Sensitivity Analysis of Individual Treatment Effects: A Robust Conformal Inference Approach

Ying Jin*, Zhimei Ren*, and Emmanuel J. Candès

1Department of Statistics, Stanford University
2Department of Statistics, University of Chicago
3Department of Mathematics, Stanford University

Abstract

We propose a model-free framework for sensitivity analysis of individual treatment effects (ITEs), building upon ideas from conformal inference. For any unit, our procedure reports the $\Gamma$-value, a number which quantifies the minimum strength of confounding needed to explain away the evidence for ITE.

Our approach rests on the reliable predictive inference of counterfactuals and ITEs in situations where the training data is confounded. Under the marginal sensitivity model of Tan (2006), we characterize the shift between the distribution of the observations and that of the counterfactuals. We first develop a general method for predictive inference of test samples from a shifted distribution; we then leverage this to construct covariate-dependent prediction sets for counterfactuals. No matter the value of the shift, these prediction sets (resp. approximately) achieve marginal coverage if the propensity score is known exactly (resp. estimated). We describe a distinct procedure also attaining coverage, however, conditional on the training data. In the latter case, we prove a sharpness result showing that for certain classes of prediction problems, the prediction intervals cannot possibly be tightened. We verify the validity and performance of the new methods via simulation studies and apply them to analyze real datasets.

1 Introduction

Understanding the effect of a treatment is arguably one of the main research lines in causal inference. Over the past few decades, there has been a rich literature in identifying, estimating and conducting inference on the mean value of causal effects; parameters of interest include the average treatment effect (ATE) or the conditional average treatment effect (CATE). These quantities, however, might fail to provide reliable uncertainty quantification for individual responses: the knowledge that a drug might be effective for a whole population ‘on average’ does not imply that it is effective on a particular patient. Taking the intrinsic variability of the responses into account, inference on the individual treatment effect (ITE) may be better suited for reliable decision-making. To quantify the uncertainty in individual treatment effects, Lei and Candès (2020) offered a novel viewpoint. Rather than constructing confidence intervals for parameters—e.g. the ATE—they proposed designing prediction intervals for potential outcomes, namely, for counterfactuals and ITEs. Briefly, Lei and Candès constructed well calibrated prediction intervals by building upon the conformal inference framework (Vovk et al., 2005, 2009). In that work, the typical mismatch between the counterfactuals and the observations due to the selection mechanism is resolved with the strong ignorability assumption (Imbens and Rubin, 2015); that is to say, the treatment assignment mechanism is independent of the potential outcomes conditional on a set of observed covariates. The strong ignorability assumption is automatically satisfied in randomized experiments and commonly used in the causal inference literature (Rubin, 1978; Rosenbaum and Rubin, 1983b; Imbens and Rubin, 2015). In observational studies, however, the strong ignorability assumption is not testable (Imbens and Rubin, 2015, Chapter 12) and hard to justify in general. In practice, failing to account for possible confounding in observational data can yield misleading conclusions (Rutter, 2007; Fewell et al., 2007; Gaudino et al., 2018).

*Author names listed alphabetically.
1.1 Γ-values

In this paper, we seek to understand the robustness of causal conclusions on ITEs against potential unmeasured confounding. To this end, the procedure we propose starts from a sequence of hypothesized confounding strengths whose precise meaning will be made clear shortly; for each hypothesized strength, a prediction interval is constructed for the ITE. The procedure then screens the prediction intervals, and for each unit, reports the smallest confounding strength with which the prediction interval contains zero: we call this the Γ-value. Informally, the Γ-value describes the strength of unmeasured confounding necessary to explain away the predicted effect.

Imagine we want to test for a positive ITE on a treated unit. For a range of hypothesized confounding strengths, our procedure constructs one-sided prediction intervals for the ITE at the $1 - \alpha = 0.9$ confidence level. The Γ-value is then the smallest confounding strength with which the lower bound of the prediction interval is smaller than zero. Figure 1 shows the survival function of the Γ-values calculated on a real dataset measuring the academic performance of students subject or not to mindset interventions (all the details are in Section 6.2). We see that 20% of the students have Γ-values greater than 1.05; roughly speaking, for these students the confounding strength needs to be as large as 1.05 to explain away the evidence for positive ITEs. We also see that 7.20% of the students have Γ-values greater than 2 and some students have Γ-values as large as 5, showing strong evidence for positive ITEs.

Formally, the Γ-value can be used to draw conclusions on the ITE with a pre-specified confounding strength. For example, if we believe the confounding strength is no larger than 2, we can claim an individual has positive ITE as long as its Γ-value is greater than 2. Our method guarantees that if the magnitude of confounding is at most 2, the probability of incorrectly ‘classifying’ a unit as having a positive ITE is at most $\alpha = 0.1$ (or any other fraction).

Figure 2 plots the Γ-values as a function of the achievement levels of the schools the students belong to. Once more, our procedure provides valid inference on a single ITE. This means that if the strength of confounding is at most 2, the chance that an individual with a negative ITE has a Γ-value larger than 2 is at most $\alpha$. Taking a step further, one might be interested in the inference on a set of selected units (e.g., the red points in Figure 2), for which evidence on multiple ITEs needs to be combined. In a companion paper, we shall consider simultaneous inference on multiple ITEs with proper error control.

1.2 Problem setup

Throughout, we work under the potential outcome framework (Neyman, 1923; Imbens and Rubin, 2015). Let $X \in \mathcal{X}$ denote the observed covariates, $T \in \{0, 1\}$ the assigned treatment, and $Y(1), Y(0) \in \mathbb{R}$ the potential outcomes. We assume there is an unobserved confounder $U \in \mathcal{U}$ satisfying

$$\quad (Y(1), Y(0)) \perp\!\!\!\perp T \mid X, U,$$

(1)
in which \( U \) can be a random vector. As pointed out by Yadlowsky et al. (2018), a confounder satisfying (1) always exists since one can take \( U = (Y(1), Y(0)) \). In contrast, the strong ignorability assumption states

\[
(Y(1), Y(0)) \perp\!\!\!\perp T \mid X. \tag{2}
\]

As well known, the latter assumes that we have measured sufficiently many features so that the potential outcomes are independent of the treatment conditional on the covariates \( X \).

Suppose there are i.i.d. samples \( \{(X_i, U_i, T_i, Y_i(0), Y_i(1))\}_{i \in \mathcal{D}} \) from some distribution \( \mathbb{P} \). We adopt the commonly used stable unit treatment value assumption (SUTVA) (see e.g., Cox (1958); Rubin (1978, 1990); Imbens and Rubin (2015)), so that we observe

\[
Y_i = Y_i(T_i) = T_i \cdot Y_i(1) + (1 - T_i) \cdot Y_i(0). 
\]

This means that the observed dataset consists of the random variables \( (X_i, T_i, Y_i)_{i \in \mathcal{D}} \).

Without further assumptions, the potential outcomes and the treatment assignment mechanism can arbitrarily depend on \( U \), making the estimation of treatment effects impossible. For example, imagine we would like to assess the effect of a drug on patients. We are interested in \( Y(1) \) (e.g., the survival time of the patient if the drug is taken), and have available observational data recording the treatment assignment \( T \) and outcome \( Y \). Consider a confounded setting, where the drug is assigned to patients based on an undocumented factor \( U \), namely, the patient’s condition when admitted to the hospital, so that only those in critical condition get treated. Since \( U \) is highly correlated with \( Y(1) \), the survival times of treated patients will likely be smaller than those in the whole population (which is our inferential target), making the task of identifying the effectiveness of the drug extremely difficult. As such, we shall work with confounders that only have limited effect on the treatment assignment mechanism; the concept of “limited effect” is formalized by the sensitivity models introduced below.

### 1.3 Sensitivity models

A sensitivity model characterizes the degree to which the data distribution violates the strong ignorability assumption. There has been a rich literature in designing different types of sensitivity models (see e.g. Zhao et al. (2017) and the references therein). In this paper, we work under the marginal sensitivity model (Tan, 2006; Zhao et al., 2017) on the unidentifiable super-population, characterized by the following marginal \( \Gamma \)-selection condition:

**Definition 1.1 (Marginal \( \Gamma \)-selection).** A distribution \( \mathbb{P} \) over \( (X, U, T, Y(0), Y(1)) \) satisfies the marginal \( \Gamma \)-selection condition if for \( \mathbb{P} \)-almost all \( x \in \mathcal{X} \) and \( u \in \mathcal{U} \),

\[
\frac{1}{\Gamma} \leq \frac{\mathbb{P}(T = 1 \mid X = x, U = u)/\mathbb{P}(T = 0 \mid X = x, U = u)}{\mathbb{P}(T = 1 \mid X = x)/\mathbb{P}(T = 0 \mid X = x)} \leq \Gamma. \tag{3}
\]

Under the marginal \( \Gamma \)-selection condition, no matter how one changes the value of the confounder, the odds of being treated conditional on the covariates and the confounder will at most be off by a factor of \( \Gamma \) when compared to the odds of being treated conditional only on the covariate. Therefore, the effect of confounders on the selection bias is bounded.

The above marginal sensitivity model is closely related to Rosenbaum’s sensitivity model (Rosenbaum, 1987) and its generalizations (Yadlowsky et al., 2018), characterized by the following \( \Gamma \)-selection condition:
Definition 1.2 (Γ-selection). A distribution \( \mathbb{P} \) over \((X, U, T, Y(0), Y(1))\) satisfies the \( \Gamma \)-selection condition if for \( \mathbb{P} \)-almost all \( x \in X \) and \( u, u' \in U \),

\[
\frac{1}{\Gamma} \leq \frac{\mathbb{P}(T = 1 | X = x, U = u)}{\mathbb{P}(T = 0 | X = x, U = u)} \leq \Gamma.
\]

As pointed out by Zhao et al. (2017, Prop. 7.1), the \( \Gamma \)-selection condition is stronger than the marginal \( \Gamma \)-selection condition in the sense that a distribution \( \mathbb{P} \) over \((X, U, T, Y(0), Y(1))\) satisfying the \( \Gamma \)-selection condition must also satisfy the marginal \( \Gamma \)-selection condition.

In the following, we let \( \mathbb{P}^{\text{sup}} \) denote the unknown super-population over \((X, U, T, Y(0), Y(1))\) that generates the partial observations \( D \). For any \( \Gamma \geq 1 \), \( \mathcal{P}(\Gamma) \) is the set of super-populations that satisfy the marginal \( \Gamma \)-selection condition.

1.4 Prediction intervals for counterfactuals

The crux of our approach is to construct reliable prediction intervals for counterfactuals when the observations satisfy the marginal sensitivity model. In Section 2, we propose a generic robust weighted conformal procedure, which is applied to counterfactual prediction in Section 3. Suppose we are interested in \( Y(1) \) and \((X_{n+1}, Y_{n+1}(1))\) is a test sample from the super-population (the results apply to other types of counterfactuals as well). Given a nominal level \( 1 - \alpha \) and a fixed confounding level \( \Gamma \geq 1 \), the prediction interval \( \hat{C}(X_{n+1}, \Gamma) \) we construct from the confounded data ensures

\[
\mathbb{P}(Y_{n+1}(1) \in \hat{C}(X_{n+1}, \Gamma)) \geq 1 - \alpha - \hat{\Delta}
\]
as long as \( \mathbb{P}^{\text{sup}} \in \mathcal{P}(\Gamma) \); here, the probability is over the confounded observations \((X_i, T_i, Y_i)_{i \in D} \) and the test sample \((X_{n+1}, Y_{n+1}(1))\). The error term \( \hat{\Delta} = 0 \) if the propensity score \( \hat{e}(x) = \mathbb{P}(T = 1 | X = x) \) of the observed data is known exactly, and otherwise depends on the estimation of the propensity score.

In practice, researchers may want to control the risk of falsely rejecting a hypothesis on an individual treatment effect given the data at hand, \( D \). Section 4 offers a sister procedure with probably approximately correct (PAC)-type guarantee. Once more, suppose \( \mathbb{P}^{\text{sup}} \in \mathcal{P}(\Gamma) \). Then given any \( \delta, \alpha > 0 \) and any \( \Gamma \geq 1 \), we can construct a prediction interval \( \hat{C}(X_{n+1}, \Gamma) \) such that

\[
\mathbb{P}(Y_{n+1}(1) \in \hat{C}(X_{n+1}, \Gamma) | D) \geq 1 - \alpha - \hat{\Delta}
\]
holds with probability at least \( 1 - \delta \) over the randomness of \( D \). As before, the error term \( \hat{\Delta} \) depends on the estimation of the propensity score \( \hat{e}(x) \). Since any distribution \( \mathbb{P} \) satisfying the \( \Gamma \)-selection condition must also satisfy the marginal \( \Gamma \)-selection condition, our methods also provide valid prediction intervals for counterfactuals under Rosenbaum’s sensitivity model.

1.5 Related work

The idea of sensitivity analysis dates back to Cornfield et al. (1959) who studied the causal effect of smoking on developing lung cancer. The authors concluded that if an unmeasured confounder—hormone in their example—were to rule out the causal association between smoking and lung cancer, it needed to be so strongly associated with smoking that no such factors could reasonably exist. The approach of Cornfield et al. (1959) requires that both the outcome and the confounder are binary and that there are no covariates. Whereas Bross (1966, 1967) used the same conditions later on, subsequent works substantially relaxed these assumptions. Rosenbaum and Rubin (1983a) proposed a sensitivity model to work with categorical covariates. Later, under Rosenbaum’s sensitivity model, a series of works (Rosenbaum, 1987; Gastwirth et al., 1998; Rosenbaum, 2002b,a) further extended sensitivity analysis to broader settings by studying samples with matching covariates. Imbens (2003), Ding and VanderWeele (2016) and VanderWeele and Ding (2017) also considered unmeasured confounders with ‘limited’ effect, but under different sensitivity models. More recently, Tan (2006) proposed the marginal sensitivity model, and Zhao et al. (2017) proposed a construction of bounds and confidence intervals for the ATE under this model. Their result was recently sharpened by Dorn and Guo (2021). Bringing a distributionally robust optimization perspective to the
sensitivity analysis problem, Yadlowsky et al. (2018) studied the estimation of CATE under Rosenbaum’s sensitivity model.

Our contribution is to provide robustness for the inference procedure against a proper level of confounding. This bears similarity with several works conducting ‘safe’ policy evaluation and policy learning under certain sensitivity models (see e.g., Namkoong et al. (2020); Kallus and Zhou (2021)). In contrast to the estimation and learning tasks, we provide well-calibrated uncertainty quantification for counterfactuals, which calls for a different set of techniques.

Another closely related line of work is conformal inference, which is the tool we employ (and improve) towards robust quantification of uncertainty. Conformal inference was pioneered and developed by Vladimir Vovk and his collaborators in a series of papers (see e.g., Vovk et al. (2005, 2009); Gammerman and Vovk (2007); Shafer and Vovk (2008); Vovk (2012, 2013)). In recent years, the technique has been broadly used for establishing statistical guarantees for learning algorithms (see e.g., Lei and Wasserman (2014); Lei et al. (2018); Lei (2019); Romano et al. (2020); Cauchois et al. (2021)). In particular, Lei and Candès (2020) studied the counterfactual prediction problem with conformal inference tools under the strong ignorability condition.

Lastly, we note that the robust prediction perspective is related to Cauchois et al. (2020), which also studies the construction of robust prediction sets. That said, the setting considered there is substantially different from ours; we will expand on this in Section 2. Park et al. (2021) constructs PAC-type prediction sets under an identifiable covariate shift, with some robustness features. We provide in Section 4 a robust PAC-type procedure as well; however, our methods apply to partially identifiable distributional shifts and are distinct from the rejection sampling strategy used in Park et al. (2021).

1.6 Outline of the paper
The rest of the paper is organized as follows:

• Sections 2 to 4 concern the development of robust counterfactual inference procedures. In Section 2, we develop a general robust weighted conformal inference procedure; we show in Section 3 how to apply it to construct valid counterfactual prediction sets. We propose a distinct procedure in Section 4 with PAC-type coverage, and establish a sharpness result.

• Section 5 expresses sensitivity analysis as a sequence of hypotheses testing problems, and gives a statistical interpretation of the Γ-value. Simulation studies explain how the Γ-value relates to the true effect size and actual confounding level.

• Section 6 evaluates the proposed method on a semi-synthetic dataset to examine its validity and applicability. Finally, our sensitivity analysis framework is used to draw causal conclusions on a real dataset.

2 Robust weighted conformal inference
We begin by considering a generic predictive inference problem under distributional shift. We will connect this to counterfactual inference under a marginal sensitivity model in Section 3.

Suppose we have i.i.d. training data \((X_i, Y_i)_{i \in D}\) from some distribution \(\mathbb{P}\), and an independent test sample \((X_{n+1}, Y_{n+1})\) from some possibly different distribution \(\tilde{\mathbb{P}}\). We consider a general setting where \(\tilde{\mathbb{P}}\) is “within bounded distance” from \(\mathbb{P}\), in the sense that, for some fixed functions \(\ell(\cdot)\) and \(u(\cdot)\), it belongs to the identification set defined as

\[
P(\mathbb{P}, \ell, u) = \left\{ \tilde{\mathbb{P}} : \ell(x) \leq \frac{d\tilde{\mathbb{P}}}{d\mathbb{P}}(x, y) \leq u(x) \text{ \(\mathbb{P}\)-almost surely} \right\}.
\]

The task is to provide a calibrated prediction interval \(\hat{\mathcal{C}}(X_{n+1})\) for \(Y_{n+1}\).

Equation (4) actually identifies a new class of distributional robustness problems. As we shall see later in Section 3.1, our model (4) is motivated by sensitivity analysis and is quite distinct from other models in
the literature. For instance, Cauchois et al. (2020) considers a setting in which the target distribution \( \mathbb{P} \) is assumed to be within an \( f \)-divergence ball with radius \( \rho \) centered around \( \mathbb{P} \), so that the identification set is

\[
Q(\mathbb{P}, \rho) = \left\{ \mathbb{P} : D_f(\mathbb{P} \| \mathbb{P}) \leq \rho \right\}.
\]

Instead of bounding the overall shift in (5), the constraint in (4) actually allows freedom in the shift of \( X \); to be sure, the set (4) can be small as long as \( \ell(x) \) and \( w(x) \) are close. For counterfactual prediction under the strong ignorability condition in Lei and Candès (2020), the identification set (4) happens to be a singleton even if \( \mathbb{P}_X \) and \( \mathbb{P}_X \) are drastically different, while (5) would require a large \( \rho \) to hold. More generally, when there is a (approximately) known large shift in the marginal distribution \( \mathbb{P}_X \) but a relatively small shift in the conditional \( \mathbb{P}_{Y|X} \), (4) provides a tighter range of the target distributions. Finally, the pointwise constraint in (4) (as opposed to the average form) makes it naturally compatible with the weighted conformal inference framework of Tibshirani et al. (2019).

2.1 Warm up: weighted conformal inference

Before introducing our method, it is best to start by a brief recap of the weighted (split) conformal inference procedure. Assume the likelihood ratio \( w(x, y) = \frac{d\mathbb{P}}{d\mathbb{P}_x}(x, y) \) is known exactly. The dataset \( \mathcal{D} \) is first randomly split into a training fold \( \mathcal{D}_{\text{train}} \) of cardinality \( n_{\text{train}} \) and a calibration fold \( \mathcal{D}_{\text{calib}} \) of cardinality \( n \). We use \( \mathcal{D}_{\text{train}} \) to train any nonconformity score function \( V : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) which measures how well \( (x, y) \) “conforms” to the calibration samples: the smaller \( V(x, y) \), the better \( (x, y) \) conforms to the calibration samples; see e.g., Gupta et al. (2019) for examples of nonconformity scores. We then define \( V_i = V(X_i, Y_i) \) for \( i \in \mathcal{D}_{\text{calib}} \). For any hypothetical value \( (x, y) \in \mathcal{X} \times \mathcal{Y} \) of the new data point, we assign weights to the samples as

\[
p_i^w(x, y) := \frac{w(X_i, Y_i)}{\sum_{j=1}^{n} w(X_j, Y_j) + w(x, y)}, \quad i = 1, \ldots, n,
\]

\[
p_{n+1}^w(x, y) := \frac{w(x, y)}{\sum_{j=1}^{n} w(X_j, Y_j) + w(x, y)}.
\]

For any random variable \( Z \), define the quantile function as

\[
\text{Quantile}(q, Z) = \inf\{z : \mathbb{P}(Z \leq z) \geq q\},
\]

and let \( \delta_{\alpha} \) denote a point mass at \( \alpha \). Then a level \( (1-\alpha) \) prediction interval is given by

\[
\hat{C}(X_{n+1}) = \{ y : V(X_{n+1}, y) \leq \hat{V}_{1-\alpha}(y) \},
\]

where

\[
\hat{V}_{1-\alpha}(y) = \text{Quantile}(1 - \alpha, \sum_{i=1}^{n} p_i^w(X_{n+1}, y) \cdot \delta_{\hat{\ell}_i} + p_{n+1}^w(X_{n+1}, y) \cdot \delta_{\infty}).
\]

The prediction interval (6) is shown by Tibshirani et al. (2019) to obey \( \mathbb{P}(Y_{n+1} \in \hat{C}(X_{n+1})) \geq 1 - \alpha \), and it is computable when \( w(x, y) \) is a known function of \( x \) only. In our context, \( w(x, y) \) depends on \( x \) only when \( \mathcal{P}(\mathbb{P}, \ell, u) = \{\mathbb{P}\} \) is a singleton—this is exactly the case in Lei and Candès (2020), where the strong ignorability condition (2) is assumed.

2.2 Robust weighted conformal inference procedure

Now suppose we have a pair of functions \( \hat{\ell} \) and \( \hat{u} : \mathcal{X} \to \mathbb{R}^+ \) with \( \hat{\ell}(x) \leq \hat{u}(x) \) for all \( x \in \mathcal{X} \). In general, we expect \( \hat{\ell}(x) \) (resp. \( \hat{u}(x) \)) to serve as a pointwise lower (resp. upper) bound on the unknown likelihood ratio \( w(x, y) \), although our theoretical guarantee does not depend on this.

Proceeding as before and denoting \( \mathcal{D}_{\text{calib}} = \{1, \ldots, n\} \), we train a nonconformity score function \( V : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) on \( \mathcal{D}_{\text{train}} \). We also allow \( \hat{\ell}(\cdot) \) and \( \hat{u}(\cdot) \) to be obtained from \( \mathcal{D}_{\text{train}} \). Let \( [1], [2], \ldots, [n] \) be a permutation of \( \{1, 2, \ldots, n\} \) such that \( V_{[1]} \leq V_{[2]} \leq \cdots \leq V_{[n]} \). Defining \( \ell_i = \hat{\ell}(X_i) \) and \( u_i = \hat{u}(X_i) \) for \( 1 \leq i \leq n \), and \( u_{n+1} = \hat{u}(X_{n+1}) \), we construct the prediction interval

\[
\hat{C}(X_{n+1}) = \{ y : V(X_{n+1}, y) \leq V_{[k]} \},
\]

where

\[
\hat{V}_{1-\alpha}(y) = \text{Quantile}(1 - \alpha, \sum_{i=1}^{n} p_i^w(X_{n+1}, y) \cdot \delta_{\ell_i} + p_{n+1}^w(X_{n+1}, y) \cdot \delta_{\infty}).
\]
where
\[ k^* = \min \{ k : \tilde{F}(k) \geq 1 - \alpha \}, \quad \tilde{F}(k) = \frac{\sum_{i=1}^{k} \ell_i}{\sum_{i=1}^{k} \ell_i + \sum_{i=k+1}^{n} u_i + u_{n+1}}. \] (8)

The thresholding function \( \tilde{F}(k) \) in (8) is monotone in \( k \), hence a linear search suffices to find \( k^* \). We summarize the procedure in Algorithm 1.

**Algorithm 1** Robust conformal prediction: the marginal procedure

**Input:** Calibration data \( D_{\text{calib}} \), bounds \( \tilde{\ell}(\cdot), \hat{u}(\cdot) \), non-conformity score function \( V : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \), test covariate \( x \), target level \( \alpha \in (0, 1) \).

1. For each \( i \in D_{\text{calib}} \), compute \( V_i = V(X_i, Y_i) \).
2. For each \( i \in D_{\text{calib}} \), compute \( \ell_i = \tilde{\ell}(X_i) \) and \( u_i = \hat{u}(X_i) \).
3. Compute \( u_{n+1} = \hat{u}(x) \).
4. For each \( 1 \leq k \leq n \), compute \( \tilde{F}(k) \) as in (8).
5. Compute \( k^* = \min \{ k : \tilde{F}(k) \geq 1 - \alpha \} \).

**Output:** Prediction set \( \hat{C}(x) = \{ y : V(x, y) \leq V_{[k^*]} \} \).

**Remark 2.1.** Writing \( W_i = w(X_i, Y_i) \) for \( 1 \leq i \leq n \) and \( W_{n+1}(y) = w(X_{n+1}, y) \), we can check for (6) that \( \hat{V}_{1-\alpha}(y) = V_{[k^*(y)]} \), where \( k^*(y) = \min \{ k : F(k, y) \geq 1 - \alpha \} \) and
\[ F(k, y) = \frac{\sum_{i=1}^{k} W_i}{\sum_{i=1}^{n} W_i + W_{n+1}(y)}. \] (9)

For each \( k \), the threshold \( \tilde{F}(k) \) in (8) is the solution to the following optimization problem

\[
\text{minimize} \quad \frac{\sum_{i=1}^{k} W_i}{\sum_{i=1}^{n} W_i + W_{n+1}}
\text{subject to} \quad \tilde{\ell}(X_i) \leq W_i \leq \hat{u}(X_i), \quad \forall \ i \in D_{\text{calib}} \cup \{ n+1 \},
\]

which seeks a lower bound on the unknown \( F(k, y) \) in (9) if we believe \( \tilde{\ell}(x) \leq w(x, y) \leq \hat{u}(x) \) for all \((x, y) \in \mathcal{X} \times \mathcal{Y} \). Therefore, \( \hat{V}_{[k^*]} \) is a conservative estimate (upper bound) of \( \hat{V}_{1-\alpha}(y) \) in (6), and it is also the tightest upper bound one could obtain given the constraints \( \tilde{\ell}(X_i) \leq W_i \leq \hat{u}(X_i), \forall \ i \in D_{\text{calib}} \cup \{ n+1 \} \).

### 2.3 Theoretical guarantee

To state the coverage guarantee of Algorithm 1, we start with some notations. We write \( a_+ = \max(a, 0) \) and \( a_- = \max(-a, 0) \) for any \( a \in \mathbb{R} \). For any random variable \( U \), define \( \|U\|_r = (\mathbb{E}[|U|^r])^{1/r} \) as the \( L_r \) norm for any \( r \geq 1 \), and \( \|U\|_\infty = \mathbb{E}[^{\text{ess sup}}|U|] \) as the \( L_\infty \) norm. Throughout the paper, all the statements are conditional on \( D_{\text{train}} \), so that \( \ell(\cdot), \hat{u}(\cdot) \) and \( V(\cdot, \cdot) \) can be viewed as fixed functions.

**Theorem 2.2.** Assume \((X_i, Y_i)_{i \in D_{\text{calib}}} \overset{\text{i.i.d.}}{\sim} P\), and the independent test point \((X_{n+1}, Y_{n+1}) \sim P\) has likelihood ratio \( w(x, y) = \frac{dP}{dP}(x, y) \). Then for any target level \( \alpha \in (0, 1) \), the output of Algorithm 1 satisfies
\[
\hat{P}(Y_{n+1} \in \hat{C}(X_{n+1})) \geq 1 - \alpha - \hat{\Delta},
\] where the probability is over \( D_{\text{calib}} \) and \((X_{n+1}, Y_{n+1})\), and
\[
\hat{\Delta} = \|1/\tilde{\ell}(X)\|_q \cdot \left( \|\ell(X) - w(X, Y)\|_p + \|\hat{u}(X) - w(X, Y)\|_p \right) + \frac{1}{n} \left\| w(X, Y) \right\|^{1/p} \cdot \| \hat{u}(X) - w(X, Y) \|_p. \] (10)
Given \( q \geq 1, \) \( p \) is chosen such that \( 1/p + 1/q = 1 \) with the convention that \( p = \infty \) for \( q = 1. \) The expectation in \( L_p, L_q \) is taken over an independent sample \( (X,Y) \sim \mathbb{P}. \)

Clearly, if \( \hat{\ell}(X) \leq w(X,Y) \leq \hat{u}(X) \) a.s., \( \Delta = 0 \) and

\[
\mathbb{P}(Y_{n+1} \in \hat{C}(X_{n+1})) \geq 1 - \alpha.
\]

The proof of Theorem 2.2 is deferred to Appendix B.2. Almost sure bounds on the likelihood ratio imply exact coverage. Otherwise, coverage is off by at most \( \Delta. \) First, \( \|1/\hat{\ell}(X)\|_q \) is bounded when \( \ell(\cdot) \) is bounded away from zero. Second, the remaining terms (between brackets) are small if \( \hat{\ell}(X) \) (resp. \( \hat{u}(X) \)) is below (resp. above) the likelihood ratio most of the time. In particular, for all target distributions within \( (4), \) if \( \hat{\ell}(\cdot) \) and \( \hat{u}(\cdot) \) are estimators for \( \ell(\cdot) \) and \( u(\cdot) \), one additive term can be decomposed as

\[
\| (\hat{\ell}(X) - w(X,Y))_+ \|_p = \left\| \{ (\hat{\ell}(X) - \ell(X)) - (w(X,Y) - \ell(X)) \}_+ \right\|_p,
\]

which is small as long as the estimation error does not exceed the population gap most of the time. Our numerical experiments demonstrate that \( \Delta \) is reasonably small even with non-negligible estimation errors.

**Remark 2.3.** The miscoverage bound in Theorem 2.2 holds for any distributional shift and any postulated bounds \( \ell(\cdot) \) and \( \hat{u}(\cdot). \) The results also hold if the bounds take the general form \( \ell(x,y) \) and \( \hat{u}(x,y). \) Therefore, our procedure may be of use in a very broad range of settings.

### 3 Valid counterfactual inference under the sensitivity model

With the generic methodology in place, we return to counterfactual inference under unmeasured confounding. We shall characterize distributional shifts of interest, translate the target distribution into a set like \( (4) \) and show how Algorithm 1 can be applied.

Recall that we have a partially revealed and possibly confounded dataset \( (X_i, T_i, Y_i)_{i \in \mathcal{D}} \) generated by an unknown super population \( \mathbb{P}^{sup}. \) Given an independent new unit from \( \mathbb{P}^{sup} \) with only the covariate \( X_{n+1} \) observed, we would like to construct a prediction interval that covers \( Y_{n+1}(1) \) with probability at least \( 1 - \alpha; \) the probability is over the randomness of the training sample \( \mathcal{D} \) and the new unit. The main challenge is that the distribution of \( (X_{n+1}, Y_{n+1}(1)) \) may differ from that of the observations we have access to; that is, the training distribution is \( \mathbb{P}_{\text{train}} = \mathbb{P}_{X,Y(1)|T=1}, \) while the target distribution is \( \mathbb{P}_{\text{target}} = \mathbb{P}_{X,Y(1)}. \)

#### 3.1 Bounding the distributional shift

In the previous example, the likelihood ratio takes the form \( w(x,y) = \frac{d\mathbb{P}_{X,Y(1)}}{d\mathbb{P}_{X,Y(1)|T=1}}(x,y). \) A key observation in Lei and Candès (2020) is that, under the strong ignorability condition \( (2), \) \( w(x,y) \) is an identifiable function of \( x, \) i.e., the target distribution can be identified from the observed (training) distribution with a covariate shift. This fact is used to construct prediction intervals for counterfactuals with finite-sample guarantees by leveraging the weighted conformal inference procedure.

In the presence of unmeasured confounding, \( w(x,y) \) can no longer be expressed as a function of \( x. \) However, under the marginal \( \Gamma \)-selection condition \( (3), \) \( w(x,y) \) can be bounded from above and below by functions of \( x; \) that is, the unknown target distribution falls within a set of the form \( (4). \) The following lemma is a key ingredient for establishing the boundedness result.

**Lemma 3.1.** Suppose a distribution \( \mathbb{P} \) over \( (X,U,T,Y(0),Y(1)) \) satisfies the marginal \( \Gamma \)-selection condition. Then for any \( t \in \{0,1\}, \) it holds for \( \mathbb{P} \)-almost all \( x \in \mathcal{X}, y \in \mathcal{Y} \) that

\[
\frac{1}{\Gamma} \leq \frac{d\mathbb{P}_{Y(t)|X,T=t}}{d\mathbb{P}_{Y(t)|X,T=1-t}}(x,y) \leq \Gamma.
\]
The proof of Lemma 3.1 is in Appendix B.1. Returning to $w(x,y)$, by Bayes’ rule we have
\[
\frac{dP_{X,Y(1)}}{dP_{X,Y(1)|T=1}} = P(T = 1) \cdot \left(1 + \frac{dP_{Y(1)|X,T=1}}{dP_{Y(1)|X,T=0}} \cdot \frac{1 - e(X)}{e(X)}\right)
\tag{12}
\]
Applying Lemma 3.1 to (12), we obtain
\[
P(T = 1) \cdot \left(1 + \frac{1}{\Gamma} \cdot \frac{1 - e(X)}{e(X)}\right) \leq \frac{dP_{X,Y(1)}}{dP_{X,Y(1)|T=1}} \leq P(T = 1) \cdot \left(1 + \Gamma \cdot \frac{1 - e(X)}{e(X)}\right).
\]
We have thus bounded the likelihood ratio $w(x,y)$ by functions of the covariate $x$.

The above reasoning broadly applies to other types of inferential targets: we might consider *average treatment effect on the treated (ATT)*-type inference on $Y(1)$; that is, to construct a prediction interval such that $P(Y_{n+1}(1) \in \hat{C}(X_{n+1}) | T = 1) \geq 1 - \alpha$. In this case, the likelihood ratio is simply $w(x,y) = \frac{dP_{X,Y(1)|T=1}}{dP_{X,Y(1)}}(x,y) = 1$. Alternatively, we might be interested in the *average treatment effect on the control (ATC)*-type inference on $Y(1)$; that is, to construct $\hat{C}(X_{n+1})$ such that $P(Y_{n+1}(1) \in \hat{C}(X_{n+1}) | T = 0) \geq 1 - \alpha$. In this case, the likelihood ratio is $\frac{dP_{X,Y(1)|T=0}}{dP_{X,Y(1)}}$ and the lower and upper bounds are
\[
\ell(x) = P(T = 1) \cdot \frac{1}{\Gamma} \cdot \frac{1 - e(x)}{e(x)}, \quad u(x) = P(T = 1) \cdot \Gamma \cdot \frac{1 - e(x)}{e(x)}
\]
More generally, one might also wish to conduct inference on a different population, i.e., the target distribution admits a different distribution of covariates whereas the joint distribution of $(Y(0), Y(1), U, T)$ given $X$ stays invariant. To be specific, we assume
\[
\text{training distribution: } P_{X,U,T,Y(0),Y(1)} = P_X \times P_{U,T,Y(0),Y(1)|X},
\]
\[
\text{target distribution: } P_{X,U,T,Y(0),Y(1)} = Q_X \times P_{U,T,Y(0),Y(1)|X}.
\]
The corresponding upper and lower bounds on the likelihood ratio are
\[
\ell(x) = P(T = 1) \cdot \frac{dQ_X}{dP_X}(x) \cdot \left(1 + \frac{1}{\Gamma} \cdot \frac{1 - e(x)}{e(x)}\right), \quad u(x) = P(T = 1) \cdot \frac{dQ_X}{dP_X}(x) \cdot \left(1 + \Gamma \cdot \frac{1 - e(x)}{e(x)}\right).
\]
The aforementioned types of inferential target can also be applied to $Y(0)$ following the same arguments. We summarize the bounds for various inferential targets in Table 1, which recovers Table 1 in Lei and Candès (2020) when $\Gamma = 1$.

| Counterfactual | Bound | ATE-type | ATT-type | ATC-type | General |
|----------------|-------|----------|----------|----------|---------|
| $Y(1)$         | $\ell(x)$ | $p_1 \cdot (1 + \frac{1}{\Gamma r(x)})$ | 1 | $p_1 \cdot \frac{dQ_X}{dP_X}(x) \cdot (1 + \frac{1}{\Gamma r(x)})$ | $p_1 \cdot \frac{dQ_X}{dP_X}(x) \cdot (1 + \frac{1}{\Gamma r(x)})$ |
|                | $u(x)$   | $p_1 \cdot (1 + \frac{1}{\Gamma r(x)})$ | 1 | $p_1 \cdot \frac{dQ_X}{dP_X}(x) \cdot (1 + \frac{1}{\Gamma r(x)})$ | $p_1 \cdot \frac{dQ_X}{dP_X}(x) \cdot (1 + \frac{1}{\Gamma r(x)})$ |
| $Y(0)$         | $\ell(x)$ | $p_0 \cdot \frac{1}{\Gamma r(x)}$ | $\frac{p_0}{p_1} \cdot \frac{r(x)}{\Gamma}$ | 1 | $p_0 \cdot \frac{dQ_X}{dP_X}(x) \cdot (1 + \frac{r(x)}{\Gamma})$ |
|                | $u(x)$   | $p_0 \cdot (1 + \Gamma r(x))$ | $\frac{p_0}{p_1} \cdot \Gamma r(x)$ | 1 | $p_0 \cdot \frac{dQ_X}{dP_X}(x) \cdot (1 + \Gamma r(x))$ |

Table 1: Summary of the upper and lower bounds of the likelihood ratio for different inferential targets. For $t \in \{0,1\}$, $p_t = P(T = t)$ and $r(x) = e(x) / (1 - e(x))$ is the odds ratio of the propensity score. The training distribution for $Y(t)$ is always $P_{X,Y(t)|T=t}$. For target distributions, ATE-type refers to $P_{X,Y(t)}$; ATT-type refers to $P_{X,Y(t)|T=1}$; ATC-type refers to $P_{X,Y(t)|T=0}$; General refers to $Q_X \times P_{Y(t)|X}$.
3.2 Robust counterfactual inference

To apply Algorithm 1 to counterfactual prediction with a pre-specified confounding level $\Gamma$, we take the upper and lower bounds as presented in Table 1. For instance, for ATE-type predictive inference for $Y(1)$, the likelihood ratio $w(x,y)$ is bounded by $\ell(x)$ and $u(x)$ which take the form:

$$\ell(x) = p_1 \cdot \left(1 + \frac{1 - e(x)}{\Gamma \cdot e(x)}\right), \quad u(x) = p_1 \cdot \left(1 + \Gamma \cdot \frac{1 - e(x)}{e(x)}\right).$$

We then construct $\hat{\ell}(x)$ and $\hat{u}(x)$ by plugging in an estimator $\hat{e}(x)$ of $e(x)$ trained on $D_{\text{train}}$. Taking $\Gamma = 1$, our procedure recovers the approach of Lei and Candès (2020), where $\hat{\ell}(x) = \hat{u}(x)$ and both equal the likelihood ratio function; our finite-sample bound reduces to a bound similar to Lei and Candès (2020, Theorem 3) (the forms of the two bounds are slightly different, hence not directly comparable in general).

The finite-sample guarantee in Theorem 2.2 shows that the accuracy of $\hat{e}(x)$ itself (hence that of $\hat{\ell}(x)$ and $\hat{u}(x)$) may not matter much for valid coverage; what matters is whether or not $\hat{\ell}(x)$ is below $w(x,y)$ and $\hat{u}(x)$ above $w(x,y)$. In our simulation studies, we empirically evaluate $\|\hat{\ell}(X) - \ell(X)\|_1$, $\|\hat{u}(X) - u(X)\|_1$ and $\hat{\Delta}$ (see Figure 4). Even if $\|\hat{\ell}(X) - \ell(X)\|_1$ and $\|\hat{u}(X) - u(X)\|_1$ can be large (especially for large $\Gamma$), the gap $\hat{\Delta}$ remains reasonably small.

3.3 Numerical experiments

We illustrate the performance of the novel procedure in a simulation setting similar to that in Yadlowsky et al. (2018). Given a sample size $n_{\text{train}} = n_{\text{calib}} \in \{500, 2000, 5000\}$ and a covariate dimension $p \in \{4, 20\}$, we generate the covariates and unobserved confounders with

$$X \sim \text{Unif}[0,1]^p, \quad U \mid X \sim N\left(0,1 + \frac{1}{2} \cdot (2.5X_1)^2\right).$$

The counterfactual of interest is $Y(1)$ generated as

$$Y(1) = \beta^T X + U, \quad \text{where} \quad \beta = (-0.531, 0.126, -0.312, 0.018, 0, \ldots, 0)^T \in \mathbb{R}^p.$$ 

In other words, the fluctuation of $Y(1)$ from its conditional mean is entirely driven by $U$. With i.i.d. data $(X_i, Y_i, U_i)$ generated from the fixed super-population, treatment assignments $T_i$ are generated from treatment mechanisms satisfying (3) with different confounding levels $\Gamma \in \{1,1.5,2,2.5,3,5\}$. Specifically, we design the propensity scores as

$$e(x) = \text{logit}(\beta^T x), \quad e(x,u) = a(x) I\{|u| > t(x)\} + b(x) I\{|u| \leq t(x)\},$$

for the same $\beta \in \mathbb{R}^p$. Above,

$$a(x) = \frac{e(x)}{e(x) + \Gamma (1 - e(x))}, \quad b(x) = \frac{e(x)}{e(x) + (1 - e(x))/\Gamma},$$

are the lower and upper bounds on $e(x,u)$ under the marginal $\Gamma$-selection model. The threshold $t(x)$ is designed to ensure $\mathbb{E}[e(X,U) \mid X] = e(X)$. The training data $D$ are $\{(X_i, Y_i(1))\}$ for those $T_i = 1$. By (13), the setting is designed to be adversarial so as to show the performance of our method in a nearly worst case.

For each configuration of $(n_{\text{calib}}, p, \Gamma, \alpha)$, we run Algorithm 1 with ground truth $\ell(\cdot)$, $u(\cdot)$ and with estimated $\hat{\ell}(\cdot)$, $\hat{u}(\cdot)$. To obtain estimated bound functions, we fit the propensity score $\hat{e}(x)$ on $D_{\text{train}}$ using regression forests from the grf R-package, and set $\hat{\ell}(x) = \hat{p}_1 (1 + (1 - \hat{e}(x))/(\Gamma \cdot \hat{e}(x)))$, $\hat{u}(x) = \hat{p}_1 (1 + \Gamma \cdot (1 - \hat{e}(x))/\hat{e}(x))$ with $\hat{p}_1$ being the empirical proportion of $T_i = 1$. We compute the average coverage on one test sample over $N = 1000$ independent runs.

The proposed approaches work for any nonconformity score function and any training method. In our experiments, we follow the Conformalized Quantile Regression algorithm (CQR) (Romano et al., 2019) to compute the nonconformity score: $D_{\text{train}}$ is employed to train a conditional quantile function $\hat{q}(x,\beta)$ for $Y(1)$.
conditional on $X$ by quantile random forests (Meinshausen and Ridgeway, 2006). Then for a target level $\alpha \in (0,1)$, the nonconformity score is defined as
\[ V(x, y) = \max \{ \tilde{q}(x, \alpha/2) - y, y - \tilde{q}(x, 1 - \alpha/2) \}. \]
We run the procedures for a target $\alpha \in \{0.1, 0.2, \ldots, 0.9\}$ with the corresponding nonconformity scores.
The empirical coverage when $\ell(\cdot)$ and $\tilde{u}(\cdot)$ are estimated is summarized in Figure 3, with its counterpart with ground truth in Figure 15 in Appendix C.1 showing quite similar performance.

![Figure 3: Empirical coverage of Algorithm 1 when $\ell(\cdot)$ and $\tilde{u}(\cdot)$ are estimated. Each column corresponds to a sample size $n = n_{\text{calib}}$, while each row corresponds to a dimension $p$. Within each subplot, each line corresponds to a confounding level $\Gamma$. The solid lines are for Algorithm 1. The dashed lines assume no confounding and are shown for comparison.](image)

**Validity** In Figure 3, the solid lines are all above the 45°-line, showing the validity of the proposed procedure over the whole spectrum of sample sizes. We also see that confounding must be taken into consideration to reach valid counterfactual conclusions.

**Sharpness** In all the configurations, especially when the target coverage is close to 0.5, the actual coverage is quite close to the target, which shows the sharpness of the prediction interval in this setting.

**Robustness to estimation error** As illustrated in the decomposition (11), the gap between $\ell(x)$ and $w(x, y)$ (as well as that between $w(x, y)$ and $u(x)$) provides some buffer for the estimation error in $\ell(\cdot)$ and $\tilde{u}(\cdot)$. To be concrete, we numerically evaluate the gap $\hat{\Delta}$ with $(q, p) = (\infty, 1)$ as well as the estimation error $\|\hat{\ell}(X) - \ell(X)\|_1$ and $\|\hat{u}(X) - u(X)\|_1$ in Figure 4. We see that although the estimation error of the lower and upper bounds can sometimes be large, the realized gap $\hat{\Delta}$ is often very close to zero.
Figure 4: Empirical gap and estimation errors. The plots in the second row zoom in on the gaps. Each plot corresponds to a sample size \( n = n_{\text{calib}} \) and a dimension \( p \). The long-dashed lines are \( \|\hat{u}(X) - u(X)\|_1 \), the short-dashed lines are \( \|\hat{\ell}(X) - \ell(X)\|_1 \), and the solid lines are \( \hat{\Delta} \) defined in Theorem 2.2.

4 PAC-type robust conformal inference

In this section, we construct robust prediction sets with guaranteed coverage on the test sample conditional on the training data. Such guarantee has been considered by Bates et al. (2021a,b) and might be appealing to the practitioners—it ensures that unless one gets really unlucky with the training set \( D \), the anticipated coverage of the prediction set on the test sample conditional on \( D \) achieves the desired level.

4.1 The procedure

We state our approach in the generic setting, starting with some basic notations. Throughout, we follow the sample splitting routine as before, and all statements are conditional on \( D_{\text{train}} \). Suppose we have a pair of functions \( \hat{\ell} \) and \( \hat{u} : \mathcal{X} \to \mathbb{R}^+ \) with \( \hat{\ell}(x) \leq \hat{u}(x) \) for all \( x \in \mathcal{X} \). Again, we expect them to bound the unknown likelihood ratio in a pointwise fashion, although this is not required for getting theoretical guarantees.

For any function \( f : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) and any target distribution \( \tilde{\mathbb{P}} \), we define the cumulative distribution function (c.d.f.) induced by \( \tilde{\mathbb{P}} \) as

\[
F(t; f ; \tilde{\mathbb{P}}) := \tilde{\mathbb{P}}(f(X_{n+1}, Y_{n+1}) \leq t) = \int \mathbb{1}_{\{f(x,y) \leq t\}} \ d\tilde{\mathbb{P}}(x,y), \quad \forall \ t \in \mathbb{R}.
\]

Our approach is based on a general non-decreasing function \( G(\cdot) : \mathbb{R} \to [0, 1] \). We expect \( G(\cdot) \) to serve as a conservative envelope function for the unknown target distribution of the non-conformity score, i.e.,

\[
G(t) \leq F(t; V; \tilde{\mathbb{P}}) \quad \text{for all} \ t \in \mathbb{R}.
\]

(14)

We now construct \( G(\cdot) \) explicitly:

\[
G(t) = \max \left\{ E \left[ \mathbb{1}_{\{V(X,Y) \leq t\}} \hat{\ell}(X) \right], 1 - E \left[ \mathbb{1}_{\{V(X,Y) > t\}} \hat{u}(X) \right] \right\}, \quad t \in \mathbb{R},
\]

(15)

where \( E \) is taken with respect to an independent copy \( (X,Y) \sim \mathbb{P} \). By construction, \( G(\cdot) \) satisfies (14) when \( \hat{\ell}(x) \) and \( \hat{u}(x) \) are lower and upper bounds on \( w(x,y) \).

Given a constant \( \delta \in (0,1) \), suppose we can construct a non-decreasing confidence lower bound \( \hat{G}_n(\cdot) \) for \( G(\cdot) \) such that for any fixed \( t \in \mathbb{R} \) or random variable \( t \in \sigma(D_{\text{train}}) \), it holds that

\[
\mathbb{P}_D \left( \hat{G}_n(t) \leq G(t) \right) \geq 1 - \delta,
\]

(16)
where \( P_{\mathcal{D}} \) is taken with respect to \( \mathcal{D}_{\text{calib}} \). We then define the prediction interval as

\[
\hat{C}(X_{n+1}) = \left\{ y : V(X_{n+1}, y) \leq \inf \{ t : \hat{G}_n(t) \geq 1 - \alpha \} \right\}.
\]

The procedure is summarized in Algorithm 2.

**Algorithm 2** Robust conformal prediction: the PAC procedure

**Input:** Calibration data \( \mathcal{D}_{\text{calib}} \), bounds \( \tilde{\ell}(\cdot), \tilde{u}(\cdot) \), non-conformity score function \( V : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R} \), test covariate \( x \), target level \( \alpha \in (0, 1) \), confidence level \( \delta \in (0, 1) \).

1. Construct the conservative envelope distribution function \( \hat{G}_n(t) \) for \( t \in \mathbb{R} \).
2. Compute \( \hat{\ell}(X_i) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{V_i \leq \hat{\ell}(X_i)\}} \tilde{G}_n(\hat{\ell}(X_i)), 1 - \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{V_i > \hat{\ell}(X_i)\}} \tilde{u}(X_i) \right\} - M \sqrt{\frac{\log(2/\delta)}{2n}}.

Hoeffding’s inequality then ensures \( P_{\mathcal{D}}(\hat{G}_n(t) \leq G(t)) \geq 1 - \delta \) for any fixed \( t \in \mathbb{R} \). One may also construct \( \hat{G}_n(\cdot) \) by the Waudby-Smith–Ramdas bound (Waudby-Smith and Ramdas, 2021); details are deferred to Proposition A.1 in Appendix A.1. When \( \tilde{\ell}(\cdot) \) and \( \tilde{u}(\cdot) \) are obtained from \( \mathcal{D}_{\text{train}} \), the upper bounds on \( \|\tilde{\ell}\|_{\infty} \) and \( \|\tilde{u}\|_{\infty} \) could be obtained from the training process.

### 4.2 Theoretical guarantee

**Theorem 4.1.** Assume that \( (X_i, Y_i)_{i \in \mathbb{D}_{\text{calib}}} \overset{i.i.d.}{\sim} P \) and the independent test point \( (X_{n+1}, Y_{n+1}) \sim \tilde{P} \) has likelihood ratio \( w(x, y) = \frac{dp}{dp}(x, y) \). Fix a target level \( \alpha \in (0, 1) \) and a confidence level \( \delta \in (0, 1) \). Suppose \( \hat{G}_n(\cdot) \) satisfies (16) for \( G(\cdot) \) in (15). Then the output of Algorithm 2 satisfies

\[
P(\hat{Y}_{n+1} \in \hat{C}(X_{n+1}) \mid \mathcal{D}_{\text{calib}}) \geq 1 - \alpha - \hat{\Delta}
\]

with probability at least \( 1 - \delta \) over \( \mathcal{D}_{\text{calib}} \), and

\[
\hat{\Delta} = \max \left\{ \mathbb{E}\left[ \left( \hat{\ell}(X) - w(X, Y) \right)^{+} \right], \mathbb{E}\left[ \left( \hat{u}(X) - w(X, Y) \right)^{-} \right] \right\}.
\]

Here the expectations are over an independent copy \( (X, Y) \sim P \).

If \( \hat{\ell}(X) \leq w(X, Y) \leq \hat{u}(X) \) a.s., then \( \hat{\Delta} = 0 \) and

\[
P(\hat{Y}_{n+1} \in \hat{C}(X_{n+1}) \mid \mathcal{D}_{\text{calib}}) \geq 1 - \alpha.
\]

The proof of Theorem 4.1 is deferred to Appendix B.3. Almost sure bounds on the likelihood ratio yields exact coverage. Otherwise, coverage is off by at most \( \hat{\Delta} \). Again, \( \hat{\Delta} \) is small if \( \hat{\ell}(X) \) (resp. \( \hat{u}(X) \)) is below (resp. above) \( w(X, Y) \) most of the time. This is demonstrated in the simulation results presented in Figure 6.

Just as before, the miscoverage bound in Theorem 4.1 holds for any distributional shift and any inputs \( \hat{\ell}(\cdot) \) and \( \hat{u}(\cdot) \). The conclusion also applies to inputs of the form \( \hat{\ell}(x, y) \) and \( \hat{u}(x, y) \) without modification.

**Application to counterfactual prediction** To apply Algorithm 2 to counterfactual prediction under a pre-specified confounding level \( \Gamma \), We plug in the estimated \( \hat{c}(x) \) to obtain \( \hat{\ell}(x) \) and \( \hat{u}(x) \) according to Table 1. As before, \( \hat{\Delta} \) can be small as long as \( \hat{\ell}(x) \) (resp. \( \hat{u}(x) \)) falls below (resp. above) \( w(x, y) \) most of the time, even if \( \hat{c}(x) \) has a non-negligible estimator error.
4.3 Sharpness

Besides validity, one may also be concerned with the sharpness of the method—indeed, one can always construct a valid but arbitrarily conservative prediction interval. Ideally, we desire a valid prediction set whose coverage is not too much larger than the prescribed level.

In this section, we take a close look at the sharpness of Algorithm 2 by identifying the worst-case distributional shift. We study the sharpness of our method in two problems: robust predictive inference and counterfactual inference under unmeasured confounding. They are treated in the same way when developing the validity results, but they actually have distinct identification sets and sharpness results.

To remove the nuisance in estimation, we fix the nonconformity score function and consider the asymptotic formulation. The key difference is that the covariate shift is identifiable while only the shift in the observable:

\[ \mathbb{E} = \max \left\{ \mathbb{E} \left[ \mathbf{I}(Y \leq t) \ell(X) \right], 1 - \mathbb{E} \left[ \mathbf{I}(Y > t) u(X) \right] \right\}, \]

(20)

where \( \mathbb{E} \) is the expectation over \((X, Y) \sim \mathbb{P})\).

The conservative distribution function \( G(\cdot) \) constructed in (14) coincides with the actual worst-case distribution function provided in (20). Therefore, ruling out the estimation errors, the PAC-type procedure proposed in Section 4 is sharp.

4.3.2 Sharpness as a counterfactual inference problem

Returning to the counterfactual inference problem, the sharpness is a bit more subtle than in the robust prediction formulation. The key difference is that the covariate shift is identifiable while only the shift in \( \mathbb{P}_{Y \mid X} \) varies, leading to a potentially smaller identification set.

For clarity, we denote the unknown super-population as \((X, Y(0), Y(1), U, T) \sim \mathbb{P}^{\text{sup}}\) and the observed distribution as \((X, Y, T) \sim \mathbb{P}^{\text{obs}}\). For a super-population \( \mathbb{P}^{\text{sup}} \) to be meaningful, it should agree with \( \mathbb{P}^{\text{obs}} \) on the observable:

\[ \mathbb{P}^{\text{sup}}_{X, Y, T} = \mathbb{P}^{\text{obs}}_{X, Y, T}, \]

(21)

which is called the data-compatibility condition in Dorn and Guo (2021). Along with the marginal sensitivity model, (21) characterizes the set of meaningful target distributions. Let us consider the counterfactual inference of \( Y(1) \) for units in the control group. Letting \( \mathbb{P} = \mathbb{P}_{X, Y(1)} = \mathbb{P}^{\text{obs}}_{X, Y(1) \mid T=1} \) be the training distribution, we have the following sharp characterization of the identification set.
Proposition 4.3 (Identification set). For the counterfactual inference of $Y(1) \mid T = 0$ under confounding level $\Gamma \geq 1$, we define the data-compatible identification set as
\[
P = \left\{ \tilde{P} = \sup_{X,Y(1) \mid T = 0} P \mid \sup P \text{ satisfies (3) and (21)} \right\}. \tag{22}\]
Then we have $P = \mathcal{P}(\tilde{P}, f, \ell_0, u_0)$, where
\[
\mathcal{P}(\tilde{P}, f, \ell_0, u_0) = \left\{ \tilde{P} : \frac{d\tilde{P}}{dP}(x) = f(x), \ \ell_0(x) \leq \frac{d\tilde{P}Y(1) \mid X}{d\tilde{P}X}(y \mid x) \leq u_0(x) \ \tilde{P}\text{-almost surely} \right\}. \tag{23}\]
Writing $e(x) = \mathbb{P}^\text{obs}(T = 1 \mid X = x)$, $p_0 = \mathbb{P}^\text{obs}(T = 0)$ and $p_1 = \mathbb{P}^\text{obs}(T = 1)$, we have $\ell_0(x) = 1/\Gamma$, $u_0(x) = \Gamma$, and $f(x) = p_1(1 - e(x))/[p_0 \cdot e(x)]$.

Employing similar arguments, each inferential target mentioned in Section 3.1 corresponds to an identification set similar to (23), where the $X$-likelihood ratio is identifiable from the training distribution, and the conditional likelihood ratio can be bounded by identifiable functions $\ell_0$ and $u_0$.

In light of Proposition 4.3, we are interested in $F(\cdot; \mathcal{P}(\tilde{P}, f, \ell_0, u_0))$ with general functions $f, \ell_0, u_0$. For any $x \in X$ and any $\beta \in [0,1]$, we denote the $\beta$-conditional quantile function of $\tilde{P} = \mathbb{P}^\text{obs}_{X,Y(1) \mid T = 1}$ (up to a.s. equivalence) as
\[
q(\beta; x, \tilde{P}) = \inf \{ z : \mathbb{P}(Y \leq z \mid X = x) \geq \beta \}.
\]

Proposition 4.4. For each $t \in \mathbb{R}$, the worst-case distribution function in (23) is
\[
F(t; \mathcal{P}(\tilde{P}, f, \ell_0, u_0)) = \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} w^*(X,Y)], \tag{24}\]
where the expectation is with respect to generic random variables $(X,Y) \sim \tilde{P}$, and
\[
w^*(x,y) = f(x) \cdot [\ell_0(x) \mathbb{I}_{\{V(x,y) < q(\tau(x):x;\tilde{P})\}} + \gamma_0(x) \mathbb{I}_{\{V(x,y) = q(\tau(x):x;\tilde{P})\}} + u_0(x) \mathbb{I}_{\{V(x,y) > q(\tau(x):x;\tilde{P})\}}]. \tag{25}\]
Here $\tau(x) = (u_0(x) - 1)/(u_0(x) - \ell_0(x))$ and $\gamma_0(x)$ is chosen as nonzero when $\mathbb{P}(V(x,Y) = q(\tau(x):x;\tilde{P}) \mid X = x) > 0$ such that $\mathbb{E}[w^*(x,Y) \mid X = x] = f(x)$ for $\tilde{P}$-almost all $x \in X$.

As indicated by Proposition 4.4, the worst-case likelihood ratio function $w^*(x,y)$ is separated into two regions: one taking the lower bound $\ell(x)$ and the other taking the upper bound $u(x)$. This is similar to (19) with the proviso that the boundary $q(\tau(x):x;\tilde{P})$ is more complicated.

It is possible to attain sharpness with a few more efforts. Under the marginal $\Gamma$-selection (3), one can check that $\tau(x) \equiv \tau$ for some constant $\tau \in (0,1)$. Therefore, letting $G(t) = F(t; \mathcal{P}(\tilde{P}, f, \ell_0, u_0))$ as in (24) yields a sharper procedure. If a tight lower bound $\hat{G}_q(t)$ for $G(t)$ could be constructed, the worst-case coverage would equal $1 - \alpha$ asymptotically. Such modifications are beyond the scope of our current work.

4.4 Numerical experiments
We apply Algorithm 2 to the same settings as of Section 3.3 with a fixed confidence level $\delta = 0.05$ and the W-S-R bound as detailed in Proposition A.1. The empirical coverage is evaluated on 10000 test samples for $N = 1000$ independent runs. The 0.05-th quantile of empirical coverage for various target level $1 - \alpha$ are summarized in Figure 5, where estimated $\hat{\ell}(\cdot)$ and $\hat{u}(\cdot)$ are used. Results with the ground truth $\ell(\cdot)$ and $u(\cdot)$ are in Figure 16 in Appendix C.2. The marginal coverage is presented in Figures 17 and 18 in Appendix C.2.

Validity In Figure 5, the 0.05-th quantiles of empirical coverage all lie above the 45°-line, which confirms the validity of the proposed procedure.

Sharpness The quantile-versus-target lines in Figure 5 almost overlap with the 45°-line, since by design the data generating distribution is a near-worst case. This shows the sharpness of our method and is in accordance with the theoretical justification in Section 4.3.
Figure 5: 0.05-th quantile of empirical coverage in Algorithm 2 when $\hat{\ell}(\cdot)$ and $\hat{u}(\cdot)$ are estimated. Each subplot corresponds to a configuration of sample size $n = n_{\text{calib}}$ and dimension $p$. Within each subplot, each line corresponds to a confounding level $\Gamma$.

Robustness to estimation error Similar to Algorithm 1, the PAC-type algorithm shows robustness to the estimation error. In Figure 6, we numerically evaluate the gap $\hat{\Delta}$ in (17) as well as the estimation errors $\|\hat{\ell}(X) - \ell(X)\|_1$ and $\|\hat{u}(X) - u(X)\|_1$. Even though the estimations error (dashed lines) can be nonnegligibly off, the actual gap $\hat{\Delta}$ defined in Theorem 4.1 is small.

Figure 6: Empirical gap and estimation errors. The plots in the second row zoom in on the gaps. Each plot corresponds to a sample size $n = n_{\text{calib}}$ and a dimension $p$. The long-dashed lines are $\|\hat{u}(X) - u(X)\|_1$, the short-dashed lines are $\|\hat{\ell}(X) - \ell(X)\|_1$, and the solid lines are $\hat{\Delta}$ defined in Theorem 4.1.
5 Sensitivity analysis of ITEs

We are now ready to present our framework of sensitivity analysis for ITEs. In the following, we first show the construction of prediction sets for ITEs, and then invert the prediction sets to output the \( \Gamma \)-values. Finally we show the statistical meaning of the \( \Gamma \)-values from a hypothesis testing perspective.

5.1 Robust predictive inference for ITEs

We consider two cases: 1) if only one outcome is missing, we use the prediction set for the counterfactual to form that for the ITE; 2) if both outcomes are missing, we combine prediction sets for both \( Y(1) \) and \( Y(0) \) to form that for the ITE.

**One outcome missing**  Given a test sample \( X_{n+1} \) with \( T_{n+1} = w \), for \( w \in \{0, 1\} \), the potential outcome \( Y_{n+1}(w) \) is observed while \( Y_{n+1}(1-w) \) is missing. Using the method introduced in Algorithm 1 or 2, we construct a prediction set \( \widehat{C}_{1-w}(X_{n+1}, \Gamma, 1-\alpha) \) for \( Y_{n+1}(1-w) \) with coverage level \( 1-\alpha \) conditional on \( T_{n+1} = w \) and the sensitivity parameter \( \Gamma \). We then create the prediction set for ITE as

\[
\widehat{C}(X_{n+1}, \Gamma) = \begin{cases} 
Y_{n+1}(1) - \widehat{C}_0(X_{n+1}, \Gamma, 1-\alpha), & \text{if } w = 1, \\
\widehat{C}_1(X_{n+1}, \Gamma, 1-\alpha) - Y_{n+1}(0), & \text{if } w = 0.
\end{cases}
\]  

**Both outcomes missing**  When both outcomes are missing, the task is more challenging and we use a Bonferroni correction to construct the predictive set for ITEs. Let \( X_{n+1} \) be a test sample with both \( Y_{n+1}(1) \) and \( Y_{n+1}(0) \) missing. Using Algorithms 1 or 2, we construct prediction set \( \widehat{C}_w(X_{n+1}, \Gamma, 1-\alpha/2, \delta/2) \) at confounding level \( \delta/2 \) is the input confidence level if Algorithm 2 is used. Then we let

\[
\widehat{C}(X_{n+1}, \Gamma) = \left\{ y - z : y \in \widehat{C}_1(X_{n+1}, \Gamma, 1-\alpha/2, \delta/2) \text{ and } z \in \widehat{C}_0(X_{n+1}, \Gamma, 1-\alpha/2, \delta/2) \right\}.
\]  

The coverage guarantee of the prediction sets in the above two cases directly follows from the validity of counterfactual prediction intervals; Propositions A.2 and A.3 are included for completeness.

In practice, though, the Bonferroni correction (27) might be too conservative. Lei and Candès (2020, Section 4.2) introduced a nested method that efficiently combines the counterfactual intervals to form the interval for the ITE; their method can also be applied here.

5.2 The \( \Gamma \)-value: inverting nested prediction sets

For a new unit, we consider the set of hypotheses indexed by \( \Gamma \in [1, \infty) \):

\[
H_0(\Gamma) : \ Y_{n+1}(1) - Y_{n+1}(0) \in C \text{ and } P^{\text{asp}} \in P(\Gamma).
\]  

If we reject \( H_0(\Gamma) \), we are saying that either \( Y(1) - Y(0) \notin C \) or the observational data has at least confounding level \( \Gamma \). The pre-specified set \( C \) determines the hypothesis one wishes to test, or equivalently, the causal conclusion one wishes to make. For example, setting \( C = \{0\} \), we are testing whether or not the ITE is exactly zero; setting \( C = (-\infty, 0] \), we wish to test whether or not the ITE is negative.

The hypothesis (28) involves the random variable \( Y_{n+1}(1) - Y_{n+1}(0) \), and there are two ways to treat such hypotheses: we may either regard it as a deterministic hypothesis, which means the condition in (28) holds almost surely, or as a random hypothesis such that \( H_0(\Gamma) \) is true with some probability. In both cases, the type-I error is defined as rejecting a true hypothesis. That is, if we treat them as random hypotheses, a type-I error is \( H_0(\Gamma) \) being true and rejected at the same time.

Hereafter, for the true super population \( P^{\text{asp}} \), we denote

\[
\Gamma^* = \inf \{ \Gamma : P^{\text{asp}} \in P(\Gamma) \},
\]

and assume without loss of generality that \( P^{\text{asp}} \in P(\Gamma^*) \). Our goal is to test the set of hypotheses \( \{H_0(\Gamma)\}_{\Gamma \geq 1} \) simultaneously—a multiple testing problem. Put

\[
H_0 = \{ \Gamma : H_0(\Gamma) \text{ is true} \}.
\]
In the case of deterministic hypotheses, \( H_0 \) is either an empty set (if \( Y_{n+1}(1) - Y_{n+1}(0) \in C \) a.s. is false) or an interval \([\Gamma^*, \infty)\) (if \( Y_{n+1}(1) - Y_{n+1}(0) \in C \) a.s. is true). In the case of random hypotheses, \( H_0 \) is a random set—\( H_0 \) is an empty set if \( Y_{n+1}(1) - Y_{n+1}(0) \notin C \), or an interval \([\Gamma^*, \infty)\) when \( Y_{n+1}(1) - Y_{n+1}(0) \in C \).

Let \( \hat{C}(X_{n+1}, \Gamma) \) be the prediction set for the ITE constructed as in Section 5.1 with the confounding level \( \Gamma \geq 1 \) and the target coverage \( 1 - \alpha \). In the case of one missing outcome, \( \hat{C}(X_{n+1}, \Gamma) \) implicitly depends on the observed outcome as well. Note that the prediction sets are nested in \( \Gamma \) in the following sense: for each fixed coverage level \( \alpha \in (0, 1) \) (and confidence level \( \delta \) if necessary), it holds that \( \hat{C}(X_{n+1}, \Gamma) \subset \hat{C}(X_{n+1}, \Gamma') \) for any \( \Gamma' \geq \Gamma \geq 1 \). Moving on, we define the rejection set as

\[
\mathcal{R} = \{ \Gamma: C \cap \hat{C}(X_{n+1}, \Gamma) = \emptyset \}.
\]

That is, we reject all \( H_0(\Gamma) \) for which \( \hat{C}(X_{n+1}, \Gamma) \) does not overlap with the target set \( C \). We now consider the critical value defined as \( \hat{\Gamma} := \sup \mathcal{R} \), with the convention that \( \hat{\Gamma} = 1 \) if \( \mathcal{R} = \emptyset \). \( \hat{\Gamma} \) is the formal definition of the \( \Gamma \)-value we introduced in Section 1.1. The \( \Gamma \)-value is a quantity specific to a unit (instead of a population quantity). Due to the variability in ITE, it might not converge to a constant value as the training sample size goes to infinity.

**Proposition 5.1** (Simultaneous control). Fix a target level \( \alpha \) (and a confidence level \( \delta \) if necessary). For any \( \Gamma \geq 1 \), let \( \hat{C}(X_{n+1}, \Gamma) \) be the output of Algorithm 1 or 2 with the confounding level \( \Gamma \). The marginal probability of making a false rejection can be controlled as

\[
\text{mErr} := \mathbb{P}(\mathcal{R} \cap H_0 \neq \emptyset) \leq \mathbb{P}(Y_{n+1}(1) - Y_{n+1}(0) \notin \hat{C}(X_{n+1}, \Gamma^*)) ,
\]

where the probability \( \mathbb{P} \) is taken over \( D_{\text{calib}} \) and the new sample on both sides. Furthermore, the \( D_{\text{calib}} \)-conditional probability of making an error satisfies

\[
\text{dErr} := \mathbb{P}(\mathcal{R} \cap H_0 \neq \emptyset \mid D_{\text{calib}}) \leq \mathbb{P}(Y_{n+1}(1) - Y_{n+1}(0) \notin \hat{C}(X_{n+1}, \Gamma^*) \mid D_{\text{calib}}).
\]

By Proposition 5.1, as long as the predictive inference achieves valid coverage at any fixed confounding level, without any adjustment of multiple testing, we achieve simultaneous control over the sequence of testing problems.

The perspective of hypothesis testing provides an interpretation of the \( \Gamma \)-value: the risk of \( Y_{n+1}(1) - Y_{n+1}(0) \in C \) being true but rejected at \( \hat{\Gamma} \geq \Gamma^* \) is (approximately) under \( \alpha \). In the case of testing deterministic hypotheses, when \( Y(1) - Y(0) \in C \) almost surely, \( \hat{\Gamma} \) is a \((1 - \alpha)\) lower confidence bound for \( \Gamma^* \). It is in accordance with the common practice of sensitivity analysis to find a critical value \( \hat{\Gamma} \) that inverts a causal conclusion and check whether \( \hat{\Gamma} \) is too large to be true in order to assess the robustness of such conclusion.

### 5.3 Types of null hypotheses

With the general recipe of assessing robustness of causal conclusions on ITE, we now provide concrete examples of the target set \( C \) and the corresponding forms of \( \hat{C}(X_{n+1}, \Gamma) \).

**Sharp null** One might be interested in the sharp null, i.e., whether the individual treatment effect is zero. In this case, one could let \( C = \{0\} \), and the prediction set can take any form. Rejecting \( H_0(\Gamma) \) is saying that \( Y_{n+1}(1) \neq Y_{n+1}(0) \) unless the true confounding level satisfies \( \Gamma^* > \Gamma \).

**Directional null** If we presume the stochastic nature of ITEs, the sharp null might be implausible. In this case, one may be interested in the directional null with \( Y_{n+1}(1) - Y_{n+1}(0) \leq 0 \), which is equivalent to choosing \( C = (-\infty, 0] \). Rejecting \( H_0(\Gamma) \) here is saying that the individual treatment effect is positive unless \( \Gamma^* > \Gamma \). More generally, one might consider \( C = (-\infty, a] \) for some \( a \in \mathbb{R} \) to test whether the ITE is above a certain value. To make sense of the multiple testing procedure, one-sided prediction intervals are constructed for ITE, i.e., \( \hat{C}(X_{n+1}, \Gamma) = [\hat{Y}(X_{n+1}, \Gamma), \infty) \) for some \( \hat{Y}(X_{n+1}, \Gamma) \in \mathbb{R} \). It can be achieved by one-sided prediction intervals \( \hat{C}_0(X_{n+1}, \Gamma, 1 - \alpha, 1 - \delta) = (-\infty, \hat{Y}_0(X_{n+1}, \Gamma)] \) if \( Y_{n+1}(0) \) is missing and \( \hat{C}_1(X_{n+1}, \Gamma, 1 - \alpha, 1 - \delta) = [\hat{Y}_1(X_{n+1}, \Gamma), \infty) \) if \( Y_{n+1}(1) \) is missing, with a Bonferroni correction as introduced in Section 5.1 if both outcomes are missing. The \( \Gamma \)-value is hence the smallest \( \Gamma \) such that the two prediction intervals overlap.
### 5.4 Numerical experiments

We focus on the ATT-type inference for the directional null hypothesis:

\[ H_0(\Gamma) : Y(1) - Y(0) \leq 0 \quad \text{and} \quad \mathbb{P}^{\sup} \in \mathcal{P}(\Gamma). \]

The test sample is from \( \mathbb{P}_{X,Y(0),Y(1)|T=1} \), for which we observe \((X_{n+1}, Y_{n+1}(1))\) and would like to predict \(Y_{n+1}(0)\).

We fix \( n_{\text{train}} = n_{\text{calib}} = 2000 \) and \( p = 4 \). The covariates \( X \), unobserved confounders \( U \) and counterfactual \( Y(0) \) (instead of \( Y(1) \)) are generated in the same way as in Section 3.3. The treatment mechanism \( e(x,u) \) is also the same as in (13) with confounding level \( \Gamma \in \{1.2, 1.4, \ldots, 2\} \). The training data are \((X_i, Y_i(0))\) for those \( T_i = 0 \). We generate \( Y(1) \) in two ways: 1) \( Y(1) - Y(0) \equiv a \) (fixed ITE) and 2) \( Y(1) - Y(0) = a \cdot U \) (random ITE). Here \( a \) ranges in \( \{-1, -0.5, 0, 0.5, 1\} \).

Fixing level \( \alpha = 0.1 \) and \( \delta = 0.05 \) (for Algorithm 2), for each fixed \( \Gamma \geq 1 \), we construct a one-sided ATT-type prediction interval for \( Y(0) \), which takes the form \( \hat{C}(X_{n+1}, \Gamma) = (-\infty, \hat{Y}(X_{n+1}, \Gamma)) \). The prediction interval is obtained via the non-conformity score

\[ V(x,y) = y - \hat{q}(x, 1 - \alpha). \]

We reject no hypotheses if \( Y_{n+1}(1) \leq \hat{Y}(X_{n+1}, 1) \); otherwise, we reject all \( H_0(\Gamma) \) such that \( Y_{n+1}(1) > \hat{Y}(X_{n+1}, \Gamma) \), hence the rejection set is \( \mathcal{R} = [1, \hat{\Gamma}] \) for some \( \hat{\Gamma} > 1 \), which we define as the \( \Gamma \)-value.

#### 5.4.1 FWER control

We evaluate the empirical FWER, which is the proportion of making a false rejection among \( \{H_0(\Gamma)\}_{\Gamma \geq 1} \), averaged over all test samples in all \( N = 1000 \) independent runs. The results with estimated \( \hat{\ell}(\cdot) \) and \( \hat{u}(\cdot) \) are presented in Figures 7 and 8, showing control of the FWER even when the likelihood ratio bounds are estimated; we omit the case of fixed ITE at \( a > 0 \) since the hypotheses \( H_0(\Gamma) \) are always false. The results with the ground truth \( \ell(\cdot) \) and \( u(\cdot) \) are in Appendix C.3.

![Figure 7: Empirical FWER of Algorithm 1. The effect size \( a \) ranges in \( \{-1, -0.5, 0, 0.5, 1\} \). The solid lines are averaged over \( N = 1000 \) runs, while the 0.25-th and 0.75-th quantiles form the shaded area.](image)

#### 5.4.2 \( \Gamma \)-values

We plot the estimated survival function \( \hat{\Gamma} \) defined as \( S(\Gamma) = \mathbb{P}(\hat{\Gamma} > \Gamma) \), which characterizes the proportion of test units that are identified as positive ITE with each confounding level \( \Gamma \). Figure 9 presents the results from one run of the procedure with Algorithm 1, where we focus on the random ITE: \( Y(1) - Y(0) = a \cdot U \).

To see how to interpret these plots, let us consider the example where \( a = 1 \) and the true confounding level is 1.6. We can see that around 10% of the samples have a \( \Gamma \)-value greater than 2.5, and 5% have a \( \Gamma \)-value greater than 5, showing strong evidence for positive ITEs. Note also that the ITE is always zero when \( a = 0 \), and the \( \Gamma \)-value should be a 90% lower confidence bound for the true confounding level. In Figure 9, we indeed observe that for around 90% of the samples, the \( \Gamma \)-value is below the true confounding level (see the green curves).
Figure 8: 0.05-th quantile of empirical FWER using Algorithm 2 with estimated $\hat{\ell}(\cdot)$ and $\hat{u}(\cdot)$, with the effect size $a$ ranging in $\{-1, -0.5, 0, 0.5, 1\}$ for fixed ITE (left) and random ITE (right).

Figure 9: Empirical evaluation of $S(\Gamma)$ reported by (one run of) the sensitivity analysis procedure with Algorithm 1. The red dashed vertical lines are the true confounding levels.

With random ITEs, both the magnitude of actual ITE and the gap between observed outcomes in treated and control groups increase with the effects size $a$. Within each subplot, the reported $\Gamma$-values become larger as the effect size increases. Thresholding at the true confounding level $\Gamma$, we see that larger magnitude of true effects also makes it easier to detect positive ITEs at the correct confounding level $\Gamma$.

The results from one run of Algorithm 2 are in Figure 10. The patterns are similar to Figure 9 in general, except that it is sometimes sharper than Algorithm 1 and provides slightly stronger evidence against unmeasured confounding.

Figure 10: Empirical evaluation of $S(\Gamma)$ reported by (one run of) the sensitivity analysis procedure with Algorithm 2. The red dashed vertical lines are the true confounding levels.

In Figure 10, some test units have large $\Gamma$-values especially when the effect size is positive. Such strong evidence would happen if there is a large gap between the observed $Y(1)$ and the typical behavior of $Y(0)$ predicted with the training data—thus, the only way our procedures can output a prediction interval that
We also track the empirical false discovery proportion

\[ \text{FDP}(\Gamma) = \frac{|\{j \in D_{\text{test}} : \hat{\Gamma} > \Gamma, Y_j(1) \leq Y_j(0)\}|}{|\{j \in D_{\text{test}} : \hat{\Gamma} > \Gamma\}|}, \quad \Gamma \geq 1 \]

for random ITE with \( a \neq 0 \), which is the proportion of false rejections among test units that are rejected at confounding level \( \Gamma \). With both the two procedures, we find that FDP(\( \Gamma \)) is always zero—the units that survive certain levels of adjustment for confounding all have positive ITE. It could be explained by the conservativeness of the procedure: to survive the adjustment, the observed \( Y(1) \) needs to be larger than the whole \( 1 - \alpha \) prediction interval for \( Y(0) \). Therefore, a unit that survives the adjustment is much more likely to have a positive ITE, leading to vanishing FDPs.

### 6 Real data analysis

#### 6.1 Counterfactual prediction on a semi-real dataset

We consider an observational study dataset from Carvalho et al. (2019), based on which we generate counterfactual prediction. We consider an observational study dataset from Carvalho et al. (2019), based on which we generate counterfactual prediction of

\[ Y(1) = \hat{\mu}_0(X_i) + \tau(X_i) + U_i, \quad Y(0) = \hat{\mu}_0(X_i) - U_i, \quad U_i \sim N(0, 0.2^2), \quad i = 1, \ldots, n, \]

where the conditional treatment effect function \( \tau(x) \) is specified the same way as in equation (1) of Carvalho et al. (2019). The propensity scores are specified as \( e(X_i) := \hat{c}(X_i) \). For each confounding level \( \Gamma \in \{1, 2, 3\} \), both \( e(X_i, U_i) \) and \( T_i \) are generated the same way as in Section 3.3.

We then conduct counterfactual inference on the synthetic dataset \( D_{\text{obs}} = \{Y_i, X_i, T_i\}_{1 \leq i \leq n} \). We randomly split \( D_{\text{obs}} \) into three folds with \( 1 : 2 : 1 \) sizes. The treated samples in the first fold are used as \( D_{\text{train}} \). The treated samples in the second fold are used as \( D_{\text{calib}} \), so that \( D = D_{\text{train}} \cup D_{\text{calib}} \). All samples in the third fold (where we have ground truth even for those in the control group) are used as test samples. The process is repeated \( N = 1000 \) times, where there are approximately \( |D_{\text{calib}}| = 1900 \) calibration samples fed into the procedures and 2500 test samples.

Figure 11 summarizes the empirical coverage using Algorithm 1 and estimated \( \hat{\ell}(\cdot), \hat{u}(\cdot) \). The output of Algorithm 1 always achieves valid coverage. The solid lines are close to the 45°-line, showing the tightness of our procedure in this setting.

The empirical coverage of Algorithm 2 with estimated \( \hat{\ell}(\cdot), \hat{u}(\cdot) \) is summarized in Figure 12, which validate the PAC-type guarantee (referring to the lower boundary of the shaded area in each plot, which is the 0.05-th quantile of empirical coverage). Due to the conservativeness of the confidence lower bound constructed by the WSR inequality, the average coverage of Algorithm 2 is a bit higher than the target for targets around 0.5. However, the 0.05-th quantile (lower boundary of the shaded area) is still very close to the target.

It is also worth pointing out that the shaded bands indicate the quantiles of the empirical coverage on test samples, which could be understood as an estimate of \( \hat{c}(D) := P(Y_{n+1} \in \hat{C}(X_{n+1}) | D) \). Although PAC-type guarantee is not theoretically provided by Algorithm 1, most of the time, \( \hat{c}(D) \) is above the target in this example (referring to the lower boundary of the shaded area, which is the 0.05-th quantile of \( \hat{c}(D) \)). The widths of the 0.05-th and the 0.95-th quantiles also provide empirical evidence that \( \hat{c}(D) \) from Algorithm 1 might be less variable than Algorithm 2. The theoretical analysis of this phenomenon might deserve future investigation.
Figure 11: Empirical coverage on the test sample. Each plot corresponds to a confounding level $\Gamma$. The points are average empirical coverage. The shaded bands correspond to the 0.05-th and 0.95-th quantiles of coverage on test samples. The solid lines correspond to Algorithm 1. The dashed lines assume no confounding and are shown for comparison. In this case, counterfactual prediction intervals are invalid.

Figure 12: Empirical coverage of Algorithm 2. Each plot corresponds to a confounding level $\Gamma$. The shaded bands corresponds to the 0.05-th and 0.95-th quantiles of coverage on test samples.

6.2 Sensitivity analysis on a real dataset

We finally apply the sensitivity analysis procedure to the treated units in the same dataset (Carvalho et al., 2019). Two types of null hypotheses are considered:

1. $H_{-0}(\Gamma): Y(1) - Y(0) \leq 0$ and $\Gamma^* \leq \Gamma$. Rejecting the null suggests a positive ITE.

2. $H_{+0}(\Gamma): Y(1) - Y(0) \geq 0$ and $\Gamma^* \leq \Gamma$. Rejecting this null suggests a negative ITE.

We randomly subsample $1/3$ of the original data as $D_{\text{train}}$. Among the remaining, those with $T = 0$ are used as $D_{\text{calib}}$, and those with $T = 1$ as the test sample $|D_{\text{test}}|$. On average, we have $|D_{\text{train}}| \approx 2329$, $|D_{\text{calib}}| \approx 4650$ and $|D_{\text{test}}| \approx 2250$. We conduct sensitivity analysis on the dataset with $\alpha = 0.1$ and $\delta = 0.05$ (the details are as in Section 5.4).

The empirical survival function of the $\Gamma$-values resulting from testing $H_{-0}^-(\Gamma)$ is plotted in Figure 13, which shows the evidence for positive ITEs. To illustrate the variability of the procedures, we present the estimated functions for all $N = 10$ independent runs, hence the multiple curves in each subplot.

Averaged over multiple independent runs, there are 19.60% or 20.46% of the treated test samples that we find at $\Gamma = 1$ as positive ITEs, using Algorithm 1 and 2, respectively. There are 6.80% or 9.65% of the test sample that we find at $\Gamma = 2$ as positive ITEs. At $\Gamma = 3$, the proportion is 3.54% with Algorithm 1 and 6.95% with Algorithm 2. With Algorithm 1, around 2% of the test sample have a $\Gamma$-value greater than 5. With Algorithm 2, about 2.5% of the test sample have $\Gamma$-values greater than 10, and some test samples have a $\Gamma$-value as large as 25, showing robust evidence of a positive ITE. Our framework guarantees that the mistake (i.e., rejecting an actually negative ITE at a too large confounding level) we make on all units is bounded by $\alpha = 0.1$ on average.
Figure 13: Empirical evaluation of $S(\Gamma)$ resulting from testing $\{H^{-}_0(\Gamma)\}$ with Algorithm 1 (left) and 2 (right).

On the other hand, we report the proportion of test units such that $H^+_0(\Gamma)$ is rejected for all $\Gamma \geq 1$ in Figure 14, which shows the evidence for negative ITEs.

Averaged over multiple runs, there are 3.58% and 3.58% of ITEs of the treated test sample that we find as negative at $\Gamma = 1$, using Algorithm 1 and 2, respectively. At $\Gamma = 2$, these proportions are 0.38% with Algorithm 1 and 1.01% with Algorithm 2. Algorithm 2 produces a little stronger evidence against unmeasured confounding, but it is slightly less stable. In general, very few of the samples have $\Gamma$-values larger than 2 using both algorithms.

### 7 Discussion

We proposed a model-free framework for sensitivity analysis of ITEs, building upon reliable counterfactual inference with potentially confounded observational data. We close the paper by discussing possible extensions of the current work.

One extension is to test the confounding level with a little more information. If we have some budget to obtain a small amount of experimental data, it would be interesting to use these experimental data to test the existence or level of unmeasured confounding in the observational data. Another interesting question is whether the experimental data can be used to calibrate the value of $\Gamma$. Taking a step further, the calibrated $\Gamma$ might also be used to provide valid counterfactual inference for units in the observational study.

Other extensions might be based on the identification of distributional shifts in (23) and (24), which can be of interest for other tasks. For example, the recent work of Dorn and Guo (2021) studies sharp bounds on average treatment effect (ATE) under the marginal $\Gamma$-selection condition (3), in which the identification
set is the same as (22). The worst-case distribution function in (24) achieves the sharp lower bound on the (conditional) expectation of $V(X, Y)$ when $(X, Y) \sim \tilde{P}$. Therefore, setting $V(x, y) = y$ (resp. $V(x, y) = -y$), one could identify the super-population $\tilde{P}$ that achieves the lower (resp. upper) bound on $\mathbb{E}[Y(t) \mid X]$, $t \in \{0, 1\}$. In policy evaluation problems, the task is to estimate $V(\pi) = \tilde{E}[\pi(X)Y(1) + (1 - \pi(X))Y(0)]$ for some policy $\pi : X \rightarrow [0, 1]$ with possibly confounded observational data. Utilizing (23) and (24) along with a coupling argument, one could construct a super-population $\tilde{P}$ that achieves the sharp lower bounds on $\mathbb{E}[Y(1) \mid X]$ and $\mathbb{E}[Y(0) \mid X]$ simultaneously, which leads to the sharp lower bound on $\mathbb{E}[\pi(X)Y(1) + (1 - \pi(X))Y(0) \mid X]$, hence on $V(\pi)$. In fact, it can also be shown that all policies attain their worst-case performance under one single super-population. Such result might be used to learn a policy whose worst-case performance is most favorable.

**Code availability and reproducibility**

The code for reproducing the simulations in Section 3.3, 4.4 and real data analysis in Section 6 is publicly available at https://github.com/ying531/cfsensitivity_paper. An R-package to implement the procedures proposed in this paper can be found at https://github.com/zhimeir/cfsensitivity.

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A Additional results

A.1 Constructing $\hat{G}_n(\cdot)$ in the PAC-type procedure

In this part, we provide the construction of $\hat{G}_n(t)$ in Section 4.1 with Waudby-Smith–Ramdas bound (Waudby-Smith and Ramdas, 2021). The proof is a slight modification of Waudby-Smith and Ramdas (2021) and included in Appendix B.4 for completeness.

Proposition A.1 (Waudby-Smith–Ramdas lower confidence bound for c.d.f.s). Suppose $\sup_x \bar{u}(x) \leq M$ for some constant $M > 0$. For $t \in \mathbb{R}$ being any constant or any random variable in $\sigma(D_{\text{train}})$, and any $\delta \in (0,1)$, we define $\bar{G}_n(t) = \max \{ \hat{G}^L_n(t), \hat{G}^U_n(t) \}$, where

$$\hat{G}^L_n(t) = M \cdot \inf \left\{ g \geq 0 : \max_{1 \leq i \leq n} K^L_i(g) \leq 2/\delta \right\},$$

$$\hat{G}^U_n(t) = 1 - M + M \cdot \inf \left\{ g \geq 0 : \max_{1 \leq i \leq n} K^U_i(g) \leq 2/\delta \right\}.$$  

For any $g \geq 0$, the thresholding functions for $i = 1, \ldots, n$ are defined as

$$K^L_i(g) = \prod_{j=1}^i \left( 1 + \nu^L_j \cdot \left[ \mathbb{I}(V_j \leq t) \hat{\ell}(X_j)/M - g \right] \right),$$

$$K^U_i(g) = \prod_{j=1}^i \left( 1 + \nu^U_j \cdot \left[ 1 - \mathbb{I}(V_j > t) \hat{\ell}(X_j)/M - g \right] \right),$$

where $\nu^L_j = \min \{ 1, \sqrt{2 \log(2/\delta)/[n(\hat{\sigma}^L_{j-1})^2]} \}$, $\nu^U_j = \min \{ 1, \sqrt{2 \log(2/\delta)/[n(\hat{\sigma}^U_{j-1})^2]} \}$, and

$$(\hat{\sigma}^L_i)^2 = \frac{1}{4} + \sum_{j=1}^i \left( \mathbb{I}(V_j \leq t) \frac{\hat{\ell}(X_j)}{M} - \hat{\mu}^L_j \right)^2, \quad \hat{\mu}^L_i = \frac{1}{2} + \sum_{j=1}^i \mathbb{I}(V_j \leq t) \frac{\hat{\ell}(X_j)}{M},$$

$$(\hat{\sigma}^U_i)^2 = \frac{1}{4} + \sum_{j=1}^i \left( 1 - \mathbb{I}(V_j > t) \frac{\hat{\ell}(X_j)}{M} - \hat{\mu}^U_j \right)^2, \quad \hat{\mu}^U_i = \frac{1}{2} + \sum_{j=1}^i \left( 1 - \mathbb{I}(V_j > t) \frac{\hat{\ell}(X_j)}{M} \right).$$

Then it holds that $\mathbb{P}_{D_{\text{calib}}}(\hat{G}_n(t) \leq G(t)) \geq 1 - \delta$ for $G(t)$ defined in (15).

A.2 Validity of prediction intervals for ITE

In this part, we provide the coverage guarantee for prediction of ITEs omitted in Section 5.1.

Proposition A.2. Consider a new test sample where we observe $(X_{n+1}, T_{n+1}, Y_{n+1}(T_{n+1}))$, with $T_{n+1} = w$ for $w \in \{0,1\}$. Let $D$ be the calibration data generated from $\mathbb{P}^{\sup}$ under confounding level $\Gamma$. If $\hat{C}_{1-w}(X_{n+1}, \Gamma, 1 - \alpha)$ is constructed by Algorithm 1, then

$$\mathbb{P}(Y_{n+1}(1) - Y_{n+1}(0) \in \hat{C}(X_{n+1}, \Gamma) \mid T_{n+1} = w) \geq 1 - \alpha - \hat{\Delta},$$

for the prediction set $\hat{C}(X_{n+1}, \Gamma, 1 - \alpha)$ in (26), where the probability is over $D_{\text{calib}}$ as well as the test point, and $\hat{\Delta}$ is the gap of coverage for $Y_{n+1}(1-w)$ in Theorem 2.2. If $\hat{C}_{1-w}(X_{n+1}, \Gamma, 1 - \alpha)$ is constructed by Algorithm 2 with confidence level $\delta \in (0,1)$, then with probability at least $1-\delta$ with respect to $D_{\text{calib}}$, we have

$$\mathbb{P}(Y_{n+1}(1) - Y_{n+1} \in \hat{C}(X_{n+1}, \Gamma) \mid T_{n+1} = w, D_{\text{calib}}) \geq 1 - \alpha - \hat{\Delta},$$

where $\hat{\Delta}$ is the gap of coverage for $Y_{n+1}(1-w)$ in Theorem 4.1.

Proposition A.3. Consider a new test sample $X_{n+1}$. Let $D$ be the observations for which $\mathbb{P}^{\sup}$ is under confounding level $\Gamma$. If for $w \in \{0,1\}$, $\hat{C}_w(X_{n+1}, \Gamma, 1 - \alpha/2, \delta/2)$ is constructed by Algorithm 1, then

$$\mathbb{P}(Y_{n+1}(1) - Y_{n+1}(0) \in \hat{C}(X_{n+1}, \Gamma)) \geq 1 - \alpha - \hat{\Delta}_1 - \hat{\Delta}_0,$$
where the probability is over $D$ as well as the test point; $\hat{\Delta}_0$, $\hat{\Delta}_1$ is the coverage gap in Theorem 2.2 for counterfactual prediction of $Y_{n+1}(1), Y_{n+1}(0)$ when the bound functions are estimated. If $\hat{C}_{1-w}(X_{n+1}, \Gamma, 1 - \alpha/2, \delta/2)$ is constructed by Algorithm 2, then with probability at least 1 - $\delta$ with respect to $D_{\text{calib}}$, we have

$$P(Y_{n+1}(1) - Y_{n+1} \in \hat{C}(X_{n+1}, \Gamma) \mid D_{\text{calib}}) \geq 1 - \alpha - \hat{\Delta}_1 - \hat{\Delta}_0,$$

where $\hat{\Delta}_0$ and $\hat{\Delta}_1$ are the coverage gaps in Theorem 2.2 for counterfactual prediction of $Y_{n+1}(1), Y_{n+1}(0)$ when the bound functions are estimated.

### B Technical proofs

#### B.1 Proof of Lemma 3.1

**Proof of Lemma 3.1.** For any measurable subset $A \subset \mathcal{U}$, any $u \in A$ and any $x \in \mathcal{X}$, by the marginal $\Gamma$-selection condition (3),

$$1 \Gamma \cdot P(T = 0 \mid X = x, U = u) \leq P(T = 1 \mid X = x, U = u) \cdot \frac{P(T = 0 \mid X = x)}{P(T = 1 \mid X = x)} \leq \Gamma \cdot P(T = 0 \mid X = x, U = u) \leq 1 \Gamma \cdot \hat{\Gamma}(1) \leq \Gamma$$

Marginalizing over $u \in A$ yields

$$1 \Gamma \leq P(U \in A \mid X = x, T = 1) \leq \Gamma$$

for $P$-almost $x \in \mathcal{X}$. Since (31) holds for any measurable set in $\mathcal{U}$, we have

$$1 \Gamma \leq \frac{dP(U \mid X, T = 1)}{dP(U \mid X, T = 0)}(u, x) \leq \Gamma,$$

for $P$-almost all $u \in \mathcal{U}$ and $x \in \mathcal{X}$. Meanwhile, for any measurable set $B \subset \mathcal{Y}$, by the tower property, we have for any $t \in \{0, 1\}$ that

$$P(Y(1) \in B, T = t \mid X) = E\left[ E\left[ \mathbb{1}_{\{Y(1) \in B\}} \mid X, U \right] \mid X \right] = E\left[ E\left[ \mathbb{1}_{\{Y(1) \in B\}} \mid X, U \right] \cdot E[\mathbb{1}_{\{T = t\}} \mid X, U] \mid X \right].$$

Rewriting (30), we have $P$-almost surely that

$$1 \Gamma \cdot E[\mathbb{1}_{\{T = 0\}} \mid X, U] \cdot \frac{E[\mathbb{1}_{\{T = 1\}} \mid X]}{E[\mathbb{1}_{\{T = 0\}} \mid X]} \leq E[\mathbb{1}_{\{T = 1\}} \mid X, U] \leq \Gamma \cdot E[\mathbb{1}_{\{T = 0\}} \mid X, U] \cdot \frac{E[\mathbb{1}_{\{T = 1\}} \mid X]}{E[\mathbb{1}_{\{T = 0\}} \mid X]}.$$

Multiplying all sides by $E[\mathbb{1}_{\{Y(1) \in B\}} \mid X, U]$ and using (32), we know

$$1 \Gamma \cdot P(Y(1) \in B, T = 0 \mid X) \cdot \frac{E[\mathbb{1}_{\{T = 1\}} \mid X]}{E[\mathbb{1}_{\{T = 0\}} \mid X]} \leq P(Y(1) \in B, T = 1 \mid X) \leq \Gamma \cdot P(Y(1) \in B, T = 0 \mid X) \cdot \frac{E[\mathbb{1}_{\{T = 1\}} \mid X]}{E[\mathbb{1}_{\{T = 0\}} \mid X]}$$

holds $P$-almost surely, and for $P$-almost all $x \in \mathcal{X}$,

$$1 \Gamma \cdot \frac{1 - e(x)}{e(x)} \leq \frac{P(Y(1) \in B, T = 0 \mid X = x)}{P(Y(1) \in B, T = 1 \mid X = x)} \leq \Gamma \cdot \frac{1 - e(x)}{e(x)},$$

Note that

$$\frac{P(Y(1) \in B \mid X = x, T = 1)}{P(Y(1) \in B \mid X = x, T = 0)} = \frac{P(Y(1) \in B, T = 1 \mid X = x)}{P(Y(1) \in B, T = 0 \mid X = x)} \cdot \frac{1 - e(x)}{e(x)}.$$
Consequently,

\[
\frac{1}{\Gamma} \leq \frac{\mathbb{P}(Y(1) \in B \mid X = x, T = 1)}{\mathbb{P}(Y(1) \in B \mid X = x, T = 0)} \leq \Gamma
\]

holds for \( \mathbb{P} \)-almost all \( x \in \mathcal{X} \). By the arbitrariness of \( B \), we have

\[
\frac{1}{\Gamma} \leq \frac{d\mathbb{P}(Y(1) \mid X, T = 1)}{d\mathbb{P}(Y(1) \mid X, T = 0)}(x, y) \leq \Gamma.
\]

Repeating the above steps for \( Y(0) \) we conclude the proof of Lemma 3.1. \( \square \)

### B.2 Proof of Theorem 2.2

**Proof of Theorem 2.2.** Fixing any \( \overline{P} \in \mathbb{P}(\mathbb{P}, \ell, u) \), we denote the likelihood ratio \( w(x, y) = \frac{d\overline{P}}{d\mathbb{P}}(x, y) \). Recall that the calibration data is \( \{(X_i, Y_i)\}_{i \in D_{\text{calib}}} \) with \( D_{\text{calib}} = \{1, \ldots, n\} \), and the test data point is \( (X_{n+1}, Y_{n+1}) \sim \overline{P} \). We denote the random variables \( Z_i = (X_i, Y_i) \) and realized values \( z_i = (x_i, y_i) \) for \( i = 1, \ldots, n \).

As a starting point, we elaborate on the weighted conformal inference introduced in Tibshirani et al. (2019), which paves the way for the analysis of marginal coverage later on. Following Tibshirani et al. (2019), the random variables \( \{Z_i\}_{i=1}^{n+1} \) are weighted exchangeable, meaning that the density of their joint distribution can be factorized as

\[
f(z_1, \ldots, z_{n+1}) = \prod_{i=1}^{n+1} w_i(z_i) \cdot g(z_1, \ldots, z_{n+1}),
\]

(33)

where \( g \) is some permutation-invariant function, i.e., \( g(z_{\sigma(1)}, \ldots, z_{\sigma(n+1)}) = g(z_1, \ldots, z_{n+1}) \) for any permutation \( \sigma \) of \( 1, \ldots, n+1 \). Specifically, here \( w_i(z) = 1 \) for \( 1 \leq i \leq n \) and \( w_{n+1}(z) = w(x, y) \). For a set of values \( z_1, \ldots, z_{n+1} \) where there may be repeated elements, we denote the unordered set \( z = [z_1, \ldots, z_{n+1}] \) and the event

\[
\mathcal{E}_z = \{ [Z_1, \ldots, Z_{n+1}] = [z_1, \ldots, z_{n+1}] \}.
\]

Let \( \Pi_{n+1} \) be the set of all permutations of \( \{1, \ldots, n+1\} \). Writing \( v_i = V(x_i, y_i) = V(z_i) \), for each \( 1 \leq i \leq n+1 \), it holds that

\[
\mathbb{P}(V_{n+1} = v_i \mid \mathcal{E}_z) = \mathbb{P}(Z_{n+1} = z_i \mid \mathcal{E}_z) = \frac{\sum_{\sigma \in \Pi_{\sigma(1), \ldots, \sigma(n+1)}} f(z_{\sigma(1)}, \ldots, z_{\sigma(n+1)})}{\sum_{\sigma \in \Pi} f(z_{\sigma(1)}, \ldots, z_{\sigma(n+1)})},
\]

where \( \mathbb{P} \) is induced by the joint distribution of \( D_{\text{train}} \cup D_{\text{calib}} \cup Z_{n+1} \). By the factorization (33), we have

\[
\frac{\sum_{\sigma \in \Pi_{\sigma(1), \ldots, \sigma(n+1)}} f(z_{\sigma(1)}, \ldots, z_{\sigma(n+1)})}{\sum_{\sigma \in \Pi} f(z_{\sigma(1)}, \ldots, z_{\sigma(n+1)})} = \frac{\sum_{\sigma \in \Pi_{\sigma(1), \ldots, \sigma(n+1)}} w_{n+1}(z_{\sigma(1)}, \ldots, z_{\sigma(n+1)})}{\sum_{\sigma \in \Pi} w_{n+1}(z_{\sigma(1)}, \ldots, z_{\sigma(n+1)})} = \frac{w_{n+1}(z_i)}{\sum_{j=1}^{n+1} w_{n+1}(z_j)}.
\]

Therefore, the distribution of \( V_{n+1} \) conditional on the event \( \mathcal{E}_z \) is

\[
V_{n+1} \mid \mathcal{E}_z \sim \sum_{i=1}^{n+1} \delta_{v_i} p^w_i, \quad \text{where} \quad p^w_i = \frac{w_{n+1}(z_i)}{\sum_{j=1}^{n+1} w_{n+1}(z_j)} = \frac{w(x_i, y_i)}{\sum_{j=1}^{n+1} w(x_j, y_j)}.
\]

Here \( \delta_{v_i} \) denotes the point mass at \( \{v_i\} \). For any unordered set \( z = [z_1, \ldots, z_n, z_{n+1}] \) and the corresponding \( k^* \) as defined in (7), it holds that

\[
\mathbb{P}(Y_{n+1} \in \hat{C}(X_{n+1}) \mid \mathcal{E}_z) = \mathbb{P}(V_{n+1} \leq v_{[k^*]} \mid \mathcal{E}_z) = \sum_{i=1}^{n+1} p^w_i \mathbb{1}_{\{v_i \leq v_{[k^*]}\}} = \frac{\sum_{i=1}^{n+1} w(x_i, y_i) \mathbb{1}_{\{v_i \leq v_{[k^*]}\}}}{\sum_{j=1}^{n+1} w(x_j, y_j)}.
\]
By the tower property of conditional expectations, we have
\[
\mathbb{P}(Y_{n+1} \in \tilde{C}(X_{n+1})) = \mathbb{E}\left[\mathbb{P}(Y_{n+1} \in \tilde{C}(X_{n+1}) \mid \mathcal{E}_n)\right] = \mathbb{E}\left[\frac{\sum_{i=1}^{n+1} w(X_i, Y_i) \mathbb{I}_{\{V_i \leq V_{i+1}\}}}{\sum_{i=1}^{n+1} w(X_i, Y_i)}\right].
\] (34)

Equipped with the above preparations, we show the coverage guarantee in our setting. By definition (7), we know
\[
V_{[k^*]} = \inf\left\{v : \frac{\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq v\}}}{\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} + \sum_{i=1}^{n} \tilde{u}(X_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} + \tilde{u}(X_{n+1})} \geq 1 - \alpha\right\},
\]
hence
\[
\mathbb{E}\left[\frac{\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}}}{\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} + \sum_{i=1}^{n} \tilde{u}(X_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} + \tilde{u}(X_{n+1})} \right] \geq 1 - \alpha
\]
since the inner random variable is always no smaller than 1 − α. Combined with (34) and by the non-negativity of \(w(X_i, Y_i)\), we have
\[
\mathbb{P}(Y_{n+1} \in \tilde{C}(X_{n+1})) - (1 - \alpha) \geq \mathbb{E}\left[\frac{\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}}}{\sum_{i=1}^{n+1} w(X_i, Y_i)} \right] - \mathbb{E}\left[\frac{\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}}}{\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} + \sum_{i=1}^{n} \tilde{u}(X_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} + \tilde{u}(X_{n+1})} \right] = \mathbb{E}\left[(\text{ii}) \mid (\text{i})\right],
\]
where we denote
\[
(i) = -w(X_{n+1}, Y_{n+1}) \cdot \sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} + \tilde{u}(X_{n+1}) \cdot \sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}}
\]
\[+ \left[\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} \tilde{u}(X_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} - \sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right]
\]
and
\[
(ii) = \left[\sum_{i=1}^{n+1} w(X_i, Y_i) \right] \left[\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} + \sum_{i=1}^{n} \tilde{u}(X_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} + \tilde{u}(X_{n+1}) \right].
\]

We first establish a lower bound for the term (i). To this end, we define the random variables
\[
\tilde{\ell}_i = \max \left\{w(X_i, Y_i), \tilde{\ell}(X_i)\right\} \quad \text{and}
\]
\[
\tilde{u}_i = \min \left\{w(X_i, Y_i), \tilde{u}(X_i)\right\}, \quad i = 1, \ldots, n + 1.
\]
By the above definition, it holds that \(0 \leq \tilde{u}_i \leq \tilde{u}(X_i)\) and \(\tilde{\ell}_i \geq \tilde{\ell}(X_i) \geq 0\). We also define the differences
\[
\Delta \tilde{\ell}_i = \tilde{\ell}_i - w(X_i, Y_i) = \left[\tilde{\ell}(X_i) - w(X_i, Y_i)\right]_+ \quad \text{and}
\]
\[
\Delta \tilde{u}_i = \tilde{u}_i - w(X_i, Y_i) = -\left[\tilde{u}(X_i) - w(X_i, Y_i)\right]_-, \quad i = 1, \ldots, n + 1.
\]
Using the above notation, we have
\[
\left[\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} \tilde{u}(X_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} \right] - \left[\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right]
\]
\[\geq \left[\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} (w(X_i, Y_i) + \Delta \tilde{u}_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} \right]
\]
\[- \left[\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} (w(X_i, Y_i) + \Delta \tilde{\ell}_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right]
\]
\[= \left[\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} \Delta \tilde{u}_i \mathbb{I}_{\{V_i > V_{[k^*]}\}} \right] - \left[\sum_{i=1}^{n} w(X_i, Y_i) \mathbb{I}_{\{V_i > V_{[k^*]}\}} \right] \left[\sum_{i=1}^{n} \Delta \tilde{\ell}_i \mathbb{I}_{\{V_i \leq V_{[k^*]}\}} \right].
\]
Following similar arguments, we have

\[-w(X_{n+1}, Y_{n+1}) \cdot \sum_{i=1}^{n} \tilde{\ell}(X_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}} + \hat{u}(X_{n+1}) \cdot \sum_{i=1}^{n} w(X_i, Y_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}}\]

\[\geq -w(X_{n+1}, Y_{n+1}) \cdot \sum_{i=1}^{n} (w(X_i, Y_i) + \Delta \tilde{\ell}_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}} + (w(X_{n+1}, Y_{n+1}) + \Delta \bar{u}_{n+1}) \cdot \sum_{i=1}^{n} w(X_i, Y_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}}\]

\[= -w(X_{n+1}, Y_{n+1}) \cdot \sum_{i=1}^{n} \Delta \tilde{\ell}_i \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}} + \Delta \bar{u}_{n+1} \cdot \sum_{i=1}^{n} w(X_i, Y_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}}\]

By construction, we know that \(\Delta \tilde{\ell}_i \geq 0\) and \(\Delta \bar{u}_i \leq 0\) for \(i = 1, \ldots, n + 1\). Putting the lower bounds together, we obtain

\[(i) \geq \left[ \sum_{i=1}^{n+1} w(X_i, Y_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}} \right] \left[ \sum_{i=1}^{n+1} \Delta \bar{u}_i + \sum_{i=1}^{n+1} \Delta \tilde{\ell}_i \mathbf{1}_{\{V_i > V_{\hat{\ell}+1}\}} \right]

- \left[ \sum_{i=1}^{n+1} w(X_i, Y_i) \mathbf{1}_{\{V_i > V_{\hat{\ell}+1}\}} \right] \left[ \sum_{i=1}^{n+1} \Delta \tilde{\ell}_i \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}} \right]

\[\geq \left[ \sum_{i=1}^{n+1} w(X_i, Y_i) \right] \left[ \sum_{i=1}^{n+1} \Delta \bar{u}_i \right] - \left[ \sum_{i=1}^{n+1} w(X_i, Y_i) \right] \left[ \sum_{i=1}^{n+1} \Delta \tilde{\ell}_i \right].\]

Since the term (ii) is non-negative, we have the lower bound

\[\mathbb{E} \left[ \frac{(i)}{(ii)} \right] \geq \frac{\sum_{i=1}^{n+1} w(X_i, Y_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}} - \sum_{i=1}^{n+1} \hat{\ell}(X_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}}}{\sum_{i=1}^{n+1} w(X_i, Y_i) - \sum_{i=1}^{n+1} \hat{\ell}(X_i)} \geq \mathbb{E} \left[ \frac{\sum_{i=1}^{n+1} w(X_i, Y_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}} - \sum_{i=1}^{n+1} \hat{\ell}(X_i) \mathbf{1}_{\{V_i \leq V_{\hat{\ell}+1}\}}}{\sum_{i=1}^{n+1} w(X_i, Y_i) - \sum_{i=1}^{n+1} \hat{\ell}(X_i)} \right].\]

Above, step (a) follows from the fact that \(\hat{u}(X_i) \geq \hat{\ell}(X_i) \geq 0\), and step (b) is due to the non-negativity of \(w(X_i, Y_i)\). By Hölder’s inequality,

\[\mathbb{E} \left[ \sum_{i=1}^{n+1} \frac{\hat{\ell}(X_i) - w(X_i, Y_i)_{+}}{\sum_{i=1}^{n+1} \hat{\ell}(X_i)} \right] \leq \left\| \frac{1}{n} \sum_{i=1}^{n} \left( \hat{\ell}(X_i) - w(X_i, Y_i) \right) \right\|_p \cdot \left\| \frac{n}{\sum_{i=1}^{n+1} \hat{\ell}(X_i)} \right\|_q\]

\[\leq \left\| \hat{\ell}(X_i) - w(X_i, Y_i) \right\|_p \cdot \left\| \frac{n}{\sum_{i=1}^{n+1} \hat{\ell}(X_i)} \right\|_q\]

\[\leq \left\| \hat{\ell}(X_i) - w(X_i, Y_i) \right\|_p \cdot \left\| \frac{1}{\hat{\ell}(X_i)} \right\|_q\],

where step (a) follows from Minkowski’s inequality, and the step (b) follows from

\[\sum_{i=1}^{n} \frac{n}{\hat{\ell}(X_i)} \leq \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\hat{\ell}(X_i)}\]
as implied by Cauchy-Schwarz inequality. Similarly,

\[
\mathbb{E}\left[\frac{\sum_{i=1}^{n+1} [\hat{u}(X_i) - u(X_i,Y_i)]}{\sum_{i=1}^{n+1} \ell(X_i)}\right] \leq \left(\frac{1}{n}\right)^p \left\|\hat{u}(X_i) - u(X_i)\right\|_p \left\|\frac{1}{\ell(X_i)}\right\|_q^{1/p} + \frac{1}{n} \left\|\hat{u}(X_{n+1}) - u(X_{n+1})\right\|_p \left\|\frac{1}{\ell(X_i)}\right\|_q^{1/p},
\]

where the \(L_p\) norm for \(X_{n+1}\) is with respect to \(\hat{P}\), hence

\[
\frac{1}{n} \left\|\hat{u}(X_{n+1}) - u(X_{n+1})\right\|_p = \left\|\frac{w(X_i,Y_i)^{1/p}}{n} \cdot (\hat{u}(X_i) - u(X_i))\right\|_p.
\]

Combining the above results, we have

\[
\mathbb{P}(Y_{n+1} \in \hat{C}(X_{n+1})) \geq 1 - \alpha - \tilde{\Delta} \cdot \left\|\frac{1}{\ell(X_i)}\right\|_q,
\]

where

\[
\tilde{\Delta} = \left\|\frac{1}{\ell(X_i)}\right\|_p + \left\|\hat{u}(X_i) - u(X_i)\right\|_p + \left\|\frac{w(X_i,Y_i)^{1/p}}{n} \cdot (\hat{u}(X_i) - u(X_i))\right\|_p,
\]

which completes the proof of Theorem 2.2. \(\square\)

**B.3 Proof of Theorem 4.1**

*Proof of Theorem 4.1.* Throughout the proof, all statements are conditional on \(D_{\text{train}}\). By the independence of \(\mathcal{D}_{\text{calib}} \cup \{(X_{n+1}, Y_{n+1})\}\), the scores \(\{V(X_i,Y_i)\}_{i \in \mathcal{D}_{\text{calib}}}\) are i.i.d. and independent of \(V(X_{n+1}, Y_{n+1})\).

Recall that \(G(\cdot)\) is defined in (15). To begin with, we define

\[
\hat{q} = \inf \left\{t: G(t) \geq 1 - \alpha\right\}, \quad \hat{q}_n = \inf \left\{t: \hat{G}_n(t) \geq 1 - \alpha\right\}.
\]

For any fixed \(\epsilon > 0\), we have

\[
\mathbb{P}(\hat{q}_n \leq \hat{q} - \epsilon) = \mathbb{P}(\hat{G}_n(\hat{q} - \epsilon) \geq 1 - \alpha) \\
\leq \mathbb{P}(G(\hat{q} - \epsilon) \geq \hat{G}_n(\hat{q} - \epsilon) \geq 1 - \alpha) + \mathbb{P}(G(\hat{q} - \epsilon) < \hat{G}_n(\hat{q} - \epsilon) \geq 1 - \alpha) \leq \delta.
\]

Here the last inequality follows from the fact that \(G(\hat{q} - \epsilon) < 1 - \alpha\) for any fixed \(\epsilon > 0\) and \(\mathbb{P}(G(\hat{q} - \epsilon) < \hat{G}_n(\hat{q} - \epsilon) \geq 1 - \alpha) \leq \delta\) by (16) with \(t = \hat{q} - \epsilon\). Therefore, by the continuity of probability measures, we have

\[
\mathbb{P}(\hat{q}_n \geq \hat{q}) = 1 - \lim_{\epsilon \to 0^+} \mathbb{P}(\hat{q}_n \leq \hat{q} - \epsilon) \geq 1 - \delta.
\]

Moreover, on the event \(\{\hat{q}_n \geq \hat{q}\}\), by the definition of \(\hat{C}(X_{n+1})\), it holds for any \(\hat{P} \in \mathcal{P}(\mathbb{P}, \ell, u)\) that

\[
\hat{P}(Y_{n+1} \in \hat{C}(X_{n+1}) | \mathcal{D}_{\text{calib}}) = \hat{P}(V(X_{n+1}, Y_{n+1}) \leq \hat{q}_n | \mathcal{D}_{\text{calib}}) \\
\geq \hat{P}(V(X_{n+1}, Y_{n+1}) \leq \hat{q} | \mathcal{D}_{\text{calib}}) \\
= \mathbb{E}\left[\mathbb{I}_{\{V(X,Y) \leq \hat{q}\}} w(X,Y) | \mathcal{D}_{\text{calib}}\right],
\]

where the expectation is with respect to \((X,Y) \sim \mathbb{P}\) independent of \(\mathcal{D}_{\text{calib}}\). By the definition of \(G(t)\)

\[
\hat{q} = \inf \left\{t: \max \left\{\mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} \ell(X)], 1 - \mathbb{E}[\mathbb{I}_{\{V(X,Y) > t\}} \ell(X)]\right\} \geq 1 - \alpha\right\} = \min\{\hat{q}_1, \hat{q}_2\},
\]

where \((X,Y) \sim \mathbb{P}\) is an independent copy and we define

\[
\hat{q}_1 = \inf \left\{t: \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} \ell(X)] \geq 1 - \alpha\right\}, \\
\hat{q}_2 = \inf \left\{t: 1 - \mathbb{E}[\mathbb{I}_{\{V(X,Y) > t\}} \ell(X)] \geq 1 - \alpha\right\}.
\]
For constants $\hat{q}_1, \hat{q}_2$, we have
\[
\mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_1\}} w(X,Y) \mid \mathcal{D}_{\text{calib}}]
= \min \left\{ \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_1\}} w(X,Y) \mid \mathcal{D}_{\text{calib}}], \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_2\}} w(X,Y) \mid \mathcal{D}_{\text{calib}}] \right\}.
\]

We analyze the two terms separately. Firstly,
\[
\mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_1\}} w(X,Y) \mid \mathcal{D}_{\text{calib}}]
= \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_1\}} \hat{\ell}(X) \mid \mathcal{D}_{\text{calib}}] - \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_1\}} (\hat{\ell}(X) - w(X,Y)) \mid \mathcal{D}_{\text{calib}}]
\geq 1 - \alpha - \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_1\}} (\hat{\ell}(X) - w(X,Y)) \mid \mathcal{D}_{\text{calib}}]
\geq 1 - \alpha - \mathbb{E}[(\hat{\ell}(X) - w(X,Y))]_+],
\]
where the step (a) follows from the definition of $\hat{q}_1$. Similarly,
\[
\mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq \hat{q}_2\}} w(X,Y) \mid \mathcal{D}_{\text{calib}}]
\geq 1 - \alpha - \mathbb{E}[(\hat{\ell}(X) - w(X,Y))]_+],
\]
where the first equality follows from the fact that $w(x,y)$ is a likelihood ratio, and the first inequality follows from the definition of $\hat{q}_2$. Putting them together, on the event $\{\hat{q}_n \geq \hat{q}\}$ which happens with probability at least $1 - \delta$ with respect to $\mathcal{D}_{\text{calib}}$, it holds that
\[
\tilde{P}(Y_{n+1} \in \hat{C}(X_{n+1}) \mid \mathcal{D}_{\text{calib}}) \geq 1 - \alpha - \tilde{\Delta},
\]
where the gap is
\[
\tilde{\Delta} = \max \left\{ \mathbb{E}[(\hat{\ell}(X) - w(X,Y))]_+, \mathbb{E}[(\hat{\ell}(X) - w(X,Y))]_- \right\},
\]
and the expectations are with respect to an independent copy $(X,Y) \sim \mathbb{P}$. Therefore, we conclude the proof of Theorem 4.1. \hfill \square

B.4 Proof of Proposition A.1

Proof of Proposition A.1. Let $t \in \mathbb{R}$ be any fixed constant or any random variable in $\sigma(\mathcal{D}_{\text{train}})$, and fix any $\delta \in (0, 1)$. We condition on $\mathcal{D}_{\text{train}}$ throughout the proof, so that $V$, $\hat{\ell}$ and $\hat{u}$ can be viewed as fixed and $t$ can be viewed as constant.

Since $\hat{G}_n(t) = \max \{ \hat{G}^t_n(t), \hat{G}^\ell_n(t) \}$, by the definition (15), it suffices to show that
\[
\mathbb{P}_{\mathcal{D}_{\text{calib}}}(\hat{G}^t_n(t) \leq \mathbb{E}\left[\mathbb{I}_{\{V_i \leq t\}} \hat{\ell}(X_i)\right]) \geq 1 - \delta/2
\]
and
\[
\mathbb{P}_{\mathcal{D}_{\text{calib}}}(\hat{G}^\ell_n(t) \leq 1 - \mathbb{E}\left[\mathbb{I}_{\{V_i > t\}} \hat{u}(X_i)\right]) \geq 1 - \delta/2.
\]

Now let
\[
f(X_i) = \mathbb{I}_{\{V_i \leq t\}} \hat{\ell}(X_i)/M, \quad h(X_i) = 1 - \mathbb{I}_{\{V_i > t\}} \hat{u}(X_i)/M,
\]
so that $f(X_i)$ and $h(X_i)$, $1 \leq i \leq n$, are i.i.d. random variables in $[0,1]$. We rescale the bounds into $\hat{f}_n = \hat{G}^t_n(t)/M$ and $\hat{h}_n = (\hat{G}^\ell_n(t) - 1 + M)/M$, hence by the tower property of conditional expectations, it suffices to show that
\[
\mathbb{P}_{\mathcal{D}_{\text{calib}}}(\hat{f}_n \leq \mathbb{E}[f(X_i)]) \geq 1 - \delta/2 \quad \text{and} \quad \mathbb{P}_{\mathcal{D}_{\text{calib}}}(\hat{h}_n \leq \mathbb{E}[h(X_i)]) \geq 1 - \delta/2.
\]
We show the desired result for \( f(\cdot) \) and that for \( h(\cdot) \) naturally applies.

Consider the filtration \( \{ F_i \}_{i \geq 1} \), where the \( \sigma \)-algebra \( F_i = \sigma(X_1, Y_1, \ldots, X_i, Y_i) \). Then by definition, \( \hat{\sigma}^t_i \) and \( \hat{\mu}^t_i \) are measurable with respect to \( F_i \), and \( \{ \nu^t_i \}_{i \geq 1} \) is a predictable sequence with respect to \( \{ F_i \}_{i \geq 1} \).

Thus letting
\[
  f_0 = \mathbb{E}[f(X)] = \mathbb{E}[1_{\{V \leq t\}} \ell(X)] / M,
\]
we have
\[
  \mathbb{E}[K^t_i(f_0) | F_{i-1}] = K^t_{i-1}(f_0) \cdot \left( 1 + \nu^t_i \cdot \mathbb{E}[f(X_i) - f_0 | F_{i-1}] \right) = K^t_{i-1}(f_0).
\]

Thus \( \{ K^t_i(f_0) \}_{i=1}^n \) is a martingale. Meanwhile, since \( f(X_i) \in [0,1] \), we know \( f(X_i) - f_0 \geq -1 \). Hence \( K^t_i(f_0) \geq 0 \) for all \( i \in [n] \). Therefore by Ville’s inequality,
\[
  \mathbb{P}_{\text{calib}} \left( \max_{1 \leq i \leq n} K^t_i(f_0) > \frac{2}{\delta} \right) \leq \frac{\delta}{2}.
\]

Also note that \( K_i(g) \) is a decreasing function in \( g \in \mathbb{R} \), hence
\[
  \mathbb{P}_{\text{calib}} \left( \hat{f}_n > \mathbb{E}[f(X_i)] \right) \leq \mathbb{P} \left( \max_{1 \leq i \leq n} K_i(f_0) > \frac{2}{\delta} \right) \leq \delta/2,
\]

Therefore, we conclude the proof of the desired results. \( \square \)

### B.5 Proof of Proposition 4.2

**Proof of Proposition 4.2.** Throughout the proof, we denote the generic random variables \((X, Y) \sim \mathbb{P}\) and \( V = V(X, Y) \). Denoting the right-hand side of (20) as \( F^*(t) \), we are to show that

(i) \( F^*(\cdot) : \mathbb{R} \to [0,1] \) is a distribution function.

(ii) \( F^*(t) \) is a lower bound for \( F(t; \mathcal{P}(\mathbb{P}, \ell, u)) \) for all \( t \in \mathbb{R} \).

(iii) \( F^*(t) \) can be achieved by some element in \( \mathcal{P}(\mathbb{P}, \ell, u) \).

First of all, (i) is straightforward by noting that \( F^*(\cdot) \) is right-continuous due to the continuity of probability measures and \( \lim_{t \to -\infty} F^*(t) = 0, \lim_{t \to +\infty} F^*(t) = 1 \). Also, similar to the arguments in the proof of Theorem 4.1, for any \( \mathbb{P} \in \mathcal{P}(\mathbb{P}, \ell, u) \), we have
\[
  F(t; V; \mathbb{P}) = \mathbb{E} \left[ 1_{\{V(X,Y) \leq t\}} \frac{d\mathbb{P}}{d\mathbb{P}(X,Y)}(X,Y) \right] \geq \mathbb{E} \left[ 1_{\{V(X,Y) \leq t\}} \ell(X) \right],
\]
\[
  F(t; V; \mathbb{P}) = 1 - \mathbb{E} \left[ 1_{\{V(X,Y) > t\}} \frac{d\mathbb{P}}{d\mathbb{P}(X,Y)}(X,Y) \right] \geq 1 - \mathbb{E} \left[ 1_{\{V(X,Y) > t\}} u(X) \right],
\]
hence (ii) follows. For (iii), we are to construct one distribution \( \mathbb{P}^* \in \mathcal{P}(\mathbb{P}, \ell, u) \) so that \( F(\cdot; V, \mathbb{P}^*) = F^*(\cdot) \).

If \( \mathbb{E}[u(X)] = 1 \), then since \( \mathbb{E}[w(X,Y)] = 1 \) for the likelihood ratio function, the collection \( \mathcal{P}(\mathbb{P}, \ell, u) = \{ \mathbb{P}^* \} \) is a singleton with \( \frac{d\mathbb{P}^*}{d\mathbb{P}}(x,y) = u(x) \), and
\[
  F(t; \mathcal{P}(\mathbb{P}, \ell, u)) = F(t; \mathbb{P}^*) = \mathbb{E} \left[ 1_{\{V(X,Y) \leq t\}} u(X) \right] = F^*(t),
\]
where the last equality follows from \( \ell(x) \leq u(x) \). Then \( \mathbb{P}^* \) satisfies (iii). Similarly, for the case where \( \mathbb{E}[\ell(X)] = 1 \), the collection \( \mathcal{P}(\mathbb{P}, \ell, u) = \{ \mathbb{P}^* \} \) is a singleton with \( \frac{d\mathbb{P}^*}{d\mathbb{P}}(x,y) = \ell(x) \), and
\[
  F(t; \mathcal{P}(\mathbb{P}, \ell, u)) = F(t; \mathbb{P}^*) = \mathbb{E} \left[ 1_{\{V(X,Y) \leq t\}} \ell(X) \right] = F^*(t),
\]
hence \( \mathbb{P}^* \) satisfies (iii). In the sequel, we consider the case where \( \mathbb{E}[\ell(X)] < 1 < \mathbb{E}[u(X)] \). We define
\[
  H(t) := \mathbb{E}[\ell(X) \cdot 1_{\{V \leq t\}} + u(X) \cdot 1_{\{V > t\}}].
\]
By the construction and the continuity of probability measures, we have
\[
\lim_{t \to \infty} H(t) = \mathbb{E}[\ell(X)] < 1 < \mathbb{E}[u(X)] = \lim_{t \to -\infty} H(t).
\]
We additionally define \( t^* = \inf\{t \in \mathbb{R} : H(t) \leq 1\} \). Note that \( t^* < \infty \) and \( H(t^*) \leq 1 \) by the right continuity of \( H(t) \). We also define the left limit of \( H(t) \) at \( t^* \) as
\[
H_-(t^*) = \lim_{t \uparrow t^*} H(t),
\]
and define the weight as
\[
\gamma = \frac{1 - H(t^*)}{H_-(t^*) - H(t^*)} - I_{H_-(t^*) > 1}
\]
Here by the definition of \( t^* \), we have \( H_-(t^*) \geq 1 \geq H(t^*) \), and the left limit takes the form
\[
H_-(t^*) = \mathbb{E}[\ell(X) \cdot 1_{\{V < t^*\}} + u(X) \cdot 1_{\{V \geq t^*\}}].
\]
We now construct the worst-case distribution \( \mathbb{P}^* \) by
\[
\frac{d\mathbb{P}^*}{d\mathbb{P}}(x, y) = \gamma \cdot [\ell(x) 1_{\{V(x,y) < t^*\}} + u(x) 1_{\{V(x,y) \geq t^*\}}] + (1 - \gamma) \cdot [\ell(x) 1_{\{V(x,y) \leq t^*\}} + u(x) 1_{\{V(x,y) > t^*\}}].
\]
We denote the likelihood ratio \( w^*(x,y) = \frac{d\mathbb{P}^*}{d\mathbb{P}}(x,y) \) as constructed above. Note that
\[
\mathbb{P}^*(X \times Y) = \mathbb{E}[w^*(X,Y)] = \gamma \cdot H_-(t^*) + (1 - \gamma) \cdot H(t^*) = 1,
\]
and also \( \ell(x) \leq w^*(x,y) \leq u(x) \) for all \( x \in X \). Therefore \( \mathbb{P}^* \) is a probability measure and is an element of \( \mathcal{P}(\mathbb{P}, \ell, u) \). In the following, we check that \( F(t; \nu, \mathbb{P}^*) = F^*(t) \) for all \( t \in \mathbb{R} \). Recall that we work with the case \( \mathbb{E}[\ell(X)] < 1 < \mathbb{E}[u(X)] \). For any constant \( t < t^* \), by the construction of \( w^* \),
\[
F(t; V, \mathbb{P}^*) = \mathbb{E}[w^*(X,Y) 1_{\{V(X,Y) \leq t\}}]
= \gamma \cdot \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t\}}] + (1 - \gamma) \cdot \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t\}}] = \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t\}}] = F^*(t),
\]
where the last equality follows from the fact that
\[
\mathbb{E}[\ell(X) 1_{\{V \leq t\}}] > 1 - \mathbb{E}[u(X) 1_{\{V > t\}}]
\]
since \( H(t) > 1 \) for \( t < t^* \). When \( t = t^* \), note that
\[
\mathbb{E}[\ell(X) 1_{\{V \leq t^*\}}] - 1 + \mathbb{E}[u(X) 1_{\{V > t^*\}}] = H(t^*) - 1 \leq 0,
\]
hence the right-hand side of (20) admits the form
\[
F^*(t^*) = 1 - \mathbb{E}[u(X) 1_{\{V \geq t^*\}}].
\]
Meanwhile, by the construction of \( w^*(x,y) \), we have
\[
F(t^*; V, \mathbb{P}^*) = \mathbb{E}[w^*(X,Y) 1_{\{V(X,Y) \leq t^*\}}]
= \gamma \cdot \mathbb{E}[\ell(X) 1_{\{V(X,Y) < t^*\}} + u(X) 1_{\{V(X,Y) = t^*\}}] + (1 - \gamma) \cdot \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t^*\}}]
= \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t^*\}}] - \gamma \cdot \mathbb{E}[\ell(X) 1_{\{V(X,Y) = t^*\}} - u(X) 1_{\{V(X,Y) = t^*\}}]
= \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t^*\}}] - \gamma \cdot (H_-(t^*) - H(t^*))
= \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t^*\}}] + 1 - H(t^*) = 1 - \mathbb{E}[u(X) 1_{\{V \geq t^*\}}] = F^*(t^*).
\]
Similarly, when \( t > t^* \), by the construction of \( w^*(x,y) \) we have
\[
F(t^*; V, \mathbb{P}^*) = 1 - \mathbb{E}[w^*(X,Y) 1_{\{V(X,Y) > t^*\}}]
= 1 - \gamma \cdot \mathbb{E}[u(X) 1_{\{V(X,Y) > t^*\}}] + (1 - \gamma) \cdot \mathbb{E}[u(X) 1_{\{V(X,Y) > t^*\}}]
= 1 - \mathbb{E}[u(X) 1_{\{V \geq t^*\}}] = F^*(t),
\]
where the last equality follows from the fact that \( H(t) \leq 1 \) thus \( 1 - \mathbb{E}[u(X) 1_{\{V(X,Y) > t^*\}}] \geq \mathbb{E}[\ell(X) 1_{\{V(X,Y) \leq t^*\}}] \). Combining the three cases, we arrive at \( F^*(\cdot) = F(\cdot; V, \mathbb{P}^*) \), hence (20) follows and we conclude the proof of Proposition 4.2.
B.6 Proof of Proposition 4.3

Proof of Proposition 4.3. The proof proceeds by showing that \( \mathcal{P} \subset \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \) and \( \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \subset \mathcal{P} \), which together lead to the desired result.

**Step 1:** \( \mathcal{P} \subset \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \). Let \( \mathbb{P}^{\text{sup}} \) be any super-population that satisfies (3) and (21). Due to the partial observation of potential outcomes, the observed distribution admits the decomposition

\[
\mathbb{P}_{X,Y,T}^{\text{obs}} = \mathbb{P}_{T=1}^{\text{obs}} \times \mathbb{P}_{X,Y(1)|T=1}^{\text{obs}} + \mathbb{P}_{T=0}^{\text{obs}} \times \mathbb{P}_{X,Y(0)|T=0}^{\text{obs}}.
\]

Therefore, the data-compatibility condition (21) is equivalent to

\[
\mathbb{P}_{X|T=w}^{\text{sup}} = \mathbb{P}_{X(T=w)}^{\text{obs}}, \quad \mathbb{P}_{X,Y(1)|T=1}^{\text{sup}} = \mathbb{P}_{X,Y(1)|T=1}^{\text{obs}}, \quad \mathbb{P}_{X,Y(0)|T=0}^{\text{sup}} = \mathbb{P}_{X,Y(0)|T=0}^{\text{obs}},
\]

where the latter two are further equivalent to

\[
\mathbb{P}_{X|T=w}^{\text{sup}} = \mathbb{P}_{X(T=w)}^{\text{obs}}, \quad \mathbb{P}_{X,Y(1)|T=1}^{\text{sup}} = \mathbb{P}_{X,Y(1)|T=1}^{\text{obs}}, \quad \mathbb{P}_{X,Y(0)|T=0}^{\text{sup}} = \mathbb{P}_{X,Y(0)|T=0}^{\text{obs}}.
\]

Recall that \( \bar{\mathbb{P}} = \mathbb{P}_{X,Y(1)|T=0}^{\text{sup}} \) and \( \mathbb{P} = \mathbb{P}_{X,Y(1)|T=1}^{\text{obs}} \). Then we have

\[
\frac{d\bar{\mathbb{P}}_X}{d\mathbb{P}_X} = \frac{d\mathbb{P}_{X|T=0}^{\text{sup}}}{d\mathbb{P}_{X|T=0}^{\text{obs}}} = \frac{d\mathbb{P}_{X|T=1}^{\text{obs}}}{d\mathbb{P}_{X|T=1}^{\text{sup}}} = \frac{\mathbb{P}_{T=1}^{\text{obs}}}{\mathbb{P}_{T=0}^{\text{obs}}} = \frac{\mathbb{P}_{T=1}}{\mathbb{P}_{T=0}} = f(X),
\]

where the second equality follows from (35) and the third equality follows from the Bayes rule. On the other hand, the shift of conditional distribution is

\[
\frac{d\bar{\mathbb{P}}_{Y(1)|X}}{d\mathbb{P}_{Y(1)|X}} = \frac{d\mathbb{P}_{Y(1)|X,T=0}^{\text{sup}}}{d\mathbb{P}_{Y(1)|X,T=1}^{\text{obs}}} \in [1/\Gamma, \Gamma]
\]

according to Lemma 3.1. Therefore, \( \mathbb{P}^{\text{sup}} \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \) by the definition. Hence we have \( \mathcal{P} \subset \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \).

**Step 2:** \( \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \subset \mathcal{P} \). For this part, we are to show that for any \( \bar{\mathbb{P}} \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \), there exists some \( \mathbb{P}^{\text{sup}} \) satisfying (3) and (21) such that \( \bar{\mathbb{P}} = \mathbb{P}^{\text{sup}}_{X,Y(1)|T=0} \). Fixing an arbitrary probability distribution \( \bar{\mathbb{P}} \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \), we define the function

\[
w(y|x) = \frac{d\bar{\mathbb{P}}_{Y(1)|X}}{d\mathbb{P}_{Y(1)|X}}(y|x),
\]

so that \( w(y|x) \in [1/\Gamma, \Gamma] \) for \( \mathbb{P}^{\text{obs}} \)-almost all \( (x, y) \in \mathcal{X} \times \mathcal{Y} \). Also, since \( \bar{\mathbb{P}} \) is a distribution, we have

\[
\mathbb{E}[w(Y(1)|X=x)|X=x] = \bar{\mathbb{P}}(Y(1)|X=x) = 1
\]

for \( \mathbb{P} \)-almost all \( x \in \mathcal{X} \), and the conditional expectation is induced by \( (X,Y(1)) \sim \mathbb{P} = \mathbb{P}_{X,Y(1)|T=1}^{\text{obs}} \).

Applying Lemma B.1 with \( r(x,y) = w(y|x) \) and \( t = 1 \), we know there exists a distribution \( \mathbb{P}^{\text{sup}} \) over \( (X,Y(0),Y(1),U,T) \) for some confounder \( U \) that satisfies (21) and (3), and

\[
\frac{d\mathbb{P}_{Y(1),X|T=0}^{\text{sup}}}{d\mathbb{P}_{Y(1),X|T=1}}(y|x) = w(y|x).
\]

Since \( \mathbb{P}^{\text{sup}} \) satisfies (21), we have \( \mathbb{P}^{\text{sup}}_{Y(1),X|T=1} = \mathbb{P}_{Y(1),X|T=1}^{\text{obs}} = \mathbb{P}_{Y(1)|X} \) where we recall the definition of \( \mathbb{P} \), the distribution at hand. Hence

\[
w(y|x) = \frac{d\mathbb{P}_{Y(1),X|T=0}^{\text{sup}}}{d\mathbb{P}_{Y(1)|X}}(y|x) = \frac{d\mathbb{P}_{Y(1)|X}}{d\mathbb{P}_{Y(1)|X}}(y|x).
\]
Therefore, we have \( \bar{\mathbb{P}}_{Y(1) \mid X} = \mathbb{P}^\text{sup}_{Y(1) \mid X \mid T = 0} \). Furthermore, since \( \mathbb{P}^\text{sup} \) satisfies (21), we know
\[
\frac{\text{d}\mathbb{P}^\text{sup}_{X \mid T = 0}}{\text{d}\mathbb{P}^\text{obs}_{X \mid T = 0}} = \frac{\text{d}\mathbb{P}^\text{obs}_{X \mid T = 0}}{\text{d}\mathbb{P}^\text{obs}_{X \mid T = 1}} = f(X) = \frac{\text{d}\bar{\mathbb{P}}_X}{\text{d}\mathbb{P}_X},
\]
where the second equality follows from the Bayes rule and the last equality follows from the fact that \( \bar{\mathbb{P}} \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \). Thus, we have \( \bar{\mathbb{P}}_X = \mathbb{P}^\text{sup}_{X \mid T = 0} \). Putting the two parts together, we have \( \bar{\mathbb{P}} = \mathbb{P}^\text{sup}_{X,Y(1) \mid T = 0} \).

By the arbitrariness of \( \bar{\mathbb{P}} \), we arrive at \( \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \subset \mathcal{P} \).

Combining the two steps, we conclude the proof of Proposition 4.3. \(\Box\)

B.7 Sharpness of the identification set

Lemma B.1 (Sharpness of Lemma 3.1). Given \( t \in \{0, 1\} \), a marginal distribution \( \mathbb{P}^\text{obs} \) over \((X, Y, T)\) and a function \( r(x, y) \in [1/\Gamma, \Gamma] \) such that
\[
\mathbb{E}^\text{obs}[r(X, Y(t)) \mid X, T = t] = 1, \quad \mathbb{P}^\text{obs}-\text{almost surely},
\]
there exists a distribution \( \mathbb{P}^\text{sup} \) over \((X, Y(0), Y(1), U, T)\) for some confounder \( U \) such that

(i) \( \mathbb{P}^\text{sup}_{X,Y,T} = \mathbb{P}^\text{obs}_{X,Y,T} \) for \( Y = Y(T) \);

(ii) \( \mathbb{P}^\text{sup} \) satisfies the marginal \( \Gamma \)-selection condition;

(iii) the likelihood ratio is exactly \( r(x, y) \), so that \( r(x, y) = \frac{\text{d}\mathbb{P}^\text{sup}_{Y(0) \mid X,T = 1-t}}{\text{d}\mathbb{P}^\text{sup}_{Y(1) \mid X,T = t}}(x, y) \) for \( \mathbb{P}^\text{sup}-\text{almost all} \) \( x, y \).

hold simultaneously.

Proof of Lemma B.1. Fix any marginal distribution \( \mathbb{P}^\text{obs} \) over \((X, Y, T)\) for \( Y = Y(T) \), and a function \( r(x, y) \in [1/\Gamma, \Gamma] \) satisfying the given condition. We show the result for \( t = 1 \), while that for \( t = 0 \) follows exactly the same arguments.

The construction of \( \mathbb{P}^\text{sup} \) To begin with, we let the confounder be the counterfactual itself, so that \( U = Y(1) \). The joint distribution is thus
\[
\mathbb{P}^\text{sup}_{(X,Y(1),Y(0)) \mid T} = \mathbb{P}^\text{sup}_{X,T} \times \mathbb{P}^\text{sup}_{(Y(1),Y(0)) \mid X,T},
\]
We set the two parts separately. Firstly, we set \( \mathbb{P}^\text{sup}_{X,T} = \mathbb{P}^\text{obs}_{X,T} \) for the distribution on \((X, T)\). The joint distribution of potential outcomes given \((X, T)\) admits
\[
\mathbb{P}^\text{sup}_{(Y(1),Y(0)) \mid X,T} = \mathbb{P}^\text{sup}_{Y(1) \mid X,T} \times \mathbb{P}^\text{sup}_{Y(0) \mid X,T,Y(1)},
\]
Since our target is for \( Y(1) \), we take a simple coupling where \( Y(0) \) is independent of \((T,Y(1))\) conditional on \( X \), so that we set
\[
\mathbb{P}^\text{sup}_{Y(0) \mid X,T,Y(1)} = \mathbb{P}^\text{sup}_{Y(0) \mid X} = \mathbb{P}^\text{sup}_{Y(0) \mid X,T = 0} = \mathbb{P}^\text{obs}_{Y(0) \mid X,T = 0}. \tag{36}
\]
On the other hand, we set \( \mathbb{P}^\text{sup}_{Y(1) \mid X,T} \) for \( T = 0,1 \) by
\[
\mathbb{P}^\text{sup}_{Y(1) \mid X,T = 1} = \mathbb{P}^\text{obs}_{Y(1) \mid X,T = 1} \quad \text{and} \quad \frac{\text{d}\mathbb{P}^\text{sup}_{Y(1) \mid X,T = 0}}{\text{d}\mathbb{P}^\text{obs}_{Y(1) \mid X,T = 1}}(y \mid x) = r(x, y). \tag{37}
\]
So far we’ve completed the pieces of constructing \( \mathbb{P}^\text{sup} \). It remains to check that it is indeed a probability measure. By construction, \( \mathbb{P}^\text{sup}_{X,T} = \mathbb{P}^\text{obs}_{X,T} \) is a probability measure on \((X, T)\). Also, by the construction,
\[
\mathbb{P}^\text{sup}(Y(1) \in \mathcal{Y} \mid X, T = 1) = \mathbb{P}^\text{obs}(Y(1) \in \mathcal{Y} \mid X, T = 1) = 1,
\]

37
and  
\[ \mathbb{P}^{\text{sup}}(Y(1) \in \mathcal{Y} \mid X, T = 0) = \mathbb{E}^{\text{obs}} \left[ \mathbb{I}_{\{Y(1) \in \mathcal{Y}\}} \frac{d\mathbb{P}^{\text{sup}}(Y(1) \mid X, T = 0)}{d\mathbb{P}^{\text{obs}}(Y(1) \mid X, T = 1)} \right] X, T = 1 \]
\[ = \mathbb{E}^{\text{obs}} \left[ \frac{d\mathbb{P}^{\text{sup}}(Y(1) \mid X, T = 0)}{d\mathbb{P}^{\text{obs}}(Y(1) \mid X, T = 1)} \right] X, T = 1 = \mathbb{E}^{\text{obs}} \left[ r(X, Y(1)) \mid X, T = 1 \right] = 1, \]
where the first equality is by the change-of-measure formula, the second equality follows from 1 = \( \mathbb{I}_{\{Y(1) \in \mathcal{Y}\}} \), the third equality follows from the construction, and the last equality is the given condition on \( r(x, y) \). Thus, \( \mathbb{P}^{\text{sup}}(Y(1) \mid X, T = 0) \) is a probability measure. Also, by the construction of \( \mathbb{P}^{\text{sup}}(Y(1) \mid X, T = 1) \), we have  
\[ \mathbb{P}^{\text{sup}}(Y(0) \in \mathcal{Y} \mid X, T, Y(1)) = \mathbb{P}^{\text{obs}}(Y(0) \in \mathcal{Y} \mid X, T = 0) = 1, \]
hence \( \mathbb{P}^{\text{sup}}(Y(0) \mid X, T, Y(1)) \) is also a probability measure. Putting them together, we know that  
\[ \mathbb{P}^{\text{sup}}(X, T, Y(1), Y(0)) = \mathbb{P}^{\text{sup}}(X, T) \times \mathbb{P}^{\text{sup}}(Y(1) \mid X, T) \times \mathbb{P}^{\text{sup}}(Y(0) \mid X, T, Y(1)) \]
is indeed a probability measure over \((X, T, Y(1), Y(0))\).

**Verify the properties** We now proceed to verify the three stated properties. For (i), due to partial observability, the observed distribution admits the decomposition  
\[ \mathbb{P}^{\text{obs}}(X, Y, T) = \mathbb{P}^{\text{obs}}(X) \times \mathbb{P}^{\text{obs}}(Y \mid X) = \mathbb{P}^{\text{obs}}(T = 1) \times \mathbb{P}^{\text{obs}}(X, Y(1) \mid T = 1) + \mathbb{P}^{\text{obs}}(T = 0) \times \mathbb{P}^{\text{obs}}(X, Y(0) \mid T = 0). \]
Similarly, the projection on the observable of \( \mathbb{P}^{\text{sup}} \) is  
\[ \mathbb{P}^{\text{sup}}(X, T, Y) = \mathbb{P}^{\text{sup}}(X) \times \mathbb{P}^{\text{sup}}(Y \mid X) = \mathbb{P}^{\text{sup}}(T = 1) \times \mathbb{P}^{\text{sup}}(X, Y(1) \mid T = 1) + \mathbb{P}^{\text{sup}}(T = 0) \times \mathbb{P}^{\text{sup}}(X, Y(0) \mid T = 0). \]
Here by the construction of \( \mathbb{P}^{\text{sup}}(X, T) = \mathbb{P}^{\text{obs}}(X, T) \), we have \( \mathbb{P}^{\text{obs}}(Y(w) \mid X, T = w) = \mathbb{P}^{\text{sup}}(Y(w) \mid X, T = w) \) for \( w \in \{0, 1\} \). Also, \( \mathbb{P}^{\text{sup}}(Y(w) \mid X, T = w) = \mathbb{P}^{\text{sup}}(Y(w) \mid X, T = w) \) holds for \( w \in \{0, 1\} \) by (36) and (37). The equivalences altogether leads to \( \mathbb{P}^{\text{obs}}(X, Y, T) = \mathbb{P}^{\text{obs}}(X, Y, T) \). For (ii), by the Bayes rule, we have  
\[ r(x, y) = \frac{d\mathbb{P}^{\text{sup}}(T = 0 \mid | X = x, Y(1) = y)}{d\mathbb{P}^{\text{sup}}(T = 0 \mid | X = x, Y(1) = y)} \cdot \frac{\mathbb{P}^{\text{sup}}(T = 1 \mid | X = x, Y(1) = y)}{\mathbb{P}^{\text{sup}}(T = 0 \mid | X = x, Y(1) = y)} \in [1/\Gamma, \Gamma], \]
so \( \mathbb{P}^{\text{sup}} \) satisfies the marginal \( \Gamma \)-selection condition (3) hence (ii) is verified. Property (iii) has also been verified as above. So far, we’ve constructed \( \mathbb{P}^{\text{sup}} \) that satisfies all stated conditions and we conclude the proof of Lemma B.1. \( \square \)

**B.8 Proof of Proposition 4.4**

**Proof of Proposition 4.4.** For simplicity, we denote (24) as \( F^*(t) \), and aim to show that  
(i) \( F^*(t) \) is a distribution function;  
(ii) \( F^*(t) \) is a lower bound for \( F(t; V, \tilde{P}) \) for all \( t \in \mathbb{R} \) and all \( \tilde{P} \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \);  
(iii) \( F^*(t) \) can be achieved by \( \mathbb{P}^* \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \) where \( d\mathbb{P}^* / d\mathbb{P}(x, y) = w^*(x, y) \) as defined in (25).

To verify (i), we note that \( F^*(t) \) is right continuous by the continuity of probability measures, as well as \( \lim_{t \to -\infty} F^*(t) = 0 \) and \( \lim_{t \to +\infty} F^*(t) = 1 \). To show (ii), we are to show that for any \( \tilde{P} \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \), it holds \( \mathbb{P} \)-almost surely that  
\[ \mathbb{E} \left[ \mathbb{I}_{\{V(X, Y) \leq t\}} w^*(X, Y) \mid X \right] \leq \tilde{P}(V(X, Y) \leq t \mid X) = \mathbb{E} \left[ \mathbb{I}_{\{V(X, Y) \leq t\}} \frac{d\tilde{P}}{d\mathbb{P}}(X, Y) \mid X \right]. \]
Fixing any \( \tilde{\mathbb{P}} \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \), we denote the conditional likelihood as \( w_0(y \mid x) = \frac{d\tilde{\mathbb{P}}_Y \mid _X / d\mathbb{P}_Y \mid _X(y \mid x)}{d\mathbb{P}/d\mathbb{P}(x,y) = f(x) \cdot w_0(y \mid x)} \). Hence for any \( t \in \mathbb{R} \),
\[
\mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} w^*(X,Y) \mid X] = \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} w^*(X,Y) \mid X] - \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} w_0(X,Y) \mid X] + \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} (w^*(X,Y) - w_0(X,Y)) \mid X] \cdot \mathbb{I}_{\{t \geq q(\tau(x); x, \mathcal{P})\}}.
\]
We treat the two terms in the last summation separately. By the definition of \( w^*(x,y) \),
\[
\mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} (w^*(X,Y) - w_0(X,Y)) \mid X] \cdot \mathbb{I}_{\{t \geq q(\tau(x); x, \mathcal{P})\}} = f(X) \cdot \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} (\ell_0(X) - w_0(y \mid X)) \mid X] \cdot \mathbb{I}_{\{t \geq q(\tau(x); x, \mathcal{P})\}} \leq 0.
\]
Meanwhile, since \( 1 = \mathbb{E}[w_0(y \mid X) \mid X] = \mathbb{E}[w^*(X,Y)/f(X) \mid X] = 1 \) holds \( \mathbb{P} \)-almost surely, we have
\[
\mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} (w^*(X,Y) - w_0(X,Y)) \mid X] \cdot \mathbb{I}_{\{t \geq q(\tau(x); x, \mathcal{P})\}}
\]
\[
= f(X) \cdot \mathbb{E}[\mathbb{I}_{\{V(X,Y) > t\}} (w_0(Y \mid X) - w^*(X,Y)/f(X)) \mid X] \cdot \mathbb{I}_{\{t \geq q(\tau(x); x, \mathcal{P})\}}
\]
\[
= f(X) \cdot \mathbb{E}[\mathbb{I}_{\{V(X,Y) > t\}} (w_0(Y \mid X) - w_0(X)) \mid X] \cdot \mathbb{I}_{\{t \geq q(\tau(x); x, \mathcal{P})\}} \leq 0.
\]
Summing them up and by the tower property of conditional expectations, it holds for any \( t \in \mathbb{R} \) that
\[
F^*(t) = \mathbb{E}[\mathbb{I}_{\{V(X,Y) \leq t\}} w^*(X,Y)] \leq \tilde{\mathbb{P}}(V(X,Y) \leq t),
\]
which verifies property (ii). Finally, we define \( \mathbb{P}^* \) by \( d\mathbb{P}^* / d\mathbb{P}(x,y) = w^*(x,y) \). Then since \( \mathbb{E}[w^*(X,Y)/f(X) \mid X = x] = 1 \), the marginal likelihood ratio satisfies \( d\mathbb{P}^* / d\mathbb{P}_X = f(x) \), hence \( d\mathbb{P}_Y \mid _X / d\mathbb{P}_Y \mid _X(x,y) = w^*(x,y)/f(x) \).
To verify \( \mathbb{P}^* \in \mathcal{P}(\mathbb{P}, f, \ell_0, u_0) \), it remains to show \( \ell_0(x) \leq \gamma_0(x) \leq u_0(x) \) when it is nonzero, i.e., \( \mathbb{P}(V(x,Y) = q(\tau(x); x, \mathcal{P}) \mid X = x) > 0 \). In this case,
\[
\gamma_0(x) = \frac{1 - \ell_0(x) \cdot \mathbb{P}(V(x,Y) < q(\tau(x); x, \mathcal{P}) \mid X = x) - u_0(x) \cdot \mathbb{P}(V(x,Y) > q(\tau(x); x, \mathcal{P}) \mid X = x)}{\mathbb{P}(V(x,Y) = q(\tau(x); x, \mathcal{P}) \mid X = x)}.
\]
Note that \( \mathbb{P}(V(x,Y) < q(\tau(x); x, \mathcal{P}) \mid X = x) \leq \tau(x) = (u_0(x) - 1)/(u_0(x) - \ell_0(x)) \), hence
\[
1 - \ell_0(x) \cdot \mathbb{P}(V(x,Y) < q(\tau(x); x, \mathcal{P}) \mid X = x)
\]
\[
\leq u_0(x) - u_0(x) \cdot \mathbb{P}(V(x,Y) < q(\tau(x); x, \mathcal{P}) \mid X = x)
\]
\[
= u_0(x) \cdot \mathbb{P}(V(x,Y) > q(\tau(x); x, \mathcal{P}) \mid X = x)
\]
\[
= u_0(x) \cdot \mathbb{P}(V(x,Y) = q(\tau(x); x, \mathcal{P}) \mid X = x) + u_0(x) \cdot \mathbb{P}(V(x,Y) = q(\tau(x); x, \mathcal{P}) \mid X = x),
\]
which leads to \( \gamma_0(x) \leq u_0(x) \). On the other hand, by the definition of quantiles, we have \( \mathbb{P}(V(x,Y) \leq q(\tau(x); x, \mathcal{P}) \mid X = x) \geq \tau(x) = (u_0(x) - 1)/(u_0(x) - \ell_0(x)) \). Hence
\[
\ell_0(x) \cdot \mathbb{P}(V(x,Y) < q(\tau(x); x, \mathcal{P}) \mid X = x) + \ell_0(x) \cdot \mathbb{P}(V(x,Y) = q(\tau(x); x, \mathcal{P}) \mid X = x)
\]
\[
= \ell_0(x) \cdot \mathbb{P}(V(x,Y) \leq q(\tau(x); x, \mathcal{P}) \mid X = x)
\]
\[
\leq 1 - u_0(x) + u_0(x) \cdot \mathbb{P}(V(x,Y) \leq q(\tau(x); x, \mathcal{P}) \mid X = x)
\]
\[
= 1 - u_0(x) \cdot \mathbb{P}(V(x,Y) > q(\tau(x); x, \mathcal{P}) \mid X = x),
\]
which leads to \( \gamma_0(x) \geq \ell_0(x) \). Therefore, we conclude the proof of Proposition 4.4.

\[\square\]

B.9 Proofs of Proposition 5.1

Proof of Proposition 5.1. Recall that \( \Gamma^* \) is the smallest sensitivity parameter such that \( \mathbb{P}^{\text{sup}} \in \mathcal{P}(\Gamma^*) \). By the definition of \( \mathcal{R} \) in (29) and the nested property of the prediction sets, we know \( \mathcal{R} = \{1, \tilde{\Gamma}\} \) if \( C \cap \tilde{C}(X_{n+1}, 1) = \emptyset \), where
\[
\tilde{\Gamma} = \sup\{\Gamma \geq 1 : C \cap \tilde{C}(X_{n+1}, \gamma) = \emptyset\},
\]

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and $\mathcal{R} = \emptyset$ otherwise. Also, by the nested nature of $H_0(\Gamma)$, we know $H_0 = [\Gamma^*, \infty)$ when $Y_{n+1}(1) - Y_{n+1}(0) \in C$ and $H_0 = \emptyset$ otherwise. Hence

$$m_{\text{Err}} = \mathbb{P}(\mathcal{R} \cap H_0 \neq \emptyset)$$

$$= \mathbb{P}\left(\{Y_{n+1}(1) - Y_{n+1}(0) \in C\} \cap \{\exists \Gamma \geq \Gamma^*, C \cap \hat{C}(X_{n+1}, \Gamma) = \emptyset\}\right)$$

$$\leq \mathbb{P}\left(\{Y_{n+1}(1) - Y_{n+1}(0) \in C\} \cap \{C \cap \hat{C}(X_{n+1}, \Gamma^*) = \emptyset\}\right)$$

$$\leq \mathbb{P}(Y_{n+1}(1) - Y_{n+1}(0) \notin \hat{C}(X_{n+1}, \Gamma^*)).$$

Following exactly the same arguments, we have

$$d_{\text{Err}} = \mathbb{P}(\mathcal{R} \cap H_0 \neq \emptyset \mid D_{\text{calib}})$$

$$= \mathbb{P}\left(\{Y_{n+1}(1) - Y_{n+1}(0) \in C\} \cap \{\exists \Gamma \geq \Gamma^*, C \cap \hat{C}(X_{n+1}, \Gamma) = \emptyset\} \mid D_{\text{calib}}\right)$$

$$\leq \mathbb{P}\left(\{Y_{n+1}(1) - Y_{n+1}(0) \in C\} \cap \{C \cap \hat{C}(X_{n+1}, \Gamma^*) = \emptyset\} \mid D_{\text{calib}}\right)$$

$$\leq \mathbb{P}(Y_{n+1}(1) - Y_{n+1}(0) \notin \hat{C}(X_{n+1}, \Gamma^*) \mid D_{\text{calib}}),$$

completing the proof of Proposition 5.1.

\section*{C Additional simulation results}

\subsection*{C.1 Additional results for Section 3.3}

In this part, we provide additional simulation results on the counterfactual prediction task in Section 3.3.

![Figure 15: Empirical (average) coverage of Algorithm 1 when $\ell(\cdot)$ and $u(\cdot)$ are known. The details are otherwise the same as in Figure 3.](image)

\subsection*{C.2 Additional simulation results for Section 4.4}

In this part, we provide additional simulation results on the counterfactual prediction task in Section 4.4.
Figure 16: 0.05-th quantile of empirical coverage on test samples in Algorithm 2 when $\ell(\cdot), u(\cdot)$ are known. The details are otherwise the same as in Figure 5.

Figure 17: Empirical (average) coverage of Algorithm 2 when $\ell(\cdot)$ and $u(\cdot)$ are known. The details are otherwise the same as in Figure 5.
C.3 Additional results for Section 5.4

In this part, we collect the results in Section 5.4 of procedures with known bound functions.

Figure 19: Empirical FWER for fixed ITE (left) and random ITE (right) with Algorithm 1. The details are otherwise the same as in Figure 7.

Figure 20: Empirical FWER for fixed ITE (left) and random ITE (right) with Algorithm 2. The details are otherwise the same as in Figure 7.