A Few Observations on Sample-Conditional Coverage in Conformal Prediction

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Abstract

We revisit the problem of constructing predictive confidence sets for which we wish to obtain some type of conditional validity. We provide new arguments showing how "split conformal" methods achieve near desired coverage levels with high probability, a guarantee conditional on the validation data rather than marginal over it. In addition, we directly consider (approximate) conditional coverage, where, e.g., conditional on a covariate X belonging to some group of interest, we would like a guarantee that a predictive set covers the true outcome Y. We show that the natural method of performing quantile regression on a held-out (validation) dataset yields minimax optimal guarantees of coverage here. Complementing these positive results, we also provide experimental evidence that interesting work remains to be done to develop computationally efficient but valid predictive inference methods.

1 Introduction and background

In conformal prediction [29, 19, 20, 3], we wish to perform predictive inference on the outcome Y coming from pairs $(X, Y) \in \mathcal{X} \times \mathcal{Y}$. The basic approach yields confidence sets $C(x) \subset \mathcal{Y}$, where given a sample $(X_i, Y_i)_{i=1}^n$, an estimated confidence set $\widehat{C}$ provides the (marginal) coverage

$$\mathbb{P}\left(Y_{n+1} \in \widehat{C}(X_{n+1})\right) \ge 1 - \alpha. \tag{1}$$

Typically, to do this, we assume the existence of a scoring function $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ and define confidence sets of the form $C_\tau(x) := \{y \mid s(x, y) \le \tau\}$. For example, when predicting $Y \in \mathbb{R}$ in regression, given a predictor $f : \mathcal{X} \to \mathbb{R}$ the absolute error $s(x, y) = |f(x) - y|$ yields the familiar confidence set $C_\tau(x) = \{y \in \mathbb{R} \mid |y - f(x)| \le \tau\} = [f(x) - \tau, f(x) + \tau]$ of values y near $f(x)$.

The classical (split-conformal) approach [29, 3] uses the sample to find the threshold $\widehat{\tau}$ larger than the observed scores on about $1 - \alpha$ fraction of the data, then notes that $s(X_{n+1}, Y_{n+1})$ is likely to be smaller than this threshold. More formally, if (X_i, Y_i) are exchangeable and we let $S_i = s(X_i, Y_i)$, then for the order statistics $S_{(1)} \le S_{(2)} \le \cdots \le S_{(n+1)}$, we have

$$\mathbb{P}\left(S_{n+1} > S_{(\lceil (1-\alpha)(n+1) \rceil)}\right) \le \alpha,$$

because the probability that S_{n+1} is in the α-largest fraction of the observed scores is at most α. Then a bit of bookkeeping [e.g. 25, Lemma 2] shows that the slightly enlarged empirical quantile

$$\widehat{\tau} := \mathsf{Quant}_{(1-\alpha)(1+1/n)}(S_1, \ldots, S_n),$$

provides the guarantee

$$\mathbb{P}\left(S_{n+1} > \widehat{\tau}\right) \le \alpha.$$

Written differently, the confidence set

$$\widehat{C}(x) := \{y \in \mathcal{Y} \mid s(x, y) \le \widehat{\tau}\}$$

satisfies

$$\mathbb{P}(Y_{n+1} \in \widehat{C}(X_{n+1})) = \mathbb{P}\left(s(X_{n+1}, Y_{n+1}) \le \widehat{\tau}\right) = \mathbb{P}\left(S_{n+1} \le \widehat{\tau}\right) \ge 1 - \alpha.$$

1.1 On X-conditional coverage

We might ask for more than the marginal guarantee (1) in a few ways. The first is to target X-*conditional coverage*, where given a new datapoint X_{n+1}, we wish to achieve

$$\mathbb{P}(Y_{n+1} \in \widehat{C}(X_{n+1}) \mid X_{n+1}) \geq 1 - \alpha.$$

But there are fundamental challenges here. Let us say a set valued mapping $\widehat{C}_n : \mathcal{X} \rightrightarrows \mathcal{Y}$ achieves distribution-free conditional $(1-\alpha)$ coverage if for any P, when $(X_i, Y_i) \stackrel{\text{iid}}{\sim} P$ and $\widehat{C}_n$ is a function of $(X_i, Y_i)_{i=1}^n$, then for P-almost-all x,

$$\mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid X_{n+1} = x) \geq 1 - \alpha. \tag{2}$$

Unfortunately, such a distribution-free guarantee is impossible. Focusing on the case that $\mathcal{Y} = \mathbb{R}$ for simplicity, so that confidence sets $\widehat{C}(x) \subset \mathbb{R}$, Vovk [28, Proposition 4] shows that the Lebesgue measure $\mathsf{Leb}(\widehat{C}(x))$ is almost always infinite (see also Barber et al. [3]):

Corollary 1.1. *Let $\mathcal{X}$ be a metric space and assume that $X \in \mathcal{X}$ has continuous distribution. If $\widehat{C}$ provides distribution free $(1-\alpha)$ conditional coverage, then for P-almost all $x \in \mathcal{X}$,*

$$\mathbb{P}(\mathsf{Leb}(\widehat{C}(x)) = +\infty) \geq 1 - \alpha.$$

Similar results apply when the marginals over X are not too discrete [10, Corollary 7.1].

These failures motivate relaxing the conditional coverage condition (2). Perhaps the simplest approach considers *group-conditional coverage*, where for groups $G \subset \mathcal{X}$, one targets the guarantee

$$\mathbb{P}(Y_{n+1} \in \widehat{C}(X_{n+1}) \mid X_{n+1} \in G) \geq 1 - \alpha. \tag{3}$$

Barber et al. [3, Sec. 4] show how to achieve the coverage (3) by considering worst-case coverage over all groups G of interest; Jung et al. [16] consider variations on this guarantee.

Gibbs, Cherian, and Candès [11] develop a compelling relaxation extending this idea. To begin, note that conditional coverage $\mathbb{P}(Y \in \widehat{C}(x) \mid X = x) = 1 - \alpha$ is equivalent to the condition

$$\mathbb{E}\left[w(X)\left(1\left\{Y \in \widehat{C}(X)\right\} - (1-\alpha)\right)\right] = 0 \tag{4}$$

for all bounded (measurable) functions $w : \mathcal{X} \to \mathbb{R}$. Indeed, the tower property of conditional expectations shows that equality (4) holds if and only if

$$\mathbb{E}\left[w(X)\left(\mathbb{P}(Y \in \widehat{C}(X) \mid X) - (1-\alpha)\right)\right] = 0, \quad \text{i.e.} \quad \mathbb{E}\left[\left|\mathbb{P}(Y \in \widehat{C}(X) \mid X) - (1-\alpha)\right|\right] = 0,$$

where we take $w(x) = \mathrm{sign}(\mathbb{P}(Y \in \widehat{C}(X) \mid X = x) - (1-\alpha))$, so $\mathbb{P}(Y \in \widehat{C}(X) \mid X) = 1 - \alpha$ with probability 1. Similarly, we obtain the one-sided inequality (2) if and only if

$$\mathbb{E}\left[w(X) 1\left\{Y \in \widehat{C}(X)\right\}\right] \geq (1-\alpha)\mathbb{E}[w(X)]$$

for all nonnegative bounded w. Taking $w(x) = 1\{x \in G\}$ for groups $G \subset \mathcal{X}$ shows that this guarantee implies the group-conditional coverage (3); relaxing the condition (4) by considering subclasses of weighting functions $\mathcal{W} \subset \{\mathcal{X} \to \mathbb{R}\}$ leads to the following definition [11]:

Definition 1.1. *A confidence set $C : \mathcal{X} \rightrightarrows \mathcal{Y}$ achieves $\mathcal{W}$-*weighted $((1-\alpha), \epsilon)$ coverage *if*

$$\left|\mathbb{E}\left[w(X)\left(1\{Y \in C(X)\} - (1-\alpha)\right)\right]\right| \leq \epsilon$$

for all $w \in \mathcal{W}$.

In Definition 1.1, we take the confidence set mapping C to be fixed; Gibbs et al. allow $\widehat{C}$ to be random, in which case (in their definition) the expectation is taken also over the $\widehat{C}$ itself. Because we study coverage conditional on a sample used to construct $\widehat{C}$, we maintain Definition 1.1.

Gibbs et al.'s main two examples are cases in which $\mathcal{W}$ corresponds to a vector space of the form $\mathcal{W} = \{w \mid w(x) = \langle v, \phi(x) \rangle\}$ for some feature mapping $\phi : \mathcal{X} \to \mathbb{R}^d$, and when $\mathcal{W}$ corresponds to a reproducing kernel Hilbert space. At prediction time—on a new example X_{n+1}—they perform *full conformal inference* [29], where implicitly for each $t \in \mathbb{R}$, they solve

$$\widehat{h}_{n+1,t} = \operatorname*{argmin}_{h \in \mathcal{W}} \sum_{i=1}^{n} \ell_\alpha(h(X_i) - S_i) + \ell_\alpha(h(X_{n+1}) - t)$$

for the quantile loss $\ell_\alpha(t) = \alpha \left[t\right]_+ + (1-\alpha) \left[-t\right]_+$, then define the implicit confidence set

$$\widehat{C}_n(X_{n+1}) \coloneqq \left\{ y \in \mathcal{Y} \mid s(X_{n+1}, y) \le \widehat{h}_{n+1, s(X_{n+1},y)}(X_{n+1}) \right\}. \tag{5}$$

A careful duality calculation [11, Sec. 4] shows how to compute $\widehat{C}_n$ by solving a linear program over $O(n+d)$ variables using $(X_i)_{i=1}^{n+1}$ and S_1^n, and Gibbs et al. show the set (5) satisfies

$$\left| \mathbb{E}\left[w(X_{n+1}) 1\left\{ Y_{n+1} \notin \widehat{C}_n(X_{n+1}) \right\} - w(X_{n+1})(1-\alpha) \right] \right| \le \epsilon_{\text{int}}(w)$$

for all functions $w \in \mathcal{W}$, where $\epsilon_{\text{int}}(w)$ is an interpolation error term (which they control and is of typically small order in n). Defining $\mathbb{P}_w(A) = \mathbb{E}_P[w(X) 1\{A\}] / \mathbb{E}_P[w(X)]$ to be the w-weighted probability of an event A for $w \ge 0$, this inequality demonstrates that

$$\mathbb{P}_w(Y_{n+1} \in \widehat{C}(X_{n+1})) \ge 1 - \alpha - \epsilon_{\text{int}}(w) \tag{6}$$

for all $w \ge 0, w \in \mathcal{W}$, a more nuanced guarantee than the marginal coverage (1).

One challenge with this full conformal approach is that computing the prediction set $\widehat{C}_n$ requires solving a sometimes costly optimization. This suggests split-conformal approaches that provide adaptive confidence sets of the form

$$\widehat{C}_n(x) \coloneqq \left\{ y \in \mathcal{Y} \mid s(x, y) \le \widehat{h}_n(x) \right\},$$

where $\widehat{h}_n$ is chosen based only on the sample $(X_i, Y_i)_{i=1}^n$—hence the name "split conformal"—making the set $\widehat{C}_n$ easy to compute [25, 8]. In spite of their ease of computation, it has been challenging to demonstrate that these sets can achieve coverage; for example, Romano et al. [25] and Cauchois et al. [8] apply another level of conformalization to fit a constant threshold $\widehat{\tau}_n$ and use $\widehat{C}_n(x) = \{y \in \mathcal{Y} \mid s(x, y) \le \widehat{h}_n(x) + \widehat{\tau}_n\}$. We revisit these types of sets and show a few new convergence and coverage guarantees for them, including new optimality guarantees.

1.2 Sample-conditional coverage

Inequalities (1) and (6) provide guarantees marginal over the entire sampling procedure, drawing $(X_i, Y_i) \stackrel{\text{iid}}{\sim} P$ for $i = 1, 2, \ldots, n+1$. While conditional coverage (on X_{n+1}) is impossible, it is possible to achieve *sample-conditional*-coverage. For this, let P_n denote the empirical distribution of $(X_i, Y_i)_{i=1}^n$ (or simply the sample itself). Then we seek a guarantee of the form

$$\mathbb{P}\left(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid P_n \right) \ge 1 - \alpha - o(1)$$

with high probability over the sampling generating $\widehat{C}_n$, which is of course a function of P_n. Because of their reliance on individual examples, full-conformal procedures cannot achieve such conditional guarantees [6], though the split-conformal procedures we review can straightforwardly guarantee them. Our main purpose is to provide new arguments for this and to extend the arguments to show how split-conformal methods can achieve approximate weighted-conditional coverage (Definition 1.1) with high probability and optimal error ϵ. For example, recalling the weighted probability (6), we will show that with high probability over the sample P_n,

$$\mathbb{P}_w(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid P_n) \geq 1 - \alpha - O(1)\sqrt{\frac{\alpha(1-\alpha)}{\mathbb{E}_P[w(X)]} \cdot \frac{d \log n}{n}}$$

simultaneously for all $w \geq 0$ in d-dimensional classes of functions $\mathcal{W}$.

We recapitulate the basic arguments to achieve sample-conditional coverage with naive split-conformal confidence sets $\widehat{C}_n(x) = \{y \mid s(x, y) \leq \widehat{\tau}_n\}$ for a fixed threshold $\widehat{\tau}_n$. Vovk [28, Section 3] shows that the event $\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\} = \{s(X_{n+1}, Y_{n+1}) > \widehat{\tau}_n\}$ has small probability via an argument working with individual failures $s(X_i, Y_i) > t$ for a particular threshold t. We provide two related arguments to obtain sample-conditional coverage here. The first uses elementary calculations and recapitulates Vovk's argument for completeness but using our notation; the second uses a concentration and VC-dimension calculation to preview our coming approaches.

To state things formally, let $S_i = s(X_i, Y_i)$ $i = 1, \ldots, n$, where $(X_i, Y_i) \stackrel{\text{iid}}{\sim} P$ for some fixed distribution P. Let $\alpha \in (0, 1)$ be a desired confidence level, and define the empirical $(1 - \alpha)$ quantile

$$\widehat{\tau}_n \coloneqq \inf \{t \in \mathbb{R} \mid P_n(S \leq t) \geq 1 - \alpha\},$$

where we recall that P_n denotes the empirical distribution. Then given this quantile, we define the confidence set

$$\widehat{C}_n(x) \coloneqq \{y \in \mathcal{Y} \mid s(x, y) \leq \widehat{\tau}_n\}.$$

Proposition 1 (Vovk [28], Proposition 2)**.** *Let the construction above hold. Then for any $\gamma > 0$, with probability at least $1 - e^{-2n\gamma^2}$ over the sample P_n,*

$$\mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid P_n) \geq 1 - \alpha - \gamma. \tag{7}$$

Jung et al. [16] consider this sample-conditional coverage with the additional desideratum of group-conditional-coverage (3), showing that under some assumptions on the smoothness of the underlying distribution of $s(x, Y)$ given $X = x$, it is approximately achievable. We revisit their approach in Section 3, providing new and sharper guarantees on its behavior, without any assumptions on the underlying distribution, allowing analogues of the guarantee (7) in approximate conditional senses. Bian and Barber [6] also consider such sample-conditional coverage, showing that it is impossible to achieve without stronger assumptions for many predictive methods.

2 Sample conditional coverage revisited

We begin by revisiting the sample-conditional coverage guarantees of Proposition 1. It admits a quite elementary proof relying only on Hoeffding's concentration inequality, making it a natural point of departure for developing more sophisticated coverage guarantees. We thus provide this elementary proof, then demonstrate the result using uniform convergence techniques. These uniform convergence guarantees—which form the basis for providing guarantees for approximate weighted coverage (Definition 1.1) also provide a two-sided bound on sample-conditional coverage:

Corollary 2.1. *Assume the scores $S_i = s(X_i, Y_i)$ are distinct with probability 1. Then for any $\gamma > 0$, with probability at least $1 - 2e^{-2n\gamma^2}$ over the sample P_n,*

$$1 - \alpha - \gamma \le \mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid P_n) \le 1 - \alpha + \frac{1}{n} + \gamma.$$

The simplicity of the guarantee (7) means it admits elegant extensions as well. For example, we can extend the argument to give a bound that more carefully tracks the desired confidence α:

Proposition 2. *Let $\delta \in (0, 1)$ and define*

$$\gamma_n(\delta) := \frac{4 \log \frac{1}{\delta}}{3n} + \sqrt{\left(\frac{4}{3n} \log \frac{1}{\delta}\right)^2 + \frac{2\alpha(1-\alpha)}{n} \log \frac{1}{\delta}} \le \frac{8 \log \frac{1}{\delta}}{3n} + \sqrt{\frac{2\alpha(1-\alpha)}{n} \log \frac{1}{\delta}}.$$

Then with probability at least $1 - \delta$ over the draw of the sample P_n,

$$1 - \alpha - \gamma_n(\delta) \le \mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid P_n).$$

If additionally the scores S have a density, then with probability at least $1 - 2\delta$,

$$1 - \alpha - \gamma_n(\delta) \le \mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid P_n) \le 1 - \alpha + \gamma_n(\delta).$$

Roughly, we see that the simple quantile-based confidence set achieves coverage

$$1 - \alpha \pm O_P(1) \sqrt{\frac{\alpha(1-\alpha)}{n}}.$$

When α is small—which is the typical case—this is always sharper than the naive guarantee (7). The central limit theorem shows this is as accurately as we could hope to even estimate the coverage level of a predictor; moreover, as we discuss following Theorem 3, it is minimax (rate) optimal. In the remainder of the section, we provide two proofs of Proposition 1, along with Corollary 2.1. In Section 2.3, we prove Proposition 2 using Bernstein-type concentration guarantees.

2.1 An elementary proof of Proposition 1

For the scalar random variable S, define the β-quantile

$$q^\star(\beta) := \inf \{t \in \mathbb{R} \mid \mathbb{P}(S \le t) \ge \beta\}. \tag{8}$$

Because the CDF is right continuous, we have $\mathbb{P}(S \le q^\star(\beta)) \ge \beta$, and $\mathbb{P}(S > q^\star(\beta)) = 1 - \mathbb{P}(S \le q^\star(\beta)) \le 1 - \beta$. For $\gamma > 0$ and any $\tau \in \mathbb{R}$, the inequality

$$\mathbb{P}(S_{n+1} > \tau) > \alpha + \gamma, \quad \text{i.e.} \quad \mathbb{P}(S_{n+1} \le \tau) < 1 - \alpha - \gamma,$$

implies that $\tau < q^\star(1 - \alpha - \gamma)$.

Consider the event that $\widehat{\tau}_n < q^\star(1 - \alpha - \gamma)$. For this to occur, it must be the case that

$$\frac{1}{n} \sum_{i=1}^{n} 1\{S_i < q^\star(1 - \alpha - \gamma)\} \ge 1 - \alpha. \tag{9}$$

But this event is unlikely: define the Bernoulli indicator variables $B_i = 1\{S_i < q^\star(1 - \alpha - \gamma)\}$. Then $\mathbb{E}[B_i] \le 1 - \alpha - \gamma$, and Hoeffding's inequality implies that $\overline{B}_n = \frac{1}{n} \sum_{i=1}^n B_i$ satisfies

$$\begin{aligned} \mathbb{P}\left(P_n(S < q^\star(1 - \alpha - \gamma)) \ge 1 - \alpha\right) &= \mathbb{P}\left(\overline{B}_n \ge 1 - \alpha\right) \\ &\le \mathbb{P}\left(\overline{B}_n - \mathbb{E}[\overline{B}_n] \ge \gamma\right) \le \exp(-2n\gamma^2). \end{aligned}$$

That is,

$$\mathbb{P}\left(\widehat{\tau}_n < q^\star(1-\alpha-\gamma)\right) \le \exp\left(-2n\gamma^2\right)$$

for any $\gamma > 0$, and so we must have

$$\mathbb{P}\left(S_{n+1} > \widehat{\tau}_n \mid P_n\right) \le \alpha + \gamma \ \text{ with probability at least } 1 - e^{-2n\gamma^2}.$$

Rearranging and recalling that $Y_{n+1} \notin \widehat{C}_n(X_{n+1})$ if and only if $s(X_{n+1}, Y_{n+1}) > \widehat{\tau}_n$, i.e., if $S_{n+1} > \widehat{\tau}_n$ gives the result.

2.2 A proof of Proposition 1 using uniform convergence

Our alternative approach to the proof of Proposition 1 uses the bounded differences inequality and a uniform concentration guarantee. First, for any estimated threshold $\widehat{\tau}_n$, we have the trivial inequality

$$\begin{aligned}\mathbb{P}(S_{n+1} > \widehat{\tau}_n \mid P_n) &= \mathbb{P}(S_{n+1} > \widehat{\tau}_n \mid P_n) - P_n(S > \widehat{\tau}_n) + P_n(S > \widehat{\tau}_n) \\ &\le \sup_{\tau \in \mathbb{R}} \left|P(S > \tau) - P_n(S > \tau)\right| + P_n(S > \widehat{\tau}_n).\end{aligned}$$

Then because we choose $\widehat{\tau}_n$ so that $P_n(S \le \widehat{\tau}_n) \ge 1 - \alpha$, we obtain

$$\mathbb{P}(S_{n+1} > \widehat{\tau}_n \mid P_n) \le \alpha + \sup_{\tau \in \mathbb{R}} \left|P(S > \tau) - P_n(S > \tau)\right|. \tag{10a}$$

If the values S_i are distinct, then $P_n(S \le \widehat{\tau}_n) \le 1 - \alpha + \frac{1}{n}$, and so a completely similar calculation yields

$$\mathbb{P}(S_{n+1} > \widehat{\tau}_n \mid P_n) \ge \alpha - \frac{1}{n} - \sup_{\tau \in \mathbb{R}} \left|P(S > \tau) - P_n(S > \tau)\right|. \tag{10b}$$

In either case, if we can control the deviation $|P(S > \tau) - P_n(S > \tau)|$ uniformly across τ, we will have evidently proved the desired result.

We consider two arguments, the first yielding sharper constants, while the second generalizes to weighted coverage. For the first, we apply the Dvoretsky-Kiefer-Wolfowitz inequality [21]:

$$\mathbb{P}\left(\sup_{\tau \in \mathbb{R}} \left|P(S > \tau) - P_n(S > \tau)\right| \ge t\right) \le 2e^{-2nt^2}$$

for all $t \ge 0$. Combining the equations (10), we thus obtain that

$$\mathbb{P}(S_{n+1} > \widehat{\tau}_n \mid P_n) \le \alpha + \gamma \ \text{ with probability at least } 1 - 2e^{-2n\gamma^2}.$$

If the scores are distinct, the corresponding lower bound is immediate, giving Corollary 2.1.

The final alternative argument to control the uniform deviations in the bounds (10) underpins our more sophisticated guarantees in the sequel, relying on uniform concentration guarantees and the Vapnik-Chervonenkis (VC) dimension. First, recall the classical bounded differences inequality [22, 30], where we say a function $f : \mathcal{X}^n \to \mathbb{R}$ satisfies c_i-bounded differences if

$$\left|f(x_1^{i-1}, x_i, x_i, x_{i+1}^n) - f(x_1^{i-1}, x_i', x_{i+1}^n)\right| \le c_i \ \text{ for all } x_1^{i-1}, x_{i+1}^n, x_i, x_i' \in \mathcal{X}.$$

Lemma 2.1 (Bounded differences)**.** *Let $X_1, \ldots, X_n$ be independent random variables and f satisfy c_i-bounded differences. Then for all $t \ge 0$,*

$$\max\left\{\mathbb{P}(f(X_1^n) - \mathbb{E}[f(X_1^n)] \ge t), \mathbb{P}(f(X_1^n) - \mathbb{E}[f(X_1^n)] \le -t)\right\} \le \exp\left(-\frac{2t^2}{\sum_{i=1}^n c_i^2}\right).$$

We then observe that $f(P_n) := \sup_{\tau \in \mathbb{R}} |P(S > \tau) - P_n(S > \tau)|$ trivially satisfies bounded differences. Indeed, let P_n' differ from P_n in a single observation. Then defining $\|P - P_n\|_\infty = \sup_\tau |P(S > \tau) - P_n(S > \tau)|$ for shorthand, we obtain

$$\left| \|P - P_n\|_\infty - \|P - P_n'\|_\infty \right| \le \|P_n - P_n'\|_\infty \le \frac{1}{n}$$

by the triangle inequality and that only one example may change. Lemma 2.1 then implies

$$\mathbb{P}\left(\|P - P_n\|_\infty \ge \mathbb{E}[\|P - P_n\|_\infty] + t\right) \le e^{-2nt^2}$$

for $t \ge 0$, so that we need only control $\mathbb{E}[\|P - P_n\|_\infty]$. For this, we perform a standard symmetrization argument [e.g. 27, Ch. 2.3]: let $P_n^0 = \frac{1}{n}\sum_{i=1}^n \varepsilon_i \mathbf{1}_{S_i}$, where $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathsf{Uni}\{\pm 1\}$ are i.i.d. Rademacher variables and $\mathbf{1}_{S_i}$ denotes a point mass on S_i. By introducing independent copies of S_i and applying Jensen's inequality [27, Lemma 2.3.1], we have the bound

$$\mathbb{E}\left[\|P_n - P\|_\infty\right] \le 2\mathbb{E}\left[\|P_n^0\|_\infty\right] = 2\mathbb{E}\left[\sup_{\tau \in \mathbb{R}} \left| \frac{1}{n} \sum_{i=1}^n \varepsilon_i 1\{S_i > \tau\} \right| \right].$$

Because the class of functions $s \mapsto 1\{s > \tau\}$ has VC-dimension at most 1, Dudley's entropy integral (see, e.g. [27, Corollary 2.2.8 and Thm. 2.6.7] or [30, Eq. (5.5.1)]) shows that

$$\mathbb{E}\left[\|P_n^0\|_\infty\right] \le \frac{c}{\sqrt{n}}$$

for a numerical constant c. We then obtain that for any $\gamma \ge 0$,

$$\mathbb{P}\left(S_{n+1} > \widehat{\tau}_n \mid P_n\right) \le \alpha + \frac{c}{\sqrt{n}} + \gamma \quad \text{w.p. } 1 - e^{-2n\gamma^2}$$

by the inequalities (10), where c is a numerical constant.

2.3 Proof of Proposition 2

Recall the quantile mapping $q^\star$ from the definition (8) and that for fixed $\gamma \in [0, \alpha]$, the event $\widehat{\tau}_n < q^\star(1 - \alpha - \gamma)$ can occur only if $P_n(S < q^\star(1 - \alpha - \gamma)) \ge 1 - \alpha$. Then defining $B_i = 1\{S_i < q^\star(1 - \alpha - \gamma)\}$ and recalling inequality (9), we obtain

$$\mathbb{P}(\widehat{\tau}_n < q^\star(1 - \alpha - \gamma)) \le \mathbb{P}(\overline{B}_n \ge 1 - \alpha) = \mathbb{P}(\overline{B}_n - \mathbb{E}[\overline{B}_n] \ge 1 - \alpha - \mathbb{E}[\overline{B}_n]).$$

Define $p(\gamma) = \mathbb{E}[B_i] = \mathbb{P}(S < q^\star(1 - \alpha - \gamma)) < 1 - \alpha - \gamma$, so that $t = t(\gamma) := 1 - \alpha - p(\gamma) > \gamma$. Then $\mathrm{Var}(B_i) = p(\gamma)(1 - p(\gamma)) = (\alpha + t)(1 - \alpha - t)$, and Bernstein's inequality implies

$$\begin{aligned}
\mathbb{P}(\overline{B}_n - \mathbb{E}[\overline{B}_n] \ge t) &\le \exp\left(-\frac{nt^2}{2(1 - \alpha - t)(\alpha + t) + \frac{2}{3}t}\right) \\
&= \exp\left(-\frac{nt^2}{2(1 - \alpha)\alpha + (\frac{8}{3} - 4\alpha)t - t^2}\right) \le \exp\left(-\frac{nt^2}{2(1 - \alpha)\alpha + \frac{8}{3}t}\right).
\end{aligned}$$

Notably, $t \mapsto \frac{nt^2}{2(1-\alpha)\alpha + \frac{8}{3}t}$ is increasing in t, so that

$$\mathbb{P}(\widehat{\tau}_n < q^\star(1 - \alpha - \gamma)) \le \exp\left(-\frac{n\gamma^2}{2(1 - \alpha)\alpha + \frac{8}{3}\gamma}\right).$$

If the scores S have a density, $\mathbb{P}(S \le q^\star(\beta)) = \beta$ for any $\beta \in (0,1)$. Then we may also consider the event that $\widehat{\tau}_n > q^\star(1-\alpha+\gamma)$. For this to occur, we require

$$P_n(S < q^\star(1-\alpha+\gamma)) \le 1-\alpha,$$

and defining $B_i = 1\{S_i < q^\star(1-\alpha+\gamma)\}$, we have $\mathbb{E}[B_i] = 1-\alpha+\gamma$ and so

$$\begin{aligned}\mathbb{P}(\overline{B}_n \le 1-\alpha) = \mathbb{P}(\overline{B}_n - \mathbb{E}[\overline{B}_n] \le -\gamma) &\le \exp\left(-\frac{n\gamma^2}{2(1-\alpha+\gamma)(\alpha-\gamma)+\frac{2}{3}\gamma}\right) \\ &\le \exp\left(-\frac{n\gamma^2}{2(1-\alpha)\alpha+\frac{2}{3}\gamma}\right)\end{aligned}$$

for $\gamma \in [0,\alpha]$. Combining the two cases, for $\gamma \ge 0$ we have

$$\max\left\{\mathbb{P}\left(\widehat{\tau}_n < q^\star(1-\alpha-\gamma)\right), \mathbb{P}\left(\widehat{\tau}_n > q^\star(1+\alpha+\gamma)\right)\right\} \le \exp\left(-\frac{n\gamma^2}{2\alpha(1-\alpha)+\frac{8}{3}\gamma}\right).$$

Solving to guarantee the right hand side is at most δ yields

$$\gamma_n := \frac{4\log\frac{1}{\delta}}{3n} + \sqrt{\left(\frac{4}{3n}\log\frac{1}{\delta}\right)^2 + \frac{2\alpha(1-\alpha)}{n}\log\frac{1}{\delta}}.$$

Applying a union bound implies Proposition 2.

3 Approaching conditional coverage

Keeping in mind the ideas in Sections 1.1 and 1.2, we revisit conditional coverage, but we do so conditional on the sample P_n as well. To do this, we revisit Jung et al. and Gibbs et al.'s approaches [16, 11], considering quantile estimation via the quantile loss [17], which for $\alpha > 0$ is

$$\ell_\alpha(t) := \alpha\,[t]_+ + (1-\alpha)\,[-t]_+\,.$$

For a random variable Y, the $(1-\alpha)$-quantile $\mathsf{Quant}_{1-\alpha}(Y) := \inf\{t \mid \mathbb{P}(Y \le t) \ge 1-\alpha\}$ minimizes $L(t) := \mathbb{E}[\ell_\alpha(t-Y)]$. This is easy to see when Y has a density, in which case we can take derivatives (ignoring the measure-0 set of points where $\ell_\alpha(t-Y)$ is non-differentiable [5]) to obtain

$$L'(t) = \alpha\mathbb{P}(t-Y>0) - (1-\alpha)\mathbb{P}(t-Y\le 0) = \mathbb{P}(Y<t) - (1-\alpha) = 0$$

if and only if $\mathbb{P}(Y < t) = 1-\alpha$; that is, $\mathsf{Quant}_{1-\alpha}(Y)$ is always *a* minimizer. (When Y has point masses, a minor extension of this argument shows that $\mathsf{Quant}_{1-\alpha}(Y)$ remains a minimizer.)

Following Gibbs et al. [11] and Jung et al. [16], consider a multi-dimensional quantile regression of attempting to predict $S \in \mathbb{R}$ from $X \in \mathcal{X}$. Let $\phi : \mathcal{X} \to \mathbb{R}^d$ be a feature mapping, and consider the population loss $L(\theta) := \mathbb{E}[\ell_\alpha(\langle\theta, \phi(X)\rangle - S)]$. Then (for motivation) assuming that S has a density conditional on $X = x$, we see that

$$\begin{aligned}\nabla L(\theta) &= \alpha\mathbb{E}\left[1\{\langle\theta,\phi(X)\rangle - S > 0\}\,\phi(X)\right] - (1-\alpha)\mathbb{E}\left[1\{\langle\theta,\phi(X)\rangle - S \le 0\}\,\phi(X)\right] \\ &= \mathbb{E}\left[\left(1\{S < \langle\theta,\phi(X)\rangle\} - (1-\alpha)\right)\phi(X)\right].\end{aligned}$$

Now let

$$\theta^\star \in \operatorname{argmin} L(\theta)$$

be a population minimizer. Then, as Gibbs et al. [11] note, for *any* $u \in \mathbb{R}^d$, we have

$$0 = \langle u, \nabla L(\theta^\star) \rangle = \mathbb{E}\left[(\mathbb{P}(S < \langle \theta^\star, \phi(X) \rangle \mid X) - (1-\alpha)) \cdot \langle u, \phi(X) \rangle \right].$$

This connects transparently to confidence set mappings [11, 16]: taking

$$S = s(X, Y) \quad \text{and} \quad C_{\theta^\star}(x) := \{ y \in \mathcal{Y} \mid s(x, y) \le \langle \theta^\star, \phi(X) \rangle \},$$

we have

$$0 = \mathbb{E}\left[(\mathbb{P}(Y \in C(X) \mid X) - (1-\alpha)) \langle u, \phi(X) \rangle \right] = 0 \ \text{ for all } u \in \mathbb{R}^d.$$

In turn, this implies the population coverage guarantee

Corollary 3.1. *Assume the distribution of S conditional on $X = x$ has no atoms for each $x \in \mathcal{X}$. Let $\theta^\star$ minimize $L(\theta) = \mathbb{E}[\ell_\alpha(\langle \theta, \phi(X) \rangle - s(X, Y))]$. Then $C_{\theta^\star}$ provides $((1-\alpha), 0)$-weighted coverage (Definition 1.1) for the class $\mathcal{W} := \{ w \mid w(x) = \langle u, \phi(x) \rangle \}_{u \in \mathbb{R}^d}$ of linear functions of $\phi(x)$.*

Two questions arise: first, whether the corollary extends to S which may have atoms. A (trivial) workaround is to simply add a tiny amount of random noise to each S_i. Otherwise, it is generally possible only to provide a one-sided bound, where we weight with nonnegative functions w (we provide this in the sequel). The more interesting question is how we can extend these guarantees to provide sample-conditional coverage. Adapting the arguments we use in Section 2.2 to prove Proposition 1 and Corollary 2.1 allows us to address this.

3.1 An estimated confidence set

The population-level confidence set $C_{\theta^\star}(x) = \{ y \mid s(x, y) \le \langle \theta^\star, \phi(x) \rangle \}$ immediately suggests developing an empirical analogue [11, 16]. Thus, we turn to an analysis of the empirical confidence set, considering the estimator

$$\widehat{\theta}_n \in \operatorname*{argmin}_\theta \mathbb{E}_{P_n} \left[\ell_\alpha(\langle \theta, \phi(X) \rangle - S) \right], \tag{11}$$

which Jung et al. [16] consider for the special case that the feature mapping $\phi(x) = [1\{x \in G\}]_{G \in \mathcal{G}}$ is an indicator vector for groups $G \subset \mathcal{X}$. This gives the confidence set

$$\widehat{C}_n(x) := \left\{ y \in \mathcal{Y} \mid s(x, y) \le \langle \widehat{\theta}, \phi(x) \rangle \right\}.$$

We first sketch an argument that this set provides a desired approximate weighted coverage. By convexity,

$$0 \in \sum_{i=1}^n \partial \ell_\alpha \left(\langle \widehat{\theta}, \phi(X_i) \rangle - S_i \right) \phi(X_i),$$

which is equivalent to the statement that for some scalars (really, dual variables) η_i satisfying

$$\eta_i = \begin{cases} \alpha & \text{if } \langle \widehat{\theta}, \phi(X_i) \rangle > S_i \\ -(1-\alpha) & \text{if } \langle \widehat{\theta}, \phi(X_i) \rangle < S_i \\ \in [-(1-\alpha), \alpha] & \text{if } \langle \widehat{\theta}, \phi(X_i) \rangle = S_i \end{cases} \tag{12}$$

we have

$$0 = \sum_{i=1}^n \eta_i \phi(X_i).$$

Let us proceed heuristically for now by taking "discrete" values for the η_i. If we assume that

$$\eta_i = \alpha 1\{\langle \widehat{\theta}, \phi(X_i)\rangle > S_i\} - (1-\alpha)1\{\langle \widehat{\theta}, \phi(X_i)\rangle \le S_i\} = 1\{S_i < \langle \widehat{\theta}, \phi(X_i)\rangle\} - (1-\alpha),$$

then

$$0 = \sum_{i=1}^n \phi(X_i)\left(1\left\{S_i \le \langle \widehat{\theta}, \phi(X_i)\rangle\right\} - (1-\alpha)\right) = \sum_{i=1}^n \phi(X_i)\left(1\left\{Y_i \in \widehat{C}_n(X_i)\right\} - (1-\alpha)\right),$$

the empirical version of Corollary 3.1. If we could argue that this (heuristic) empirical average concentrates around its expectation, we would obtain

$$\mathbb{E}\left[\phi(X_{n+1})\left(1\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} - \alpha\right) \mid P_n\right] \approx \frac{1}{n}\sum_{i=1}^n \phi(X_i)\left(1\left\{S_i > \langle \widehat{\theta}, \phi(X_i)\rangle\right\} - \alpha\right) = 0,$$

weighted coverage for a new example (X_{n+1}, Y_{n+1}).

To make this argument rigorous, we employ a bit of empirical process theory and measure concentration. For now and for simplicity, we assume that $\phi(x)$ is bounded in ℓ_2, so that $\|\phi(x)\|_2 \le b_\phi$ for all x, and let $\mathbb{B}_2 = \{u \in \mathbb{R}^d \mid \|u\|_2 \le 1\}$ be the ℓ_2-ball.

Theorem 1. *Assume the boundedness conditions above and that $n \ge d$. Let $\widehat{\theta}$ be the empirical minimizer (11) of the α-quantile loss, let $\widehat{h}(x) = \langle \widehat{\theta}, \phi(x)\rangle$, and define the confidence set*

$$\widehat{C}_n(x) := \left\{y \in \mathcal{Y} \mid s(x,y) \le \widehat{h}(x)\right\}.$$

Then there exists a constant $c \le 2 + \alpha/\sqrt{d}$ such that for $t \ge 0$, with probability at least $1 - e^{-nt^2}$ over the draw of the sample P_n,

$$\mathbb{E}\left[\langle u, \phi(X_{n+1})\rangle\left(1\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} - (1-\alpha)\right) \mid P_n\right] \ge -cb_\phi\left(\sqrt{\frac{d}{n}\log\frac{n}{d}} + t\right)$$

simultaneously for all $u \in \mathbb{B}_2$ satisfying $\langle u, \phi(x)\rangle \ge 0$ for all $x \in \mathcal{X}$.

If additionally the scores S_i are distinct with probability 1, then with the same probability,

$$\mathbb{E}\left[\langle u, \phi(X_{n+1})\rangle\left(1\left\{Y_{n+1} \in \widehat{C}_n(X_{n+1})\right\} - (1-\alpha)\right) \mid P_n\right] \le 3b_\phi\left(\sqrt{\frac{d}{n}\log\frac{n}{d}} + t + \frac{d}{3n}\right).$$

simultaneously for all $u \in \mathbb{B}_2$.

We defer the proof of Theorem 1 to Section 3.2.

Translating things to guarantee (nearly) exact coverage and distinct scores even when the naive scores may not be distinct, we can randomize, though we will assume the randomization scale makes it unlikely to modify results (e.g., perturbing by noise at a scale of 10^{-10}). In this case, let U_i, $i = 1, 2, \ldots, n+1$ be i.i.d. random variables with a density on $\mathbb{R}$, and define the scores $S_i = s(X_i, Y_i)$ as usual and perturbed scores $S_i + U_i$; then (abusing notation) let $\widehat{\theta}_n$ be an empirical estimator

$$\widehat{\theta}_n \in \operatorname*{argmin}_\theta \mathbb{E}_{P_n}\left[\ell_\alpha\left(\langle \theta, \phi(X)\rangle - S - U\right)\right].$$

We obtain the following corollary.

Corollary 3.2. *Let $\widehat{\theta}_n$ be as above and define $\widehat{h}(x) = \langle \widehat{\theta}_n, \phi(x) \rangle$. Define the confidence set*

$$\widehat{C}_n(x, u) := \left\{ y \in \mathcal{Y} \mid s(x, y) \le \widehat{h}(x) + u \right\}.$$

Then there exists a numerical constant $c \le 3$ such that for $t \ge 0$, with probability at least $1 - e^{-nt^2}$, the randomized confidence set $\widehat{C}_n(\cdot, U)$ achieves $((1-\alpha), \epsilon_n)$-weighted coverage (Definition 1.1) for the class $\mathcal{W} := \{w(x) = \langle u, \phi(x) \rangle\}_{u \in \mathbb{B}_2}$ with

$$\epsilon_n \le c b_\phi \left(\sqrt{\frac{d \log \frac{n}{d}}{n}} + \frac{d}{n} + t \right).$$

As another corollary to Theorem 1, let us assume that $\mathcal{G} = \{G_1, \ldots, G_d\}$ consists of sets G_i partitioning $\mathcal{X}$, and define the feature indicator $\phi_{\mathcal{G}}(x) = (1, 1\{x \in G_1\}, \ldots, 1\{x \in G_d\})$. With this particular choice, we obtain the following result:

Corollary 3.3. *Let $\widehat{\theta}$ be as in Theorem 1 and $\phi = \phi_{\mathcal{G}}$ be the group feature function. Then simultaneously for all groups G_j,*

$$\mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid X_{n+1} \in G_j, P_n) \ge 1 - \alpha - \frac{4}{\mathbb{P}(X_{n+1} \in G_j)} \left(\sqrt{\frac{d}{n} \log \frac{n}{d}} + t \right)$$

with probability at least $1 - e^{-nt^2}$.

We will sharpen this inequality via more sophisticated arguments in the sequel.

It is instructive here, however, to compare this guarantee to that the full-conformal approach (5), which depends on X_{n+1}, provides. The construction (5) appears appears to obtain better coverage than the more basic approaches here [11, Fig. 3], but it can be more computationally challenging [11, Fig. 6]. Indeed, Gibbs et al. [11] show that a randomized version of their procedure (5) achieves

$$\mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}) \mid X_{n+1} \in G) = 1 - \alpha \quad \text{for all } G \in \mathcal{G}.$$

This can be substantially sharper than the guarantee Corollary 3.3 provides, as our sample-conditional coverage guarantees are not quite so exact; we revisit these points in experiments.

3.2 Proof of Theorem 1

We use the empirical process notation $P_n f = \frac{1}{n} \sum_{i=1}^n f(X_i)$ for shorthand. Recall that for a convex function f, the directional derivative $f'(x; u) = \lim_{t \downarrow 0} \frac{f(x+tu) - f(x)}{t}$ exists and satisfies $f'(x; u) = \sup\{\langle g, u \rangle \mid g \in \partial f(x)\}$. Thus, by definition of optimality,

$$P_n \ell'_\alpha(\langle \widehat{\theta}, \phi(X) \rangle - S; u) \ge 0$$

for all u. Let u be such that $\langle u, \phi(x) \rangle \ge 0$ for all $x \in \mathcal{X}$. Then

$$\ell'_\alpha(\langle \theta, \phi(x) \rangle - s; u) = \langle \phi(x), u \rangle \left[\alpha 1\{\langle \theta, \phi(x) \rangle \ge s\} - (1-\alpha) 1\{\langle \theta, \phi(x) \rangle < s\} \right].$$

Then by the first-order optimality condition we obtain

$$\begin{aligned} 0 &\le \left\langle u, \alpha P_n \phi(X) 1\left\{ \langle \widehat{\theta}, \phi(X) \rangle \ge S \right\} - (1-\alpha) P_n \phi(X) 1\left\{ \langle \widehat{\theta}, \phi(X) \rangle < S \right\} \right\rangle \\ &= \left\langle u, \alpha P_n \phi(X) - P_n \phi(X) 1\left\{ \langle \widehat{\theta}, \phi(X) \rangle < S \right\} \right\rangle. \end{aligned}$$

Suppose that we demonstrate that

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \phi(X_i) 1\{S_i > \langle \theta, \phi(X_i) \rangle\} - \mathbb{E}_P[\phi(X) 1\{S > \langle \theta, \phi(X) \rangle\}] \right\|_2 \le \epsilon$$

uniformly over $\theta \in \mathbb{R}^d$. Then we would obtain

$$0 \le \left\langle u, P_n \phi(X) \left(\alpha - 1\left\{ S > \langle \widehat{\theta}, \phi(X) \rangle \right\} \right) \right\rangle \le \mathbb{E}_P \left[\langle u, \phi(X) \rangle \left(\alpha - 1\left\{ S > \langle \widehat{\theta}, \phi(X) \rangle \right\} \right) \right] + \epsilon,$$

for all $u \in \mathbb{B}_2$ with $\langle u, \phi(x) \rangle \ge 0$ for all $x \in \mathcal{X}$, that is,

$$\mathbb{E}_P \left[\langle u, \phi(X) \rangle \left(1\left\{ Y \notin \widehat{C}(X) \right\} - \alpha \right) \right] \le \epsilon, \tag{13}$$

as $y \notin \widehat{C}(x)$ if and only if $s(x, y) > \langle \widehat{\theta}, \phi(x) \rangle$. With appropriate ϵ, this will give the first claim of the theorem.

To that end, we abstract a bit and let $\mathcal{H} \subset \{\mathcal{X} \to \mathbb{R}\}$ be (for now) any collection of functions, and consider the process defined by

$$Z_n(h) := \frac{1}{n} \sum_{i=1}^{n} \phi(X_i) 1\{S_i > h(X_i)\}.$$

When $\mathcal{H}$ is a VC-class, for each coordinate j, functions of the form $\phi_j(x) 1\{s > h(x)\}$ are VC-subgraph [27, Lemma 2.6.18]. So (at least abstractly) we expect Z_n to concentrate around its expectations at a reasonable rate. The following technical lemma, whose proof we provide in Appendix A.1, provides one variant of this.

Lemma 3.1. *Let $\mathbb{B}_2 = \{u : \|u\|_2 \le 1\}$ and $\mathcal{H}$ have VC-dimension k. Then*

$$\mathbb{E} \left[\sup_{h \in \mathcal{H}, u \in \mathbb{B}_2} \langle u, Z_n(h) - \mathbb{E}[Z_n(h)] \rangle \right] \le 2 \sqrt{\frac{k \log \frac{ne}{k}}{n}} \mathbb{E} \left[\frac{1}{n} \sum_{i=1}^{n} \|\phi(X_i)\|^2 \right]^{1/2}.$$

The trivial inequality $\mathbb{E}[\sup_{u \in \mathbb{B}_\phi} \langle u, P_n \phi(X) - \mathbb{E}[\phi(X)] \rangle] \le \frac{1}{\sqrt{n}} \mathbb{E}[\|\phi(X)\|_2^2]^{1/2}$ addresses terms involving $P_n \phi(X) \alpha$ above.

We can extend the lemma by homogeneity to capture arbitrary vectors. To do so, note that if we change a single example (X_i, S_i), then $\langle u, Z_n(h) \rangle$ changes by at most $n^{-1} \sup_x \langle u, \phi(x) \rangle \le n^{-1} \|u\|_2 \sup_x \|\phi(x)\|_2$. Using homogeneity, for any scalar t there exists $u \in \mathbb{R}^d$ such that $\langle u, Z_n(h) - \mathbb{E}[Z_n(h)] \rangle \ge \|u\|_2 t$ if and only if there exists $u \in \mathbb{S}^{d-1}$ such that $\langle u, Z_n(h) - \mathbb{E}[Z_n(h)] \rangle \ge t$. So if $b_\phi = \sup_{x \in \mathcal{X}} \|\phi(x)\|_2$, we obtain by bounded differences (Lemma 2.1) and homogeneity that

$$\mathbb{P} \left(\sup_{u \ne 0, h \in \mathcal{H}} \frac{\langle u, Z_n(h) - \mathbb{E}[Z_n(h)] \rangle}{\|u\|_2} \ge b_\phi t + \mathbb{E} \left[\sup_{u \in \mathbb{S}^{d-1}, h \in \mathcal{H}} \langle u, Z_n(h) - \mathbb{E}[Z_n(h)] \rangle \right] \right) \le e^{-nt^2}.$$

Summarizing, we have proved the following proposition.

Proposition 3. *Let $\mathcal{H}$ have VC-dimension k. Then for $t \ge 0$,*

$$\mathbb{P} \left(\sup_{u \ne 0, h \in \mathcal{H}} \frac{\langle u, Z_n(h) - \mathbb{E}[Z_n(h)] \rangle}{\|u\|_2} \ge 2 b_\phi \sqrt{\frac{k \log \frac{n}{k}}{n}} + b_\phi t \right) \le e^{-nt^2}.$$

By taking $\mathcal{H} = \{h : h(x) = \langle \theta, \phi(x) \rangle\}_{\theta \in \mathbb{R}^d}$, which has VC-dimension d, in Proposition 3, we have thus shown that inequality (13) holds with

$$\epsilon = 2b_\phi \sqrt{\frac{d \log \frac{n}{d}}{n}} + b_\phi t + \frac{b_\phi \alpha}{\sqrt{n}}$$

with probability at least $1 - e^{-nt^2}$, which is the first claim of Theorem 1.

Now we turn to the second claim of Theorem 1, which applies when the scores S_i are distinct with probability 1. Recall the definition (12) of the subgradient terms g_i, and define the index sets $\mathcal{I}_+ = \{i \mid \langle \widehat{\theta}, \phi(X_i) \rangle > S_i\}$, $\mathcal{I}_- = \{i \mid \langle \widehat{\theta}, \phi(X_i) \rangle < S_i\}$, and $\mathcal{I}_0 = \{i \mid \langle \widehat{\theta}, \phi(X_i) \rangle = S_i\}$. Then

$$\begin{aligned}
&\sum_{i=1}^n \phi(X_i) \left(1\left\{S_i > \langle \widehat{\theta}, \phi(X_i) \rangle\right\} - \alpha\right) \\
&= \sum_{i \in \mathcal{I}_+ \cup \mathcal{I}_-} \phi(X_i) \left(1\left\{S_i > \langle \widehat{\theta}, \phi(X_i) \rangle\right\} - \alpha\right) + \sum_{i \in \mathcal{I}_0} \phi(X_i) \left(1\left\{S_i > \langle \widehat{\theta}, \phi(X_i) \rangle\right\} - \alpha\right) \\
&= -\sum_{i \in \mathcal{I}_+ \cup \mathcal{I}_-} \phi(X_i) g_i - \sum_{i \in \mathcal{I}_0} \phi(X_i) g_i - \sum_{i \in \mathcal{I}_0} \phi(X_i) \left(\alpha - g_i\right) = \sum_{i \in \mathcal{I}_0} \left(g_i - \alpha\right) \phi(X_i),
\end{aligned}$$

where we used that $\sum_{i=1}^n g_i \phi(X_i) = 0$ by construction. Now, we leverage our assumption that S_i are distinct with probability 1. We see immediately that $\text{card}(\mathcal{I}_0) \le d$, because with distinct values S_i we may satisfy (at most) d linear equalities, and so

$$\left\| \frac{1}{n} \sum_{i=1}^n \phi(X_i) \left(1\left\{S_i > \langle \widehat{\theta}, \phi(X_i) \rangle\right\} - \alpha\right) \right\|_2 \le \frac{\text{card}(\mathcal{I}_0)}{n} b_\phi \le \frac{d}{n} b_\phi.$$

Because Proposition 3 controls the fluctuations of the process $\theta \mapsto \phi(x) 1\{s > \langle \phi(x), \theta \rangle\}$, we obtain that with probability at least $1 - e^{-nt^2}$,

$$\begin{aligned}
&\left\| \mathbb{E}\left[\phi(X) 1\left\{S > \langle \widehat{\theta}, \phi(X) \rangle\right\}\right] - \alpha \mathbb{E}[\phi(X)] \right\|_2 \\
&\le \left\| \frac{1}{n} \sum_{i=1}^n \phi(X_i) \left(1\left\{S_i > \langle \widehat{\theta}, \phi(X_i) \rangle\right\} - \alpha\right) \right\|_2 + 2b_\phi \sqrt{\frac{d}{n} \log \frac{n}{d}} + \frac{b_\phi \alpha}{\sqrt{n}} + b_\phi t \\
&\le b_\phi \frac{d}{n} + 3b_\phi \sqrt{\frac{d}{n} \log \frac{n}{d}} + b_\phi t.
\end{aligned}$$

This completes the proof of the theorem.

4 Sharper and rate-optimal approximate conditional bounds

The bounds Theorem 1 provides do not reflect the sharper coverage possible in the purely marginal case that Proposition 2 provides. By leveraging empirical process variants of the Bernstein concentration inequalities we use to prove Proposition 2, we can achieve sharper bounds on weighted coverage, where the sharper bounds depend on the expectations and variances of the linear functionals $x \mapsto \langle u, \phi(x) \rangle$ themselves. As a consequence of our results, in terms of achieving approximate conditional coverage (i.e., weighted coverage as in Definition 1.1), the empirical estimator (11) is minimax rate optimal; we discuss this after Theorem 3.

To state our results, assume that $\mathbb{B} \subset \mathbb{R}^d$ is an arbitrary but bounded set of vectors, and define

$$b_\phi(u) := \sup_{x \in \mathcal{X}} |\langle u, \phi(x) \rangle| \quad \text{and} \quad b_\phi := \sup_{u \in \mathbb{B}} b_\phi(u).$$

We can then extend Proposition 2 to weighted conditional coverage (Def. 1.1), conditional on the sample. We defer their proofs, presenting the building blocks common to both in Section 4.1, then specializing in Sections 4.2 and 4.3, respectively.

Theorem 2. *Let $K_n = 1 + \log_2 n$. Then there exists a numerical constant $c < \infty$ such that for all $t \geq 0$, with probability at least $1 - 2K_n e^{-t} - e^{-d \log n - t}$,*

$$\begin{aligned} &\mathbb{E}\left[\langle u, \phi(X_{n+1}) \rangle \left(1\{Y_{n+1} \notin \widehat{C}(X_{n+1})\} - \alpha\right) \mid P_n\right] \\ &\leq c \left[\sqrt{b_\phi(u)\alpha \cdot \mathbb{E}[\langle u, \phi(X) \rangle]} \sqrt{\frac{d \log n + t}{n}} + b_\phi \frac{d \log n + t}{n}\right] \end{aligned}$$

simultaneously for all $u \in \mathbb{B}$ such that $\langle u, \phi(x) \rangle \geq 0$ for all x. If additionally the scores S_i are distinct with probability 1, then with the same probability,

$$\begin{aligned} &\mathbb{E}\left[\langle u, \phi(X_{n+1}) \rangle \left(1\{Y_{n+1} \notin \widehat{C}(X_{n+1})\} - \alpha\right) \mid P_n\right] \\ &\geq -c \left[\sqrt{b_\phi(u)\alpha \cdot \mathbb{E}[\langle u, \phi(X) \rangle]} \sqrt{\frac{d \log n + t}{n}} + b_\phi \frac{d \log n + t}{n}\right] \end{aligned}$$

simultaneously for all $u \in \mathbb{B}$ such that $\langle u, \phi(x) \rangle \geq 0$ for all x.

Simplifying the statement and ignoring higher-order terms, we can obtain a guarantee for weighted coverage (6): for the class $\mathcal{W} = \{w(x) = \langle u, \phi(x) \rangle\}_{u \in \mathbb{R}^d}$, with probability $1 - e^{-t}$,

$$\mathbb{P}_w(Y_{n+1} \in \widehat{C}_{n+1}) \geq 1 - \alpha - O(1) \left[\sqrt{\frac{\alpha}{\mathbb{E}[w(X)]}} \cdot \sqrt{\frac{d \log n + t}{n}}\right]$$

simultaneously for $w \geq 0$ with the normalization that $w(x) = \langle u, \phi(x) \rangle$ for a u satisfying $b_\phi(u) = 1$.

Applying the theorem to group indicators, meaning that we have a collection of groups $\mathcal{G} \subset 2^{\mathcal{X}}$, and the feature mapping $\phi(x) = (1\{x \in G\})_{G \in \mathcal{G}}$, we have the following corollary.

Corollary 4.1. *Assume that $\phi(x) = (1\{x \in G\})_{G \in \mathcal{G}}$, and let $d = \mathrm{card}(\mathcal{G})$. Then with probability at least $1 - 3 \log_2 n e^{-t}$,*

$$\mathbb{P}(Y_{n+1} \notin \widehat{C}(X_{n+1}) \mid X_{n+1} \in G, P_n) \leq \alpha + c \left[\sqrt{\frac{\alpha}{\mathbb{P}(X_{n+1} \in G)} \frac{d \log n + t}{n}} + \frac{d \log n + t}{\mathbb{P}(X_{n+1} \in G) \cdot n}\right]$$

simultaneously for all $G \in \mathcal{G}$.

The result follows immediately upon considering the standard basis vectors $u = e_i$. Comparing this to Corollary 3.3, we see a much sharper deviation guarantee.

When the scores $S = s(X, Y)$ are distinct with probability 1, we achieve two sided bounds extending Theorem 2, as in Proposition 2. The next theorem provides an exemplar result.

Theorem 3. *Let the conditions of Theorem 2 hold, except assume that S_i are distinct with probability 1, and that the mapping $\phi(x)$ includes a constant bias term $\phi_1(x) = 1$. Then there exists a numerical constant $c < \infty$ such that for all $t \geq 0$, with probability at least $1 - 2K_n e^{-t} - e^{-d \log n - t}$, simultaneously for all $u \in \mathbb{B}$,*

$$\left|\mathbb{E}\left[\langle u, \phi(X)\rangle \left(1\{Y_{n+1} \notin \widehat{C}(X_{n+1})\} - \alpha\right) \mid P_n\right]\right| \leq c\left[b_\phi(u)\sqrt{\alpha}\sqrt{\frac{d \log n + t}{n}} + b_\phi \frac{d \log n + t}{n}\right].$$

The conclusion is weaker than that of Theorem 2, as it replaces $\sqrt{b_\phi(u)\mathbb{E}[\langle u, \phi(X)\rangle]}$ with $b_\phi(u)$.

These convergence guarantees are sharp to within logarithmic factors, and appear to capture the correct dependence on α and the weight functions $\mathcal{W}$. Indeed, assume that the estimated confidence set $\widehat{C}_n$ takes the form $\widehat{C}_n(x) = \{y \mid s(x, y) \leq \widehat{h}(x)\}$ or $\widehat{C}_n(x) = \{y \mid \widehat{a}(x) \leq s(x, y) \leq \widehat{b}(x)\}$ for *some* estimated functions $\widehat{h}$, $\widehat{a}$, or $\widehat{b}$. Areces et al. [1] show that for *any* class of functions $\mathcal{W}$ mapping $\mathcal{X}$ to $\{\pm 1\}$ with VC-dimension d, there exists a sampling distribution P for which $S \mid X$ has a continuous density and such that with constant probability over the draw of P_n,

$$\left|\mathbb{E}\left[w(X_{n+1})1\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} - w(X_{n+1})\alpha \mid P_n\right]\right| \geq c\sqrt{\frac{d\alpha(1-\alpha)}{n}},$$

where $c > 0$ is a universal constant. To compare this with Theorems 2 and 3, let $\{G_1, \ldots, G_d\}$, $G_j \subset \mathcal{X}$, be a partition of $\mathcal{X}$ into d groups, and define the group feature mapping $\phi(x) = [1\{x \in G_j\}]_{j=1}^d$. Then the class of linear functionals $\mathcal{W} = \{w \mid w(x) = \langle u, \phi(x)\rangle\}_{u \in \mathbb{R}^d}$ has VC-dimension d, as does its restriction $\mathcal{W}_1 = \{w \mid w(x) = \langle u, \phi(x)\rangle\}_{u \in \{\pm 1\}^d}$, where $w \in \mathcal{W}_1$ satisfies $w(x) \in \{\pm 1\}$. Theorems 2 and 3, conversely, demonstrate that for $\mathbb{B}_1 = \{u \mid \|u\|_1 \leq 1\}$, we have

$$\left|\mathbb{E}\left[w(X_{n+1})\left(1\left\{Y_{n+1} \notin \widehat{C}_n(X_{n+1})\right\} - \alpha\right) \mid P_n\right]\right| \leq c\sqrt{\frac{\alpha(1-\alpha)}{n}} \cdot \sqrt{d \log n + t}$$

with probability at least $1 - e^{-t}$ simultaneously for all $w(x) = \langle u, \phi(x)\rangle$ for some $u \in \mathbb{B}_1$, as long as $\alpha < \frac{1}{2}$ (where we use $1 - \alpha \geq \frac{1}{2}$ and wrap constants together for a cleaner statement).

4.1 Proof of Theorems 2 and 3: building blocks

Our proof leverages a combination of Talagrand's concentration inequalities for empirical processes, a VC-dimension calculation, and localized Rademacher complexities [4, 18]. We begin with the form of Talagrand's empirical process inequality with constants due to Bousquet [7].

Lemma 4.1 (Talagrand's empirical process inequality)**.** *Let $\mathcal{F}$ be a countable class of functions with $Pf = 0$ and $\|f\|_\infty \leq b$ for $f \in \mathcal{F}$. Let $Z = \sup_{f \in \mathcal{F}} P_n f$ and $\sigma^2 = \sigma^2(\mathcal{F}) = \sup_{f \in \mathcal{F}} Pf^2$. Define $v^2 \coloneqq \sigma^2 + 2b\mathbb{E}[Z]$. Then for $t \geq 0$,*

$$\mathbb{P}\left(Z \geq \mathbb{E}[Z] + \sqrt{2v^2 t} + b\frac{t}{3}\right) \leq e^{-nt}.$$

Because we will consider functions of the form $f(x, s) = \langle u, \phi(x)\rangle 1\{\langle \theta, \phi(x)\rangle > s\}$, we also require some control over the complexity of such rank-one-like products.

Lemma 4.2. *Let $\mathcal{H}$ and $\mathcal{G}$ be classes of functions with VC-dimensions d_1 and d_2, respectively. Then the classes of functions*

$$\mathcal{F} \coloneqq \{f \mid f(x) = g(x)1\{h(x) > 0\}\} \quad \textit{and} \quad \mathcal{F}_+ \coloneqq \{f \mid f(x) = g(x)1\{h(x) > 0\} - cg(x)\}$$

where c is a constant have VC-dimension $O(1)(d_1 + d_2)$.

Proof For a set of points $x_1, \ldots, x_n$, let $\mathcal{S}(x_1^n, \mathcal{H}) = \{1\{h(x_i) > 0\}\}_{i=1}^n$ be the set of "sign" vectors that h realizes. By definition of the VC-dimension and the Sauer-Shelah lemma, this set has cardinality at most $\sum_{i=0}^{d_1} \binom{n}{i} \le (\frac{ne}{d_1})^{d_1}$. Similarly, the set of signs

$$\mathcal{S}(x_1^n, \mathcal{F}) = \{\text{sign}(g(x_i)) \cdot 1\{h(x_i) > 0\}\}_{i=1}^n$$

has cardinality at most $\sum_{i=0}^{d_1} \binom{n}{i} \cdot \sum_{i=0}^{d_2} \binom{n}{i} \le (\frac{ne}{d_1})^{d_1} (\frac{ne}{d_2})^{d_2}$. If n is large enough that

$$\left(\frac{ne}{d_1}\right)^{d_1} \cdot \left(\frac{ne}{d_2}\right)^{d_2} < 2^n,$$

then certainly $\mathcal{F}$ cannot shatter n points; this occurs once $n \ge c \cdot (d_1 + d_2)$ for some numerical constant c. For the second class the argument is similar. $\square$

For the next lemma, our main technical building block for convergence, we consider the class of functions $\mathcal{F}$ indexed by $u \in \mathbb{B}$ and $h \in \mathcal{H}$, where $\mathcal{H}$ is a class with VC-dimension at most d, with

$$f(x, s) = f_{u,h}(x, s) \coloneqq \langle u, \phi(x) \rangle 1\{s > h(x)\}\,. \tag{14}$$

Each of these functions evidently satisfies $|f(x, s)| \le b_\phi$. The variance proxy

$$v^2(u, h) \coloneqq v^2(f_{u,h}) = P f_{u,h}(X, S)^2 = \mathbb{E}[\langle \phi(X), u \rangle^2 1\{S > h(X)\}] \tag{15}$$

and its empirical variant

$$v_n^2(u, h) = P_n f_{u,h}(X, S)^2 = \frac{1}{n} \sum_{i=1}^n \langle \phi(X_i), u \rangle^2 1\{S_i > h(X_i)\}\,.$$

will allow us to bound deviations of $P_n f$ from Pf relative to $v^2(f)$.

For later use, we recall the *empirical Rademacher complexity* of a function class $\mathcal{F}$,

$$\mathfrak{R}_n(\mathcal{F}) \coloneqq \frac{1}{n} \mathbb{E}\left[\sup_{f \in \mathcal{F}} \sum_{i=1}^n \varepsilon_i f(X_i) \mid X_1^n\right],$$

where $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathsf{Uni}\{\pm 1\}$ are random signs. In some cases, we will require *localized Rademacher complexities* [4, 18] around a class $\mathcal{F}_r \coloneqq \{f \mid Pf^2 \le r^2\}$, which contains functions of small variance, allowing us to "relativize" bounds. Bartlett et al. [4, Proof of Corollary 3.7] demonstrate the following.

Lemma 4.3. *Let $\mathcal{F}$ be a star-convex collection of functions, meaning that $f \in \mathcal{F}$ implies $\lambda f \in \mathcal{F}$ for $\lambda \in [0, 1]$, and assume that $\sup_x |f(x)| \le b$ and $\mathcal{F}$ has VC-dimension d. Then*

$$\mathbb{E}\left[\mathfrak{R}_n(\mathcal{F}_r)\right] \le \frac{b_\phi}{n} + cr\sqrt{\frac{d}{n} \log \frac{b_\phi}{r}} \quad \textit{if} \quad r^2 > b_\phi^2 \frac{d}{n} \log \frac{n}{d}, \tag{16}$$

where $c < \infty$ is a numerical constant.

We will combine the VC-bound in Lemma 4.2, the version of Talagrand's empirical process inequality in Lemma 4.1, and a localization argument on Rademacher complexities via inequality (16) to prove the following lemma in Appendix A.2.

Lemma 4.4. *Let $\mathcal{F}$ be the class of functions (14). Let $K_n = 1 + \log_2 n$. Then for all $t \ge 0$, with probability at least $1 - K_n e^{-t}$ over the draw of the sample P_n,*

$$|(P_n - P)f| \le c\left[v(f)\sqrt{\frac{d\log n + t}{n}} + b_\phi \frac{d\log n + t}{n}\right]$$

simultaneously for all $f \in \mathcal{F}$, where $c < \infty$ is a numerical constant. In addition, with the same probability,

$$|(P_n - P)\langle u, \phi(X)\rangle| \le c\left[\sqrt{P\langle u, \phi\rangle^2}\sqrt{\frac{d\log n + t}{n}} + b_\phi \frac{d\log n + t}{n}\right]$$

simultaneously for all $u \in \mathbb{B}$.

Next we present a version of a result appearing as [30, Theorem 14.12] (the result there assumes functions are mean-zero, but an inspection of the proof shows this is unnecessary); see also the results of [23] and [9, Proof of Proposition 1]. These show that second moments satisfy one-sided concentration bounds with high probability as soon as we have the fourth moment condition

$$\mathbb{E}[f^4(X,S)] \le b^2 \mathbb{E}[f^2(X,S)] \quad \text{for all } f \in \mathcal{F}. \tag{17}$$

For the setting we consider, where $\mathcal{F}$ consists of product functions (14), inequality (17) immediately holds with $b = b_\phi$, though tighter constants may be possible.

Lemma 4.5. *There exist numerical constants $0 < c$ and $C < \infty$ such that the following holds. Let inequality (17) hold and for $\mathcal{F}_r = \{f \mid Pf^2 \le r^2\}$, let r satisfy $\mathbb{E}[\mathfrak{R}_n(\mathcal{F}_r)] \le \frac{r^2}{Cb}$. Then with probability at least $1 - e^{-cnr^2/b^2}$,*

$$P_n f^2 \ge \frac{1}{2} P f^2 \quad \textit{simultaneously for all } f \textit{ s.t. } v(f) \ge r.$$

Inequality (16) shows the conclusions of of Lemma 4.5 hold if the radius r satisfies

$$r\sqrt{\frac{d}{n}\log\frac{n}{d}} \lesssim \frac{r^2}{b_\phi} \quad \text{or} \quad r^2 \gtrsim b_\phi^2 \cdot \frac{d}{n}\log\frac{n}{d}.$$

We then obtain the following consequence:

Lemma 4.6. *Let $r^2 \gtrsim b_\phi^2 \frac{d}{n}\log\frac{n}{d}$. Then with probability at least $1 - e^{-cnr^2/b_\phi^2}$,*

$$P_n\langle u, \phi(X)\rangle^2 1\{S > h(X)\} \ge \frac{1}{2} P\langle u, \phi(X)\rangle^2 1\{S > h(X)\}$$

simultaneously over $u \in \mathbb{B}$ and h such that $P\langle u, \phi(X)\rangle^2 1\{S > h(X)\} \ge r^2$.

Now, let $\widehat{h} = \langle \widehat{\theta}, \phi(\cdot)\rangle$, where $\widehat{\theta}$ solves the problem (11). Then simultaneously for all $u \in \mathbb{B}$, with probability at least $1 - K_n e^{-t}$,

$$\left|(P_n - P)\langle u, \phi(X)\rangle 1\left\{S > \widehat{h}(X)\right\}\right| \le c\left[v(\widehat{h}, u)\sqrt{\frac{d\log n + t}{n}} + b_\phi \frac{d\log n + t}{n}\right] \tag{18}$$

by Lemma 4.4. Moreover, for $r^2 \gtrsim b_\phi^2 \frac{d}{n}\log\frac{n}{d}$, either $v(\widehat{h}, u) \le r$ or

$$v^2(\widehat{h}, u) \le 2P_n\langle \phi(X), u\rangle^2 1\left\{S > \widehat{h}(X)\right\}$$

by Lemma 4.6 (with the appropriate probability $1 - e^{-cr^2/b_\phi^2}$).

4.2 Proof of Theorem 2: nonnegative weights

We now specialize our development to the particular cases that $\langle u, \phi(x)\rangle \ge 0$ for all $x \in \mathcal{X}$. First, we leverage the particular structure of the quantile loss to give a non-probabilistic bound on the empirical weights.

Lemma 4.7. *Let u be such that $\langle u, \phi(x)\rangle \ge 0$ for all $x \in \mathcal{X}$. Then*

$$P_n\langle \phi(X), u\rangle 1\Big\{S > \widehat{h}(X)\Big\} \le \alpha P_n\langle \phi(X), u\rangle.$$

If additionally S_i are all distinct, then

$$P_n\langle \phi(X), u\rangle 1\Big\{S > \widehat{h}(X)\Big\} \ge \alpha P_n\langle \phi(X), u\rangle - b_\phi(u)\frac{d}{n}.$$

Proof The directional derivative $\ell'_\alpha(t;1) \coloneqq \lim_{\delta\downarrow 0} \frac{\ell_\alpha(t+\delta)-\ell_\alpha(t)}{\delta} = 1\{t \ge 0\} - (1-\alpha)$. Then

$$\begin{aligned} P_n\langle \phi(X), u\rangle 1\Big\{S > \widehat{h}(X)\Big\} &= P_n\langle \phi(X), u\rangle \left(1 - \alpha - 1\Big\{S \le \widehat{h}(X)\Big\}\right) + P_n\langle u, \phi(X)\rangle\alpha \\ &= P_n\langle \phi(X), u\rangle \left(-\ell'_\alpha(\widehat{h}(X) - S; 1)\right) + \alpha P_n\langle u, \phi(X)\rangle. \end{aligned}$$

Letting $L_n(h) = P_n\ell_\alpha(h(X) - S)$, we now use that directional derivatives are positively homogeneous [14] and that by assumption $\widehat{h}$ minimizes $P_n\ell_\alpha(h(X) - S)$ over functions of the form $h(x) = \langle \theta, \phi(x)\rangle$ to obtain

$$P_n\langle \phi(X), u\rangle \left(-\ell'_\alpha(\widehat{h}(X) - S; 1)\right) = -P_n\ell'_\alpha(\widehat{h}(X) - S; \langle \phi(X), u\rangle) = -L'_n(\widehat{h}(X); u).$$

But of course, as $\widehat{h}$ minimizes L_n, we have $L'_n(\widehat{h}(X); u) \ge 0$ for all u, and so

$$P_n\langle \phi(X), u\rangle 1\Big\{S > \widehat{h}(X)\Big\} \le \alpha P_n\langle u, \phi(X)\rangle.$$

If S_i are all distinct, then considering the left directional derivative, we also have

$$P_n\langle \phi(X), u\rangle 1\Big\{S \ge \widehat{h}(X)\Big\} \ge \alpha P_n\langle u, \phi(X)\rangle.$$

If $\mathcal{I}_0 = \{i \mid \widehat{h}(X_i) = S_i\}$, then $\mathrm{card}(\mathcal{I}_0) \le d$, and so

$$0 \ge P_n\langle \phi(X), u\rangle \left(1\Big\{S > \widehat{h}(X)\Big\} - 1\Big\{S \ge \widehat{h}(X)\Big\}\right) = -P_n\langle \phi(X), u\rangle 1\Big\{S = \widehat{h}(X)\Big\} \ge -b_\phi(u)\frac{d}{n}.$$

Rearranging and performing a bit of algebra, we obtain the second claim of the lemma. □

From the lemma, we see that

$$\begin{aligned} &P\langle u, \phi(X)\rangle \left(1\Big\{S > \widehat{h}(X)\Big\} - \alpha\right) \\ &= (P - P_n)\langle u, \phi(X)\rangle \left(1\Big\{S > \widehat{h}(X)\Big\} - \alpha\right) + P_n\langle u, \phi(X)\rangle \left(1\Big\{S > \widehat{h}(X)\Big\} - \alpha\right) \\ &\le (P - P_n)\langle u, \phi(X)\rangle 1\Big\{S > \widehat{h}(X)\Big\} - \alpha(P - P_n)\langle u, \phi(X)\rangle \qquad (19) \end{aligned}$$

by Lemma 4.7. Additionally, the lemma implies that

$$P_n\langle\phi(X),u\rangle^2 1\left\{S>\widehat{h}(X)\right\}\le b_\phi(u)P_n\langle\phi(X),u\rangle 1\left\{S>\widehat{h}(X)\right\}\le b_\phi(u)\alpha P_n\langle\phi(X),u\rangle.$$

We use this to control the first term in the expansion (19) by combining these bounds with inequality (18) and considering that $v(\widehat{h},u)\le r$ or $v(\widehat{h},u)>r$ where $r^2=O(1)b_\phi^2\frac{d}{n}\log\frac{n}{d}$. In the latter, we have $v^2(\widehat{h},u)\le cb_\phi(u)\alpha P_n\langle\phi(X),u\rangle$. We have therefore shown that for any $r^2\gtrsim\frac{d}{n}\log\frac{n}{d}$, with probability at least $1-K_ne^{-t}-e^{-nr^2}$, for all $u\in\mathbb{B}$ with $\langle u,\phi(x)\rangle\ge 0$,

$$\begin{aligned}&\left|(P_n-P)\langle u,\phi(X)\rangle 1\left\{S>\widehat{h}(X)\right\}\right| \qquad (20)\\&\le c\left[\left(\sqrt{b_\phi(u)\alpha P_n\langle u,\phi(X)\rangle}+b_\phi r\right)\sqrt{\frac{d\log n+t}{n}}+b_\phi\frac{d\log n+t}{n}\right].\end{aligned}$$

Applying Lemma 4.4 to the quantity $P_n\langle u,\phi(X)\rangle$ shows that simultaneously for all $u\in\mathbb{B}$,

$$|(P_n-P)\langle u,\phi(X)\rangle|\le c\left[\sqrt{b_\phi(u)P\langle u,\phi(X)\rangle}\sqrt{\frac{d\log n+t}{n}}+b_\phi\frac{d\log n+t}{n}\right]$$

with probability at least $1-K_ne^{-t}$. Substituting this into the bounds (19) and (20), and ignoring lower-order terms (because $\alpha\le 1$), we obtain the guarantee that for all $t\ge 0$ and $r^2\gtrsim\frac{d}{n}\log\frac{n}{d}$, then with probability at least $1-2K_ne^{-t}-e^{-nr^2}$, for all u such that $P\langle u,\phi(X)\rangle\ge b_\phi\frac{d\log n+t}{n}$,

$$\mathbb{E}\left[\langle u,\phi(X)\rangle\left(1\left\{S>\widehat{h}(X)\right\}-\alpha\right)\mid P_n\right]\le c\left[\left(\sqrt{\alpha b_\phi(u)P\langle u,\phi(X)\rangle}+b_\phi r\right)\sqrt{\frac{d\log n+t}{n}}+b_\phi\frac{d\log n+t}{n}\right]$$

and for all u such that $P\langle u,\phi(X)\rangle\le b_\phi\frac{d\log n+t}{n}$,

$$\mathbb{E}\left[\langle u,\phi(X)\rangle\left(1\left\{S>\widehat{h}(X)\right\}-\alpha\right)\mid P_n\right]\le cb_\phi\left[r\sqrt{\frac{d\log n+t}{n}}+\frac{d\log n+t}{n}\right].$$

Combining the inequalities and replacing r^2 with $\frac{d\log n+t}{n}$ gives the first claim of Theorem 2.

For the second claim, when the scores S_i are distinct, note simply that we may replace inequality (19) with

$$\begin{aligned}&P\langle u,\phi(X)\rangle\left(1\left\{S>\widehat{h}(X)\right\}-\alpha\right)\\&=(P-P_n)\langle u,\phi(X)\rangle\left(1\left\{S>\widehat{h}(X)\right\}-\alpha\right)+P_n\langle u,\phi(X)\rangle\left(1\left\{S>\widehat{h}(X)\right\}-\alpha\right)\\&\ge(P-P_n)\langle u,\phi(X)\rangle 1\left\{S>\widehat{h}(X)\right\}-\alpha(P-P_n)\langle u,\phi(X)\rangle-b_\phi(u)\frac{d}{n}.\end{aligned}$$

The remainder of the argument is, *mutatis mutandis*, identical to the proof of the first claim of the theorem.

4.3 Proof of Theorem 3: distinct scores

Because of the distinctness of S_i and that we assume $\phi_1(x)=1$ (that is, we include the constant offset), the optimality conditions for the quantile loss imply that

$$\frac{d}{n}\ge\sum_{i=1}^n 1\left\{S_i>\widehat{h}(X_i)\right\}-\alpha\ge-\frac{d}{n}.$$

So if $b_\phi(u) \coloneqq \sup_{x\in\mathcal{X}} |\langle u, \phi(x)\rangle|$, then

$$P_n\langle \phi(X), u\rangle^2 1\left\{S > \widehat{h}(X)\right\} \le b_\phi^2(u)\left(\alpha + \frac{d}{n}\right).$$

Applying inequality (18), we find that with probability at least $1 - K_n e^{-t} - e^{-cnr^2/b_\phi^2}$,

$$\left|(P_n - P)\langle u, \phi(X)\rangle 1\left\{S > \widehat{h}(X)\right\}\right| \le c\left[\left(b_\phi(u)\sqrt{\alpha} + r\right)\sqrt{\frac{d\log n + t}{n}} + b_\phi \frac{d\log n + t}{n}\right].$$

The deviations $\alpha(P_n - P)\langle u, \phi(X)\rangle$ are of smaller order than this by Lemma 4.4.

5 Experimental Results

Our main purpose thus far has been to re-investigate conditional quantile estimation procedures, providing theoretical bounds for their performance; there is already substantial practical experience with these methods. Nonetheless, we can incorporate a few recent theoretical results to enhance the practical performance of the proposed conformalization procedures, allowing some additional performance gains, while simultaneously exhibiting the need for future work. We consider mostly the difference between the full conformal approach that Gibbs et al. [11] develop and the split-conformal approaches that simply minimize the empirical loss (11). Our theoretical results provide no guidance to lower-order corrections to the desired level α to guarantee (exact) marginal coverage rather than approximate sample-conditional coverage, and so we proceed a bit heuristically here, using theoretical results to motivate modifications of the level α that do not change the sample-conditional coverage results we provide, but which turn out to be empirically effective.

To motivate our tweaks, recall the classical (unconditional) conformal approach to achieve exact finite-sample marginal coverage $\mathbb{P}(Y_{n+1} \in \widehat{C}_n(X_{n+1}))$, where the confidence confidence set $\widehat{C}_n(x) = \{y \mid s(x,y) \le \widehat{\tau}_n\}$. Setting $\widehat{\tau}_n = \mathsf{Quant}_{(1+1/n)(1-\alpha)}(S_1^n)$, the slightly enlarged quantile, guarantees $(1-\alpha)$ coverage; this follows by letting $S_{(i,n)}$ be the order statistics of S_1^n and $S_{(i,n+1)}$ those of S_1^{n+1}, and noting that the score $S_{n+1} \le S_{(k,n)}$ if and only if $S_{n+1} \le S_{(k,n+1)}$ [25, Lemma 2], so the inflation by $\frac{n+1}{n}$ is necessary. Equivalently, if we wish to achieve coverage $(1-\alpha_{\mathrm{des}})$ using the estimator (11) with feature mapping $\phi(x) = 1$ fit at level α, then α must solve $(1-\alpha) = (1+\frac{1}{n})(1-\alpha_{\mathrm{des}})$, that is, $\alpha = 1 - (1+\frac{1}{n})(1-\alpha_{\mathrm{des}}) = (1+\frac{1}{n})\alpha_{\mathrm{des}} - \frac{1}{n}$. That is, quantile regression under-covers.

When $\phi : \mathcal{X} \to \mathbb{R}^d$, it is then natural to heuristically imagine that the order statistics ought to "swap orders" by at most roughly d items and so we ought to target coverage $\frac{n+d}{n}(1-\alpha_{\mathrm{des}})$; unfortunately, it escapes our ability to prove such a result currently. Nonetheless, we consider a "naive" adaptation of the confidence level, setting α to solve

$$(1-\alpha) = \left(1 + \frac{d}{n}\right)(1-\alpha_{\mathrm{des}}), \quad \text{or} \quad \alpha = \left(1+\frac{d}{n}\right)\alpha_{\mathrm{des}} - \frac{d}{n}, \tag{21}$$

and then choosing $\widehat{\theta}$ to minimize (11) with this α, which we term the "naive" choice. Bai et al. [2] give an alternative perspective, where they show that the actual marginal coverage achieved by quantile regression at level α in the high-dimensional scaling $d, n \to \infty$ with $d/n \to \kappa \in (0,1)$ is

$$(1-\alpha) - \frac{d}{n}\left(\frac{1}{2} - \alpha\right) + o(d/n)$$

for $\alpha < \frac{1}{2}$, at least when the covariates are Gaussian. Solving this and ignoring the higher-order term, we recognize that to achieve desired coverage α, we ought (according to this heuristic) to compute the estimator (11) using α solving

$$(1 - \alpha_{\rm des}) = (1 - \alpha) - \frac{d}{n}\left(\frac{1}{2} - \alpha\right) \quad \text{or} \quad \alpha = \frac{\alpha_{\rm des} - \frac{d}{2n}}{1 - \frac{d}{n}}. \tag{22}$$

We call the choice (22) the "scaling" choice. Neither of the rescalings (21) or (22) have any effect on the convergence guarantees our theory provides, as they are of lower order.

5.1 Synthetic datasets

We perform two synthetic experiments that give a sense of the coverage properties of the methods we have analyzed. These exploratory experiments help provide justification for the heuristic corrections to the desired level α we set in the real data experiments.

5.1.1 Level rescaling on a simple synthetic dataset

For our first experiment, we consider the simple setting of a standard Gaussian linear model, where we observe

$$y_i = \langle w^\star, x_i \rangle + \varepsilon_i, \quad \varepsilon_i \stackrel{\rm iid}{\sim} \mathsf{N}(0, 1) \;\; \text{and} \;\; x_i \stackrel{\rm iid}{\sim} \mathsf{N}(0, I_d).$$

We mimic the experiment Gibbs et al. [11, Fig. 3] provide, but we investigate the coverage properties of the coverage set from the estimator (11) with uncorrected α and level α corrected either naively (21) or via the scaling correction (22). In all cases, we use the feature map $\phi(x) = (1, 1\{x_1 > 0\}, \ldots, 1\{x_d > 0\}) \in \{0, 1\}^{d+1}$ indicating nonnegative coordinates. Figure 1 displays the results of this experiment for 1000 trials, where in each trial, we draw $w^\star \sim \mathsf{Uni}(\mathbb{S}^{d-1})$, fit a regression estimator $\widehat{w}$ on a training dataset of size $n_{\rm train} = 100$ using least squares, then conformalize this predictor using a validation set of size n and evaluate its coverage on a test dataset of size $n_{\rm test} = 10 n_{\rm train} = 1000$. We vary the ratio n/d of the validation dataset, keeping $d = 20$ fixed. From the figure, it is clear that the uncorrected confidence set using $\alpha = \alpha_{\rm des} = .1$ undercovers, especially when the ratio $n/d < 20$ or so. The naive correction (21) appears to be a bit conservative, while the scaling correction (22) is more effective.

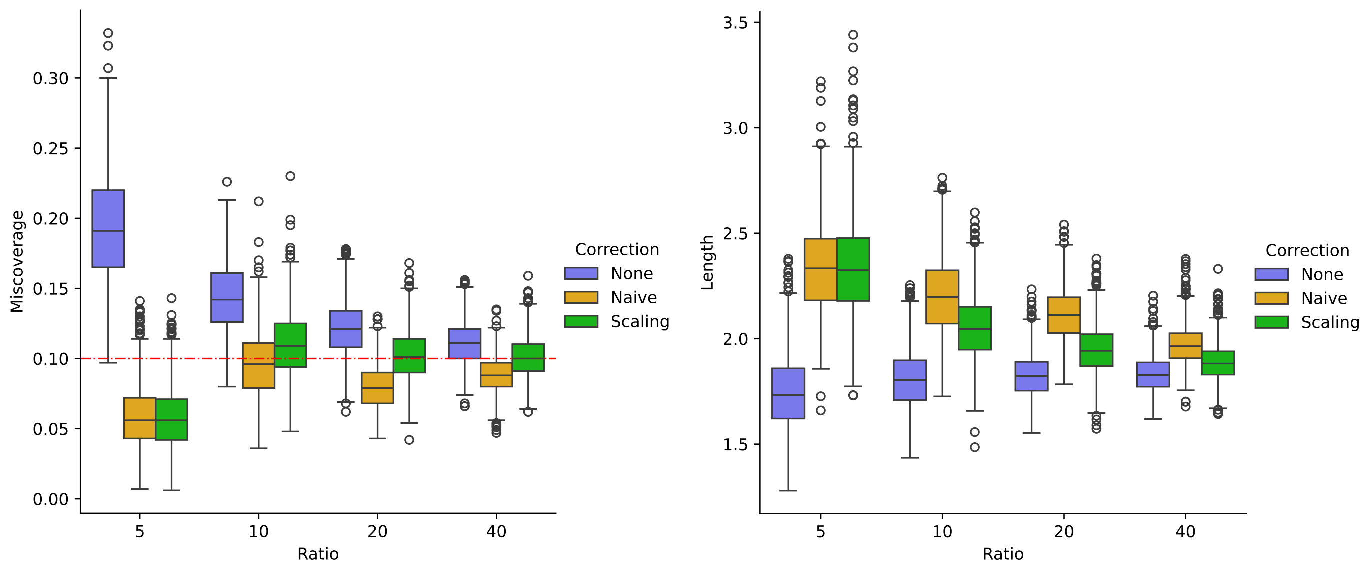
5.1.2 Full conformal versus split-conformal predictions

We briefly look at the coverage properties of the full conformalization method (5) from the paper [11], comparing with split-conformal methods (11), on a synthetic regression dataset we design to have asymmetric mean-zero heteroskedastic noise. We generate pairs $(X_i, Y_i) \in \mathbb{R}^2$ according to $Y = f(x) + \varepsilon(x)$, discretizing $x \in [0, 1]$ into bins $B_i = \{x \mid \frac{i}{k} \le x < \frac{i+1}{k}\}$, $i = 0, \ldots, k-1$, for $k = 5$. Within each experiment, we draw $U_0, U_1 \stackrel{\rm iid}{\sim} \mathsf{Uni}[-1, 1]$ and $\phi_0, \phi_1 \stackrel{\rm iid}{\sim} \mathsf{Uni}[\frac{\pi}{4}, 4\pi]$ to define

$$f(x) = U_0 \cos(\phi_0 \cdot x) + U_1 \sin(\phi_1 \cdot x).$$

Within the ith region $\frac{i}{k} \le x < \frac{i+1}{k}$ we set $\lambda_{0,i} = \exp(3 - \frac{3}{k} i)$ and $\lambda_{1,i} = \exp(4 - \frac{3}{k} i)$, i.e., evenly spaced in $\{e^3, \ldots, e^0\}$ and $\{e^4, \ldots, e^1\}$, and draw

$$\varepsilon(x) \sim \begin{cases} \mathsf{Exp}(\lambda_{0,i}) & \text{with probability } \frac{\lambda_{0,i}}{\lambda_{0,i} + \lambda_{1,i}} = \frac{1}{1+e} \\ -\mathsf{Exp}(\lambda_{1,i}) & \text{otherwise,} \end{cases}$$



(a) (b)

Figure 1. Impact of the correction to α used in fitting the conformal predictor (11) for a desired level $\alpha_{\text{des}} = .1$, i.e., 90% coverage. The "None" correction uses $\alpha = \alpha_{\text{des}}$, "Naive" uses the correction (21), and "Scaling" uses the correction (22). (a) Coverage rates with the desired coverage marked as the red line. (b) Width of predictive intervals $\widehat{C}(x) = \{y \in \mathbb{R} \mid |\widehat{f}(x) - y| \le \widehat{\theta}^\top \phi(x)\}$.

so that $\mathbb{E}[\varepsilon(x) \mid x] = 0$ but the noise is skewed upward, with variance increasing in i.

Figure 2 shows the results of this experiment over 200 independent trials, where in each experiment we draw a new mean function f and fit it using a degree 5 polynomial regression on a training set of size $n_{\text{train}} = 200$. The conformalization methods use a group-indicator featurization $\phi(x) = (1, 1\{x \in B_1\}, \ldots, 1\{x \in B_k\})$ and confidence sets $C(x) = \{y \mid \theta_0^\top \phi(x) \le y \le \theta_1^\top \phi(x)\}$. Within each trial, we compute miscoverage proportions $\mathbb{P}(Y \not\in \widehat{C}(X) \mid X \in B_i)$ for each bin i on a test set of size 500, drawing a new function f. We vary the size of the validation data $n_{\text{val}} = \{10k, 20k, 40k, 80k, 160k\}$, and use the scaling correction (22) to set α for the split-conformal method. The figure plots results for validation sizes $40k$ and $160k$; from the figure—which is consistent with our other sample sizes and experiments—we see that when the validation size is large relative to the dimension of the mapping ϕ, both methods are similar; for smaller ratios, the offline method undercovers slightly within the groups, though its marginal coverage remains near perfect in spite of the very non-Gaussian data.

We remark in passing that the full conformal method requires roughly $10\times$ the amount of time to compute predictions as the split conformal method requires to both fit a quantile prediction model and make its predictions. Once the split-conformal quantile model is available—it has been fit—this difference becomes roughly a factor of 2000–4000 in our experiments. For some applications, this may be immaterial; for others, it may be a substantial expense, suggesting that a decision between the offline method and the online procedure may boil down to one of computational feasibility.

5.2 Prediction on CIFAR-100

We also perform an exploratory experiment on the CIFAR-100 dataset, a 100-class image classification dataset consisting of 60,000 training examples and a 10,000 example test set. We use the

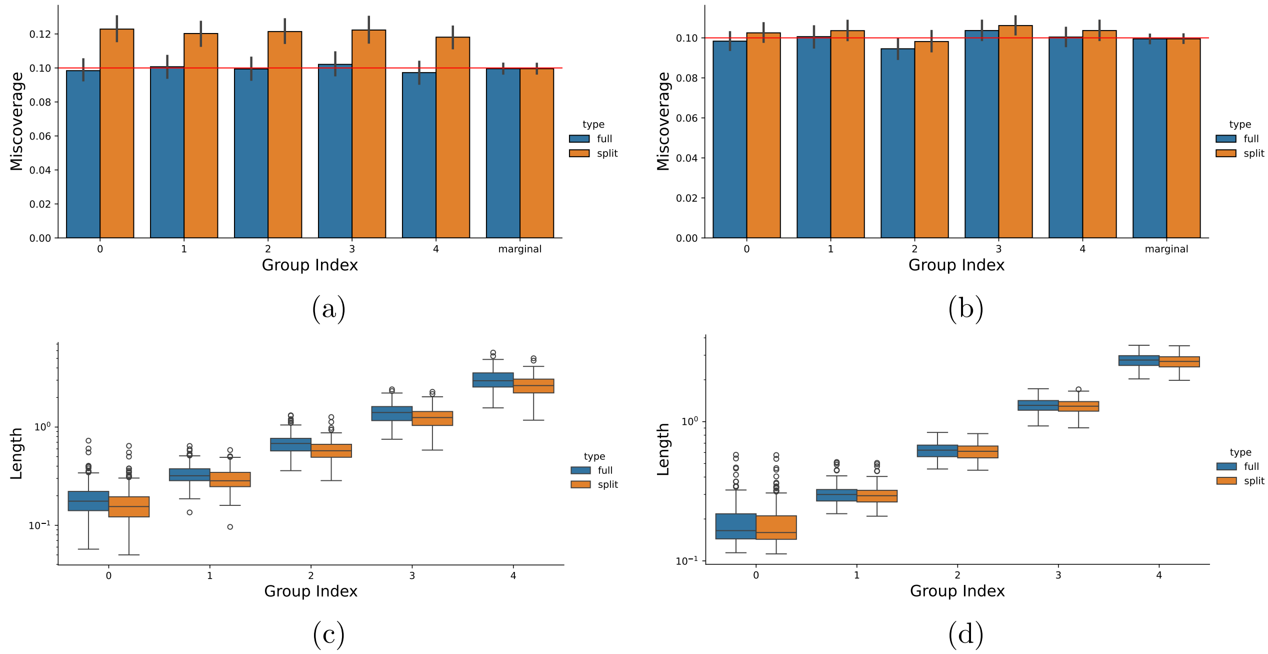


Figure 2. Comparison of full- and split-conformal methods on the simulated sinusoidal data of Sec. 5.1.2 with $n_{\text{train}} = 200$ training examples and target miscoverage $\alpha = .1$. Plots (a) and (c) use validation sample sizes $n_{\text{val}} = 20k = 100$, while (b) and (d) use $n_{\text{val}} = 160k = 800$. Plots (a) and (b) show miscoverage $\mathbb{P}(Y \notin \widehat{C}(X) \mid X \in B_i)$ by group B_i; plots (c) and (d) prediction interval lengths.

output features of a 50 layer ResNet, pre-trained on the ImageNet dataset [12, 13], as a $d = 2048$-dimensional input into a multiclass logistic regression classifier. We repeat the following experiment 10 times:

1. Uniformly randomly split the training examples into a validation set of size 10,000 and a model training set of size 50,000, on which we fit a linear classifier $s : \mathbb{R}^d \to \mathbb{R}^k$, where $s_y(x) = \langle \beta_y, x \rangle$ is the score assigned to class y, using multinomial logistic regression.

2. Draw a random matrix $W \in \mathbb{R}^{d \times d_0}$, where $d_0 = 10$ and $W_{ij} \stackrel{\text{iid}}{\sim} \mathsf{N}(0, 1)$, and use the validation data with score function $s(x, y) = s_y(x)$ and the lower-dimensional mapping $\phi(x) = W^\top x$ to predict quantiles via $\widehat{h}(x) = \langle \widehat{\theta}, \phi(x) \rangle$.

3. Compare the coverage of the full-conformal method, standard split conformal with a static threshold, meaning confidence sets of the form $\widehat{C}(x) = \{y \in [k] \mid s(x, y) \le \widehat{\tau}\}$, and split conformal with the threshold function $\widehat{h}(x)$ fit on the validation data. To perform the comparison, we draw subsamples from the test $Z_{\text{test}} = \{(x_i, y_i)\}_{i=1}^{n_{\text{test}}}$ by defining groups G of the form

$$G_{j,>} = \{(x, y) \in Z_{\text{test}} \mid \langle w_j, x \rangle \ge \mathsf{Quant}_{.8}(\{\langle w_j, x_i \rangle\}_{i=1}^{n_{\text{test}}})\} \quad \text{and}$$
$$G_{j,<} = \{(x, y) \in Z_{\text{test}} \mid \langle w_j, x \rangle \le \mathsf{Quant}_{.2}(\{\langle w_j, x_i \rangle\}_{i=1}^{n_{\text{test}}})\}$$

for each row $w_j^\top$ of the random dimension reduction matrix W from step 2.

Figure 3 displays the results of this experiment. In the figure, we notice three main results: first, the static thresholded sets $\widehat{C}(x) = \{y \mid s(x, y) \le \widehat{\tau}\}$ have substantially more variability in coverage on the random slices of the dataset. Second, the split conformal method and full conformal

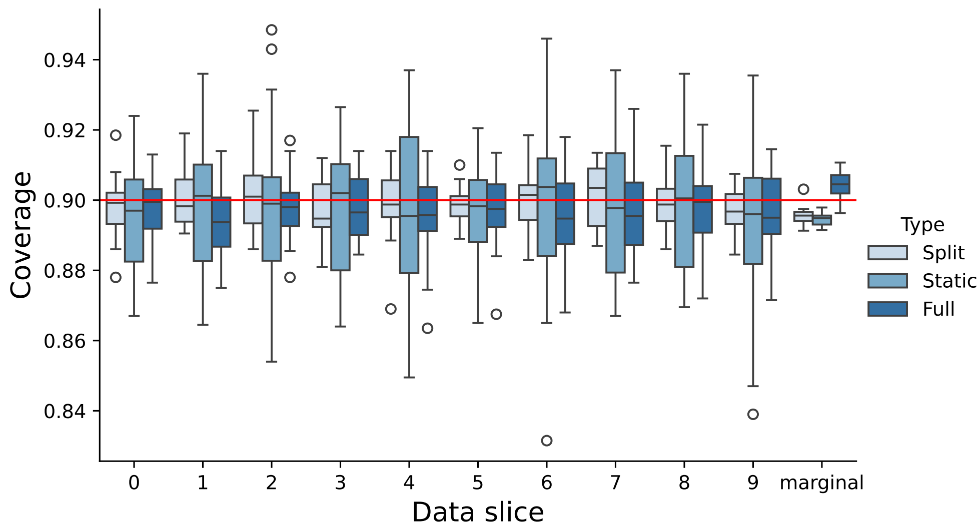


Figure 3. Coverage of full conformal, split conformal, and static split conformal methods on random 20% "slices" of CIFAR-100 data.

methods have similar coverage on each of the slices, with some slices exhibiting more variability of the full conformal methodology and some with the split conformal methodology, but all around the nominal (desired) 90% coverage level. Finally, the split conformal methods slightly undercover marginally, while the full conformal method slighlty overcovers marginally.

6 Conclusion and discussion

The results in our experiments, though they are relatively small scale, appear to be consistent with other experiments we do not present for brevity. In brief: split conformal methods with confidence sets using adaptive thresholds of the form $\widehat{C}(x) = \{y \mid s(x,y) \le \widehat{h}(x)\}$ can indeed provide stronger coverage than non-adaptive thresholds. Moreover, they are *much* faster to compute with than full conformal methods—in the experiment in Figure 3, the split conformal method was roughly 8000$\times$ faster than the full conformal method. Additionally, they enjoy strong sample-conditional stability as well as minimax optimality.

In spite of this, when the adaptive threshold $\widehat{h}(x)$ comes from a class of functions that is high-dimensional relative to the size of the data available for calibration, these methods can undercover, as they exhibit downard bias in their coverage. This bias is easy to correct for a static threshold $\widehat{C}(x) = \{y \mid s(x,y) \le \widehat{\tau}\}$ by simply using a slightly larger quantile, however, it is unclear how to address it in adaptive scenarios. This makes obtaining a data-adaptive way to compute the coverage bias, either marginally or along various splits of the validation data, substantially interesting and a natural direction for future work. Identifying such an offline correction without relying, as our heuristic development in Section 5.1, could make these procedures substantially more practical, by both enjoying the test-time speed of split conformal methods and the coverage accuracy of full-conformal procedures.

A Technical proofs

A.1 Proof of Lemma 3.1

When $\mathbb{B}_2$ is the ℓ_2-ball,

$$\mathbb{E}\left[\sup_{h\in\mathcal{H},u\in\mathbb{B}_2}\langle u, Z_n(h)-\mathbb{E}[Z_n(h)]\rangle\right] = \mathbb{E}\left[\sup_{h\in\mathcal{H}}\|Z_n(h)-\mathbb{E}[Z_n(h)]\|_2\right].$$

Performing a typical symmetrization argument, we let $P_n^0 = \frac{1}{n}\sum_{i=1}^n \varepsilon_i \mathbf{1}_{X_i,S_i}$ be the symmetrized empirical measure, where $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathsf{Uni}\{\pm 1\}$ are i.i.d. Rademacher variables, and define the symmetrized process $Z_n^0(h) = \frac{1}{n}\sum_{i=1}^n \varepsilon_i\phi(X_i)1\{S_i > h(X_i)\}$. Then for the (random) set of vectors $\mathcal{V}_n = \{(1\{S_1 > h(X_1)\},\ldots,1\{S_n > h(X_n)\})\}_{h\in\mathcal{H}} \subset \{0,1\}^n$

$$\mathbb{E}\left[\sup_{h\in\mathcal{H}}\|Z_n(h)-\mathbb{E}[Z_n(h)]\|_2\right] \le 2\mathbb{E}\left[\sup_{h\in\mathcal{H}}\left\|Z_n^0(h)\right\|_2\right] \le 2\mathbb{E}\left[\max_{v\in\mathcal{V}_n}\left\|\frac{1}{n}\sum_{i=1}^n \varepsilon_i\phi(X_i)v_i\right\|_2\right].$$

Now, we recognize that because the vectors ϕ lie in a Hilbert space, we enjoy certain dimension free concentration guarantees. In particular, we have for any fixed $v \in \{0,1\}^n$ that

$$\mathbb{P}\left(\left\|\sum_{i=1}^n \varepsilon_i\phi(X_i)v_i\right\|_2 \ge t \mid X_1^n\right) \le 2\exp\left(-\frac{t^2}{2\Phi_n^2}\right),$$

where $\Phi_n^2 \coloneqq \sum_{i=1}^n \|\phi(X_i)\|_2^2$ by Pinelis [24, Theorem 3.5] (see also [15, Corollary 10]). In particular, using that for U a nonnegative random variable $\mathbb{E}[U] = \int_0^\infty \mathbb{P}(U \ge u)du$, we obtain

$$\begin{aligned}\mathbb{E}\left[\max_{v\in\mathcal{V}_n}\left\|\sum_{i=1}^n \varepsilon_i\phi(X_i)v_i\right\|_2 \mid X_1^n\right] &\le \int_0^\infty \mathbb{P}\left(\max_{v\in\mathcal{V}_n}\left\|\sum_{i=1}^n \varepsilon_i\phi(X_i)v_i\right\|_2 \ge t \mid X_1^n\right)dt \\ &\le t_0 + 2\,\mathrm{card}(\mathcal{V}_n)\int_{t_0}^\infty \exp\left(-\frac{t^2}{2\Phi_n^2}\right)dt.\end{aligned}$$

Recognizing the Gaussian tail bound that

$$\int_c^\infty e^{-\frac{t^2}{2\sigma^2}}dt = \sqrt{2\pi\sigma^2}\int_{c/\sigma}^\infty \frac{1}{\sqrt{2\pi}}e^{-z^2/2}dz \le \sqrt{2\pi\sigma^2}\min\left\{\frac{1}{\sqrt{2\pi}}\frac{\sigma}{c},1\right\}\exp\left(-\frac{c^2}{2\sigma^2}\right)$$

by Mills' ratio, we see that for any $t_0 \ge 0$,

$$\mathbb{E}\left[\max_{v\in\mathcal{V}_n}\left\|\sum_{i=1}^n \varepsilon_i\phi(X_i)v_i\right\|_2 \mid X_1^n\right] \le t_0 + 2\,\mathrm{card}(\mathcal{V}_n)\cdot\frac{\Phi_n^2}{t_0}\exp\left(-\frac{t_0^2}{2\Phi_n^2}\right).$$

Finally, recognize that $\mathcal{V}_n$ has cardinality at most $(\frac{en}{k})^k$ by the Sauer-Shelah lemma because $\mathcal{H}$ has VC-dimension k. Consequently, we may take $t_0^2 = 2\log\mathrm{card}(\mathcal{V}_n)\Phi_n^2$ to obtain the bound

$$\mathbb{E}\left[\max_{v\in\mathcal{V}_n}\left\|\sum_{i=1}^n \varepsilon_i\phi(X_i)v_i\right\|_2 \mid X_1^n\right] \le \sqrt{2\log\mathrm{card}(\mathcal{V}_n)}\Phi_n + \frac{\Phi_n}{\sqrt{2\log\mathrm{card}(\mathcal{V}_n)}} \le 2\sqrt{k\log\frac{ne}{k}}\cdot\Phi_n.$$

Take expectations over X_1^n.

A.2 Proof of Lemma 4.4

For $r \ge 0$, define the localized class

$$\mathcal{F}_r := \left\{ f \in \mathcal{F} \mid Pf^2 = \mathbb{E}[\langle v, \phi(X)\rangle^2 1\{S > h(X)\}] \le r^2 \right\}.$$

Note that $\mathcal{F}_r$ always includes the 0 function and is star-convex, because if $f \in \mathcal{F}_r$, then $\lambda f \in \mathcal{F}_r$ for $\lambda \in [0,1]$. Recalling inequality (16), the second term dominates the first, and so

$$\mathbb{E}\left[\mathfrak{R}_n(\mathcal{F}_r)\right] \le cr\sqrt{\frac{d}{n}\log\frac{n}{d}} \quad \text{if} \quad r^2 \ge b_\phi^2 \frac{d}{n}\log\frac{n}{d}.$$

Define the random variable $Z_n(r) := \sup_{f\in\mathcal{F}_r}(P_n - P)f = \sup_{f\in\mathcal{F}_r}|(P_n - P)f|$, the equality following by symmetry of $\mathcal{F}_r$. Then Talagrand's concentration inequality (Lemma 4.1) implies that

$$\mathbb{P}\left(Z_n(r) \ge \mathbb{E}[Z_n(r)] + \sqrt{2(r^2 + 2b_\phi \mathbb{E}[Z_n(r)])t} + \frac{b_\phi}{3}t\right) \le e^{-nt}$$

for all $t \ge 0$. Applying a standard symmetrization argument and inequality (16), we thus obtain that for $r^2 \ge b_\phi^2 \frac{d}{n}\log\frac{n}{d}$, with probability at least $1 - e^{-t}$,

$$Z_n(r) \le cr\sqrt{\frac{d\log n}{n}} + c\sqrt{\frac{r^2}{n^2} + \frac{b_\phi^2}{n} r\sqrt{\frac{d\log n}{n}}}\sqrt{t} + \frac{b_\phi t}{3n}.$$

As the last step, we apply a peeling argument [30, 26]: consider the intervals

$$E_k := \left(2^{k-1}\frac{b_\phi^2 d\log n}{n}, 2^k \frac{b_\phi^2 d\log n}{n}\right] \quad k = 1, 2, \ldots, K_n := \left\lceil \log_2 \frac{n}{d\log n}\right\rceil.$$

Let $\mathcal{F}^k = \{f \in \mathcal{F} \mid Pf^2 \in E_k\}$, where $\mathcal{F}^0 = \{f \in \mathcal{F} \mid Pf^2 \le \frac{d\log n}{n}\}$. Then evidently $\cup_{k=0}^{K_n}\mathcal{F}^k = \mathcal{F}$, and letting $r_k^2 = 2^k b_\phi^2 \frac{d\log n}{n}$, we have $\mathcal{F}_{r_k} \subset \mathcal{F}^k$. So by a union bound, with probability at least $1 - (K_n + 1)e^{-t}$,

$$Z_n(r_k) \le cr_k\sqrt{\frac{d\log n}{n}} + c\sqrt{\frac{r_k^2}{n^2} + \frac{b_\phi}{n}\sqrt{\frac{r_k^2 d\log n}{n}}}\sqrt{t} + \frac{b_\phi}{3n}t \quad \text{for } k = 1, \ldots, K_n \tag{23a}$$

and

$$Z_n(r_0) \le c\frac{d\log n}{n} + \sqrt{\frac{r_0^2}{n^2} + \frac{b_\phi}{n}\frac{d\log n}{n}}\sqrt{t} + \frac{b_\phi t}{3n}. \tag{23b}$$

Recall the definition $v^2(f) := Pf^2 = \mathrm{Var}(f) + (Pf)^2$. Then $f \in \mathcal{F}^k$ implies $\frac{1}{2}r_k \le v(f) \le r_k$, so that on the event that all the inequalities (23) hold, then simultaneously for all f satisfying $v^2(f) \ge \frac{d\log n}{n}$, then

$$|(P_n - P)f| \le cv(f)\sqrt{\frac{d\log n}{n}} + c\sqrt{\frac{v^2(f)}{n^2} + \frac{b_\phi}{n}\sqrt{v^2(f)\frac{d\log n}{n}}}\sqrt{t} + \frac{b_\phi}{3n}t,$$

while for all f with $v^2(f) \le \frac{d\log n}{n}$ we have

$$|(P_n - P)f| \le c\frac{d\log n}{n} + c\sqrt{\frac{d\log n}{n^3} + \frac{b_\phi}{n}\frac{d\log n}{n}}\sqrt{t} + \frac{b_\phi}{3n}t.$$

(To obtain the absolute bounds, we have used that $f \in \mathcal{F}$ implies $-f \in \mathcal{F}$ and each set $\mathcal{F}_r$ and $\mathcal{F}^k$ is symmetric.) Finally, we note that

$$\begin{aligned}\sqrt{\frac{v^2(f)}{n^2} + \frac{b_\phi}{n}\sqrt{v^2(f)\frac{d\log n}{n}}} &\le \sqrt{\frac{v^2(f)}{n^2} + \frac{b_\phi^2 d\log n}{2n^2} + \frac{v^2(f)}{2n}} \\ &\le \frac{b_\phi\sqrt{d\log n}}{\sqrt{2}n} + \frac{v(f)}{\sqrt{n}},\end{aligned}$$

which implies the first statement of Lemma 4.4.

The second statement follows via the same argument.

References

[1] F. Areces, C. Cheng, J. Duchi, and R. Kuditipudi. Two fundamental limits for uncertainty quantification in predictive inference. 2024.

[2] Y. Bai, S. Mei, H. Wang, and C. Xiong. Understanding the under-coverage bias in uncertainty estimation. *arXiv:2106.05515 [cs.LG]*, 2021.

[3] R. F. Barber, E. J. Candès, A. Ramdas, and R. J. Tibshirani. The limits of distribution-free conditional predictive inference. *Information and Inference*, 10(2):455–482, 2021.

[4] P. L. Bartlett, O. Bousquet, and S. Mendelson. Local Rademacher complexities. *Annals of Statistics*, 33(4):1497–1537, 2005.

[5] D. P. Bertsekas. Stochastic optimization problems with nondifferentiable cost functionals. *Journal of Optimization Theory and Applications*, 12(2):218–231, 1973.

[6] M. Bian and R. F. Barber. Training-conditional coverage for distribution-free predictive inference. *arXiv:2205.03647 [math.ST]*, 2022.

[7] O. Bousquet. *Concentration inequalities and empirical processes theory applied to the analysis of learning algorithms*. PhD thesis, L'Ecole Polytechnique, 2002.

[8] M. Cauchois, S. Gupta, and J. Duchi. Knowing what you know: valid and validated confidence sets in multiclass and multilabel prediction. *Journal of Machine Learning Research*, 22(81): 1–42, 2021.

[9] J. Duchi and F. Ruan. Solving (most) of a set of quadratic equalities: Composite optimization for robust phase retrieval. *Information and Inference*, iay015, 2018.

[10] J. C. Duchi, S. Gupta, K. Jiang, and P. Sur. Predictive inference in multi-environment scenarios. *Statistical Science*, to appear, 2024.

[11] I. Gibbs, J. Cherian, and E. Candès. Conformal prediction with conditional guarantees. *arXiv:2305.12616 [stat.ME]*, 2023.

[12] K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 770–778, 2016.

[13] K. He, X. Zhang, S. Ren, and J. Sun. Identity mappings in deep residual networks. In *European Conference on Computer Vision*, pages 630–645, 2016.

[14] J. Hiriart-Urruty and C. Lemaréchal. *Convex Analysis and Minimization Algorithms I.* Springer, New York, 1993.

[15] S. R. Howard, A. Ramdas, J. McAuliffe, and J. Sekhon. Time-uniform Chernoff bounds via nonnegative supermartingales. *Probability Surveys*, 17:257–317, 2020.

[16] C. Jung, G. Noarov, R. Ramalingam, and A. Roth. Batch multivalid conformal prediction. In *Proceedings of the Eleventh International Conference on Learning Representations*, 2023.

[17] R. Koenker and G. Bassett Jr. Regression quantiles. *Econometrica: Journal of the Econometric Society*, 46(1):33–50, 1978.

[18] V. Koltchinskii. Local Rademacher complexities and oracle inequalities in risk minimization. *Annals of Statistics*, 34(6):2593–2656, 2006.

[19] J. Lei and L. Wasserman. Distribution-free prediction bands for non-parametric regression. *Journal of the Royal Statistical Society, Series B*, 76(1):71–96, 2014.

[20] J. Lei, M. G'Sell, A. Rinaldo, R. J. Tibshirani, and L. Wasserman. Distribution-free predictive inference for regression. *Journal of the American Statistical Association*, 113(523):1094–1111, 2018.

[21] P. Massart. The tight constant in the Dvoretzky-Kiefer-Wolfowitz inequality. *Annals of Probability*, 18(3):1269–1283, 1990.

[22] C. McDiarmid. On the method of bounded differences. *Surveys in Combinatorics*, pages 148–188, 1989.

[23] S. Mendelson. Learning without concentration. In *Proceedings of the Twenty Seventh Annual Conference on Computational Learning Theory*, 2014.

[24] I. Pinelis. Optimum bounds for the distributions of martingales in Banach spaces. *Annals of Probability*, 22(4):1679–1706, 1994.

[25] Y. Romano, E. Patterson, and E. J. Candès. Conformalized quantile regression. In *Advances in Neural Information Processing Systems 32*, 2019.

[26] S. van de Geer. *Empirical Processes in M-Estimation.* Cambridge University Press, 2000.

[27] A. W. van der Vaart and J. A. Wellner. *Weak Convergence and Empirical Processes: With Applications to Statistics.* Springer, New York, 1996.

[28] V. Vovk. Conditional validity of inductive conformal predictors. In *Proceedings of the Asian Conference on Machine Learning*, volume 25 of *Proceedings of Machine Learning Research*, pages 475–490, 2012.

[29] V. Vovk, A. Grammerman, and G. Shafer. *Algorithmic Learning in a Random World.* Springer, 2005.

[30] M. J. Wainwright. *High-Dimensional Statistics: A Non-Asymptotic Viewpoint.* Cambridge University Press, 2019.