

Semi-supervised Regression Analysis with Model Misspecification and High-dimensional Data

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Abstract: The accessibility of vast volumes of unlabeled data has sparked growing interest in semi-supervised learning (SSL) and covariate shift transfer learning (CSTL). In this paper, we present an inference framework for estimating regression coefficients in conditional mean models within both SSL and CSTL settings, while allowing for the misspecification of conditional mean models. We develop an augmented inverse probability weighted (AIPW) method, employing regularized calibrated estimators for both propensity score (PS) and outcome regression (OR) nuisance models, with PS and OR models being sequentially dependent. We show that when the PS model is correctly specified, the proposed estimator achieves consistency, asymptotic normality, and valid confidence intervals, even with possible OR model misspecification and high-dimensional data. Moreover, by suppressing detailed technical choices, we demonstrate that previous methods can be unified within our AIPW framework. Our theoretical findings are verified through extensive simulation studies and a real-world data application.

Key words and phrases: Augmented inverse probability weighted estimator, Covariate shift transfer learning, High-dimensional data, Semi-supervised learning.

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1. Introduction

In recent years, vast volumes of unlabeled data have become increasingly accessible, sparking growing interest in how to leverage these data in both academic research and industrial applications. One of the active areas of research is semi-supervised learning (SSL). In addition, covariate shift transfer learning (CSTL) also exploits information from unlabeled data. Both have various application scenarios like computer vision (Sohn et al., 2020; Zhou and Levine, 2021; Zheng et al., 2022), natural language process (Chen and Huang, 2016; Ruder et al., 2019; Zhao et al., 2022), causal inference (Alvari et al., 2019; Aloui et al., 2023; Zhang et al., 2023), health-care data analysis (Castro et al., 2020; Liu et al., 2023; Tang et al., 2024), etc.

In both SSL and CSTL settings, we have access to a labeled dataset $\mathcal{L}$ and an unlabeled dataset $\mathcal{U}$, where the labeled dataset $\mathcal{L}$ contains observations with both the covariates $\mathbf{X}$ and the outcome Y , while the unlabeled dataset $\mathcal{U}$ consists solely of observations with the covariates $\mathbf{X}$. The training set $\mathcal{T}$ is the union of $\mathcal{L}$ and $\mathcal{U}$. Nevertheless, there is a key distinction between the classic SSL and CSTL setups (Chapelle et al., 2006; Liu et al., 2023). In CSTL, the conditional distributions of Y given $\mathbf{X}$ in the labeled and unlabeled datasets are assumed to be the same, whereas the marginal distributions of $\mathbf{X}$ are different (hence the term covariate shift), and the estimator is ultimately evaluated on unlabeled data. However, under the classic SSL setup, it is assumed that the distributions of labeled data, unlabeled

data, and population are the same, making no difference in evaluating the estimator on which distribution. To accommodate both SSL and CSTL, we consider a more general setting. We only assume the conditional distribution of Y given $\mathbf{X}$ is the same in labeled and unlabeled data, while marginal distributions of $\mathbf{X}$ are permitted to be different. Estimators evaluated on the population and unlabeled data are both considered.

While there is a long history of SSL (Chapelle et al., 2006; Zhu, 2008) and CSTL (Quiñonero-Candela et al., 2009), a growing literature has considered inference procedures only recently. Notable advancements have been made in estimating the population mean $\mathbb{E}(Y)$ (Zhang et al., 2019; Zhang and Bradic, 2021) and regression coefficients or fixed linear combinations in (generalized) linear models regressing Y against a sub-vector of $\mathbf{X}$ (Chakraborty, 2016; Liu et al., 2023) or in linear models regressing Y against full $\mathbf{X}$ (Chakraborty and Cai, 2018; Chakraborty et al., 2019; Deng et al., 2023; Zhang et al., 2023; Chen and Zhang, 2023). See Section 5.1 and Supplement Section S2 for further information. Inferences of quantile regression (Chakraborty et al., 2022), explained variance (Cai and Guo, 2020), and model performance metrics such as true and false positive rates (Gronsbell and Cai, 2017) have also attracted interest.

In this article, we focus on the inference of regression coefficients in (conditional) mean models for Y against a sub-vector of $\mathbf{X}$ in SSL settings, hence called semi-supervised regression analysis. We demonstrate a unified framework for estimating

and inferring these coefficients, particularly in cases where the (conditional) mean model and outcome regression (OR) model $\mathbb{E}[Y|\mathbf{X}]$ may be misspecified. Previous SSL and CSTL methods that considered this type of problems, such as Chakraborty (2016), Chakraborty and Cai (2018), Zhang et al. (2019), Zhang and Bradic (2021) and Liu et al. (2023), can largely be accommodated in the augmented inverse probability weighting (AIPW) framework (Robins et al., 1994; Tan, 2020a; Wu et al., 2024). See Section 5 and Section 8 for further details.

Despite significant advancements made, there remain limitations in the previous AIPW methods. Methods developed in SSL settings usually treat the problem as the one where data are missing completely at random (MCAR) (Chakraborty, 2016; Chakraborty and Cai, 2018; Zhang et al., 2019; Zhang and Bradic, 2021). This restricts their application scenarios and overlooks the significance of constructing the propensity score (PS) model. In contrast, our setting is in general a missing-at-random (MAR) problem (Little and Rubin, 2019), and the estimation of the PS model is no longer negligible. In the setting of MCAR, the PS remains a constant, whereas in the setting of MAR, the PS varies with the covariates $\mathbf{X}$. In MAR problems, similarly as in Tan (2020a), the estimation of PS and OR models needs to be carefully handled in a way different from regularized least squares or maximum likelihood as in previous papers, so that $\sqrt{N}$ -consistent estimation can be achieved with possible misspecification of the OR model, where N is the sample size of $\mathcal{T}$.

In summary, we mainly make two contributions. First, we present an inference

framework that accommodates several previous settings, including the estimation of population mean and regression coefficients in conditional mean models of Y given any sub-vector of $\mathbf{X}$ under both SSL and CSTL setups. Second, we propose a novel AIPW method that enables $\sqrt{N}$ -consistent and asymptotically normal estimation and achieves valid confidence intervals under suitable sparsity conditions, when the PS model is correctly specified but the OR model may be misspecified. This robustness to model misspecification is achieved by carefully exploiting the connection between PS and OR models and designing estimating equations for nuisance parameters, differently from regularized least-squares or maximum-likelihood estimation. Previous related methods (Chakraborty et al., 2019) achieve $\sqrt{N}$ -consistency when both PS and OR models are correctly specified and the estimated PS and OR functions converge to the *true values* at fast enough rates (specifically, the product of estimation errors is smaller than $N^{-1/2}$). In contrast, our proposed estimator is shown to be $\sqrt{N}$ -consistent even when the estimated OR function converges to a *target value* different from the true value and the estimated PS function converges to the true value, both slower than $N^{-1/2}$ (but faster than $N^{-1/4}$), with misspecified OR model and correctly specified PS model. Hence the aforementioned product of estimation errors may be greater than $N^{-1/2}$.

This work is also related to the causal inference problem under the strong ignorability assumption (Rosenbaum and Rubin, 1983). Specifically, the SSL problem is similar to estimating the average treatment effect (ATE) and the conditional ATE

(CATE) (Zimmert and Lechner, 2019; Fan et al., 2022; Wu et al., 2024). The CSTL problem can be viewed as an analog to the estimation of the average treatment effect on the treated (ATT).

The rest of this paper is organized as follows. In section 2, we present our setup and define the target parameters of interest. In Section 3, we construct a novel AIPW estimator for the target parameter. We show theoretical properties of the proposed estimator in Section 4, and compare them with the previous literature in Section 5. Numerical implementation is introduced in Section 6. An application to a crime study is presented in Section 7. Extension of proposed methods to the CSTL setting is given in Section 8 followed by concluding discussions in Section 9.

2. Setup and preliminaries

2.1 Data and target parameters

Let $Y \in \mathbb{R}$ be a response variable and $\mathbf{X} = (1, X_1, \dots, X_d)^\top \in \mathbb{R}^{d+1}$ be a covariate vector with the first element being the constant 1. In addition, let $R \in \{0, 1\}$ be the indicator of whether Y is observed: $R = 1$ if observed and $R = 0$ if missing. Assume that $\{(\mathbf{X}_i, Y_i, R_i) : i = 1, \dots, N\}$ is an independent and identically distributed (i.i.d.) sample from a joint distribution of $(\mathbf{X}, Y, R)$, denoted as $\mathbb{P}$. The observed dataset, $\{(\mathbf{X}_i, R_i Y_i, R_i) : i = 1, \dots, N\}$, can be split into a labeled dataset $\mathcal{L} = \{(\mathbf{X}_i, Y_i, R_i = 1), i = 1, \dots, n\}$ and an unlabeled dataset $\mathcal{U} = \{(\mathbf{X}_i, R_i = 0), i =$

$n + 1, \dots, N\}$. For $\mathbf{Z} \in \mathbb{R}^m$, a sub-vector of $\mathbf{X}$, it is of interest to fit a regression model for the conditional mean $\mathbb{E}(Y|\mathbf{Z})$:

$$\mathbb{E}(Y|\mathbf{Z}) = \psi(\beta^{*\top} \mathbf{Z}), \quad (2.1)$$

where $\mathbb{E}(\cdot)$ denotes the expectation under $\mathbb{P}$, β^* is a parameter vector, and $\psi(\cdot)$ is an (increasing) inverse link function, such as the identity function $\psi(u) = u$ and logit function $\psi(u) = 1/\{1+\exp(-u)\}$. When $\mathbf{Z}$ is a strict sub-vector of $\mathbf{X}$, the parameter β^* can be seen to capture the marginal (or full) effect of $\mathbf{Z}$ on Y , as any indirect effect of $\mathbf{Z}$ on Y through other covariates in $\mathbf{X}$ is marginalized out conceptually. This is similar to marginal structural models (Robins, 1999; Wu et al., 2024). In comparison, the coefficient sub-vector associated with $\mathbf{Z}$ in the full regression of Y on $\mathbf{X}$ can be seen to represent the direct effect of $\mathbf{Z}$ on Y after accounting for the influence of other covariates in $\mathbf{X}$ on Y .

Model (2.1) is allowed to be misspecified, that is, $\mathbb{E}(Y|\mathbf{Z})$ may not be in the form $\psi(\beta^\top \mathbf{Z})$. With possible model misspecification, β^* is defined as the solution to

$$\mathbb{E} [\{Y - \psi(\beta^\top \mathbf{Z})\} \mathbf{Z}] = 0. \quad (2.2)$$

For a generalized linear model with $\psi(\cdot)$ as the canonical inverse link, the estimating equation (2.2) leads to maximum likelihood estimation, so that $\psi(\beta^{*\top} \mathbf{Z})$ can be

interpreted as the best likelihood-based approximation to $\mathbb{E}(Y|\mathbf{Z})$ using model (2.1).

The regression model (2.1) is flexible. The target parameter β^* accommodates a variety of estimands in the previous literature.

- (a) If we set $\mathbf{Z} = 1$ and $\psi(u) = u$, then $\beta^* = \mathbb{E}(Y)$. The problem corresponds to the semi-supervised estimation of the population mean (Zhang et al., 2019; Zhang and Bradic, 2021).
- (b) If we set $\mathbf{Z}$ to be a univariate covariate, for example, $\mathbf{Z} = X_1$, then β^* corresponds to the regression coefficient in the regression model of Y given the particular covariate X_1 . This problem was studied by Liu et al. (2023) and Wu et al. (2024).
- (c) If we set $\mathbf{Z} = \mathbf{X}$, then β^* corresponds to the coefficient vector in the regression model of Y given the full covariate vector $\mathbf{X}$ (Chakraborty, 2016; Chakraborty and Cai, 2018; Chakraborty et al., 2019; Deng et al., 2023; Zhang et al., 2023).

The description above is general, without specifying dependency of the dimensions of $\mathbf{X}$ and $\mathbf{Z}$ on N . Nevertheless, for our statistical theory (Section 4), we allow the dimension of $\mathbf{X}$ to increase as N increases, but the dimension of $\mathbf{Z}$ is fixed, and we study inference about the entire vector β^* . Hence our work is distinct from Chakraborty et al. (2019) in case (c) where $\mathbf{Z} = \mathbf{X}$ is high-dimensional and then the estimation objective is inferences about individual elements of β^* . See Supplement Section S2 for a detailed comparison of our work and several papers men-

tioned in case (c). On the other hand, for Chakraborty (2016) and Chakraborty and Cai (2018) in case (c), $\mathbf{Z} = \mathbf{X}$ is fixed-dimensional and inference about β^* is studied by incorporating kernel smoothing in fitting the OR function. Hence such settings can be properly accommodated by our theory with fixed-dimensional $\mathbf{Z}$ but high-dimensional $\mathbf{X}$ as basis functions (denoted as $\mathbf{F}$ or $\mathbf{G}$ later) for OR fitting.

In addition to the parameter vector β^* , it may also be of interest to consider target parameters defined within unlabeled data corresponding to the CSTL setting, as studied in several recent papers (Liu et al., 2023; He et al., 2024). To incorporate this setting, we consider a regression model for the conditional mean in the unlabeled data: $\mathbb{E}(Y|R = 0, \mathbf{Z}) = \psi(\beta^{0*T} \mathbf{Z})$. With possible model misspecification, β^{0*} is defined as the solution to

$$\mathbb{E}[(1 - R) \{Y - \psi(\beta^T \mathbf{Z})\} \mathbf{Z}] = 0. \quad (2.3)$$

To illustrate the main ideas, we focus on the estimation of β^* , and defer the associated results for the estimation of β^{0*} to Section 8.

2.2 General assumptions

Without imposing any assumption, we cannot obtain a consistent estimator of β^* due to the missingness of Y in the unlabeled data. Below, we introduce the identifiability assumption.

Assumption 1. $Y \perp\!\!\!\perp R \mid \mathbf{X}$.

Assumption 1 is crucial for the identifiability of β^* and β^{0*} . It ensures that $\mathbb{E}(Y|\mathbf{X}, R = 1) = \mathbb{E}(Y|\mathbf{X}, R = 0)$, indicating that the conditional mean of Y is the same for both unlabeled and labeled data after accounting for the full covariates $\mathbf{X}$. This establishes the connection between the labeled and unlabeled data. Moreover, Assumption 1 implies that $\mathbb{P}(R = 1|\mathbf{X}, Y) = \mathbb{P}(R = 1|\mathbf{X})$, meaning that the label indicator R depends solely on the covariates $\mathbf{X}$, i.e., R is missing at random (Molenberghs et al., 2015; Imbens and Rubin, 2015). It should be noted that Assumption 1 does not imply $Y \perp\!\!\!\perp R \mid \mathbf{Z}$ when $\mathbf{Z} \neq \mathbf{X}$. If $Y \perp\!\!\!\perp R \mid \mathbf{Z}$ and the regression models are correctly specified, then $\beta^* = \beta^{0*}$. Otherwise, the equality may not hold.

Despite bearing many similarities, Assumption 1 differs from the classic SSL setup in the missing mechanism represented by the probabilistic behavior of R . SSL assumes the missing-completely-at-random mechanism (MCAR) (Chakraborty, 2016; Chakraborty and Cai, 2018; Zhang et al., 2019; Zhang and Bradic, 2021), that is, $R \perp\!\!\!\perp (\mathbf{X}, Y)$, thus $\mathbb{P}(R = 1|\mathbf{X})$ is a constant, independent of $\mathbf{X}$. In contrast, we allow R to probabilistically depend on $\mathbf{X}$. In addition, we make the following technical assumption.

Assumption 2. $\pi^*(\mathbf{X}) = \mathbb{P}(R = 1|\mathbf{X}) > c$ almost surely, for some constant $0 < c < 1$ independent of N and d .

This condition is introduced to ensure that each unit has a positive probability

of belonging to $\mathcal{L}$. Then the labeled dataset $\mathcal{L}$ is of a non-negligible size compared with N . By Assumption 2, the ratio n/N may randomly fluctuate but, as $N \rightarrow \infty$, converges to a value in the interval $(0, 1]$, equal to $\mathbb{E}(n/N) = \mathbb{P}(R = 1)$. This distinguishes our sampling process from the stratified sampling process widely used in the previous literature (Chakraborty, 2016; Chakraborty and Cai, 2018; Zhang et al., 2019; Zhang and Bradic, 2021), where the sizes of labeled and unlabeled datasets, n and $N - n$, are deterministic. For the asymptotic analysis, they assume that both n and N tend to ∞ such that n/N converges to a value in $[0, 1]$, including zero. See Section 5 for a detailed discussion.

2.3 AIPW estimating equations

For estimating β^* , we introduce the augmented inverse probability weighting (AIPW) estimating equations. Essentially the same AIPW estimating equation has been used in the previous literature, albeit under somewhat different settings than ours. See Section 5 for a connection and comparison of our method with the previous methods.

With the true PS model $\pi^*(\mathbf{X}) = \mathbb{P}(R = 1|\mathbf{X})$, under Assumption 1, we have $\mathbb{E}[\{R/\pi^*(\mathbf{X})\}\{Y - \psi(\beta^T \mathbf{Z})\}\mathbf{Z}] = \mathbb{E}[\{Y - \psi(\beta^T \mathbf{Z})\}\mathbf{Z}]$. Then a sample estimating equation for β^* is $\tilde{\mathbb{E}}[\{R/\hat{\pi}(\mathbf{X})\}\{Y - \psi(\beta^T \mathbf{Z})\}\mathbf{Z}] = 0$, where $\hat{\pi}(\mathbf{X})$ is an estimator of $\pi^*(\mathbf{X})$ and $\tilde{\mathbb{E}}$ denotes the sample mean, defined as $\tilde{\mathbb{E}}(U) = N^{-1} \sum_{i=1}^N U_i$ for a variable U . Let $\hat{\beta}_{\text{IPW}}$ be a solution to the previous estimating equation. If the PS model is correctly specified, then under certain regularity conditions, $\hat{\pi}(\mathbf{X}) \xrightarrow{\mathbb{P}} \pi^*(\mathbf{X})$ and

$\hat{\beta}_{\text{IPW}} \xrightarrow{\mathbb{P}} \beta^*$; If the PS model is misspecified, $\hat{\pi}(\mathbf{X}) \not\xrightarrow{\mathbb{P}} \pi^*(\mathbf{X})$ and $\hat{\beta}_{\text{IPW}} \not\xrightarrow{\mathbb{P}} \beta^*$.

To mitigate the possible inconsistency of $\hat{\beta}_{\text{IPW}}$, the AIPW method introduces an augmented term. Specifically, let $m^*(X) = \mathbb{E}[Y|\mathbf{X}]$ be the true OR function and $\hat{m}(\mathbf{X})$ be a corresponding estimator, the AIPW estimating equation is

$$\tilde{\mathbb{E}} \left[\frac{R}{\hat{\pi}(\mathbf{X})} \{Y - \psi(\beta^T \mathbf{Z})\} \mathbf{Z} + \left\{ 1 - \frac{R}{\hat{\pi}(\mathbf{X})} \right\} \{\hat{m}(\mathbf{X}) - \psi(\beta^T \mathbf{Z})\} \mathbf{Z} \right] = 0. \quad (2.4)$$

Let $\hat{\beta}_{\text{AIPW}}$ be the solution to equation (2.4). If the PS model is misspecified, the augmented term $\tilde{\mathbb{E}}[\{1 - R/\hat{\pi}(\mathbf{X})\} \{\hat{m}(\mathbf{X}) - \psi(\beta^T \mathbf{Z})\} \mathbf{Z}]$ corrects the bias of $\tilde{\mathbb{E}}[\{R/\hat{\pi}(\mathbf{X})\} \{Y - \psi(\beta^T \mathbf{Z})\} \mathbf{Z}]$ by introducing the estimator $\hat{m}(\mathbf{X})$. In addition, if the PS model is correctly specified, the augmented term improves the estimation efficiency of β^* by leveraging the association between $\mathbf{X}$ and Y . It can be shown that the left side of equation (2.4) converges in probability to that of equation (2.2), if either $\hat{\pi}(\mathbf{X}) \xrightarrow{\mathbb{P}} \pi^*(\mathbf{X})$ or $\hat{m}(\mathbf{X}) \xrightarrow{\mathbb{P}} m^*(\mathbf{X})$, which is the property of double robustness.

In the classic SSL setup, estimating β^* is considered to be an MCAR problem, where $\hat{\pi}(\mathbf{X})$ is a constant, independent of $\mathbf{X}$, and the estimator $\hat{m}(\mathbf{X})$ is usually defined using an OR model by (unweighted) least squares, maximum likelihood, or variations (Chakraborty, 2016; Chakraborty and Cai, 2018; Zhang et al., 2019). However, our semi-supervised regression is formulated as a MAR problem, where $\hat{\pi}(\mathbf{X})$ depends on $\mathbf{X}$. In such a scenario, as shown in the next section, the estimators

$\hat{\pi}(\mathbf{X})$ and $\hat{m}(\mathbf{X})$ for the PS and OR functions can be defined in a sequential manner, different from least squares or maximum likelihood, in order to obtain desirable properties with possible model misspecification.

3. Method

We develop a novel AIPW method that achieves $\sqrt{N}$ -consistency in the setting of sparse high-dimensional PS and OR models, even if the estimation of the PS model exhibits convergence rates slower than $N^{-1/2}$ and the OR model is misspecified.

3.1 Model specification for nuisance parameters

AIPW estimation based on the estimating equation (2.4) requires constructing the estimators $\hat{\pi}(\mathbf{X})$ and $\hat{m}(\mathbf{X})$ for $\pi^*(\mathbf{X})$ and $m^*(\mathbf{X})$, using some PS and OR models. In contrast with the previous literature, we introduce a dependency between $\hat{\pi}(\mathbf{X})$ and $\hat{m}(\mathbf{X})$ by carefully specifying basis functions and incorporating weighted estimation.

Specifically, let $\mathbf{F}(\mathbf{X}) = \{1, f_1(\mathbf{X}), \dots, f_p(\mathbf{X})\}^\top$ be a vector of known functions of $\mathbf{X}$. We allow p to be high-dimensional, tending to infinity as N increases. As in Tan (2020a), we propose using logistic regression as a working model for the PS function $\pi^*(\mathbf{X})$,

$$\mathbb{P}(R = 1|\mathbf{X}) = \pi(\mathbf{X}; \gamma) = [1 + \exp\{-\gamma^\top \mathbf{F}(\mathbf{X})\}]^{-1}, \quad (3.1)$$

where γ is an unknown coefficient parameter.

Remark 1. In several related works on classic SSL and stratified sampling setups, making efforts to estimate the PS may not be necessary. Firstly, in the classic SSL setup, the true PS is a constant, leading to a constant PS model. Secondly, in the stratified sampling setup, the proportion n/N is fixed and known, which corresponds to a known PS function. Thus, researchers concentrate on specifying OR models.

Next, we turn to modeling the OR function $m^*(\mathbf{X})$. The working model for $m^*(\mathbf{X})$ is specified as

$$\mathbb{E}[Y|\mathbf{X}] = m(\mathbf{X}; \alpha) = \psi\{\alpha^\top \mathbf{G}(\mathbf{X})\}, \quad (3.2)$$

where $\mathbf{G}(\mathbf{X}) = \{1, g_1(\mathbf{X}), \dots, g_q(\mathbf{X})\}^\top$ is a vector of known functions of $\mathbf{X}$ and q can be high-dimensional. In contrast to the previous literature, to ensure valid inference even when the OR model is misspecified, we carefully specify a choice of $\mathbf{G}(\mathbf{X})$ as follows:

$$\mathbf{G}(\mathbf{X}) = [\mathbf{F}(\mathbf{X})^\top, \{\mathbf{Z} \otimes \mathbf{F}(\mathbf{X})\}^\top]^\top, \quad (3.3)$$

where $\mathbf{Z} \otimes \mathbf{F}(\mathbf{X})$ consists of all interactions between $\mathbf{Z}$ and $\mathbf{F}(\mathbf{X})$ (i.e., all products of individual components from $\mathbf{Z}$ and $\mathbf{F}(\mathbf{X})$). Equation (3.3) represents the minimal choice for $\mathbf{G}(\mathbf{X})$, and additional covariates can also be incorporated, such as nonlinear terms of $\mathbf{Z}$ and $\mathbf{F}(\mathbf{X})$. Under sparsity conditions, these additional

terms can be readily accommodated.

3.2 Estimation procedures

The proposed method consists of the following three steps: (a) estimating the parameter γ in the PS model (3.1); (b) estimating the parameter α in the OR model (3.2); (c) estimating the target parameter β .

For estimating γ , we utilize a regularized calibrated estimator (Tan, 2020b), defined as

$$\hat{\gamma} = \underset{\gamma \in \mathbb{R}^{p+1}}{\operatorname{argmin}} L_{\text{RCAL}}(\gamma) = \underset{\gamma \in \mathbb{R}^{p+1}}{\operatorname{argmin}} \{\ell_{\text{CAL}}(\gamma) + \lambda_{\gamma} \|\gamma_{1:p}\|_1\}, \quad (3.4)$$

where $\ell_{\text{CAL}}(\gamma) = \tilde{\mathbb{E}}[R \exp\{-\gamma^T \mathbf{F}(\mathbf{X})\} + (1-R)\gamma^T \mathbf{F}(\mathbf{X})]$, λ_{γ} is a pre-specified tuning parameter, $\|\cdot\|_1$ denotes the L_1 -norm, and for any vector ν , $\nu_{i:j}$ is the sub-vector of ν consisting of its i -th to j -th elements (both ends included). For a possibly misspecified model $\pi(\mathbf{X}; \gamma)$, under suitable regularity conditions, $\hat{\gamma}$ converges in probability to its target value $\bar{\gamma}$ defined by $\bar{\gamma} = \underset{\gamma \in \mathbb{R}^{p+1}}{\operatorname{argmin}} \mathbb{E}[R \exp\{-\gamma^T \mathbf{F}(\mathbf{X})\} + (1-R)\gamma^T \mathbf{F}(\mathbf{X})]$.

For estimating α , we adopt a regularized weighted maximum likelihood estimator (Tan, 2020a), defined as

$$\hat{\alpha} = \underset{\alpha \in \mathbb{R}^{q+1}}{\operatorname{argmin}} L_{\text{RWL}}(\alpha; \hat{\gamma}) = \underset{\alpha \in \mathbb{R}^{q+1}}{\operatorname{argmin}} \{\ell_{\text{WL}}(\alpha; \hat{\gamma}) + \lambda_{\alpha} \|\alpha_{1:q}\|_1\}, \quad (3.5)$$

where $\ell_{\text{WL}}(\alpha; \hat{\gamma}) = \tilde{\mathbb{E}}(Rw(\mathbf{X}; \hat{\gamma})[-Y\alpha^T \mathbf{G}(\mathbf{X}) + \Psi\{\alpha^T \mathbf{G}(\mathbf{X})\}])$, $w(X, \hat{\gamma}) = \{1 -$

$\pi(\mathbf{X}, \hat{\gamma})\}/\pi(\mathbf{X}, \hat{\gamma})$, $\Psi(u) = \int_0^u \psi(t)dt$ is the antiderivative of ψ and λ_α is a tuning parameter. Similar to the target value $\bar{\gamma}$, we define the target value of α as $\bar{\alpha} = \operatorname{argmin}_{\alpha \in \mathbb{R}^{q+1}} \mathbb{E}(Rw(\mathbf{X}; \bar{\gamma}) [-Y\alpha^\top \mathbf{G}(\mathbf{X}) + \Psi\{\alpha^\top \mathbf{G}(\mathbf{X})\}])$.

After obtaining the estimators of γ and α , the proposed calibrated AIPW estimator of β , denoted as $\hat{\beta}$, is the solution to

$$\tilde{\mathbb{E}}\{\tau(\mathbf{O}, \hat{\alpha}, \beta, \hat{\gamma})\} = 0, \quad (3.6)$$

where $\mathbf{O} = (\mathbf{X}, \mathbf{Z}, Y, R)$ and $\tau(\mathbf{O}, \alpha, \beta, \gamma) = \{R/\pi(\mathbf{X}; \gamma)\}\{Y - \psi(\alpha^\top \mathbf{G})\}\mathbf{Z} + \{\psi(\alpha^\top \mathbf{G}) - \psi(\beta^\top \mathbf{Z})\}\mathbf{Z}$. Our estimating equations (3.6) share the same form as the estimating equations (2.4). However, there is a crucial distinction between our method and previous related methods based on (2.4). In previous methods, the PS and OR models are specified and fitted independently of each other, typically both by least squares, maximum likelihood, or variations. In our method, the PS and OR models are specified and fitted in a sequentially dependent manner. This design allows our estimator $\hat{\beta}$ to achieve $\sqrt{N}$ -consistency in the presence of misspecified OR models.

4. Theoretical analysis

In this section, we present the theoretical analysis of the proposed estimator $\hat{\beta}$. In Section 4.1, we examine theoretical properties of estimators $\hat{\gamma}$ and $\hat{\alpha}$ in PS and OR models. Then, we study the asymptotic properties of the proposed estimator $\hat{\beta}$ in

Section 4.2. Finally, in Section 4.3, we extend our analysis to the classic SSL setting (stratified sampling with constant PS).

4.1 Properties of the estimators for nuisance parameters

For simplicity, we denote $\mathbf{F}(\mathbf{X})$ and $\mathbf{G}(\mathbf{X})$ as $\mathbf{F}$ and $\mathbf{G}$, respectively. All the regularity Assumptions are given in the Supplement. In addition, let $|\cdot|$ denote the cardinality of a set. We first present the properties of $\hat{\gamma}$ based on Tan (2020a) [Theorems 1 and 3].

Proposition 1. *Suppose that Assumption S1 in the Supplement is satisfied, and λ_γ in (3.4) is specified by $\lambda_\gamma = A_0\lambda_0$, where $A_0 > 1$ is a constant defined in Assumption S1. Then, with probability at least $1 - 8\epsilon$,*

$$D_{\text{CAL}}^\dagger(\hat{\gamma}^\text{T}\mathbf{F}, \bar{\gamma}^\text{T}\mathbf{F}) + (A_0 - 1)\lambda_0\|\hat{\gamma} - \bar{\gamma}\|_1 \leq M_0|S_{\bar{\gamma}}|\lambda_0^2, \quad (4.1)$$

where $M_0 > 0$ is a constant, and $D_{\text{CAL}}^\dagger(\hat{\gamma}^\text{T}\mathbf{F}, \bar{\gamma}^\text{T}\mathbf{F})$ is the symmetrized Bregman Divergence w.r.t $\ell_{\text{CAL}}(\gamma)$, i.e., $D_{\text{CAL}}^\dagger(\hat{\gamma}^\text{T}\mathbf{F}, \bar{\gamma}^\text{T}\mathbf{F}) = -\tilde{\mathbb{E}}[R\{\exp(-\hat{\gamma}^\text{T}\mathbf{F}) - \exp(-\bar{\gamma}^\text{T}\mathbf{F})\}(\hat{\gamma}^\text{T}\mathbf{F} - \bar{\gamma}^\text{T}\mathbf{F})]$.

Note that $D_{\text{CAL}}^\dagger(\hat{\gamma}^\text{T}\mathbf{F}, \bar{\gamma}^\text{T}\mathbf{F}) \geq 0$, then equation (4.1) implies that $\|\hat{\gamma} - \bar{\gamma}\|_1 \leq \{M_0/(A_0 - 1)\}|S_{\bar{\gamma}}|\lambda_0$, which indicates that the L_1 -convergence rate of the proposed regularized calibrated estimator $\hat{\gamma}$ is $|S_{\bar{\gamma}}|\lambda_0$, where $|S_{\bar{\gamma}}|$ is the nonzero size of $\bar{\gamma}$ and $\lambda_0 = c_\gamma\sqrt{\ln\{(1+p)/\epsilon\}/N}$ for some constant c_γ . For example, taking $\epsilon = 1/(1+p)$

4.2 Large sample properties of the proposed estimator

gives $\lambda_0 = c_\gamma \sqrt{2 \ln(1+p)/N}$, which leads to $\|\hat{\gamma} - \bar{\gamma}\|_1 = O(|S_{\bar{\gamma}}| \sqrt{\ln(1+p)/N})$.

Proposition 2. *Suppose Assumptions S1 and S2 in the Supplement are satisfied. If $\ln\{(1+p)/\epsilon\}/N < 1$ and λ_α in (3.5) is specified as $A_1 \lambda_1$, where $A_1 > 1$ is a constant defined in Assumption S2. Then with probability at least $1 - 10\epsilon$,*

$$D_{\text{WL}}^\dagger(\hat{\alpha}^\text{T} \mathbf{G}, \bar{\alpha}^\text{T} \mathbf{G}, \bar{\gamma}) + \exp(\eta_{01})(A_1 - 1)\lambda_1 \|\hat{\alpha} - \bar{\alpha}\|_1 \leq M_{11}|S_{\bar{\gamma}}|\lambda_0^2 + M_{12}|S_{\bar{\alpha}}|\lambda_1^2, \quad (4.2)$$

where η_{01} is a constant defined in Lemma S9, M_{11} and M_{12} are constants defined in Section S6.2 of Supplement; $D_{\text{WL}}^\dagger(\hat{\alpha}^\text{T} \mathbf{G}, \bar{\alpha}^\text{T} \mathbf{G}, \bar{\gamma})$ is the symmetrized Bregman divergence given by

$$D_{\text{WL}}^\dagger(\hat{\alpha}^\text{T} \mathbf{G}, \bar{\alpha}^\text{T} \mathbf{G}, \bar{\gamma}) = \tilde{\mathbb{E}}[Rw(\mathbf{X}; \bar{\gamma})\{\psi(\hat{\alpha}^\text{T} \mathbf{G}) - \psi(\bar{\alpha}^\text{T} \mathbf{G})\}(\hat{\alpha}^\text{T} \mathbf{G} - \bar{\alpha}^\text{T} \mathbf{G})]. \quad (4.3)$$

Proposition 2 gives the convergence rate of $\hat{\alpha}$. Since $D_{\text{WL}}^\dagger(\hat{\alpha}^\text{T} \mathbf{G}, \bar{\alpha}^\text{T} \mathbf{G}, \bar{\gamma}) \geq 0$ and $\lambda_1 \geq \lambda_0$ (Assumption S2(vi)), $\|\hat{\alpha} - \bar{\alpha}\|_1 \leq c_m(|S_{\bar{\gamma}}| + |S_{\bar{\alpha}}|)\lambda_1$ for some constant $c_m > 0$.

4.2 Large sample properties of the proposed estimator

In this subsection, we present the properties of the proposed estimator $\hat{\beta}$.

Theorem 1. Suppose Assumptions 1, 2, and S1 – S3 in the Supplement are satisfied, and the PS model (3.1) is correctly specified with $\pi(\cdot; \bar{\gamma}) = \pi^*(\cdot)$. If $\ln((1+p)/\epsilon)/N <$

1, then the following results hold.

(i) The estimator $\hat{\beta}$ is consistent and asymptotically normal, and $\sqrt{N}(\hat{\beta} - \beta^*) \xrightarrow{d} N(0, \Sigma)$, where $\xrightarrow{d}$ denotes convergence in distribution, $\Sigma = \Gamma^{-1} \Lambda \Gamma^{-1}$ with $\Gamma = \mathbb{E}\{\psi_1(\beta^{*\top} \mathbf{Z}) \mathbf{Z} \mathbf{Z}^\top\}$, and $\Lambda = \mathbb{E}\{\tau(\mathbf{O}, \bar{\alpha}, \beta^*, \bar{\gamma}) \tau(\mathbf{O}, \bar{\alpha}, \beta^*, \bar{\gamma})^\top\}$.

(ii) A consistent estimator of Σ is $\hat{\Sigma} = \hat{\Gamma}^{-1} \hat{\Lambda} \hat{\Gamma}^{-1}$, where $\hat{\Gamma} = \tilde{\mathbb{E}}\{\psi_1(\hat{\beta}^\top \mathbf{Z}) \mathbf{Z} \mathbf{Z}^\top\}$ and $\hat{\Lambda} = \tilde{\mathbb{E}}\{\tau(\mathbf{O}, \hat{\alpha}, \hat{\beta}, \hat{\gamma}) \tau(\mathbf{O}, \hat{\alpha}, \hat{\beta}, \hat{\gamma})^\top\}$. Thus, for a constant vector $\mathbf{c}$ with the same dimension of β , an asymptotic $(1 - \eta)$ confidence interval for $\mathbf{c}^\top \beta^*$ is $\mathbf{c}^\top \hat{\beta} \pm z_{\eta/2} \sqrt{\mathbf{c}^\top \hat{\Sigma} \mathbf{c} / N}$, where $z_{\eta/2}$ is the $(1 - \eta/2)$ quantile of the standard normal distribution.

Theorem 1 shows that if the PS model is correct, and $\alpha \rightarrow \bar{\alpha}$ at certain rate (faster than $N^{-1/4}$), regardless of whether the OR working model is correct, the proposed estimator $\hat{\beta}$ is $\sqrt{N}$ -consistent and asymptotically normal, and the proposed CIs based on $\hat{\Sigma}$ are valid. In Section S1 of Supplement, we provide a detailed discussion to explain how these properties are achieved and why, for a general choice of $\mathbf{Z}$, the correct specification of the PS model is assumed, although either PS model or OR model is assumed to be correct in related work (Tan, 2020a).

In contrast, the estimator $\hat{\beta}_{\text{IPW}}$ is not $\sqrt{N}$ -consistent in general, even with a correctly specified PS model, because in high-dimensional settings, the convergence rate of $\hat{\pi}(\mathbf{X})$ is typically slower than $N^{-1/2}$, leading to a slower convergence rate of $\hat{\beta}_{\text{IPW}}$. Similarly, when the PS model is correctly specified but the OR model is misspecified, the convergence rate of the AIPW estimator with the PS and OR

functions being estimated using conventional regularized maximum likelihood as in double machine learning (Chernozhukov et al., 2018) may also be slower than $N^{-1/2}$. Such double-machine learning estimators are only shown to achieve $\sqrt{N}$ -consistency when both PS and OR models are correctly specified and the estimated PS and OR functions converge to the *true values* at fast enough rates (specifically, the product of estimation errors is smaller than $N^{-1/2}$).

4.3 Extension to stratified sampling with constant PS

To facilitate comparison with existing methods described in Section 5, we extend the theoretical analysis of the proposed estimator to the classic SSL setting (stratified sampling with constant PS), where the sizes of labeled and unlabeled datasets, n and $N - n$, are deterministic. For fixed n and N , the observed data are generated as follows:

- The labeled dataset $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n) \stackrel{\text{i.i.d.}}{\sim} \mathbb{P}(\mathbf{X}, Y | R = 1)$.
- The unlabeled dataset $(\mathbf{X}_{n+1}, \dots, \mathbf{X}_N) \stackrel{\text{i.i.d.}}{\sim} \mathbb{P}(\mathbf{X}, Y | R = 0)$.

Moreover, by letting $\mathbf{F} = 1$, $\hat{\pi}(\mathbf{X}) = \pi(\mathbf{X}; \hat{\gamma}) = n/N$ (constant PS) and allowing a general choice of $\mathbf{G}$ instead of (3.3), our AIPW estimator, denoted as $\hat{\beta}^s$, can be rewritten as a solution to the following estimating equation:

$$\frac{1}{n} \sum_{i=1}^n \{Y_i - \psi(\hat{\alpha}^\top \mathbf{G}_i)\} \mathbf{Z}_i + \frac{1}{N} \sum_{i=1}^N \{\psi(\hat{\alpha}^\top \mathbf{G}_i) - \psi(\beta^\top \mathbf{Z}_i)\} \mathbf{Z}_i = 0. \quad (4.4)$$

Due to the constant $\hat{\pi}(\mathbf{X})$, our estimator $\hat{\alpha}$ reduces to the regularized unweighted maximum likelihood or least squares estimator. The following proposition for $\hat{\beta}^s$ can be readily derived.

Proposition 3. *Suppose that the conditions of Theorem 1 are satisfied with $\mathbf{F} = 1$, $\pi^*(\mathbf{X}) \equiv n/N$, and a general choice of $\mathbf{G}$, where Assumption S3(v) reduces to $|S_{\bar{\alpha}}| \ln(q+1) = o_p(\sqrt{n})$. Then we have $\sqrt{n}(\hat{\beta}^s - \beta^*) \xrightarrow{d} N(0, \Sigma^s)$, where $\Sigma^s = \mathbf{\Gamma}^{-1} \mathbf{\Lambda}^s \mathbf{\Gamma}^{-1}$, with $\mathbf{\Gamma}$ defined as in Theorem 1 and $\mathbf{\Lambda}^s = \mathbb{E}([Y - \{(N-n)/N\}\psi(\bar{\alpha}^T \mathbf{G}) - (n/N)\psi(\beta^{*T} \mathbf{Z})]^2 \mathbf{Z} \mathbf{Z}^T) + \{(N-n)n/N^2\} \mathbb{E}[\{\psi(\bar{\alpha}^T \mathbf{G}) - \psi(\beta^{*T} \mathbf{Z})\}^2 \mathbf{Z} \mathbf{Z}^T]$.*

For comparison, by letting $\mathbf{F} = 1$ and $\pi^*(\mathbf{X}) \equiv n/N$ in Theorem 1, the variance matrix Σ for $\hat{\beta}$ such that $\sqrt{N}(\hat{\beta} - \beta^*) \xrightarrow{d} N(0, \Sigma)$ is $\Sigma = \mathbf{\Gamma}^{-1} \mathbf{\Lambda} \mathbf{\Gamma}^{-1}$, where $\mathbf{\Lambda} = \mathbb{E}([(N/n)\{Y - \psi(\bar{\alpha}^T \mathbf{G})\}^2 + \{\psi(\bar{\alpha}^T \mathbf{G}) - \psi(\beta^{*T} \mathbf{Z})\}^2] \mathbf{Z} \mathbf{Z}^T) + 2\mathbb{E}(\{Y - \psi(\bar{\alpha}^T \mathbf{G})\} \{\psi(\bar{\alpha}^T \mathbf{G}) - \psi(\beta^{*T} \mathbf{Z})\}) \mathbf{Z} \mathbf{Z}^T)$. By direct calculation (see Section S8 of Supplement), we have $\Sigma/N = \Sigma^s/n$, which means the asymptotic variances of $\hat{\beta}^s$ and $\hat{\beta}$ are the same. Hence, in the classic SSL with constant PS, the asymptotic variances of our estimators, $\hat{\beta}$ under random sampling or $\hat{\beta}^s$ under stratified sampling, are equivalent to each other.

5. Comparison with previous methods

We first summarize various previous methods, all of which can be integrated into the AIPW estimation framework. We also compare the asymptotic variances of our

methods with previous ones. See Supplement Section S2 for a detailed comparison of our paper with several related papers with regression of Y on high-dimensional $\mathbf{Z} = \mathbf{X}$ as mentioned in Section 2.1.

5.1 Unified framework

Various methods have been proposed in the classic SSL setting, i.e., stratified sampling with constant PS ($\mathbf{F} = 1$) as in Section 4.3 (Chakraborty, 2016; Chakraborty and Cai, 2018; Zhang et al., 2019; Zhang and Bradic, 2021). From an AIPW point of view, the major difference among previous methods lies in the choices of OR working models. For example, Zhang et al. (2019) and Zhang and Bradic (2021) proposed linear OR working models for the estimation of $\mathbb{E}(Y)$, i.e., with $\mathbf{Z} = 1$. Chakraborty (2016) and Chakraborty and Cai (2018) proposed using non-parametric or semi-parametric OR working models, such as kernel smoothing or partially linear model, for regression analysis with $\mathbf{Z}$ a sub-vector of $\mathbf{X}$.

If we disregard the specific choice of the OR working model, the previous methods can be incorporated into the AIPW estimating framework. In our notation, the previous estimators can be reformulated as solutions of

$$\frac{1}{n} \sum_{i=1}^n \{Y_i - \psi(\hat{\alpha}^T \mathbf{G}_i)\} \mathbf{Z}_i + \frac{1}{N} \sum_{i=1}^N \{\psi(\hat{\alpha}^T \mathbf{G}_i) - \psi(\beta^T \mathbf{Z}_i)\} \mathbf{Z}_i = 0, \quad (5.1)$$

for different choices of $\mathbf{Z}_i$ and $\psi(\cdot)$. Specifically, Zhang et al. (2019) and Zhang and

Bradic (2021) correspond to the case of $\mathbf{Z} = 1$ and $\psi(\cdot)$ is the identity function in (5.1), while Chakraborty (2016) corresponds to the case where $\mathbf{Z}$ is any sub-vector of $\mathbf{X}$ and $\psi(\cdot)$ is an arbitrary inverse link function. Suppose a constant PS model is used with $\pi^*(\mathbf{X}) \equiv n/N$, then the AIPW estimating equation (3.6) or, in the simplified form, (4.4) in Section 4.3, coincides with (5.1).

In addition, Chakraborty and Cai (2018) adopted a variation of AIPW estimating equations. By the assumption $\lim_{n,N \rightarrow \infty} n/N \rightarrow 0$ and controlling kernel smoothing in fitting OR working models, they made it possible to drop the labeled part and only retain the augmented term of unlabeled data in (5.1). Their estimating equations can be reformulated in our notation as $\{1/(N-n)\} \sum_{i=n+1}^N \{\psi(\hat{\alpha}^\top \mathbf{G}_i) - \psi(\beta^\top \mathbf{Z}_i)\} \mathbf{Z}_i = 0$, with $\psi(\cdot)$ to be identity function and $\mathbf{Z} = \mathbf{X}$, corresponding to full linear regression.

5.2 Variance comparison

Under stratified sampling with constant PS, both estimators of Zhang et al. (2019) and Zhang and Bradic (2021) of $\mathbb{E}(Y)$ achieve asymptotic normality and their asymptotic variance is $\text{Var}(Y - \bar{\alpha}^\top \mathbf{G}) + (n/N)\text{Var}(\bar{\alpha}^\top \mathbf{G})$. Under this setting, by Proposition 3 with $\mathbf{Z} = 1$, our AIPW estimator has the asymptotic variance $\mathbb{E}\{(Y - \bar{\alpha}^\top \mathbf{G})^2 + (n/N)(\bar{\alpha}^\top \mathbf{G} - \beta^*)^2 + 2(n/N)(Y - \bar{\alpha}^\top \mathbf{G})(\bar{\alpha}^\top \mathbf{G} - \beta^*)\}$, where $\beta^* = \mathbb{E}(Y) = \mathbb{E}(\bar{\alpha}^\top \mathbf{G})$ and $\mathbb{E}\{(Y - \bar{\alpha}^\top \mathbf{G})\mathbf{G}\} = 0$ by definition of $\bar{\alpha}$ and the fact that $\mathbf{G}$ includes 1. Then $\mathbb{E}\{(Y - \bar{\alpha}^\top \mathbf{G})(\bar{\alpha}^\top \mathbf{G} - \beta^*)\} = \mathbb{E}\{(Y - \bar{\alpha}^\top \mathbf{G})(\bar{\alpha}^\top \mathbf{G})\} = 0$, and our

asymptotic variance reduces to $\text{Var}(Y - \bar{\alpha}^T \mathbf{G}) + (n/N)\text{Var}(\bar{\alpha}^T \mathbf{G})$ matching results in Zhang et al. (2019) and Zhang and Bradic (2021).

Under stratified sampling with constant PS, the estimators of regression coefficients in conditional mean models proposed by Chakraborty (2016) and Chakraborty and Cai (2018) achieve asymptotic normality under the assumption that $\lim_{n,N \rightarrow \infty} n/N \rightarrow 0$. Their asymptotic variances satisfy

$$\mathbf{\Gamma}^{-1} \text{Var}[\{Y - \psi(\bar{\alpha}^T \mathbf{G})\} \mathbf{Z}] \mathbf{\Gamma}^{-1}. \quad (5.2)$$

In this setup, by Proposition 3, our estimator has the asymptotic variance $\mathbf{\Gamma}^{-1} \text{Var}[\{Y - \psi(\bar{\alpha}^T \mathbf{G})\} \mathbf{Z}] \mathbf{\Gamma}^{-1} + (n/N) \mathbf{\Gamma}^{-1} \mathbb{E}[\{\psi(\bar{\alpha}^T \mathbf{G}) - \psi(\beta^{*T} \mathbf{Z})\}^2 \mathbf{Z} \mathbf{Z}^T] \mathbf{\Gamma}^{-1} + 2(n/N) \mathbf{\Gamma}^{-1} \mathbb{E}[\{Y - \psi(\bar{\alpha}^T \mathbf{G})\} \{\psi(\bar{\alpha}^T \mathbf{G}) - \psi(\beta^{*T} \mathbf{Z})\} \mathbf{Z} \mathbf{Z}^T] \mathbf{\Gamma}^{-1}$, which, compared with (5.2), in general has additional term $(n/N) \mathbf{\Gamma}^{-1} \left\{ \mathbb{E}[\{\psi(\bar{\alpha}^T \mathbf{G}) - \psi(\beta^{*T} \mathbf{Z})\}^2] + 2 \mathbb{E}[\{Y - \psi(\bar{\alpha}^T \mathbf{G})\} \{\psi(\bar{\alpha}^T \mathbf{G}) - \psi(\beta^{*T} \mathbf{Z})\}] \mathbf{Z} \mathbf{Z}^T \right\} \mathbf{\Gamma}^{-1}$.

The additional term reduces to 0 under the condition $\lim_{n,N \rightarrow \infty} n/N \rightarrow 0$, implying that our result aligns with those of Chakraborty (2016) and Chakraborty and Cai (2018) with the same condition.

6. Numerical implementation and simulation

We design experiments to evaluate the finite-sample performance of the proposed method and compare it with several alternative methods: the IPW method with

Lasso-regularized maximum likelihood estimation for the PS model, AIPW methods with Lasso-regularized maximum likelihood estimation for both the PS and OR models without cross-fitting as in Tan (2020a), and AIPW methods with cross-fitting and Lasso-regularized maximum likelihood estimation for both the PS and OR models (Chernozhukov et al., 2018; Zhang and Bradic, 2021). These competing estimators are denoted as IPW, AIPW_{RML} , and AIPW_{CF} , respectively. For the PS and OR models, the basis functions $\mathbf{F}$ and $\mathbf{G}$ are specified as follows.

- $\text{AIPW}_{\text{RCAL}}$: Given $\mathbf{X} = (1, X_1, \dots, X_d)^\top$, let $\{\xi_i\}_{i=1}^k$ be k points equally spaced within $(-a, a)$, where $d = 3$, $k = 49$, and $a = 3$. Let $f_{ij}(\mathbf{X}) = (X_i - \xi_j)_+$, $i = 1, \dots, d, j = 1, \dots, k$. Let $\mathbf{F} = \{1, f_{11}(\mathbf{X}), \dots, f_{1n_k}(\mathbf{X}), \dots, f_{d1}(\mathbf{X}), \dots, f_{dn_k}(\mathbf{X})\}^\top$ be basis functions in the PS model, and $\mathbf{G} = \{\mathbf{F}^\top, (\mathbf{Z} \otimes \mathbf{F})^\top\}^\top$ be basis functions in the OR model. The dimension of $\mathbf{F}$ is 148. For $\mathbf{Z} = 1, X_1, \mathbf{X}$, the dimensions of $\mathbf{G}$ are 148, 285 and 589, respectively.
- IPW: Let $\mathbf{F}$ be the basis functions for the PS model.
- AIPW_{RML} : Let $\mathbf{F}$ and $\mathbf{G} = \mathbf{F}$ be the basis functions for both PS and OR models, respectively.
- AIPW_{CF} : Let $\mathbf{F}$ and $\mathbf{G} = \mathbf{F}$ be the basis functions for both PS and OR models, respectively.

We consider the estimators of population mean for $\mathbf{Z} = 1$, regression coefficients in the mean model for $\mathbf{Z} = X_1$ and $\mathbf{Z} = \mathbf{X}$, respectively. The data generating mechanisms and the associated numerical results are presented in Section S9

of Supplement. We evaluate methods with five metrics: Bias (Monte Carlo bias), $\sqrt{\text{Var}}$ (Monte Carlo standard deviation), $\sqrt{\text{EVar}}$ (square root of the mean of variance estimates), CP90 (coverage proportions of the 90% CIs), and CP95 (coverage proportions of the 95% CIs). The simulation results demonstrate that the proposed method $\text{AIPW}_{\text{RCAL}}$ has the smallest $\sqrt{\text{Var}}$ and $\sqrt{\text{EVar}}$, and Bias. Moreover, CP90 and CP95 of the proposed method are more aligned with their nominal values of 0.90 and 0.95, respectively. This indicates the effectiveness of the proposed method in terms of estimating both the population mean and regression coefficients. See Section S9.3 of Supplement for more details.

7. Application

7.1 Data description

The Communities and Crime dataset comprises 1994 records of crime-related information from communities in the USA, which combine socio-economic data from the 1990 US Census, law enforcement data from the 1990 US LEMAS survey, and crime data from the 1995 FBI UCR. Each record includes a response `ViolentCrimesPerPop` (total number of violent crimes per 100,000 population) and 127 covariates, encompassing both location information, such as `state` as well as `county`, and socio-economic factors, such as `PctTeen2Par` (percent of kids age 12-17 in two parent households), `HousVacant` (number of vacant households), `PctHousNoPhone` (per-

cent of occupied housing units without phone) and **PopDens** (population density in persons per square mile). In this study, we are interested in examining the influence of univariate covariates on the response. We consider the case where $\mathbf{Z} = (1, X_i)^\top$ for a particular univariate covariate X_i as discussed in Section 2.1 and denote $\beta^* = (\beta_0, \beta_1)$.

Due to the presence of numerous missing values in high-dimensional covariates, we eliminate covariates with high missing ratios. See details of the pre-processing procedure in Section S10.1 of Supplement. After pre-processing, the analytical dataset consists of 1993 observations and 26 covariates (i.e., $d = 26$). The shift in covariates $\mathbf{X}$ is naturally introduced by the different states where the communities are located. We set label indicator R for communities in New Jersey (Code 34) to be 1 and that for communities in other states to be 0 and remove the associated response data if $R = 0$, resulting in 211 labeled observations and 1782 unlabeled observations. The covariate shift of the joint distribution of $\mathbf{X}$ was confirmed to exist using a Gaussian kernel two-sample test with maximum mean discrepancy (You, 2023). Additionally, we assess the shift of each individual covariate by a bootstrap version of the Kolmogorov–Smirnov test (Sekhon, 2011). For results of those tests, please see Section S10.2 of Supplement.

We randomly take 90% of labeled data and 90% of unlabeled data to form the training set with the remaining data used for the testing set. From the remaining 26 covariates, we select four representative ones: **PctTeen2Par**, **HousVacant**,

PctHousNoPhone and **PopDens**, which illustrate different aspects of the socio-economic characteristics of communities. Notice that the covariate shift exists in all four covariates.

We compare the proposed method with IPW, AIPW_{RML} and AIPW_{CF} methods with piecewise linear basis functions introduced in Section 6. The PS and OR working models are estimated the same way as described in Section S9.2 of Supplement. For details of the procedures for designing basis functions, please see Section S10.3 of Supplement.

7.2 Results

Table 1 presents the estimates of the regression coefficients $\hat{\beta}_1$ along with the prediction mean squared error (MSE), which are calculated using the test data. It reveals that the point estimates of the regression coefficient are similar across the different methods. Notably, our estimators achieve the lowest prediction MSE except **PctTeen2Par**, highlighting the superior performance of our methods in minimizing predictive errors.

Table 1: Summary of $\hat{\beta}_1$ and prediction MSE

	$\hat{\beta}_1$				prediction MSE			
	$\text{AIPW}_{\text{RCAL}}$	IPW	AIPW_{RML}	AIPW_{CF}	$\text{AIPW}_{\text{RCAL}}$	IPW	AIPW_{RML}	AIPW_{CF}
PctTeen2Par	-0.137	-0.172	-0.147	-0.256	0.034	0.032	0.034	0.044
HousVacant	0.107	0.261	0.073	0.133	0.046	0.085	0.046	0.047
PctHousNoPhone	0.123	0.245	0.103	0.050	0.036	0.058	0.039	0.047
PopDens	0.045	0.069	0.048	0.039	0.050	0.052	0.052	0.055

Moreover, signs of estimates of coefficients are the same among different meth-

ods for each covariate Z of interest. and they coincide with common sense and previous studies. For example, the coefficients of `PctTeen2Par` are negative, since it is believed to have protective effects in assaults (Luo and Qi, 2017); the coefficients of `HousVacant` is positive, and criminological theories predict a positive association between vacancy and crime since empty structures of houses could provide locations for some crimes (e.g., prostitution, drug dealing), and the absence of residents may prevent social organization and reduce guardianship (Roth, 2019). Moreover, AIPW_{RML} and ours are close in all cases, while IPW estimators and AIPW_{CF} estimators are far from others in some cases.

In Figure 1, we compare the 95% CIs of $\text{AIPW}_{\text{RCAL}}$, AIPW_{RML} and AIPW_{CF} . From the CIs, we see that for AIPW_{RML} and our estimators all four single effects are significant. CIs of our estimators and of AIPW_{RML} 's have similar lengths and are overlapped, except `HousVacant`. The reason of the small difference is that the estimates of β_0 are a bit different. CIs of AIPW_{CF} are much longer; for `PctHousNoPhone` and `PopDens`, the estimates are not significant. Both phenomena show that AIPW_{CF} is not as efficient as other two methods.

8. Extension to estimation of β^{0*}

Consider the estimation of β^{0*} , defined as a solution to estimating equations (2.3). Under Assumption 1, $\mathbb{E}[R\{1 - \pi^*(\mathbf{X})\}/\pi^*(\mathbf{X})\{Y - \psi(\beta^{\text{T}}\mathbf{Z})\}|\mathbf{Z}] = \mathbb{E}[\{1 - R\}\{Y - \psi(\beta^{\text{T}}\mathbf{Z})\}|\mathbf{Z}]$. Then a natural sample estimating equation for β^{0*} is $\tilde{\mathbb{E}}[R\{1 -$

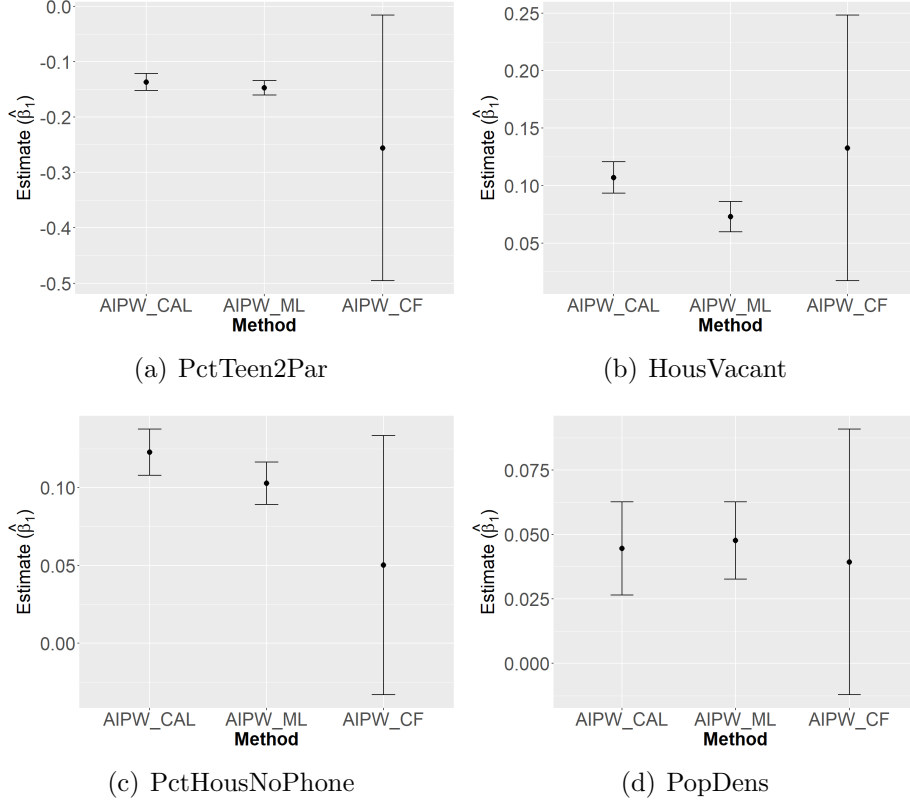


Figure 1: Comparison of 95% CIs of $AIPW_{RCAL}$, $AIPW_{RML}$ and $AIPW_{CF}$

$\hat{\pi}(\mathbf{X})\}/\hat{\pi}(\mathbf{X})\{Y - \psi(\beta^T \mathbf{Z})\}\mathbf{Z}] = 0$. We augment the estimating equations similarly as described in Section 2.3 and obtain the sample AIPW estimating equations:

$$\tilde{\mathbb{E}} \left[\frac{R\{1 - \hat{\pi}(\mathbf{X})\}}{\hat{\pi}(\mathbf{X})} \{Y - \psi(\beta^T \mathbf{Z})\} \mathbf{Z} + \left\{ 1 - \frac{R}{\hat{\pi}(\mathbf{X})} \right\} \{\hat{m}(\mathbf{X}) - \psi(\beta^T \mathbf{Z})\} \mathbf{Z} \right] = 0. \quad (8.1)$$

For the PS and OR models, we adopt a similar construction as in Section 3. Our AIPW estimator for β^{0*} , $\hat{\beta}^0$, is defined as the solution to the estimating equations $\tilde{\mathbb{E}}\{\tau^0(\mathbf{O}, \hat{\alpha}, \beta, \hat{\gamma})\} = 0$, where $\tau^0(\mathbf{O}, \alpha, \beta, \gamma) = ([R\{1 - \pi(\mathbf{X}; \gamma)\}]/\pi(\mathbf{X}; \gamma))\{Y -$

$\psi(\beta^T \mathbf{Z})\} + [\{\pi(\mathbf{X}; \gamma) - R\}/\pi(\mathbf{X}; \gamma)]\{\psi(\alpha^T \mathbf{G}) - \psi(\beta^T \mathbf{Z})\})\mathbf{Z}$. The asymptotic properties of β^{0*} is given in Theorem 2.

Theorem 2. Under Assumptions 1–2 and S1 – S3 in the Supplement, if the PS model (3.1) is correctly specified with $\pi(\cdot; \bar{\gamma}) = \pi^*(\cdot)$, and $\ln\{(1+p)/\epsilon\}/N < 1$, we have that

(i) the estimator $\hat{\beta}^0$ is consistent and asymptotically normal, and $\sqrt{N}(\hat{\beta}^0 - \beta^{0*}) \xrightarrow{d} N(0, \Sigma^0)$, where $\Sigma^0 = \Gamma^{0-1} \Lambda^0 \Gamma^{0-1}$ with $\Gamma^0 = \mathbb{E}[\{1 - \pi(\mathbf{X}; \bar{\gamma})\}\psi_1(\beta^{0*\top} \mathbf{Z}) \mathbf{Z} \mathbf{Z}^\top]$ and $\Lambda^0 = \mathbb{E}\{\tau^0(\mathbf{O}, \bar{\alpha}, \beta^*, \bar{\gamma})\tau^0(\mathbf{O}, \bar{\alpha}, \beta^*, \bar{\gamma})^\top\}$.

(ii) a consistent estimator of Σ^0 is $\hat{\Sigma}^0 = \hat{\Gamma}^{0-1} \hat{\Lambda}^0 \hat{\Gamma}^{0-1}$, where $\hat{\Gamma}^0 = \tilde{\mathbb{E}}\{\psi_1(\hat{\beta}^{0\top} \mathbf{Z}) \mathbf{Z} \mathbf{Z}^\top\}$ and $\hat{\Lambda}^0 = \tilde{\mathbb{E}}\{\tau^0(\mathbf{O}, \hat{\alpha}, \hat{\beta}^{0\top}, \hat{\gamma})\tau^0(\mathbf{O}, \hat{\alpha}, \hat{\beta}^{0\top}, \hat{\gamma})^\top\}$. Thus, for a constant vector $\mathbf{c}$ with the same dimension of β , an asymptotic $(1 - \eta)$ confidence interval for $\mathbf{c}^\top \beta^{0*}$ is $\mathbf{c}^\top \hat{\beta}^{0\top} \pm z_{\eta/2} \sqrt{\mathbf{c}^\top \hat{\Sigma}^0 \mathbf{c}/N}$.

Theorem 2 shows that if the PS model is correct, regardless of the correctness of OR working models, the proposed estimator $\hat{\beta}^0$ is consistent, asymptotically normal, and the proposed CIs based on $\hat{\Sigma}^0$ are valid. Similarly to the estimation of β^* , conclusions in Theorem 2 also hold in low-dimensional settings with a reduced form of Assumptions S1 to S3.

We point out that the method of Liu et al. (2023) for CSTL can be viewed as an AIPW estimator of β^{0*} under the stratified sampling setting, where the labeled and unlabeled datasets $\mathcal{L}$ and $\mathcal{U}$ are treated as two independent samples of fixed sizes

n and $N - n$. They employed partial linear models for both PS and OR working models. By replacing their choices of semi-parametric nuisance models with our parametric models, the estimator of β^{0*} in Liu et al. (2023) can be reformulated as the solution to the following estimating equations:

$$\frac{1}{n} \sum_{i=1}^n w(\mathbf{X}_i; \hat{\gamma}^s) [\{Y_i - \psi(\hat{\alpha}^T \mathbf{G}_i)\} \mathbf{Z}_i] + \frac{1}{N - n} \sum_{i=n+1}^N [\{\psi(\hat{\alpha}^T \mathbf{G}_i) - \psi(\beta^T \mathbf{Z}_i)\} \mathbf{Z}_i] = 0. \quad (8.2)$$

where $w(\mathbf{X}_i; \hat{\gamma}^s) = \exp(-\hat{\gamma}^{sT} \mathbf{F}_i)$ and $\mathbf{F}_i$ is the abbreviation of $\mathbf{F}(\mathbf{X}_i)$; $\hat{\gamma}^s = (\hat{\gamma}_0^s, \hat{\gamma}_{1:p}^{sT})^T$ is an estimator of the parameter γ^s in an exponential tilt model, defined as

$$dG_1 = \exp(\gamma_0^s + \gamma_{1:p}^{sT} \mathbf{F}_{1:p}) dG_0, \quad (8.3)$$

where G_0 and G_1 are two probability distributions for the unlabeled and labeled data in $\mathbf{F}_{1:p}$ and $\gamma_0^s = -\ln \left\{ \int \exp(\gamma_{1:p}^{sT} \mathbf{F}_{1:p}) dG_0 \right\}$ to ensure that $\int dG_1 = 1$. The exponential tilt model (8.3) can be shown to be equivalent to the logistic PS model (3.1), where the coefficients are related as follows (Prentice and Pyke, 1979; Qin, 1998; Tian et al., 2023):

$$\gamma_0 = \gamma_0^s + \ln \left(\frac{\rho_m}{1 - \rho_m} \right), \quad \gamma_{1:p} = \gamma_{1:p}^s, \quad (8.4)$$

where $\rho_m = \mathbb{P}(R = 1)$, the true value of the proportion of missing data. When

analyzing the asymptotic property in stratified sampling settings, we assume n/N to be constant and, consequently, assume that $\rho_m = n/N$. On the other hand, our estimating equations (8.1) can be rewritten as

$$\frac{1}{N} \sum_{i=1}^n w(\mathbf{X}_i; \hat{\gamma}) [\{Y_i - \psi(\hat{\alpha}^T \mathbf{G}_i)\} \mathbf{Z}_i] + \frac{1}{N} \sum_{i=n+1}^N [\{\psi(\hat{\alpha}^T \mathbf{G}_i) - \psi(\beta^T \mathbf{Z}_i)\} \mathbf{Z}_i] = 0, \quad (8.5)$$

where $\hat{\gamma} = (\hat{\gamma}_0, \hat{\gamma}_{1:p})^T$ is an estimator of the parameter γ in logistic PS model (3.1). If the estimators $\hat{\gamma}^s$ and $\hat{\gamma}$ satisfy the same relationship as (8.4), i.e., $\hat{\gamma}_0 = \hat{\gamma}_0^s + \ln\{n/(N - n)\}$ and $\hat{\gamma}_{1:p} = \hat{\gamma}_{1:p}^s$, then one can see that $\{(N - n)/n\}w(\mathbf{X}_i; \hat{\gamma}^s) = \exp(-\hat{\gamma}^T \mathbf{F}_i) = w(\mathbf{X}_i; \hat{\gamma})$, and the two equations (8.2) and (8.5) match each other. Thus, the different forms of (8.2) and (8.5) can be explained by the relationship of the coefficient estimates between the exponential tilt model (8.3) and the logistic regression model (3.1).

9. Discussion

We present a new AIPW method for the inference of regression coefficients in (conditional) mean models in SSL and CSTL settings. We demonstrate that various previous methods can be unified in our AIPW framework by suppressing detailed technical choices. Our AIPW estimator achieves asymptotic normality, and valid CIs can be obtained, whether or not the OR working model is correctly specified, with high-dimensional data. Finite sample performances of the proposed method

are confirmed by a simulation study and an application to a real-world dataset.

Currently, the proposed CIs can only achieve single robustness to the misspecification of the OR model. Doubly robust CIs can be developed using the approach of Ghosh and Tan (2022), albeit at the cost of increasing technical and numerical complexities. In addition, how to handle the case where $\lim_{n,N \rightarrow \infty} n/N \rightarrow 0$ under the random sampling process is also technically challenging, since the “positivity assumption” (Assumption 2) typical in missing data theory is violated. New analysis needs to be developed to address the problem.

Supplementary Material

The online Supplementary Material contains a heuristic discussion on conditions for the proposed estimator to be $\sqrt{N}$ -consistent and asymptotic normal, a comparison of our paper with several related papers with regression of Y on high-dimensional $\mathbf{Z} = \mathbf{X}$ and papers under stratified sampling settings, detailed proofs of theorems as well as propositions, and details of the numerical implementation and application.

Acknowledgements

The authors thank the assistant editor and the anonymous reviewers for their helpful comments and valuable suggestions. Peng Wu was supported by the National Natural Science Foundation of China (No. 12301370), the funding from the Beijing Municipal Education Commission for the Emerging Interdisciplinary Platform for

Digital Business at Beijing Technology and Business University, the Beijing Key Laboratory of Applied Statistics and Digital Regulation.

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