Attribute-adaptive statistical inference for finite populations under distribution shift

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Abstract

Parameters of sub-populations can be more relevant than super-population ones. For example, a healthcare provider might be interested in the effect of a treatment plan on a subset of their patients; a video subscription service might be interested in the satisfaction of its current customers; or policymakers might care about the impact of a policy in a state with a given population. In these cases, one is interested in a finite population, as opposed to an infinite super-population. Such finite population can be characterized by fixing some attributes that are intrinsic to them, leaving unexplained variation like measurement error as random. More generally, inference for a population with fixed attributes can be modeled as inferring parameters of a conditional distribution given these attributes. It is desirable that confidence intervals are conditionally valid for the realized population, instead of marginalizing over many draws of such populations.

We provide a statistical inference framework for parameters of populations with fixed attributes. By leveraging the attribute information, we derive estimators and confidence intervals that are closely related to a specific finite population. When the data is from the population of interest, our confidence intervals attain asymptotic conditional validity given the attributes, and are typically shorter than those for super-population inference. In addition, we develop procedures to infer parameters of new populations with differing covariate distributions; the confidence intervals are also conditionally valid under mild conditions. Our methods extend to situations where the fixed information has weaker structure or is only partially observed. We demonstrate the validity and applicability of our methods on simulated and real-world data.

1 Introduction

Statistical inference targets populations of various resolutions, from super-population to individuals. In causal inference for example, traditionally, average treatment effects describe properties of a hypothetical super-population. Driven by the need of individualization in domains like precision medicine (Kosorok and Laber, 2019), there is a surge of interest in conditional average treatment effects to provide unit-specific information that varies with individual characteristics.

This paper studies a situation that lies between unit-specific and super-population inference. For instance, to decide whether to deploy a novel treatment plan, it is sensible for a healthcare provider to focus on its own patients. The population of interest might be best described as a finite set of units, as opposed to one particular unit or a hypothetical super-population. One could imagine these patients as drawn from a super-population, a reasonable characterization if no other knowledge is available. However, if some information such as their demographics is known, averaging over many draws of such information – a super-population perspective – might become inappropriate; instead, one should view the demographic information as fixed or conditioned on the realized values to describe this specific population.

To model this scenario, we allow practitioners to choose certain information about these units as fixed. Thus, the population follows the conditional distribution given such information. Our estimand is then a parameter of the conditional distribution, termed conditional parameter. It is argued in Abadie et al. (2014)
that in some cases conditional parameters can be more relevant than super-population parameters. Let us continue with the healthcare example and consider two settings where conditional parameters are of interest.

The first setting is described in Abadie et al. (2014) as “the sample is from the population of interest”. Suppose the healthcare provider is interested in its patients’ health conditions after deploying the treatment plan on them, for which a measurement has been collected. One could view some attributes that are intrinsic to these patients as fixed; depending on the application, the attributes may or may not be fully observed. In this way, the data are from the conditional distribution given these attributes, while other unexplained variation such as measurement error remains. Conditioning on relevant information provides a more precise characterization of these patients than the super-population: intuitively, the conditional distribution informs what would happen if the patients’ health measurements are drawn anew while holding their attributes fixed, as opposed to new draws of both the health measurements and the attributes.

The upper panel of Figure 1 visualizes the super-population (blue) versus a realized sub-population (red), also showing other potential sub-populations (grey). The super-population characterizes the overall distribution. However, once certain attributes are fixed, the finite population is actually represented by the red-shaded conditional distribution; in contrast, the super-population marginalizes over all potential sub-populations that may not be that relevant for the current one. The task is then to infer parameters of this conditional distribution. We call this setting inference for the population at hand. In this case, quantifying the uncertainty for the (red) sub-population leads to distinct confidence intervals than super-population inference.

Another setting that is new to the literature is where the sub-population of interest differs from the sample. After collecting data from the first batch of patients, the healthcare provider might also like to predict the effect of the new treatment plan on a set of new patients before deploying it on them, i.e., without observing their responses. Again, the health conditions of this specific group of patients are relevant for this decision; we suppose the healthcare provider has observed a few attributes of these new patients. The unknown health condition of these patients is then from the conditional distribution given the attributes. Parameters of this conditional distribution could also be interpreted as the expected behavior of this fixed population based on the available information. In Fig. 1, the green curve on the lower panel represents the super-population the new units are from. With newly observed attributes, the population of interest is the purple-shaded sub-population. The goal is thus to transfer the knowledge to the new population, or equivalently, to infer parameters of the new conditional distribution. We call this setting transductive inference.

Targeting specific sub-populations leads to estimators that differ from super-population ones in transductive inference. In the following example, we give a sneak peek on the performance of a procedure that will be formally developed in Section 3.2.

**Example 1.1** (Super-population versus targeted sub-population estimation). This example is motivated by Arceneaux et al. (2006) who studied the effect of get-out-the-vote mails on voter turnout. We consider a
scenario where a local politician is interested in using such mails in a particular region. Thus, in this setting the target is the average treatment effect in the sub-population, conditionally on observed attributes. The outcomes are drawn according to (Nie and Wager, 2021, Section 4.1), with the causal effect shifted upwards by .3 to bring the simulation in line with the real-world outcomes. We repeatedly generate training data from the super-population and covariates of a small disjoint target population \((n = 100)\), and compute covariate-adjusted difference-in-means estimators, either for the average treatment effect (super-population) or the conditional treatment effect (sub-population). We depict the results over 1000 runs in Figure 2; each point in the plot stands for one of the potential sub-populations in Fig. 1. The transductive estimator uses covariates to target the sub-population and thus achieves much higher accuracy for estimating the conditional parameter. Such targeted information, equipped with its reliable coverage guarantee we are to introduce, could support decision-making for specific sub-populations.

Fixing certain attributes motivates conditional inference guarantee. A marginally valid confidence interval covers the target with a prescribed probability, averaged across many draws of the attributes. However, ideally confidence intervals should be valid for the specific population we are interested in, that means, conditional on the attributes. In an illustrative example in Section A of the supplementary material, we find that super-population inference lacks conditional validity even without transfer; in contrast, our inference is conditionally valid for the specific population of interest. For example, our method builds a confidence interval around each conditional transductive estimator in Fig. 2 that is valid for the sub-population.

Our contribution. In this paper, we provide a framework for statistical inference about populations with fixed attributes. Distinct from conventional super-population inference, our estimand targets a specific sub-population. We develop a set of tools to construct confidence intervals that attain a new type of conditional inference guarantee in the two inferential scenarios.

- In the first setup which is close to that of Abadie et al. (2014); Buja et al. (2016, 2019), we provide conditionally valid inference for a large class of estimands, that means, inference that is valid given the attributes, instead of marginalizing over new draws. Our framework also allows for arbitrarily fixed attributes or fixed unobserved attributes.

- In the new transductive inference setting, we extend our tools to construct conditionally valid confidence intervals for parameters of new populations. Notably, we allow the new attributes to follow a different distribution; when the distributional shift is unknown, we achieve conditional validity even in cases where nuisance components are estimated with slow rates.

In both cases, compared to super-population inference, our framework leads to shorter confidence intervals and more reliable inference with conditional coverage. To our knowledge, this is the first work to deal with
both conditional inference and distribution shift in a general setting (see Section 2.3 for a more extensive discussion on related work). To address all these problems in a single framework, throughout the main text, we use a sampling-based justification by assuming the attributes are i.i.d. drawn and then conditioned on.

We provide two R-packages at https://github.com/ying531. The procedures allow transporting any generalized linear model to a new (conditional) distribution, with (conditionally) valid confidence intervals. The most basic use-case is

```r
fit = lm(Y ~ ., data = data) // conditional inference
cond_inf(fit)
// transductive inference
transfer(fit, newdata = Z.new)
```

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 Sections 3.2 and 3.3, we develop conditionally valid inference for a new population potentially under unknown covariate shift. In Sections 4 and 5, We demonstrate the performance of our methods on simulated and real-world data.

2 Inferential targets

2.1 Conditional parameters

We now formally define the conditional parameter as our estimand, which characterizes a conditional distribution. Conditional parameters have a long history in statistics and econometrics; we give an overview of the literature in Section 2.3.

Let us begin with a recap on classical settings (van der Vaart, 1998; Tsiatis, 2007). For a super-population $P$ from which a random variable $D \in \mathbb{D}$ is drawn, an unknown parameter $\theta_0 \in \Theta \subset \mathbb{R}^p$ of dimension $p$ is defined as a solution to

$$E[s(D, \theta)] = 0 \quad (1)$$

for some score function $s: \mathbb{D} \times \Theta \to \mathbb{R}^p$, where $E$ denotes the expectation under $P$. Here and in the following, we adopt the common assumption in the literature (van der Vaart, 1998) that the solution to equation (1) is unique. Therefore, $\theta_0$ is a deterministic quantity that characterizes the super-population $P$; inference for $\theta_0$ 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 Abadie et al. (2014); Buja et al. (2016, 2019), we suppose $(D_1, Z_1), \ldots, (D_n, Z_n)$ are i.i.d. from an unknown distribution $P$, where $D_i \in \mathbb{D}$ are the full data, and $Z_i \in \mathbb{Z}$ are the attributes we condition on. Given the attributes $Z_n = (Z_1, \ldots, Z_n)$, the data $D_n = (D_1, \ldots, D_n)$ are from the conditional distribution given $Z_n$. The i.i.d. assumption on the attributes is not essential for conditional inference and could be relaxed later on; for now, we keep it for consistency across all scenarios. We define the $Z_n$-conditional parameter $\theta_n^{\text{cond}} = \theta_n^{\text{cond}}(Z_n)$ as the solution to

$$\sum_{i=1}^n E[s(D_i, \theta) \mid Z_i] = 0, \quad (2)$$

which is assumed to be unique. Note that $\theta_n^{\text{cond}}$ depends on $Z_n$. From a marginal perspective, $\theta_n^{\text{cond}}$ is random and varies with the sample size. $\theta_n^{\text{cond}}$ characterizes the distribution of $D_n$ given that $Z_n$ are fixed at their realized values, as opposed to $\theta_0$ that characterizes the unconditional distribution (super-population). Conditional parameter can also be seen as a generalization of the super-population parameter in the sense that $\theta_0 = \theta_n^{\text{cond}}(\emptyset)$. 

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well-specified model, we would have $Z$ can be viewed as the regression coefficient for a set of subjects with fixed regressors, averaging over measurements and emissions for the population reacts to the treatment. Consider random variables $(T,X,Y)$ react differently to treatments. In this case, conditional inference can be used to understand how a specific subject is sampled from the conditional distribution given $(Z_i)$. If $Z_i = X_i$, the parameter $θ^n_{cond}$ 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 $Y_i = X_i^\top \theta + e_i$ for $E[e_i | X_i] = 0$, i.e., well-specified model, we would have $θ^n_{cond} = \theta_0$. In practice, however, this is usually not held, and the conditional parameter might vary with the realization of $X_i$. More generally, $Z$ might also be a variable outside 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. Conditioning on $Z$ can change the parameters if it is correlated with both the predictors and the residuals.

Example 2.3 (Finite-sample causal inference). Finite-sample treatment effects are a common target of causal inference (Imbens and Rubin, 2015). 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 subject is sampled from a superpopulation $\mathbb{P}$, 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 (Imbens and Rubin, 2015), for each unit we observe $D = (T, X, Y)$, where $Y = TY(1) + (1 - T)Y(0)$. The (super-population) average treatment effect $θ_0 = E[Y(1) - Y(0)]$ is the solution to equation (1) where $s(D, θ) = Y(1) - Y(0) - θ$. 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 $θ^n_{cond} = \frac{1}{n} \sum_{i=1}^{n} (Y_i(1) - Y_i(0))$, characterizes the population where potential outcomes of the subjects are fixed. This is commonly the target in finite-sample causal inference (Splawa-Neyman et al., 1990; Hinkelmann and Kempthorne, 1994; Freedman et al., 2008; Rosenbaum, 2010; Imbens and Rubin, 2015). 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 $θ^n_{cond} = \frac{1}{n} \sum_{i=1}^{n} E[Y_i(1) - Y_i(0) | X_i]$ which could also be interpreted as the best prediction for the treatment effects of the population given $\{X_i\}_n^{i=1}$. Here $τ(x) = E[Y(1) - Y(0) | X = x]$ is the conditional average treatment effect (CATE) and indicates treatment effect heterogeneity on the covariate level. Finally, conditioning on the empty set, we obtain $θ_0$ that represents the super-population the units are sampled from.

2.2 Conditional inference

Conditional parameters can describe a population at hand, or a new population with some observed attributes. As we focus on a specific sub-population, it is desirable that confidence intervals are conditionally valid for the specific sub-population, instead of marginalizing over all potential sub-populations. We now formalize these two settings and preview the conditional inference guarantees we are to provide.
Conditional inference for the population at hand. As discussed earlier, the healthcare provider might be interested in the health of its own patients, holding some intrinsic information as fixed and averaging over other variation. When inferring the population at hand, we observe i.i.d. data \( \{(D_i, Z_i)\}_{i=1}^n \) from a super-population \( \mathbb{P} \), where \( Z_i = \{Z_i^j\}_{j=1}^m \) are the conditioning variables (e.g., the attributes of the patients that are viewed as fixed), and \( D_i = \{D_i^j\}_{j=1}^m \) are the observations (e.g., the observed health conditions). The conditional parameter \( \hat{\theta}_n^{\text{cond}} = \hat{\theta}_n^{\text{cond}}(Z_n) \) defined in (2) provides a more precise characterization for the current patients than the super-population quantity; the latter instead characterizes the overall health of an hypothetical infinite patient base. In Section 3.1, we construct a confidence interval \( \hat{C}(D_n, Z_n) \) obeying

\[
\mathbb{P}\left(\hat{\theta}_n^{\text{cond}} \in \hat{C}(D_n, Z_n) \mid Z_n\right) \rightarrow 1 - \alpha \tag{3}
\]

in probability as \( n \rightarrow \infty \). Put another way, our inference on \( \theta_n^{\text{cond}} \) is valid conditional on any realized attributes. In our motivating example, the conditional guarantee (3) means the validity given the current patients; it is in contrast to marginal guarantees where the coverage is valid marginalized over many draws of patients. We also extend conditionally valid inference to situations where \( Z_n \) is fixed at any value without being i.i.d., and where it is more reasonable to condition on some unobserved attributes \( X_n \).

Transductive inference for a new population. The healthcare provider might also be interested in estimating the health condition of another subgroup of its patients, based on measurements of the first subgroup of patients. We formalize this problem as follows.

We denote the target data as \( \{(D_i^\text{new}, Z_i^\text{new})\}_{i=1}^m \) from a super-population \( \mathbb{Q} \), where \( Z_i^\text{new} = \{Z_i^\text{new}^j\}_{j=1}^m \) are the new attributes we condition on, and \( D_i^\text{new} = \{D_i^\text{new}^j\}_{j=1}^m \) are the unobserved data (e.g., the health measurements of the target units). The source units \( \{(D_i, Z_i)\}_{i=1}^n \) are i.i.d. from a super-population \( \mathbb{P} \) (e.g., the health measurements and attributes of the source units). For transductive inference, we always impose the super-population assumption on the attributes to ensure sufficient structure. The quantity of interest is \( \theta_m^{\text{cond,new}} = \theta_m^{\text{cond}}(Z_m^\text{new}) \) as a functional of the conditional distribution of \( D_m^\text{new} \) given \( Z_m^\text{new} \). In Sections 3.2 and 3.3, we construct a confidence interval \( \hat{C}(D_n, Z_n, Z_m^\text{new}) \) that obeys

\[
\mathbb{P}\left(\theta_m^{\text{cond,new}} \in \hat{C}(D_n, Z_n, Z_m^\text{new}) \mid Z_m^\text{new}, Z_n\right) \rightarrow 1 - \alpha
\]

in probability as \( m, n \rightarrow \infty \). In particular, we allow \( \mathbb{Q} \) to admit a covariate shift \( w(z) = \frac{d\mathbb{Q}}{d\mathbb{P}}(d, z) \) from the fully observed data, and the conditional distribution of \( D \) given \( Z \) is invariant. When \( w(z) \) is unknown and needs to be estimated from data, our procedure yields valid inference even if nuisance components are estimated at slow 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, the conditional parameters, under similar assumptions yet with different guarantees. For example, Abadie et al. (2014) quantify the asymptotic deviation of estimators from conditional parameters for maximum likelihood and method of moment estimators; Buja et al. (2016, 2019) argue that models should be seen as approximations. These works define conditional parameters and derive marginally valid asymptotics; they argue to treat the covariates as random and focus on marginal inference. Similar considerations also arise in the econometrics literature (Manski, 1991; Angrist, 1995) that different sources of variation may give different results. We substantially generalize their framework by providing conditionally valid inference and studying transductive inference on new populations.

Asymptotics conditional on covariates. More broadly than the above point, our setting connects to a literature of asymptotics conditional on covariates. The major difference is that we study a new transductive inference setting. Among these works, in fixed-design setting where the covariates are arbitrary and fixed, some early works (White, 1980; Goldberger, 1991) study inference under well-specified models, and Fahrmeir (1990); Kuchibhotla et al. (2018); Abadie et al. (2020) study misspecified models. Among works that operate
under i.i.d. attributes, the closest to ours is Andrews et al. (2019), which derives conditionally valid confidence intervals for linear moment models. In our work, the i.i.d. assumption on attributes is not essential for conditional inference for the population at hand; however, in our setting this assumption allows us to consistently estimate the asymptotic variance, which is shown to be impossible otherwise when attributes are arbitrarily fixed (White, 1980; Kuchibhotla et al., 2018). The i.i.d. assumption also guarantees that the proposed conditional confidence intervals are shorter than super-population confidence intervals. In the new transductive inference problem, the i.i.d. assumption on the attributes (while allowing for distributional shift) ensures a shared structure between the original and the new populations. Our transductive inference results potentially also generalize to fixed design, but for readability we will state our results under an i.i.d. assumption.

Finite-sample causal inference. In finite-sample causal inference (Splawa-Neyman et al., 1990; Hinkelmann and Kempthorne, 1994; Freedman et al., 2008; Rosenbaum, 2010; Imbens and Rubin, 2015), it is common to condition on potential outcomes and derive bounds for the asymptotic variance of estimators of causal effects. Inference conditional on potential outcomes is similar to our goal of population at hand by conditioning on unobserved variables. Finite-sample causal inference usually does not rely on super-population assumptions, which is close to our fixed-design extension. Furthermore, in this literature, conditional inference results are usually derived on a case-by-case basis, while we study a general class of estimators.

Distribution shift and missing data. Our transductive inference is connected to a vast literature of inference under covariate shift, an important condition for transferring knowledge to new populations. In a general spirit, our method is similar to AIPW estimators (Robins et al., 1994). Rotnitzky et al. (2012) and Liu et al. (2020) also study inference under unknown covariate shift with doubly-robust property. The distinction from them is that we provide conditional validity for conditional parameters instead of marginal validity for super-population quantities, leading to new targets and different variances. The estimands we study are also more general than theirs.

Classical conditional inference. A classical line of work (Hinkley, 1980; Cox and Reid, 1987) tackles inference problems by conditioning on ancillary statistics or estimators of nuisance parameters (see e.g., a review in Casella (1992)), stemming from the ideas of Fisher (1935a,b). One strand uses conditional inference to reduce the effect of nuisance parameters such as Cox and Reid (1987). We condition on attributes of the data instead of summary statistics, leading to different parameters, different interpretation and different inferential guarantees. Another strand uses conditioning to induce relevance of probabilistic analysis to the data at hand, including permutation tests (Fisher et al., 1937; Ernst et al., 2004; Edgington and Onghena, 2007) and tests for categorical data (Agresti, 2003). Conditioning on available information in our framework shares the spirits of conducting inference that is closely related to the data at hand. However, our basis of inference is quite different: we condition on sets of variables and rely on the asymptotic behavior of general semi-parametric and parametric estimators, while these works often rely on exchangeability to derive the conditional distribution of test statistics given the observations.

Mixed effect models and generalizability theory. Our approach obtains variance decompositions, which is similar to mixed effect models and generalizability theory (Pinheiro and Bates, 2006; Brennan, 2001). However, compared to this literature, we do not make restrictive modelling assumptions about the relationship between variables or the error distribution. Our conditional inference procedures apply to a large variety of parametric and semi-parametric estimators.

3 Conditional inference

3.1 Conditional inference for the population at hand

Recall the motivating example where the healthcare provider is interested in a conditional parameter that is specific to its current patients. In this part, we construct confidence interval 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). For simplicity of illustration, we present our theoretical results for \( p = 1 \) throughout the rest of the paper, while all of them can be generalized to fixed-\( p \) settings with variances replaced by covariance matrices.

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 asymptotics, see for example van der Vaart (1998) or Tsiatis (2007). Under regularity conditions, the conditional parameter (2) satisfies

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

We establish sufficient conditions for equations (4) and (5) to hold when \( (D_i, Z_i) \) are i.i.d. from some super-population, whose proof is deferred to Section E.1 of the supplementary material.

**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 (1) and \( \hat{\theta}_{n, \text{cond}} \) is the unique solution to (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 \( \dot{s}(D, \theta) = \nabla_{\theta} s(D, \theta) \in \mathbb{R}^{p \times p} \) the derivative matrix of \( s(D, \theta) \) at \( \theta \) and \( \ddot{s}(D, \theta) = \nabla_{\theta} \dot{s}(D, \theta) \) the derivative tensor of \( \dot{s}(D, \theta) \) at \( \theta \). Additionally, \( \dot{t}(Z, \theta) = \nabla_{\theta} t(Z, \theta) = \mathbb{E}[\dot{s}(D, \theta) \mid Z] \) and \( \ddot{t}(Z, \theta) = \nabla_{\theta} \dot{t}(Z, \theta) = \mathbb{E}[\ddot{s}(D, \theta) \mid Z] \). (iv) For each \( j, k \), \( \|\ddot{s}_{jk}(D, \theta)\| = \|\partial s(D, \theta) / \partial \theta_j \partial \theta_k\| \leq g(D) \) for some \( g \) with \( \mathbb{E}[g(D)] < \infty \). Also, the matrix \( \mathbb{E}[\ddot{s}(D, \theta_0)] \) is assumed to be non-singular. Then equations (4) and (5) hold with influence function

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

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 (van der Vaart, 1998), and has been informally stated in Buja et al. (2016). We impose the linear expansion as the following assumption for the convenience of reference later.

**Assumption 3.2.** \( \hat{\theta}_n \) and \( \hat{\theta}_{n, \text{cond}} \) obey equations (4) and (5), respectively.

**Assumption 3.3.** The influence function \( \phi(\cdot) \) defined in (6) satisfies \( \mathbb{E}[\phi(D)^4] < \infty \).

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

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

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

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

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

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 Section F.1 in the supplementary material. The asymptotic conditional validity relies on the convergence of the conditional distribution of \( \sqrt{n}(\hat{\theta}_n - \hat{\theta}_{n, \text{cond}}) \), derived from a conditional central limit theorem (Dedecker and Merlevède, 2003; Grzenda and Zieba, 2008); we include
Lemma I.1 in Section I.1 of the supplement for completeness. As a clarification note, the conditional coverage converges in probability (with respect to the attributes) to the nominal level instead of uniformly over all possible values.

It remains to construct a consistent estimator \( \hat{\sigma}^2 \) for the asymptotic variance (7). In Section B.1 of the supplementary material, we describe a detailed estimation procedure (c.f. Algorithm 3) with consistency guarantees, relying on the formula (6) and nonparametric regression for \( \varphi(Z) = \mathbb{E}[\phi(D) \mid Z] \). Abadie et al. (2014) 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 estimator is consistent under generic consistency conditions on nonparametric regression. This relaxes the technical assumptions and overcomes the computational difficulty of matching in practice.

Many results in the literature are close to Theorem 3.4. Closer to our setting, Abadie et al. (2014) considers a similar estimand and derives a same asymptotic variance. However, these results all provide marginal coverage guarantees, which can be insufficient for reliable inference for a specific population (see the illustrative example in Section A). For the special case of fixed-design OLS, Kuchibhotla et al. (2018) shows it is impossible to estimate the asymptotic variance without any assumptions; instead, our sampling justification allows for consistent estimation of the variance and leads to a feasible general conditional inference recipe.

**Remark 3.5.** Super-population inference carries out a similar protocol with an estimator of the (unconditional) asymptotic variance, usually of the form \( \sigma_0^2 := \text{Var}(\phi(D)) \). The variance (7) for conditional inference is always no greater than \( \sigma_0^2 \), as \( \sigma^2 = \text{Var}(\phi(D)) - \text{Var}(\mathbb{E}[\phi(D) \mid Z]) \leq \text{Var}(\phi(D)) \). Take the least-square parameter as an example. The linear expansion (4) and (5) hold with \( \phi(D) = (\mathbb{E}[XX^\top])^{-1} X^\top(Y - X^\top \theta_0) \in \mathbb{R}^d \). 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., \( \mathbb{E}[\epsilon \mid X] = 0 \) a.s., we have \( \sigma^2 = \sigma_0^2 \) 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 \( X \) (Abadie et al., 2014; Buja et al., 2016, 2019). If \( \mathbb{E}[X\epsilon \mid Z] \) is not a.s. zero, our confidence interval is shorter than that for super-population inference.

We finally note two generalizations of the current framework of conditional inference: non-i.i.d. attributes and conditioning on unobserved variables.

**Remark 3.6 (Non-i.i.d. attributes).** Conditional inference generalizes naturally to fixed attributes \( \{z_i\}_{i=1}^n \) without an i.i.d. structure. In Section C.1 of the supplementary material, we provide a set of results that are parallel to the current subsection, where we make no probabilistic statements on the attributes. In that case, the asymptotic variance \( \sigma_n^2 \) we derive depends on \( \{z_i\}_{i=1}^n \), whose consistent estimation requires certain assumptions. One could also use \( \sigma_n^2 \) instead of \( \sigma^2 \) for i.i.d. attributes to provide a covariate-dependent quantification of uncertainty while maintaining conditional validity; however, the difference between them is negligible. We discuss these issues in details in the supplementary material.

**Remark 3.7 (Conditioning on unobserved variables).** In our motivating example, the practitioner might instead characterize the patients by fixing a hidden intrinsic health \( Y^* \). While this variable is unobserved, we could still conduct \( \{Y^*_i\}_{i=1}^n \)-conditionally valid inference with observed attributes \( \{Z_i\}_{i=1}^n \). The resulting confidence intervals are shorter than super-population inference, yet perhaps unavoidably conservative for conditioning on unobserved variables. We provide formal results and detailed discussion in Section C.2 of the supplementary material.

### 3.2 Transductive inference across data sets from the same super-population

Prepared with the above conditional inference techniques, we now study transductive inference. This tackles situations where a healthcare provider might have deployed a novel treatment plan on a subset of its patients, and would like to infer the effect on the remaining ones. To fix ideas, we first discuss the setting where the units in both populations are drawn from the same super-population. The case with different super-populations is discussed in Section 3.3.

With access to i.i.d. observations \( \{(D_i, Z_i)\}_{i=1}^n \sim \mathbb{P} \), the i.i.d. new units \( \{(D_{\text{new}}, Z_{\text{new}})\}_{m=1}^m \sim \mathbb{P} \) are from the same distribution, where only \( Z_{\text{new}} := \{(Z_{\text{new}}^j)_{j=1}^m\} \) are observed. We are interested in the finite population, which is from a conditional distribution given \( Z_{\text{new}} \). The new conditional parameter \( \theta_m^{\text{cond,new}} := \theta_m^{\text{cond}}(Z_{\text{new}}) \) is the unique solution to \( \sum_{j=1}^m \mathbb{E}[s(D_{\text{new}}^j, \theta) \mid Z_{\text{new}}^j] = 0 \).
We assume an estimator $\hat{\theta}_n$ satisfies (4) (e.g., a $Z$-estimator specified in Proposition 3.1), and similar to (5), $\theta^\text{cond, new}_m$ satisfies the asymptotic linearity $\sqrt{m}(\hat{\theta}^\text{cond, new}_m - \theta_0) = \frac{1}{\sqrt{m}} \sum_{j=1}^{m} \varphi(Z^\text{new}_j) + o_P(1)$ for $\varphi(\cdot) := \mathbb{E}[\varphi(D_i) | Z_i = \cdot]$. We use $\hat{\theta}_n$ as a starting point and add a correction term to account for the fact that we target $\theta^\text{cond, new}_m$. Specifically, we define

$$\hat{\theta}^\text{trans}_{m,n} = \hat{\theta}_n - \frac{1}{n} \sum_{i=1}^{n} \hat{\varphi}(D_i) + \frac{1}{m} \sum_{j=1}^{m} \hat{\varphi}(Z^\text{new}_j),$$

(8)

where with a slight abuse of notation, we let $\hat{\varphi}(\cdot)$ be an estimator for $\varphi(\cdot)$ obtained from cross-fitting (Chernozhukov et al., 2018): we first randomly split $\mathcal{I} = \{1, \ldots, n\}$ into two equal-sized folds $\mathcal{I}_1$ and $\mathcal{I}_2$, then use $\{(D_i, Z_i)\}_{i \in \mathcal{I}_1}$ to obtain an estimator $\hat{\varphi}(k)$ for $\varphi(\cdot)$ for each $k = 1, 2$.\footnote{A special case of Algorithm 5, Appendix B.1 by taking weight $w(z) \equiv 1$ provides a detailed algorithm for estimating $\varphi$.} We define $\hat{\varphi}(Z_i) = \hat{\varphi}(k)(Z_i)$ for $i \notin \mathcal{I}_k$, and $\hat{\varphi}(Z^\text{new}_j) = (\hat{\varphi}(1)(Z^\text{new}_j) + \hat{\varphi}(2)(Z^\text{new}_j))/2$ for all $j$.

To gain some more intuition on the bias correction term, note the asymptotic expansion

$$\hat{\theta}_n - \theta^\text{cond, new}_m = \frac{1}{n} \sum_{i=1}^{n} \varphi(D_i) - \frac{1}{m} \sum_{j=1}^{m} \varphi(Z^\text{new}_j) + o_P(1/\sqrt{n} + 1/\sqrt{m}).$$

Conditioned on $Z_n$ and $Z^\text{new}_m$, the conditional mean of the first term is $\frac{1}{n} \sum_{i=1}^{n} \varphi(Z_i)$, and that of the second is $\frac{1}{m} \sum_{j=1}^{m} \varphi(Z^\text{new}_j)$. These could be viewed as the conditional bias of $\hat{\theta}_n$ for $\theta^\text{cond, new}_m$, and motivates our correction term in (8). Intuitively, correcting for this conditional bias ensures that the resulting $\hat{\theta}^\text{trans}_{m,n}$ centers around $\theta^\text{cond, new}_m$ conditional on $Z^\text{new}_m$ and $Z_n$.

The following result shows asymptotic conditional validity of confidence intervals based on the bias-corrected estimator. Its proof can be found in Section F.2 of the supplementary material.

**Theorem 3.8.** Suppose $\hat{\theta}_n$ satisfies (4), $\sqrt{m}(\theta^\text{cond, new}_m - \theta_0) = \frac{1}{\sqrt{m}} \sum_{j=1}^{m} \varphi(Z^\text{new}_j) + o_P(1)$, and Assumption 3.3 holds. Assume an estimator $\hat{\sigma}^2$ converges in probability to $\sigma^2$ in (7), and $\max_{k=1,2} \|\hat{\varphi}(k)(\cdot) - \varphi(\cdot)\|_{L_2(\mathcal{P})}$ converges in probability to 0. Let $\hat{\theta}^\text{trans}_{m,n}$ be defined in (8). Then

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

converges in probability to $1 - \alpha$ as $n \to \infty$.

From a practical perspective, the above theorem enables targeted inference of sub-population parameters in settings where both groups follow the same distribution. For example, a company can run an experiment on a representative subset of the users, and then generalize the results to the other users based on some covariate information.

Let us discuss some mathematical consequences of this theorem. First, the length of confidence interval for transductive inference is asymptotically the same as conditional inference, without any additional uncertainty from the new population. Thus, roughly speaking, in this setting, we do not pay any price for the parameter transfer in terms of asymptotic variance. Furthermore, such inference guarantee does not require any convergence rate of $\hat{\varphi}(\cdot)$; this is because the attributes in two groups follow the same distribution, hence the cross-fitted $\hat{\varphi}(\cdot)$ is able to accurately cancel out the variation in attributes. Similar ideas apply to settings with covariate shifts, which we study in the following.

### 3.3 Transductive inference with covariate shift

In transductive inference, the first batch of patients and the target population might follow different distributions. In the following, we show that when the two distributions only differ in the covariate distribution, one could still reliably infer parameters for the new population. From now on, we assume the new i.i.d. data $\{(D^\text{new}_j, Z^\text{new}_j)\}_{j=1}^{m} \sim \mathcal{Q}$ with a perhaps unknown covariate shift $w(z) = d\mathcal{Q}/d\mathcal{P}(d,z)$, and assume $w(z) < \infty$ for $\mathcal{P}$-almost all $z$ to ensure transferrability. The identical distribution setting is a special case with $w(z) \equiv 1$. 
Remark 3.9. Covariate shift is a popular setting in machine learning (Quinonero-Candela et al., 2008) and social sciences (Egami and Hartman, 2021; Tipton et al., 2014). In our context, it ensures identifiability of the new conditional parameter. It holds when the two populations are selected only based on the attributes, similar to the unconfoundedness assumption in causal inference (Imbens and Rubin, 2015). In addition, \( w(z) < \infty \) resembles the overlap condition in causal inference, which rules out any sample space that is never observed under \( \mathbb{F} \).

Recall that the new conditional parameter \( \theta_{m}^{\text{cond,new}} \) is the (unique) solution to

\[
\sum_{j=1}^{m} E[s(D_{j}^{new}, \theta) \mid Z_{j}^{new}] = 0,
\]

with the conditional expectation induced by \( \mathbb{Q} \). Given that \( \mathbb{P}_{D \mid Z} = \mathbb{Q}_{D \mid Z} \) are invariant, one might consider solving (9) for \( \theta_{m}^{\text{cond,new}} \) by estimating \( E[s(D, \theta) \mid Z = z] \) for every \( \theta \); however, estimating infinitely many conditional expectations is infeasible in general. In addition, this approach poses challenges to statistical inference since estimation of the conditional expectations might result in slow convergence rates. We will now describe a procedure that estimates the new conditional parameter with \( \sqrt{n} \)-convergence rate even when the distribution shift is unknown.

At a high level, our approach relies on the fact that \( \theta_{m}^{\text{cond,new}} \) is close to \( \theta_{0}^{\text{new}} \), the new super-population parameter, which is defined as the unique solution to

\[
E[w(Z) s(D, \theta)] = E_{\mathbb{Q}}[s(D^{\text{new}}, \theta)] = 0,
\]

where the first expectation is over \( (D, Z) \sim \mathbb{P} \) and the second expectation is over \( D^{\text{new}} \sim \mathbb{Q} \). We will use the asymptotic linearity of \( \theta_{m}^{\text{cond,new}} \) to correct for conditional bias and construct conditionally valid confidence intervals.

Let \( \hat{w}(\cdot) \) be an estimator of \( w(\cdot) \); if \( w \) is known, one can simply set \( \hat{w} = w \). We assume \( \hat{w} \) is obtained from another independent set of data. Alternatively, one could use cross-fitting (Chernozhukov et al., 2018) to yield the same guarantees under similar conditions only using the data at hand. However, since this increases the complexity of notation and exposition, we defer the details to Appendix D.1 when \( w(\cdot) \) is known, and Appendix D.2 when \( w(\cdot) \) is estimated.

To account for the covariate shift, we begin with a reweighted estimator \( \hat{\theta}_{n}^{\text{trans}} \) that is close to \( \theta_{0}^{\text{new}} \), defined as the unique solution to

\[
\sum_{i=1}^{n} \hat{w}(Z_{i}) s(D_{i}, \theta) = 0.
\]

It can be shown that \( \hat{\theta}_{n}^{\text{trans}} \) and \( \theta_{m}^{\text{cond,new}} \) are asymptotically linear around \( \theta_{0}^{\text{new}} \) under mild assumptions. For simplicity of exposition, we will state these as assumptions; in Section E.2 of the supplementary material, we provide justifications under sup-norm consistency of \( \hat{w} \) and mild regularity conditions that are similar to those in Proposition 3.1.

Assumption 3.10. As \( m, n \to \infty \), \( \sup_{z} \left| \hat{w}(z) - w(z) \right| \to 0 \) in probability, and

\[
\sqrt{n}(\hat{\theta}_{n}^{\text{trans}} - \theta_{0}^{\text{new}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \psi(D_{i}) \hat{w}(Z_{i}) + o_{P}(1),
\]

\[
\sqrt{m}(\theta_{m}^{\text{cond,new}} - \theta_{0}^{\text{new}}) = \frac{1}{\sqrt{m}} \sum_{j=1}^{m} \eta(Z_{j}^{\text{new}}) + o_{P}(1),
\]

where \( \psi(d) = -\left( E_{\mathbb{Q}}[s(D^{\text{new}}, \theta_{0}^{\text{new}})] \right)^{-1} s(d, \theta_{0}^{\text{new}}) \), and \( \eta(z) = E[\psi(D_{j}^{\text{new}}) \mid Z_{j}^{\text{new}} = z] \).

Similar to the preceding subsection, we add a bias correction term to \( \hat{\theta}_{n}^{\text{trans}} \) and construct

\[
\hat{\theta}_{m,n}^{\text{trans}} = \hat{\theta}_{n}^{\text{trans}} - \hat{c}_{\text{trans}}, \quad \hat{c}_{\text{trans}} := \frac{1}{n} \sum_{i=1}^{n} \hat{\eta}(Z_{i}) \hat{w}(Z_{i}) - \frac{1}{m} \sum_{j=1}^{m} \hat{\eta}(Z_{j}^{\text{new}}).
\]
Again, for ease of illustration, we assume \( \hat{\eta}(\cdot) \) is an estimator for \( \eta(\cdot) \) obtained elsewhere, such that it is independent of all the data we have. A rigorous treatment without referring to external datasets is in Sections D.1 and D.2 in the supplementary material.

The following theorem established conditional inference guarantee that is robust to estimation error: we obtain \( n^{-1/2} \)-rate inference, as long as the product of the errors in the estimation of \( \hat{\omega} \) and \( \hat{\eta} \) is no greater than \( O(n^{-1/2}) \). As a special case, when \( \omega(\cdot) \) is known, we achieve conditionally valid inference under \( L_2 \)-consistency of \( \hat{\eta} \) similar to Theorem 3.8. In the rigorous treatment with cross-fitting, the same result holds under similar convergence rates of the estimated covariate shift and influence functions; these are shown to be achievable under generic conditions for nonparametric regression, see Proposition B.5 of Section B.2 in the supplementary material. The proof of Theorem 3.11 is in Section F.3 of the supplementary material.

**Theorem 3.11.** Suppose Assumption 3.10 holds, and \( m \geq 4n \epsilon^2 \). Assume \( \| \hat{\eta}(\cdot) - \eta(\cdot) \|_{L_2(\Omega)} = o_P(1), \| w(\cdot) \|_{L_2(\Omega)} = o_P(1), \| \hat{\omega}(\cdot) - \omega(\cdot) \|_{L_2(\Omega)} = o_P(1) \). If an estimator \( \hat{\sigma}^2_{\text{shift}} \) converges in probability to

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

and the variance is induced by \( (D_1, Z_1) \sim \mathbb{P} \), then the random variable

\[
P\left( \hat{\theta}_{m,n}^{\text{trans,new}} \in \left[ \hat{\theta}_{m,n}^{\text{trans}} - \tilde{\sigma}_{\text{shift}} \cdot z_{1-\alpha/2}/\sqrt{n}, \hat{\theta}_{m,n}^{\text{trans}} + \tilde{\sigma}_{\text{shift}} \cdot z_{1-\alpha/2}/\sqrt{n} \right] \mid Z_{m,n}^{\text{new}}, Z_n \right)
\]

converges in probability to \( 1 - \alpha \) as \( n \to \infty \), where \( \hat{\sigma}_{m,n}^{\text{trans}} \) is defined in equation (12).

Theorem 3.11 shows how to conduct estimation and inference of sub-population parameters under distribution shift. For instance, after running an experiment on a set of patients, a hospital could infer its effect on a new set of patients who have a different covariate distribution.

Perhaps surprisingly, even with distribution shift, the asymptotic variance \( \sigma^2_{\text{shift}}/n \) does not depend on \( m \); this is due to the fact that bias correction is statistically an easy task. We pay some price for the transfer to the new super-population since the variance term is weighted with \( w(\cdot) \); however, we do not pay any price in efficiency for the transfer to the new sub-population.

To complete the whole picture, it remains to construct a consistent estimator for \( \sigma^2_{\text{shift}} \) defined in (13). In Section B.1 of the supplementary material, we detail a stand-alone estimation procedure for \( \sigma^2_{\text{shift}} \) (Algorithm 6) that does not rely on external datasets. An intermediate step relies on estimating \( \hat{\eta}(\cdot) \); we offer a detailed procedure (Algorithm 5) in Section B.1 with rigorous guarantee, which is also useful for the cross-fitting approach for transductive inference. Theoretical analysis for these algorithms is in Section B.2 of the supplementary material.

**Remark 3.12** (Transfer to super-populations). We have described how to conduct inference for the sub-population parameter \( \hat{\theta}_{m,n}^{\text{cond,new}} \), the parameter for the new distribution conditionally on \( Z_1^{\text{new}}, \ldots, Z_{m,n}^{\text{new}} \). One might also be interested in the super-population parameter of the new distribution or may want to condition on a different set of variables. The proposed approach can be extended to this setting by adjusting the confidence intervals appropriately. More details are given in Section C.3 of the supplementary material.

### 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

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

\[
(\varepsilon_1, \varepsilon_2)^\top \sim N(0, \Sigma), \quad \Sigma_{11} = \Sigma_{22} = 1, \quad \Sigma_{12} = \Sigma_{21} = 1/2,
\]

\[
Y = X_1 + \left| X_1 \right| + X_3 + \varepsilon', \quad \varepsilon' \sim N(0, \nu^2).
\]
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 \( \theta_n^{\text{cond}} = \arg\min_{\theta \in \mathbb{R}^p} \sum_{i=1}^{n} \mathbb{E}[(Y_i - \beta^T X_i)^2 | Z_i] \), 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

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

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 \( \{Z_i\}_{i=1}^{n} = \{(X_{i1}, X_{i2})\}_{i=1}^{n} \); 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. The asymptotic variance is estimated with Algorithm 3 in the supplementary material, where we use \texttt{loess} function in R for the nonparametric regression. The procedure is repeated for \( N_X = 800 \) draws of the conditioning set.

We summarize the \( N_X \) unconditional coverage for \( \theta_n^{\text{cond}} \) in Figure 3: each subplot corresponds to a configuration of \( \nu \). Both figures confirm the conditional validity of our procedure (the boxplots mark median and quartile quantiles of the unconditional coverage). In particular, the estimation error of variance for the second entry with smaller sample sizes leads to overcoverage on the right-hand side of Fig. 3. It shows the robustness of our procedure to the estimation error of \( \varphi(\cdot) \): in cases where the estimation of \( \varphi(\cdot) \) is inaccurate, the algorithm tends to overestimate the variance, so that the procedure still provides valid coverage. This is because using Algorithm 3 (see details in the supplementary material), when \( \hat{\varphi}(\cdot) \) converges to a function \( \varphi(\cdot) \), our output \( \hat{\sigma}^2 \) converges to \( \mathbb{E}[(\varphi(D) - \varphi(Z))^2] \geq \mathbb{E}[(\varphi(D) - \varphi(Z))^2] = \sigma^2 \), as \( \varphi(Z) \) is the least-square projection of \( \varphi(D) \) onto the space of measurable functions of \( Z \).

![Figure 3](image3.png)

Figure 3: Conditional coverage of \( \theta_n^{\text{cond}} \) for first (left) and second (right) entry. Red dashed lines are nominal level.

We compute the ratio of estimated standard deviation (i.e., that of confidence interval lengths) for conditional inference and super-population inference in Figure 4. We see that conditional inference often

![Figure 4](image4.png)

Figure 4: Ratio of estimated standard deviation of conditional v.s. super-population inference. Red dashed lines equal 1.

leads to shorter confidence intervals once the estimation error is reasonably small.

### 4.2 Transductive inference under covariate shift

In this part, we evaluate the performance of transductive inference procedures on simulated data. Our results show that the conditional coverage is close to the nominal level even with estimated covariate shift.
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 3.3 for \( N_Y = 500 \) times. We follow algorithms in Section B.1 in the supplementary material to construct \( \hat{\sigma}^2_{\text{shift}}, \hat{\theta}_{m,n}^{\text{trans}} \) and the confidence intervals, where the meta algorithm 1 uses the \texttt{loess} function in R. When covariate shift is estimated, we let \( \hat{w}(\cdot) = \frac{\hat{\epsilon}(\cdot)}{1 - \hat{\epsilon}(\cdot)} \cdot \frac{1 - \hat{\rho}}{\hat{\rho}} \), where \( T_i = 1 \{i \text{ is in the new dataset}\} \), and \( \hat{\epsilon}(x) \) (resp. \( \hat{\rho} \)) estimates \( P(T_i = 1 \mid x_i = x) \) (resp. \( P(T_i = 1) \)) by pooling the two datasets, and \( \hat{\rho}(x) \) 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 \( \hat{\theta}_{m,n}^{\text{trans, new}} \) associated with the first (left) and second (right) entry of OLS parameter is in Figure 5. 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 \( \nu \); 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.

### Figure 5: Conditional coverage of \( \hat{\theta}_{m,n}^{\text{cond, new}} \) for first (left) and second (right) entry. Red dashed lines are nominal level.

5 Real data analysis

Besides the real data analysis we show in the introduction, we also 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 Kuenzel (2019), 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.

Our framework constructs conditionally valid confidence intervals for the mean price of a subset of cars. This is suitable when a dealer or agent is interested in whether to sell its own cars through this platform. This situation, as we introduced at the beginning of this paper, is in between predicting an individual price or inferring the overall mean price 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 focus on the particularly difficult task of inferring the price of old cars (Kuenzel, 2019). 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 $\{(Y_j^{\text{new}}, X_j^{\text{new}})\}_{1 \leq j \leq m}$; 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 $Y_j^{\text{new}}$, 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

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

Specifically, with $T_i = 1$ indicating $(X_i, Y_i^*)$ is in the new (shifted) dataset, the weight function is obtained by

$$
\hat{w}(\cdot) = \frac{\hat{c}(\cdot)}{1 - \hat{c}(\cdot)} \cdot \frac{1 - \hat{p}}{\hat{p}},
$$

where $\hat{c}(x)$ estimates $\mathbb{P}(T_i = 1 | X_i = x)$ and $\hat{p}$ estimates $\mathbb{P}(T_i = 1)$ 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 6.

![Figure 6](image_url)

Figure 6: 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.

Our procedure works well especially for reasonably large original dataset and moderate proportion $r$ of the shifted dataset. The coverage improves as the sample size gets larger, especially when the proportion of shifted data is not too large or too small (so that old cars appear reasonably often 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 might lead to the undercoverage, as can be observed in the first plot in Figure 6.

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A Conditional versus marginal inference

Continuing the example of a healthcare provider (for simplicity, let us say they are hospitals in a city) estimating health conditions discussed in the introduction, suppose there are \( N = 1000 \) hospitals \( j = 1, \ldots, N \), each having \( n = 10000 \) fixed patients with i.i.d. attributes \( Z_{ij} \sim P_Z, i = 1, \ldots, n \). For simplicity, we assume that the fixed population is defined by fixing their attributes, so that the observations are \( Y_{ij} = f_j(Z_{ij}) + \epsilon_{ij} \), where \( \epsilon_{ij} \sim N(0, 1) \) is i.i.d. measurement noise and unexplained variation, and \( f_j(z) \) is the average health of a patient 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 \( \epsilon_{ij} \) are repeatedly drawn. For simplicity, we assume the marginal variance \( \sigma_m = \text{sd}(Y_{ij}) \) and measurement noise \( \sigma_e = \text{sd}(\epsilon_{ij}) \) are known.

![Coverage of superpopulation parameter](image1)
![Coverage of conditional parameter](image2)

Figure 7: Left: coverage of super-population confidence intervals across hospitals (37 hospitals with coverage < .75 are not shown). Right: coverage of conditional confidence intervals across hospitals. In both cases, the marginal coverage is .95. Details of the simulation are in Section A

In super-population inference, each hospital can construct 95% confidence intervals for the super-population parameter \( \mathbb{E}[Y_{ij}] \) via \( \frac{1}{n} \sum_{i=1}^{n} Y_{ij} \pm 1.96 \sigma_m / \sqrt{n} \). We show the histogram of coverage across the hospitals in the left-hand side of Figure 7, where we observe under-coverage for some hospitals. Indeed, 26% of hospitals have coverage below .95, and the average coverage among these hospitals is only .85. Furthermore, if these hospitals would repeat similar examinations many times, their confidence intervals would consistently suffer from under-coverage. On the other hand, the confidence intervals of some other hospitals will consistently over-cover if similar examinations are repeated many times. Such lack of conditional coverage illustrates the risk of super-population inference, which is especially pressing in high-stakes applications such as healthcare.

Mathematically, the issue is that for each hospital \( j \), the customers defined by \( \{ Z_{ij} \}_{i=1}^{n} \) are fixed and only the remaining variation in \( \{ \epsilon_{ij} \}_{i=1}^{n} \) is 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 the hospitals). In this situation, however, it would be more desirable to have coverage close to .95 for each hospital, i.e., 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 intrinsic health risk of the fixed patients in hospital \( j \), ruling out the measurement error. In our framework, 95% confidence intervals can be constructed via \( \frac{1}{n} \sum_{i=1}^{n} Y_{ij} \pm 1.96 \sigma_e / \sqrt{n} \). The histogram of coverage of these confidence intervals are shown on the right-hand side of Figure 7, where we observe coverage consistently close to .95 for all hospitals. By switching to conditional parameters, the confidence intervals are more relevant and more reliable for the patients in each hospital. We also note that conditional confidence intervals are shorter than those for
super-population inference.

We finally remark a few over-simplified aspects in this stylized example. Firstly, replacing \( \sigma \) with a consistent or conservative estimator preserves conditional validity under mild conditions. Secondly, one may want to condition on unobserved variables. To be more precise, one may want to infer some health indicator \( Y^* = \mathbb{E}[Y | Z^*] \) (where \( Z^* \) is an unobserved variable that is finer than \( Z \)), we still allow for \( Y^* \)-conditionally valid (yet conservative) inference for the corresponding conditional parameter \( \frac{1}{n} \sum_{i=1}^{n} Y_{ij}^* \). More details are discussed in Section 3.1.

\[ \square \]

### B Algorithms and convergence guarantees

#### B.1 Algorithms for inference procedures

In this section, we describe concrete algorithms for estimating \( \varphi(\cdot) \), \( \eta(\cdot) \), \( \sigma^2 \) and \( \sigma^2_{\text{shift}} \). Corresponding theory can be found in Section B.2. Similar to the main text, the estimation of variances is discussed for the one-dimensional parameters, while the arguments naturally carry over to the estimation of covariance matrix for multi-dimensional parameters, 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 case for multivariate covariates (attributes).

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

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

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

\[
    M(s, w, \theta) = -\left( \mathbb{E}[w(Z_i)\hat{s}(D_i, \theta)] \right)^{-1} \in \mathbb{R}^{P \times P}, \quad (D_i, Z_i) \sim \mathbb{P}. \tag{14}
\]

Our general recipe is to estimate \( M(s, w, \theta) \) and \( \mathbb{E}[s(D_i, \theta) | Z_i = z] \) 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 \( h(\cdot): \mathbb{D} \rightarrow \mathbb{R}^P \), dataset \( \{(D_i, Z_i)\}_{i \in I} \) independent of \( h(\cdot) \).

**Output:** Function \( \hat{G}(h, I)(\cdot): Z \rightarrow \mathbb{R}^P \).

**Algorithm 2 Meta Algorithm: Matrix Estimation.**

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

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

**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 \( \{(D_i, Z_i)\}_{i \in I} \) is detailed in Algorithm 3. Roughly speaking, we first obtain estimators for \( \phi(D_i), i \in I_1 \); then we estimate \( \varphi(\cdot) = \mathbb{E}[\phi(Z = \cdot)] \) only using data in one fold \( I_1 \) and apply to another independent fold \( I_2 \), which are finally used to estimate \( \sigma^2 \). The sub-routine of estimating \( \phi(\cdot) \) is detailed in Algorithm 7 below.

**Estimation for transductive inference in Sections 3.2 and 3.3.** Transductive inference requires a consistent estimator for \( \sigma^2_{\text{shift}} \) defined in equation (13), and an estimator for \( \eta(\cdot) \) only using one fold \( I_k \). 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., Sugiyama et al. (2012) for a comprehensive review.
Algorithm 3 Estimate $\sigma^2$.

**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 $I_2$. // Estimate $\phi(D_i)$ for $i \in I_2$
2: Set $\hat{\theta}$ as solution to $\sum_{i \in I_1} s(D_i, \theta) = 0$. // Estimate $\phi(\cdot)$ with only $I_1$
3: Obtain $\hat{M} := \hat{M}(s, 1, \hat{\theta}, I_2)$ using Algorithm 2. // Apply to $I_2$
4: Set $\hat{\phi}_i = \hat{M}(s, \hat{\theta})$ for all $i \in I_2$.
5: Obtain $\hat{\sigma}^2 = \frac{1}{|I_2|} \sum_{i \in I_2} (\hat{\phi}_i - \hat{\phi})^2$.

Output: $\hat{\sigma}^2$.

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 $\hat{e}(z) = \hat{P}(T = 1 | Z = z)$ using pooled data by any regression or classification algorithm.

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

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 $s: \mathbb{D} \times \Theta \rightarrow \mathbb{R}^p$, weight $w: \mathbb{Z} \rightarrow \mathbb{R}$.

1: Split indices $I$ into equally-sized $I_1$, $I_2$ and $I_3$. // Obtain weight function
2: if $w$ is given then
3: Set $\hat{w} = w$
4: else
5: Estimate weight function $\hat{w}(\cdot): \mathbb{Z} \rightarrow \mathbb{R}$ 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 $\hat{s}(\cdot) = s(\cdot, \hat{\theta}): \mathbb{D} \rightarrow \mathbb{R}^p$. // Estimate $\mathbb{E}[s(D, \theta_0^{\text{new}}) | Z = \cdot]$
10: Obtain $\hat{t}(\cdot) := \hat{G}(\hat{s}, I_3)(\cdot): \mathbb{Z} \rightarrow \mathbb{R}^p$ using Algorithm 1.

Output: function $\eta(s, w, \hat{\theta}, I^{\text{new}})(\cdot): \mathbb{Z} \rightarrow \mathbb{R}^p$, where $\hat{\eta}(z) = \hat{M}(z)$.
In Algorithm 5, we describe in details the estimation of \( \eta(\cdot) \) using any fold \( I \) and \( I^{\text{new}} \). Note that when \( w(\cdot) \) is known, it is directly used to construct \( \hat{\theta}^{\text{trans}}_{m,n} \) for Theorem D.2, so that \( I^{\text{new}} \) is in fact not used. Otherwise, we set aside a part of \( I \) to estimate it and construct \( \hat{\theta}^{\text{trans,shift}}_{m,n} \) in Theorem D.6.

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 \( i \in I_3 \); then we use only \( I_1, I_2 \) to estimate \( \eta(\cdot) \) and apply to estimate \( \eta(Z_i), i \in I_3 \), which are used to estimate \( \sigma^2_{\text{shift}} \).

**Algorithm 6 Estimate \( \sigma^2_{\text{shift}} \).**

**Input:** Datasets \( \{(D_i, Z_i)\}_{i \in I}, \{(D^\text{new}_j, Z^\text{new}_j)\}_{j \in I^{\text{new}}} \), score function \( s: \mathcal{D} \times \Theta \to \mathbb{R}^p \), weight function \( w: \mathcal{Z} \to \mathbb{R} \).

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

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

We note that the estimation of \( \varphi(\cdot) = -(\mathbb{E}[s(D, \theta_0)])^{-1} \mathbb{E}[s(D, \theta_0) \mid Z = \cdot] \) with data \( \{(D_i, Z_i)\}_{i \in I} \) could be viewed as a special case of Algorithm 5 by taking \( w(z) \equiv 1 \). Nevertheless, we include a stand-alone algorithm here for convenience of reference. 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 \( s: \mathcal{D} \times \Theta \to \mathbb{R}^p \).

1. Split indices \( I \) into equally-sized \( I_1 \) and \( I_2 \).
2. Set \( \hat{\theta} \) as solution to \( \sum_{i \in I_1} s(D_i, \hat{\theta}) = 0. \)
3. Obtain \( \hat{M} := \hat{M}(s, 1, \hat{\theta}, I_2) \) using Algorithm 2.
4. Set \( \hat{s}(\cdot) = s(\cdot, \hat{\theta}): \mathcal{D} \to \mathbb{R}^p \).
5. Obtain \( \hat{f}(\cdot) := \hat{G}(\hat{s}, I_2)(\cdot): \mathcal{Z} \to \mathbb{R}^p \) using Algorithm 1.

**Output:** Function \( \varphi(s, I)(\cdot) = \hat{M}(\cdot): \mathcal{Z} \to \mathbb{R}^p \).

**B.2 Estimation guarantees**

In this section, we provide estimation guarantees for algorithms in Section B.1 with explicit and detailed conditions. We state conditions for parameters in \( \mathbb{R}^p \) for generality; the targets are still the variance estimation for one-dimensional parameters, which can be generalized to covariance matrix estimation under the same conditions we state.

We begin with generic assumptions on the meta Algorithms 1 and 2. For any function \( f(\cdot) \), we let \( \mathcal{G}(f)(z) = \mathbb{E}[f(D) \mid Z = z] \) be the conditional mean function, viewing \( f \) as fixed; also, recall that \( \mathcal{G}(f, I) \) is the output of Algorithm 1 using data \( I \). Also, recall that \( \hat{M}(s, w, \theta, I) \) is the output of Algorithm 2 using data \( I \) and \( M(s, w, \theta) \) in (14) is its estimation target.

**Assumption B.1.** For any fixed input function \( f \) and dataset \( I \), the output of Algorithm 1 satisfies that \( \| \mathcal{G}(f,I)(\cdot) - \mathcal{G}(f)(\cdot) \|_{L_2(\mathcal{P})} = O_P(\mathcal{R}_r(|I|)) \) for some rate function \( \mathcal{R}_r(\cdot): \mathbb{N} \to \mathbb{R}^+ \).
Assumption B.2. For any fixed input \( w, \theta \) and dataset \( I \), the output of Algorithm 2 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 (Nadaraya, 1964; Watson, 1964), local polynomial regression (Cleveland, 1979; Cleveland and Devlin, 1988), smoothing spline (Green and Silverman, 1993) and modern machine learning methods including regression trees (Breiman et al., 1984) and random forests (Ho, 1995), to name a few.

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

Assumption B.3. The matrix \( M(s, w, \theta) \) satisfies that \( \|M(s, 1, \theta) - M(s, 1, \theta')\|_{\infty} = O(\|\theta - \theta'\|_2) \) and \( \|M(s, w, \theta) - M(s, w', \theta)\|_{\infty} = O(\|w(z) - w'(z)\|_{L_2(P)}) \) for any weight functions \( w, w' \) and any \( \theta, \theta' \in \Theta \).

Also, \( \|s(\cdot, \theta) - s(\cdot, \theta')\|_{L_2(P)} = O(\|\theta - \theta'\|_2) \) 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 B.4 is in Appendix H.2.

Proposition B.4 (Consistency of \( \hat{\sigma}^2 \)). Suppose Assumptions B.1, B.2 and B.3 hold, and the regularity conditions of Proposition 3.1 hold for \( \hat{\theta} \) in Algorithm 3. Also suppose \( \mathcal{R}_m(n), \mathcal{R}_r(n) \to 0 \) 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 D.2, 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 D.6, we further need the convergence rate for estimating \( \eta(\cdot) \). We analyze \( \hat{\eta}(\cdot) \), the output of Algorithm 5, under generic rates of the meta algorithms as follows. The proof of Proposition B.5 is in Appendix H.3.

Proposition B.5 (Convergence rate of \( \hat{\eta} \)). Suppose Assumptions B.1, B.2, B.3 and the regularity conditions in Propositions E.1 and E.2 hold. Let \( I, I^\text{new} \) be any inputs of Algorithm 5. If \( w(\cdot) \) is known, the output of Algorithm 5 satisfies

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

If \( \hat{\eta}(\cdot) \) is estimated, assume \( \sup_z |\hat{\eta}(z)| = O_P(1) \) and the regularity conditions in Proposition E.2 also hold for \( \hat{\theta} \). Then the output of Algorithm 5 satisfies

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

As a direct implication, Assumption D.5 holds if

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

Note that in Algorithm 5, \( I^\text{new} \) is only possibly used to estimate \( w(\cdot) \). Consequently, the convergence rate of \( \hat{\eta}(\cdot) \) depends on \( I^\text{new} \) only through \( \|\hat{\eta}(\cdot) - w(\cdot)\|_{L_2(P)} \).

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

Proposition B.6 (Consistency of \( \hat{\sigma}^2_{\text{shift}} \)). Let \( I, I^\text{new} \) be any inputs of Algorithm 6. Suppose Assumptions B.1, B.2 and B.3 hold, and the regularity conditions in Proposition E.2 hold for \( \hat{\theta} \) in Algorithm 6. Assume \( \mathcal{R}_m(n) \to 0 \) and \( \mathcal{R}_r(n) \to 0 \) as \( n \to \infty \). If \( \sup_z |\hat{\eta}(z) - w(z)| = o_P(1) \), \( \sup_z |w(z)| < \infty \), then the output of Algorithm 6 obeys \( \hat{\sigma}^2_{\text{shift}} \to \sigma^2_{\text{shift}} \) in probability as \( |I| \to \infty \).

Finally, we note that \( \varphi(\cdot) \) can be estimated with Algorithm 5 by setting \( w(\cdot) \equiv 1 \). For completeness, we include the following consistency result for \( \hat{\varphi}(\cdot) \), whose proof is in Appendix H.1.

Proposition B.7 (Consistency of \( \hat{\varphi} \)). Suppose Assumptions B.1 and B.2 hold, and the regularity conditions in Proposition 3.1 hold for \( \hat{\theta} \). Assume \( M(s, 1, \theta) - M(s, 1, \theta') \|_{\infty} = O(\|\theta - \theta'\|_2) \) and \( \|s(\cdot, \theta) - s(\cdot, \theta')\|_{L_2(P)} = O(\|\theta - \theta'\|_2) \) for any \( \theta, \theta' \in \Theta \). Then the output of Algorithm 5 with \( w(\cdot) \equiv 1 \), denoted as \( \hat{\varphi}(\cdot) \), satisfies

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

C.1 Fixed-attributes results

In this section, we provide a set of results for fixed attributes, i.e., the attributes \( \{z_i\}_{i=1}^n \) are fixed a priori and not drawn i.i.d. from a super-population. These results generalize the counterparts in Section 3.1.

We start by describing the setup. Let \( \{z_i\}_{i=1}^n \) be the fixed attributes of \( n \) units. We assume the observed dataset \( \{D_i\}_{i=1}^n \) are mutually independent with \( D_i \sim P_D|Z=z_i \). Our target is still the parameter that characterizes the (conditional) distribution of these fixed units. For ease of illustration, we use the language of M-estimators. Let \( \ell: \mathbb{D} \times \Theta \rightarrow \mathbb{R} \) be a loss function, and define the conditional parameter as

\[
\hat{\theta}_{n \text{cond}} = \arg \min_{\theta \in \Theta} L_n(\theta), \quad L_n(\theta) := \frac{1}{n} \sum_{i=1}^n E[\ell(D_i, \theta) | z_i].
\]

Then \( \hat{\theta}_{n \text{cond}} \) only depends on \( \{z_i\}_{i=1}^n \) and is fixed. Parallel to Section 3.1, we assume access to an estimator

\[
\hat{\theta}_n = \arg \min_{\theta \in \Theta} \hat{L}_n(\theta), \quad \hat{L}_n(\theta) := \frac{1}{n} \sum_{i=1}^n \ell(D_i, \theta).
\]

We first establish the asymptotic linearity for the deviation of \( \hat{\theta}_n \) from \( \theta_{n \text{cond}} \) and a few conditions for the loss function and observations are needed. For simplicity, since \( \{z_i\}_{i=1}^n \) are fixed, all probabilities and expectations are then implicitly conditional on \( \{z_i\}_{i=1}^n \). The proof of Proposition C.2 is in Appendix G.1.

Assumption C.1. (i) \( \hat{\theta}_n \) and \( \theta_{n \text{cond}} \) are both unique minimizers for their targets; (ii) \( \ell(d, \cdot) \) is convex and twice continuously differentiable for every \( d \); (iii) \( \nabla \ell(d, \cdot) \) and \( \nabla^2 \ell(d, \cdot) \) are \( m_n(d) \)-Lipschitz on \( \Theta \) and \( \frac{1}{n} \sum_{i=1}^n E[m_n(D_i)^2] \leq M \) for constant \( M < \infty \); (iv) \( \text{Var}(\nabla \hat{L}_n(\theta_{n \text{cond}})) \geq c_2 I_{p \times p} \) and \( \nabla^2 L_n(\theta_{n \text{cond}}) \geq c_2 I_{p \times p} \) for constant \( c_2 > 0 \); (v) \( \frac{1}{n} \sum_{i=1}^n E[|\nabla \ell(D_i, \theta_{n \text{cond}})||\theta|] < \infty \) for \( q > 2 \).

Proposition C.2. Suppose Assumption C.1 holds. Then \( \sqrt{n}(\hat{\theta}_n - \theta_{n \text{cond}}) = o_p(1) \) and it holds that

\[
\sqrt{n}(\hat{\theta}_n - \theta_{n \text{cond}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^n -[\nabla^2 L_n(\theta_{n \text{cond}})]^{-1} \nabla \ell(D_i, \theta_{n \text{cond}}) + o_p(1).
\]

The following theorem then establishes the asymptotics for \( \theta_{n \text{cond}} \), whose proof is also in Appendix G.1.

Theorem C.3. Define \( \Sigma_n^{1/2} = [\nabla^2 L_n(\theta_{n \text{cond}})]^{-1} \text{Var}(\nabla \hat{L}_n(\theta_{n \text{cond}}))^{1/2} \). Then \( \sqrt{n}(\hat{\theta}_n - \theta_{n \text{cond}}) \xrightarrow{d} N(0, \Sigma_n^{1/2}) \) as \( n \rightarrow \infty \).

To form (conditional) confidence intervals, it remains to construct a consistent estimator for \( \Sigma_n^{1/2} \). For simplicity, we show a concrete approach for \( p = 1 \), while the multi-dimensional case follows similar ideas. Denote \( \ell(d, \cdot) = \nabla_\theta \ell(d, \theta) \) and \( \hat{\ell}(d, \cdot) = \nabla_\theta \hat{\ell}(d, \theta) \). The asymptotics in Theorem C.3 reduce to

\[
\sigma_n := \Sigma_n^{1/2} = \left( \frac{1}{n} \sum_{i=1}^n E[\ell(D_i, \hat{\theta}_{n \text{cond}})] \right)^{-1} \left( \frac{1}{n} \sum_{i=1}^n \text{Var}(\hat{\ell}(D_i, \hat{\theta}_{n \text{cond}}) | z_i) \right)^{1/2}.
\]

The following algorithm returns an estimator for \( \sigma_n \) by running a nonparametric regression on \( \{z_i\}_{i=1}^n \).

We establish the consistency of Algorithm 8 under mild conditions, and its robustness if such conditions fail. The proof of Proposition C.4 is in Appendix G.1.

Proposition C.4. Suppose Assumption C.1 holds, and \( \frac{1}{n} \sum_{i=1}^n (\hat{\ell}(z_i) - \mu(z_i))^2 = o_P(1) \) for some fixed function \( \mu: \mathbb{Z} \rightarrow \mathbb{R} \). Also, suppose \( \text{E}[\ell(D_i, \theta_{n \text{cond}}) | z_i] = \mu^*(z_i) \) for some function \( \mu^*: \mathbb{Z} \rightarrow \mathbb{R} \). Then the output of Algorithm 8 satisfies that (i) \( \hat{\theta}_n - \mu_{n \text{cond}} = o_P(1) \) when \( \mu^* = \mu \), and (ii) otherwise, \( \hat{\theta}_n - \hat{\sigma}_n = o_P(1) \) for some \( \hat{\sigma}_n \geq \sigma_n \) which also only depends on \( \{z_i\}_{i=1}^n \).
Algorithm 8 Estimate $\sigma_n$.

**Input:** Dataset $\{(D_i, z_i)\}_{i=1}^n$, loss function $\ell : \mathbb{D} \times \Theta \to \mathbb{R}$.

1. Set $\hat{\theta}_n$ as solution to $\sum_{i=1}^n \ell(D_i, \theta) = 0$.
2. Compute $\tilde{M} = \frac{1}{n} \sum_{i=1}^n \ell(D_i, \hat{\theta}_n)$.
3. Obtain $\tilde{\ell}(\cdot) = \mathcal{G}(\hat{s}, \mathcal{Z})(\cdot) : \mathcal{Z} \to \mathbb{R}^p$ using Algorithm 1 for $\hat{s}(\cdot) = \tilde{\ell}(\cdot; \hat{\theta}_n) : \mathbb{D} \to \mathbb{R}$.

**Output:** estimator $\hat{\sigma}_n = \tilde{M}^{-1/2} \sum_{i=1}^n [\hat{s}(D_i) - \tilde{\ell}(z_i)]^2$.

In words, the above proposition shows the consistency of $\hat{\sigma}_n$ if the nonparametric regression of $\tilde{\ell}(D_i, \hat{\theta}_n)$ on $z_i$ is consistent for the truth $\mu^*(z_i) = \mathbb{E}[\tilde{\ell}(D_i, \theta_{n \text{ cond}}) | z_i]$. If the regression is instead run with $\tilde{\ell}(D_i, \theta_{n \text{ cond}})$, the well-established theory of nonparametric regression such as kernel regression or smoothing splines guarantees the diminishing $L_2$ error if the underlying function $\mu^*$ is well-behaved. Considering the order $O(n^{-1/2})$ deviation of $\tilde{\ell}(D_i, \hat{\theta}_n)$ from $\tilde{\ell}(D_i, \theta_{n \text{ cond}})$, the consistency requirement of Proposition B.4 is mild. In addition, even though the regression is not consistent but converges to some deterministic function (an even more mild condition), Algorithm 8 returns an upper bound for $\sigma_n$, which would lead to a conservative yet valid confidence interval.

Finally, as we mentioned in Remark 3.6, one could also use $\sigma_n^2$ derived here instead of $\sigma^2$ for the i.i.d. setting (7), as the regularity conditions above hold with high probability for i.i.d. drawn attributes. Compared to $\sigma^2$, $\sigma_n^2$ might provide attribute-dependent characterization for the statistical uncertainty.

However, we do not see the similarity between $\sigma^2$ and $\sigma_n^2$ for i.i.d. attributes. In this case, we have $\sigma_n^2 = \sigma^2 + O_P(1/\sqrt{n})$, their contributions to constructing the confidence interval differ by a magnitude that is of the same order as, hence indistinguishable from, the error in the asymptotic linearity (Assumption 3.2) we rely on. Furthermore, in practice, the estimation of $\sigma_n^2$ in Algorithm 8 and of $\sigma^2$ in Algorithm 3 does not make much difference. The main distinction is that the i.i.d. assumption allows for sample splitting in the estimation of $\sigma^2$, which simplifies theoretical analysis and our theoretical guarantee only relies on generic consistency conditions of nonparametric regression. Instead, Algorithm 8 applies all the data in every step; hence, it needs slightly stronger and less generic conditions on the regression outputs. The practical choice between $\sigma_n^2$ or $\sigma^2$ could also be viewed as a tradeoff between confidence in the i.i.d. assumption and confidence in regression accuracy.

C.2 Conditioning on unobserved variables

In this part, we generalize the conditional inference framework to situations where some unobserved variables are fixed. Again, we assume $\{(D_i, Z_i)\}_{i=1}^n$ are i.i.d. from a super-population $\mathbb{P}$. Suppose a data scientist would like to view some unobserved variable $X_n = \{X_i\}_{i=1}^n$ as fixed, which are also i.i.d. from the super-population and then conditioned on. While we could also relax the i.i.d. assumption to fixed-attributes settings, such extension follows similar ideas as Appendix C.1 hence we omit here for brevity.

Following Section 2.1, the conditional parameter $\theta_{n \text{ cond}} = \theta_{n \text{ cond}}(X_n)$ is the unique solution to

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

As we only observe attributes $\{Z_i\}_{i=1}^n$, we could use the procedures proposed in Sections 3.1 and B.1 to obtain an estimator $\hat{\sigma}_Z^2$ for the (observed) asymptotic variance $\sigma_Z^2 = \mathbb{E}[(\phi(D) - \varphi(Z))^2]$. The following theorem states the conditional validity of inference based on $\hat{\sigma}_Z^2$, whose proof is in Appendix G.2.

**Theorem C.5.** Suppose $\hat{\sigma}_Z^2 \xrightarrow{P} \sigma_Z^2$, and Assumptions 3.2 and 3.3 hold with $Z$ replaced by $X$. If $\mathbb{E}[(\mathbb{E}[\phi(D) | X])^2] \geq \mathbb{E}[(\mathbb{E}[\phi(D) | Z])^2]$, then for any $\alpha \in (0, 1)$, it holds that

$$\mathbb{P}(\theta_{n \text{ cond}}(X_n) \in [\hat{\theta}_n - z_{1-\alpha/2} \hat{\sigma}_Z / \sqrt{n}, \hat{\theta}_n + z_{1-\alpha/2} \hat{\sigma}_Z / \sqrt{n}] | X_n)$$ 

converges in probability to $1 - \beta$ for some fixed $\beta \leq \alpha$ as $n \to \infty$. 

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The only additional requirement for conditionally valid (and perhaps conservative) inference given unobserved attributes is that $\mathbb{E}(\mathbb{E}[\phi(D) \mid X])^2 \geq \mathbb{E}(\mathbb{E}[\phi(D) \mid Z])^2$. Roughly speaking, it requires the covariate $Z$ to explain away less variation in $\phi(D)$ than the unobserved variable $X$. For instance, one might want to condition on more information than the observed, and view the observed attributes $Z$ as partially defining the fixed population. In this situation (which might be the only case where one would like to condition on unobserved attributes), this condition is naturally satisfied. In fact, this situation is related Example 2.3 when we condition on the partially observed $\{(Y_i(0), Y_i(1))\}_{i=1}^n$ for finite-population treatment effect $\frac{1}{n} \sum_{i=1}^n (Y_i(1) - Y_i(0))$; methods in the literature often proceed with conservative estimators for the asymptotic variance, which is similar to our setting here.

C.3 Transferring a subset of observed attributes

The proposed transductive inference procedures generalize to settings where the conditioning set is smaller than that for the covariate shift. That is, the covariate shift holds for the whole set $Z$ of observed attributes, while one might think a subset $X$ should be viewed as fixed to characterize the new population. We discuss the extension of our framework to this setting in this part.

Formally, we assume $X \subset Z$ where $Z$ is observable, and there is a (possibly unknown) covariate shift $\frac{dQ}{dP}(d,z) = w(z)$. As usual, we denote $X^\text{new}_m = \{X^\text{new}_j\}_{j=1}^n$ as the new conditioning attributes. The target is the new conditional parameter $\theta^\text{cond}_m(X^\text{new})$ with respect to a subset of observed attributes. This setting is challenging because the invariance of conditional distribution does not necessarily hold for $X$. However, as we will see, the proposed estimator still allows for conditionally valid transductive inference.

Let $\hat{\theta}_m^\text{trans}$ be the estimator defined in (12) of the main text, which is obtained from $Z_n \cup Z^\text{new}_m$. The following theorem shows that slightly modifying the asymptotic variance leads to valid inference; for completeness, we discuss both the simplified exposition in the main text and the cross-fitted procedures in Appendix D.1 and D.2. The proof is in Appendix G.3.

**Theorem C.6.** Under the setup of Section 3.3, suppose all conditions in Theorem 3.11 hold; under the setup of Appendix D.1, suppose the conditions in Theorem D.2 hold; under the setup of Appendix D.1, suppose the conditions in Theorem D.6 hold. Let $\hat{\theta}_m^\text{trans}$ be the estimator built with $Z_n$ and $Z^\text{new}_m$ in any of these cases. Suppose $(\sigma'_{\text{shift}})^2$ converges in probability to

$$(\sigma'_{\text{shift}})^2 = \text{Var} \{w(Z_i)(\psi(D_i) - \eta(Z_i))\} + n/m \cdot \text{Var} \{\eta(Z^\text{new}_j) - \mathbb{E}[\eta(Z^\text{new}_j) \mid X^\text{new}_j]\}.$$

Then for any fixed $\alpha \in (0,1)$, it holds that

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

converges in probability to $1 - \alpha$ as $m,n \to \infty$.

D Details of cross-fitting for transductive inference

D.1 Details of cross-fitting for transductive inference with known covariate shift

This section contains details of cross-fitting for transductive inference under known covariate shift $w(\cdot)$ that we omit for clarity in Section 3.3. Instead of referring to external datasets, we split the data to decouple the estimation of nuisance components, and reuse the folds to achieve the same statistical efficiency.

We first split the index set $\mathcal{I} = \{1, \ldots, n\}$ of $\{(D_i, Z_i)\}_{i=1}^n$ into equally-sized halves $\mathcal{I}_1$ and $\mathcal{I}_2$. Then for $k = 1, 2$, we obtain estimator $\hat{\eta}^k_\mathcal{I} \cdot$ for $\eta(\cdot) = \mathbb{E}[\psi(D^\text{new}_j) \mid Z^\text{new}_j = \cdot]$, using only the data in $\mathcal{I}_k$.\footnote{One can set $\hat{\eta}^k_\mathcal{I}$ as the output of Algorithm 5 (c.f. Section B.1) with inputs $w$ and $\mathcal{I}_k$. Since in Algorithm 5, the new attributes are only used to estimate the weight function (if it is unknown), here we do not need them as input for estimating $\eta(\cdot)$.}

We then define the estimator

$$\hat{\theta}_m^\text{trans} = \hat{\theta}_m^\text{trans} - c^\text{trans},$$

(16)
where $\hat{\theta}_n^{\text{trans}}$ is the unique solution to
\[
\sum_{i=1}^{n} w(Z_i)s(D_i, \theta) = 0,
\]
i.e., setting $\hat{w}(\cdot) = w(\cdot)$ in (11). The correction term is defined as
\[
\hat{c}^{\text{trans}} = \frac{1}{2|I_1|} \sum_{i \in I_1} \bar{\eta}_i^{\text{trans}}(Z_i)w(Z_i) + \frac{1}{2|I_2|} \sum_{i \in I_2} \bar{\eta}_i^{\text{trans}}(Z_i)w(Z_i) - \frac{1}{2m} \sum_{k=1}^{2m} \sum_{j=1}^{m} \bar{\eta}_k^{\text{trans}}(Z_j^{\text{new}}).
\]

We construct a confidence interval centered around $\hat{\theta}_n^{\text{trans}}$ in Theorem D.2. We assume the $L_2(Q)$ consistency of $\bar{\eta}_i^{\text{trans}}$; note that similar to the i.i.d. setting in Section 3.2, we do not require any convergence rates of $\bar{\eta}_i^{\text{trans}}$.

**Assumption D.1.** $\|\bar{\eta}_k^{\text{trans}}(\cdot) - \eta(\cdot)\|_{L_2(P)}$ and $\|\bar{\eta}_k^{\text{trans}}(\cdot) - \eta(\cdot)\|_{L_2(Q)}$ converges in probability to zero for $k = 1, 2$.

The following theorem states the asymptotic conditional validity of our cross-fitting procedure, whose proof is deferred to Section F.4 in this supplementary material.

**Theorem D.2.** Suppose Assumption 3.10 in the main text holds for $\bar{w} = w$, Assumption D.1 holds, and $m \geq cn$ for some constant $c > 0$. If an estimator $\hat{\sigma}_{\text{shift}}$ converges in probability to $\sigma_{\text{shift}} > 0$ for $\sigma^2$ defined in (13). Then the random variable
\[
P\left(\chi_m^{\text{cond,new}} \in \left[\hat{\theta}_m^{\text{trans}} - \hat{\sigma}_{\text{shift}} \cdot z_{1-\alpha/2}/\sqrt{n}, \hat{\theta}_m^{\text{trans}} + \hat{\sigma}_{\text{shift}} \cdot z_{1-\alpha/2}/\sqrt{n}\right] \mid Z_m^{\text{new}}, Z_n\right)
\]
converges in probability to $1 - \alpha$ as $n \to \infty$, where $\hat{\theta}_m^{\text{trans}}$ is defined in equation (16).

In Theorem D.2, the asymptotic linearity with $\bar{w} = w$ in the main text has been justified in Proposition E.1. Similar to Theorem 3.8, the asymptotic variance does not depend on $m$, and the result only depends on the $L_2$-consistency of $\bar{\eta}_i^{\text{trans}}$. Finally, one could estimate $\hat{\sigma}_{\text{shift}}^2$ using Algorithm 6 without referring to external datasets.

### D.2 Details of cross-fitting for transductive inference with estimated covariate shift

In this section, we provide details for cross-fitting in transductive inference when the covariate shift $w(\cdot)$ in Section 3.3 is unknown. Procedures here do not refer to any external datasets.

We employ cross-fitting (Chernozhukov et al., 2018) to decouple the estimation of $w(\cdot)$ and other quantities. The index set $\mathcal{I} = \{1, \ldots, n\}$ of the original dataset $\{(D_i, Z_i)\}_{i=1}^{n}$ is randomly split into three equally-sized folds, denoted as $\mathcal{I}_1$, $\mathcal{I}_2$ and $\mathcal{I}_3$. The index set $\mathcal{I}^{\text{new}} = \{1, \ldots, m\}$ of the new dataset $Z_m^{\text{new}} = \{Z_j^{\text{new}}\}_{j=1}^{m}$ 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 $\mathcal{I}_\ell$ and $\mathcal{I}^{\text{new}}$ to obtain an estimator $\hat{w}_\ell(\cdot)$ of the covariate shift. Then we use all remaining data $\mathcal{I} \setminus \mathcal{I}_\ell$ to obtain $\hat{\theta}_n^{\text{new,}(\ell)}$, which is a unique solution to
\[
\sum_{i \notin \mathcal{I}_\ell} \hat{w}_\ell(Z_i)s(D_i, \theta) = 0.
\]

Next, for each $k \neq \ell$, we obtain an estimator $\hat{\eta}_k^{\ell}(\cdot)$ for $\eta(\cdot)$ using only $\mathcal{I}_k$ and $\mathcal{I}_k^{\text{new}}$. We define the $\ell$-th correction term as
\[
\hat{c}^{(\ell)} = \sum_{k \neq \ell} \frac{3}{2m} \sum_{i \in \mathcal{I}_k \setminus \mathcal{I}_\ell} \hat{w}(Z_i)\hat{\eta}_k^{\ell}(Z_i) - \sum_{k \neq \ell} \frac{3}{2m} \sum_{j \notin \mathcal{I}_k^{\text{new}} \cup \mathcal{I}_\ell^{\text{new}}} \hat{\eta}_k^{\ell}(Z_j^{\text{new}}).
\]

---

3We give an example in Algorithm 4 for estimating $w(\cdot)$ using any fold $\mathcal{I}$ of original data and any fold $\mathcal{I}^{\text{new}}$ of new covariates.

4To be specific, $\hat{\eta}_k^{\ell}(\cdot)$ is the output $\eta(s, z, \mathcal{I}_k, \mathcal{I}_k^{\text{new}})(\cdot)$ from Algorithm 5 that only depends on $\mathcal{I}_k$ and $\mathcal{I}_k^{\text{new}}$. 
We note that the high-level idea of the above correction term is similar to our simplified expression in Section 3.3; the only difference is that we carefully split and reuse the data to achieve good statistical property. Finally, we define the transductive estimator as

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

(18)

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 \( O(1/m + 1/n) \). Similar to Assumption 3.10 in the main text, we assume consistency of \( \hat{\sigma} \). Finally, we define the transductive estimator as Section 3.3; the only difference is that we carefully split and reuse the data to achieve good statistical property. We note that the high-level idea of the above correction term is similar to our simplified expression in

**Assumption D.3.** For \( \ell = 1, 2, 3 \), \( \sup_{z} |\hat{w}_{\ell}(z) - w(z)| \to 0 \) in probability as \( n \to \infty \).

For ease of exposition, we impose the linear expansion of \( \hat{\theta}_{n}^{\text{new,}(\ell)} \) as follows. In Proposition E.2 in Section E.3 of this supplementary material, we show that Assumption D.4 holds under Assumption D.3 and regularity conditions similar to previous cases.

**Assumption D.4.** For \( \ell = 1, 2, 3 \), \( \hat{\theta}_{n}^{\text{new,}(\ell)} \) is the unique solution to (17). Also, letting \( \theta_{0}^{\text{new}} \) be the unique solution to (10), assume the following asymptotic linearity holds:

\[ \sqrt{\frac{2n/3}{3}}(\hat{\theta}_{n}^{\text{new,}(\ell)} - \theta_{0}^{\text{new}}) = \frac{1}{\sqrt{\frac{2n/3}{3}}} \sum_{i \notin I_{\ell}} \hat{w}_{\ell}(Z_{i})\psi(D_{i}) + o_{P}(1), \]  

(19)

\[ \sqrt{m}(\theta_{m}^{\text{cond,new}} - \theta_{0}^{\text{new}}) = \frac{1}{\sqrt{m}} \sum_{j=1}^{m} \eta(Z_{j}^{\text{new}}) + o_{P}(1), \]

where \( \psi(d) = -(E_{Q}[\hat{s}(D_{\text{new}}, \theta_{0}^{\text{new}})])^{-1} s(d, \theta_{0}^{\text{new}}), \) and \( \eta(z) = E[\psi(D_{j}^{\text{new}}) | Z_{j}^{\text{new}} = z] \).

In the linear expansion (19), \( \sqrt{2n/3} \) 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 also assume (slow) convergence rates of the estimated covariate shift and influence functions. Detailed conditions for it to hold can be found in the analysis of our estimation procedures, see Proposition B.5 of Section B.2.

**Assumption D.5.** \( \|w(\cdot)[\hat{\eta}_{\ell}^{X}(\cdot) - \eta(\cdot)]\|_{L_{2}(P)} \to 0 \) in probability, \( E_{P}[w(Z_{i})^{4}\psi(D_{i})] < \infty \) and \( \|\hat{w}_{\ell}(\cdot) - w(\cdot)\|_{L_{2}(P)} \cdot \|\hat{\eta}_{\ell}^{X}(\cdot) - \eta(\cdot)\|_{L_{2}(P)} = o_{P}(1/\sqrt{n}) \) for \( k = 1, 2 \) and \( \ell = 1, 2, 3 \).

The following theorem proved in Appendix F.5 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 no grater than \( O(n^{-1/2}) \).

**Theorem D.6.** Suppose Assumptions D.3, D.4 and D.5 hold, and \( m \geq cn \) for some fixed \( c > 0 \). If an estimator \( \hat{\sigma}_{\text{shift}} \to \sigma_{\text{shift}} \) in probability for the variance \( \sigma_{\text{shift}}^{2} \) defined in (13), then

\[ \mathbb{P} \left( \theta_{m,n}^{\text{cond,new}} \in \left[ \hat{\theta}_{m,n}^{\text{trans,shift}} - \hat{\sigma}_{\text{shift}} \cdot z_{1-\alpha/2}/\sqrt{n}, \hat{\theta}_{m,n}^{\text{trans,shift}} + \hat{\sigma}_{\text{shift}} \cdot z_{1-\alpha/2}/\sqrt{n} \right] | Z_{j}^{\text{new}}, Z_{n} \right), \]

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 \( \hat{\theta}_{m,n}^{\text{trans,shift}} \) is defined in equation (18).

As before, a noteworthy feature of this result is that asymptotically the variance does not depend on \( m \). The inference procedure in Theorem D.6 relies on the construction of \( \hat{\sigma}_{\text{shift}}, \hat{w}_{\ell}(\cdot) \) and \( \hat{\eta}_{\ell}^{X}(\cdot) \). In Section B.1, we provide a stand-alone procedure to obtain \( \hat{\sigma}_{\text{shift}} \) with a single fold \( I_{k} \) (c.f. Algorithm 5) and a detailed procedure to estimate \( \sigma_{\text{shift}}^{2} \) (c.f. Algorithm 6).
E Details for asymptotic linearity

E.1 Asymptotic linearity for conditional inference

Proof of Proposition 3.1. We first show the consistency of \( \hat{\theta}_n \to \theta^0 \) and \( \theta_n^{\text{cond}} \to \theta^0 \), where the convergence in probability is in each entry. The consistency of \( \hat{\theta}_n \) follows directly from the classical results (van der Vaart, 1998, Theorem 5.9). Similarly, we note that \( \theta_n^{\text{cond}} \) is the unique solution to (1) with the score function replaced by \( t(Z_i, \theta) \). Thus, under the given conditions we have the consistency of \( \theta_n^{\text{cond}} \) following (van der Vaart, 1998, Theorem 5.9).

We now employ the Taylor expansion argument to obtain the asymptotic linearity (4) and (5). Recall that \( s(D, \theta) : \mathcal{D} \times \Omega \to \mathbb{R}^p \). Expanding \( \sum_{i=1}^n s(D_i, \theta_n) \) at \( \theta^0 \) yields

\[
0 = \frac{1}{\sqrt{n}} \sum_{i=1}^n s(D_i, \theta^0) + \frac{1}{\sqrt{n}} \sum_{i=1}^n \bar{s}(D_i, \theta^0)(\hat{\theta}_n - \theta^0) + \frac{1}{2\sqrt{n}} \sum_{i=1}^n (\hat{\theta}_n - \theta^0) \bar{s}^\top(D_i, \hat{\theta}_n)(\hat{\theta}_n - \theta^0),
\]

where the random vector \( \hat{\theta}_n \) lies within the segment between \( \theta^0 \) and \( \hat{\theta}_n \). Rearranging the terms, we have

\[
-\frac{1}{\sqrt{n}} \sum_{i=1}^n s(D_i, \theta^0) = \left( \frac{1}{n} \sum_{i=1}^n s(D_i, \theta^0) + \frac{1}{2n} \sum_{i=1}^n (\hat{\theta}_n - \theta^0) \bar{s}^\top(D_i, \hat{\theta}_n) \right) \cdot \sqrt{n}(\hat{\theta}_n - \theta^0).
\]

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

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

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

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

That is, the asymptotic linearity (4) holds with

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

On the other hand, recall the observation that \( \theta_n^{\text{cond}} \) is the unique solution to (1) with the score function replaced by \( t(Z_i, \theta) \). Meanwhile, condition (iv) implies also \( \| s_t(Z, \theta) \| \leq \mathbb{E}[g(D) \mid Z] \) due to Jensen’s inequality; and \( \mathbb{E}[t(Z, \theta^0) \mid Z] = E[s(D, \theta^0)] \) due to the tower property of conditional expectations and the exchangeability of expectation and derivative in (iv). Following exactly the same arguments, we have

\[
\sqrt{n}(\theta_n^{\text{cond}} - \theta^0) = -\frac{1}{\sqrt{n}} \sum_{i=1}^n (\mathbb{E}[s(D, \theta^0)])^{-1}t(Z_i, \theta^0) + o_P(1)
\]

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

That is, the asymptotic linearity (5) holds with the same \( \phi(D) \). Therefore, we complete the proof of Proposition 3.1.

E.2 Justification for asymptotic linearity in main text

In this part, we show that the asymptotic linearity in Assumption 3.10 of the main text holds under the consistency of \( \hat{\omega} \) and regularity conditions that are similar to Proposition 3.1 in the main text.
Proposition E.1. Suppose conditions (ii), (iii) in Proposition 3.1 hold also at \( \theta = \theta_{0}^{\text{new}} \) and the following two conditions hold: (i') \( \theta_{0}^{\text{new}} \) is the unique solution to (10), \( \theta_{\text{cond,new}}^{m} \) is the unique solution to (9) and \( \theta_{n}^{\text{trans}} \) is the unique solution to (11). (iv') For each \( j, k \), \( \| s_{j,k}(D, \theta) \| = \| \theta s(D, \theta) / \partial \theta_{j} \partial \theta_{k} \| \leq g(D) \), where \( g(D) \) and \( g(D)w(Z) \) are both integrable. Also, both \( \mathbb{E}[s(D, \theta_{0}^{\text{new}})] \) and \( \mathbb{E}[w(Z)s(D, \theta_{0}^{\text{new}})] \) are non-singular matrices. Then Assumption 3.10 holds if \( \sup_{z} |\hat{w}(z) - w(z)| \) converges to zero in probability.

Proof of Proposition E.1. Since \( \hat{w} \) is obtained from an external dataset, we condition on the training process of \( \hat{w} \); in this way, we view \( \hat{w}(\cdot) \) as fixed. Also, without loss of generality we suppose \( \sup_{\theta} |\hat{s}(D, \theta_{0}^{\text{new}}) - s(D, \theta)| \) converges to zero as \( n \to \infty \).

We first show \( \theta_{n}^{\text{trans}} \xrightarrow{P} \theta_{0}^{\text{new}} \). To this end, we utilize Theorem 5.9 of van der Vaart (1998) and define

\[
\hat{S}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \hat{w}(Z_i) s(D_i, \theta), \quad S(\theta) = \mathbb{E}[w(Z)s(D, \theta)],
\]

so that it suffices to show (a) \( \sup_{\theta \in \Theta} |\hat{S}(\theta) - S(\theta)| \to 0 \) in probability, and (b) for any \( \epsilon > 0 \), there exists some \( \delta > 0 \) such that \( \inf_{\| \theta - \theta_{0}^{\text{new}} \| > \delta} |S(\theta) - S(\theta_{0}^{\text{new}})| > \epsilon \). Firstly, for any fixed \( \theta \in \Theta \), we have

\[
|\hat{S}(\theta) - S(\theta)| \leq \frac{1}{n} \sum_{i=1}^{n} |\hat{w}(Z_i) - w(Z_i)| \cdot |s(D_i, \theta)| + \left| \frac{1}{n} \sum_{i=1}^{n} w(Z_i) s(D_i, \theta) - S(\theta) \right|
\]

where

\[
\frac{1}{n} \sum_{i=1}^{n} |\hat{w}(Z_i) - w(Z_i)| \cdot |s(D_i, \theta)| \leq \sup_{z} |\hat{w}(z) - w(z)| \cdot \frac{1}{n} \sum_{i=1}^{n} |s(D_i, \theta)| = o_{P}(1)
\]

by the consistency assumption 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 van der Vaart (1998)). Thus we have \( \theta_{n}^{\text{trans}} \to \theta_{0}^{\text{new}} \) in probability as \( n \to \infty \).

We now employ a Taylor expansion argument to show the asymptotic linearity. Expanding \( \hat{S}(\theta_{n}^{\text{trans}}) \) at \( \theta_{0}^{\text{new}} \) yields

\[
0 = \sum_{i=1}^{n} \hat{w}(Z_i)s(D_i, \theta_{0}^{\text{new}}) + \sum_{i=1}^{n} \hat{w}(Z_i)\hat{s}(D_i, \theta_{0}^{\text{new}})(\hat{\theta}_{n}^{\text{trans}} - \theta_{0}^{\text{new}})
\]

\[
+ \frac{1}{2} \sum_{i=1}^{n} \hat{w}(Z_i)(\hat{\theta}_{n}^{\text{trans}} - \theta_{0}^{\text{new}})^{\top}(\hat{\theta}_{n}^{\text{trans}} - \theta_{0}^{\text{new}}).
\]

Utilizing the fact that each entry of \( \hat{s}(D_i, \theta_{0}^{\text{new}}) \) is controlled by an integrable \( g(D_i) \), the random variable

\[
\frac{1}{n} \sum_{i=1}^{n} \hat{w}(Z_i)\hat{s}(D_i, \theta_{0}^{\text{new}}) = \frac{1}{n} \sum_{i=1}^{n} (\hat{w}(Z_i) - w(Z_i))\hat{s}(D_i, \theta_{0}^{\text{new}}) + \frac{1}{n} \sum_{i=1}^{n} w(Z_i)\hat{s}(D_i, \theta_{0}^{\text{new}})
\]

is of order \( O_{P}(1) \), hence

\[
\frac{1}{2n} \sum_{i=1}^{n} \hat{w}(Z_i)(\hat{\theta}_{n}^{\text{trans}} - \theta_{0}^{\text{new}})^{\top}\hat{s}(D_i, \theta_{0}^{\text{new}}) = o_{P}(1).
\]

The above \( O_{P}(1) \) and \( o_{P}(1) \) are both in the entry-wise sense. Reorganizing the Taylor expansion,

\[
-\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \hat{w}(Z_i)s(D_i, \theta_{0}^{\text{new}}) = \left( O_{P}(1) + \frac{1}{n} \sum_{i=1}^{n} \hat{w}(Z_i)\hat{s}(D_i, \theta_{0}^{\text{new}}) \right) \cdot \sqrt{n}(\hat{\theta}_{n}^{\text{trans}} - \theta_{0}^{\text{new}}).
\]
Following similar arguments as before, we also have

$$ \frac{1}{n} \sum_{i=1}^{n} \hat{w}(Z_i) \hat{s}(D_i, \theta_{0}^{\text{new}}) = \mathbb{E}[w(Z_i)\hat{s}(D_i, \theta_{0}^{\text{new}})] + o_P(1). $$

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

$$ \sqrt{n}(\hat{\theta}_n^{\text{trans}} - \theta_0^{\text{new}}) = -\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \mathbb{E}[w(Z_i)\hat{s}(D_i, \theta_{0}^{\text{new}})] \right)^{-1} \hat{w}(Z_i)\hat{s}(D_i, \theta_0^{\text{new}}) + o_P(1), $$

which is equivalent to the linear expansion for $\hat{\theta}_n^{\text{trans}}$ in Assumption 3.10 by the definition of $\psi(\cdot)$.

We now show the linear expansion of $\theta_{m}^{\text{cond,new}}$. Note that the conditions in Proposition E.1 imply the same conditions as Proposition 3.1 when we substitute $(D_i, Z_i) \sim \mathbb{P}$ with $(D_i^{\text{new}}, Z_i^{\text{new}}) \sim \mathbb{Q}$. Thus, applying the same arguments as those in the proof of Proposition 3.1 leads to the linear expansion of $\theta_{m}^{\text{cond,new}}$ in Assumption 3.10 of the main text. Therefore, we complete the proof of Proposition E.1.

\[\blacksquare\]

### E.3 Justification for asymptotic linearity with cross-fitting in Section D.2

In this part, we justify the asymptotic linearity for cross-fitted estimators in Assumption D.4 of Section D.2; we show that it holds under consistency of $\hat{w}_i$ (Assumption D.3) and mild regularity conditions.

**Proposition E.2.** Suppose Assumption D.3, conditions (ii), (iii) in Proposition 3.1 and conditions (iv') in Proposition E.1 hold. Also, suppose the following condition hold: (i") $\theta_{0}^{\text{new}}$ is the unique solution to (10), $\theta_{m}^{\text{cond,new}}$ is the unique solution to (9) and $\theta_{n}^{\text{new},(f)}$ is the unique solution to (17). Then Assumption D.4 holds.

**Proof of Proposition E.2.** The proof is quite similar to that of Proposition E.1, except for the notational complexity and the change in sample size due to cross-fitting. The asymptotic linearity of $\theta_{m}^{\text{cond,new}}$ has been proved in Proposition E.1. We thus only need to prove (19) for $\theta_{n}^{\text{new},(f)}$.

We first show the consistency of $\theta_{n}^{\text{new},(f)} \xrightarrow{P} \theta_0^{\text{new}}$. Without loss of generality, the sample size is $|\mathcal{I} \setminus \mathcal{I}_c| = 2n/3$. To this end, we utilize Theorem 5.9 of van der Vaart (1998), so that it suffices to show (a) $\sup_{\theta \in \Theta} |\tilde{S}(\theta) - S(\theta)| \to 0$ in probability, and (b) for any $\epsilon > 0$, there exists some $\delta > 0$ such that $\inf_{\theta \neq \theta_0^{\text{new}}} |S(\theta) - S(\theta_0^{\text{new}})| > \epsilon$, where we define

$$ \tilde{S}(\theta) = \frac{3}{2n} \sum_{i \notin \mathcal{I}_c} \hat{w}_i(Z_i) s(D_i, \theta), \quad S(\theta) = \mathbb{E}[w(Z)s(D, \theta)]. $$

Firstly, for any fixed $\theta \in \Theta$, we have

$$ \left| \tilde{S}(\theta) - S(\theta) \right| \leq \frac{3}{2n} \sum_{i \notin \mathcal{I}_c} \left| \hat{w}_i(Z_i) - w(Z_i) \right| \cdot |s(D_i, \theta)| + \frac{3}{2n} \sum_{i \notin \mathcal{I}_c} w(Z_i) s(D_i, \theta) - S(\theta), $$

where

$$ \frac{3}{2n} \sum_{i \notin \mathcal{I}_c} \left| \hat{w}_i(Z_i) - w(Z_i) \right| \cdot |s(D_i, \theta)| \leq \sup_z \left| \hat{w}_i(z) - w(z) \right| \cdot \frac{3}{2n} \sum_{i \notin \mathcal{I}_c} |s(D_i, \theta)| = o_P(1) $$

by Assumption D.3 and the integrability of $s(D_i, \theta)$. The second term also converges to zero by the law of large numbers. Hence $|\tilde{S}(\theta) - S(\theta)| = o_P(1)$ for any fixed $\theta \in \Theta$. By compactness of $\Theta$ in condition (ii) of Proposition 3.1 as well as the continuity of $\tilde{S}(\theta)$ 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 van der Vaart (1998)). Thus we have $\theta_{n}^{\text{new},(f)} \xrightarrow{P} \theta_0^{\text{new}}$ in probability as $n \to \infty$. 

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Following similar arguments as before, we also have

\[ P \text{ (1)} \quad \frac{3}{2n} \sum_{i \in I_i} \hat{w}_i(Z_i)s(D_i, \theta_0^{\text{new}}) = \frac{3}{2n} \sum_{i \in I_i} (\hat{w}_i(Z_i) - w(Z_i)) s(D_i, \theta_0^{\text{new}}) + \frac{3}{2n} \sum_{i \in I_i} w(Z_i)s(D_i, \theta_0^{\text{new}}) \]

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

\[ \frac{3}{4n} \sum_{i \in I_i} \hat{w}_i(Z_i)(\hat{\theta}_n^{\text{new},(l)} - \theta_0^{\text{new}})^\top \hat{s}(D_i, \theta_0^{\text{new}}) = o_P(1). \]

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

\[ \frac{1}{\sqrt{2n/3}} \sum_{i \in I_i} \hat{w}_i(Z_i)s(D_i, \theta_0^{\text{new}}) = \left( o_P(1) + \frac{3}{2n} \sum_{i \in I_i} \hat{w}_i(Z_i)s(D_i, \theta_0^{\text{new}}) \right) \cdot \sqrt{2n/3}(\hat{\theta}_n^{\text{new},(l)} - \theta_0^{\text{new}}). \]

Following similar arguments as before, we also have

\[ \frac{3}{2n} \sum_{i \in I_i} \hat{w}_i(Z_i)s(D_i, \theta_0^{\text{new}}) = E[w(Z_i)s(D_i, \theta_0^{\text{new}})] + o_P(1). \]

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

\[ \sqrt{2n/3}(\hat{\theta}_n^{\text{new},(l)} - \theta_0^{\text{new}}) = -\frac{1}{\sqrt{2n/3}} \sum_{i \in I_i} \left( E[w(Z_i)s(D_i, \theta_0^{\text{new}})] \right)^{-1} \hat{w}_i(Z_i)s(D_i, \theta_0^{\text{new}}) + o_P(1), \]

which is equivalent to (19) by the definition of \( \psi(\cdot) \). Therefore, we complete the proof of Proposition E.2. \( \square \)

**F Proofs for main results**

**F.1 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 F.1.** Suppose Assumptions 3.2 and 3.3 hold. For any fixed \( x \in \mathbb{R} \), the random variable \( P(\sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) \leq x \mid Z_n) \) 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 (7).

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

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

For notational simplicity, we write

\[ d_n = \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) - \frac{1}{\sqrt{n}} \sum_{i=1}^n \zeta_i, \quad \text{where} \quad \zeta_i = \phi(D_i) - E[\phi(D_i) \mid Z_i], \quad i = 1, \ldots, n, \]

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where \( d_n = o_P(1) \) follows from the given conditions. Hence Lemma 1.4 implies that for any fixed \( \epsilon > 0 \),
\[
\mathbb{P}\left( |d_n| > \epsilon \mid \mathcal{Z}_n \right) = o_P(1). \quad (20)
\]
On the other hand, we denote the conditional law of the essential term as
\[
\mathcal{L}_n = \mathcal{L}\left( \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \phi(D_i) - \mathbb{E}[\phi(D_i) \mid \mathcal{Z}_i] \right) \mid \mathcal{Z}_n \right).
\]
By the conditional CLT in Lemma I.1, taking \( g(X_i) = \phi(D_i) \) and the filtration \( \mathcal{F}_n = \sigma(\mathcal{Z}_n) = \sigma(\{\mathcal{Z}_i\}_{i=1}^{n}) \), we know that the conditional law \( \mathcal{L}_n \) converges almost surely to \( N(0, \sigma^2) \) with \( \sigma^2 \) defined in equation (7).

That is, for any \( x \in \mathbb{R} \), we have
\[
\mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) + d_n \leq x \mid \mathcal{Z}_n \right) \xrightarrow{a.s.} \Phi\left( \frac{x}{\sigma} \right),
\]
where \( \Phi(\cdot) \) is the cumulative distribution function of standard normal distribution. By equation (20), for any constant \( \epsilon > 0 \), it holds that
\[
\mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) \leq x \mid \mathcal{Z}_n \right) = \mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) \leq x, |d_n| \leq \epsilon \mid \mathcal{Z}_n \right) + \mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) \leq x, |d_n| > \epsilon \mid \mathcal{Z}_n \right)
\leq \mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) + d_n \leq x + \epsilon \mid \mathcal{Z}_n \right) + \mathbb{P}(\{|d_n| > \epsilon \mid \mathcal{Z}_n\}) = \Phi\left( \frac{x + \epsilon}{\sigma} \right) + o_P(1). \quad (21)
\]
On the other hand, we have
\[
\mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) \leq x \mid \mathcal{Z}_n \right)
\geq \mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) + d_n \leq x - \epsilon, |d_n| \leq \epsilon \mid \mathcal{Z}_n \right)
\geq \mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) + d_n \leq x - \epsilon \mid \mathcal{Z}_n \right) - \mathbb{P}(\{|d_n| > \epsilon \mid \mathcal{Z}_n\}) = \Phi\left( \frac{x - \epsilon}{\sigma} \right) + o_P(1). \quad (22)
\]
By the arbitrariness of \( \epsilon > 0 \) in equations (21) and (22), for any fixed \( x \in \mathbb{R} \), it holds that
\[
\mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) \leq x \mid \mathcal{Z}_n \right) = \Phi\left( \frac{x}{\sigma} \right) + o_P(1).
\]
Therefore, we conclude the proof of Proposition F.1.

The proof of Theorem 3.4 is as follows.

Proof of Theorem 3.4. By Proposition F.1, for any fixed \( x \in \mathbb{R} \),
\[
\mathbb{P}\left( \sqrt{n}(\hat{\theta}_n - \theta_n^{\text{cond}}) \leq x \mid \mathcal{Z}_n \right) = \Phi(x/\sigma) + o_P(1).
\]
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
\[
\Delta^{\pm}(\epsilon) = \mathbb{P}\left( \sqrt{n}|\hat{\theta}_n - \theta_n^{\text{cond}}| \leq z^{\pm}(\epsilon) \mid \mathcal{Z}_n \right) - \left( 2\Phi\left( z^{\pm}(\epsilon)/\sigma \right) - 1 \right),
\]
we have \( \Delta^{+}(\epsilon), \Delta^{-}(\epsilon) = o_P(1) \) by Proposition F.1. Since the estimator \( \hat{\sigma} \xrightarrow{P} \sigma \), we have
\[
\mathbb{P}\left( \sqrt{n}|\hat{\theta}_n - \theta_n^{\text{cond}}| \leq z_{1-\alpha/2}. \hat{\sigma} \mid \mathcal{Z}_n \right) - (1 - \alpha)
\geq \mathbb{P}\left( \sqrt{n}|\hat{\theta}_n - \theta_n^{\text{cond}}| \leq z_{1-\alpha/2}. (\sigma - \epsilon) \mid \mathcal{Z}_n \right) - (1 - \alpha) + \mathbb{P}(\hat{\sigma} < \sigma - \epsilon \mid \mathcal{Z}_n)
= 2\Phi(z^{-}(\epsilon)/\sigma) - 1 - (1 - \alpha) + \mathbb{P}(\hat{\sigma} < \sigma - \epsilon \mid \mathcal{Z}_n) + \Delta^{-}(\epsilon), \quad (23)
\]
where the conditional probability \( P(\hat{\sigma} < \sigma - \epsilon \mid Z_n) = o_P(1) \) by Lemma I.4. On the other hand, for any fixed constant \( \epsilon > 0 \), we have
\[
P\left( \sqrt{n} |\hat{\theta}_n - \theta^\text{cond}_n| \leq z_{1-\alpha/2} \cdot \hat{\sigma} \mid Z_n \right)
\leq P\left( \sqrt{n} |\hat{\theta}_n - \theta^\text{cond}_n| \leq z_{1-\alpha/2} \cdot (\sigma + \epsilon) \mid Z_n \right) + P(\hat{\sigma} > \sigma + \epsilon \mid Z_n)
= 2\Phi\left( \frac{z^+ (\epsilon)}{\sigma} \right) - 1 - (1 - \alpha) + P(\hat{\sigma} < \sigma + \epsilon \mid Z_n) + \Delta^+ (\epsilon),
\]
where \( P(\hat{\sigma} > \sigma + \epsilon \mid Z_n) = o_P(1) \) by Lemma I.4. Thus for any fixed constant \( \delta > 0 \), we can choose some fixed \( \epsilon > 0 \) such that \( 2\Phi(\frac{z^- (\epsilon)}{\sigma}) - 1 - (1 - \alpha) > -\delta/2 \) and \( 2\Phi(\frac{z^+ (\epsilon)}{\sigma}) - 1 - (1 - \alpha) < \delta/2 \). Combining equations (23) and (24), we have
\[
P\left( P\left( \sqrt{n} |\hat{\theta}_n - \theta^\text{cond}_n| \leq z_{1-\alpha/2} \cdot \hat{\sigma} \mid Z_n \right) - (1 - \alpha) \right) > \delta
\leq P(P(\hat{\sigma} < \sigma - \epsilon \mid Z_n) + \Delta^- (\epsilon) < -\delta/2) + P(P(\hat{\sigma} < \sigma + \epsilon \mid Z_n) + \Delta^+ (\epsilon) > \delta/2) \to 0.
\]
By the arbitrariness of \( \delta > 0 \), we complete the proof of Theorem 3.4.

F.2 Proof of Theorem 3.8

Proof of Theorem 3.8. We note that all the methods and conditions in Theorem 3.8 can be viewed as a special case for those in Section D.1 with \( w(z) \equiv 1 \). Thus, Theorem 3.8 could be viewed as a corollary for Theorem D.2, whose proof is in Section F.4 in this supplementary material.

F.3 Proof of Theorem 3.11

Proof of Theorem 3.11. Throughout this proof, we condition on the training process of \( \hat{w} \) and \( \hat{\eta} \), so that they are deterministic functions. All probabilities and expectations are with respect to the i.i.d. samples in the two datasets. By Assumption 3.10 and the fact that \( m \geq \epsilon n \), we have
\[
\hat{\theta}^\text{trans}_{m,n} - \theta^\text{cond}_{m,new}
= \frac{1}{n} \sum_{i=1}^{n} \psi(D_i) \hat{w}(Z_i) - \frac{1}{n} \sum_{i=1}^{n} \hat{\eta}(Z_i) \hat{w}(Z_i) + \frac{1}{m} \sum_{j=1}^{m} (\hat{\eta}(Z^\text{new}_j) - \eta(Z^\text{new}_j)) + o_P(1/\sqrt{n})
= \frac{1}{n} \sum_{i=1}^{n} (\psi(D_i) - \eta(Z_i)) \hat{w}(Z_i) - \frac{1}{n} \sum_{i=1}^{n} (\hat{\eta}(Z_i) - \eta(Z_i)) (\hat{w}(Z_i) - w(Z_i))
+ \frac{1}{m} \sum_{j=1}^{m} (\hat{\eta}(Z^\text{new}_j) - \eta(Z^\text{new}_j)) - \frac{1}{n} \sum_{i=1}^{n} (\hat{\eta}(Z_i) - \eta(Z_i)) w(Z_i) + o_P(1/\sqrt{n}).
\]
We now treat these three terms separately. Firstly, term (i) can be decomposed as
\[
(i) = \frac{1}{n} \sum_{i=1}^{n} (\psi(D_i) - \eta(Z_i)) (\hat{w}(Z_i) - w(Z_i)) + \frac{1}{n} \sum_{i=1}^{n} (\psi(D_i) - \eta(Z_i)) w(Z_i),
\]
where each i.i.d. copy in the first summation obeys
\[
\mathbb{E}\left[ (\psi(D_i) - \eta(Z_i)) (\hat{w}(Z_i) - w(Z_i)) \right] = \mathbb{E}\left[ \mathbb{E}[\psi(D_i) - \eta(Z_i) \mid Z_i] \cdot (\hat{w}(Z_i) - w(Z_i)) \right] = 0.
\]
By Markov’s inequality, we have
\[
\frac{1}{n} \sum_{i=1}^{n} (\psi(D_i) - \eta(Z_i)) (\hat{w}(Z_i) - w(Z_i))
= O_P\left( \|\psi(D) - \eta(Z)\|_{L_2(\mathbb{P})} \cdot \|\hat{w}(Z) - w(Z)\|_{L_2(\mathbb{P})} / \sqrt{n} \right) = o_P(1/\sqrt{n})
\]
due to the consistency condition on \( \hat{w} \). Secondly, by the product rate of \( \hat{\eta} \) and \( \hat{w} \), term (ii) can be bounded by Cauchy-Schwarz inequality as 

\[
|\text{(ii)}| \leq O_P\left(\|\hat{w}(\cdot) - w(\cdot)\|_{L_2(P)} \cdot \|\hat{\eta}(\cdot) - \eta(\cdot)\|_{L_2(P)}\right) = o_P(1/\sqrt{n}).
\]

Noting the covariate shift between \( Z_i \) and \( Z_j^{\text{new}} \), we know that

\[
E[\hat{\eta}(Z_j^{\text{new}}) - \eta(Z_j^{\text{new}})] = E[(\hat{\eta}(Z_i) - \eta(Z_i))w(Z_i)].
\]

Subtracting both sides from term (iii), we obtain

\[
(iii) = \frac{1}{m} \sum_{j=1}^{m} \left( \hat{\eta}(Z_j^{\text{new}}) - \eta(Z_j^{\text{new}}) - \hat{\eta}(Z_j^{\text{new}}) - \eta(Z_j^{\text{new}}) \right)
- \frac{1}{n} \sum_{i=1}^{n} \left( (\hat{\eta}(Z_i) - \eta(Z_i))w(Z_i) - E[(\hat{\eta}(Z_i) - \eta(Z_i))w(Z_i)] \right).
\]

In the first summation, the i.i.d. copies are mean zero with variance bounded by \( \|\hat{\eta}(Z_j^{\text{new}}) - \eta(Z_j^{\text{new}})\|_{L_2(Q)} = o_P(1) \). By Markov’s inequality, the first summation is bounded by \( o_P(1/\sqrt{n}) \). Similarly, the second summation is also bounded by \( o_P(1/\sqrt{n}) \). Thus, we have (iii) = \( o_P(1/\sqrt{n}) \). Combining the three terms together, we obtain

\[
\sqrt{n}(\hat{\theta}_{m,n}^{\text{trans}} - \theta_{m,n}^{\text{cond,new}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \psi(D_i) - \eta(Z_i) \right)w(Z_i) + o_P(1).
\]

Applying the conditional CLT in Lemma 1.1 to \( g(X_i) = \psi(D_i)w(Z_i) \) and the filtration

\[
\mathcal{F}_n = \sigma\{\{Z_i\}_{i=1}^{n} \cup \{Z_j^{\text{new}}\}_{j=1}^{m}\},
\]

we know that conditional on (almost all) \( Z_m^{\text{new}} \cup Z_n \), \( \sqrt{n}(\hat{\theta}_{m,n}^{\text{trans}} - \theta_{m,n}^{\text{cond,new}}) \) converges in distribution to \( N(0, \sigma_{\text{shift}}^2) \). Finally, by the consistency of \( \sigma_{\text{shift}}^2 \) and the Slutsky’s theorem, we obtain the conditional validity of the confidence intervals. We thus complete the proof of Theorem D.2.

\[\square\]

## F.4 Proof of Theorem D.2

**Proof of Theorem D.2.** Recall that \( \eta(\cdot) = E[\psi(D) \mid Z = z] \); by the invariance of conditional distribution of \( D \) given \( Z \), we have \( E[\psi(D_i) \mid Z_i] = \eta(Z_i) \) and \( E[\psi(D_j^{\text{new}}) \mid Z_j^{\text{new}}] = \eta(Z_j^{\text{new}}) \) for all \( i \in [n] \) and all \( j \in [m] \). In the following, we are to show that

\[
\hat{\theta}_{m,n}^{\text{trans}} - \theta_{m,n}^{\text{cond,new}} = \frac{1}{n} \sum_{i=1}^{n} w(Z_i) \left( \psi(D_i) - \eta(Z_i) \right) + o_P\left(1/\sqrt{n \min(n,m)}\right).
\]

By the asymptotic linearity in Assumption 3.10 (with \( \hat{w} := w \)), we have

\[
\hat{\theta}_{n} - \theta_{m,n}^{\text{cond,new}} = \frac{1}{n} \sum_{i=1}^{n} w(Z_i) \psi(D_i) - \frac{1}{m} \sum_{j=1}^{m} \eta(Z_j^{\text{new}}) + o_P\left(1/\sqrt{n} + 1/\sqrt{m}\right).
\]

By the definition of \( \hat{\theta}_{m,n}^{\text{trans}} \) in equation (16), we have the decomposition

\[
\hat{\theta}_{m,n}^{\text{trans}} - \theta_{m,n}^{\text{cond,new}} = \hat{\theta}_{n} - \theta_{m,n}^{\text{cond,new}} - \hat{\theta}_{n} + \hat{\theta}_{m,n}^{\text{trans}} - \theta_{m,n}^{\text{cond,new}}
= \frac{1}{n} \sum_{i=1}^{n} w(Z_i) \psi(D_i) - \hat{\theta}_{n} + \frac{1}{m} \sum_{j=1}^{m} \eta(Z_j^{\text{new}}) + o_P\left(1/\sqrt{n} + 1/\sqrt{m}\right).
\]

By the definition of \( \hat{\theta}_{m,n}^{\text{trans}} \) in equation (16), we have the decomposition

\[
\hat{\theta}_{m,n}^{\text{trans}} - \theta_{m,n}^{\text{cond,new}} = \hat{\theta}_{n} - \theta_{m,n}^{\text{cond,new}} - \hat{\theta}_{n} + \hat{\theta}_{m,n}^{\text{trans}} - \theta_{m,n}^{\text{cond,new}}
= \frac{1}{n} \sum_{i=1}^{n} w(Z_i) \left( \psi(D_i) - \eta(Z_i) \right) + o_P\left(1/\sqrt{n} + 1/\sqrt{m}\right) + (i) + (ii).
\]
where

\[(i) = \frac{1}{n} \sum_{i=1}^{n} w(Z_i) \eta(Z_i) - \frac{1}{2|I_1|} \sum_{i \in I_1} w(Z_i) \hat{\eta}^{T_2}(Z_i) - \frac{1}{2|I_2|} \sum_{i \in I_2} w(Z_i) \hat{\eta}^{T_1}(Z_i)\]

\[+ \frac{1}{2} \mathbb{E}_P[w(Z) \hat{\eta}^{T_2}(Z) \mid I_1] + \frac{1}{2} \mathbb{E}_P[w(Z) \hat{\eta}^{T_2}(Z) \mid I_2],\]

\[(ii) = \frac{1}{2m} \sum_{j=1}^{m} \{\hat{\eta}^{T_1}(Z_j^{\text{new}}) + \hat{\eta}^{T_2}(Z_j^{\text{new}})\} - \frac{1}{m} \sum_{j=1}^{m} \eta(Z_j^{\text{new}}) - \frac{1}{2} \mathbb{E}_Q[\hat{\eta}^{T_1}(Z) \mid I_1] - \frac{1}{2} \mathbb{E}_Q[\hat{\eta}^{T_2}(Z) \mid I_2].\]

Here the decomposition utilizes the fact that

\[\mathbb{E}_P[w(Z_i) \hat{\eta}^{T_k}(Z_i) \mid I_k] = \mathbb{E}_Q[\hat{\eta}^{T_k}(Z_j^{\text{new}}) \mid I_k]\]

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

In the sequel, we bound the terms (i) and (ii) separately. Since \(I_1\) and \(I_2\) are (approximately) equal-sized with \(|I_1| + |I_2| = n\), we have

\[(i) = \frac{1}{2|I_1|} \sum_{i \in I_1} w(Z_i) \eta(Z_i) - \frac{1}{2|I_1|} \sum_{i \in I_1} w(Z_i) \hat{\eta}^{T_2}(Z_i) + \frac{1}{2} \mathbb{E}_P[w(Z) \hat{\eta}^{T_2}(Z) \mid I_2] + O_P(1/n).\]

For the term (i,a), we note that for \(i \in I_1\) where \((D_i, Z_i) \sim \mathbb{P}\),

\[\mathbb{E}[w(Z_i) \eta(Z_i) \mid I_2] = \mathbb{E}_Q[\eta(Z)] = 0.\]

Hence we can write (i,a) = \(\frac{1}{2|I_1|} \sum_{i \in I_1} \xi_i\), where

\[\xi_i = w(Z_i)(\eta(Z_i) - \hat{\eta}^{T_2}(Z_i)) - \mathbb{E}[w(Z_i) \eta(Z) - w(Z_i) \hat{\eta}^{T_2}(Z) \mid I_2].\]

Conditional on \(I_2\), \(\{\xi_i\}_{i \in I_1}\) are i.i.d. with mean zero, since the estimation of \(\hat{\eta}^{T_2}\) does not use data in \(I_1\). Therefore, we have

\[\mathbb{E}[(i,a)^2 \mid I_2] = \frac{1}{4|I_1|} \mathbb{E}[\xi_i^2 \mid I_2] \leq \frac{1}{4|I_1|} \|w(\cdot)(\eta(\cdot) - \hat{\eta}^{T_2}(\cdot))\|_{L_2(\mathbb{P})}^2,\]

where \(\|w(\cdot)(\eta(\cdot) - \hat{\eta}^{T_2}(\cdot))\|_{L_2(\mathbb{P})}^2 = \mathbb{E}[(w(Z)(\eta(Z) - \hat{\eta}^{T_2}(Z))^2)]\) for an independent copy \(Z \sim \mathbb{P}\). Thus, by Assumption D.1, we have \(n \cdot \mathbb{E}[(i,a)^2 \mid I_2] = o_P(1)\). Referring to Lemma 1.4 for non-negative random variables \(n \cdot (i,a)^2\) and the filtration composed of \(I_2\), 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

\[\hat{\theta}^{\text{trans}, \text{new}}_{m,n} - \theta^{\text{cond}, \text{new}}_m = \frac{1}{n} \sum_{i=1}^{n} w(Z_i)(\psi(D_i) - \eta(Z_i)) + o_P\left(1/\sqrt{n} + 1/\sqrt{m}\right).\]
Assumption D.5, we have
\[ \hat{\theta} \]
Furthermore, note that the estimation of \( \hat{\theta} \)

Invoking Lemma I.5 and by symmetry of \( \mathcal{D} \)

We bound the two terms (i) and (ii) separately. Since the folds \( \mathcal{D}, \mathcal{I}_{\ell,1}, \mathcal{I}_{\ell,2} \) are disjoint, conditional on \( \mathcal{I}_{\ell} \cup \mathcal{I}_{\ell,1} \cup \mathcal{I}_{\ell,2}, \{ \Delta_w(Z_i) \Delta_{\eta}^\ell(Z_i) \}_{i \in I_{\ell,2}} \) are i.i.d. random variables. By Cauchy-Schwarz inequality and Assumption D.5, we have

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

Invoking Lemma I.5 and by symmetry of \( \mathcal{I}_{\ell,1} \) and \( \mathcal{I}_{\ell,2} \), we know that

\[ \left| \langle i \rangle \right| = \left| \frac{3}{2n} \sum_{i \in I_{\ell,1}} \Delta_w(Z_i) \Delta_{\eta}^\ell(Z_i) + \frac{3}{2n} \sum_{i \in I_{\ell,2}} \Delta_w(Z_i) \Delta_{\eta}^\ell(Z_i) \right| = o_P(1/\sqrt{n}). \]

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

\[ \mathbb{E} \left[ \Delta_{\eta}^k(Z_i) \bigg| \mathcal{I}_{\ell} \cup \mathcal{I}_{\ell,new} \cup \mathcal{I}_{\ell,k} \right] = \mathbb{E}_Q \left[ \Delta_{\eta}^k(Z_j) \bigg| \mathcal{I}_{\ell} \cup \mathcal{I}_{\ell,k} \cup \mathcal{I}_{\ell,new} \cup \mathcal{I}_{\ell,k} \right] \]
for \( i \in \mathcal{I}_{\ell,3-k} \) and \( j \in \mathcal{I}_{\ell,3-k} \), \( k = 1, 2 \). Then we have

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

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

\[
n \cdot E \left[ \left( \frac{3}{2n} \sum_{i \in \mathcal{I}_{\ell,1}} \left( w(Z_i) \Delta_{\eta}^{(2)}(Z_i) - E^{(2)}_\Delta \right) \right)^2 \right]_{\mathcal{I}_\ell \cup \mathcal{I}_\ell^{\text{new}} \cup \mathcal{I}_{\ell,2} \cup \mathcal{I}_{\ell,\text{new}}^{\text{new}}}
= 3/2 \cdot \| w(\cdot) \Delta_{\eta}^{(2)}(\cdot) \|_{L^2(P)}^2 = o_P(1)
\]

by Assumption D.5. Invoking Lemma 1.5 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

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

(25)

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

\[
n \cdot E \left[ \frac{3}{2n} \sum_{i \in \mathcal{I}_{\ell}} \Delta_w(Z_i)(\psi(D_i) - \eta(Z_i)) \right]_{\mathcal{I}_\ell \cup \mathcal{I}_\ell^{\text{new}}}
= 3/2 \cdot \| \Delta_w(Z_i)(\psi(D_i) - \eta(Z_i)) \|_{L^2(P)}^2
\leq 3/2 \cdot \sup_z | \tilde{w}_\ell(z) - w(z) |^2 \cdot \| \psi(D_i) - \eta(Z_i) \|_{L^2(P)}^2 = o_P(1).
\]

The last equation follows from \( \sup_z | \tilde{w}_\ell(z) - w(z) | = o_P(1) \) in Assumption D.5 as well as the fact that \( \psi(D_i) \) and \( \eta(Z_i) \) both have finite \( L^2(P) \) norms. Invoking Lemma 1.5, we know

\[
\frac{3}{2n} \sum_{i \in \mathcal{I}_{\ell}} \Delta_w(Z_i)(\psi(D_i) - \eta(Z_i)) = o_P(1/\sqrt{n}).
\]

(26)

Combining equations (25) and (26), we have

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

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

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

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

\[
\sqrt{n}(\tilde{\theta}_m^{\text{trans}, \text{shift}} - \hat{\theta}_m^{\text{cond}, \text{new}}) = \frac{1}{\sqrt{n}} \sum_{i=1}^n w(Z_i)(\psi(D_i) - \eta(Z_i)) + o_P(1).
\]
Finally, applying the conditional central limit theorem of Lemma I.1 to \( w(Z_i)(\psi(D_i) - \eta(Z_i)) \) which has finite fourth moment, and invoking Lemma I.4, it holds for any \( x \in \mathbb{R} \) that

\[
P\left( \sqrt{n}(\hat{\theta}_{m,n}^{\text{trans,shift}} - \theta_{m,n}^{\text{cond,new}}) \leq x \mid Z_{m,n}^{\text{new}}, Z_n \right) = \Phi(x/\sigma_{\text{shift}}) + o_P(1).
\]

Since \( \sigma_{\text{shift}} \to \sigma_{\text{shift}} \) in probability, with exactly the same arguments as those in the proof of Theorem 3.4, we obtain the desired result in Theorem D.6.

\[\square\]

G Proof of extension results

G.1 Proof of fixed-attributes results

**Proof of Proposition C.2.** We first show that \( \hat{\theta}_n \to_P \theta_{\text{cond}} \). By the optimality of \( \theta_{\text{cond}} \), we have the first-order condition \( \nabla L_n(\theta_{\text{cond}}) = 0 \), i.e., \( \sum_{i=1}^n \mathbb{E} [\nabla \ell(D_i, \theta) \mid z_i] = 0 \) with the exchangeability of gradient and expectation under Assumption C.1. By definition, we have \( \nabla^2 \hat{L}_n(\theta_{\text{cond}}) - \nabla^2 L_n(\theta_{\text{cond}}) = \frac{1}{n} \sum_{i=1}^n (\nabla^2 \ell(D_i, \theta_{\text{cond}}) - \mathbb{E}[\nabla^2 \ell(D_i, \theta_{\text{cond}}) \mid z_i]) \), which converges (elementwise) to zero by the law of large numbers. In particular, it holds with probability tending to 1 that

\[
\nabla^2 \hat{L}_n(\theta_{\text{cond}}) - \nabla^2 L_n(\theta_{\text{cond}}) \succeq -c_2/2 \cdot I_{p \times p}.
\]

Recalling condition (iv), we now invoke Lemma I.6 on the event that \( (27) \) holds, and take \( f = \hat{L}_n, \theta = \hat{\theta}_n, \theta_0 = \theta_{\text{cond}}, \) and \( \lambda = c_2/2, c = c_1 \). By the fact that \( \hat{L}_n(\hat{\theta}_n) \leq \hat{L}_n(\theta_{\text{cond}}) \), we have

\[
\min \{ \| \hat{\theta} - \theta_{\text{cond}} \|^2, c_1 \| \hat{\theta} - \theta_{\text{cond}} \| \} \leq \frac{2}{\lambda} (\hat{L}_n(\hat{\theta}_n) - \hat{L}_n(\theta_{\text{cond}}) - \nabla \hat{L}_n(\theta_{\text{cond}}) \top (\hat{\theta}_n - \theta_{\text{cond}})) \\
\leq \frac{2}{\lambda} \| \nabla \hat{L}_n(\theta_{\text{cond}}) \| \cdot \| \hat{\theta} - \theta_{\text{cond}} \|.
\]

We further note by the law of large numbers that \( \nabla \hat{L}_n(\theta_{\text{cond}}) - \nabla L_n(\theta_{\text{cond}}) = o_P(1) \) with entrywise convergence. Thus, \( \| \nabla \hat{L}_n(\theta_{\text{cond}}) \| = o_P(1) \), and the above inequality leads to \( \| \hat{\theta}_n - \theta_{\text{cond}} \| = o_P(1) \).

We then use Taylor expansion of \( \nabla \hat{L}_n \) around \( \hat{\theta}_n \) to show the asymptotic linearity. As \( \nabla \hat{L}_n(\hat{\theta}_n) = 0 \),

\[
-\nabla \hat{L}_n(\theta_{\text{cond}}) = \nabla^2 \hat{L}_n(\hat{\theta}_n)(\hat{\theta}_n - \theta_{\text{cond}}),
\]

where \( \hat{\theta}_n \) lies on the segment between \( \hat{\theta}_n \) and \( \theta_{\text{cond}} \). Thus, condition (iii) in Assumption C.1 implies

\[
\| \nabla^2 \hat{L}_n(\theta_{\text{cond}}) \|_{op} \leq \frac{1}{\sqrt{n}} \sum_{i=1}^n m_n(D_i)^2 \| \hat{\theta}_n - \theta_{\text{cond}} \| \leq \frac{1}{\sqrt{n}} \sum_{i=1}^n m_n(D_i)^2 \| \hat{\theta}_n - \theta_{\text{cond}} \| = o_P(1).
\]

Also, the law of large numbers implies \( \| \nabla^2 \hat{L}_n(\theta_{\text{cond}}) - \nabla^2 L_n(\theta_{\text{cond}}) \|_{op} = o_P(1) \), which further implies \( \| \nabla^2 \hat{L}_n(\hat{\theta}_n) - \nabla^2 L_n(\theta_{\text{cond}}) \|_{op} = o_P(1) \). Combining this fact with \( (28) \), we have

\[
-\frac{1}{\sqrt{n}} \sum_{i=1}^n \nabla \ell(D_i, \theta_{\text{cond}}) = (\nabla^2 L_n(\theta_{\text{cond}}) + o_P(1)) \cdot \sqrt{n}(\hat{\theta}_n - \theta_{\text{cond}}),
\]

which completes the proof of Proposition C.2.

\[\square\]

**Proof of Theorem C.3.** By Proposition C.2, one has

\[
\Sigma_n^{-1/2} \sqrt{n}(\hat{\theta}_n - \theta_{\text{cond}}) = -\text{Var}(\sqrt{n} \nabla \hat{L}_n(\theta_{\text{cond}}))^{-1/2} \frac{1}{\sqrt{n}} \sum_{i=1}^n \nabla \ell(D_i, \theta_{\text{cond}}) + o_P(1).
\]

Note that \( \nabla \ell(D_i, \theta_{\text{cond}}) \) are mutually independent. By condition (v) in Assumption C.1 and invoking the Lyapunov’s Central Limit Theorem (Billingsley, 1995), we obtain the asymptotic normal distribution and completes the proof of Theorem C.3.

\[\square\]
Proof of Proposition C.4. We first show that \( \widetilde{M}^{-1} = \left( \frac{1}{n} \sum_{i=1}^{n} E[\tilde{\ell}(D_i, \theta_{n}^{\text{cond}})] \right)^{-1} + o_P(1) \). By condition (iii) in Assumption C.1, we have \( \left| \frac{1}{n} \sum_{i=1}^{n} \tilde{\ell}(D_i, \theta_{n}^{\text{cond}}) \right| \leq \frac{1}{n} \sum_{i=1}^{n} m_n(D_i) \cdot |\theta_n - \theta_{n}^{\text{cond}}| = o_P(1) \) since \( |\theta_n - \theta_{n}^{\text{cond}}| = o_P(1) \) from Proposition C.2. The law of large numbers thus implies the desired result by noting that \( \frac{1}{n} \sum_{i=1}^{n} E[\tilde{\ell}(D_i, \theta_{n}^{\text{cond}})] = o_P(1) \). Hence \( \widetilde{M}^{-1} = \left( \frac{1}{n} \sum_{i=1}^{n} E[\tilde{\ell}(D_i, \theta_{n}^{\text{cond}})] \right)^{-1} + o_P(1) \) as the latter is strictly positive definite by condition (iv).

Furthermore, by condition (iii) of Assumption C.1 as well as Proposition C.2, we have

\[
\frac{1}{n} \sum_{i=1}^{n} (\hat{\ell}(D_i) - \tilde{\ell}(D_i, \theta_{n}^{\text{cond}}))^2 = \frac{1}{n} \sum_{i=1}^{n} (\tilde{\ell}(D_i, \hat{\theta}_n) - \tilde{\ell}(D_i, \theta_{n}^{\text{cond}}))^2 \\
\leq \frac{1}{n} \sum_{i=1}^{n} m_n(D_i)^2 \cdot (\hat{\theta}_n - \theta_{n}^{\text{cond}})^2 = o_P(\hat{\theta}_n - \theta_{n}^{\text{cond}})^2 = o_P(1).
\]

As \( \frac{1}{n} \sum_{i=1}^{n} (\hat{\ell}(z_i) - \mu(z_i))^2 = o_P(1) \) for a fixed function \( \mu: \mathbb{Z} \to \mathbb{R} \), Cauchy-Schwarz inequality implies

\[
\frac{1}{n} \sum_{i=1}^{n} (\hat{\ell}(D_i) - \tilde{\ell}(z_i) - \tilde{\ell}(D_i, \theta_{n}^{\text{cond}}) + \mu(z_i))^2 = o_P(1),
\]

which further leads to

\[
\frac{1}{n} \sum_{i=1}^{n} (\hat{\ell}(D_i) - \tilde{\ell}(z_i))^2 = \frac{1}{n} \sum_{i=1}^{n} (\hat{\ell}(D_i, \theta_{n}^{\text{cond}}) - \mu(z_i))^2 + o_P(1).
\]

Writing \( \mu^*(z_i) = E[\hat{\ell}(D_i, \theta_{n}^{\text{cond}}) | z_i] \), condition (v) in Assumption C.1 and Markov’s inequality implies

\[
\frac{1}{n} \sum_{i=1}^{n} (\hat{\ell}(D_i, \theta_{n}^{\text{cond}}) - \mu^*(z_i))^2 = \frac{1}{n} \sum_{i=1}^{n} E[(\hat{\ell}(D_i, \theta_{n}^{\text{cond}}) - \mu^*(z_i))^2] + o_P(1),
\]

where \( E[(\hat{\ell}(D_i, \theta_{n}^{\text{cond}}) - \mu^*(z_i))^2] = Var(\hat{\ell}(D_i, \theta_{n}^{\text{cond}}) | z_i) \). Finally, we have \( \frac{2}{n} \sum_{i=1}^{n} \hat{\ell}(D_i, \theta_{n}^{\text{cond}}) - \mu^*(z_i) \cdot [\mu(z_i) - \mu^*(z_i)] = o_P(1) \) since each term in the summation is mean zero and the moment condition (v) holds. Thus

\[
\frac{1}{n} \sum_{i=1}^{n} \hat{\ell}(D_i, \theta_{n}^{\text{cond}}) - \mu(z_i)^2 = \frac{1}{n} \sum_{i=1}^{n} \hat{\ell}(D_i, \theta_{n}^{\text{cond}}) - \mu^*(z_i)^2 + \frac{1}{n} \sum_{i=1}^{n} [\mu(z_i) - \mu^*(z_i)]^2 \\
= \frac{1}{n} \sum_{i=1}^{n} Var(\hat{\ell}(D_i, \theta_{n}^{\text{cond}}) | z_i) + \frac{1}{n} \sum_{i=1}^{n} [\mu(z_i) - \mu^*(z_i)]^2 + o_P(1).
\]

Combining with the consistency of \( \widetilde{M}^{-1} \), we know that \( \hat{\sigma}_n - \sigma_n = o_P(1) \) if \( \mu^* = \mu \), and \( \hat{\sigma}_n - \sigma_n = o_P(1) \) for some \( \sigma_n \geq \sigma_n \) otherwise. This completes the proof of Proposition C.4.

G.2 Proof of results for conditioning on unobserved attributes

Proof of Theorem C.5. Following exactly the same arguments as Proposition 3.1, we obtain the linear expansion in Assumption 3.2 with \( Z \) replaced by \( X \), which implies

\[
\hat{\theta}_n - \theta_{n}^{\text{cond}}(X_n) = \frac{1}{n} \sum_{i=1}^{n} (\phi(D_i) - E[\phi(D_i) | X_i]) + o_P(1/\sqrt{n}).
\]

Using the same arguments in the proof of Proposition F.1, we know that for any fixed \( x \in \mathbb{R} \), the random variable \( P\{\sqrt{n}(\hat{\theta}_n - \theta_{n}^{\text{cond}}(X_n)) \leq x | X_n \} \) converges in probability to \( \Phi(x/\sigma_X) \), where \( \Phi \) is the c.d.f. of standard Gaussian distribution, and \( \sigma_X := E[(\phi(D) - E[\phi(D) | X])^2] \).

We then slightly modify the proof of Theorem 3.4 to show the desired results. To be specific, for any fixed \( x \in \mathbb{R} \) and any fixed constant \( \epsilon > 0 \), we write \( z^- = z_{1-\alpha/2} - \sigma_Z - \epsilon \) and \( z^+ = z_{1-\alpha/2} + \epsilon \). Denoting \( \Delta^+(\epsilon) = P\{\sqrt{n}(\hat{\theta}_n - \theta_{n}^{\text{cond}}(X_n)) \leq z^+ \mid X_n \} - 2\Phi(z^+|\sigma_X) - 1 \), we have \( \Delta^+(\epsilon), \Delta^-(\epsilon) = o_P(1) \) similar to Proposition F.1. Since \( \hat{\sigma}_Z \xrightarrow{p} \sigma_Z \), following similar arguments as (23) and (24) in the proof of Theorem 3.4, we have

\[
P\{\sqrt{n}(\hat{\theta}_n - \theta_{n}^{\text{cond}}(X_n)) \leq z_{1-\alpha/2} \cdot \hat{\sigma}_Z \mid X_n \} \geq 2\Phi\left(\frac{z_n - \epsilon}{\sigma_X}\right) - 1 + P(\hat{\sigma}_Z < \sigma_Z - \epsilon \mid X_n) + \Delta^-(\epsilon),
\]

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where \( P(\tilde{\sigma}_Z < \sigma_Z - \epsilon \mid X_n) = o_P(1) \) by Lemma I.4. On the other hand, we similarly have
\[
P\left( \sqrt{n} \tilde{\theta}_n - \theta_m^{\text{cond}}(X_n) \right) \leq z_{1-\alpha/2} \cdot \tilde{\sigma}_Z \mid X_n \right) \leq 2 \Phi\left( \frac{z_{(\epsilon)}}{\sigma_X} \right) - 1 + P(\tilde{\sigma}_Z < \sigma_Z + \epsilon \mid X_n) + \Delta^+(\epsilon),
\]
where \( P(\tilde{\sigma}_Z > \sigma_Z + \epsilon \mid X_n) = o_P(1) \) by Lemma I.4. For any fixed \( \delta > 0 \), we can choose some fixed \( \epsilon > 0 \) such that \( 2 \Phi(z^{-}(\epsilon)/\sigma_X) - 1 + (1 - \beta)/2 \) and \( 2 \Phi(z^{+}(\epsilon)/\sigma_X) - 1 + (1 - \beta)/2 \) for
\[
\tilde{\sigma}_Z = 1 - \Phi\left( \frac{\sigma_Z}{\sigma_X} \cdot z_{1-\alpha} \right)
\]
Combining the above, we have \( P(\sqrt{n} \tilde{\theta}_n - \theta_m^{\text{cond}}(X_n) \leq z_{1-\alpha/2} \cdot \tilde{\sigma}_Z \mid X_n) - (1 - \beta) > \delta \) \( \rightarrow 0 \), hence prove the convergence in probability. Finally, we note that \( \sigma_Z^2 = \text{Var}(\phi(D)) - \text{E}(\text{E}[\phi(D) \mid Z])^2 \) and \( \sigma_X^2 = \text{Var}(\phi(D)) - \text{E}(\text{E}[\phi(D) \mid X])^2 \). If \( \text{E}(\text{E}[\phi(D) \mid X])^2 \geq \text{E}(\text{E}[\phi(D) \mid Z])^2 \), we have \( \sigma_Z \geq \sigma_X \) hence \( \beta \leq \alpha \), thus completing the proof of Theorem C.5.

G.3 Proof of transferring to subsets

Proof of Theorem C.6. In any of the setups in Theorem C.6, we have shown that (c.f. the respective proofs)
\[
\hat{\theta}_{\text{trans}}^{\text{new}} - \theta_0^{\text{new}} = \frac{1}{n} \sum_{i=1}^n w(Z_i)(\psi(D_i) - \eta(Z_i)) + \frac{1}{m} \sum_{j=1}^m \eta(Z_j^{\text{new}}) + o_P(1/\sqrt{n}).
\]
Under regularity conditions that are similar to Proposition E.1, we have the following asymptotic linear expansion of \( \theta_m^{\text{cond}}(X_m^{\text{new}}) \) that is similar to Assumption 3.10:
\[
\theta_m^{\text{cond}}(X_m^{\text{new}}) - \theta_0^{\text{new}} = \frac{1}{m} \sum_{j=1}^m \text{E}\left[\psi(D_j^{\text{new}}) \mid X_j^{\text{new}}\right] + o_P(1/\sqrt{m}).
\]
Here since \( X \subset Z \), we note by the tower property of conditional expectations that almost surely
\[
\text{E}\left[\psi(D_j^{\text{new}}) \mid X_j^{\text{new}}\right] = \text{E}\left[\eta(Z_j^{\text{new}}) \mid X_j^{\text{new}}\right],
\]
Combining the above results, we have
\[
\hat{\theta}_{\text{trans}}^{\text{new}} - \theta_m^{\text{cond}}(X_m^{\text{new}}) = \frac{1}{n} \sum_{i=1}^n w(Z_i)(\psi(D_i) - \eta(Z_i)) + \frac{1}{m} \sum_{j=1}^m \left\{ \eta(Z_j^{\text{new}}) - \text{E}\left[\eta(Z_j^{\text{new}}) \mid X_j^{\text{new}}\right] \right\} + o_P(1/\sqrt{n}).
\]
Each term in the above summation is mean zero conditional on \( X_m^{\text{new}} \). Thus, applying the conditional CLT in Lemma I.1 to the filtration \( F_k = \sigma\{X_j^{\text{new}}\}_{j=1}^k \), and dealing with the \( o_P(1/\sqrt{n}) \) term similar to the proof of Theorem 3.4, we complete the proof of Theorem C.6.

H Proofs of estimation

H.1 Proof of Proposition B.7

Proof of Proposition B.7. 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 B.2, 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 \( \|M(s, 1, \hat{\theta}) - M(s, 1, \theta_0)\|_\infty = O(\|\hat{\theta} - \theta_0\|_2) = O(|I|^{-1/2}) \). Hence

\[
\|\hat{M} - M(\theta_0)\|_\infty \leq O_P(\mathcal{R}_m(|I|) + |I|^{-1/2}).
\] (29)

By Assumption B.1, we have \( \|\mathcal{G}(\hat{s}, I_2) - \mathcal{G}(\hat{s})\|_{L_2(P)} = O_P(\mathcal{R}_r(|I|)) \). Meanwhile, writing \( \mathcal{G}(s) = \mathbb{E}[s(D, \theta_0) \mid Z = \cdot] \), by the definition of \( \mathcal{G}() \), we have

\[
\|\mathcal{G}(\hat{s}) - \mathcal{G}(s)\|_{L_2(P)} = \left\| \mathbb{E}[s(D, \hat{\theta}) - s(D, \theta_0) \mid Z = \cdot] \right\|_{L_2(P)} \leq \|s(\cdot, \hat{\theta}) - s(\cdot, \theta_0)\|_{L_2(P)} = O(\|\hat{\theta} - \theta_0\|_2) = O_P(|I|^{-1/2}),
\]

where \( \|s(\cdot, \hat{\theta}) - s(\cdot, \theta)\|_{L_2(P)} \) views \( \hat{\theta} \) as fixed and the \( L_2 \)-norm is with respect to \( D \sim P \). Putting them together, the estimated conditional mean function satisfies

\[
\|\hat{\mu}(\cdot) - \mathcal{G}(s)\|_{L_2(P)} \leq \|\mathcal{G}(\hat{s}, I_2) - \mathcal{G}(\hat{s})\|_{L_2(P)} + \|\mathcal{G}(\hat{s}) - \mathcal{G}(s)\|_{L_2(P)} \leq O_P(\mathcal{R}_r(|I|) + |I|^{-1/2}).
\] (30)

Altogether, we have

\[
\|\hat{\mu}(\cdot) - \varphi(\cdot)\|_{L_2(P)} = \|\hat{M} \cdot \mathcal{G}(s)\|_{L_2(P)} \leq \|\hat{M} - M(\theta_0)\|_{\infty} \cdot \|\mathcal{G}(s)\|_{L_2(P)} \leq p \cdot \|\hat{M} - M(\theta_0)\|_{\infty} \cdot \|\hat{\mu}(\cdot)\|_{L_2(P)} + p \cdot \|M(\theta_0)\|_{\infty} \cdot \|\hat{\mu}(\cdot) - \mathcal{G}(s)\|_{L_2(P)} \leq p \cdot O_P(\mathcal{R}_m(|I|) + \mathcal{R}_r(|I|) + |I|^{-1/2}),
\]

where the last inequality follows from (29) and (30) and the fact that

\[
\|\hat{\mu}(\cdot)\|_{L_2(P)} \leq \|\mathcal{G}(s)\|_{L_2(P)} + O_P(\mathcal{R}_r(|I|) + |I|^{-1/2}) = O_P(1).
\]

We thus complete the proof of Proposition B.7. \( \square \)

**H.2 Proof of Proposition B.4**

**Proof of Proposition B.4.** 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,

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

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

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

Employing Lemma I.4, we have

\[
2 \frac{1}{|I_2|} \sum_{i \in I_2} \left( \hat{M}s(D_i, \hat{\theta}) - M s(D_i, \theta_0) \right)^2 = 2 \hat{M}^2 - \frac{1}{|I_2|} \sum_{i \in I_2} \left( s(D_i, \hat{\theta}) - s(D_i, \theta_0) \right)^2 = o_P(1).
\]
Following the same arguments as in the proof of Proposition B.7, we have $\hat{M} = M + o_P(1)$, hence
\[
\frac{2}{|I_2|} \sum_{i \in I_2} \left( \hat{M} s(D_i, \theta_0) - M s(D_i, \theta_0) \right)^2 = 2(\hat{M} - M)^2 + \frac{1}{|I_2|} \sum_{i \in I_2} s(D_i, \theta_0)^2 = o_P(1).
\]

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 B.7, we have
\[
\mathbb{E}\left[ \frac{1}{|I_2|} \sum_{i \in I_2} \Delta \phi_i^2 \right] = \left\| \hat{\varphi} - \varphi(\cdot) \right\|_{L_2(\mathbb{P})} = o_P(1),
\]
which, combined with Lemma I.4, leads to $\frac{1}{|I_2|} \sum_{i \in I_2} \Delta \varphi_i^2 = o_P(1)$. 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,
\[
\hat{\sigma}^2 = \frac{1}{|I_2|} \sum_{i \in I_2} (\phi(D_i) - \phi(Z_i)) \leq \frac{1}{|I_2|} \sum_{i \in I_2} (\phi(D_i) - \varphi(Z_i))^2 + \frac{1}{|I_2|} \sum_{i \in I_2} (\varphi(Z_i) - \varphi(Z_i))^2 + 2 \sqrt{\frac{1}{|I_2|} \sum_{i \in I_2} (\phi(D_i) - \varphi(Z_i))^2} \cdot \sqrt{\frac{1}{|I_2|} \sum_{i \in I_2} (\varphi(Z_i) - \varphi(Z_i))^2} = \sigma^2 + o_P(1),
\]
where the last equality follows from the law of large numbers.

\[ \square \]

H.3 Proof of Proposition B.5

Proof of Proposition B.5. To begin with, we write
\[
\mathcal{G}(s) = \mathbb{E}[s(D, \theta_0^{new}) \mid Z = \cdot] = \mathbb{E}[s(D^{new}, \theta_0^{new}) \mid Z^{new} = \cdot]
\]
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 $\eta(z) = M(s, w, \theta_0^{new})\mathcal{G}(s)(z)$.

We first prove the result with ground truth of $w(\cdot)$. In this case, with regularity conditions we know $\| \hat{\theta} - \theta_0^{new} \|_2 = O_P(|I_2|^{-1/2}) = O_P(|I|^{-1/2})$. Thus, following exactly the same arguments as in the proof of Proposition B.7, we have
\[
\left\| \hat{\varphi}(\cdot) - \mathcal{G}(s)(\cdot) \right\|_{L_2(\mathbb{P})} \leq O_P(\mathcal{R}_r(|I|) + |I|^{-1/2}).
\]

On the other hand, by Algorithm 5, we know
\[
\| \hat{M} - M(s, w, \theta_0^{new}) \|_\infty = \| \hat{M}(s, w, \hat{\theta}, I_3) - M(s, w, \theta_0^{new}) \|_\infty \leq \| \hat{M}(s, w, \hat{\theta}, I_3) - M(s, w, \hat{\theta}) \|_\infty + \| M(s, w, \hat{\theta}) - M(s, w, \theta_0^{new}) \|_\infty.
\]

Since $\hat{\theta}$ is independent of $I_3$, by Assumption B.2, we have
\[
\| \hat{M}(s, w, \hat{\theta}, I_3) - M(s, w, \hat{\theta}) \|_\infty \leq O_P(\mathcal{R}_m(|I_3|)) = O_P(\mathcal{R}_m(|I|)).
\]

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The given conditions also imply
\[ \| M(s, w, \hat{\theta}) - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \leq O\left(\| \hat{\theta} - \theta_0^{\text{new}} \|_2 \right) = O_P\left( |\mathcal{I}|^{-1/2} \right). \]

Putting them together, we have
\[ \| \hat{M} - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \leq O_P\left( R_m(|\mathcal{I}|) + |\mathcal{I}|^{-1/2} \right). \]

Following the same arguments as in the proof of Proposition B.7, we obtain the desired result (15).

We now consider the result for estimated \( \hat{w}(\cdot) \). Since it is obtained from \( \mathcal{I}_1 \), it is independent of subsequent estimation steps. By similar regularity conditions as Proposition E.2, we know that
\[ \| \hat{\theta} - \theta_0^{\text{new}} \|_2 = \left\| \frac{1}{|\mathcal{I}_2|} \sum_{i \in \mathcal{I}_2} \hat{w}(Z_i) \psi(D_i) \right\|_2 + O_P\left( |\mathcal{I}_2|^{-1/2} \right) = O_P\left( |\mathcal{I}_2|^{-1/2} \right) = O_P\left( |\mathcal{I}|^{-1/2} \right). \]

With estimated \( \hat{w} \), by Algorithm 5, we know
\[ \| \hat{M} - M(s, w, \theta_0^{\text{new}}) \|_{\infty} = \| \hat{M}(s, \hat{w}, \hat{\theta}, \mathcal{I}_3) - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \leq \| \hat{M}(s, \hat{w}, \hat{\theta}, \mathcal{I}_3) - M(s, \hat{w}, \hat{\theta}) \|_{\infty} + \| M(s, \hat{w}, \hat{\theta}) - M(s, w, \theta_0^{\text{new}}) \|_{\infty}. \]

Here by Assumption B.2, since \( \mathcal{I}_3 \) is independent of \( \hat{w} \) and \( \hat{\theta} \), the estimation error is bounded as
\[ \| \hat{M}(s, w, \hat{\theta}, \mathcal{I}_3) - M(s, \hat{w}, \hat{\theta}) \|_{\infty} \leq O_P\left( R_m(|\mathcal{I}_3|) \right) = O_P\left( R_m(|\mathcal{I}|) \right). \]

By the stability assumptions of \( M(s, w, \theta) \), we have
\[ \| M(s, \hat{w}, \hat{\theta}) - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \leq \| M(s, \hat{w}, \hat{\theta}) - M(s, w, \hat{\theta}) \|_{\infty} + \| M(s, w, \hat{\theta}) - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \leq O_P\left( \| \hat{w}(\cdot) - w(\cdot) \|_{L_2[\mathcal{P}]} \right) + O_P\left( \| \hat{\theta} - \theta_0^{\text{new}} \|_2 \right) \leq O_P\left( \| \hat{w}(\cdot) - w(\cdot) \|_{L_2[\mathcal{P}]} + |\mathcal{I}|^{-1/2} \right). \]

hence
\[ \| \hat{M} - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \leq O_P\left( \| \hat{w}(\cdot) - w(\cdot) \|_{L_2[\mathcal{P}]} + R_m(|\mathcal{I}|) + |\mathcal{I}|^{-1/2} \right) (31) \]

On the other hand, since \( \mathcal{I}_3 \) is independent of the function \( \hat{s}(\cdot) = s(\cdot, \hat{\theta}) \), we know \( \| \mathcal{G}(\hat{s}, \mathcal{I}_3)(\cdot) - \mathcal{G}(\hat{s})(\cdot) \|_{L_2[\mathcal{P}]} \leq O_P\left( R_r(|\mathcal{I}_3|) \right) = O_P\left( R_r(|\mathcal{I}|) \right). \) Also, the stability of \( s(\cdot, \cdot) \) implies
\[ \| \mathcal{G}(\hat{s})(\cdot) - \mathcal{G}(s)(\cdot) \|_{L_2[\mathcal{P}]} \leq \| \hat{s}(\cdot, \hat{\theta}) - s(\cdot, \hat{\theta}) \|_{L_2[\mathcal{P}]} = O(\| \hat{\theta} - \theta_0 \|_2) = O_P\left( |\mathcal{I}|^{-1/2} \right). \]

Therefore, the error in \( \hat{f}(\cdot) \) can be bounded as
\[ \| \hat{f}(\cdot) - \mathcal{G}(s)(\cdot) \|_{L_2[\mathcal{P}]} \leq \| \mathcal{G}(\hat{s}, \mathcal{I}_3)(\cdot) - \mathcal{G}(\hat{s})(\cdot) \|_{L_2[\mathcal{P}]} + \| \mathcal{G}(\hat{s})(\cdot) - \mathcal{G}(s)(\cdot) \|_{L_2[\mathcal{P}]} \leq O_P\left( \| \hat{w}(\cdot) - w(\cdot) \|_{L_2[\mathcal{P}]} + |\mathcal{I}|^{-1/2} \right). (32) \]

Following similar arguments as the case with ground truth of \( w(\cdot) \), we combine the bounds (31) and (32) and obtain
\[ \| \eta(s, \mathcal{I})(\cdot) - \eta(\cdot) \|_{L_2[\mathcal{P}]} \leq \left\| \left( \hat{M} - M(s, w, \theta_0^{\text{new}}) \right) \hat{f}(\cdot) \right\|_{L_2[\mathcal{P}]} + \left\| M(s, w, \theta_0^{\text{new}}) \left( \hat{f}(\cdot) - \mathcal{G}(s)(\cdot) \right) \right\|_{L_2[\mathcal{P}]} \leq p \cdot \| \hat{M} - M(s, w, \theta_0^{\text{new}}) \|_{\infty} \cdot \| \hat{f}(\cdot) \|_{L_2[\mathcal{P}]} + p \cdot \| M(s, w, \theta_0^{\text{new}}) \|_{\infty} \cdot \| \hat{f}(\cdot) - \mathcal{G}(s)(\cdot) \|_{L_2[\mathcal{P}]} \leq p \cdot O_P\left( \| \hat{w}(\cdot) - w(\cdot) \|_{L_2[\mathcal{P}]} + R_m(|\mathcal{I}|) + R_r(|\mathcal{I}|) + |\mathcal{I}|^{-1/2} \right), \]

which completes the proof of Proposition B.5. 

\[ \square \]
H.4 Proof of Proposition B.6

Proof of Proposition B.6. Firstly, we write $M = -(E[w(Z)s(D, \theta_0^\text{new})])^{-1}$, so that $\psi(d) = M s(d, \theta_0^\text{new})$. Following the same arguments as in the proof of Proposition B.5, we have $\hat{M} = M + o_p(1)$ under the diminishing rate of $R_m(1) \to 0$ as $|I| \to \infty$. By the regularity conditions, we have $\|\hat{\theta} - \theta_0^\text{new}\|_2 = o_p(1)$.

Writing $\Delta \hat{\psi}_i = \hat{\psi}_i - \psi(D_i)$, we have

$$\frac{1}{|I_3|} \sum_{i \in I_3} \Delta \hat{\psi}_i^2 = \frac{1}{|I_3|} \sum_{i \in I_3} (\hat{M}s(D_i, \hat{\theta}) - M s(D_i, \theta_0^\text{new}))^2$$

$$\leq \frac{2}{|I_3|} \sum_{i \in I_3} (\hat{M}s(D_i, \hat{\theta}) - \hat{M}s(D_i, \theta_0^\text{new}))^2 + \frac{2}{|I_3|} \sum_{i \in I_3} (\hat{M}s(D_i, \theta_0^\text{new}) - M s(D_i, \theta_0^\text{new}))^2.$$ 

Since $\hat{\theta}$ is independent of $I_3$, we know

$$\mathbb{E} \left[ \frac{1}{|I_3|} \sum_{i \in I_3} (s(D_i, \hat{\theta}) - s(D_i, \theta_0^\text{new}))^2 \right]_{I_1 \cup I_2} = \|s(\cdot, \theta) - s(\cdot, \theta_0^\text{new})\|_{L_2(P)}^2 = o_p(1).$$

Hence Lemma 1.4 yields

$$\frac{2}{|I_3|} \sum_{i \in I_3} (\hat{M}s(D_i, \hat{\theta}) - \hat{M}s(D_i, \theta_0^\text{new}))^2 = 2\hat{M}^2 \cdot \frac{1}{|I_3|} \sum_{i \in I_3} (s(D_i, \hat{\theta}) - s(D_i, \theta_0^\text{new}))^2 = o_p(1).$$

Also, since $\hat{M} - M = o_p(1)$, we have

$$2(M - \hat{M})^2 \cdot \frac{1}{|I_3|} \sum_{i \in I_3} (s(D_i, \theta_0^\text{new}) - s(D_i, \theta_0^\text{new}))^2 = o_p(1),$$

which further leads to $\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 \Delta \hat{\psi}_i^2 = o_p(1)$ since $\|w(\cdot)\|_{\infty} < \infty$. On the other hand, by the rate conditions and the convergence result of $\hat{\eta}$ in Proposition B.5, we know that $\|\hat{\eta}(\cdot) - \eta(\cdot)\|_{L_2(P)} = o_p(1)$. Since $I_3$ is independent of $\hat{\eta}$, writing $\Delta \hat{\eta}_i = \hat{\eta}_i - \eta(Z_i)$,

$$\mathbb{E} \left[ \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 \Delta \hat{\eta}_i^2 \right]_{I_1 \cup I_2} \leq \|w(\cdot)\|_{\infty} \cdot \|\hat{\eta}(\cdot) - \eta(\cdot)\|_{L_2(P)}^2 = o_p(1).$$

Invoking Lemma 1.4 yields $\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 \Delta \hat{\eta}_i^2 = o_p(1)$. Therefore,

$$\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\hat{\psi}_i - \hat{\eta}_i)^2 - \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\hat{\psi}_i - \eta(Z_i))^2$$

$$\leq \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\Delta \hat{\psi}_i - \Delta \eta_i)^2$$

$$+ 2 \sqrt{\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\hat{\psi}_i - \eta(Z_i))^2} \cdot \sqrt{\frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\Delta \hat{\psi}_i - \Delta \eta_i)^2} = o_p(1).$$

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

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

$$= \frac{1}{|I_3|} \sum_{i \in I_3} w(Z_i)^2 (\psi(D_i) - \eta(Z_i))^2 + o_p(1) = \hat{\sigma}_{\text{shift}}^2 + o_p(1),$$

which completes the proof. \qed
I Auxiliary Results

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

I.1 Auxiliary results for conditional laws

Lemma I.1. Let \( g(\cdot) \) be a function such that \( E[|g(X_i)|^2] < \infty \), 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

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

converges almost surely to \( \Phi(x/\sigma) \), where \( \Phi \) is the cumulative distribution function of standard normal distribution, and

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

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

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

converges almost surely to \( \Phi(x/\sigma) \).

Proof of Lemma I.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 \( \zeta_i := g(X_i) - \mathbb{E}[g(X_i) \mid Z_i] \). 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

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

By Lemma I.2, we know that the conditional law \( \mathcal{L}_n \) converges almost surely to \( N(0, \sigma^2) \), which completes the proof of equation (33). Since the conditional probabilities are bounded within \([0, 1]\), equation (34) follows from dominated convergence theorem. Therefore we conclude the proof of Lemma I.1.

Lemma I.2. Under the same assumption as Lemma I.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 I.1.

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

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

Since the random variables \( \{\mathbb{E}[\zeta_i^2 \mid Z_j]\}_{i=1}^n \) are i.i.d., by the law of large numbers, it holds that

\[
\sum_{m=1}^n \left( -\frac{t^2}{2n}\mathbb{E}[\zeta_j^2 \mid Z_j] \right) \xrightarrow{a.s.} -\frac{t^2}{2}\mathbb{E}[\zeta_j^2] = -\frac{t^2}{2}\sigma^2,
\]

where \( \sigma^2 \) is defined in Lemma I.1. Note that \( |e^{ix} - 1 - ix + x^2/2| \leq \min\{|x|^2, |x|^3/6\} \) for any \( x \in \mathbb{R} \), thus

\[
|R_{n,j}| = \left| \mathbb{E}\left[ e^{it \zeta_j} - 1 - \frac{it}{\sqrt{n}} \zeta_j + \frac{t^2}{2n} \zeta_j^2 \mid Z_j \right] \right|
\]

\[
\leq \mathbb{E}\left[ \min\left\{ \frac{t^2}{2n} \zeta_j^2, \frac{t^3}{6n^{3/2}} |\zeta_j|^3 \right\} \mid Z_j \right] \leq \frac{t^3}{6n^{3/2}} \mathbb{E}[|\zeta_j|^3 \mid Z_j].
\]
Under the finite fourth-moment condition, by the law of large numbers we have

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

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

$$\sum_{j=1}^{n} |z_{n,j}|^2 \leq \frac{t^4}{2n^2} \sum_{i=1}^{n} (\mathbb{E}[|z_j|^2 \mid Z_j])^2 + 2 \sum_{j=1}^{n} R_{n,j}^2 \leq \frac{t^4}{2n^2} \sum_{j=1}^{n} \mathbb{E}[|z_j|^4 \mid Z_j] + 2 \sum_{j=1}^{n} R_{n,j}^2$$ (35)

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 (35) and Lemma I.3, we conclude the proof of Lemma I.2.

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

**Lemma I.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 $n \to \infty$.

### I.2 Auxiliary technical lemmas

**Lemma I.4.** Suppose a sequence of random variables $E_n$ satisfies $E_n = o_P(1)$ as $n \to \infty$. Then for any $\sigma$-algebras $\mathcal{F}_n$ and any constant $\epsilon > 0$, it holds that $\mathbb{P}(\{|E_n| > \epsilon \mid \mathcal{F}_n\}) = o_P(1)$.

**Proof of Lemma I.4.** Note that $\mathbb{E}[\mathbb{P}(\{|E_n| > \epsilon \mid \mathcal{F}_n\})] = \mathbb{P}(\{|E_n| > \epsilon\})$. Thus for any $\delta > 0$, we have

$$\mathbb{P}(\{|E_n| > \epsilon \mid \mathcal{F}_n\} > \delta) \leq \frac{1}{\delta} \mathbb{P}(\{|E_n| > \epsilon\}) \to 0.$$

Therefore we have $\mathbb{P}(\{|E_n| > \epsilon \mid \mathcal{F}_n\}) = o_P(1)$ and completes the proof of Lemma I.4.

**Lemma I.5.** Let $\mathcal{F}_n$ be a sequence of $\sigma$-algebra, and let $A_n \geq 0$ be a sequence of nonnegative random variables. If $\mathbb{E}(A_n \mid \mathcal{F}_n) = o_P(1)$, then $A_n = o_P(1)$.

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

$$B_n := \mathbb{P}(A_n > \epsilon \mid \mathcal{F}_n) \leq \frac{\mathbb{E}[A_n \mid \mathcal{F}_n]}{\epsilon} = o_P(1),$$

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

We cite without proof the following result on convex functions; see, e.g., Ex 2.5 in Duchi (2021).

**Lemma I.6.** If $f : \Theta \to \mathbb{R}$ is convex in $\Theta \subset \mathbb{R}^p$ and $\nabla^2 f(\theta) \succeq \lambda I_{p \times p}$ for all $\theta \in \Theta$ with $\|\theta - \theta_0\| \leq c$ for constants $\lambda, c$, then $f(\theta) \geq f(\theta_0) + \nabla f(\theta_0)^T (\theta - \theta_0) + \lambda/2 \cdot \min\{\|\theta - \theta_0\|^2, c\|\theta_0 - \theta\|\}$. 

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