
Conformal Off-Policy Prediction in Contextual Bandits

Muhammad Faaiz Taufiq*
Department of Statistics
University of Oxford

Jean-Francois Ton*†
AI-Lab-Research
Bytedance AI Lab

Rob Cornish
Department of Statistics
University of Oxford

Yee Whye Teh
Department of Statistics
University of Oxford

Arnaud Doucet
Department of Statistics
University of Oxford

Abstract

Most off-policy evaluation methods for contextual bandits have focused on the expected outcome of a policy, which is estimated via methods that at best provide only asymptotic guarantees. However, in many applications, the expectation may not be the best measure of performance as it does not capture the variability of the outcome. In addition, particularly in safety-critical settings, stronger guarantees than asymptotic correctness may be required. To address these limitations, we consider a novel application of conformal prediction to contextual bandits. Given data collected under a behavioral policy, we propose *conformal off-policy prediction* (COPP), which can output reliable predictive intervals for the outcome under a new target policy. We provide theoretical finite-sample guarantees without making any additional assumptions beyond the standard contextual bandit setup, and empirically demonstrate the utility of COPP compared with existing methods on synthetic and real-world data.

1 Introduction

Before deploying a decision-making policy to production, it is usually important to understand the plausible range of outcomes that it may produce. However, due to resource or ethical constraints, it is often not possible to obtain this understanding by testing the policy directly in the real-world. In such cases we have to rely on observational data collected under a different policy than the target. Using this observational data to evaluate the target policy is known as off-policy evaluation (OPE).

Traditionally, most techniques for OPE in contextual bandits focus on evaluating policies based on their **expected** outcomes; see e.g., Kuzborskij et al. [2021]; Wang et al. [2017]; Thomas et al. [2015]; Swaminathan and Joachims [2015a,b]; Dudík et al. [2014]. However, this can be problematic as methods that are only concerned with the average outcome do not take into account any notions of variance, for example. Therefore, in risk-sensitive settings such as econometrics, where we want to minimize the potential risks, metrics such as CVaR (Conditional Value at Risk) might be more appropriate [Keramati et al., 2020]. Additionally, when only small sample sizes of observational data are available, the average outcomes under finite data can be misleading, as they are prone to outliers and hence, metrics such as medians or quantiles are more robust in these scenarios [Altschuler et al., 2019].

Notable exceptions in the OPE literature are Huang et al. [2021]; Chandak et al. [2021]. Instead of estimating bounds on the expected outcomes, Huang et al. [2021]; Chandak et al. [2021] establish

*Denotes equal contribution, where ordering was determined through coin flip. Corresponding authors muhammad.taufiq@stats.ox.ac.uk and jeanfrancois@bytedance.com.

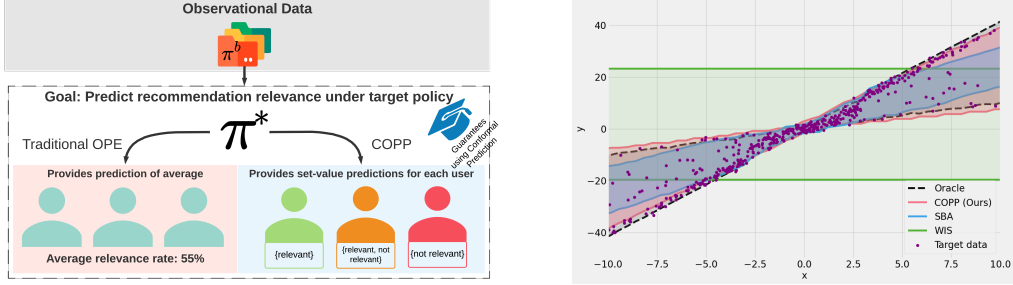


Figure 1: **Left (a):** Conformal Off-Policy Prediction against standard off-policy evaluation methods. **Right (b):** 90% predictive intervals for Y against X for COPP, competing methods and the oracle.

finite-sample bounds for a general class of metrics (e.g., Mean, CVaR, CDF) on the outcome. Their methods can be used to estimate quantiles of the outcomes under the target policy and are therefore robust to outliers. However, the resulting bounds do not depend on the covariates X (not adaptive w.r.t. X). This can lead to overly conservative intervals, as we will show in our experiments and can become uninformative when the data are heteroscedastic (see Fig. 1b).

In this paper, we propose Conformal Off-Policy Prediction (COPP), a novel algorithm that uses Conformal Prediction (CP) [Vovk et al., 2005] to construct predictive interval/sets for outcomes in contextual bandits (see Fig. 1a) using an observational dataset. COPP enjoys both finite-sample theoretical guarantees and adaptivity w.r.t. the covariates X , and, to the best of our knowledge, is the first such method based on CP that can be applied to stochastic policies and continuous action spaces.

In summary, our contributions are: (i) We propose an application of CP to construct predictive intervals for bandit outcomes that is more general (applies to stochastic policies and continuous actions) than previous work. (ii) We provide theoretical guarantees for COPP, including finite-sample guarantees on marginal coverage and asymptotic guarantees on conditional coverage. (iii) We show empirically that COPP outperforms standard methods in terms of coverage and predictive interval width when assessing new policies.

1.1 Problem Setup

Let \mathcal{X} be the covariate space (e.g., user data), \mathcal{A} the action space (e.g., recommended items) and \mathcal{Y} the outcome space (e.g., relevance to the user). We allow both \mathcal{A} and \mathcal{Y} to be either discrete or continuous. In our setting, we are given logged observational data $\mathcal{D}_{obs} = \{x_i, a_i, y_i\}_{i=1}^{n_{obs}}$ where actions are sampled from a behavioural policy π^b , i.e. $A \mid x \sim \pi^b(\cdot \mid x)$ and $Y \mid x, a \sim P(\cdot \mid x, a)$. We assume that we do not suffer from unmeasured confounding. At test time, we are given a state x^{test} and a new policy π^* . While π^b may be unknown, we assume the target policy π^* to be known.

We consider the task of rigorously quantifying the performance of π^* without any distributional assumptions on X or Y . Many existing approaches estimate $\mathbb{E}_{\pi^*}[Y]$, which is useful for comparing two policies directly as they return a single number. However, the expectation does not convey fine-grained information about how the policy performs for a specific value of X , nor does it account for the uncertainty in the outcome Y .

Here, we aim to construct intervals/sets on the outcome Y which are (i) adaptive w.r.t. X , (ii) capture the variability in the outcome Y and (iii) provide finite-sample guarantees. Current methods lack at least one of these properties (see Sec. 5). One way to achieve these properties is to construct a set-valued function of x , $\hat{C}(x)$ which outputs a *subset* of \mathcal{Y} . Given any finite dataset \mathcal{D}_{obs} , this subset is guaranteed to contain the true value of Y with any pre-specified probability, i.e.

$$1 - \alpha \leq \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (Y \in \hat{C}(X)) \leq 1 - \alpha + o_{n_{obs}}(1) \quad (1)$$

where n_{obs} is the size of available observational data and $P_{X,Y}^{\pi^*}$ is the joint distribution of (X, Y) under target policy π^* . In practice, $\hat{C}(x)$ can be used as a diagnostic tool downstream for a granular assessment of likely outcomes under a target policy. The probability in (1) is taken over the joint distribution of (X, Y) , meaning that (1) holds marginally in X (marginal coverage) and not for a given $X = x$ (conditional coverage). In Sec. 4.2, we provide additional regularity conditions under which

not only marginal but also conditional coverage holds. Next, we introduce the Conformal Prediction framework, which allows us to construct intervals $\hat{C}(x)$ that satisfy (1) along with properties (i)-(iii).

2 Background

Conformal prediction [Vovk et al., 2005; Shafer and Vovk, 2008] is a methodology that was originally used to compute distribution-free prediction sets for regression and classification tasks. Before introducing COPP, which applies CP to contextual bandits, we first illustrate how CP can be used in standard regression.

2.1 Standard Conformal Prediction

Consider the problem of regressing $Y \in \mathcal{Y}$ against $X \in \mathcal{X}$. Let \hat{f} be a model trained on the *training* data $\mathcal{D}_{tr} = \{X_i^0, Y_i^0\}_{i=1}^m \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}$ and let the *calibration* data $\mathcal{D}_{cal} = \{X_i, Y_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}$ be independent of \mathcal{D}_{tr} . Given a desired coverage rate $1 - \alpha \in (0, 1)$, we construct a band $\hat{C}_n : \mathcal{X} \rightarrow \{\text{subsets of } \mathcal{Y}\}$, based on the calibration data such that, for a new i.i.d. test data $(X, Y) \sim P_{X,Y}$,

$$1 - \alpha \leq \mathbb{P}_{(X,Y) \sim P_{X,Y}}(Y \in \hat{C}_n(X)) \leq 1 - \alpha + \frac{1}{n+1}, \quad (2)$$

where the probability is taken over X, Y and $\mathcal{D}_{cal} = \{X_i, Y_i\}_{i=1}^n$ and is conditional upon \mathcal{D}_{tr} .

In order to obtain \hat{C}_n satisfying (2), we introduce a non-conformity score function $V_i = s(X_i, Y_i)$, e.g., $(\hat{f}(X_i) - Y_i)^2$. We assume here $\{V_i\}_{i=1}^n$ have no ties almost surely. Intuitively, the non-conformity score V_i uses the outputs of the predictive model \hat{f} on the calibration data, to measure how far off these predictions are from the ground truth response. Higher scores correspond to worse fit between x and y according to \hat{f} . We define the empirical distribution of the scores $\{V_i\}_{i=1}^n \cup \{\infty\}$

$$\hat{F}_n := \frac{1}{n+1} \sum_{i=1}^n \delta_{V_i} + \frac{1}{n+1} \delta_{\infty} \quad (3)$$

with which we can subsequently construct the conformal interval \hat{C}_n that satisfies (2) as follows:

$$\hat{C}_n(x) := \{y : s(x, y) \leq \eta\} \quad (4)$$

where η is an empirical quantile of $\{V_i\}_{i=1}^n$, i.e. $\eta = \text{Quantile}_{1-\alpha}(\hat{F}_n)$ is the $1 - \alpha$ quantile.

Intuitively, for roughly $100 \cdot (1 - \alpha)\%$ of the calibration data, the score values will be below η . Therefore, if the new datapoint (X, Y) and \mathcal{D}_{cal} are i.i.d., the probability $\mathbb{P}(s(X, Y) \leq \eta)$ (which is equal to $\mathbb{P}(Y \in \hat{C}_n(X))$ by (4)) will be roughly $1 - \alpha$. Exchangeability of the data is crucial for the above to hold. In the next section we will explain how Tibshirani et al. [2019] relax the exchangeability assumption.

2.2 Conformal Prediction under covariate shift

Tibshirani et al. [2019] extend the CP framework beyond the setting of exchangeable data, by constructing valid intervals even when the calibration data and test data are not drawn from the same distribution. The authors focus on the *covariate shift* scenario i.e. the distribution of the covariates changes at test time:

$$\begin{aligned} (X_i, Y_i) &\stackrel{\text{i.i.d.}}{\sim} P_{X,Y} = P_X \times P_{Y|X}, \quad i = 1, \dots, n \\ (X, Y) &\sim \tilde{P}_{X,Y} = \tilde{P}_X \times P_{Y|X}, \text{ independently} \end{aligned}$$

where the ratio $w(x) := d\tilde{P}_X/dP_X(x)$ is known. The key realization in Tibshirani et al. [2019] is that the requirement of *exchangeability* in CP can be relaxed to a more general property, namely *weighted exchangeability* (see Def. A.1). They propose a weighted version of conformal prediction, which shifts the empirical distribution of non-conformity scores, \hat{F}_n , at a point x , using weights $w(x)$. This adjusts \hat{F}_n for the covariate shift, before picking the quantile η :

$$\hat{F}_n^x := \sum_{i=1}^n p_i^w(x) \delta_{V_i} + p_{n+1}^w(x) \delta_{\infty} \quad \text{where,}$$

$$p_i^w(x) = \frac{w(X_i)}{\sum_{j=1}^n w(X_j) + w(x)}, p_{n+1}^w(x) = \frac{w(x)}{\sum_{j=1}^n w(X_j) + w(x)}.$$

In standard CP (without covariate shift), the weight function satisfies $w(x) = 1$ for all x , and we recover (3). Next, we construct the conformal prediction intervals \hat{C}_n as in standard CP using (4) where η now depends on x due to $p_i^w(x)$. The resulting intervals, \hat{C}_n , satisfy:

$$\mathbb{P}_{(X,Y) \sim \tilde{P}_{X,Y}}(Y \in \hat{C}_n(X)) \geq 1 - \alpha$$

As mentioned previously in Sec. 1.1, the above demonstrates marginal coverage guarantees over test point X and calibration dataset \mathcal{D}_{cal} , not conditional on a given $X = x$ or a fixed \mathcal{D}_{cal} . We will discuss this nuance later on in Sec. 4.2. In addition, previous work by Vovk shows that conditioned on a single calibration dataset, standard CP can achieve coverage that is ‘close’ to the required coverage with high probability. However, this has not been extended to the case where the distribution shifts. This is out of the scope of this paper and an interesting future direction.

Algorithm 1: Conformal Off-Policy Prediction (COPP)

Inputs: Observational data $\mathcal{D}_{obs} = \{X_i, A_i, Y_i\}_{i=1}^{n_{obs}}$, conf. level α , a score function $s(x, y) \in \mathbb{R}$, new data point x^{test} , target policy π^* ;

Output: Predictive interval $\hat{C}_n(x^{test})$;

Split \mathcal{D}_{obs} into training data (\mathcal{D}_{tr}) and calibration data (\mathcal{D}_{cal}) of sizes m and n respectively;

Use \mathcal{D}_{tr} to estimate weights $\hat{w}(\cdot, \cdot)$ using (7);

Compute $V_i := s(X_i, Y_i)$ for $(X_i, A_i, Y_i) \in \mathcal{D}_{cal}$;

Let $\hat{F}_n^{x,y}$ be the weighted distribution of scores $\hat{F}_n^{x,y} := \sum_{i=1}^n p_i^{\hat{w}}(x, y) \delta_{V_i} + p_{n+1}^{\hat{w}}(x, y) \delta_\infty$

where $p_i^{\hat{w}}(x, y) = \frac{\hat{w}(X_i, Y_i)}{\sum_{j=1}^n \hat{w}(X_j, Y_j) + \hat{w}(x, y)}$ and $p_{n+1}^{\hat{w}}(x, y) = \frac{\hat{w}(x, y)}{\sum_{j=1}^n \hat{w}(X_j, Y_j) + \hat{w}(x, y)}$;

For x^{test} construct: $\hat{C}_n(x^{test}) := \{y : s(x^{test}, y) \leq \text{Quantile}_{1-\alpha}(\hat{F}_n^{x^{test}, y})\}$

Return $\hat{C}_n(x^{test})$

Thus Tibshirani et al. [2019] show that the CP algorithm can be extended to the setting of covariate shift with the resulting predictive intervals satisfying the coverage guarantees when the weights are known. The extension of these results to approximate weights was proposed in Lei and Candès [2021] and is generalized to our setting in Sec. 4.

3 Conformal Off-Policy Prediction (COPP)

In the contextual bandits introduced in Sec. 1.1, we assume that the observational data $\mathcal{D}_{obs} = \{x_i, a_i, y_i\}_{i=1}^{n_{obs}}$ is generated from a behavioural policy π^b . At inference time we are given a new target policy π^* and want to provide intervals on the outcomes Y for covariates X that satisfy (1).

The key insight of our approach is to consider the following joint distribution of (X, Y) :

$$\begin{aligned} P^{\pi^b}(x, y) &= P(x) \int P(y|x, a) \pi^b(a|x) da = P(x) P^{\pi^b}(y|x) \\ P^{\pi^*}(x, y) &= P(x) \int P(y|x, a) \pi^*(a|x) da = P(x) P^{\pi^*}(y|x) \end{aligned}$$

Therefore, the change of policies from π^b to π^* causes a shift in the joint distributions of (X, Y) from $P_{X,Y}^{\pi^b}$ to $P_{X,Y}^{\pi^*}$. More precisely, a shift in the conditional distribution of $Y|X$. As a result, our problem boils down to using CP in the setting where the conditional distribution $P_{Y|X}^{\pi^b}$ changes to $P_{Y|X}^{\pi^*}$ due to the different policies, while the covariate distribution P_X remains the same.

Hence our problem is not concerned about covariate shift as addressed in Tibshirani et al. [2019], but instead uses the idea of *weighted exchangeability* to extend CP to the setting of policy shift. To account for this distributional mismatch, our method shifts the empirical distribution of non-conformity scores

at a point (x, y) using the weights $w(x, y) = dP_{X,Y}^{\pi^*} / dP_{X,Y}^{\pi^b}(x, y) = dP_{Y|X}^{\pi^*} / dP_{Y|X}^{\pi^b}(x, y)$:

$$\hat{F}_n^{x,y} := \sum_{i=1}^n p_i^w(x, y) \delta_{V_i} + p_{n+1}^w(x, y) \delta_{\infty}, \quad (5)$$

$$p_i^w(x, y) = \frac{w(X_i, Y_i)}{\sum_{j=1}^n w(X_j, Y_j) + w(x, y)}, p_{n+1}^w(x, y) = \frac{w(x, y)}{\sum_{j=1}^n w(X_j, Y_j) + w(x, y)}.$$

The intervals are then constructed as below which we call Conformal Off-Policy Prediction (Alg. 1).

$$\hat{C}_n(x^{test}) := \{y : s(x^{test}, y) \leq \eta(x^{test}, y)\} \text{ where } \eta(x, y) := \text{Quantile}_{1-\alpha}(\hat{F}_n^{x,y}). \quad (6)$$

Remark. The weights $w(x, y)$ in (5) depend on x and y , as opposed to only x . In particular, finding the set of y 's satisfying (6) becomes more complicated than for the standard covariate shifted CP which only requires a single computation of $\eta(x)$ for a given x as shown in (4). In our case however, we have to create a k sized grid of potential values of y for every x to find $\hat{C}_n(x)$. This operation is embarrassingly parallel and hence does not add much computational overhead compared to the standard CP, especially because CP mainly focuses on scalar predictions.

3.1 Estimation of weights $w(x, y)$

So far we have been assuming that we know the weights $w(x, y)$ exactly. However, in most real-world settings, this will not be the case. Therefore, we must resort to estimating $w(x, y)$ using observational data. In order to do so, we first split the observational data into training (\mathcal{D}_{tr}) and calibration (\mathcal{D}_{cal}) data. Next, using \mathcal{D}_{tr} , we estimate $\hat{\pi}^b(a | x) \approx \pi^b(a | x)$ and $\hat{P}(y | x, a) \approx P(y | x, a)$ (which is independent of the policy). We then compute a Monte Carlo estimate of weights using the following:

$$\hat{w}(x, y) = \frac{\frac{1}{h} \sum_{k=1}^h \hat{P}(y|x, A_k^*)}{\frac{1}{h} \sum_{k=1}^h \hat{P}(y|x, A_k)} \approx \frac{\int P(y|x, a) \pi^*(a|x) da}{\int P(y|x, a) \pi^b(a|x) da}, \quad (7)$$

where $A_k \sim \hat{\pi}^b(\cdot | x)$, $A_k^* \sim \pi^*(\cdot | x)$ and h is the number of Monte Carlo samples.

Why not construct intervals using $\hat{P}(y|x, a)$ directly? We could directly construct predictive intervals $\hat{C}_n(x)$ over outcomes by sampling $Y_j \stackrel{\text{i.i.d.}}{\sim} \hat{P}^{\pi^*}(y|x) = \int \hat{P}(y|x, a) \pi^*(a|x) da$. However, the coverage of these intervals directly depends on the estimation error of $\hat{P}(y|x, a)$. This is not the case in COPP, as the coverage does not depend on $\hat{P}(y|x, a)$ directly but rather on the estimation of $\hat{w}(x, y)$ (see Prop. 4.2). We hypothesize that this indirect dependence of COPP on $\hat{P}(y|x, a)$ makes it less sensitive to the estimation error. In Sec. 6, our empirical results support this hypothesis as COPP provides more accurate coverage than directly using $\hat{P}(y|x, a)$ to construct intervals. Lastly, in Appendix B.5.2 we show how we can avoid estimating $\hat{P}(y|x, a)$ by proposing an alternative method for estimating the weights directly. We leave this for future work.

4 Theoretical Guarantees

4.1 Marginal Coverage

In this section we provide theoretical guarantees on marginal coverage $\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n(X))$ for the cases where the weights $w(x, y)$ are known exactly as well as when they are estimated. Using the idea of *weighted exchangeability*, we extend [Tibshirani et al., 2019, Theorem 2] to our setting.

Proposition 4.1. *Let $\{X_i, Y_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}^{\pi^b}$ be the calibration data. For any score function s , and any $\alpha \in (0, 1)$, define the conformal predictive interval at a point $x \in \mathbb{R}^d$ as $\hat{C}_n(x) := \{y \in \mathbb{R} : s(x, y) \leq \eta(x, y)\}$ where $\eta(x, y) := \text{Quantile}_{1-\alpha}(\hat{F}_n^{x,y})$, and $\hat{F}_n^{x,y}$ is as defined in (5) with exact weights $w(x, y)$. If $P^{\pi^*}(y|x)$ is absolutely continuous w.r.t. $P^{\pi^b}(y|x)$, then \hat{C}_n satisfies $\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n(X)) \geq 1 - \alpha$.*

Proposition 4.1 assumes exact weights $w(x, y)$, which is usually not the case. For CP under covariate shift, Lei and Candès [2021] showed that even when the weights are approximated, i.e., $\hat{w}(x, y) \neq w(x, y)$, we can still provide finite-sample upper and lower bounds on the coverage, albeit slightly modified with an error term Δ_w (see (8)). We show that this result can be extended to our setting when the weight function $w(x, y)$ is approximated as in Sec. 3.1.

Proposition 4.2. *Let \hat{C}_n be the conformal predictive intervals obtained as in Proposition 4.1, with weights $w(x, y)$ replaced by approximate weights $\hat{w}(x, y) = \hat{w}(x, y; \mathcal{D}_{tr})$, where the training data, \mathcal{D}_{tr} , is fixed. Assume that $\hat{w}(x, y)$ satisfies $(\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [\hat{w}(X, Y)^r])^{1/r} \leq M_r < \infty$ for some $r \geq 2$. Define Δ_w as,*

$$\Delta_w := \frac{1}{2} \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} | \hat{w}(X, Y) - w(X, Y) |. \quad (8)$$

$$\text{Then, } \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (Y \in \hat{C}_n(X)) \geq 1 - \alpha - \Delta_w.$$

If, in addition, non-conformity scores $\{V_i\}_{i=1}^n$ have no ties almost surely, then we also have

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (Y \in \hat{C}_n(X)) \leq 1 - \alpha + \Delta_w + cn^{1/r-1},$$

for some positive constant c depending only on M_r and r .

Proposition 4.2 provides finite-sample guarantees with approximate weights $\hat{w}(\cdot, \cdot)$. Note that if the weights are known exactly then the above proposition can be simplified by setting $\Delta_w = 0$. In the case where the weight function is estimated consistently, we recover the exact coverage asymptotically. A natural question to ask is whether the consistency of $\hat{w}(x, y)$ implies the consistency of $\hat{P}(y|x, a)$; in which case one could use $\hat{P}(y|x, a)$ directly to construct the intervals. We prove that this is not the case in general and provide detailed discussion in Appendix B.5.

4.2 Conditional Coverage

So far we only considered marginal coverage (1), where the probability is over both X and Y . Here, we provide results on conditional coverage $\mathbb{P}_{Y \sim P_{Y|X}^{\pi^*}} (Y \in \hat{C}_n(X) \mid X)$ which is a strictly stronger notion of coverage than marginal coverage [Foygel Barber et al., 2021]. Vovk [2012]; Lei and Wasserman [2014] prove that exact conditional coverage cannot be achieved without making additional assumptions. However, we show that, in the case where Y is a continuous random variable and we can estimate the quantiles of $P_{Y|X}^{\pi^*}$ consistently, we get an approximate conditional coverage guarantee using the below proposition.

Proposition 4.3 (Asymptotic Conditional Coverage). *Let m, n be the number of training and calibration data respectively, $\hat{q}_{\beta, m}(x) = \hat{q}_{\beta, m}(x; \mathcal{D}_{tr})$ be an estimate of the β -th conditional quantile $q_{\beta}(x)$ of $P_{Y|X=x}^{\pi^*}$, $\hat{w}_m(x, y) = \hat{w}_m(x, y; \mathcal{D}_{tr})$ be an estimate of $w(x, y)$ and $\hat{C}_{m, n}(x)$ be the conformal interval resulting from algorithm 1 with score function $s(x, y) = \max\{y - \hat{q}_{\alpha_{hi}}(x), \hat{q}_{\alpha_{lo}}(x) - y\}$ where $\alpha_{hi} - \alpha_{lo} = 1 - \alpha$. Assume that the following hold:*

1. $\lim_{m \rightarrow \infty} \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} |\hat{w}_m(X, Y) - w(X, Y)| = 0$.
2. *there exists $r, b_1, b_2 > 0$ such that $P^{\pi^*}(y \mid x) \in [b_1, b_2]$ uniformly over all (x, y) with $y \in [q_{\alpha_{lo}}(x) - r, q_{\alpha_{lo}}(x) + r] \cup [q_{\alpha_{hi}}(x) - r, q_{\alpha_{hi}}(x) + r]$,*
3. $\exists k > 0$ s.t. $\lim_{m \rightarrow \infty} \mathbb{E}_{X \sim P_X} [H_m^k(X)] = 0$ where $H_m(x) = \max\{|\hat{q}_{\alpha_{lo}, m}(x) - q_{\alpha_{lo}}(x)|, |\hat{q}_{\alpha_{hi}, m}(x) - q_{\alpha_{hi}}(x)|\}$

Then for any $t > 0$, we have that $\lim_{m, n \rightarrow \infty} \mathbb{P}_{Y \sim P_{Y|X}^{\pi^*}} (Y \in \hat{C}_{m, n}(X) \mid X) \leq 1 - \alpha - t = 0$.

Remark. One caveat of Prop. 4.3 is that Assumption 3 is rather strong. In general, consistently estimating the quantiles under the target policy π^* is not straightforward given that we only have access to observational data from π^b . While one can use a weighted pinball loss to estimate quantiles under π^* , consistent estimation of these quantiles would require a consistent estimate of the weights (see Appendix C). Hence, unlike [Lei and Candès, 2021, Theorem 1], our Prop. 4.3 is not a “doubly robust” result.

Towards Group Balanced Coverage. As pointed out by Angelopoulos and Bates [2021], we may want predictive intervals that have the same coverage across different groups, e.g., across male and female users [Romano et al., 2020]. Standard CP will not necessarily achieve this, as the coverage guarantee (1) is over the entire population of users. However, we can use COPP on each subgroup separately to obtain group balanced coverage. A more detailed discussion on how to construct such intervals has been included in Appendix B.4.

5 Related Work

Conformal Prediction: A number of works have explored the use of CP under distribution shift. The works of Tibshirani et al. [2019] and Lei and Candès [2021] are particularly notable as they extend CP to the general setting of *weighted exchangeability*. In particular, Lei and Candès [2021] use CP for counterfactual inference where the goal is to obtain predictive intervals on the outcomes of treatment and control groups. The authors formulate the counterfactual setting into that of covariate shift in the input space \mathcal{X} and show that under certain assumptions, finite-sample coverage can be guaranteed.

Fundamentally, our work differs from Lei and Candès [2021] by framing the problem as a shift in the conditional $P_{Y|X}$ rather than as a shift in the marginal P_X . The resulting methodology we obtain from this then differs from Lei and Candès [2021] in a variety of ways. For example, while Lei and Candès [2021] assume a deterministic target policy, COPP can also be applied to stochastic target policies, which have been used in a variety of applications, such as recommendation systems or RL applications [Swaminathan et al., 2017; Su et al., 2020; Farajtabar et al., 2018]. Likewise, unlike Lei and Candès [2021], COPP is applicable to continuous action spaces, e.g., doses of medication administered.

In addition, when the target policy is deterministic, there is an important methodological difference between COPP and Lei and Candès [2021]. In particular, Lei and Candès [2021] construct the intervals on outcomes by splitting calibration data w.r.t. actions. In contrast, it can be shown that COPP uses the entire calibration data when constructing intervals on outcomes. This is a consequence of integrating out the actions in the weights $w(x, y)$ (7), and empirically leads to smaller variance in coverage compared to Lei and Candès [2021]. See B.1 for the experimental results comparing COPP to Lei and Candès [2021] for deterministic policies.

Osama et al. [2020] propose using CP to *construct* robust policies in contextual bandits with discrete actions. Their methodology uses CP to choose actions and does not involve evaluating target policies. Hence, the problem being considered is orthogonal to ours. There has also been concurrent work adapting CP to individual treatment effect (ITE) sensitivity analysis model [Jin et al., 2021; Yin et al., 2021]. Similar to our approach, these works formulate the sensitivity analysis problem as one of CP under the joint distribution shift $P_{X,Y}$. While our methodologies are related, the application of CP explored in these works, i.e. ITE estimation under unobserved confounding, is fundamentally different.

Uncertainty in contextual bandits: Recall from the introduction, that most works in this area have focused on quantifying uncertainty in expected outcome (policy value) [Dudík et al., 2014; Kuzborskij et al., 2021]. Despite providing finite sample-guarantees on the expectation, these methods do not account for the variability in the outcome itself and in general are not adaptive w.r.t. X , i.e. they do not satisfy properties (i), (ii) from Sec. 1.1. Huang et al. [2021]; Chandak et al. [2021] on the other hand, propose off-policy assessment algorithms for contextual bandits w.r.t. a more general class of risk objectives such as Mean, CVaR etc. Their methodologies can be applied to our problem, to construct predictive intervals for off-policy outcomes. However, unlike COPP, these intervals are not adaptive w.r.t. X , i.e. do not satisfy property (i) in Sec. 1.1. Moreover, they do not provide upper bounds on coverage probability, which often leads to overly conservative intervals, as shown in our experiments. Lastly, while distributional perspective has been explored in reinforcement learning [Bellemare et al., 2017], no finite sample-guarantees are available to the best of our knowledge.

6 Experiments

Baselines for comparison. Given our problem setup, there are no established baselines. Instead, we compare our proposed method COPP to the following competing methods, which were constructed to capture the uncertainty in the outcome distribution and take into account the policy shift.

Table 1: Toy experiment results with required coverage 90%. While WIS intervals provide required coverage, the mean interval length is huge compared to COPP (see table 1b).

(a) Mean Coverage as a function of policy shift with 2 standard errors over 10 runs.

Coverage	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$
COPP (Ours)	0.90 \pm 0.01	0.90 \pm 0.01	0.91 \pm 0.01
WIS	0.89 \pm 0.01	0.91 \pm 0.02	0.94 \pm 0.02
SBA	0.90 \pm 0.01	0.88 \pm 0.01	0.87 \pm 0.01
COPP (GT weights Ours)	0.90 \pm 0.01	0.90 \pm 0.01	0.90 \pm 0.01
CP (no policy shift)	0.90 \pm 0.01	0.87 \pm 0.01	0.85 \pm 0.01
CP (union)	0.96 \pm 0.01	0.96 \pm 0.01	0.96 \pm 0.01

(b) Mean Interval Length as a function of policy shift with 2 standard errors over 10 runs.

Interval Lengths	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$
COPP (Ours)	9.08 \pm 0.10	9.48 \pm 0.22	9.97 \pm 0.38
WIS	24.14 \pm 0.30	32.96 \pm 1.80	43.12 \pm 3.49
SBA	8.78 \pm 0.12	8.94 \pm 0.10	8.33 \pm 0.09
COPP (GT weights Ours)	8.91 \pm 0.09	9.25 \pm 0.12	9.59 \pm 0.20
CP (no policy shift)	9.00 \pm 0.10	9.00 \pm 0.10	9.00 \pm 0.10
CP (union)	10.66 \pm 0.18	11.04 \pm 0.2	11.4 \pm 0.26

Weighted Importance Sampling (WIS) CDF estimator. Given observational dataset $\mathcal{D}_{obs} = \{x_i, a_i, y_i\}_{i=1}^{n_{obs}}$, Huang et al. [2021] proposed a non-parametric WIS-based estimator for the empirical CDF of Y under π^* , $\hat{F}_{WIS}(t) := \frac{\sum_{i=1}^{n_{obs}} \hat{\rho}(a_i, x_i) \mathbb{1}(y_i \leq t)}{\sum_{i=1}^{n_{obs}} \hat{\rho}(a_i, x_i)}$ where $\hat{\rho}(a, x) := \frac{\pi^*(a|x)}{\hat{\pi}^b(a|x)}$ are the importance weights. We can use \hat{F}_{WIS} to get predictive intervals $[y_{\alpha/2}, y_{1-\alpha/2}]$ where $y_\beta := \text{Quantile}_\beta(\hat{F}_{WIS})$. The intervals $[y_{\alpha/2}, y_{1-\alpha/2}]$ do not depend on x .

Sampling Based Approach (SBA). As mentioned in Sec. 3.1, we can directly use the estimated $\hat{P}(y | x, a)$ to construct the predictive intervals as follows. For a given x^{test} , we generate $A_i \stackrel{\text{i.i.d.}}{\sim} \pi^*(\cdot | x^{test})$, and $Y_i \sim \hat{P}(\cdot | x^{test}, A_i)$ for $i \leq \ell$. We then define the predictive intervals for x^{test} using the $\alpha/2$ and $1 - \alpha/2$ quantiles of $\{Y_i\}_{i \leq \ell}$. While SBA is not a standard baseline, it is a natural comparison to make to answer the question of “why not construct the intervals using $\hat{P}(y|x, a)$ directly”?

6.1 Toy Experiment

We start with synthetic experiments and an ablation study, in order to dissect and understand our proposed methodology in more detail. We assume that our policies are stationary and there is overlap between the behaviour and target policy, both of which are standard assumptions [Huang et al., 2021; Su et al., 2019; Xie et al., 2019].

6.1.1 Synthetic data experiments setup

In order to understand how COPP works, we construct a simple experimental setup where we can control the amount of “policy shift” and know the ground truth. In this experiment, $X \in \mathbb{R}$, $A \in \{1, 2, 3, 4\}$ and $Y \in \mathbb{R}$, where X and $Y | x, a$ are normal random variables. Further details and additional experiments on continuous action spaces are given in Appendix D.1.

Behaviour and Target Policies. We define a family of policies $\pi_\epsilon(a | x)$, where we use the parameter $\epsilon \in (0, 1/3)$ to control the policy shift between target and behaviour policies. Exact form of $\pi_\epsilon(a | x)$ is given in D.1. For the behaviour policy π^b , we use $\epsilon^b = 0.3$ (i.e. $\pi^b(a | x) \equiv \pi_{0.3}(a | x)$), and for target policies π^* , we use $\epsilon^* \in \{0.1, 0.2, 0.3\}$. Using the true behaviour policy, π^b , we generate observational data $\mathcal{D}_{obs} = \{x_i, a_i, y_i\}_{i=1}^{n_{obs}}$ which is then split into training (\mathcal{D}_{tr}) and calibration (\mathcal{D}_{cal}) datasets, of sizes m and n respectively.

Estimation of ratios, $\hat{w}(x, y)$. Using the training dataset \mathcal{D}_{tr} , we estimate $P(y|x, a)$ as $\hat{P}(y|x, a) = \mathcal{N}(\mu(x, a), \sigma(x, a))$, where $\mu(x, a), \sigma(x, a)$ are both neural networks (NNs). Similarly, we use NNs to estimate the behaviour policy $\hat{\pi}^b$ from \mathcal{D}_{tr} . Next, to estimate $\hat{w}(x, y)$, we use (7) with $h = 500$.

Score. For the score function, we use the same formulation as in Romano et al. [2019], i.e. $s(x, y) = \max\{\hat{q}_{\alpha_{lo}}(x) - y, y - \hat{q}_{\alpha_{hi}}(x)\}$, where $\hat{q}_\beta(x)$ denotes the β quantile estimate of $P_{Y|X=x}^{\pi^b}$ trained using pinball loss.

Lastly, our weights $w(x, y)$ depend on x and y and hence we use a grid of 100 equally spaced out y ’s in our experiments to determine the predictive interval which satisfies $\hat{C}_n(x) := \{y : s(x, y) \leq \text{Quantile}_{1-\alpha}(\hat{F}_n^{x,y})\}$. This is parallelizable and hence does not add much computational overhead.

Results. Table 1a shows the coverages of different methods as the policy shift $\Delta_\epsilon = \epsilon^b - \epsilon^*$ increases. The behaviour policy $\pi^b = \pi_{0.3}$ is fixed and we use $n = 5000$ calibration datapoints, across 10 runs.

Table 2: Mean Coverage as a function of policy shift Δ_ϵ and 2 standard errors over 10 runs. COPP attains the required coverage of 90%, whereas the competing methods, WIS and SBA, are over-conservative i.e. coverage above 90%. In addition, when we do not account for the policy shift, standard CP becomes progressively worse with increasing policy shift.

	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$	$\Delta_\epsilon = 0.3$	$\Delta_\epsilon = 0.4$
COPP (Ours)	0.90 ± 0.00	0.90 ± 0.02	0.90 ± 0.01	0.89 ± 0.01	0.91 ± 0.01
WIS	1.00 ± 0.00	1.00 ± 0.00	0.92 ± 0.00	0.94 ± 0.00	0.91 ± 0.00
SBA	0.99 ± 0.00	0.99 ± 0.00	0.98 ± 0.00	0.97 ± 0.00	0.96 ± 0.00
CP (no policy shift)	0.91 ± 0.02	0.92 ± 0.02	0.93 ± 0.01	0.94 ± 0.01	0.96 ± 0.01

Table 1a shows, how COPP stays very close to the required coverage of 90% across all target policies compared to WIS and SBA. WIS intervals are overly conservative i.e. above the required coverage, while the SBA intervals suffer from under-coverage i.e. below the required coverage. These results supports our hypothesis from Sec. 3.1, which stated that COPP is less sensitive to estimation errors of $\hat{P}(y|x, a)$ compared to directly using $\hat{P}(y|x, a)$ for the intervals, i.e. SBA.

Next, Table 1b shows the mean interval lengths and even though WIS has reasonable coverage for $\Delta_\epsilon = 0.0$ and 0.1 , the average interval length is huge compared to COPP. Fig. 1b shows the predictive intervals for one such experiment with $\pi^* = \pi_{0.1}$ and $\pi^b = \pi_{0.3}$. We can see that SBA intervals are overly optimistic, while WIS intervals are too wide and are not adaptive w.r.t. X . COPP produces intervals which are much closer to the oracle intervals.

6.1.2 Ablation Study.

To isolate the effect of weight estimation error and policy shift, we conduct an ablation study, comparing COPP with estimated weights to COPP with Ground Truth (GT) weights and standard CP (assuming no policy shift). Table 1a shows that at $\Delta_\epsilon = 0$, i.e. no policy shift, standard CP achieves the required coverage as expected. However the coverage of standard CP intervals decreases as the policy shift Δ_ϵ increases. COPP, on the other hand, attains the required coverage of 90%, by adapting the predictive intervals with increasing policy shift. Table 1b shows that the average interval length of COPP increases with increasing policy shift Δ_ϵ . Furthermore, Table 1a illustrates that while COPP achieves the required coverage for different target policies, on average it is slightly more conservative than using COPP with GT weights. This can be explained by the estimation error in $\hat{w}(x, y)$. Additionally, to investigate the effect of integrating out the actions in (7), we also perform CP for each action a separately (as in Lei and Candès [2021]) and then take the union of the intervals across these actions. In the union method, the probability of an action being chosen is not taken into account, (i.e., intervals are independent of π^*) and hence the coverage is overly conservative as expected.

Lastly, we investigate how increasing the number of calibration data n affects the coverage for all the methodologies. We observe that coverage of COPP is closer to the required coverage of 90% compared to the competing methodologies. Additionally, the coverage of COPP converges to the required coverage as n increases; see Appendix D.1.1 for detailed experimental results.

6.2 Experiments on Microsoft Ranking Dataset

We now apply COPP onto a real dataset i.e. the Microsoft Ranking dataset 30k [Qin and Liu, 2013; Swaminathan et al., 2017; Bietti et al., 2018]. Due to space constraints, we have added additional extensive experiments on UCI datasets in Appendix D.3.

Dataset. The dataset contains relevance scores for websites recommended to different users, and comprises of 30,000 user-website pairs. For each user-website pair, the data contains a 136-dimensional feature vector, which consists of user’s attributes corresponding to the website, such as length of stay or number of clicks on the website. Furthermore, for each user-website pair, the dataset also contains a relevance score, i.e. how relevant the website was to the user.

First, given a user, we sample (with replacement) 5 websites from the data corresponding to that user. Next, we reformulate this into a contextual bandit where $a_i \in \{1, 2, 3, 4, 5\}$ corresponds to the action of recommending the a_i ’th website to the user i . x_i is obtained by combining the 5 user-website feature vectors corresponding to the user i i.e. $x_i \in \mathbb{R}^{5 \times 136}$. $y_i \in \{0, 1, 2, 3, 4\}$ corresponds to

the relevance score for the a_i 'th website, i.e. the recommended website. The goal is to construct prediction sets that are guaranteed to contain the true relevance score with a probability of 90%.

Behaviour and Target Policies. We first train a NN classifier model, \hat{f}_θ , mapping each 136-dimensional user-website feature vector to the softmax scores for each relevance score class. We use this trained model \hat{f}_θ to define a family of policies which pick the most relevant website as predicted by \hat{f}_θ with probability ϵ and the rest uniformly with probability $(1 - \epsilon)/4$ (see Appendix D.2 for more details). Like the previous experiment, we use ϵ to control the shift between behaviour and target policies. For π^b , we use $\epsilon^b = 0.5$ and for π^* , $\epsilon^* \in \{0.1, 0.2, 0.3, 0.4, 0.5\}$.

Estimation of ratios $\hat{w}(X, Y)$. To estimate the $\hat{P}(y | x, a)$ we use the trained model \hat{f}_θ as detailed in Appendix D.2. To estimate the behaviour policy $\hat{\pi}^b$, we train a neural network classifier model $\mathcal{X} \rightarrow \mathcal{A}$, and we use (7) to estimate the weights $\hat{w}(x, y)$.

Score. The space of outcomes \mathcal{Y} in this experiment is discrete. We define $\hat{P}^{\pi^b}(y | x) = \sum_{i=1}^5 \hat{\pi}^b(A = i | x) \hat{P}(y | x, A = i)$. Using similar formulation as in Angelopoulos and Bates [2021], we define the score:

$$s(x, y) = \sum_{y'=0}^4 \hat{P}^{\pi^b}(y' | x) \mathbb{1}(\hat{P}^{\pi^b}(y' | x) \geq \hat{P}^{\pi^b}(y | x)).$$

Since \mathcal{Y} is discrete, we no longer need to construct a grid of y values on which to compute $\text{Quantile}_{1-\alpha}(\hat{F}_n^{x,y})$. Instead, we will simply compute this quantity on each $y \in \mathcal{Y}$, when constructing the predictive sets $\hat{C}_n(x^{test})$.

Results. Table 2 shows the coverages of different methodologies across varying target policies π_{ϵ^*} . The behaviour policy $\pi^b = \pi_{0.5}$ is fixed and we use $n = 5000$ calibration datapoints, across 10 runs. Table 2 also shows that the coverage of WIS and SBA sets is dependent upon the policy shift, with both being overly conservative across the different target policies as compared to COPP. Recall that the WIS sets do not depend on x^{test} and as a result we get the same set for each test data point. This becomes even more problematic when Y is discrete – if, for each label y , $\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y = y) > 10\%$, then WIS sets (with the required coverage of 90%) are likely to contain every label $y \in \mathcal{Y}$. In comparison, COPP is able to stay much closer to the required coverage of 90% across all target policies. We have also added standard CP without policy shift as a sanity check, and observed that the sets get increasingly conservative as the policy shift increases.

Finally, we also plotted how the coverage changes as the number of calibration data n increases. We observe again that the coverage of COPP is closer to the required coverage of 90% compared to the competing methodologies. Due to space constraints, we have added the plots in Appendix D.2.

Class-balanced conformal prediction. Using the methodology described in Sec. 4.2, we construct predictive sets, $\hat{C}_n^{\mathcal{Y}}(x)$, which offer label conditioned coverage guarantees (see B.4), i.e. for all $y \in \mathcal{Y}$,

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n^{\mathcal{Y}}(X) | Y = y) \geq 1 - \alpha.$$

We empirically demonstrate that $\hat{C}_n^{\mathcal{Y}}$ provides label conditional coverage, while \hat{C}_n obtained using alg. 1 may not. Due to space constraints, details on construction of $\hat{C}_n^{\mathcal{Y}}$ as well as experimental results have been included in Appendix D.2.1.

7 Conclusion and Limitations

In this paper, we propose COPP, an algorithm for constructing predictive intervals on off-policy outcomes, which are adaptive w.r.t. covariates X . We theoretically prove that COPP can guarantee finite-sample coverage by adapting the framework of conformal prediction to our setup. Our experiments show that conventional methods cannot guarantee any user pre-specified coverage, whereas COPP can. For future work, it would be interesting to apply COPP to policy training. This could be a step towards robust policy learning by optimising the worst case outcome [Stutz et al., 2022].

We conclude by mentioning several limitations of COPP. Firstly, we do not guarantee conditional coverage in general. We outline conditions under which conditional coverage holds asymptotically

(Prop. 4.3), however, this relies on somewhat strong assumptions. Secondly, our current method estimates the weights $w(x, y)$ through $P(y \mid x, a)$, which can be challenging. We address this limitation in Appendix B.5.2, where we propose an alternative method to estimate the weights directly, without having to model $P(y \mid x, a)$. Lastly, reliable estimation of our weights $\hat{w}(x, y)$ requires sufficient overlap between behaviour and target policies. The results from COPP may suffer in cases where this assumption is violated, which we illustrate empirically in Appendix D.1.2. We believe these limitations suggest interesting research questions that we leave to future work.

Acknowledgements

We would like to thank Andrew Jesson, Sahra Ghalebikesabi, Robert Hu, Siu Lun Chau and Tim Rudner for useful feedback. JFT is supported by the EPSRC and MRC through the OxWaSP CDT programme (EP/L016710/1). MFT acknowledges his PhD funding from Google DeepMind. RC and AD are supported by the Engineering and Physical Sciences Research Council (EPSRC) through the Bayes4Health programme [Grant number EP/R018561/1].

References

- Jason Altschuler, Victor-Emmanuel Brunel, and Alan Malek. Best arm identification for contaminated bandits. *Journal of Machine Learning Research*, 20(91):1–39, 2019.
- Anastasios N. Angelopoulos and Stephen Bates. A gentle introduction to conformal prediction and distribution-free uncertainty quantification. *arXiv preprint arXiv:2107.07511*, 2021.
- Marc G Bellemare, Will Dabney, and Rémi Munos. A distributional perspective on reinforcement learning. In *International Conference on Machine Learning*, pages 449–458, 2017.
- Alberto Bietti, Alekh Agarwal, and John Langford. A contextual bandit bake-off. *arXiv preprint arXiv:1802.04064*, 2018.
- Yash Chandak, Scott Niekum, Bruno Castro da Silva, Erik Learned-Miller, Emma Brunskill, and Philip S Thomas. Universal off-policy evaluation. *arXiv preprint arXiv:2104.12820*, 2021.
- Miroslav Dudík, Dumitru Erhan, John Langford, and Lihong Li. Doubly robust policy evaluation and optimization. *Statistical Science*, 29(4), 2014.
- Mehrdad Farajtabar, Yinlam Chow, and Mohammad Ghavamzadeh. More robust doubly robust off-policy evaluation. In *International Conference on Machine Learning*, pages 1447–1456. PMLR, 2018.
- Rina Foygel Barber, Emmanuel J Candès, Aaditya Ramdas, and Ryan J Tibshirani. The limits of distribution-free conditional predictive inference. *Information and Inference: A Journal of the IMA*, 10(2):455–482, 2021.
- Audrey Huang, Liu Leqi, Zachary C. Lipton, and Kamyar Azizzadenesheli. Off-policy risk assessment in contextual bandits. *arXiv preprint arXiv:2104.08977*, 2021.
- Ying Jin, Zhimei Ren, and Emmanuel J Candès. Sensitivity analysis of individual treatment effects: A robust conformal inference approach. *arXiv preprint arXiv:2111.12161*, 2021.
- Ramtin Keramati, Christoph Dann, Alex Tamkin, and Emma Brunskill. Being optimistic to be conservative: Quickly learning a cvar policy. In *AAAI Conference on Artificial Intelligence*, volume 34, pages 4436–4443, 2020.
- Ilya Kuzborskij, Claire Vernade, András György, and Csaba Szepesvári. Confident off-policy evaluation and selection through self-normalized importance weighting. In *International Conference on Artificial Intelligence and Statistics*, pages 640–648, 2021.
- Jing Lei and Larry Wasserman. Distribution-free prediction bands for non-parametric regression. *Journal of the Royal Statistical Society: Series B*, pages 71–96, 2014.
- Lihua Lei and Emmanuel J Candès. Conformal inference of counterfactuals and individual treatment effects. *Journal of the Royal Statistical Society: Series B*, pages 911–938, 2021.

- Muhammad Osama, Dave Zachariah, and Peter Stoica. Learning robust decision policies from observational data. *arXiv preprint arXiv:2006.02355*, 2020.
- Tao Qin and Tie-Yan Liu. Introducing LETOR 4.0 datasets. *arXiv preprint arXiv:1306.2597*, 2013.
- Yaniv Romano, Evan Patterson, and Emmanuel J. Candès. Conformalized quantile regression. In *Advances in Neural Information Processing Systems*, volume 32, pages 3543–3553, 2019.
- Yaniv Romano, Rina Foygel Barber, Chiara Sabatti, and Emmanuel J. Candès. With malice toward none: Assessing uncertainty via equalized coverage. *Harvard Data Science Review*, 2(2), 4 2020.
- Glenn Shafer and Vladimir Vovk. A tutorial on conformal prediction. *Journal of Machine Learning Research*, 9(3), 2008.
- David Stutz, Krishnamurthy Dvijotham, Ali Taylan Cemgil, and Arnaud Doucet. Learning optimal conformal classifiers. *International Conference on Representation Learning*, 2022.
- Yi Su, Maria Dimakopoulou, Akshay Krishnamurthy, and Miroslav Dudík. Doubly robust off-policy evaluation with shrinkage. *CoRR*, abs/1907.09623, 2019. URL <http://arxiv.org/abs/1907.09623>.
- Yi Su, Maria Dimakopoulou, Akshay Krishnamurthy, and Miroslav Dudík. Doubly robust off-policy evaluation with shrinkage. In *International Conference on Machine Learning*, pages 9167–9176. PMLR, 2020.
- Adith Swaminathan and Thorsten Joachims. Batch learning from logged bandit feedback through counterfactual risk minimization. *Journal of Machine Learning Research*, 16(52):1731–1755, 2015a.
- Adith Swaminathan and Thorsten Joachims. The self-normalized estimator for counterfactual learning. In *Advances in Neural Information Processing Systems*, volume 28, 2015b.
- Adith Swaminathan, Akshay Krishnamurthy, Alekh Agarwal, Miroslav Dudík, John Langford, Damien Jose, and Imed Zitouni. Off-policy evaluation for slate recommendation. In *Advances in Neural Information Processing Systems*, 2017.
- Philip S. Thomas, Georgios Theodorou, and Mohammad Ghavamzadeh. High-confidence off-policy evaluation. In *AAAI Conference on Artificial Intelligence*, 2015.
- Ryan J. Tibshirani, Rina Foygel Barber, Emmanuel J. Candès, and Aaditya Ramdas. Conformal prediction under covariate shift. In *Advances in Neural Information Processing Systems*, 2019.
- Vladimir Vovk. Conditional validity of inductive conformal predictors. In Steven C. H. Hoi and Wray Buntine, editors, *Proceedings of the Asian Conference on Machine Learning*, volume 25 of *Proceedings of Machine Learning Research*, pages 475–490, Singapore Management University, Singapore, 04–06 Nov 2012. PMLR. URL <https://proceedings.mlr.press/v25/vovk12.html>.
- Vladimir Vovk, Alexander Gammerman, and Glenn Shafer. *Algorithmic Learning in a Random World*. Springer Science & Business Media, 2005.
- Yu-Xiang Wang, Alekh Agarwal, and Miroslav Dudík. Optimal and adaptive off-policy evaluation in contextual bandits. In *International Conference on Machine Learning*, page 3589–3597, 2017.
- Tengyang Xie, Yifei Ma, and Yu-Xiang Wang. Towards optimal off-policy evaluation for reinforcement learning with marginalized importance sampling. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019. URL <https://proceedings.neurips.cc/paper/2019/file/4ffb0d2ba92f664c2281970110a2e071-Paper.pdf>.
- Mingzhang Yin, Claudia Shi, Yixin Wang, and David M Blei. Conformal sensitivity analysis for individual treatment effects. *arXiv preprint arXiv:2112.03493*, 2021.

A Proofs

A.1 Proof of Proposition 4.1

This proof is a direct adaptation of [Tibshirani et al., 2019, Lemma 3], and has only been included for the sake of completeness.

In this proof, we use the notion of *weighted exchangeability* as defined in Section 3.2 of Tibshirani et al. [2019].

Definition A.1 (Weighted exchangeability). Random variables V_1, \dots, V_n are said to be *weighted exchangeable* with weight functions w_1, \dots, w_n , if the density f of their joint distribution can be factorized as

$$f(v_1, \dots, v_n) = \prod_{i=1}^n w_i(v_i) g(v_1, \dots, v_n) \quad (9)$$

where g is any function that does not depend on the ordering of its inputs, i.e. $g(v_{\sigma(1)}, \dots, v_{\sigma(n)}) = g(v_1, \dots, v_n)$ for any permutation σ of $1, \dots, n$.

Lemma A.2. Let $Z_i = (X_i, Y_i) \in \mathbb{R}^d \times \mathbb{R}$, $i = 1, \dots, n+1$, be such that $\{(X_i, Y_i)\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}^{\pi^b}$ and $(X_{n+1}, Y_{n+1}) \sim P_{X,Y}^{\pi^*}$. Then Z_1, \dots, Z_{n+1} are weighted exchangeable with weights $w_i \equiv 1$, $i \leq n$ and $w_{n+1}(X, Y) = dP_{X,Y}^{\pi^*}/dP_{X,Y}^{\pi^b}(X, Y)$.

Proof. The proof below is merely a verification that our proposed weights still retain the coverage guarantees and is mainly taken from Tibshirani et al. [2019]. Hence, we follow the same strategy as in Tibshirani et al. [2019], with the exception that we have the weights as in Lemma A.2, hence inducing a lot of simplifications. As in Tibshirani et al. [2019], we assume for simplicity that V_1, \dots, V_{n+1} are distinct almost surely, however the result holds in general case as well. We define f as the joint distribution of the random variables $\{X_i, Y_i\}_{i=1}^{n+1}$. We also denote E_z as the event of $\{Z_1, \dots, Z_{n+1}\} = \{z_1, \dots, z_{n+1}\}$ and let $v_i = s(z_i) = s(x_i, y_i)$, then for each i :

$$\mathbb{P}\{V_{n+1} = v_i | E_z\} = \mathbb{P}\{Z_{n+1} = z_i | E_z\} = \frac{\sum_{\sigma: \sigma(n+1)=i} f(z_{\sigma(1)}, \dots, z_{\sigma(n+1)})}{\sum_{\sigma} f(z_{\sigma(1)}, \dots, z_{\sigma(n+1)})} \quad (10)$$

Now using the fact that Z_1, \dots, Z_{n+1} are weighted exchangeable:

$$\begin{aligned} \frac{\sum_{\sigma: \sigma(n+1)=i} f(z_{\sigma(1)}, \dots, z_{\sigma(n+1)})}{\sum_{\sigma} f(z_{\sigma(1)}, \dots, z_{\sigma(n+1)})} &= \frac{\sum_{\sigma: \sigma(n+1)=i} \prod_{j=1}^{n+1} w_j(z_{\sigma(j)}) g(z_{\sigma(1)}, \dots, z_{\sigma(n+1)})}{\sum_{\sigma} \prod_{j=1}^{n+1} w_j(z_{\sigma(j)}) g(z_{\sigma(1)}, \dots, z_{\sigma(n+1)})} \\ &= \frac{w_{n+1}(z_i) g(z_1, \dots, z_{n+1})}{\sum_{j=1}^{n+1} w_{n+1}(z_j) g(z_1, \dots, z_{n+1})} \\ &= p_i^w(z_{n+1}) \end{aligned} \quad (11)$$

where we recall that

$$p_i^w(x, y) := \frac{w(X_i, Y_i)}{\sum_{j=1}^n w(X_j, Y_j) + w(x, y)}.$$

We get simplifications in (11) due to the weights defined in Lemma A.2, i.e. $w_i \equiv 1$ for $i \leq n$ and $w_{n+1}(x, y) = w(x, y) = dP_{X,Y}^{\pi^*}/dP_{X,Y}^{\pi^b}(x, y)$. Next, just as in Tibshirani et al. [2019] we can view:

$$V_{n+1} = v_i | E_z \sim \sum_{i=1}^{n+1} p_i^w(z_{n+1}) \delta_{v_i} \quad (12)$$

which implies that:

$$\mathbb{P}\{V_{n+1} \leq \text{Quantile}_{\beta}(\sum_{i=1}^{n+1} p_i^w(z_{n+1}) \delta_{v_i}) | E_z\} \geq \beta.$$

This is equivalent to

$$\mathbb{P}\{V_{n+1} \leq \text{Quantile}_\beta(\sum_{i=1}^{n+1} p_i^w(Z_{n+1})\delta_{v_i})|E_z\} \geq \beta$$

and, after marginalizing, one has

$$\mathbb{P}\{V_{n+1} \leq \text{Quantile}_\beta(\sum_{i=1}^{n+1} p_i^w(Z_{n+1})\delta_{v_i})\} \geq \beta$$

This is equivalent to the claim in Proposition 4.1. \square

A.2 Proof of Proposition 4.2

The following proof is an adaptation of [Lei and Candès, 2021, Proposition 1] to our setting.

Before detailing the main proof, we introduce a preliminary result which will be used in the proof of Proposition 4.2.

Lemma A.3. *Let $\hat{w}(x, y)$ be an estimate of the weights $w(x, y) = dP_{X,Y}^{\pi^*}/dP_{X,Y}^{\pi^b}(x, y)$, and $(\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}}[\hat{w}(X, Y)^r])^{1/r} \leq M_r < \infty$ for some $r \geq 2$. Let $(X_i, Y_i) \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}^{\pi^b}$ and \mathcal{A} denote the event that*

$$\sum_{i=1}^n \hat{w}(X_i, Y_i) \leq n/2.$$

Then,

$$\mathbb{P}(\mathcal{A}) \leq \frac{c_1 M_r^2}{n}$$

where c_1 is an absolute constant, and the probability is taken over $\{X_i, Y_i\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}^{\pi^b}$.

Proof of Lemma A.3

The condition $\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}}[\hat{w}(X, Y)^r] < \infty \implies \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^b}}(\hat{w}(X, Y) < \infty) = 1$ and $\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}}[\hat{w}(X, Y)] < \infty$. WLOG assume $\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}}[\hat{w}(X, Y)] = 1$. Recall that $p_i^{\hat{w}}(x, y) := \frac{\hat{w}(X_i, Y_i)}{\sum_{i=1}^n \hat{w}(X_i, Y_i) + \hat{w}(x, y)}$, and therefore, $p_i^{\hat{w}}(x, y)$ are invariant to weight scaling. Since $\mathbb{E}_{(X_i, Y_i) \sim P_{X,Y}^{\pi^b}}[\hat{w}(X_i, Y_i)]^2 \leq M_r^2$ and $\mathbb{E}_{(X_i, Y_i) \sim P_{X,Y}^{\pi^b}}(\hat{w}(X_i, Y_i)) = 1$, using Chebyshev's inequality

$$\begin{aligned} \mathbb{P}\left(\sum_{i=1}^n \hat{w}(X_i, Y_i) \leq n/2\right) &= \mathbb{P}\left(\sum_{i=1}^n (\hat{w}(X_i, Y_i) - 1) \leq -n/2\right) \\ &\leq \mathbb{P}\left(\left|\sum_{i=1}^n (\hat{w}(X_i, Y_i) - 1)\right| \geq n/2\right) \\ &\leq \frac{4}{n^2} \mathbb{E}\left[\left(\sum_{i=1}^n \hat{w}(X_i, Y_i) - \mathbb{E}[\hat{w}(X_i, Y_i)]\right)^2\right] \\ &= \frac{4}{n^2} \{n\mathbb{E}|\hat{w}(X_1, Y_1) - \mathbb{E}[\hat{w}(X_1, Y_1)]|^2\} \end{aligned} \tag{13}$$

$$\begin{aligned} &\leq \frac{16}{n^2} n\mathbb{E}|\hat{w}(X_1, Y_1)|^2 \\ &\leq \frac{c_1 M_r^2}{n} \end{aligned} \tag{14}$$

where to get from (13) to (14) we use:

$$\begin{aligned} \mathbb{E}|\hat{w}(X_1, Y_1) - \mathbb{E}[\hat{w}(X_1, Y_1)]|^2 &\leq 2\mathbb{E}[\hat{w}(X_1, Y_1)^2 + \mathbb{E}[\hat{w}(X_1, Y_1)]^2] \\ &\leq 4\mathbb{E}[\hat{w}(X_1, Y_1)^2]. \end{aligned}$$

□

We can now prove Proposition 4.2.

Proof. The condition $\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [\hat{w}(X,Y)^r] < \infty \implies \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^b}} (\hat{w}(X,Y) < \infty) = 1$ and $\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [\hat{w}(X,Y)] < \infty$. **WLOG** assume $\mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [\hat{w}(X,Y)] = 1$. Let $\tilde{P}_{X,Y}^{\pi^*}$ be a probability measure with

$$d\tilde{P}_{X,Y}^{\pi^*}(x,y) := \hat{w}(x,y) dP_{X,Y}^{\pi^b}(x,y)$$

and $(\tilde{X}, \tilde{Y}) \sim \tilde{P}_{X,Y}^{\pi^*}$ that is independent of the data. By Hölder's inequality,

$$\begin{aligned} \mathbb{E}_{(\tilde{X}, \tilde{Y}) \sim \tilde{P}_{X,Y}^{\pi^*}} [\hat{w}(\tilde{X}, \tilde{Y})] &= \int_{\tilde{x}, \tilde{y}} \frac{d\tilde{P}^{\pi^*}(\tilde{x}, \tilde{y})}{dP^{\pi^b}(\tilde{x}, \tilde{y})} d\tilde{P}^{\pi^*}(\tilde{x}, \tilde{y}) \\ &= \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [\hat{w}(X,Y)^2] \leq M_r^2 < \infty \end{aligned}$$

Note using Proposition 4.1 with (\tilde{X}, \tilde{Y}) denoting (X_{n+1}, Y_{n+1}) for simplicity

$$\begin{aligned} &\mathbb{P}(\tilde{Y} \in \hat{C}(\tilde{X}, \tilde{Y})) \\ &= \mathbb{E}_{(\tilde{X}, \tilde{Y}) \sim \tilde{P}_{X,Y}^{\pi^*}} \left[\mathbb{P} \left(s(\tilde{X}, \tilde{Y}) \leq \text{Quantile}_{1-\alpha} \left(\sum_{i=1}^n p_i^{\hat{w}}(\tilde{X}, \tilde{Y}) \delta_{V_i} + p_{n+1}^{\hat{w}}(\tilde{X}, \tilde{Y}) \delta_{\infty} \right) \mid \mathcal{E}(\tilde{V}) \right) \right] \end{aligned} \quad (15)$$

where $\mathcal{E}(\tilde{V})$ denotes the unordered set of V_1, \dots, V_{n+1} . Marginalising over $\{(X_i, Y_i)\}_{i=1}^n$, we obtain

$$(15) \leq \mathbb{E} \left(1 - \alpha + \max_{i \in [n+1]} p_i^{\hat{w}}(\tilde{X}, \tilde{Y}) \right) \quad (16)$$

where the expectation is over $\{(X_i, Y_i)\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} P_{X,Y}^{\pi^b}$ and $(\tilde{X}, \tilde{Y}) \sim \tilde{P}_{X,Y}^{\pi^*}$. Let \mathcal{A} denote the event that

$$\sum_{i=1}^n \hat{w}(X_i, Y_i) \leq n/2.$$

using Lemma A.3 and $\mathbb{E}[\hat{w}(\tilde{X}, \tilde{Y})] \leq M_r^2$, we get that

$$\begin{aligned} \mathbb{E} \left[\max_{i \in [n+1]} p_i^{\hat{w}}(\tilde{X}, \tilde{Y}) \right] &= \mathbb{E} \left[\frac{\max\{\hat{w}(\tilde{X}, \tilde{Y}), \max_i \hat{w}(X_i, Y_i)\}}{\hat{w}(\tilde{X}, \tilde{Y}) + \sum_{i=1}^n \hat{w}(X_i, Y_i)} \right] \\ &\leq \mathbb{E} \left[\frac{\max\{\hat{w}(\tilde{X}, \tilde{Y}), \max_i \hat{w}(X_i, Y_i)\}}{\hat{w}(\tilde{X}, \tilde{Y}) + \sum_{i=1}^n \hat{w}(X_i, Y_i)} \mathbb{1}_{\mathcal{A}^c} \right] + \mathbb{P}(\mathcal{A}) \\ &\leq \mathbb{E} \left[\frac{2 \max\{\hat{w}(\tilde{X}, \tilde{Y}), \max_i \hat{w}(X_i, Y_i)\}}{n} \mathbb{1}_{\mathcal{A}^c} \right] + \frac{c_1 M_r^2}{n} \\ &\leq \frac{2}{n} \left(\mathbb{E}[\hat{w}(\tilde{X}, \tilde{Y})] + \mathbb{E} \max_i \hat{w}(X_i, Y_i) \right) + \frac{c_1 M_r^2}{n} \\ &\leq \frac{2}{n} \left(\mathbb{E}[\hat{w}(\tilde{X}, \tilde{Y})] + \left(\sum_{i=1}^n \mathbb{E}[\hat{w}(X_i, Y_i)^r] \right)^{1/r} \right) + \frac{c_1 M_r^2}{n} \\ &\leq \frac{2}{n} \left(M_r^2 + n^{1/r} M_r \right) + \frac{c_1 M_r^2}{n}. \end{aligned}$$

This implies that

$$\mathbb{P}_{(X,Y) \sim \tilde{P}_{X,Y}^{\pi^*}} (Y \in \hat{C}(X)) \leq 1 - \alpha + cn^{1/r-1}$$

for some constant c that only depends on M_r and r . Note that

$$|\mathbb{P}_{(X,Y) \sim \tilde{P}_{X,Y}^{\pi^*}} (Y \in \hat{C}(X)) - \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (Y \in \hat{C}(X))| \leq d_{\text{TV}}(\tilde{P}^{\pi^*}, P^{\pi^*}) \quad (17)$$

where d_{TV} is the total variation norm which satisfies

$$\begin{aligned} d_{TV}(\tilde{P}^{\pi^*}, P^{\pi^*}) &= \frac{1}{2} \int |\hat{w}(x, y) dP^{\pi^b}(x, y) - dP^{\pi^*}(x, y)| \\ &= \frac{1}{2} \int |\hat{w}(x, y) dP^{\pi^b}(x, y) - w(x, y) dP^{\pi^b}(x, y)| \\ &= \frac{1}{2} \mathbb{E}_{(X, Y) \sim P_{X, Y}^{\pi^b}} [|\hat{w}(X, Y) - w(X, Y)|] = \Delta_w. \end{aligned} \quad (18)$$

Putting together (17) and (18), we get

$$\mathbb{P}_{(X, Y) \sim P_{X, Y}^{\pi^*}}(Y \in \hat{C}(X)) \leq 1 - \alpha + \Delta_w + cn^{1/r-1}. \quad (19)$$

For the lower bound, using Proposition 4.1 we get that

$$\begin{aligned} \mathbb{P}_{(\tilde{X}, \tilde{Y}) \sim \tilde{P}_{\tilde{X}, \tilde{Y}}^{\pi^*}}(\tilde{Y} \in \hat{C}(\tilde{X}, \tilde{Y})) &= \mathbb{P}\left(s(\tilde{X}, \tilde{Y}) \leq \text{Quantile}_{1-\alpha}\left(\sum_{i=1}^n p_i^{\hat{w}}(\tilde{X}, \tilde{Y}) \delta_{V_i} + p_{n+1}^{\hat{w}}(\tilde{X}, \tilde{Y}) \delta_{\infty}\right)\right) \\ &\geq 1 - \alpha. \end{aligned} \quad (20)$$

Using (17) we thus obtain

$$\begin{aligned} \mathbb{P}_{(X, Y) \sim P_{X, Y}^{\pi^*}}(Y \in \hat{C}(X)) &\geq \mathbb{P}_{(X, Y) \sim \tilde{P}_{X, Y}^{\pi^*}}(Y \in \hat{C}(X)) - d_{TV}(\tilde{P}^{\pi^*}, P^{\pi^*}) \\ &\geq 1 - \alpha - \Delta_w. \end{aligned} \quad (21)$$

□

A.3 Proof of Proposition 4.3

For notational convenience, we suppress the subscripts m and n in $\hat{q}, \hat{w}, \hat{C}$. Moreover, we use \hat{w}_i to denote $\hat{w}(X_i, Y_i)$ and $\eta(x, y)$ to denote $\text{Quantile}_{1-\alpha}(\sum_{i=1}^n \hat{p}_i(x, y) \delta_{V_i} + \hat{p}_{n+1}(x, y) \delta_{\infty})$.

Proof. We use $(\tilde{X}, \tilde{Y}) \sim P_{X, Y}^{\pi^*}$ in place of (X_{n+1}, Y_{n+1}) and let $\epsilon < r/2$. By the definition of $\hat{C}(\tilde{X})$, we directly have

$$\begin{aligned} \mathbb{P}(\tilde{Y} \in \hat{C}(\tilde{X}) \mid \tilde{X}) &= \mathbb{P}(s(\tilde{X}, \tilde{Y}) \leq \eta(\tilde{X}, \tilde{Y}) \mid \tilde{X}) \\ &\geq \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq \eta(\tilde{X}, \tilde{Y}) - H(\tilde{X}) \mid \tilde{X}) \end{aligned} \quad (22)$$

where $s^*(\tilde{X}, \tilde{Y}) := \max\{\tilde{Y} - q_{\alpha_{hi}}(\tilde{X}), q_{\alpha_{lo}}(\tilde{X}) - \tilde{Y}\}$ and the probability is taken over $\{(X_i, Y_i)\}_{i=1}^n \stackrel{\text{i.i.d.}}{\sim} P_{X, Y}^{\pi^b}$ and $\tilde{Y} \sim P_{Y|X=\tilde{X}}^{\pi^*}$. We then get

$$\begin{aligned} (22) &\geq \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq -\epsilon - H(\tilde{X}) \mid \tilde{X}) - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \\ &\geq \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq -\epsilon - H(\tilde{X}) \mid \tilde{X}) \left(\mathbb{1}(H(\tilde{X}) \leq \epsilon) + \mathbb{1}(H(\tilde{X}) > \epsilon) \right) - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \end{aligned} \quad (23)$$

$$\begin{aligned} &\geq \left(\mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq 0 \mid \tilde{X}) - b_2\{\epsilon + H(\tilde{X})\} \right) \mathbb{1}(H(\tilde{X}) \leq \epsilon) \\ &\quad + \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq -\epsilon - H(\tilde{X}) \mid \tilde{X}) \mathbb{1}(H(\tilde{X}) > \epsilon) - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \end{aligned} \quad (24)$$

$$\begin{aligned} &\geq \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq 0 \mid \tilde{X}) \mathbb{1}(H(\tilde{X}) \leq \epsilon) - b_2\{\epsilon + H(\tilde{X}) \mathbb{1}(H(\tilde{X}) \leq \epsilon)\} \\ &\quad + \left(\mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq 0 \mid \tilde{X}) - \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \in (-\epsilon - H(\tilde{X}), 0)) \right) \mathbb{1}(H(\tilde{X}) > \epsilon) \\ &\quad - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \\ &\geq \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq 0 \mid \tilde{X}) - b_2\{\epsilon + H(\tilde{X}) \mathbb{1}(H(\tilde{X}) \leq \epsilon)\} - \mathbb{1}(H(\tilde{X}) > \epsilon) \\ &\quad - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \end{aligned} \quad (25)$$

where, to get from (23) to (24), we use the condition $2\epsilon < r$ and Assumption 2

$$(25) \geq \mathbb{P}(s^*(\tilde{X}, \tilde{Y}) \leq 0 \mid \tilde{X}) - b_2\{\epsilon + H(\tilde{X})\} - \mathbb{1}(H(\tilde{X}) > \epsilon) - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \quad (26)$$

$$= 1 - \alpha - b_2\{\epsilon + H(\tilde{X})\} - \mathbb{1}(H(\tilde{X}) > \epsilon) - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}). \quad (27)$$

Next, we derive an upper bound on $\mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X})$. Let G denote the CDF of the random distribution $\sum_{i=1}^n \hat{p}_i(x, y)\delta_{V_i} + \hat{p}_{n+1}(x, y)\delta_\infty$. Then, $\eta(\tilde{X}, \tilde{Y}) < -\epsilon$ implies $G(-\epsilon) \geq 1 - \alpha$ and thus $\mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \leq \mathbb{P}(G(-\epsilon) \geq 1 - \alpha \mid \tilde{X})$ a.s. Moreover, we have

$$\begin{aligned} \mathbb{P}(G(-\epsilon) \geq 1 - \alpha \mid \tilde{X}) &= \mathbb{P}\left(\frac{\sum_{i=1}^n \hat{w}_i \mathbb{1}(V_i \leq -\epsilon)}{\sum_{i=1}^n \hat{w}_i + \hat{w}(\tilde{X}, \tilde{Y})} \geq 1 - \alpha \mid \tilde{X}\right) \\ &\leq \mathbb{P}\left(\frac{\sum_{i=1}^n \hat{w}_i \mathbb{1}(V_i \leq -\epsilon)}{\sum_{i=1}^n \hat{w}_i} \geq 1 - \alpha \mid \tilde{X}\right) \end{aligned} \quad (28)$$

$$= \mathbb{P}\left(\frac{\sum_{i=1}^n \hat{w}_i \mathbb{1}(V_i \leq -\epsilon)}{\sum_{i=1}^n \hat{w}_i} \geq 1 - \alpha\right) \quad (29)$$

where, to get from (28) to (29) we use the independence of $\{(X_i, Y_i)\}_{i=1}^n$ and \tilde{X} . Now we observe that

$$\frac{\sum_{i=1}^n \hat{w}_i \mathbb{1}(V_i \leq -\epsilon)}{n} = \frac{\sum_{i=1}^n (\hat{w}_i - w_i) \mathbb{1}(V_i \leq -\epsilon)}{n} + \frac{\sum_{i=1}^n w_i \mathbb{1}(V_i \leq -\epsilon)}{n}.$$

As $n \rightarrow \infty$, the strong law of large numbers yields

$$\begin{aligned} \left| \frac{\sum_{i=1}^n (\hat{w}_i - w_i) \mathbb{1}(V_i \leq -\epsilon)}{n} \right| &\xrightarrow{a.s.} \left| \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [(\hat{w}(X, Y) - w(X, Y)) \mathbb{1}(s(X, Y) \leq -\epsilon)] \right| \\ &\leq \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [|\hat{w}(X, Y) - w(X, Y)| \mathbb{1}(s(X, Y) \leq -\epsilon)] \\ &\leq \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [|\hat{w}(X, Y) - w(X, Y)|] \xrightarrow{m \rightarrow \infty} 0 \end{aligned} \quad (30)$$

from Assumption 1 and

$$\frac{\sum_{i=1}^n w_i \mathbb{1}(V_i \leq -\epsilon)}{n} \xrightarrow{a.s.} \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [w(X, Y) \mathbb{1}(s(X, Y) \leq -\epsilon)] = \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (s(X, Y) \leq -\epsilon). \quad (31)$$

Using the triangle inequality,

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (s(X, Y) \leq -\epsilon) \leq \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (s^*(X, Y) \leq -\epsilon/2) + \mathbb{P}(H(X) \geq \epsilon/2) \quad (32)$$

$$\begin{aligned} &\leq \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}} (s^*(X, Y) \leq 0) - \epsilon b_1/2 + 2^k \mathbb{E}[H^k(X)]/\epsilon^k \quad (33) \\ &= 1 - \alpha - \epsilon b_1/2 + 2^k \mathbb{E}[H^k(X)]/\epsilon^k \xrightarrow{m \rightarrow \infty} 1 - \alpha - \epsilon b_1/2. \end{aligned}$$

To get from (32) to (33), we use Assumption 2 and Markov's inequality. Similarly, we have

$$\frac{\sum_{i=1}^n \hat{w}_i}{n} = \frac{\sum_{i=1}^n (\hat{w}_i - w_i)}{n} + \frac{\sum_{i=1}^n w_i}{n}$$

so, as $n \rightarrow \infty$,

$$\begin{aligned} \left| \frac{\sum_{i=1}^n (\hat{w}_i - w_i)}{n} \right| &\xrightarrow{a.s.} \left| \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [(\hat{w}(X, Y) - w(X, Y))] \right| \\ &\leq \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [|\hat{w}(X, Y) - w(X, Y)|] \xrightarrow{m \rightarrow \infty} 0, \end{aligned} \quad (34)$$

and

$$\frac{\sum_{i=1}^n w_i}{n} \xrightarrow{a.s.} \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [w(X, Y)] = 1. \quad (35)$$

Putting this all together using the continuous mapping theorem, we get that, almost surely,

$$\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} \frac{\sum_{i=1}^n \hat{w}_i \mathbb{1}(V_i \leq -\epsilon)}{\sum_{i=1}^n \hat{w}_i} = \lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} \frac{\sum_{i=1}^n \hat{w}_i \mathbb{1}(V_i \leq -\epsilon)/n}{\sum_{i=1}^n \hat{w}_i/n} = 1 - \alpha - \epsilon b_1/2. \quad (36)$$

Since convergence almost surely implies convergence in probability, we have

$$\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} \mathbb{P} \left(\frac{\sum_{i=1}^n \hat{w}_i \mathbb{1}(V_i \leq -\epsilon)}{\sum_{i=1}^n \hat{w}_i} \geq 1 - \alpha \right) = 0. \quad (37)$$

This implies that, for any $\epsilon > 0$, $\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) = 0$ almost surely.

Using Markov's inequality and Assumption 3

$$\mathbb{P}(H(X) > \epsilon) \leq \mathbb{E}[H^k(X)]/\epsilon^k \xrightarrow{m \rightarrow \infty} 0. \quad (38)$$

So as $m \rightarrow \infty$, $H(X) \xrightarrow{\mathcal{P}} 0$. Similarly, $\mathbb{1}(H(X) > \epsilon) \xrightarrow{\mathcal{P}} 0$ as $m \rightarrow \infty$.

Recall (using 27) that, for any $\epsilon \in (0, r/2)$, almost surely,

$$\mathbb{P}(\tilde{Y} \in \hat{C}(\tilde{X}) \mid \tilde{X}) - (1 - \alpha - b_2\epsilon) \geq -b_2H(\tilde{X}) - \mathbb{1}(H(\tilde{X}) > \epsilon) - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}). \quad (39)$$

For given $t > 0$, pick $\epsilon < \min(r/2, t/2b_2)$. Then,

$$\mathbb{P}(\tilde{Y} \in \hat{C}(\tilde{X}) \mid \tilde{X}) - (1 - \alpha - t/2) \geq -b_2H(\tilde{X}) - \mathbb{1}(H(\tilde{X}) > \epsilon) - \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}). \quad (40)$$

Each term on the right hand side of (40) converges in probability to 0 as $m, n \rightarrow \infty$, and therefore using continuous mapping theorem

$$b_2H(\tilde{X}) + \mathbb{1}(H(\tilde{X}) > \epsilon) + \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \xrightarrow{\mathcal{P}} 0.$$

This implies

$$\begin{aligned} \mathbb{P}(\mathbb{P}(\tilde{Y} \in \hat{C}(\tilde{X}) \mid \tilde{X}) \leq 1 - \alpha - t) \\ \leq \mathbb{P}(b_2H(\tilde{X}) + \mathbb{1}(H(\tilde{X}) > \epsilon) + \mathbb{P}(\eta(\tilde{X}, \tilde{Y}) < -\epsilon \mid \tilde{X}) \geq t/2) \rightarrow 0. \end{aligned}$$

Therefore,

$$\lim_{m \rightarrow \infty} \lim_{n \rightarrow \infty} \mathbb{P}(\mathbb{P}(\tilde{Y} \in \hat{C}(\tilde{X}) \mid \tilde{X}) \leq 1 - \alpha - t) = 0. \quad (41)$$

□

B Conformal Off-Policy Prediction (COPP)

B.1 Further comments on the differences between Lei and Candès [2021] and COPP

In this subsection, we elaborate on the differences between our work and Lei and Candès [2021].

Firstly, Lei and Candès [2021] consider a setup in which the distribution of X is shifted, and construct intervals on the outcome under a specific (deterministic) action, i.e. $Y(a)$. In contrast, we consider a setup in which the distribution of $Y|X$ is shifted due to a change in the policy which is non trivial, and construct bounds on the outcome under this new policy (which could be stochastic). Additionally, since the theory in our methodology relies on the ratio of the joint distribution $P_{X,Y}$, our framework can be straightforwardly extended to the case where both, the conditional $P_{Y|X}$ and the covariate distribution P_X shift.

Secondly, as already mentioned in section 5, Lei and Candès [2021] can only be applied to the case where we have a deterministic target policy and a discrete action space, whereas COPP generalizes to the stochastic policy and continuous action space. This limitation of Lei and Candès [2021] can be partially addressed by employing the “union method” as described in the main text, which consists of constructing CP intervals for each action separately before taking the union of the intervals. However, we showed in our experiments that this leads to overly conservative intervals i.e. coverage above the required $1 - \alpha$ in Table 1a. This is because the predictive interval does not depend on the target policy, since every action is treated identically when taking the union. This approach is moreover unsuitable for continuous action spaces, whereas COPP applies without modification.

Thirdly, as stated in in section 5, even in the case when we only consider deterministic target policies, there is an important methodological difference between COPP and Lei and Candès [2021]. Lei and Candès [2021] construct the intervals on $Y(a)$ by only using calibration data with $A = a$ (see eq. 3.4 in Lei and Candès [2021]). In contrast, it can be shown that COPP uses the entire calibration data when constructing intervals on $Y(a)$. This is a consequence of integrating out the actions in the weights $w(x, y)$ (sec 3.1). This empirically leads to smaller variance in coverage compared to Lei and Candès [2021] as evidenced by the experimental results in B.2.

Finally, in our paper we are *not* interested in a linear combination of the $Y(a)$ as in Lei and Candès [2021], who consider the linear combination of the form $Y(1) - Y(0)$. Instead, as described in section 1.1, we are interested in the outcome Y under the new target policy π^* (sometimes denoted as $Y(\pi^*)$ in the literature), which cannot be expressed as a linear combination of $Y(a)$. As a result, there does not appear to be a straightforward application of [Lei and Candès, 2021, Section 4.3] to our setup which relies on the linear combination assumption to be applicable.

B.2 Comparison with Lei and Candès [2021] on deterministic target policies.

In order to further clarify the distinction between COPP and Lei and Candès [2021], we conducted additional experiments when the target policy is deterministic i.e. $\pi^*(A|X) = \mathbb{1}\{A = a\}$. In the main text we modified Lei and Candès [2021] to our setting of stochastic policies by constructing the conformal intervals through the union of the CP sets across the actions. Here we aim to apply COPP to the setting of Lei and Candès [2021], i.e. deterministic target policy.

As mentioned in in the main text, given that we are integrating out the action in Eq. 7, we are essentially able to use the full dataset when constructing the CP intervals. To see this explicitly, consider the case where $Y | X, A$ is a normal random variable (as in our toy experiment). In this case, it can be straightforwardly shown that the weights $w(x_i, y_i)$ will be non-zero, and therefore, when constructing the COPP intervals using (5), we are able to use all the calibration datapoints.

This is contrary to Lei and Candès [2021], who only consider calibration data with $A = a$, when constructing the CP intervals for $Y(a)$. Below, we use the same experimental setup as our toy experiment in section 6.1 (see section D.1 for more details) with the difference here that we now consider deterministic target policies. In figure 2 we plot the coverage for given deterministic target policies against the number of calibration datapoints. In this figure, we refer to the methodology of Lei and Candès [2021] as *LC21*. Here, we use the behavioural policy $\pi_{0.3}$ and a deterministic target policy which takes a single fixed action $a \in \{1, 2, 3, 4\}$ at test time. In the title of each subfigure, $Y(a)$ corresponds to the outcome for the target policy $\pi^*(A = a | X) = \mathbb{1}(A = a)$.

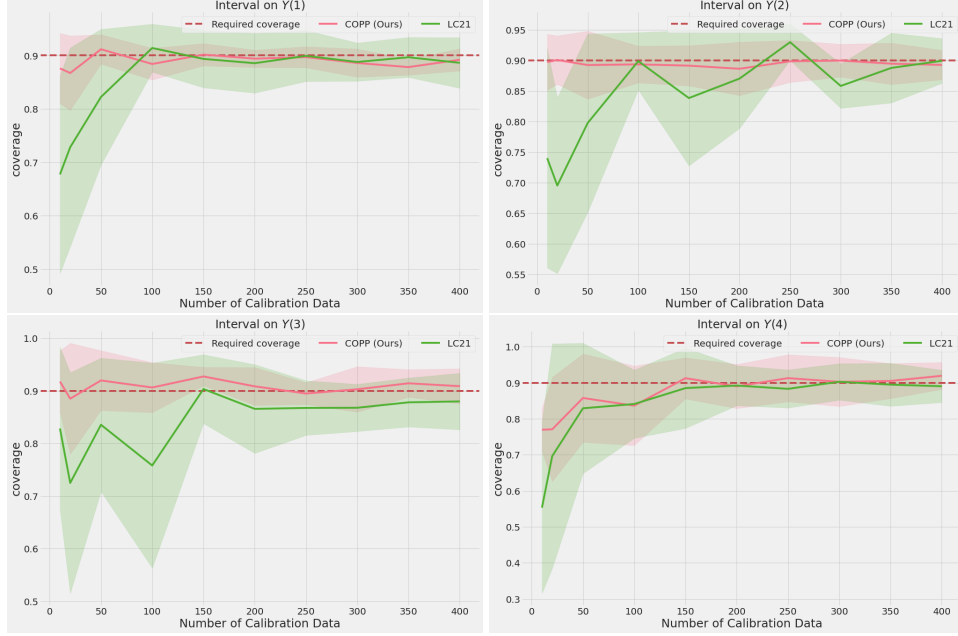


Figure 2: Results for synthetic data experiment with $\pi^b = \pi_{0.3}$ and deterministic target policies.

Results: We first note in Figure 2 that the coverage of COPP intervals has a lower variance than Lei and Candès [2021]. Given that COPP is able to use all the data when constructing the CP intervals, as opposed to Lei and Candès [2021] which only uses a subset, our bounds have lower variance while also attaining the coverage guarantees. We observe this difference particularly in the case when we have little calibration data. Given that Lei and Candès [2021] have to split the data into 4 different splits (we have 4 different actions), the calibration data for each action is relatively small, whereas we are able to use the whole dataset to construct our CP intervals.

B.3 Motivation of using stochastic policies for bandits

One of the key difference between our method and that of Lei and Candès [2021] is that our method can be applied to the setting where the target policy is stochastic. In many settings, deterministic target policies might not be applicable such as in the settings of recommendation systems or RL where exploration is needed [Swaminathan et al., 2017; Su et al., 2020]. For example, COPP can be used to compare different recommendation systems given some logged data. We explore this application in our MSR experiments where the target policies correspond to different recommendation systems which are, by default, stochastic. Other applications which also make use of stochastic policies bandit problems can be found in Su et al. [2020]; Farajtabar et al. [2018].

B.4 COPP for Group-balanced coverage

As Angelopoulos and Bates [2021] point out, we may want predictive intervals that have same error rates across multiple different groups. Using our example of a recommendation system, we may want the predictive intervals to have same coverage across male and female users.

Formally, this problem can be expressed as follows. Let $\Omega = \{\Omega_1, \dots, \Omega_k\}$ be subsets of $\mathcal{X} \times \mathcal{Y}$ with $\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}((X,Y) \in \Omega_j) > 0$ for $j \in \{1, \dots, k\}$. We would like to construct predictive intervals \hat{C}_n^Ω which satisfy

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n^\Omega(X) \mid (X,Y) \in \Omega_j) \geq 1 - \alpha \text{ for all } j \in \{1, \dots, k\}.$$

CP offers us the ability to construct such intervals \hat{C}_n^Ω , by simply running algorithm 1 (main text) on each group separately. This has been visualized in figure 3.

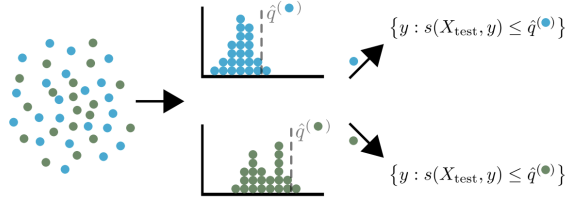


Figure 3: Figure taken from Angelopoulos and Bates [2021]. To achieve group-balanced coverage, we simply run conformal prediction separately on each group.

Formally, this procedure can be described as follows. We group scores into different groups according to each subset.

$$\{(X_i^{\Omega_j}, Y_i^{\Omega_j})\}_{i=1}^{n_j} := \{(X_i, Y_i) : (X_i, Y_i) \in \Omega_j\}_{i=1}^n \text{ and,} \\ V_i^{\Omega_j} := (X_i^{\Omega_j}, Y_i^{\Omega_j})$$

Then, within each subset, we calculate the conformal quantile,

$$\eta^{\Omega_j}(x, y) := \text{Quantile}_{1-\alpha}(\hat{F}_n^{\Omega_j}(x, y))$$

where,

$$\hat{F}_n^{\Omega_j}(x, y) := \sum_{i=1}^{n_j} p_i^{\Omega_j}(x, y) \delta_{V_i^{\Omega_j}} + p_{n+1}^{\Omega_j}(x, y) \delta_{\infty} \text{ where,} \\ p_i^{\Omega_j}(x, y) := \frac{w(X_i^{\Omega_j}, Y_i^{\Omega_j})}{\sum_{i=1}^{n_j} w(X_i^{\Omega_j}, Y_i^{\Omega_j}) + w(x, y)} \\ p_{n+1}^{\Omega_j}(x, y) := \frac{w(x, y)}{\sum_{i=1}^{n_j} w(X_i^{\Omega_j}, Y_i^{\Omega_j}) + w(x, y)}$$

Next, we construct the set \hat{C}_n^{Ω} as follows:

$$\hat{C}_n^{\Omega}(x^{test}) := \bigcup_{j=1}^k \hat{C}_n^{\Omega_j}(x^{test}) \text{ where,} \\ \hat{C}_n^{\Omega_j}(x^{test}) := \{y : (x^{test}, y) \in \Omega_j \text{ and } s(x^{test}, y) \leq \eta^{\Omega_j}(x^{test}, y)\}. \quad (42)$$

Proposition B.1 (Coverage guarantee for class-balanced conformal prediction). *Let $\Omega = \{\Omega_1, \dots, \Omega_k\}$ be subsets of $\mathcal{X} \times \mathcal{Y}$ with $\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}((X, Y) \in \Omega_j) > 0$ for $j \in \{1, \dots, k\}$. Then, the set \hat{C}_n^{Ω} defined above satisfies the coverage guarantee*

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n^{\Omega}(X) \mid (X, Y) \in \Omega_j) \geq 1 - \alpha \text{ for all } j \in \{1, \dots, k\}.$$

Proof of Proposition B.1

$$\begin{aligned} & \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n^{\Omega}(X) \mid (X, Y) \in \Omega_j) \\ & \geq \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n^{\Omega_j}(X) \mid (X, Y) \in \Omega_j) \\ & \geq \mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}((X, Y) \in \Omega_j : s(X, Y) \leq \eta^{\Omega_j}(X, Y) \mid (X, Y) \in \Omega_j) \end{aligned} \quad (43)$$

Define the measure $P_{X,Y}^j$ by restricting $P_{X,Y}^{\pi^*}$ to Ω_j , i.e.

$$P_{X,Y}^j(x, y) \propto P_{X,Y}^{\pi^*}(x, y) \mathbb{1}((x, y) \in \Omega_j)$$

Then, (43) can be written as

$$(43) = \mathbb{P}_{(X,Y) \sim P_{X,Y}^j}(s(X,Y) \leq \eta^{\Omega_j}(X,Y)) \quad (44)$$

Moreover, for $(x,y) \in \Omega_j$ we have

$$w(x,y) = \frac{P_{X,Y}^{\pi^*}(x,y)}{P_{X,Y}^{\pi^b}(x,y)} \propto \frac{P_{X,Y}^j(x,y)}{P_{X,Y}^{\pi^b}(x,y)}$$

Since $p_i^{\Omega_j}(x,y)$ is invariant to scaling of weights $w(x,y)$, replacing the weights by $\tilde{w}(x,y) = \frac{P_{X,Y}^j(x,y)}{P_{X,Y}^{\pi^b}(x,y)}$ keeps the conformal sets unchanged.

Therefore, using Proposition 4.1, the conformal sets constructed will provide coverage guarantees under the measure $P_{X,Y}^j$, i.e.

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^j}(s(X,Y) \leq \eta^{\Omega_j}(X,Y)) \geq 1 - \alpha$$

Using (44), we get that

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n^{\Omega}(X) \mid (X,Y) \in \Omega_j) \geq \mathbb{P}_{(X,Y) \sim P_{X,Y}^j}(s(X,Y) \leq \eta^{\Omega_j}(X,Y)) \geq 1 - \alpha$$

□

B.4.1 COPP for class-balanced coverage

Algorithm 2: COPP for class-balanced coverage

Inputs: Observational data $\mathcal{D}_{obs} = \{X_i, A_i, Y_i\}_{i=1}^{n_{obs}}$, conf. level α , a score function $s(x,y) \in \mathbb{R}$, new data point x^{test} , target policy π^* ;

Output: $\hat{C}_n^{\mathcal{Y}}(x^{test})$ with coverage guarantee (45);

Split \mathcal{D}_{obs} into training data (\mathcal{D}_{tr}) and calibration data (\mathcal{D}_{cal}) of sizes m and n respectively;

Use \mathcal{D}_{tr} to estimate weights $\hat{w}(\cdot, \cdot)$;

for $y \in \mathcal{Y}$ **do**

 Let $\{X_j^y, Y_j^y\}_{j=1}^{n_y}$ be the following subset of calibration data: $\{(X_i, Y_i) : Y_i = y\}$;

 Let $V_j^y := s(X_j^y, Y_j^y)$, for $j = 1, \dots, n_y$;

 Define $\hat{F}_n^{x,y} = \sum_{i=1}^{n_y} p_i^w(x,y) \delta_{V_i^y} + p_{n+1}^w(x,y) \delta_{\infty}$;

 where, $p_i^w(x,y) := \frac{w(X_i^y, Y_i^y)}{\sum_{i=1}^{n_y} w(X_i^y, Y_i^y) + w(x,y)}$, $p_{n+1}^w(x,y) := \frac{w(x,y)}{\sum_{i=1}^{n_y} w(X_i^y, Y_i^y) + w(x,y)}$;

$\eta(x,y) := \text{Quantile}_{1-\alpha}(\hat{F}_n^{x,y})$

end

Define $\hat{C}_n^{\mathcal{Y}}(x^{test}) := \{y : s(x^{test}, y) \leq \eta(x^{test}, y)\}$;

Return $\hat{C}_n^{\mathcal{Y}}(x^{test})$

In the case when Y is discrete, we construct predictive sets, $\hat{C}_n^{\mathcal{Y}}(x)$, which offer label conditioned coverage guarantees using the methodology described above,

$$\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n^{\mathcal{Y}}(X) \mid Y = y) \geq 1 - \alpha, \text{ for all } y \in \mathcal{Y} \quad (45)$$

This is a strictly stronger guarantee than marginal coverage, i.e. $\mathbb{P}_{(X,Y) \sim P_{X,Y}^{\pi^*}}(Y \in \hat{C}_n(X)) \geq 1 - \alpha$. To understand what (45) means, consider our running example of recommendation systems, where the outcome Y is whether the recommendation is relevant (0) or not (1) to the user. Then, Eq. (45) ensures that out of the users who received irrelevant recommendations, the predictive sets contain ‘not relevant’ (1) at least $100 \cdot (1 - \alpha)\%$ of the times. This can be thought of as controlling the false negative rate of irrelevant recommendations at $100 \cdot \alpha\%$. The same is true for users who receive relevant recommendations. This is particularly useful when data is imbalanced, for example when majority of the users in observational receive relevant recommendations.

B.5 Weights estimation $\hat{w}(x, y)$

B.5.1 Consistent estimation of the weights does not imply consistent estimation of $\hat{P}(y|x, a)$

In Proposition 4.1, we assume to have consistent estimator of $w(x, y)$ which begs the following question: In general, does a consistent estimate of $w(x, y)$ imply that we also obtain a consistent estimate of $P(y|x, a)$? In particular, one could then just use the estimate of $\hat{P}(y|x, a)$ to construct the predictive interval. However, we answer the above question with the negative by supplying a counter example.

Counter-example:

Let $X \in [1, +\infty)$, $a \in \mathbb{R}$ s.t. $|a| < K$ for $K \in \mathbb{R}_{>0}$.

Let $Y|X, a \sim \mathcal{N}((KX^2 + a)^{0.5}, (KX^2 - a))$.

We have $\mathbb{E}[Y^2|X, a] = \text{Var}(Y|X, a) + \mathbb{E}[Y|X, a]^2 = KX^2 + a + KX^2 - a = 2KX^2$ (independent of a)

Next let

$$\hat{P}(y|x, a) := \frac{y^2 P(y|x, a)}{2KX^2}. \quad (46)$$

Recall that

$$w(x, y) = \frac{\int P(y|x, a) \pi^*(a|x) da}{\int P(y|x, a) \pi^b(a|x) da} \quad (47)$$

Using the above definition of $\hat{P}(y|x, a)$ we have:

$$\begin{aligned} \hat{w}(x, y) &= \frac{\int \hat{P}(y|x, a) \pi^*(a|x) da}{\int \hat{P}(y|x, a) \pi^b(a|x) da} \\ &= \frac{\int P(y|x, a) \frac{Y^2}{2KX^2} \pi^*(a|x) da}{\int P(y|x, a) \frac{Y^2}{2KX^2} \pi^b(a|x) da} \\ &= w(x, y). \end{aligned}$$

Hence, $w(x, y) \equiv \hat{w}(x, y) \not\Rightarrow \hat{P}(y|x, a) \equiv P(y|x, a)$. □

More generally, if there exists a function $\Phi : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}_{\geq 0}$ such that

1. $\Phi(x, y)$ is not constant in y
2. $0 < \mathbb{E}[\Phi(X, Y) | X, A] < \infty$, and does not depend on A

Then, we can define $\tilde{P}(y|x, a) := P(y|x, a) \Phi(x, y) / \mathbb{E}[\Phi(X, Y) | X, A]$, and the weights computed using $\tilde{P}(y|x, a)$ will be the equal to $w(x, y)$ even though $\tilde{P}(y|x, a) \neq P(y|x, a)$.

B.5.2 Alternative ways to estimate $\hat{w}(x, y)$ without estimating $\hat{P}(y|x, a)$

In this section, we show how we could estimate $w(x, y)$ without having to estimate $\hat{P}(y|x, a)$. One way to obtain an estimate $\hat{w}(x, y)$ is by taking a closer look at the definition of $w(x, y)$ and rewriting the ratio.

$$\begin{aligned} w(x, y) &= \frac{P_{X,Y}^{\pi^*}(x, y)}{P_{X,Y}^{\pi^b}(x, y)} \\ &= \int \frac{P_{X,A,Y}^{\pi^*}(x, a, y)}{P_{X,A,Y}^{\pi^b}(x, a, y)} P_{A|X,Y}^{\pi^b}(a|x, y) da \\ &= \int \frac{\pi^*(a|x)}{\pi^b(a|x)} P_{A|X,Y}^{\pi^b}(a|x, y) da \\ &= \mathbb{E}_{A \sim P_{A|X=x, Y=y}^{\pi^b}} \left[\frac{\pi^*(A|x)}{\pi^b(A|x)} \right]. \end{aligned} \quad (48)$$

Lemma B.2. Let $w(x, y) = \frac{P_{X,Y}^{\pi^*}(x, y)}{P_{X,Y}^{\pi^b}(x, y)}$, then

$$w(x, y) = \arg \min_f \mathbb{E}_{X,A,Y \sim P_{X,A,Y}^{\pi^b}} \left[\left\| \frac{\pi^*(A|X)}{\pi^b(A|X)} - f(X, Y) \right\|^2 \right]. \quad (49)$$

Proof of Lemma B.2 This follows directly from the identity (48). We prove it here for sake of completeness.

$$\begin{aligned} & \mathbb{E}_{X,A,Y \sim P_{X,A,Y}^{\pi^b}} \left[\left\| \frac{\pi^*(A|X)}{\pi^b(A|X)} - f(X, Y) \right\|^2 \right] \\ &= \mathbb{E}_{X,Y \sim P_{X,Y}^{\pi^b}} \left[\mathbb{E}_{A \sim P_{A|X,Y}^{\pi^b}} \left\| \frac{\pi^*(A|X)}{\pi^b(A|X)} - f(X, Y) \right\|^2 \right] \\ &= \mathbb{E}_{X,Y \sim P_{X,Y}^{\pi^b}} \left[\text{Var}_{A \sim P_{A|X,Y}^{\pi^b}} \left[\frac{\pi^*(A|X)}{\pi^b(A|X)} \right] + \left(\mathbb{E}_{A \sim P_{A|X,Y}^{\pi^b}} \left[\frac{\pi^*(A|X)}{\pi^b(A|X)} \right] - f(X, Y) \right)^2 \right]. \quad (50) \end{aligned}$$

Where, (50) is minimized if $f(x, y) = \mathbb{E}_{A \sim P_{A|X=x,Y=y}^{\pi^b}} \left[\frac{\pi^*(A|x)}{\pi^b(A|x)} \right] = w(x, y)$. \square

Using Lemma B.2, we can thus approximate $w(x, y)$ by minimizing the loss

$$\hat{w}(x, y) = \arg \min_{f_\theta} \mathbb{E}_{X,A,Y \sim P_{X,A,Y}^{\pi^b}} \left[\left\| \frac{\pi^*(A|X)}{\pi^b(A|X)} - f_\theta(X, Y) \right\|^2 \right] \quad (51)$$

Hence we see that the ratio estimation problem can be rewritten as a regression problem where $f_\theta(x, y)$ is for example a neural network. This allows one to estimate directly, without the need for estimating $\hat{P}(y | x, a)$ first.

C Estimation of the quantiles of the target distribution

As mentioned in Section 4.2, we present here a way to estimate the quantiles of the target distribution $P_{X,Y}^{\pi^*}$ consistently when the ground truth weight function $w(x, y)$ is known. As we are interested in the quantiles, we will be using the pinball loss to train our model \hat{f}_θ defined by

$$L_\alpha(\theta, x, y) = \begin{cases} \alpha(\hat{f}_\theta(x) - y) & \text{if } (\hat{f}_\theta(x) - y) > 0, \\ (1 - \alpha)(y - \hat{f}_\theta(x)) & \text{if } (\hat{f}_\theta(x) - y) < 0. \end{cases}$$

Then we have the following objective to optimize:

$$\begin{aligned} \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^*}} [L_\alpha(\theta, X, Y)] &= \int_{X,Y} L_\alpha(\theta, x, y) P_{X,Y}^{\pi^*}(\mathrm{d}x, \mathrm{d}y) \\ &= \int_{X,Y} L_\alpha(\theta, x, y) \frac{\mathrm{d}P_{X,Y}^{\pi^*}(x, y)}{\mathrm{d}P_{X,Y}^{\pi^b}(x, y)} P_{X,Y}^{\pi^b}(\mathrm{d}x, \mathrm{d}y) \\ &= \int_{X,Y} L_\alpha(\theta, x, y) w(x, y) P_{X,Y}^{\pi^b}(\mathrm{d}x, \mathrm{d}y) \\ &= \mathbb{E}_{(X,Y) \sim P_{X,Y}^{\pi^b}} [L_\alpha(\theta, X, Y) w(X, Y)]. \end{aligned}$$

The above holds true if the true weight function is known. However in the case where we only have a consistent estimator of $w(x, y)$, it remains to be proven that the above objective will also yield a consistent estimator of the quantiles under π^* . We leave this for future work to prove as we are simply providing a possible avenue to relax the assumptions in Proposition 4.2.

D Experiments

The code for our experiments is available at <https://anonymous.4open.science/r/COPP-75F5> and we ran all our experiments on Intel(R) Xeon(R) CPU E5-2690 v4 @ 2.60GHz with 8GB RAM per core. We were able to use 100 CPUs in parallel to iterate over different configurations and seeds. However, we would like to note that our algorithms only requires 1 CPU and at most 10 mins to run, as our networks are relatively small.

D.1 Toy Experiment

D.1.1 Synthetic data experiments setup

Model. The observational data distribution is defined as follows:

$$\begin{aligned} X_i &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 9) \\ A_i \mid x_i &\sim \pi^b(\cdot \mid x_i) \text{ where } \pi^b \text{ has been defined below} \\ Y_i \mid x_i, a_i &\sim \mathcal{N}(a_i * x_i, 1) \end{aligned}$$

Behaviour and Target Policies. We define a family of policies $\pi_\epsilon(a \mid x)$ as follows:

$$\pi_\epsilon(a \mid x) := \begin{cases} \epsilon \mathbb{1}(a \in \{1, 2, 3\}) + (1 - 3\epsilon) \mathbb{1}(a = 4) & \text{if } |x| \in (3, \infty) \\ \epsilon \mathbb{1}(a \in \{1, 2, 4\}) + (1 - 3\epsilon) \mathbb{1}(a = 3) & \text{if } |x| \in (2, 3] \\ \epsilon \mathbb{1}(a \in \{1, 3, 4\}) + (1 - 3\epsilon) \mathbb{1}(a = 2) & \text{if } |x| \in (1, 2] \\ \epsilon \mathbb{1}(a \in \{2, 3, 4\}) + (1 - 3\epsilon) \mathbb{1}(a = 1) & \text{if } |x| \in [0, 1] \end{cases}$$

We use the parameter $\epsilon \in (0, 1/3)$ to control the policy shift between target and behaviour policies. For the behaviour policy π^b , we use $\epsilon^b = 0.3$, and for target policies π^* , we use $\epsilon^* \in \{0.1, 0.2, 0.3\}$. Here we use $m = 1000$ training datapoints.

Neural Network Architectures

- To approximate the behaviour policy π^b , we use a neural network with 2 hidden layers and 16 nodes in each hidden layer, and ReLU activation function.
- To approximate $P(y \mid x, a)$, we use $\mathcal{N}(\mu(x, a), \sigma(x, a))$, where μ and σ are neural networks with one-hidden layer, 32 nodes in the hidden layer, and ReLU activation function.
- For the score function, we train the quantiles $\hat{q}_{\alpha/2}$ and $\hat{q}_{1-\alpha/2}$ using quantile regression, each of which are modelled using neural networks with one-hidden layer, 32 nodes in the hidden layer, and ReLU activation functions.

Results: Coverage as a function of increase calibration data As mentioned in the main text, we have also performed experiments to investigate how much calibration data is needed for COPP as well as other methods to converge to the required 90% coverage. In the below figure 4 we have plotted the coverage as a function of n calibration data points. Our proposed method is converging much faster to the required coverage compared to the competing methods.

Additional experimental baseline using weighted quantile regression. In order to add an additional baseline that is also covariate dependent, we have added some experiments using the weighted quantile regression (WQR) as described in Sec. C on our toy experiments from Sec. 6 in the main text. Below in Table 3 and Table 4 we see the complete coverage table with the respective interval lengths. Note also that WQR does not seem to perform well as it does not have any statistical guarantees and heavily relies on good estimation of the ratio. We have added these experiments here in the appendix for completeness and did not add it in the main text as the results were not comparable to other baselines.

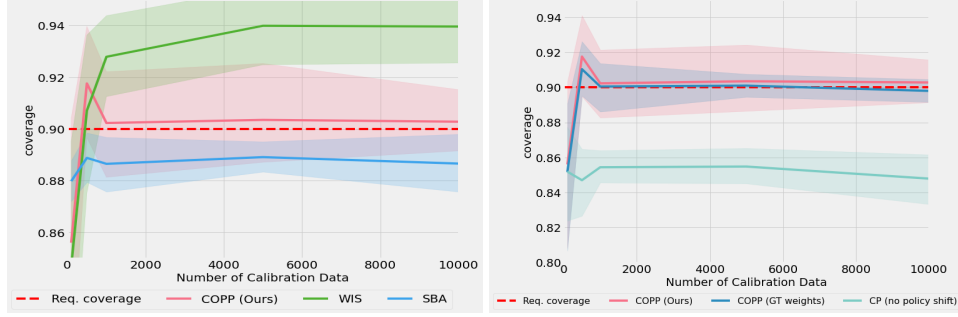


Figure 4: Results for synthetic data experiment with $\pi^b = \pi_{0.3}$ and the target policy is $\pi^* = \pi_{0.1}$. **Left:** our proposed method is able to converge to the required coverage rather quickly compared to the competing methods. **Right:** here we see that our method is on par with using the GT weights. Due to estimation error, COPP with estimated weights has slightly higher variance in terms of coverage

Table 3: Mean Coverage as a function of policy shift with 2 standard errors over 10 runs. We have added weighted quantile regression (WQR) for completeness and note that it does not seem to perform well.

Coverage	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$
COPP (Ours)	0.90 ± 0.01	0.90 ± 0.01	0.91 ± 0.01
WIS	0.89 ± 0.01	0.91 ± 0.02	0.94 ± 0.02
SBA	0.90 ± 0.01	0.88 ± 0.01	0.87 ± 0.01
COPP (GT weights Ours)	0.90 ± 0.01	0.90 ± 0.01	0.90 ± 0.01
CP (no policy shift)	0.90 ± 0.01	0.87 ± 0.01	0.85 ± 0.01
CP (union)	0.96 ± 0.01	0.96 ± 0.01	0.96 ± 0.01
WQR	0.82 ± 0.04	0.76 ± 0.03	0.70 ± 0.03

Table 4: Mean Interval Length as a function of policy shift with 2 standard errors over 10 runs. We have added weighted quantile regression (WQR) for completeness and note that it does not seem to perform well.

Interval Lengths	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$
COPP (Ours)	9.08 ± 0.10	9.48 ± 0.22	9.97 ± 0.38
WIS	24.14 ± 0.30	32.96 ± 1.80	43.12 ± 3.49
SBA	8.78 ± 0.12	8.94 ± 0.10	8.33 ± 0.09
COPP (GT weights Ours)	8.91 ± 0.09	9.25 ± 0.12	9.59 ± 0.20
CP (no policy shift)	9.00 ± 0.10	9.00 ± 0.10	9.00 ± 0.10
CP (union)	10.66 ± 0.18	11.04 ± 0.2	11.4 ± 0.26
WQR	8.55 ± 0.50	8.61 ± 0.52	8.70 ± 0.55

D.1.2 Experiments with continuous action space

As mentioned in the main text and also in Sec. B.1, our proposed method, contrary to the work of Lei and Candès [2021] is able to also handle continuous action space. Given that we are integrating out the actions when computing the weights in Eq. 7 our method trivially extends to the continuous action space, whereas Lei and Candès [2021] is only applicable for discrete action spaces, as they compute conformal intervals conditioned on a given action.

Model. The observational data distribution is defined as follows:

$$\begin{aligned}
 X_i &\stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, 4) \\
 A_i \mid x_i &\sim \mathcal{N}(x_i/4, 1) \\
 Y_i \mid x_i, a_i &\sim \mathcal{N}(a_i + x_i, 1)
 \end{aligned}$$

Target Policies. We define a family of policies $\pi_\epsilon(a \mid x)$ as follows:

$$\pi_\epsilon(a \mid x) = \mathcal{N}(x/4 + \epsilon, 1). \quad (52)$$

In our experiments, for the target policy π^* , we use $\pi^* = \pi_{\epsilon^*}$ for $\epsilon^* \in \{0, 0.5, 1, 1.5, 2, 2.5\}$.

Results. Table 5 shows the coverages of different methods as the policy shift ϵ^* increases. The behaviour policy $\pi^b = \pi_0$ is fixed and we use $n = 5000$ calibration datapoints and $m = 1000$ training points, across 10 runs. Table 5 shows, how COPP stays very close to the required coverage of 90% across all target policies with $\epsilon^* \leq 2.0$, compared to WIS and SBA. Both, WIS intervals and SBA intervals suffer from under-coverage i.e. below the required coverage. These results again support our hypothesis from Sec. 3.1, which stated that COPP is less sensitive to estimation errors of $\hat{P}(y|x, a)$ compared to directly using $\hat{P}(y|x, a)$ for the intervals i.e. SBA.

Next, Table 6 shows the mean interval lengths and even though WIS intervals are under-covered, the average interval length is huge compared to COPP. Additionally, for $\epsilon^* \in \{0, 0.5, 1, 1.5\}$, COPP with estimated weights produces results which are close to COPP intervals with ground truth weights. This shows that when the behaviour and target policies have reasonable overlap, the effect of weights estimation error on COPP results is limited. However, as ϵ^* increases to 2.0 and 2.5, the overlap between behaviour and target policies becomes low. We empirically note that this leads to high weights estimation error and consequently under-coverage in COPP with estimated weights. In contrast, COPP with ground truth weights still achieves required coverage, even though it becomes conservative when the overlap is low. Figure 5 visualises how the overlap between target and behaviour policies decreases with increasing ϵ^* . It can be seen that $\epsilon^* \in \{2, 2.5\}$ leads to very low overlap between the behaviour and target data.

Table 5: Mean Coverage as a function of policy shift with 2 standard errors over 10 runs.

Coverage	$\epsilon^* = 0.0$	$\epsilon^* = 0.5$	$\epsilon^* = 1.0$	$\epsilon^* = 1.5$	$\epsilon^* = 2.0$	$\epsilon^* = 2.5$
COPP (Ours)	0.90 \pm 0.01	0.91 \pm 0.01	0.92 \pm 0.01	0.91 \pm 0.01	0.89 \pm 0.02	0.85 \pm 0.02
WIS	0.87 \pm 0.01	0.87 \pm 0.01	0.87 \pm 0.01	0.87 \pm 0.02	0.89 \pm 0.02	0.83 \pm 0.02
SBA	0.86 \pm 0.01	0.86 \pm 0.01	0.86 \pm 0.01	0.86 \pm 0.01	0.89 \pm 0.02	0.83 \pm 0.02
COPP (GT Weights Ours)	0.90 \pm 0.01	0.91 \pm 0.01	0.91 \pm 0.01	0.90 \pm 0.01	0.96 \pm 0.02	0.93 \pm 0.02
CP (no policy shift)	0.90 \pm 0.01	0.88 \pm 0.01	0.82 \pm 0.01	0.73 \pm 0.01	0.60 \pm 0.01	0.46 \pm 0.01

Table 6: Mean Interval Length as a function of policy shift with 2 standard errors over 10 runs.

Interval Lengths	$\epsilon^* = 0.0$	$\epsilon^* = 0.5$	$\epsilon^* = 1.0$	$\epsilon^* = 1.5$	$\epsilon^* = 2.0$	$\epsilon^* = 2.5$
COPP (Ours)	4.75 \pm 0.04	5.08 \pm 0.09	5.89 \pm 0.14	6.92 \pm 0.18	7.82 \pm 0.41	8.45 \pm 0.44
WIS	9.55 \pm 0.1	9.56 \pm 0.12	9.56 \pm 0.27	9.44 \pm 0.38	9.40 \pm 0.59	9.08 \pm 0.64
SBA	4.38 \pm 0.03	4.37 \pm 0.03	4.36 \pm 0.04	4.34 \pm 0.07	4.31 \pm 0.1	4.28 \pm 0.14
COPP (GT Weights Ours)	4.73 \pm 0.05	5.07 \pm 0.09	5.87 \pm 0.14	6.82 \pm 0.13	7.57 \pm 0.19	8.07 \pm 0.22
CP (no policy shift)	4.70 \pm 0.05	4.70 \pm 0.05	4.70 \pm 0.05	4.70 \pm 0.05	4.70 \pm 0.05	4.70 \pm 0.05

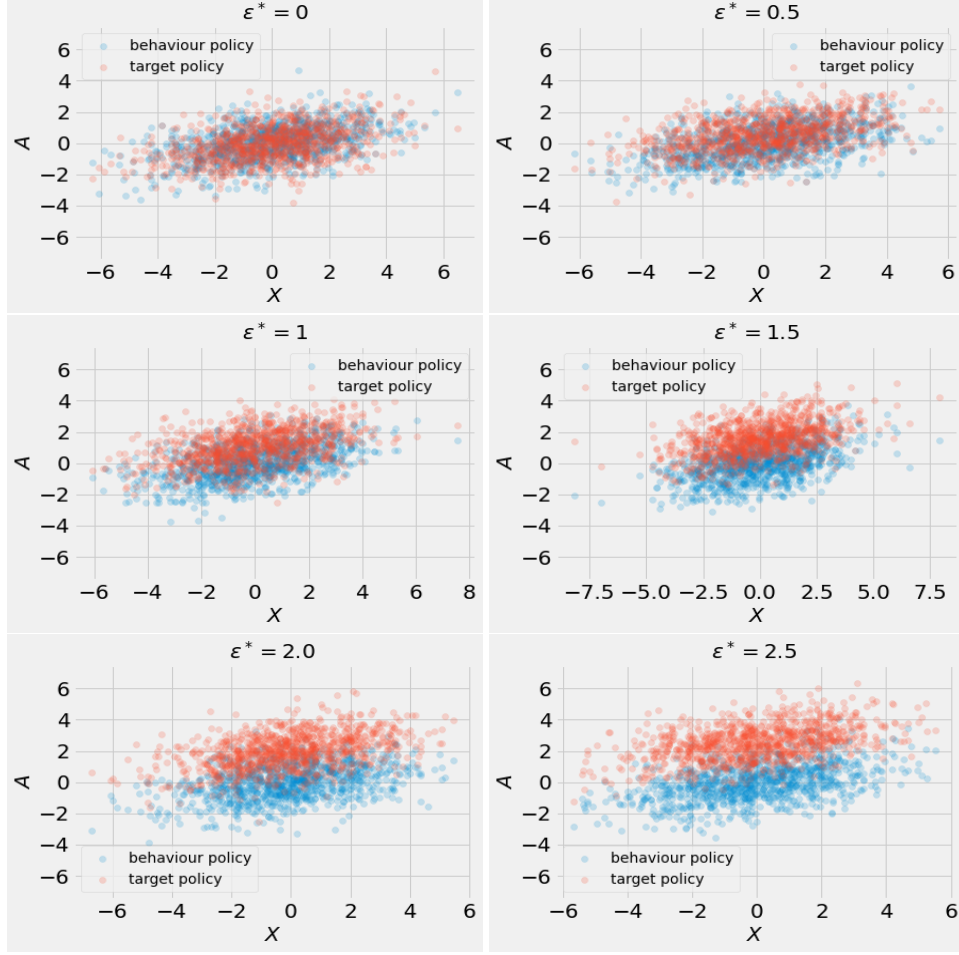


Figure 5: Plots of A against X , where $X \sim \mathcal{N}(0, 4)$ and $A | X$ is sampled from behaviour and target policies. Here, target policies are defined in (52) for $\epsilon^* \in \{0, 0.5, 1, 1.5, 2, 2.5\}$.

D.2 Experiments on Microsoft Ranking Dataset

Dataset details. The dataset contains relevance scores for websites recommended to different users, and comprises of 30,000 user-website pairs. For a user i and website j , the data contains a 136-dimensional feature vector u_i^j , which consists of user i 's attributes corresponding to website j , such as length of stay or number of clicks on the website. Furthermore, for each user-website pair, the dataset also contains a relevance score, i.e. how relevant the website was to the user.

First, given a user i we sample (with replacement) 5 websites, $\{u_i^j\}_{j=1}^5$, from the data. Next, we reformulate this into a contextual bandit where $A \in \{1, 2, 3, 4, 5\}$ corresponds to the website we recommend to a user. For a user i , we define X by combining the 5 feature vectors corresponding to the user, i.e. $X \in \mathbb{R}^{5 \times 136}$, where $x_i = (u_i^1, u_i^2, u_i^3, u_i^4, u_i^5)$. In addition, $Y \in \{0, 1, 2, 3, 4\}$ corresponds to the relevance score for the A 'th website, i.e. the recommended website. The goal is to construct prediction sets that are guaranteed to contain the true relevance score with a probability of 90%. Here we use $m = 5000$ training data points.

Behaviour and Target Policies. We first train a Neural Network (NN) classifier model mapping each 136-dimensional feature vector to the softmax scores for each relevance score class, $\hat{f}_\theta : \mathcal{U} \rightarrow [0, 1]^5$. We use this trained model \hat{f}_θ to define a family of policies such that we pick the most relevant website as predicted by \hat{f}_θ with probability ϵ and the rest uniformly with probability $(1 - \epsilon)/4$.

Formally, this has been expressed as follows. We use $\hat{f}_\theta^{\text{label}}$ to denote the relevance class predicted by \hat{f}_θ , i.e. $\hat{f}_\theta^{\text{label}}(u) := \arg \max_i \{\hat{f}_\theta(u)_i\}$.

Then,

$$\begin{aligned} \pi_\epsilon(a \mid X = (u^1, u^2, u^3, u^4, u^5)) := & \epsilon \mathbb{1}(a = \arg \max_j \{\hat{f}_\theta^{\text{label}}(u^j)\}) \\ & + (1 - \epsilon)/4 \mathbb{1}(a \neq \arg \max_j \{\hat{f}_\theta^{\text{label}}(u^j)\}) \end{aligned}$$

Estimation of ratios, $\hat{w}(X, Y)$. To estimate the $\hat{P}(y \mid x, a)$ we use the trained model \hat{f}_θ as follows:

$$\hat{P}(y \mid x = (u^1, u^2, u^3, u^4, u^5), a) = \hat{f}_\theta(u^a)_y$$

where $\hat{f}_\theta(u^a)_y$ corresponds to the softmax prediction of u^a for label y under the model \hat{f}_θ . To estimate the behaviour policy $\hat{\pi}^b$, we train a classifier model $\mathcal{X} \rightarrow \mathcal{A}$ using a neural network. We use (7) to estimate the weights $\hat{w}(x, y)$.

Neural Network Architectures

- To approximate the behaviour policy, we use a neural network with 2 hidden layers and 25 nodes in each hidden layer, ReLU activations and softmax output.
- To approximate \hat{f}_θ , we use a neural network with 2 hidden layers with 64 nodes each and ReLU activations.

Results: Coverage as a function of increase calibration data. As mentioned in the main text, we have also performed experiments to investigate how much calibration data is needed for COPP as well as other methods to converge to the required 90% coverage. In the below plot we have plotted the coverage as a function of n calibration data points. We observe that our proposed method is converging much faster to the required coverage compared to the competing methods.

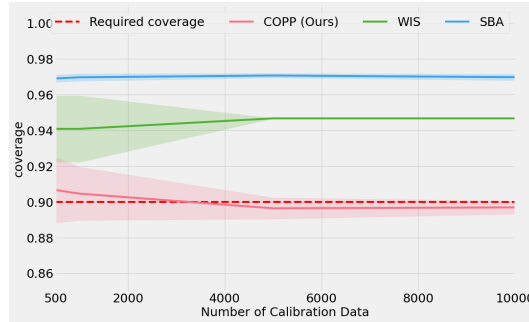


Figure 6: Results of Microsoft Ranking Dataset experiment with behaviour policy $\pi^b = \pi_{0.5}$ and the target policy is $\pi^* = \pi_{0.2}$. Our proposed method is able to converge to the required coverage rather quickly compared to the competing methods

Table 7: Coverages for COPP with and without label conditioned coverage, $\hat{C}_n^{\mathcal{Y}}$ and \hat{C}_n respectively. Overall coverage refers to marginal coverage while $Y = y$ refers to coverage conditioned on $Y = y$. Here n_{test} corresponds to the number of test data points ($\sim P^{\pi^*}$).

	n_{test}	\hat{C}_n Cov	$\hat{C}_n^{\mathcal{Y}}$ Cov
Overall	5000	0.896 ± 0.005	0.941 ± 0.003
$Y = 0$	266	0.700 ± 0.020	1.000 ± 0.000
$Y = 1$	293	0.526 ± 0.019	1.000 ± 0.000
$Y = 2$	228	0.772 ± 0.018	0.990 ± 0.029
$Y = 3$	320	0.852 ± 0.015	0.964 ± 0.035
$Y = 4$	3893	0.950 ± 0.006	0.928 ± 0.003

D.2.1 Results: COPP for Class-balanced coverage

Table 7 shows the coverages of COPP predictive sets (\hat{C}_n with marginal coverage guarantee constructed using algorithm 1) and COPP intervals with label conditioned coverage ($\hat{C}_n^{\mathcal{Y}}$ satisfying (45) constructed using algorithm 2). Extensions of WIS and SBA to the conditional case are not straightforward and hence have not been included. For \hat{C}_n , while the overall coverage is very close to the required coverage of 90%, we see that there is under-coverage for $Y = 0, 1, 2, 3$. This can be explained by the data imbalance – the number of test data points with $Y = 0, 1, 2, 3$ is significantly lower than $Y = 4$.

This under-coverage problem disappears in $\hat{C}_n^{\mathcal{Y}}$. Instead, in cases where number of data points is small, ($Y = 0, 1, 2, 3$), the predictive sets $\hat{C}_n^{\mathcal{Y}}$ are conservative (i.e. have coverage $> 90\%$). As a result, the overall coverage increases to 0.941. This is a price to be paid for label conditioned coverage – the overall coverage may increase, however, being conservative in safety-critical settings is better than being overly optimistic.

D.3 UCI Dataset experiments

Following Huang et al. [2021]; Dudík et al. [2014]; Wang et al. [2017] we apply COPP on UCI classification datasets. We can pose classification as contextual bandits by defining the covariates \mathcal{X} as the features, the action space $\mathcal{A} = \mathcal{K}$, where \mathcal{K} is the set of labels, and the outcomes are binary, i.e. $\mathcal{Y} = \{0, 1\}$, defined by $Y | X, A = \mathbb{1}(X \text{ belongs to class } A)$. Here we use $m = 1000$ training data points.

Behaviour and Target Policies. First we train a neural network classifier mapping each covariate to the softmax scores for each class, $\hat{f}_\theta : \mathcal{X} \rightarrow [0, 1]^{|\mathcal{K}|}$. We use this trained model \hat{f}_θ to define a family of policies such that we pick the most likely label as predicted by \hat{f}_θ with probability ϵ and the rest uniformly with probability. Formally, this can be expressed as follows:

$$\pi_\epsilon(a | x) := \epsilon \mathbb{1}(a = \arg \max_{k \in \mathcal{K}} \{\hat{f}_\theta(x)_k\}) + (1 - \epsilon) / (|\mathcal{K}| - 1) \mathbb{1}(a \neq \arg \max_{k \in \mathcal{K}} \{\hat{f}_\theta(x)_k\})$$

Like other experiments, we use ϵ to control the shift between behaviour and target policies. For π^b , we use $\epsilon^b = 0.5$ and for $\epsilon^* \in \{0.05, 0.3, 0.4, 0.5, 0.6, 0.7, 0.95\}$. Using this behaviour policy π^b , we generate an observational dataset $\mathcal{D}_{obs} = \{x_i, a_i, y_i\}_{i=1}^{n_{obs}}$ which is then split into training \mathcal{D}_{tr} and calibration datasets \mathcal{D}_{cal} , of sizes m and n respectively.

Estimation of ratios, $\hat{w}(X, Y)$. To estimate the $\hat{P}(y | x, a)$ we use the trained model \hat{f}_θ as follows:

$$\hat{P}(Y = 1 | x, a) = \hat{f}_\theta(x)_a$$

where $\hat{f}_\theta(x)_a$ corresponds the softmax prediction of x for label a under the model \hat{f}_θ . To estimate the behaviour policy π^b , we train a classifier model $\mathcal{X} \rightarrow \mathcal{A}$ using a neural network. We use (7) in main text to estimate weights $\hat{w}(x, y)$.

Score. We define $\hat{P}^{\pi^b}(y | x) = \sum_{i \in \mathcal{K}} \hat{\pi}^b(A = i | x) \hat{P}(y | x, A = i)$. Using similar formulation as in Angelopoulos and Bates [2021], we define the score as

$$s(x, y) = \sum_{y'=0,1} \hat{P}^{\pi^b}(y' | x) \mathbb{1}(\hat{P}^{\pi^b}(y' | x) \geq \hat{P}^{\pi^b}(y | x))$$

Neural Network Architectures

- To approximate the behaviour policy, we use a neural network with 2 hidden layers and 64 nodes in each hidden layer, ReLU activations and softmax output.
- To approximate \hat{f}_θ , we use a neural network with 2 hidden layers with 64 nodes each and ReLU activations.

Results. Tables 8-13 show the coverages across varying target policies for different classification datasets. The behaviour policy $\pi^b = \pi_{0.5}$ is fixed and we use $n = 5000$ calibration datapoints, across 10 runs with $m = 5000$ training data. The tables show that COPP is able to provide the required coverage of 90% across all target policies. Moreover, compared to COPP, SBA and WIS are overly conservative. WIS estimates are not adaptive w.r.t. X , and as a result, the predictive sets produced are uninformative (i.e. contain all outcomes) in these experiments where the outcome is binary.

We have also included a comparison of COPP using estimated behaviour policy with COPP using GT behaviour policy. The latter provides more accurate coverage, and using estimated behaviour policy provides slightly over-covered predictive sets comparatively in most cases. This can be explained by policy estimation error. Additionally, we observe that using standard CP leads to predictive sets which are not adaptive to policy shift. As a result, the standard CP predictive sets get overly conservative (optimistic) as Δ_ϵ becomes more negative (positive).

Table 8: Yeast dataset results

	$\Delta_\epsilon = -0.45$	$\Delta_\epsilon = -0.2$	$\Delta_\epsilon = -0.1$	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$	$\Delta_\epsilon = 0.45$
COPP (Ours)	0.92±0.00	0.92±0.00	0.92±0.00	0.92±0.00	0.92±0.00	0.92±0.00	0.91±0.00
WIS	0.99±0.01	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
SBA	0.98±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
COPP (GT behav policy)	0.91±0.00	0.91±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00
CP (no policy shift)	0.97±0.00	0.93±0.00	0.92±0.00	0.90±0.00	0.89±0.00	0.87±0.00	0.83±0.00

Table 9: Ecoli dataset results

	$\Delta_\epsilon = -0.45$	$\Delta_\epsilon = -0.2$	$\Delta_\epsilon = -0.1$	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$	$\Delta_\epsilon = 0.45$
COPP (OURS)	0.92±0.00	0.91±0.00	0.91±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00
WIS	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
SBA	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
COPP (GT BEHAV POLICY)	0.91±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.01
CP (NO POLICY SHIFT)	0.92±0.00	0.91±0.00	0.91±0.00	0.90±0.00	0.90±0.00	0.89±0.00	0.88±0.00

Table 10: Letter dataset results

	$\Delta_\epsilon = -0.45$	$\Delta_\epsilon = -0.2$	$\Delta_\epsilon = -0.1$	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$	$\Delta_\epsilon = 0.45$
COPP (OURS)	0.95±0.00	0.93±0.00	0.93±0.00	0.92±0.00	0.92±0.00	0.92±0.00	0.91±0.00
WIS	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
SBA	0.97±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
COPP (GT BEHAV POLICY)	0.92±0.00	0.91±0.00	0.91±0.00	0.90±0.00	0.89±0.00	0.89±0.00	0.88±0.00
CP (NO POLICY SHIFT)	0.99±0.00	0.94±0.00	0.92±0.00	0.90±0.00	0.88±0.00	0.86±0.00	0.81±0.00

Table 11: Optdigits dataset results

	$\Delta_\epsilon = -0.45$	$\Delta_\epsilon = -0.2$	$\Delta_\epsilon = -0.1$	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$	$\Delta_\epsilon = 0.45$
COPP (OURS)	0.93±0.00	0.93±0.00	0.93±0.00	0.93±0.00	0.93±0.00	0.93±0.00	0.93±0.00
WIS	0.99±0.01	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
SBA	0.97±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	0.99±0.00
COPP (GT BEHAV POLICY)	0.91±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.89±0.00	0.89±0.00
CP (NO POLICY SHIFT)	0.97±0.00	0.93±0.00	0.91±0.00	0.90±0.00	0.88±0.00	0.87±0.00	0.83±0.00

Table 12: Pendigits dataset results

	$\Delta_\epsilon = -0.45$	$\Delta_\epsilon = -0.2$	$\Delta_\epsilon = -0.1$	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$	$\Delta_\epsilon = 0.45$
COPP (OURS)	0.92±0.00	0.92±0.00	0.92±0.00	0.92±0.00	0.92±0.00	0.92±0.00	0.91±0.00
WIS	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
SBA	0.97±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	0.99±0.00
COPP (GT BEHAV POLICY)	0.91±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.89±0.00	0.89±0.00
CP (NO POLICY SHIFT)	0.99±0.00	0.94±0.00	0.92±0.00	0.90±0.00	0.88±0.00	0.86±0.00	0.81±0.00

Table 13: Satimage dataset results

	$\Delta_\epsilon = -0.45$	$\Delta_\epsilon = -0.2$	$\Delta_\epsilon = -0.1$	$\Delta_\epsilon = 0.0$	$\Delta_\epsilon = 0.1$	$\Delta_\epsilon = 0.2$	$\Delta_\epsilon = 0.45$
COPP (OURS)	0.92±0.00	0.91±0.00	0.91±0.00	0.91±0.00	0.91±0.00	0.91±0.00	0.91±0.00
WIS	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00
SBA	0.98±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	1.00±0.00	0.99±0.00
COPP (GT BEHAV POLICY)	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.90±0.00	0.89±0.00
CP (NO POLICY SHIFT)	0.97±0.00	0.93±0.00	0.92±0.00	0.90±0.00	0.88±0.00	0.87±0.00	0.83±0.00

E How the miscoverage depends on $\hat{P}(y \mid x, a)$

Proposition E.1. *Let*

$$\tilde{w}(x, y) := \frac{\int \hat{P}(y \mid x, a) \pi^*(a \mid x) da}{\int \hat{P}(y \mid x, a) \pi^b(a \mid x) da}.$$

Assume that $\hat{P}(y \mid x, a)/P(y \mid x, a) \in [1/\Gamma, \Gamma]$ for some $\Gamma \geq 1$. Then,

$$\Delta_w := \frac{1}{2} \mathbb{E}_{(X,Y) \sim P_{\tilde{X},Y}^{\pi^b}} \mid \tilde{w}(X, Y) - w(X, Y) \mid \leq \Gamma^2 - 1.$$

Proof. In this proof, we investigate the error of the weights as a function of the error in $\hat{P}(y \mid x, a)$. Therefore, to isolate this effect we ignore the Monte Carlo error, and assume known behavioural policy π^b .

Under the assumption above, we have that

$$\begin{aligned} \frac{1/\Gamma \int P(y \mid x, a) \pi^*(a \mid x) da}{\Gamma \int P(y \mid x, a) \pi^b(a \mid x) da} &\leq \tilde{w}(x, y) \leq \frac{\Gamma \int P(y \mid x, a) \pi^*(a \mid x) da}{1/\Gamma \int P(y \mid x, a) \pi^b(a \mid x) da} \\ \implies \frac{1}{\Gamma^2} w(x, y) &\leq \tilde{w}(x, y) \leq \Gamma^2 w(x, y) \end{aligned}$$

This means that,

$$\left(\frac{1}{\Gamma^2} - 1 \right) w(x, y) \leq \tilde{w}(x, y) - w(x, y) \leq (\Gamma^2 - 1) w(x, y)$$

So,

$$\mid \tilde{w}(x, y) - w(x, y) \mid \leq (\Gamma^2 - 1) w(x, y)$$

And therefore,

$$\mathbb{E}_{(X,Y) \sim P_{\tilde{X},Y}^{\pi^b}} \mid \tilde{w}(X, Y) - w(X, Y) \mid \leq (\Gamma^2 - 1) \mathbb{E}_{(X,Y) \sim P_{\tilde{X},Y}^{\pi^b}} [w(X, Y)] = \Gamma^2 - 1$$

□