ into equally-sized $\mathcal{I}_1$ and $\mathcal{I}_2$.
2. Set $\hat{\theta}$ as solution to $\sum_{i \in \mathcal{I}_1} s(D_i, \hat{\theta}) = 0$. \hspace{1cm} // Estimate $\phi(D_i)$ for $i \in \mathcal{I}_2$
3. Obtain $\hat{M} := \hat{M}(s, 1, \hat{\theta}, \mathcal{I}_2)$ using Algorithm 2.
4. Set $\hat{\phi}_i = \hat{M} s(D_i, \hat{\theta})$ for all $i \in \mathcal{I}_2$.
5. Obtain $\hat{\varphi}(\cdot) = \varphi(s, \mathcal{I}_1)(\cdot)$ from Alg. 7 (c.f. Appendix A.2). \hspace{1cm} // Estimate $\varphi(\cdot)$ with only $\mathcal{I}_1$
6. Set $\hat{\varphi}_i = \hat{\varphi}(Z_i)$ for all $i \in \mathcal{I}_2$. \hspace{1cm} // Apply to $\mathcal{I}_2$
7. Output: $\hat{\sigma}^2 = \frac{1}{|\mathcal{I}_2|} \sum_{i \in \mathcal{I}_2} (\hat{\phi}_i - \hat{\varphi}_i)^2$. 

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Algorithm 4 Estimate $w(\cdot)$.

**Input:** Datasets $\{Z_i\}_{i \in I}$, $\{Z_j^{\text{new}}\}_{j \in I^{\text{new}}}$.
1. Pool $I, I^{\text{new}}$ together, and set $T_i = 0$ for $i \in I$ and $T_j = 1$ for $j \in I^{\text{new}}$.
2. Estimate $\hat{\varepsilon}(z) = \hat{F}(T = 1 | Z = z)$ using pooled data by any regression or classification algorithm.

**Output:** function $\hat{w}(\cdot) = \frac{\hat{\varepsilon}(\cdot)}{1 - \hat{\varepsilon}(\cdot)} : Z \to \mathbb{R}$.

Algorithm 5 Estimate $\eta(\cdot)$.

**Input:** Datasets $\{(D_i, Z_i)\}_{i \in I}$, $\{(D_j^{\text{new}}, Z_j^{\text{new}})\}_{j \in I^{\text{new}}}$, score function $s : \mathbb{D} \times \Theta \to \mathbb{R}^p$, weight function $w : Z \to \mathbb{R}$.
1. Split indices $I$ into equally-sized $I_1, I_2$ and $I_3$.
2. if $w$ is given then
3. end if
4. if $w$ is given then
5. Estimate weight function $\hat{w}(\cdot) : Z \to \mathbb{R}$ with $I_1$ and $I^{\text{new}}$.
6. end if
7. Set $\hat{\theta}$ as solution to $\sum_{i \in I_2} \hat{w}(Z_i) s(D_i, \theta) = 0$. // Estimate $\theta_0^{\text{new}}$
8. Obtain $\hat{M} = \hat{M}(s, \hat{w}, \hat{\theta}, I_3)$ using Algorithm 2 // Estimate $M(s, w, \theta_0^{\text{new}})$
9. Set $\hat{s}(\cdot) = s(\cdot, \hat{\theta}) : \mathbb{D} \to \mathbb{R}^p$. // Estimate $\mathbb{E}[s(D, \theta_0^{\text{new}}) | Z = \cdot]
10. Obtain $\hat{t}(\cdot) = \hat{G}(\hat{s}, I_3)(\cdot) : Z \to \mathbb{R}^p$ using Algorithm 3.

**Output:** function $\eta(s, w, I, I^{\text{new}})(\cdot) : Z \to \mathbb{R}^p$, where $\hat{\eta}(z) = \hat{M}(z)$.

Algorithm 6 Estimate $\sigma_{\text{shift}}^2$.

**Input:** Datasets $\{(D_i, Z_i)\}_{i \in I}$, $\{(D_j^{\text{new}}, Z_j^{\text{new}})\}_{j \in I^{\text{new}}}$, score function $s : \mathbb{D} \times \Theta \to \mathbb{R}^p$, weight function $w : Z \to \mathbb{R}$.
1. Split indices $I$ into equally-sized $I_1, I_2$ and $I_3$.
2. if $w$ is given then
3. Set $\hat{w} = w$; // Obtain weight function
4. else
5. Estimate weight function $\hat{w}(\cdot) : Z \to \mathbb{R}$ with $I_1$ and $I^{\text{new}}$.
6. end if
7. Set $\hat{\theta}$ as solution to $\sum_{i \in I_2} \hat{w}(Z_i) s(D_i, \theta) = 0$. // Estimate $\psi(D_i)$ for $i \in I_3$
8. Obtain $\hat{M} = \hat{M}(s, \hat{w}, \hat{\theta}, I_3)$ using Algorithm 2 // Estimate $\eta(\cdot)$ using only $\hat{w}$ and $I_2$
9. Set $\hat{\psi}_i = \hat{M}(D_i, \hat{\theta})$ for all $i \in I_3$.
10. Obtain $\hat{\eta} = \eta(s, \hat{w}, I_2, \Theta)(\cdot)$ from Algorithm 5 // Apply to $I_3$
11. Set $\hat{\eta}_i = \hat{\eta}(Z_i)$ for all $i \in I_3$.

**Output:** $\hat{\sigma}_{\text{shift}}^2 = \frac{1}{|I_3|} \sum_{i \in I_3} \hat{w}(Z_i)^2 (\hat{\psi}_i - \hat{\eta}_i)^2$. 

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Assumption 3.14. For any fixed input \( w, \theta \) and dataset \( I \), the output of Algorithm 3 satisfies \( \| \hat{M}(s, w, \theta, I) - M(s, w, \theta) \|_\infty = O_P(\mathcal{R}_m(|I|)) \) for some rate function \( \mathcal{R}_m(\cdot) : \mathbb{N} \to \mathbb{R}^+ \), where \( \| \cdot \|_\infty \) is the entry-wise maximum.

The above assumption on the convergence rate holds for a couple of nonparametric regression methods if the input \( f(\cdot) \), viewed as a fixed function, is sufficiently smooth. For example, localized nonparametric methods like kernel regression [93, 15], local polynomial regression [72, 13], smoothing spline [24] and modern machine learning methods including regression trees [6] and random forests [27], to name a few.

To show consistency of \( \hat{\sigma}^2 \) from Algorithm 3, we additionally assume the targets are stable.

Assumption 3.15. The matrix \( M(s, w, \theta) \) satisfies that \( M(s, 1, \theta) - M(s, 1, \theta') \|_\infty = O(\| \theta - \theta' \|_2) \) and \( M(s, w, \theta) - M(s, w', \theta) \|_\infty = O(\| w(z) - w'(z) \|_{L_2(I)}) \) for any weight functions \( w, w' \) and any \( \theta, \theta' \in \Theta \). Also, \( \| s(\cdot, \theta) - s(\cdot, \theta') \|_{L_2(I)} = O(\| \theta - \theta' \|_2) \) for any \( \theta, \theta' \in \Theta \).

We show that \( \hat{\sigma}^2 \), the output of Algorithm 3, is consistent if the two generic meta algorithms have diminishing estimation error and the target functions are stable. The proof of Proposition 3.16 is in Appendix C.2.

Proposition 3.16 (Consistency of \( \hat{\sigma}^2 \)). Suppose Assumptions \[3.13, 3.14\] and \[3.15\] hold, and the regularity conditions in Proposition \[3.1\] hold for \( \theta \) in Algorithm \[3\]. Also assume \( \mathcal{R}_m(n), \mathcal{R}_r(n) \to 0 \) as \( n \to \infty \). Then the output of Algorithm \[3\] satisfies \( \hat{\sigma}^2 \to \sigma^2 \) in probability as \( |I| \to \infty \).

In Theorem 3.8 we only need the \( L_2 \)-consistency for the estimation of \( \eta(\cdot) \), as well as a consistent estimator for \( \sigma^2_{\text{shift}} \). In Theorem 3.12 we further need the convergence rate for estimating \( \eta(\cdot) \). We analyze \( \hat{\eta}(\cdot) \), the output of Algorithm 3 under generic rates of the meta algorithms as follows. The proof of Proposition 3.17 is in Appendix C.3.

Proposition 3.17 (Convergence rate of \( \hat{\eta}(\cdot) \)). Suppose Assumptions \[3.13, 3.14, 3.15\] and the regularity conditions in Propositions \[A.7, A.2\] hold. Let \( I, T^{\text{new}} \) be any inputs of Algorithm 3. If \( w(\cdot) \) is known, the output of Algorithm 3 satisfies

\[
\| \hat{\eta}(\cdot) - \eta(\cdot) \|_{L_2(I)} \leq p \cdot O_P(\mathcal{R}_m(|I|) + \mathcal{R}_r(|I|) + |I|^{-1/2}).
\]

If \( \hat{w}(\cdot) \) is estimated, assume \( \sup_z |\hat{w}(z) - w(z)| = o_P(1) \) and the regularity conditions in Proposition \[A.2\] also hold for \( \hat{\theta} \). Then the output of Algorithm 3 satisfies

\[
\| \hat{\eta}(\cdot) - \eta(\cdot) \|_{L_2(I)} \leq p \cdot O_P(\| \hat{w}(\cdot) - w(\cdot) \|_{L_2(I)} + \mathcal{R}_m(|I|) + \mathcal{R}_r(|I|) + |I|^{-1/2}).
\]

As a direct implication, Assumption 3.11 holds if

\[
\| \hat{w}(\cdot) - w(\cdot) \|_{L_2(I)} = O_P(n^{-1/4}) \quad \text{and} \quad \mathcal{R}_m(n) + \mathcal{R}_r(n) = O_P(n^{-1/4}).
\]

Note that in Algorithm 3 \( T^{\text{new}} \) is only possibly used to estimate \( w(\cdot) \). Consequently, the convergence rate of \( \hat{\eta}(\cdot) \) depends on \( T^{\text{new}} \) only through \( \| \hat{w}(\cdot) - w(\cdot) \|_{L_2(I)} \).

The output \( \hat{\sigma}^2_{\text{shift}} \) of Algorithm 6 is analyzed as follows, whose proof is in Appendix C.4.

Proposition 3.18 (Consistency of \( \hat{\sigma}^2_{\text{shift}} \)). Let \( I, T^{\text{new}} \) be any inputs of Algorithm 6. Suppose Assumptions \[3.13, 3.14\] and \[3.15\] hold, and the regularity conditions in Proposition \[A.2\] hold for \( \theta \) in Algorithm 6. Assume \( \mathcal{R}_m(n) \to 0 \) and \( \mathcal{R}_r(n) \to 0 \) as \( n \to \infty \). If \( \sup_z |\hat{w}(z) - w(z)| = o_P(1) \), \( \sup_z |w(z)| < \infty \), then the output of Algorithm 6 obeys \( \hat{\sigma}^2_{\text{shift}} \to \sigma^2_{\text{shift}} \) in probability as \( |I| \to \infty \).

4 Simulations

4.1 Conditional inference

In this section, we evaluate the conditional inference procedure in Section 3.1 with simulations. The results validate the conditional coverage and show the robustness to estimation error.
We generate data $D_i = (X_i, Y_i)$ with covariates $X \in \mathbb{R}^{10}$ and response $Y \in \mathbb{R}$ according to

$$X_1, X_2, X_5, \ldots, X_{10} \overset{i.i.d.}{\sim} N(0, 1), \quad X_3 = X_1 + \varepsilon_1, \quad X_4 = X_1 + \varepsilon_2,$$

$$(\varepsilon_1, \varepsilon_2)^\top \sim N(0, \Sigma), \quad \Sigma_{11} = \Sigma_{22} = 1, \quad \Sigma_{12} = \Sigma_{21} = 1/2, \quad Y = X_1 + |X_1| + X_3 + \varepsilon', \quad \varepsilon' \sim N(0, \nu^2).$$

Here the linear model is misspecified but the OLS projection coefficient is still well-defined. We focus on two conditional parameters: the first two entries of the ordinary least square coefficient $\theta = \arg\min_{\beta \in \mathbb{R}^p} \mathbb{E}[(Y - \beta^\top X)^2 | Z]$, where we set the conditioning set as $Z = (X_1, X_2)$. The corresponding super-population quantities are $\theta_1 = 1$ and $\theta_2 = 0$. The influence function is

$$\phi(d; \theta) = (\mathbb{E}[XX^\top])^{-1} x(y - \theta^\top x), \quad \text{where} \quad d = (x, y) \in \mathbb{R}^p \times \mathbb{R}.$$

The procedure in Section 3.1 is carried out for sample sizes $n \in \{200, 1000, 2000, 5000\}$ and $\nu \in \{0.1, 0.2, 0.5\}$ with $\alpha = 0.05$. We first generate i.i.d. observations $\{Z_i\}_{i=1}^n$; then we repeatedly sample $\{D_i\}_{i=1}^n$ conditional on $\{Z_i\}_{i=1}^n$ for $N_Y = 500$ times. We construct confidence intervals and evaluate the coverage of the two conditional parameters over $N_Y$ times. For the nonparametric regression in Algorithm 1, we use loess function in R. The procedure is repeated for $N_X = 800$ draws of conditioning set.

We summarize the $N_X$ conditional coverage for $\theta_1^{cond}$ in Figures 2 and 3; each subplot corresponds to a configuration of $\nu$. Both figures confirm the conditional validity of our procedure (the boxplots mark median and quarter quantiles of the conditional coverage). In particular, the estimation error of variance for the second entry with smaller sample sizes leads to overcoverage in Figure 3. It shows the robustness of our procedure to estimation error: in cases where the estimation of $\varphi(\cdot)$ is inaccurate, the algorithm tends to overestimate the variance, and overall the procedure still provides valid coverage.

![Conditional coverage of the first entry of $\theta_1^{cond}$.](image1)

![Conditional coverage of the second entry of $\theta_2^{cond}$.](image2)

We also compute the ratio of estimated variances for conditional inference and super-population inference in Figure 4. We see that conditional inference often leads to shorter confidence intervals once the estimation error of $\varphi(\cdot)$ is reasonably small.

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4.2 Transductive inference under covariate shift

In this part, we evaluate the performance of transductive inference procedures on simulated data. Even with estimated covariate shift, the conditional coverage is close to the nominal level.

The data-generating process and parameters of interest are the same as Section 4.1 while we set the conditioning set as \( Z = X_1 \) and the covariate shift as \( w(z) = 0.5 + 1 \{ z > 0 \} \). We set sample sizes \( n \in \{200, 1000, 2000, 5000\} \) and \( m = n \cdot \epsilon \), where \( \epsilon \in \{0.5, 1, 2\} \). We independently draw \( N_X = 500 \) times of i.i.d. attributes \( Z_{\text{new}} = (Z_{\text{new}}^j)_{1 \leq j \leq m} \). In each time, we fix the new attributes and repeatedly draw \( \{D_i, Z_i\}_{1 \leq i \leq n} \), then apply the procedures in Section 3.2 and Section 3.3 for \( N_Y = 500 \) times. We follow Section 3.4 to construct \( \hat{\sigma}^2_{\text{shift}} \), \( \hat{\theta}_{m,n}^{\text{trans}} \) and the confidence intervals, where the meta algorithm \( \hat{\theta}_{m,n}^{\text{cond,new}} \) uses the \texttt{loess} function in R. When covariate shift is estimated, we let \( \hat{\omega}(\cdot) = \frac{\hat{\epsilon}(1 - \hat{\epsilon}^2)}{1 - \hat{\epsilon}^2} \cdot \frac{1 - \hat{p}}{\hat{p}} \), where \( T_i = 1 \{i \text{ is in the new dataset}\} \), and \( \hat{c}(x) \) (resp. \( \hat{\rho} \)) estimates \( P(T_i = 1 \mid X_i = x) \) (resp. \( P(T_i = 1) \)) by pooling the two datasets, and \( \hat{c}(x) \) is obtained by \texttt{randomForest} function in R.

Given \( \alpha = 0.05 \), we evaluate the conditional coverage of the two procedures given each draw of new attributes by empirical coverage among the \( N_Y = 500 \) replicates. Coverage for \( \hat{\theta}_{m,n}^{\text{cond,new}} \) associated with the first and second entries of OLS parameter \( \hat{\theta} \) is in Figures 5 and 8 respectively.

The conditional coverage is close to the nominal level 95% with both ground truth (blue) and estimated (yellow) covariate shift. The proposed procedure works slightly better with larger noise \( \epsilon \); it is due to over-estimation of asymptotic variance. Also, the coverage is higher for large proportion of \( m/n \). This might be due to smaller approximation error of asymptotic linear expansion.

5 Real Data Analysis

We apply the transductive inference procedure in Section 3.3 to a real-world dataset for predicting car prices. The dataset is from Ebay-Kleinanzeigen and consists of around 50,000 observations. Features include continuous ones like registration year and discrete ones like brand and make. The dataset has been studied in [30], where reliable prediction of car prices is found to be challenging. In particular, it is difficult to predict the individual prices of some ‘usual’ cars, such as old cars (registered before 2000), vintage cars and race cars.

Instead of predicting individual prices or estimating the overall mean price, our framework provides an approach in-between: we can form conditionally valid confidence intervals for the mean price of a subset of cars. In the following, we conduct conditional inference for the mean of a sub-population of old cars and evaluate the performance by the conditional coverage.

We first generate a semi-synthetic dataset for evaluation. We fit a random forest model \( \hat{m}(\cdot) \) for the conditional mean \( m(x) = \mathbb{E}[Y_i \mid X_i = x] \) on the whole dataset, and view the fitted values \( \hat{m}(X_i) \) as the conditional mean, then compute the residuals \( \epsilon_i = Y_i - \hat{m}(X_i) \). To create the synthetic dataset, we randomly sample (without replacement) a population of size \( N \in \{2, 5, 10, 20, 50\} \times 10^3 \) from the original dataset. We
Figure 5: Conditional coverage of the first entry of $\theta_m^{\text{cond, new}}$. Red dashed lines are nominal level.

Figure 6: Conditional coverage of the second entry of $\theta_m^{\text{cond, new}}$. Red dashed lines are nominal level.
focus on the particularly difficult task of inferring the price of old cars [30]. We choose the old cars with registration year earlier than 2000, and take a subsample of proportion $r \in \{0.1, 0.2, \ldots, 0.9\}$ as the new (shifted) dataset $\{(Y^*_j, X^*_j)\}_{1 \leq j \leq m}$; The original dataset $\{(Y^*_i, X^*_i)\}_{1 \leq i \leq n}$ consists of the rest of the old cars and all newer cars, so that $m + n = N$. In particular, we fix the covariates and randomly resample the errors to create the observations $Y^*_i$ and $Y^*_j$, and evaluate conditional coverage.

The transductive inference procedure discussed in Section 3.3 is applied to the synthetic dataset, where the confidence interval is constructed as

$$\hat{\theta}_{\text{trans,shift}}^{\text{trans,shift}} + z_{0.025} \cdot \hat{\sigma}_{\text{shift}} / \sqrt{n}, \quad \hat{\theta}_{\text{trans,shift}}^{\text{trans,shift}} + z_{0.975} \cdot \hat{\sigma}_{\text{shift}} / \sqrt{n}. $$

Specifically, with $T_i = 1$ indicating $(X_i, Y^*_i)$ is in the new (shifted) dataset, the weight function is obtained by $\hat{w}(\cdot) = \frac{\hat{e}(\cdot)}{1 - \hat{e}(\cdot)} \cdot \frac{1 - \hat{p}}{\hat{p}}$, where $\hat{e}(x)$ estimates $P(T_i = 1 | X_i = x)$ and $\hat{p}$ estimates $P(T_i = 1)$ by pooling the two datasets. The coverage for the conditional parameter $\theta_{\text{cond, new}} = \frac{1}{m} \sum_{i=1}^{N} T_i \cdot \hat{m}(X_i)$ is evaluated over 1000 replicates; the results are summarized in Figure 7.

Figure 7: Conditional coverage versus proportions $r$ of shifted data; each subplot corresponds to a sample size $N$. The red dashed lines indicate the nominal level 0.95.

In Figure 7 our procedure generally works well, especially for reasonably large original dataset and moderate proportion $r$ of the shifted dataset. The coverage improves as the whole sample size gets larger, especially when the proportion of shifted data is not too large or too small (so that old cars appear reasonably much in both datasets). We observe that the coverage might be deteriorated when the proportion of shifted data is large (like $r = 0.9$), in which case there are fewer representative observations of old cars in the original data, so that training a model for those conditional means gets harder. On the other hand, when the sample size (for example $N = 2000$) and the proportion $r$ (like $r = 0.1$) is relatively small, the random noise in the shifted data also manifest itself through the undercoverage in the first plot in Figure 7.

Acknowledgement

The authors thank Guido Imbens and Peng Ding for helpful discussions.

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A Additional algorithm details and analysis

A.1 Deferred details

The following proposition justifies Assumption 3.6, whose proof is in Appendix B.2.

**Proposition A.1.** Suppose conditions (ii), (iii) in Proposition 3.1 hold also at \( \hat{\theta}_n^{\text{new}} \) and the following two conditions hold: (i') \( \hat{\theta}_n^{\text{cond,new}} \) is the unique solution to (3.5), \( \hat{\theta}_n^{\text{trans}} \) is the unique solution to (3.7). (iv') For each \( j,k \), \( |\hat{s}(D,\theta)| = \|\hat{d}s(D,\theta)/\partial \theta_j \hat{d}\theta_k \| \leq g(D) \), where \( g(D) \) and \( g(D)w(Z) \) are both integrable. Also, both \( \mathbb{E}[\hat{s}(D,\theta_0^{\text{new}})] \) and \( \mathbb{E}[w(Z)\hat{s}(D,\theta_0^{\text{new}})] \) are non-singular matrices. Then Assumption 3.6 holds.

The following proposition justifies Assumption 3.10, whose proof is in Appendix B.3.

**Proposition A.2.** Suppose Assumption 3.9, conditions (ii), (iii) in Proposition 3.1 and condition (iv') in Proposition A.1 hold. If \( \hat{\theta}_n^{\text{new},(\ell)} \) is the unique solution to (3.12), then Assumption 3.10 holds.

A.2 Estimation of \( \varphi \)

Based on the meta algorithms, we estimate \( \varphi(\cdot) = -(\mathbb{E}[s(D,\theta_0)])^{-1}\mathbb{E}[s(D,\theta_0) | Z = \cdot] \) with data \( \{(D_i, Z_i)\}_{i \in I} \) as follows. For notational convenience, we define \( 1(z) \equiv 1 \).

**Algorithm 7 Estimate \( \varphi(\cdot) \).**

**Input:** Dataset \( \{(D_i, Z_i)\}_{i \in I} \), score function \( s: \mathbb{D} \times \Theta \rightarrow \mathbb{R}^p \).
1. Split indices \( I \) into equally-sized \( I_1 \) and \( I_2 \).
2. Set \( \hat{\theta} \) as solution to \( \sum_{i \in I_1} s(D_i, \theta) = 0 \).
3. Obtain \( \hat{M} := \hat{M}(s, 1, \hat{\theta}, I_2) \) using Algorithm 2.
4. Set \( \hat{s}(\cdot) = s(\cdot, \hat{\theta}): \mathbb{D} \rightarrow \mathbb{R}^p \).
5. Obtain \( \hat{t}(\cdot) := \hat{G}(\hat{s}, I_2)(\cdot): \mathbb{Z} \rightarrow \mathbb{R}^p \) using Algorithm 1.

**Output:** function \( \varphi(s, I)(\cdot) = \hat{M}\hat{t}(\cdot): \mathbb{Z} \rightarrow \mathbb{R}^p \).

The proof of the following consistency result is in Appendix C.1.

**Proposition A.3 (Consistency of \( \hat{\varphi} \)).** Suppose Assumptions 3.12 and 3.14 hold, and the regularity conditions in Proposition 3.1 hold for \( \tilde{\theta} \). Assume \( M(s, 1, \theta) - M(s, 1, \theta') = O(||\theta - \theta'||_2) \) and \( |s(\cdot, \theta) - s(\cdot, \theta')|_{L^2(\nu)} = O(||\theta - \theta'||_2) \) for any \( \theta, \theta' \in \Theta \). Then the output of Algorithm 7 satisfies

\[ \|\eta(s, I)(\cdot) - \varphi(\cdot)\|_{L^2(\nu)} \leq p \cdot O_P(\mathcal{R}_m(|I|) + \mathcal{R}_r(|I|) + |I|^{-1/2}). \]

B Technical proofs

B.1 Linearity of Z-estimators

**Proof of Proposition 3.1.** We first show the consistency of \( \hat{\theta}_n \xrightarrow{p} \theta_0 \) and \( \hat{\theta}_n^{\text{cond}} \xrightarrow{p} \theta_0 \), where the convergence in probability is in each entry. The consistency of \( \hat{\theta}_n \) follows directly from the classical results [42, Theorem 5.9]. Similarly, we note that \( \hat{\theta}_n^{\text{cond}} \) is the unique solution to (2.1) with the score function replaced by \( t(Z_i, \theta) \). Thus, under the given conditions, we have the consistency of \( \hat{\theta}_n^{\text{cond}} \) following [42, Theorem 5.9].

We now employ the Taylor expansion argument to obtain the asymptotic linearity (3.1) and (3.2). Recall that \( s(D, \theta): \mathbb{D} \times \Theta \rightarrow \mathbb{R}^p \). Expanding \( \sum_{i=1}^n s(D_i, \theta_n) \) at \( \theta_0 \) yields

\[ 0 = \frac{1}{\sqrt{n}} \sum_{i=1}^n s(D_i, \theta_0) + \frac{1}{\sqrt{n}} \sum_{i=1}^n \hat{s}(D_i, \theta_0)(\hat{\theta}_n - \theta_0) + \frac{1}{2\sqrt{n}} \sum_{i=1}^n (\hat{\theta}_n - \theta_0)^\top R(D_i, \hat{\theta}_n)(\hat{\theta}_n - \theta_0), \]
where the random vector $\tilde{\theta}_n$ lies within the segment between $\theta^0$ and $\hat{\theta}_n$. Rearranging the terms, we have

$$-rac{1}{\sqrt{n}} \sum_{i=1}^{n} s(D_i, \theta^0) = \left( \frac{1}{n} \sum_{i=1}^{n} s(D_i, \theta^0) + \frac{1}{2n} \sum_{i=1}^{n} (\tilde{\theta}_n - \theta^0) \top \tilde{s}(D_i, \tilde{\theta}_n) \right) \cdot \sqrt{n} (\tilde{\theta}_n - \theta^0).$$

The law of large numbers implies $\frac{1}{n} \sum_{i=1}^{n} \tilde{s}(D_i, \theta^0) = \mathbb{E}[\tilde{s}(D, \theta^0)] + o_P(1)$, where $\mathbb{E}[\tilde{s}(D, \theta^0)]$ is non-singular according to (iv). Meanwhile, Condition (iv) implies $\|\frac{1}{n} \sum_{i=1}^{n} (\tilde{\theta}_n - \theta^0) \top \tilde{s}(D_i, \tilde{\theta}_n)\|_1 \leq \|\tilde{\theta}_n - \theta^0\|_1 \cdot \frac{1}{2n} \sum_{i=1}^{n} g(D_i) = o_P(1)$ since $\tilde{\theta}_n$ converges in probability to $\theta^0$. Hence

$$\mathbb{E}[\tilde{s}(D, \theta^0)] + o_P(1) \cdot \sqrt{n} (\tilde{\theta}_n - \theta^0) = -\frac{1}{\sqrt{n}} \sum_{i=1}^{n} s(D_i, \theta^0).$$

On the left-handed side, $o_P(1)$ means a random matrix where each entry converges in probability to zero. Thus we have

$$\sqrt{n} (\tilde{\theta}_n - \theta^0) = -\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}[\tilde{s}(D, \theta^0)])^{-1} s(D_i, \theta^0) + o_P(1).$$

That is, the asymptotic linearity (3.1) holds with

$$\phi(D) = - (\mathbb{E}[\tilde{s}(D, \theta^0)])^{-1} s(D, \theta^0).$$

On the other hand, recall the observation that $\theta^0_{n \text{cond}}$ is the unique solution to (2.1) with the score function replaced by $\tilde{t}(Z_i, \theta)$. Meanwhile, condition (iv) implies also $\|\tilde{s}_{jk}(Z, \theta)\| \leq \mathbb{E}[g(D) | Z]$ due to Jensen’s inequality; and $E[\tilde{t}(Z, \theta^0)] = E[\tilde{s}(D, \theta^0)]$ due to the tower property of conditional expectations and the exchangeability of expectation and derivative in (iv). Following exactly the same arguments, we have

$$\sqrt{n} (\theta^0_{n \text{cond}} - \theta^0) = -\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}[\tilde{t}(Z, \theta^0)])^{-1} \tilde{t}(Z_i, \theta^0) + o_P(1)$$

$$= -\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (\mathbb{E}[\tilde{s}(D, \theta^0)])^{-1} E[s(D_i, \theta^0) | Z_i] + o_P(1).$$

That is, the asymptotic linearity (3.2) holds with the same $\phi(D)$. Therefore, we complete the proof of Proposition 3.1. \qed

### B.2 Linear expansion with known covariate shift

**Proof of Proposition A.1** Firstly, note that the conditions in Proposition A.1 imply the same conditions as Proposition 3.1 when we substitute $(D_i, Z_i) \sim P$ with $(D_i^{\text{new}}, Z_i^{\text{new}}) \sim Q$. Therefore, applying the same arguments as those in the proof of Proposition 3.1 leads to the linear expansion (3.9) of $\theta^0_{n \text{cond,new}}$.

When it comes to $\hat{\theta}_n^{\text{trans}}$, note that $\hat{\theta}_n^{\text{trans}}$ is the unique solution to

$$\sum_{i=1}^{n} \tilde{s}(D_i, Z_i, \theta) = 0,$$

where $\tilde{s}(D_i, Z_i, \theta) = w(Z_i) s(D_i, \theta)$. The conditions in Proposition A.1 imply the same conditions of Proposition 3.1 for $\tilde{s}$. Therefore, following the arguments of Proposition 3.1 we have the linear expansion

$$\sqrt{n} (\hat{\theta}_n^{\text{trans}} - \theta^0_{\text{new}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \phi(D_i, Z_i) + o_P(1),$$

where

$$\phi(D_i, Z_i) = - (\mathbb{E}[\tilde{s}(D, \theta^0_{\text{new}})])^{-1} \tilde{s}(D, \theta^0).$$

It’s straightforward to see that $\phi(D_i, Z_i) = \psi(D_i) w(Z_i)$, hence completing the proof of the linear expansion (3.8) of $\hat{\theta}_n^{\text{trans}}$. \qed
B.3  Linear expansion with estimated covariate shift

Proof of Proposition A.2. We first show the consistency of \( \hat{\theta}_{n,\ell}^{\text{new}} \) for any fixed \( \theta \). Without loss of generality, the sample size is \( |I| / |I_x| = 2n / 3 \). To this end, we utilize Theorem 5.9 of [42], so that it suffices to show (a) \( \sup_{\theta \in \Theta} |S(\hat{\theta}) - S(\theta)| \rightarrow 0 \) in probability, and (b) for any \( \epsilon > 0 \), there exists some \( \delta > 0 \) such that \( \inf_{\theta - \theta_0^{\text{new}} \leq \delta} |S(\theta) - S(\theta_0^{\text{new}})| > \epsilon \), where we define

\[
\hat{S}(\theta) = \frac{3}{2n} \sum_{i \not\in I_x} \hat{w}_i(Z_i)s(D_i, \theta), \quad S(\theta) = E[w(Z)s(D, \theta)].
\]

Firstly, for any fixed \( \theta \in \Theta \), we have

\[
|\hat{S}(\theta) - S(\theta)| \leq \frac{3}{2n} \sum_{i \not\in I_x} |\hat{w}_i(Z_i) - w(Z_i)| \cdot |s(D_i, \theta)| + \left| \frac{3}{2n} \sum_{i \not\in I_x} w(Z_i)s(D_i, \theta) - S(\theta) \right|,
\]

where

\[
\frac{3}{2n} \sum_{i \not\in I_x} |\hat{w}_i(Z_i) - w(Z_i)| \cdot |s(D_i, \theta)| \leq \sup_z |\hat{w}_i(z) - w(z)| \cdot \frac{3}{2n} \sum_{i \not\in I_x} |s(D_i, \theta)| = o_P(1)
\]

by Assumption 3.9 and the integrability of \( s(D, \theta) \). The second term also converges to zero by the law of large numbers. Hence \( |\hat{S}(\theta) - S(\theta)| = o_P(1) \) for any fixed \( \theta \in \Theta \). By compactness of \( \Theta \) in condition (ii) of Proposition 3.1 as well as the continuity of \( \hat{S}(\theta) \) and \( S(\theta) \), we know that the uniform convergence in (a) holds. The compactness of \( \Theta \) and the uniqueness of solution \( \theta_0^{\text{new}} \) implies the well-separatedness condition (b) (c.f. Theorem 5.9 of [42]). Thus we have \( \hat{\theta}_{n,\ell}^{\text{new}} \rightarrow \theta_0^{\text{new}} \) in probability as \( n \rightarrow \infty \).

We now employ a Taylor expansion argument to show the asymptotic linearity. Expanding \( \hat{S}(\theta_{n,\ell}^{\text{new}}) \) at \( \theta_0^{\text{new}} \) yields

\[
0 = \sum_{i \in I_x} \hat{w}_i(Z_i) s(D_i, \theta_0^{\text{new}}) + \sum_{i \not\in I_x} \hat{w}_i(Z_i) \tilde{s}(D_i, \theta_0^{\text{new}}) (\hat{\theta}_{n,\ell}^{\text{new}} - \theta_0^{\text{new}})
\]

\[
+ \frac{1}{2} \sum_{i \not\in I_x} \hat{w}_i(Z_i) (\hat{\theta}_{n,\ell}^{\text{new}} - \theta_0^{\text{new}})^{\top} \tilde{s}(D_i, \theta_0^{\text{new}}) (\hat{\theta}_{n,\ell}^{\text{new}} - \theta_0^{\text{new}}).
\]

Here utilizing the fact that each entry of \( \tilde{s}(D_i, \theta_0^{\text{new}}) \) is controlled by an integrable \( g(D_i) \), the random variable

\[
\frac{3}{2n} \sum_{i \not\in I_x} \hat{w}_i(Z_i) \tilde{s}(D_i, \theta_0^{\text{new}}) = \frac{3}{2n} \sum_{i \not\in I_x} \left( \hat{w}_i(Z_i) - w(Z_i) \right) \tilde{s}(D_i, \theta_0^{\text{new}}) + \frac{3}{2n} \sum_{i \not\in I_x} w(Z_i) \tilde{s}(D_i, \theta_0^{\text{new}})
\]

is of order \( o_P(1) \), hence

\[
\frac{3}{4n} \sum_{i \not\in I_x} \hat{w}_i(Z_i) (\hat{\theta}_{n,\ell}^{\text{new}} - \theta_0^{\text{new}})^{\top} \tilde{s}(D_i, \theta_0^{\text{new}}) = o_P(1).
\]

The above \( o_P(1) \) and \( o_P(1) \) are both in the entry-wise sense. Reorganizing the Taylor expansion,

\[
- \frac{1}{\sqrt{2n/3}} \sum_{i \not\in I_x} \hat{w}_i(Z_i) s(D_i, \theta_0^{\text{new}}) = \left( o_P(1) + \frac{3}{2n} \sum_{i \not\in I_x} \hat{w}_i(Z_i) \tilde{s}(D_i, \theta_0^{\text{new}}) \right) \cdot \sqrt{2n/3} (\hat{\theta}_{n,\ell}^{\text{new}} - \theta_0^{\text{new}}).
\]

Following similar arguments as before, we also have

\[
\frac{3}{2n} \sum_{i \not\in I_x} \hat{w}_i(Z_i) \tilde{s}(D_i, \theta_0^{\text{new}}) = E[w(Z_i) \tilde{s}(D_i, \theta_0^{\text{new}})] + o_P(1).
\]

Since the expected matrix is invertible by condition (iv') in Proposition A.1, we know

\[
\sqrt{2n/3} (\hat{\theta}_{n,\ell}^{\text{new}} - \theta_0^{\text{new}}) = - \frac{1}{\sqrt{2n/3}} \sum_{i \not\in I_x} \left( E[w(Z_i) \tilde{s}(D_i, \theta_0^{\text{new}})] \right)^{-1} \hat{w}_i(Z_i) s(D_i, \theta_0^{\text{new}}) + o_P(1),
\]

which is equivalent to (3.14) by the definition of \( \psi(\cdot) \). Therefore, we complete the proof of Proposition A.2.
B.4 Proofs of validity of conditional inference

This section contains the proof of Theorem 3.4. Before proving Theorem 3.4, we first state and prove an intermediate result on the asymptotic distribution of $\hat{\theta}_n - \theta_{n\text{cond}}$.

**Proposition B.1.** Suppose Assumptions 3.2 and 3.3 hold. For any fixed $x \in \mathbb{R}$, the random variable $\mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) \leq x \mid Z)$ converges in probability to $\Phi(x/\sigma)$, where $\Phi$ is the cumulative distribution function (c.d.f.) of standard Gaussian distribution, and $\sigma^2$ is defined in equation (3.4).

**Proof of Proposition B.1.** By Assumptions 3.2 and 3.3 we have

$$\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \phi(D_i) - \mathbb{E}[\phi(D_i) \mid Z_i] \right) + o_P(1).$$

For notational simplicity, we write

$$d_n = \sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) - \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \zeta_i,$$

where $\zeta_i = \phi(D_i) - \mathbb{E}[\phi(D_i) \mid Z_i]$, $i = 1, \ldots, n$,

where $d_n = o_P(1)$ follows from the given conditions. Hence Lemma D.4 implies that for any fixed $\epsilon > 0$,

$$\mathbb{P}(|d_n| > \epsilon \mid Z_n) = o_P(1). \quad \text{(B.1)}$$

On the other hand, we denote the conditional law of the essential term as

$$L_n = \mathcal{L}\left( \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \phi(D_i) - \mathbb{E}[\phi(D_i) \mid Z_i] \right) \mid Z_n \right).$$

By the conditional CLT in Lemma D.1 taking $g(X_i) = \phi(D_i)$ and the filtration $\mathcal{F}_n = \sigma(Z_n) = \sigma(\{Z_i\}_{i=1}^{n})$, we know that the conditional law $L_n$ converges almost surely to $N(0, \sigma^2)$ with $\sigma^2$ defined in equation (3.4). That is, for any $x \in \mathbb{R}$, we have

$$\mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) + d_n \leq x \mid Z_n) \overset{a.s.}{\to} \Phi\left(\frac{x}{\sigma}\right),$$

where $\Phi(\cdot)$ is the cumulative distribution function of standard normal distribution. By equation (B.1), for any constant $\epsilon > 0$, it holds that

$$\mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) \leq x \mid Z_n)$$

$$= \mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) \leq x, |d_n| \leq \epsilon \mid Z_n) + \mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) \leq x, |d_n| > \epsilon \mid Z_n)$$

$$\leq \mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) + d_n \leq x + \epsilon \mid Z_n) + \mathbb{P}(|d_n| > \epsilon \mid Z_n) = \Phi\left(\frac{x + \epsilon}{\sigma}\right) + o_P(1). \quad \text{(B.2)}$$

On the other hand, we have

$$\mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) \leq x \mid Z_n)$$

$$\geq \mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) + d_n \leq x - \epsilon \mid Z_n)$$

$$\geq \mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) + d_n \leq x - \epsilon \mid Z_n) - \mathbb{P}(|d_n| > \epsilon \mid Z_n) = \Phi\left(\frac{x - \epsilon}{\sigma}\right) + o_P(1). \quad \text{(B.3)}$$

By the arbitrariness of $\epsilon > 0$ in equations (B.2) and (B.3), for any fixed $x \in \mathbb{R}$, it holds that

$$\mathbb{P}(\sqrt{n}(\hat{\theta}_n - \theta_{n\text{cond}}) \leq x \mid Z_n) = \Phi\left(\frac{x}{\sigma}\right) + o_P(1).$$

Therefore, we conclude the proof of Proposition B.1. \qed

The proof of Theorem 3.4 is as follows.
Proof of Theorem 3.4. By Proposition B.1 for any fixed $x \in \mathbb{R}$,
\[ P\left( \sqrt{n}(\hat{\theta}_n - \theta_{n, \text{cond}}) \leq x \mid Z_n \right) = \Phi(x/\sigma) + o_P(1). \]

For any fixed constant $\epsilon > 0$, we write $z^-(\epsilon) = z_{1-\alpha/2}(\sigma - \epsilon)$ and $z^+(\epsilon) = z_{1-\alpha/2}(\sigma + \epsilon)$. Denoting
\[ \Delta^\pm(\epsilon) = P\left( \sqrt{n}(\hat{\theta}_n - \theta_{n, \text{cond}}) \leq z^\pm(\epsilon) \right) = \Phi(z^\pm(\epsilon)/\sigma), \]
we have $\Delta^+(\epsilon), \Delta^-(\epsilon) = o_P(1)$ by Proposition B.1. Since the estimator $\hat{\sigma} \rightarrow \sigma$, we have
\[ P\left( \sqrt{n}(\hat{\theta}_n - \theta_{n, \text{cond}}) \leq z_{1-\alpha/2} \cdot \hat{\sigma} \mid Z_n \right) - (1 - \alpha) \geq \Phi(z^+(\epsilon)) - (1 - \alpha) + P(\hat{\sigma} < \sigma + \epsilon \mid Z_n) + \Delta^+(\epsilon), \]
where the conditional probability $P(\hat{\sigma} < \sigma - \epsilon \mid Z_n) = o_P(1)$ by Lemma D.4. On the other hand, for any fixed constant $\epsilon > 0$, we have
\[ P\left( \sqrt{n}(\hat{\theta}_n - \theta_{n, \text{cond}}) \leq z_{1-\alpha/2} \cdot \hat{\sigma} \mid Z_n \right) \leq P(\hat{\sigma} > \sigma + \epsilon \mid Z_n) \]
\[ = \Phi(z^-(\epsilon)) - (1 - \alpha) + P(\hat{\sigma} < \sigma - \epsilon \mid Z_n) + \Delta^-(\epsilon), \]
and combining equations (B.4) and (B.5), we have
\[ P\left( P\left( \sqrt{n}(\hat{\theta}_n - \theta_{n, \text{cond}}) \leq z_{1-\alpha/2} \cdot \hat{\sigma} \mid Z_n \right) - (1 - \alpha) > \delta \right) \]
\[ \leq P(\hat{\sigma} < \sigma - \epsilon \mid Z_n) + \Delta^-(\epsilon) < -\delta/2 + P(\hat{\sigma} < \sigma + \epsilon \mid Z_n) + \Delta^+(\epsilon) > \delta/2 \rightarrow 0. \]
By the arbitrariness of $\delta > 0$, we complete the proof of Theorem 3.4.

B.5 Proof of Theorem 3.8

Proof of Theorem 3.8. Recall that $\eta(z) = \mathbb{E}[\psi(D) \mid Z = z]$; by the invariance of conditional distribution of $D$ given $Z$, we have $\mathbb{E}[\psi(D_i) \mid Z_i] = \eta(Z_i)$ and $\mathbb{E}[\psi(D_{j, \text{new}}) \mid Z_{j, \text{new}}] = \eta(Z_{j, \text{new}})$ for all $i \in [n]$ and all $j \in [m]$. In the following, we are to show that
\[ \hat{\theta}_{m, n}^{\text{trans}} - \theta_{m, n}^{\text{cond, new}} = \frac{1}{n} \sum_{i=1}^{n} w(Z_i)(\psi(D_i) - \eta(Z_i)) + o_P\left(1/\sqrt{\min(n, m)}\right). \]
By equation (3.2), we have the asymptotic linearity that
\[ \hat{\theta}_{n}^{\text{trans}} - \theta_{n}^{\text{cond, new}} = \frac{1}{n} \sum_{i=1}^{n} w(Z_i)\psi(D_i) - \frac{1}{m} \sum_{j=1}^{m} \eta(Z_{j, \text{new}}) + o_P\left(1/\sqrt{n} + 1/\sqrt{m}\right). \]
By the definition of $\hat{\theta}_{m, n}^{\text{trans}}$ in equation (3.10), we have the decomposition
\[ \hat{\theta}_{m, n}^{\text{trans}} - \theta_{m, n}^{\text{cond, new}} = \hat{\theta}_{n}^{\text{trans}} - \hat{\theta}_{m}^{\text{trans}} - \theta_{m, n}^{\text{cond, new}} \]
\[ = \frac{1}{n} \sum_{i=1}^{n} w(Z_i)\psi(D_i) - \frac{1}{m} \sum_{j=1}^{m} \eta(Z_{j, \text{new}}) + o_P\left(1/\sqrt{n} + 1/\sqrt{m}\right). \]
\[ = \frac{1}{n} \sum_{i=1}^{n} w(Z_i)(\psi(D_i) - \eta(Z_i)) + o_P\left(1/\sqrt{n} + 1/\sqrt{m}\right) + (i) + (ii), \]
For the term (i,a), we note that for \( m \)

Furthermore, the arguments apply similarly to the term (ii) with sample size \( n \)

where

\[
(i) = \frac{1}{n} \sum_{i=1}^{n} w(Z_i) \eta(Z_i) - \frac{1}{2|\mathcal{I}_1|} \sum_{i \in \mathcal{I}_1} w(Z_i) \bar{\eta}^Z(Z_i) - \frac{1}{2|\mathcal{I}_2|} \sum_{i \in \mathcal{I}_2} w(Z_i) \bar{\eta}^Z(Z_i) + \frac{1}{2} \mathbb{E}_P[w(Z) \bar{\eta}^Z(Z) | \mathcal{I}_2],
\]

\[
(ii) = \frac{1}{2m} \sum_{j=1}^{m} (\bar{\eta}^{Z_j}(Z_j^{\text{new}}) + \bar{\eta}^Z(Z_j^{\text{new}})) - \frac{1}{m} \sum_{j=1}^{m} \eta(Z_j^{\text{new}}) - \frac{1}{2} \mathbb{E}_Q[\eta^Z(Z) | \mathcal{I}_1] - \frac{1}{2} \mathbb{E}_Q[\eta^Z(Z) | \mathcal{I}_2].
\]

Here the decomposition utilizes the fact that

\[ \mathbb{E}_P[w(Z_i) \bar{\eta}^Z(Z_i) | \mathcal{I}_k] = \mathbb{E}_Q[\bar{\eta}^Z(Z_j^{\text{new}}) | \mathcal{I}_k] \]

for \( i \notin \mathcal{I}_k \) and \( j \in \mathcal{T}^{\text{new}} \), \( k = 1, 2 \), which follows from the fact that \( \mathbb{P} \) and \( \mathbb{Q} \) are related with a covariate shift \( w(Z) \), and the estimation of \( \bar{\eta}^Z \) is independent of \( \mathcal{T}^{\text{new}} \) when \( w(\cdot) \) is known.

In the sequel, we bound the terms (i) and (ii) separately. Since \( \mathcal{I}_1 \) and \( \mathcal{I}_2 \) are (approximately) equal-sized with \( |\mathcal{I}_1| + |\mathcal{I}_2| = n \), we have

\[
(i) = \frac{1}{2|\mathcal{I}_1|} \sum_{i \in \mathcal{I}_1} w(Z_i) \eta(Z_i) - \frac{1}{2|\mathcal{I}_1|} \sum_{i \in \mathcal{I}_1} w(Z_i) \bar{\eta}^Z(Z_i) + \frac{1}{2} \mathbb{E}_P[w(Z) \bar{\eta}^Z(Z) | \mathcal{I}_2]
\]

\[
+ \frac{1}{2|\mathcal{I}_2|} \sum_{i \in \mathcal{I}_2} w(Z_i) \eta(Z_i) - \frac{1}{2|\mathcal{I}_2|} \sum_{i \in \mathcal{I}_2} w(Z_i) \bar{\eta}^Z(Z_i) + \frac{1}{2} \mathbb{E}_Q[w(Z) \bar{\eta}^Z(Z) | \mathcal{I}_1] + O_P(1/n).
\]

For the term (i,a), we note that for \( i \in \mathcal{I}_1 \) where \( (D_i, Z_i) \sim \mathbb{P} \),

\[ \mathbb{E}[w(Z_i) \eta(Z_i) | \mathcal{I}_2] = \mathbb{E}_Q[\eta(Z)] = 0. \]

Hence we can write \( (i,a) = \frac{1}{2|\mathcal{I}_1|} \sum_{i \in \mathcal{I}_1} \xi_i \), where

\[ \xi_i = w(Z_i)(\eta(Z_i) - \bar{\eta}^Z(Z_i)) - \mathbb{E}[w(Z_i) \eta(Z_i) - w(Z_i) \bar{\eta}^Z(Z_i) | \mathcal{I}_2]. \]

Conditional on \( \mathcal{I}_2 \), \( \{\xi_i\}_{i \in \mathcal{I}_1} \) are i.i.d. with mean zero, since the estimation of \( \bar{\eta}^Z \) does not use data in \( \mathcal{I}_1 \). Therefore, we have

\[ \mathbb{E}[\langle i,a \rangle^2 | \mathcal{I}_2] = \frac{1}{4|\mathcal{I}_1|} \mathbb{E}[\xi_i^2 | \mathcal{I}_2] \leq \frac{1}{4|\mathcal{I}_1|} \|w(\cdot)(\eta(\cdot) - \bar{\eta}^Z(\cdot))\|_{L_2(\mathbb{P})}, \]

where \( \|w(\cdot)(\eta(\cdot) - \bar{\eta}^Z(\cdot))\|_{L_2(\mathbb{P})}^2 = \mathbb{E}[\langle w(Z)(\eta(Z) - \bar{\eta}^Z(Z)) \rangle^2] \) for an independent copy \( Z \sim \mathbb{P} \). Thus, by Assumption 3.7, we have \( n \cdot \mathbb{E}[\langle i,a \rangle^2 | \mathcal{I}_2] = o_P(1) \). Referring to Lemma D.4 for non-negative random variables \( n \cdot \langle i,a \rangle^2 \) and the filtration composed of \( \mathcal{I}_2 \), we have \( (i,a) = o_P(1/\sqrt{n}) \). The same arguments also apply to the term (i,b), which lead to

\[ |(i)| = o_P(1/\sqrt{n}). \]

Furthermore, the arguments apply similarly to the term (ii) with sample size \( m \), hence

\[ |(ii)| = o_P(1/\sqrt{m}). \]

Putting them together, we have

\[ \hat{\theta}_{m,n}^{\text{trans}} - \bar{\theta}_{m,n}^{\text{cond,new}} = \frac{1}{n} \sum_{i=1}^{n} w(Z_i) (\psi(D_i) - \eta(Z_i)) + o_P(1/\sqrt{n} + 1/\sqrt{m}). \]
Applying the conditional CLT result in Lemma 4.1 to $g(X_i) = \phi(D_i)$ and filtrations

$$G_n = \sigma\left(\{Z_j^{\text{new}}\}_{j=1}^m\right) \subset F_n = \sigma\left(\{Z_i\}_{i=1}^n, \{Z_j^{\text{new}}\}_{j=1}^m\right),$$

we know that conditional on $Z_m^{\text{new}}$, $1/\sqrt{n} \sum_{i=1}^n w(Z_i) \left(\psi(D_i) - \eta(Z_i)\right)$ converges in distribution to $N(0, \sigma^2_{\text{shift}})$ almost surely. Thus, with similar arguments as in the proof of Theorem 3.4 for a consistent estimator $\hat{\sigma}^2_{\text{shift}}$, we obtain the desired results in Theorem 4.8.

### B.6 Proof of Theorem 3.12

**Proof of Theorem 3.12.** For notational simplicity, for $\ell = 1, 2, 3$, we denote $I_{\ell,1}$ and $I_{\ell,2}$ as the two remaining folds other than $I_{\ell}$, and similarly for $I_{\ell,1}^{\text{new}}$ and $I_{\ell,2}^{\text{new}}$. We also denote $\hat{\eta}_{\ell,1}$ and $\hat{\eta}_{\ell,2}$ as the estimators obtained with the two folds. For any dataset indexed by $I$, we use $I$ to represent the random variables when there is no confusion.

For any fixed $\ell$, by (3.14) and the definition of $\hat{c}(\ell)$, we have

$$\hat{\theta}^{\text{trans.},(\ell)} - \frac{3}{2m} \sum_{j \notin I_{\ell}^{\text{new}}} \eta(Z_j^{\text{new}}) = \frac{3}{2n} \sum_{i \in I_{\ell,1}} \tilde{w}_i(Z_i) \psi(D_i) - \frac{3}{2n} \sum_{i \in I_{\ell,1}} \tilde{w}_i(Z_i) \tilde{\eta}_{\ell,2}(Z_i) - \frac{3}{2n} \sum_{i \in I_{\ell,2}} \tilde{w}_i(Z_i) \tilde{\eta}_{\ell,1}(Z_i) + \frac{3}{2m} \sum_{j \in I_{\ell,1}^{\text{new}}} \tilde{\eta}_{\ell,1}(Z_j^{\text{new}}) + \frac{3}{2m} \sum_{j \in I_{\ell,2}^{\text{new}}} \tilde{\eta}_{\ell,2}(Z_j^{\text{new}}) - \frac{3}{2m} \sum_{j \notin I_{\ell}^{\text{new}}} \eta(Z_j^{\text{new}}) + o_P(1/\sqrt{n}).$$

Writing $\Delta_w(\cdot) = \tilde{w}_\ell(\cdot) - w(\cdot)$ and $\Delta^{(k)}(\cdot) = \tilde{\eta}_{\ell,k}(\cdot) - \eta(\cdot)$ for $k = 1, 2$, we have

$$\hat{\theta}^{\text{trans.},(\ell)} - \frac{3}{2m} \sum_{j \notin I_{\ell}^{\text{new}}} \eta(Z_j^{\text{new}}) = -\frac{3}{2n} \sum_{i \in I_{\ell,1}} \tilde{w}_i(Z_i) \Delta^{(2)}(Z_i) \left[\Delta_{\ell,1}(Z_i)\right] + \frac{3}{2m} \sum_{j \in I_{\ell,1}^{\text{new}}} \Delta^{(2)}(Z_j^{\text{new}}) + \frac{3}{2m} \sum_{j \in I_{\ell,2}^{\text{new}}} \Delta^{(1)}(Z_j^{\text{new}}) - \frac{3}{2n} \sum_{i \in I_{\ell,2}} \Delta_w(Z_i) \Delta^{(2)}(Z_i) - \frac{3}{2n} \sum_{i \in I_{\ell,2}} \Delta_w(Z_i) \Delta^{(1)}(Z_i)$$

We bound the two terms (i) and (ii) separately. Since the folds $D_{\ell}, I_{\ell,1}, I_{\ell,2}$ are disjoint, conditional on $I_{\ell} \cup I_{\ell,1}^{\text{new}} \cup I_{\ell,2}, \{\Delta_w(Z_i)\Delta^{(1)}(Z_i)\}_{i \in I_{\ell,2}}$ are i.i.d. random variables. By Cauchy-Schwarz inequality and Assumption 3.11, we have

$$\mathbb{E}\left[\frac{3}{2n} \sum_{i \in I_{\ell,1}} \left|\Delta_w(Z_i) \Delta^{(1)}(Z_i)\right| \left| I_{\ell} \cup I_{\ell,1}^{\text{new}} \cup I_{\ell,1}\right| \right] \leq \|\Delta_w(\cdot)\|_{L_2(P)} \cdot \|\Delta^{(1)}(\cdot)\|_{L_2(P)} = o_P(1/\sqrt{n}).$$

Invoking Lemma 4.5 and by symmetry of $I_{\ell,1}$ and $I_{\ell,2}$, we know that

$$\left|\Delta^{(1)}\right| = \left|\frac{3}{2n} \sum_{i \in I_{\ell,1}} \Delta_w(Z_i) \Delta^{(2)}(Z_i) + \frac{3}{2n} \sum_{i \in I_{\ell,2}} \Delta_w(Z_i) \Delta^{(1)}(Z_i)\right| = o_P(1/\sqrt{n}).$$

Furthermore, note that the estimation of $\hat{\eta}_{\ell,k}$ only depends on $I_{\ell,k}$ and $I_{\ell,k}^{\text{new}}$ for each $k = 1, 2$. Since $P, Q$ admit a covariate shift, we have

$$\mathbb{E}\left[w(Z_i) \Delta^{(k)}(Z_i) \left| I_{\ell} \cup I_{\ell,k} \cup I_{\ell,1}^{\text{new}} \cup I_{\ell,k}^{\text{new}}\right.\right] = \mathbb{E}_Q\left[\Delta^{(k)}(Z_j^{\text{new}}) \left| I_{\ell} \cup I_{\ell,k} \cup I_{\ell,1}^{\text{new}} \cup I_{\ell,k}^{\text{new}}\right.\right] := E^{(k)}_{\Delta}$$
for \( i \in I_{\ell,3-k} \) and \( j \in I_{\ell,3-k}^{\text{new}}, k = 1, 2 \). Then we have

\[
(ii) = -\frac{3}{2n} \sum_{i \in I_{\ell,1}} \left( w(Z_i) \Delta_{\eta}^{(2)}(Z_i) - E_{\Delta}^{(2)} \right) - \frac{3}{2n} \sum_{i \in I_{\ell,2}} \left( w(Z_i) \Delta_{\eta}^{(1)}(Z_i) - E_{\Delta}^{(1)} \right) + \frac{3}{2m} \sum_{j \in I_{\ell,2}^{\text{new}}} \left( \Delta_{\eta}^{(1)}(Z_j^{\text{new}}) + \Delta_{\eta}^{(2)}(Z_j^{\text{new}}) - E_{\Delta}^{(1)} - E_{\Delta}^{(2)} \right).
\]

Note that conditional on \( I_{\ell} \cup I_{\ell}^{\text{new}} \cup I_{\ell,2} \), the random variables \( \{ w(Z_i) \Delta_{\eta}^{(2)}(Z_i) - E_{\Delta}^{(2)} \}_{i \in I_{\ell,1}} \) are i.i.d. and mean zero. Hence

\[
n \cdot E \left[ \left( \frac{3}{2n} \sum_{i \in I_{\ell,1}} \left( w(Z_i) \Delta_{\eta}^{(2)}(Z_i) - E_{\Delta}^{(2)} \right) \right)^2 \right] = \frac{3}{2n} \cdot \| \Delta_{\eta}^{(2)}(\cdot) \|^2_{L_2(P)} = o_P(1)
\]

by Assumption 3.11. Invoking Lemma D.5 again with similar arguments for all other terms, we have

\[
| (ii) | = o_P(1/\sqrt{n} + 1/\sqrt{m}) = o_P(1/\sqrt{n}).
\]

Putting the two bounds together, we have

\[
\tilde{\theta}_n^{\text{trans.}(\ell)} - \frac{3}{2n} \sum_{i \in I_{\ell,1}} \eta(Z_i^{\text{new}}) - \frac{3}{2n} \sum_{i \in I_{\ell,2}} \hat{w}(Z_i)(\psi(D_i) - \eta(Z_i)) = o_P(1/\sqrt{n}). \tag{B.6}
\]

Furthermore, note that \( E[\psi(D_i) - \eta(Z_i) \mid Z_i] = 0 \) almost surely, hence conditional on \( I_{\ell} \cup I_{\ell}^{\text{new}} \), the random variables \( \{ \Delta_{w}(Z_i) [\psi(D_i) - \eta(Z_i)] \}_{i \in I_{\ell}} \) are i.i.d. and mean zero. Thus

\[
n \cdot E \left[ \left( \frac{3}{2n} \sum_{i \in I_{\ell}} \Delta_{w}(Z_i) (\psi(D_i) - \eta(Z_i)) \right)^2 \right] I_{\ell} \cup I_{\ell}^{\text{new}}
\]

\[
= 3/2 \cdot \| \Delta_{w}(Z_i) (\psi(D_i) - \eta(Z_i)) \|^2_{L_2(P)}
\]

\[
\leq 3/2 \cdot \sup_z | \hat{w}(z) - w(z) |^2 \cdot || \psi(D_i) - \eta(Z_i) ||_{L_2(P)} = o_P(1).
\]

The last equation follows from \( \sup_z | \hat{w}(z) - w(z) | = o_P(1) \) in Assumption 3.11 as well as the fact that \( \psi(D_i) \) and \( \eta(Z_i) \) both have finite \( L_2(P) \) norms. Invoking Lemma D.5 we know

\[
\frac{3}{2n} \sum_{i \in I_{\ell}} \Delta_{w}(Z_i) (\psi(D_i) - \eta(Z_i)) = o_P(1/\sqrt{n}). \tag{B.7}
\]

Combining equations (B.6) and (B.7), we have

\[
\tilde{\theta}_n^{\text{trans.}(\ell)} - \frac{3}{2m} \sum_{j \in I_{\ell,2}^{\text{new}}} \eta(Z_j^{\text{new}}) - \frac{3}{2n} \sum_{i \in I_{\ell}} \hat{w}(Z_i)(\psi(D_i) - \eta(Z_i)) = o_P(1/\sqrt{n}).
\]

Recalling the sample splitting protocol, averaging over \( \ell = 1, 2, 3 \), we thus have

\[
\tilde{\theta}_m^{\text{trans. split}} - \frac{1}{m} \sum_{j=1}^m \eta(Z_j^{\text{new}}) - \frac{1}{n} \sum_{i=1}^n \hat{w}(Z_i)(\psi(D_i) - \eta(Z_i)) = o_P(1/\sqrt{n}),
\]

which (since \( m \geq cn \) for some \( c > 0 \)) further leads to

\[
\sqrt{n}(\tilde{\theta}_m^{\text{trans. split}} - \hat{\theta}_m^{\text{cond. split}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \hat{w}(Z_i)(\psi(D_i) - \eta(Z_i)) + o_P(1).
\]
Finally, applying the conditional central limit theorem of Lemma D.1 to \( w(Z_i)(\psi(D_i) - \eta(Z_i)) \) which has finite fourth moment, and invoking Lemma D.4, it holds for any \( x \in \mathbb{R} \) that
\[
\mathbb{P}(\sqrt{n}(\hat{\theta}_{m,n}^{\text{shift}} - \theta_{m}^{\text{cond,new}}) \leq x \mid Z_m^{\text{new}}) = \Phi(x/\sigma_{\text{shift}}) + o_p(1).
\]
Since \( \sigma_{\text{shift}} \rightarrow \sigma_{\text{shift}} \) in probability, with exactly the same arguments as those in the proof of Theorem 3.4, we obtain the desired result in Theorem 3.12.

\[
\text{C Proofs of estimation}
\]

\[
\text{C.1 Proof of Proposition A.3}
\]

Proof of Proposition A.3. We first analyze the entry-wise error in \( \hat{M} \). Note that
\[
\hat{M} - M(\theta) = \hat{M}(s, 1, \hat{\theta}, \mathcal{I}_2) - M(s, 1, \theta_0)
\]
\[
= \hat{M}(s, 1, \hat{\theta}, \mathcal{I}_2) - M(s, 1, \hat{\theta}) + M(s, 1, \hat{\theta}) - M(s, 1, \theta_0).
\]
On the other hand, by Assumption 3.14, we have
\[
\|\hat{M}(s, 1, \hat{\theta}, \mathcal{I}_2) - M(s, 1, \hat{\theta})\|_\infty \leq O_{p}(\mathcal{R}_m(\{\mathcal{I}_2\})) = O_{p}(\mathcal{R}_m(\{\mathcal{I}\}))
\]
and
\[
\|M(s, 1, \hat{\theta}) - M(s, 1, \theta_0)\|_\infty = O(||\hat{\theta} - \theta_0||_2) = O(||\mathcal{I}||^{-1/2}).
\]
Hence
\[
\|\hat{M} - M(\theta_0)\|_\infty \leq O_{p}(\mathcal{R}_m(\{\mathcal{I}\}) + ||\mathcal{I}||^{-1/2}).
\]
(C.1)

By Assumption 3.13, we have
\[
\|G(\hat{s}, \mathcal{I}_2) - G(s)\|_{L_2(\mathcal{P})} = O_{p}(\mathcal{R}_r(\{\mathcal{I}\})).
\]
Meanwhile, writing \( G(s) = \mathbb{E}[s(D, \theta_0) \mid Z = \cdot] \), by the definition of \( G(\cdot) \), we have
\[
\|G(\hat{s}) - G(s)\|_{L_2(\mathcal{P})} = \|\mathbb{E}[s(\hat{D}, \hat{\theta}) - s(D, \theta_0) \mid Z = \cdot]\|_{L_2(\mathcal{P})}
\]
\[
\leq \|s(\cdot, \hat{\theta}) - s(\cdot, \theta_0)\|_{L_2(\mathcal{P})} = O(||\hat{\theta} - \theta_0||_2) = O(||\mathcal{I}||^{-1/2})
\]
where \( \|s(\cdot, \hat{\theta}) - s(\cdot, \theta)\|_{L_2(\mathcal{P})} \) views \( \hat{\theta} \) as fixed and the \( L_2 \)-norm is with respect to \( D \sim \mathcal{P} \). Putting them together, the estimated conditional mean function satisfies
\[
\|\hat{\mu}(\cdot) - G(s)(\cdot)\|_{L_2(\mathcal{P})} \leq \|G(\hat{s}, \mathcal{I}_2) - G(s)\|_{L_2(\mathcal{P})} + \|G(\hat{s}) - G(s)\|_{L_2(\mathcal{P})}
\]
\[
\leq O_{p}(\mathcal{R}_r(\{\mathcal{I}\}) + ||\mathcal{I}||^{-1/2}).
\]
(C.2)

Altogether, we have
\[
\|\hat{\mu}(\cdot) - \varphi(\cdot)\|_{L_2(\mathcal{P})} = \|\hat{M} \hat{\mu}(\cdot) - M(\theta_0)G(s)(\cdot)\|_{L_2(\mathcal{P})}
\]
\[
\leq \left\| (\hat{M} - M(\theta_0)) \hat{\mu}(\cdot) \right\|_{L_2(\mathcal{P})} + \|M(\theta_0)(\hat{\mu}(\cdot) - G(s)(\cdot))\|_{L_2(\mathcal{P})}
\]
\[
\leq p \cdot \|\hat{M} - M(\theta_0)\|_\infty \cdot \|\hat{\mu}(\cdot)\|_{L_2(\mathcal{P})} + p \cdot \|M(\theta_0)\|_\infty \cdot \|\hat{\mu}(\cdot) - G(s)(\cdot)\|_{L_2(\mathcal{P})}
\]
\[
\leq p \cdot O_{p}(\mathcal{R}_m(\{\mathcal{I}\}) + \mathcal{R}_r(\{\mathcal{I}\}) + ||\mathcal{I}||^{-1/2}),
\]
where the last inequality follows from (C.1) and (C.2) and the fact that
\[
\|\hat{\mu}(\cdot)\|_{L_2(\mathcal{P})} \leq \|G(s)\|_{L_2(\mathcal{P})} + O_{p}(\mathcal{R}_r(\{\mathcal{I}\}) + ||\mathcal{I}||^{-1/2}) = O_{p}(1).
\]
We thus complete the proof of Proposition A.3.
C.2 Proof of Proposition 3.16

Proof of Proposition 3.16 For simplicity, we denote \( \Delta \phi_i = \phi(D_i) - \hat{\phi}_i \) and \( \Delta \varphi_i = \varphi(Z_i) - \hat{\varphi}_i \), where \( \hat{\phi}_i \) and \( \hat{\varphi}_i \) are estimated in Algorithm 3. Firstly, by Cauchy-Schwarz inequality,

\[
\frac{1}{|I_2|} \sum_{i \in I_2} \Delta \phi_i^2 = \frac{1}{|I_2|} \sum_{i \in I_2} (\hat{M}s(D_i, \hat{\theta}) - Ms(D_i, \theta_0))^2 \\
= \frac{1}{|I_2|} \sum_{i \in I_2} (\hat{M}s(D_i, \hat{\theta}) - \hat{M}s(D_i, \theta_0) + \hat{M}s(D_i, \theta_0) - Ms(D_i, \theta_0))^2 \\
\leq \frac{2}{|I_2|} \sum_{i \in I_2} (\hat{M}s(D_i, \hat{\theta}) - \hat{M}s(D_i, \theta_0))^2 + \frac{2}{|I_2|} \sum_{i \in I_2} (\hat{M}s(D_i, \theta_0) - Ms(D_i, \theta_0))^2.
\]

Here since \( \hat{\theta} \) is independent of \( I_2 \), we have

\[
\mathbb{E} \left[ \frac{1}{|I_2|} \sum_{i \in I_2} (s(D_i, \hat{\theta}) - s(D_i, \theta_0))^2 \bigg| I_1 \right] = \left\| \mathbb{E}[s(\cdot, \hat{\theta}) - s(\cdot, \theta_0)]_{L_2(\mathbb{P})} \right\|^2 = O(\|\hat{\theta} - \theta_0\|_2) = o_P(1).
\]

Employing Lemma D.4, we have

\[
\frac{2}{|I_2|} \sum_{i \in I_2} (\hat{M}s(D_i, \hat{\theta}) - 2\hat{M}^2 \cdot \frac{1}{|I_2|} \sum_{i \in I_2} (s(D_i, \hat{\theta}) - s(D_i, \theta_0))^2 = o_P(1).
\]

Following the same arguments as in the proof of Proposition A.3, we have \( \hat{M} = M + o_P(1) \), hence

\[
\frac{2}{|I_2|} \sum_{i \in I_2} (\hat{M}s(D_i, \theta_0) - Ms(D_i, \theta_0))^2 = 2(\hat{M} - M)^2 \cdot \frac{1}{|I_2|} \sum_{i \in I_2} s(D_i, \theta_0)^2 = o_P(1).
\]

Thus \( \frac{1}{|I_2|} \sum_{i \in I_2} \Delta \phi_i^2 = o_P(1) \). On the other hand, by the construction, \( \hat{\varphi} \) is independent of \( I_2 \), hence by Proposition A.3, we have

\[
\mathbb{E} \left[ \frac{1}{|I_2|} \sum_{i \in I_2} \Delta \phi_i^2 \bigg| I_1 \right] = \left\| \hat{\varphi} - \varphi(\cdot) \right\|_{L_2(\mathbb{P})} = o_P(1),
\]

which, combined with Lemma D.4 leads to \( \frac{1}{|I_2|} \sum_{i \in I_2} \Delta \phi_i^2 = o_P(1) \). Therefore, by Cauchy-Schwarz inequality, we have

\[
\frac{1}{|I_2|} \sum_{i \in I_2} (\Delta \phi_i - \Delta \varphi_i)^2 \leq \frac{2}{|I_2|} \sum_{i \in I_2} \Delta \phi_i^2 + \frac{2}{|I_2|} \sum_{i \in I_2} \Delta \varphi_i^2 = o_P(1).
\]

Finally, by Algorithm 3 and Cauchy-Schwarz inequality,

\[
\hat{\sigma}^2 = \frac{1}{|I_2|} \sum_{i \in I_2} (\phi(D_i) - \Delta \phi_i - \varphi(Z_i) + \Delta \varphi_i)^2 \\
\leq \frac{1}{|I_2|} \sum_{i \in I_2} (\phi(D_i) - \varphi(Z_i))^2 \\
+ \frac{1}{|I_2|} \sum_{i \in I_2} (\Delta \phi_i - \Delta \varphi_i)^2 \\
+ 2 \sqrt{\frac{1}{|I_2|} \sum_{i \in I_2} (\phi(D_i) - \varphi(Z_i))^2} \cdot \sqrt{\frac{1}{|I_2|} \sum_{i \in I_2} (\Delta \phi_i - \Delta \varphi_i)^2} = \sigma^2 + o_P(1),
\]

where the last equality follows from the law of large numbers.

\( \square \)
C.3 Proof of Proposition 3.17

Proof of Proposition 3.17 To begin with, we write
\[ \mathcal{G}(s) = \mathbb{E}[s(D, \theta_0^{\text{new}}) | Z = .] = \mathbb{E}[s(D^{\text{new}}, \theta_0^{\text{new}}) | Z^{\text{new}} = .] \]
and for any fixed \( \theta \in \Theta \),
\[ M(s, w, \theta) = -\left( \mathbb{E}[w(Z)s(D, \theta)] \right)^{-1}, \]
so that the ground truth satisfies \( \eta(z) = M(s, w, \theta_0^{\text{new}})\mathcal{G}(s)(z) \).

We first prove the result with ground truth of \( w(\cdot) \). In this case, with regularity conditions we know \( \| \hat{\theta} - \theta_0^{\text{new}} \|_2 = O_P(|\mathcal{I}|^{-1/2}) = O_P(|\mathcal{I}|^{-1/2}) \). Thus, following exactly the same arguments as in the proof of Proposition A.3 we have
\[ \| \hat{\theta}(\cdot) - \mathcal{G}(s)(\cdot) \|_{L_2(\mathcal{P})} \leq O_P(R_m(\mathbb{I}) + |\mathcal{I}|^{-1/2}). \]

On the other hand, by Algorithm 5, we know
\[ \| \hat{\theta} - \theta_0^{\text{new}} \|_2 = O_P(|\mathcal{I}|^{-1/2}) = O_P(|\mathcal{I}|^{-1/2}) \]
Thus, following exactly the same arguments as in the proof of Proposition A.3 we obtain the desired result (3.16).
hence
\[ \| \hat{M} - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \leq O_P \left( \| \hat{w}(\cdot) - w(\cdot) \|_{L_2(P)} + R_m(|I|) + |I|^{-1/2} \right) \quad (C.3) \]

On the other hand, since \( I_3 \) is independent of the function \( \hat{s}(\cdot) = s(\cdot, \hat{\theta}) \), we know \( \| G(\hat{s}, I_3)(\cdot) - G(\hat{s})(\cdot) \|_{L_2(P)} \leq O_P(\mathcal{R}_r(|I_3|)) = O_P(\mathcal{R}_r(|I|)) \). Also, the stability of \( s(\cdot, \theta) \) implies
\[ \| G(\hat{s})(\cdot) - G(s)(\cdot) \|_{L_2(P)} \leq \| \hat{s}(\cdot, \hat{\theta}) - s(\cdot, \theta) \|_{L_2(P)} = O(\| \hat{\theta} - \theta_0 \|_2) = O_P(|I|^{-1/2}). \]

Therefore, the error in \( \hat{\eta}(\cdot) \) can be bounded as
\[ \| \hat{\eta}(\cdot) - G(s)(\cdot) \|_{L_2(P)} \leq \| G(\hat{s}, I_3)(\cdot) - G(\hat{s})(\cdot) \|_{L_2(P)} + \| G(\hat{s})(\cdot) - G(s)(\cdot) \|_{L_2(P)} \leq O_P(\| \hat{w}(\cdot) - w(\cdot) \|_{L_2(P)} + |I|^{-1/2}). \quad (C.4) \]

Following similar arguments as the case with ground truth of \( w(\cdot) \), we combine the bounds (C.3) and (C.4) and obtain
\[ \| \eta(s, I)(\cdot) - \eta(\cdot) \|_{L_2(P)} \leq \left( \| \hat{M} - M(s, w, \theta_0^{\text{new}}) \|_{L_2(P)} + \| M(s, w, \theta_0^{\text{new}})(\hat{\eta}(\cdot) - G(s)(\cdot)) \|_{L_2(P)} \right) \]
\[ \leq p \cdot \| \hat{M} - M(s, w, \theta_0^{\text{new}}) \|_{L_2(P)} + p \cdot \| M(s, w, \theta_0^{\text{new}})(\hat{\eta}(\cdot) - G(s)(\cdot)) \|_{L_2(P)} \]
\[ \leq p \cdot O_P(\| \hat{w}(\cdot) - w(\cdot) \|_{L_2(P)} + R_m(|I|) + \mathcal{R}_r(|I|) + |I|^{-1/2}), \]

which completes the proof of Proposition 3.17

\[ \square \]

C.4 Proof of Proposition 3.18

Proof of Proposition 3.18 Firstly, we write \( M = -\mathcal{E}(w(Z)\hat{s}(D_i, \theta_0^{\text{new}})))^{-1} \), so that \( \psi(d) = Ms(d, \theta_0^{\text{new}}) \). Following the same arguments as in the proof of Proposition 3.17, we have \( \hat{M} = M + o_P(1) \) under the diminishing rate of \( \mathcal{R}_m(|I|) \to 0 \) as \( |I| \to \infty \). By the regularity conditions, we have \( \| \hat{\theta} - \theta_0^{\text{new}} \|_2 = o_P(1) \).

Writing \( \Delta \psi_i = \psi_i - \psi(D_i) \), we have
\[ \frac{1}{|I_3|} \sum_{i \in I_3} \hat{\Delta} \psi_i^2 = \frac{1}{|I_3|} \sum_{i \in I_3} (\hat{M}s(D_i, \hat{\theta}) - Ms(D_i, \theta_0^{\text{new}}))^2 \]
\[ \leq \frac{2}{|I_3|} \sum_{i \in I_3} (\hat{M}s(D_i, \hat{\theta}) - Ms(D_i, \theta_0^{\text{new}}))^2 + \frac{2}{|I_3|} \sum_{i \in I_3} (Ms(D_i, \theta_0^{\text{new}}) - Ms(D_i, \theta_0^{\text{new}}))^2. \]

Since \( \hat{\theta} \) is independent of \( I_3 \), we know
\[ \mathbb{E} \left[ \frac{1}{|I_3|} \sum_{i \in I_3} (s(D_i, \hat{\theta}) - s(D_i, \theta_0^{\text{new}}))^2 \mid I_1 \cup I_2 \right] \]
\[ = \| s(\cdot, \hat{\theta}) - s(\cdot, \theta_0^{\text{new}}) \|_{L_2(P)}^2 = O(\| \hat{\theta} - \theta_0^{\text{new}} \|_2) = o_P(1). \]

Hence Lemma D.4 yields
\[ \frac{2}{|I_3|} \sum_{i \in I_3} (\hat{M}s(D_i, \hat{\theta}) - Ms(D_i, \theta_0^{\text{new}}))^2 = 2\hat{M}^2 \cdot \frac{1}{|I_3|} \sum_{i \in I_3} (s(D_i, \hat{\theta}) - s(D_i, \theta_0^{\text{new}}))^2 = o_P(1). \]

Also, since \( \hat{M} = M = o_P(1) \), we have
\[ 2(M - \hat{M})^2 \cdot \frac{1}{|I_3|} \sum_{i \in I_3} (s(D_i, \theta_0^{\text{new}}) - s(D_i, \theta_0^{\text{new}}))^2 = o_P(1), \]

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which further leads to \( \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 \Delta \psi_i^2 = o_P(1) \) since \( \|w(\cdot)\|_\infty < \infty \). On the other hand, by the rate conditions and the convergence result of \( \hat{\eta} \) in Proposition 3.17, we know that \( \|\hat{\eta}(\cdot) - \eta(\cdot)\|_{L_2(p)} = o_P(1) \). Since \( I_3 \) is independent of \( \hat{\eta} \), writing \( \Delta \eta_i = \hat{\eta}_i - \eta(Z_i) \),

\[
\mathbb{E} \left[ \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 \Delta \eta_i^2 \right] \leq \|w(\cdot)\|_\infty \cdot \|\hat{\eta}(\cdot) - \eta(\cdot)\|_{L_2(p)}^2 = o_P(1).
\]

Invoking Lemma D.4 yields \( \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 \Delta \eta_i^2 = o_P(1) \). Therefore,

\[
\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\hat{\psi}_i - \hat{\eta}_i)^2 - \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\psi(D_i) - \eta(Z_i))^2
\leq \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\Delta \psi_i - \Delta \eta_i)^2
\]

\[
+ 2 \sqrt{\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\psi(D_i) - \eta(Z_i))^2} \cdot \sqrt{\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\Delta \psi_i - \Delta \eta_i)^2 = o_P(1)}.
\]

Similar arguments also yield

\[
\frac{1}{|I_3|} \sum_{i \in I_3} (\hat{\psi}_i - \hat{\eta}_i)^2 = \frac{1}{|I_3|} \sum_{i \in I_3} (\psi(D_i) - \eta(Z_i))^2 + o_P(1).
\]

Combining the above two results, we have

\[
\hat{\sigma}_{\text{shift}}^2 = \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\hat{\psi}_i - \hat{\eta}_i)^2 + \sup_z |\hat{w}(z) - w(z)|^2 \cdot \frac{1}{|I_3|} \sum_{i \in I_3} (\hat{\psi}_i - \hat{\eta}_i)^2
\]

\[
= \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\psi(D_i) - \eta(Z_i))^2 + o_P(1) = \sigma_{\text{shift}}^2 + o_P(1),
\]

which completes the proof. \( \square \)

## D Auxiliary Results

In this section, we provide auxiliary technical results for the proofs in preceding sections.

### D.1 Auxiliary results for conditional laws

**Lemma D.1.** Let \( g(\cdot) \) be a function such that \( \mathbb{E}[|g(X_i)|^4] < \infty \), where \( \{(X_i, Z_i)\}_{i=1}^n \) are i.i.d. data. Define the filtration \( \mathcal{F}_n = \sigma(\{Z_i\}_{i=1}^n) \). Then for any \( x \in \mathbb{R} \), it holds that

\[
P \left( \frac{1}{\sqrt{n}} \sum_{i=1}^n (g(X_i) - \mathbb{E}[g(X_i) | Z_i]) \leq x \ \big| \ \mathcal{F}_n \right) \leq \Phi(x/\sigma),
\]

where \( \Phi \) is the cumulative distribution function of standard normal distribution, and

\[
\sigma^2 = \mathbb{E} \left[ (g(X_i) - \mathbb{E}[g(X_i) | Z_i])^2 \right].
\]

Moreover, for any filtration \( \mathcal{G}_n \subset \mathcal{F}_n \), we also have

\[
P \left( \frac{1}{\sqrt{n}} \sum_{i=1}^n (g(X_i) - \mathbb{E}[g(X_i) | Z_i]) \leq x \ \big| \ \mathcal{G}_n \right) \leq \Phi(x/\sigma),
\]

converges almost surely to \( \Phi(x/\sigma) \).
Proof of Lemma D.1. Let $\mathcal{L}_n$ denote the conditional law of $\frac{1}{\sqrt{n}} \sum_{i=1}^n \zeta_i$ given $\mathcal{F}_n$, where $\zeta_i := g(X_i) - \mathbb{E}[g(X_i) | Z_i]$. Since the data are i.i.d., $\{X_i\}_{i=1}^n$ are mutually independent conditional on $\mathcal{F}_n = \sigma(\{Z_i\}_{i=1}^n)$. Thus the characteristic function of $\mathcal{L}_n$ is

$$\varphi_{\mathcal{L}_n}(t) = \mathbb{E}[e^{it \frac{1}{\sqrt{n}} \sum_{i=1}^n \zeta_i} | \mathcal{F}_n] = \prod_{j=1}^n \mathbb{E}[e^{it \zeta_j} | \mathcal{F}_n], \quad \text{for all } t \in \mathbb{R}.$$  

By Lemma D.2, we know that the conditional law $\mathcal{L}_n$ converges almost surely to $N(0, \sigma^2)$, which completes the proof of equation (D.1). Since the conditional probabilities are bounded within $[0, 1]$, equation (D.2) follows from dominated convergence theorem. Therefore we conclude the proof of Lemma D.1.

Lemma D.2. Under the same assumption as Lemma D.1, we have $\varphi_{\mathcal{L}_n}(t)$ converges almost surely to $\exp\left(-t^2\sigma^2/2\right)$, for all $t \in \mathbb{R}$, where $\sigma^2$ is defined in Lemma D.1.

Proof of Lemma D.2. We now focus on $z_{n,j} = \mathbb{E}[e^{it \zeta_j} | Z_j] - 1$. By the tower property of conditional expectations, we have $\mathbb{E}[\zeta_j | Z_j] = 0$ for all $j \in [n]$. Therefore

$$z_{n,j} = \frac{-t^2}{2n} \mathbb{E}[\zeta_j^2 | Z_j] + R_{n,j}, \quad \text{where } R_{n,j} = \mathbb{E}\left[e^{it \zeta_j} - 1 - \frac{it}{\sqrt{n}} \zeta_j + \frac{t^2}{2n} \zeta_j^2 | Z_j\right].$$

Since the random variables $\{\mathbb{E}[\zeta_j^2 | Z_j]\}_{j=1}^n$ are i.i.d., by the law of large numbers, it holds that

$$\sum_{n=1}^{\infty} \left(-\frac{t^2}{2n} \mathbb{E}[\zeta_j^2 | Z_j]\right) \overset{a.s.}{\to} -\frac{t^2}{2} \mathbb{E}[\zeta_j^2] = -\frac{t^2}{2} \sigma^2,$$

where $\sigma^2$ is defined in Lemma D.1. Note that $|e^{it} - 1 - it + t^2/2| \leq \min\{|t|^2, |t|^3/6\}$ for any $t \in \mathbb{R}$, thus

$$|R_{n,j}| = \left|\mathbb{E}\left[e^{it \zeta_j} - 1 - \frac{it}{\sqrt{n}} \zeta_j + \frac{t^2}{2n} \zeta_j^2 | Z_j\right]\right| \leq \mathbb{E}\left[\min\left\{\frac{t^2}{2n} \zeta_j^2, \frac{t^3}{6n^{3/2}} |\zeta_j|^3\right\} | Z_j\right] \leq \frac{t^3}{6n^{3/2}} \mathbb{E}[|\zeta_j|^3 | Z_j].$$

Under the finite fourth-moment condition, by the law of large numbers we have

$$\frac{1}{n} \sum_{j=1}^{n} \mathbb{E}[|\zeta_j|^3 | Z_j] \overset{a.s.}{\to} \mathbb{E}[|\zeta_j|^3] < \infty,$$

hence $\sum_{j=1}^{n} |R_{n,j}|$ converges to zero almost surely, which leads to $\sum_{j=1}^{n} z_{n,j} \to -\frac{t^2}{2} \sigma^2$ almost surely. We now show $\sum_{j=1}^{n} |z_{n,j}|^2 \overset{a.s.}{\to} 0$. Simply note that $(x + y)^2 \leq 2x^2 + 2y^2$, so

$$\sum_{j=1}^{n} |z_{n,j}|^2 \leq \frac{t^4}{2n^2} \sum_{i=1}^{n} (\mathbb{E}[\zeta_j^4 | Z_j]) + 2 \sum_{j=1}^{n} R_{n,j}^2 \leq \frac{t^4}{2n^2} \sum_{j=1}^{n} \mathbb{E}[\zeta_j^4 | Z_j] + 2 \sum_{j=1}^{n} R_{n,j}^2 \quad (D.3)$$

which converges to zero almost surely, where the second inequality follows from Jensen’s inequality. The a.s. convergence follows from the strong law of large numbers under the moment condition in Assumption 3.3, as well as the fact that $\sum_{j=1}^{n} R_{n,j}^2 \leq \sum_{j=1}^{n} |R_{n,j}| \cdot \max_{j} |R_{n,j}| \leq (\sum_{j=1}^{n} |R_{n,j}|)^2$, which converges to zero almost surely. Combining equation (D.3) and Lemma D.3, we conclude the proof of Lemma D.2.

We quote the following well-known complex analysis result without proof.

Lemma D.3. Suppose $z_{n,k} \in \mathbb{C}$ are such that $z_n = \sum_{k=1}^{n} z_{n,k} \to z_{\infty}$ and $\eta_n = \sum_{k=1}^{n} |z_{n,k}|^2 \to 0$ as $n \to \infty$. Then $\varphi_n \prod_{k=1}^{n} (1 + z_{n,k}) \to \exp(z_{\infty})$ as $n \to \infty$.  

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D.2 Auxiliary technical lemmas

Lemma D.4. Suppose a sequence of random variables $E_n$ satisfies $E_n = o_P(1)$ as $n \to \infty$. Then for any $\sigma$-algebras $F_n$ and any constant $\epsilon > 0$, it holds that $P(|E_n| > \epsilon | F_n) = o_P(1)$.

Proof of Lemma D.4. Note that $E[ P(|E_n| > \epsilon | F_n) ] = P(|E_n| > \epsilon)$. Thus for any $\delta > 0$, we have

$$P\left( P\left( |E_n| > \epsilon | F_n \right) > \delta \right) \leq \frac{1}{\delta} P(|E_n| > \epsilon) \to 0.$$

Therefore we have $P(|E_n| > \epsilon | F_n) = o_P(1)$ and completes the proof of Lemma D.4. □

Lemma D.5. Let $F_n$ be a sequence of $\sigma$-algebra, and let $A_n \geq 0$ be a sequence of nonnegative random variables. If $E[A_n | F_n] = o_P(1)$, then $A_n = o_P(1)$.

Proof of Lemma D.5. By Markov’s inequality, for any $\epsilon > 0$, we have

$$B_n := P(A_n > \epsilon | F_n) \leq \frac{E[A_n | F_n]}{\epsilon} = o_P(1),$$

and $B_n \in [0, 1]$ are bounded random variables. For any subsequence $\{n_k\}_{k \geq 1}$ of $\mathbb{N}$, since $B_{n_k} \overset{P}{\to} 0$, there exists a subsequence $\{n_{k_i}\}_{i \geq 1} \subset \{n_k\}_{k \geq 1}$ such that $B_{n_{k_i}} \overset{a.s.}{\to} 0$ as $i \to \infty$. By the dominated convergence theorem, we have $E[B_{n_{k_i}}] \to 0$, or equivalently, $P(A_{n_{k_i}} > \epsilon) \to 0$. Therefore, for any subsequence $\{n_k\}_{k \geq 1}$ of $\mathbb{N}$, there exists a subsequence $\{n_{k_i}\}_{i \geq 1} \subset \{n_k\}_{k \geq 1}$ such that $A_{n_{k_i}} \overset{P}{\to} 0$ as $i \to \infty$. By the arbitrariness of $\{n_k\}_{k \geq 1}$, we know $A_n \overset{P}{\to} 0$ as $n \to \infty$, which completes the proof. □