Knowing what you know: valid confidence sets in multiclass and multilabel prediction∗

Maxime Cauchois†, Suyash Gupta†, and John C. Duchi†, 2

1Department of Statistics, Stanford University
2Department of Electrical Engineering, Stanford University
{maxcauch, suyash28, jduchi}@stanford.edu

Abstract

We develop conformal prediction methods for constructing valid predictive confidence sets in multiclass and multilabel problems without assumptions on the data generating distribution. A challenge here is that typical conformal prediction methods—which give marginal validity (coverage) guarantees—provide uneven coverage, in that they address easy examples at the expense of essentially ignoring difficult examples. By leveraging ideas from quantile regression, we build methods that always guarantee correct coverage but additionally provide (asymptotically optimal) conditional coverage for both multiclass and multilabel prediction problems. To address the potential challenge of exponentially large confidence sets in multilabel prediction, we build tree-structured classifiers that efficiently account for interactions between labels. Our methods can be bolted on top of any classification model—neural network, random forest, boosted tree—to guarantee its validity. We also provide an empirical evaluation suggesting the more robust coverage of our confidence sets.

Keywords Multilabel and Multiclass Classification · Conformal Inference · Quantile Regression · Graphical Models

1 Introduction

The average accuracy of a machine-learned model by itself is insufficient to trust the model’s application; instead, we should ask for valid confidence in its predictions. Valid here does not mean “valid under modeling assumptions,” or “trained to predict confidence,” but honest validity, independent of the underlying distribution. In particular, for a supervised learning task with inputs $x \in \mathcal{X}$, targets $y \in \mathcal{Y}$, and a given confidence level $\alpha \in (0, 1)$, we seek confidence sets $C(x)$ such that $P(Y \in C(X)) \geq 1 - \alpha$; that is, we cover the true target $Y$ with a given probability $1 - \alpha$.

The typical approach in supervised learning is to learn a scoring function $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ where high scores $s(x, y)$ mean that $y$ is more likely for a given $x$. Given such a score function,
a natural goal for prediction with confidence is to compute a quantile function $q_\alpha$ of the score satisfying

$$P(s(x, Y) \geq q_\alpha(x) \mid X = x) \geq 1 - \alpha,$$

(1)

where $\alpha > 0$ is some pre-fixed level of acceptable error. We could then output conditionally valid confidence sets at level $1 - \alpha$ by simply returning

$$\{y \in Y \mid s(x, y) \geq q_\alpha(x)\}$$

for each $x \in \mathcal{X}$. Unfortunately, such conditionally valid coverage is impossible without either vacuously loose thresholds [32] or strong modeling assumptions [32, 1], but this idea forms the basis for our coming approach.

To address this impossibility, conformal inference [33] resolves instead to a marginal coverage guarantee: given $n$ observations and a desired confidence level $1 - \alpha$, conformal inference methods construct confidence sets $C(x)$ such that for a new pair $(X_{n+1}, Y_{n+1})$ from the same distribution, $Y_{n+1} \in C(X_{n+1})$ with probability at least $1 - \alpha$, where the probability is jointly over $X$ and $Y$. Conformal inference algorithms can build upon arbitrary predictors, neural networks, random forests, kernel methods and treat them as black boxes, “conformalizing” them post-hoc.

This distribution-free coverage is only achievable marginally, and standard conformal predictions for classification achieve it (as we see later) by providing good coverage on easy examples at the expense of miscoverage on harder instances. We wish to provide more uniform coverage, and we address this in multiclass and multilabel problems. We combine the ideas of conformal prediction [33] with an approach to fit a quantile function $q$ on the scores $s(x, y)$ of the prediction model—an approach Romano et al. [27] originate for regression problems—and build feature-adaptive quantile predictors, which output sets of labels, allowing us to guarantee valid marginal coverage (independent of the data generating distribution) while better approximating the conditional coverage (1).

**Conformal inference in classification** We consider both multiclass (where each example belongs to a single class) and multilabel (where each example may belong to several classes) classification problems.

In the multiclass case, we propose a method that fits a quantile function on the scores, conformalizing it on held-out data. While this immediately provides valid marginal coverage, the accuracy of the quantile function—how well it approximates the conditional quantiles—determines conditional coverage performance. Under certain consistency assumptions on the learned scoring functions and quantiles as sample size increases, we show in Section 2 that we recover the conditional coverage (1) asymptotically.

The multilabel case poses new statistical and computational challenges, as a $K$-class problem entails $2^K$ potential responses. In this case, we seek efficiently representable inner and outer sets $C_{\text{in}}(x)$ and $C_{\text{out}}(x) \subset \{1, \ldots, K\}$ such that

$$\mathbb{P}(C_{\text{in}}(X) \subset Y \subset C_{\text{out}}(X)) \geq 1 - \alpha.$$

(2)

We propose two approaches to guarantee the containments (2). The first directly fits inner and outer sets by solving two separate quantile regression problems. The second begins by observing that labels are frequently correlated—think, for example, of chairs, which frequently co-occur with a table—and learns a tree-structured graphical model [19] to efficiently address such correlation. We show how to build these in top of any predictive model.
Related work and background Vovk et al. [33] introduce (split-)conformal inference, which splits the first \( n \) samples of the exchangeable pairs \( \{(X_i, Y_i)\}_{i=1}^{n+1} \) into two sets (say, each of size \( n_1 \) and \( n_2 \) respectively) where the first training set \( (I_1) \) is used to learn a scoring function \( s: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R} \) and the second validation set \( (I_2) \) to “conformalize” the scoring function and construct a confidence set over potential labels (or targets) \( \mathcal{Y} \) of the form

\[
C(x) := \{y \in \mathcal{Y} \mid s(x, y) \geq t\}
\]

for some threshold \( t \). The basic split-conformal method chooses the \((1+1/n_2)(1-\alpha)\)-empirical quantile \( \hat{Q}_{1-\alpha}^{\text{marg}} \) of the negative scores \( \{-s(X_i, Y_i)\}_{i \in I_2} \) (on the validation set) and defines the confidence sets

\[
C(x) := \{y \in \mathcal{Y} \mid s(x, y) \geq -\hat{Q}_{1-\alpha}^{\text{marg}}\}. \tag{3}
\]

The argument is beautifully simple, and shows that given any scoring function \( s \), one may use a validation set to achieve valid marginal coverage with such confidence sets: letting \( S_i = -s(X_i, Y_i) \), if \( \hat{Q}_{1-\alpha}^{\text{marg}} \) is the \((1+1/n_2)(1-\alpha)\)-quantile of \( \{S_i\}_{i \in I_2} \) and the pairs \( \{(X_i, Y_i)\}_{i=1}^{n+1} \) are exchangeable, we have

\[
\mathbb{P}(Y_{n+1} \in C(X_{n+1})) = \mathbb{P}(s(X_{n+1}, Y_{n+1}) \geq -\hat{Q}_{1-\alpha}^{\text{marg}}) = \mathbb{P}\left( \text{Rank of } S_{n+1} \text{ in } \{S_i\}_{i \in I_2 \cup \{n+1\}} \leq \left( (n_2 + 1)(1 - \alpha) \right) \right) \geq 1 - \alpha.
\]

We refer to the procedure (3) as the Marginal conformal prediction method. Such a “conformalization” scheme typically outputs a confidence set by listing all the labels that it contains, which is feasible in a \( K \)-class multiclass problem, but much more challenging in a \( K \)-class multilabel one, as the overall number of configurations (\( 2^K \)) grows exponentially. For this reason, and to the best of our knowledge, there currently exists no conformal-type method that efficiently deals with a multilabel problem.

While conformal inference guarantees marginal coverage without assumption on the distribution that generates the data, Vovk [32] shows it is virtually impossible to attain distribution-free conditional coverage, and Barber et al. [1] prove that in regression, one can only achieve a weaker form of approximately-conditional coverage without conditions on the underlying distribution. Because of this theoretical limitation, work in conformal inference often focuses on minimizing confidence set sizes or guaranteeing different types of coverage. For instance, Sadinle et al. [28] propose conformal prediction algorithms for multiclass problems that minimize the expected size of the confidence set and conformalize the scores separately for each class, providing class-wise coverage. In the same vein, Hechtlinger et al. [15] use density estimates of \( p(x \mid y) \) as conformal scores to build a “cautious” predictor, the idea being that it should output an empty set when the new sample differs too much from the original distribution. In regression problems, Romano et al. [27] conformalize a quantile predictor, which allows them to build marginally valid confidence sets that are adaptive to feature heterogeneity and empirically smaller on average than purely marginal confidence sets. We adapt this regression approach to classification tasks, learning quantile functions to construct valid—potentially conditionally valid—confidence predictions.

Notation \( \mathcal{P} \) is a set of distributions on \( \mathcal{X} \times \mathcal{Y} \), where \( \mathcal{Y} = \{0,1\}^K \) is a discrete set of labels, \( K \geq 2 \) is the number of classes, and \( \mathcal{X} \subset \mathbb{R}^d \). We assume that we observe a finite sequence \( (X_i, Y_i)_{1 \leq i \leq n} \text{ iid} \sim P \) from some distribution \( P = P_X \times P_{Y \mid X} \in \mathcal{P} \) and wish to predict a confidence set for a new example \( X_{n+1} \sim P_X \). \( \mathcal{P} \) stands over the randomness of both the new sample \( (X_{n+1}, Y_{n+1}) \) and the full procedure. Finally, we tacitly identify the one-hot vector...
$Y \in \mathcal{Y} = \{0, 1\}^K$ with the subset of $[K] = \{1, \ldots, K\}$ it represents, and the notation $\mathcal{X} \Rightarrow [K]$ indicates a set-valued mapping between $\mathcal{X}$ and $[K]$.

## 2 Conformal multiclass classification

We begin with multiclass classification problems, developing Conformalized Quantile Classification (CQC) to construct finite sample marginally valid confidence sets. CQC is similar to Romano et al.'s Conformalized Quantile Regression (CQR): we estimate a quantile function of the scores, which we use to construct valid confidence sets after conformalization. The idea is to split the data into subsets, $\mathcal{I}_1$, $\mathcal{I}_2$, and $\mathcal{I}_3$ with sample sizes $n_1, n_2$ and $n_3$ respectively, where $\mathcal{I}_3$ is disjoint from $\mathcal{I}_1 \cup \mathcal{I}_2$. The basic idea is as follows, as Fig. 1 outlines: we use the set $\mathcal{I}_1$ for fitting the scoring function with an (arbitrary) given learning algorithm $\mathcal{A}$, use $\mathcal{I}_2$ for fitting a quantile function from a family $\mathcal{Q} \subset \mathcal{X} \rightarrow \mathbb{R}$ of possible quantile functions to the resulting scores, and use $\mathcal{I}_3$ for calibration. In the algorithm, we recall the “pinball loss” \[18\] $\rho_\alpha(t) = (1 - \alpha)[-t]_+ + \alpha [t]_+$, which satisfies $\arg\min_{q \in \mathbb{R}} \mathbb{E}[\rho_\alpha(Z - q)] = \inf \{q \mid \mathbb{P}(Z \leq q) \geq \alpha \}$ for any random variable $Z$.

### Algorithm 1: Split Conformalized Quantile Classification (CQC).

**Input:** Sample $\{(X_i, Y_i)\}_{i=1}^n$, index sets $\mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3 \subset [n]$, fitting algorithm $\mathcal{A}$, quantile functions $\mathcal{Q}$, and desired confidence level $\alpha$

1. Fit scoring function via
   \[ \hat{s} := \mathcal{A}((X_i, Y_i)_{i \in \mathcal{I}_1}) \]  
2. Fit quantile function via
   \[ \hat{q}_\alpha \in \arg\min_{q \in \mathcal{Q}} \left\{ \frac{1}{|\mathcal{I}_2|} \sum_{i \in \mathcal{I}_2} \rho_\alpha (\hat{s}(X_i, Y_i) - q(X_i)) \right\} \]  
3. Calibrate by computing conformity scores $S_i = \hat{q}_\alpha(X_i) - \hat{s}(X_i, Y_i)$, defining
   \[ Q_{1-\alpha}(S, \mathcal{I}_3) := (1 + 1/n_3)(1 - \alpha) \text{ empirical quantile of } \{S_i\}_{i \in \mathcal{I}_3} \]
   and return prediction set function
   \[ \hat{C}_{1-\alpha}(x) := \{k \in [K] \mid \hat{s}(x, k) \geq \hat{q}_\alpha(x) - Q_{1-\alpha}(S, \mathcal{I}_3)\} \]

The CQC algorithm in Fig. 1 returns an estimated confidence set function $\hat{C}_{1-\alpha}$, which on a new input $X_{n+1}$, predicts the set $\hat{C}_{1-\alpha}(X_{n+1})$.

### 2.1 Finite sample validity of CQC

We begin by showing that Alg. 1 enjoys the coverage guarantees we expect, which is more or less immediate by the marginal guarantees for the method (3). We include the proof for completeness and because its cleanness highlights the ease of achieving validity. For simplicity, we typically assume that the full sample $\{(X_i, Y_i)\}_{i=1}^{n+1}$ is exchangeable, but we really only require the sample $\{(X_i, Y_i)\}_{i \in \mathcal{I}_0 \cup \{n+1\}}$ to be exchangeable conditionally on $\{(X_i, Y_i)\}_{i \in \mathcal{I}_1 \cup \mathcal{I}_2}$. In particular, if we previously learned scores $\hat{s}$ and quantile function $\hat{q}_\alpha$ on some prior independent
data—potentially even from a different distribution—, then Theorem 1 below (as well as all our next conformal theorems) remains valid if the exchangeability assumption holds for the instances in $\mathcal{I}_3 \cup \{n+1\}$.

**Theorem 1.** Assume that $\{(X_i, Y_i)\}_{i=1}^{n+1} \sim P$ are exchangeable, where $P$ is an arbitrary distribution. Then the prediction set $\hat{C}_{1-\alpha}$ of the split CQC Algorithm 1 satisfies

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

**Proof** The argument is due to Romano et al. [27, Thm. 1]. Observe that $Y_{n+1} \in \hat{C}_{1-\alpha}(X_{n+1})$ if and only if $S_{n+1} \leq Q_{1-\alpha}(S, \mathcal{I}_3)$. Define the $\sigma$-field $\mathcal{F}_{12} = \sigma\{(X_i, Y_i) \mid i \in \mathcal{I}_1 \cup \mathcal{I}_2\}$. Then

$$\mathbb{P}(Y_{n+1} \in \hat{C}_{1-\alpha}(X_{n+1}) \mid \mathcal{F}_{12}) = \mathbb{P}(S_{n+1} \leq Q_{1-\alpha}(S, \mathcal{I}_3) \mid \mathcal{F}_{12}).$$

We use the following lemma.

**Lemma 2.1** (Lemma 2, Romano et al. [27]). Let $Z_1, \ldots, Z_{n+1}$ be exchangeable random variables and $\hat{Q}_n(\cdot)$ be the empirical quantile function of $Z_1, \ldots, Z_n$. Then for any $\alpha \in (0, 1)$,

$$\mathbb{P}\{Z_{n+1} \leq \hat{Q}_n((1 + n^{-1})\alpha)\} \geq \alpha.$$

If $Z_1, \ldots, Z_n$ are almost surely distinct, then

$$\mathbb{P}\{Z_{n+1} \leq \hat{Q}_n((1 + n^{-1})\alpha)\} \leq \alpha + \frac{1}{n}.$$

Since the original sample is exchangeable, so are the conformity scores $S_i$ for $i \in \mathcal{I}_3$, conditionally on $\mathcal{F}_{12}$. Lemma 2.1 implies $\mathbb{P}(S_{n+1} \leq Q_{1-\alpha}(S, \mathcal{I}_3) \mid \mathcal{F}_{12}) \geq 1 - \alpha$, and taking expectations over $\mathcal{F}_{12}$ yields the theorem.

The conditional distribution of scores given $X$ is discrete, so the conformalized quantile confidence set may be conservative: it is possible that for any $q$ such that $P(s(X, Y) \geq q \mid X) \geq 1 - \alpha$, we have $P(s(X, Y) \geq q \mid X) \geq 1 - \epsilon$ for some $\epsilon \ll \alpha$. Conversely, as the CQC procedure 1 seeks $1 - \alpha$ marginal coverage, it may sacrifice a few examples to bring the coverage down to $1 - \alpha$. Moreover, there may be no unique quantile function for the scores. There are several possibilities to address these issues: the first is to estimate a quantile function on $\mathcal{I}_2$ (recall step (5) of the CQC method) so that we can guarantee higher coverage (which is more conservative, but is free in the $\epsilon \ll \alpha$ case). An alternative, which we outline here, is to randomize scores without changing the relative order.

To achieve exact $1 - \alpha$ asymptotic coverage and a unique quantile, we randomize by adding a continuous random variable with full support on the real line simultaneously to each sample score. Let $Z_i \overset{\text{iid}}{\sim} \pi$ for some distribution $\pi$ with continuous density that is supported on the entire real line, and let $\sigma > 0$ be a noise parameter. Then for any scoring function $s : X \times Y \rightarrow \mathbb{R}$, we define the randomized scores

$$s^\sigma(x, y, z) := s(x, y, z) + \sigma z.$$ 

Note that $s^\sigma(x, y, z) - s^\sigma(x, y', z) = s(x, y) - s(x, y')$, so that this does not change the relative ordering of label scores, only giving the score function a conditional density.

Now, consider replacing the quantile estimator (5) with the randomized estimator

$$\hat{q}_\alpha^\sigma \in \arg\min_{q \in \mathcal{Q}} \left\{ \frac{1}{n_2} \sum_{i \in \mathcal{I}_2} \rho_\alpha(\hat{s}^\sigma(X_i, Y_i, Z_i) - q(X_i)) \right\},$$

(7)
and let $S_i^\sigma := \hat{q}_n^\sigma(X_i) - \tilde{s}^\sigma(X_i, Y_i, Z_i)$ be the corresponding conformity scores. Similarly, replace the prediction set (6) with

$$\hat{C}_{1-\alpha}(x, z) := \{k \in [K] \mid \tilde{s}^\sigma(x, k, z) \geq \hat{q}_n^\sigma(x) - Q_{1-\alpha}(S^\sigma, I_3)\}.$$  \hspace{1cm} (8)

where $Q_{1-\alpha}(S^\sigma, I_3)$ is the $(1 - \alpha)(1 + 1/n_3)$-th empirical quantile of $\{S_i^\sigma\}_{i \in I_3}$. Then for a new input $X_{n+1} \in \mathcal{X}$, we simulate a new independent variable $Z_{n+1} \sim \pi$, and give the confidence set $\hat{C}_{1-\alpha}(X_{n+1}, Z_{n+1})$.

As the next theorem shows, this gives nearly perfectly calibrated coverage.

**Theorem 2.** Assume that $\{(X_i, Y_i)\}_{i=1}^{n+1} \sim P$ are exchangeable, where $P$ is an arbitrary distribution. Let the estimators (7) and (8) replace the estimators (5) and (6) in the CQC Algorithm 1, respectively. Then the prediction set $\hat{C}_{1-\alpha}$ satisfies

$$1 - \alpha \leq P\{Y_{n+1} \in \hat{C}_{1-\alpha}(X_{n+1}, Z_{n+1})\} \leq 1 - \alpha + \frac{1}{1 + n_3}.$$  

**Proof** The argument is again more or less due to Romano et al. [27]. First, we observe that $Y_{n+1} \in \hat{C}_{1-\alpha}(X_{n+1}, Z_{n+1})$ if and only if $S_{n+1}^\sigma \leq Q_{1-\alpha}(S^\sigma, I_3)$, which implies, conditionally on the $\sigma$-field $\mathcal{F}_2 = \sigma((X_i, Y_i) \mid i \in I_2)$, that

$$P\left(Y_{n+1} \in \hat{C}_{1-\alpha}(X_{n+1}, Z_{n+1}) \mid \mathcal{F}_2\right) = P\left(S_{n+1}^\sigma \leq Q_{1-\alpha}(S^\sigma, I_3) \mid \mathcal{F}_2\right).$$

As the original observations are exchangeable, so are the conformity scores $S_i^\sigma$ for $i \in I_3$, as we add independent noise to each, which guarantees the $S_i^\sigma$ are distinct almost surely. Then applying Lemma 2.1 and taking expectations gives

$$1 - \alpha \leq P(S_{n+1}^\sigma \leq Q_{1-\alpha}(S^\sigma, I_3)) \leq 1 - \alpha + \frac{1}{n_3 + 1},$$

as desired. \hfill \Box

### 2.2 Asymptotic optimality of CQC method

Under appropriate assumptions typical in proving the consistency of prediction methods, Conformalized Quantile Classification (CQC) guarantees conditional coverage asymptotically. To set the stage, assume that as $n \uparrow \infty$, the fit score functions $\hat{s}_n$ in Eq. (4) converge to a fixed $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ (cf. Assumption A1). Let

$$q_\alpha(x) := \inf\{z \in \mathbb{R} \mid \alpha \leq P(s(x, Y) \leq z \mid X = x)\}$$

be the $\alpha$-quantile function of the limiting scores $s(x, Y)$ and for $\sigma > 0$ define

$$q_\alpha^\sigma(x) := \inf\{z \in \mathbb{R} \mid \alpha \leq P(s^\sigma(x, Y, Z) \leq z \mid X = x)\},$$

where $Z \sim \pi$ (for a continuous distribution $\pi$ as in the preceding section) is independent of $x, y$, to be the $\alpha$-quantile function of the noisy scores $s^\sigma(x, Y, Z) = s(x, Y) + \sigma Z$. With these, we can make the following natural definitions of our desired asymptotic confidence sets.

**Definition 2.1.** The randomized-oracle and super-oracle confidence sets are $C_{1-\alpha}^\sigma(X, Z) := \{k \in [K] \mid s^\sigma(X, k, Z) \geq q_\alpha^\sigma(X)\}$ and $C_{1-\alpha}(X) = \{k \in [K] \mid s(X, k) \geq q_\alpha(X)\}$, respectively.
Our aim will be to show that the confidence sets of the split CQC method 1 (or its randomized variant) converge to these confidence sets under appropriate consistency conditions.

To that end, we consider the following consistency assumption.

**Assumption A1 (Consistency of scores and quantile functions).** The score functions $\hat{s}$ and quantile estimator $\hat{q}_\alpha^\sigma$ are mean-square consistent, that is,

$$\|\hat{s} - s\|_{L^2(P_X)}^2 := \int_\mathcal{X} \|\hat{s}(x, \cdot) - s(x, \cdot)\|_2^2 dP_X(x) \xrightarrow{P} 0$$

and

$$\|\hat{q}_\alpha^\sigma - q_\alpha^\sigma\|_{L^2(P_X)}^2 := \int_\mathcal{X} (\hat{q}_\alpha^\sigma(x) - q_\alpha^\sigma(x))^2 dP_X(x) \xrightarrow{P} 0$$

as $n_1, n_2, n_3 \to \infty$.

With this assumption, we have the following theorem, whose proof we provide in Appendix A.1.

**Theorem 3.** Let Assumption A1 hold. Then the confidence sets $\hat{C}_{1-\alpha}^\sigma$ satisfy

$$\lim_{n \to \infty} \mathbb{P}(\hat{C}_{1-\alpha}^\sigma(X_{n+1}, Z_{n+1}) \neq C_{1-\alpha}^\sigma(X_{n+1}, Z_{n+1})) = 0.$$

While we do not require this for Theorem 3, the ideal scenario occurs when the limiting score function $s$ is optimal (cf. [2, 36, 31]), so that $s(x, y) > s(x, y')$ whenever $P(Y = y \mid X = x) > P(Y = y' \mid X = x)$. Under this additional condition, the super-oracle confidence set $C_{1-\alpha}(X)$ in Def. 2.1 is the smallest conditionally valid confidence set at level $1 - \alpha$. Conveniently, our randomization is consistent as $\sigma \downarrow 0$: the super oracle confidence set $C_{1-\alpha}$ contains $C_{1-\alpha}^\sigma$ (with high probability). We provide the proof of the following theorem in Appendix A.2.

**Theorem 4.** The confidence sets $C_{1-\alpha}^\sigma$ satisfy

$$\lim_{\sigma \to 0} \mathbb{P}(C_{1-\alpha}^\sigma(X_{n+1}, Z_{n+1}) \subseteq C_{1-\alpha}(X_{n+1})) = 1.$$

Because we always have $\mathbb{P}(Y \in C_{1-\alpha}^\sigma(X, Z)) \geq 1 - \alpha$, Theorem 4 shows that we maintain validity while potentially shrinking the confidence sets.

## 3 The multilabel setting

In multilabel classification, we observe a single feature vector $x \in \mathcal{X}$ and wish to predict a vector $y \in \{-1, 1\}^K$ where $y_k = 1$ indicates that label $k$ is present and $y_k = 0$ indicates its absence. For example, in object detection problems [26, 30, 22], we want to detect several entities in an image, while in text classification tasks [23, 24, 17], a single document can potentially share multiple topics. To conformalize such predictions, we wish to output an aggregated set of predictions $\{\hat{y}(x)\} \subseteq \{-1, 1\}^K$—a collection of -1-1-valued vectors—that contains the true configuration $Y = (Y_1, \ldots, Y_K)$ with probability at least $1 - \alpha$.

The multilabel setting poses both statistical and computational challenges. On the statistical side, multilabel prediction engenders a multiple testing challenge: even if each task has an individual confidence set $C_k(x)$ such that $P(Y_k \in C_k(X)) \geq 1 - \alpha$, in general we can only conclude that $P(Y \in C_1(X) \times \cdots \times C_K(X)) \geq 1 - K\alpha$, though as all predictions share the same features $x$, we wish to leverage correlation through $x$. Additionally, as we discuss
in the introduction (recall Eq. (3)), we require a scoring function \( s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \). A naive scoring function, given a predictor \( \hat{y} : \mathcal{X} \to \{-1,1\}^K \), for multilabel problems is to simply use \( s(x, y) = 1 \{ \hat{y}(x) = y \} \), but this fails, as the confidence sets contain either all configurations or a single configuration. On the computational side, the total number of label configurations \((2^K)\) grows exponentially, so a “standard” multiclass-like approach outputting confidence sets \( \hat{C}(X) \subset \mathcal{Y} = \{-1,1\}^K \), although feasible for small values of \( K \), is computationally impractical even for moderate \( K \).

We instead propose using inner and outer set functions \( \hat{C}_{\text{in}}, \hat{C}_{\text{out}} : \mathcal{X} \Rightarrow [K] \) to efficiently describe a confidence set on \( \mathcal{Y} \), where we require they satisfy the coverage guarantee

\[
\mathbb{P}( \hat{C}_{\text{in}}(X) \subset Y \subset \hat{C}_{\text{out}}(X) ) \geq 1 - \alpha, \tag{9a}
\]

or equivalently, we learn two functions \( \hat{y}_{\text{in}}, \hat{y}_{\text{out}} : \mathcal{X} \to \mathcal{Y} = \{-1,1\}^K \) such that

\[
\mathbb{P}( \hat{y}_{\text{in}}(X) \preceq Y \preceq \hat{y}_{\text{out}}(X) ) \geq 1 - \alpha. \tag{9b}
\]

We thus say that coverage is valid if the inner set exclusively contains positive labels and the outer set contains at least all positive labels. For example, \( \hat{y}_{\text{in}}(x) = \mathbf{0} \) and \( \hat{y}_{\text{out}}(x) = \mathbf{1} \) are always valid, though uninformative, while the smaller the set difference between \( \hat{C}_{\text{in}}(X) \) and \( \hat{C}_{\text{out}}(X) \) the more confident we may be in a single prediction.

In the remainder of this section, we propose methods to conformalize multilabel predictors in varying generality, using tree-structured graphical models to both address correlations among labels and computational efficiency. We begin in Section 3.1 with a general method for conformalizing an arbitrary scoring function \( s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) on multilabel vectors, which guarantees validity no matter the score. We then show different strategies to efficiently implement the method, depending on the structure of available scores, in Section 3.2, showing how “tree-structured” scores allow computational efficiency while modeling correlations among the task labels \( y \). Finally, in Section 3.3, we show how to build such a tree-structured score function \( s \) from both arbitrary predictive models (e.g. \([4, 35]\)) and those more common multilabel predictors—in particular, those based on neural networks—that learn and output per-task scores \( s_k : \mathcal{X} \to \mathbb{R} \) for each task \([16, 25]\).

### 3.1 A generic split-conformal method for multilabel sets

We begin by assuming we have a general score function \( s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) for \( \mathcal{Y} = \{-1,1\}^K \) that evaluates the quality of a given set of labels \( y \in \mathcal{Y} \) for an instance \( x \); in the next subsection, we describe how to construct such scores from multilabel prediction methods, presenting our general method first. We consider the variant of the CQC method 1 in Alg. 2.
Algorithm 2: Split Conformalized Inner/Outer method for classification (CQioC)

**Input:** Sample \( \{(X_i, Y_i)\}_{i=1}^n \), disjoint index sets \( \mathcal{I}_2, \mathcal{I}_3 \subset [n] \), quantile functions \( \mathcal{Q} \), desired confidence level \( \alpha \), and score function \( s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \).

1. Fit quantile function \( \hat{q}_\alpha \in \text{argmin}_{q \in \mathcal{Q}} \{ \sum_{i \in \mathcal{I}_2} \rho_\alpha(s(X_i, Y_i) - q(X_i)) \} \), as in (5).

2. Compute conformity scores \( S_i = \hat{q}_\alpha(X_i) - s(X_i, Y_i) \), define \( \hat{Q}_{1-\alpha} \) as \( (1 + 1/|\mathcal{I}_3|) \cdot (1 - \alpha) \) empirical quantile of \( S = \{ S_i \}_{i \in \mathcal{I}_3} \), and return prediction set function

\[
\hat{C}_{\text{io}}(x) := \{ y \in \mathcal{Y} \mid \hat{y}_{\text{in}}(x) \leq y \leq \hat{y}_{\text{out}}(x) \},
\]

where \( \hat{y}_{\text{in}} \) and \( \hat{y}_{\text{out}} \) satisfy

\[
\hat{y}_{\text{in}}(x)_k = 1 \text{ if and only if } \max_{y \in \mathcal{Y} : y_k = 1} s(x, y) < \hat{q}_\alpha(x) - \hat{Q}_{1-\alpha},
\]

\[
\hat{y}_{\text{out}}(x)_k = -1 \text{ if and only if } \max_{y \in \mathcal{Y} : y_k = -1} s(x, y) < \hat{q}_\alpha(x) - \hat{Q}_{1-\alpha}. \tag{11}
\]

There are two considerations for Algorithm 2: its computational efficiency and its validity guarantees. Deferring the efficiency questions to the coming subsections, we begin with the latter. The naive approach is to simply use the “standard” or implicit conformalization approach, used for regression or classification, by defining

\[
\hat{C}_{\text{imp}}(x) := \{ y \in \mathcal{Y} \mid s(x, y) \geq \hat{q}_\alpha(x) - \hat{Q}_{1-\alpha} \}, \tag{12}
\]

where \( \hat{q}_\alpha \) and \( \hat{Q}_{1-\alpha} \) are as in the CQioC method 2. This does guarantee validity, as we have the following corollary of Theorem 1.

**Corollary 3.1.** Assume that \( \{(X_i, Y_i)\}_{i=1}^{n+1} \sim P \) are exchangeable, where \( P \) is an arbitrary distribution. Then for any confidence set \( C \supseteq \mathcal{Y} \) satisfying \( \hat{C}(x) \supset \hat{C}_{\text{imp}}(x) \) for all \( x \),

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

Instead of the inner/outer set \( \hat{C}_{\text{io}} \) in Eq. (10), we could use any confidence set \( \hat{C}(x) \supset \hat{C}_{\text{imp}}(x) \) and maintain validity. Unfortunately, as we note above, the set \( \hat{C}_{\text{imp}} \) may be exponentially complex to represent and compute, necessitating a simplifying construction, such as our inner/outer approach. Conveniently, the set (10) we construct via \( \hat{y}_{\text{in}} \) and \( \hat{y}_{\text{out}} \) satisfying the conditions (11) satisfies Corollary 3.1. Indeed, we have the following.

**Proposition 1.** Let \( \hat{y}_{\text{in}} \) and \( \hat{y}_{\text{out}} \) satisfy the conditions (11). Then the confidence set \( \hat{C}_{\text{io}}(x) \) in Algorithm 2 is the smallest set containing \( \hat{C}_{\text{imp}}(x) \) and admitting the form (10).

**Proof** The conditions (11) immediately imply

\[
\hat{y}_{\text{in}}(x)_k = \min_{y \in \hat{C}_{\text{imp}}(x)} y_k \text{ and } \hat{y}_{\text{out}}(x)_k = \max_{y \in \hat{C}_{\text{imp}}(x)} y_k,
\]

which shows that \( \hat{C}_{\text{imp}}(x) \subset \hat{C}_{\text{io}}(x) \). On the other hand, suppose that \( \hat{y}_{\text{in}}(x) \) and \( \hat{y}_{\text{out}}(x) \) are configurations inducing a confidence set \( \hat{C}(x) \) that satisfies \( \hat{C}_{\text{imp}}(x) \subset \hat{C}(x) \). Then for any label \( k \) included in \( \hat{y}_{\text{in}}(x) \), all configurations \( y \in \hat{C}_{\text{imp}}(x) \) satisfy \( y_k = 1 \), as \( \hat{C}_{\text{imp}}(x) \subset \hat{C}(x) \), so we must have \( \hat{y}_{\text{in}}(x)_k \leq \hat{y}_{\text{in}}(x)_k \). The argument to prove \( \hat{y}_{\text{out}}(x)_k \geq \hat{y}_{\text{out}}(x)_k \) is similar. \( \square \)
The expansion from $\hat{C}_{\text{imp}}(x)$ to $\hat{C}_{\text{io}}(x)$ may increase the size of the confidence set; in practice, we see it is rarely a substantial increase, as our predictors address correlation between individual labels $y_k$, making it unlikely that “opposing” configurations $y$ and $-y$ both belong to $\hat{C}_{\text{io}}(x)$. Moreover, in the case that the standard implicit confidence set $\hat{C}_{\text{imp}}$ is a singleton, so that there is only a single label vector $y \in \mathcal{Y}$ satisfying $s(x, y) \geq \hat{q}_a(x) - \hat{Q}_{1-\alpha}$, then by definition $\hat{y}_{\text{in}}(x) = \hat{y}_{\text{out}}(x)$, so that $\hat{C}_{\text{io}} = \hat{C}_{\text{imp}}$. Thus, at least when we have strong predictors, the expansion (11) has limited downside.

### 3.2 Efficient construction of inner and outer confidence sets

With the validity of any inner/outer construction verifying the conditions (11) established, we turn to two approaches to efficiently satisfy these. The first focuses on the scenario where a prediction method provides individual scoring functions $s_k : \mathcal{X} \to \mathbb{R}$ for each task $k \in [K]$ (as frequent for complex classifiers, such as random forests or deep networks [e.g. 16, 25]), while the second considers the case when we have a scoring function $s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ that is tree-structured in a sense we make precise; in the next section, we will show how to construct such tree-structured scores using any arbitrary multilabel prediction method.

**A direct inner/outer method using individual task scores** We assume here that we observe individual scoring functions $s_k : \mathcal{X} \to \mathbb{R}$ for each task. We can construct inner and outer sets using only these scores while neglecting label correlations by learning threshold functions $t_{\text{in}} \geq t_{\text{out}} : \mathcal{X} \to \mathbb{R}$, where we would like to have the (true) labels $y_k$ satisfy

$$\text{sign}(s_k(x) - t_{\text{in}}(x)) \leq y_k \leq \text{sign}(s_k(x) - t_{\text{out}}(x)).$$

In Algorithm 3, we accomplish this via quantile threshold functions on the maximal and minimal values of the scores $s_k$ for positive and negative labels, respectively.

| **Algorithm 3**: Split Conformalized Direct Inner/Outer method for Classification (CDioC). |
|---|
| **Input**: Sample $\{(X_i, Y_i)\}_{i=1}^n$, disjoint index sets $\mathcal{I}_2, \mathcal{I}_3 \subset [n]$, quantile functions $Q$, desired confidence level $\alpha$, and $K$ score functions $s_k : \mathcal{X} \to \mathbb{R}$. |
| 1. Fit threshold functions (noting the sign conventions)

$$\hat{t}_{\text{in}} = -\arg\min_{\hat{t} \in Q} \left\{ \sum_{i \in \mathcal{I}_2} \rho_{\alpha/2} \left( -\max_k \{s_k(X_i) \mid Y_{i,k} = -1\} - \hat{t}(X_i) \right) \right\}$$

$$\hat{t}_{\text{out}} = \arg\min_{\hat{t} \in Q} \left\{ \sum_{i \in \mathcal{I}_2} \rho_{\alpha/2} \left( \min_k \{s_k(X_i) \mid Y_{i,k} = 1\} - \hat{t}(X_i) \right) \right\}$$

(13)

2. Define score $s(x, y) = \min \{ \min_{k:y_k=1} s_k(x) - \hat{t}_{\text{out}}(x), \hat{t}_{\text{in}}(x) - \max_{k:y_k=-1} s_k(x) \}$ and compute conformity scores $S_i := -s(X_i, Y_i)$.

3. Let $\hat{Q}_{1-\alpha}$ be the $(1 + 1/|\mathcal{I}_3|)(1 - \alpha)$-empirical quantile of $S = \{S_i\}_{i \in \mathcal{I}_3}$ and

$$t_{\text{in}}(x) := \hat{t}_{\text{in}}(x) + \hat{Q}_{1-\alpha} \quad \text{and} \quad t_{\text{out}}(x) := \hat{t}_{\text{out}}(x) - \hat{Q}_{1-\alpha}.$$ 

4. Define $\hat{y}_{\text{in}}(x)_k = \text{sign}(s_k(x) - t_{\text{in}}(x))$ and $\hat{y}_{\text{out}}(x)_k = \text{sign}(s_k(x) - t_{\text{out}}(x))$ and return prediction set $\hat{C}_{\text{io}}$ as in Eq. (10). |
The method is a slightly modified instantiation of the CQioC method in Alg. 2 that allows easier computation. We can also see that it guarantees validity.

**Corollary 3.2.** Assume that \( \{(X_i, Y_i)\}_{i=1}^{n+1} \sim P \) are exchangeable, where \( P \) is an arbitrary distribution. Then the confidence set \( \hat{C}_{io} \) in Algorithm 3 satisfies
\[
P(Y_{n+1} \in \hat{C}_{io}(X_{n+1})) \geq 1 - \alpha.
\]

**Proof** We show that the definitions of \( \hat{y}_{in} \) and \( \hat{y}_{out} \) in Alg. 3 are special cases of the condition (11), which then allows us to apply Corollary 3.1. We focus on the inner set, as the outer is similar. Suppose in Alg. 3 that \( \hat{y}_{in}(x)_k = 1 \). Then \( s_k(x) - \hat{t}_in(x) - \hat{Q}_{1-\alpha} \geq 0 \), which implies that \( \hat{t}_in(x) - s_k(x) \leq -\hat{Q}_{1-\alpha} \), and for any \( y \in \mathcal{Y} \) satisfying \( y_k = -1 \), we have
\[
\hat{t}_in(x) - \max_{t|y=-1} s_l(x) \leq -\hat{Q}_{1-\alpha}.
\]
But of course, for the scores \( s(x, y) \) in line 2 of Alg. 3, we then immediately obtain \( s(x, y) \leq -\hat{Q}_{1-\alpha} \) for any \( y \in \mathcal{Y} \) with \( y_k = -1 \). This is the first condition (11), so that (performing, mutatis-mutandis, the same argument with \( \hat{y}_{out}(x)_k \) Corollary 3.1 then implies the validity of \( \hat{C}_{io} \) in Algorithm 3. \qed

**A prediction method for tree-structured scores** We now turn to efficient computation of the inner and outer vectors (11) when the scoring function \( s : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) is tree-structured. By this we mean that there is a tree \( \mathcal{T} = ([K], E) \), with nodes \( [K] \) and edges \( E \subseteq [K]^2 \), and an associated set of pairwise and singleton factors \( \psi_e : \{1, -1\}^2 \times \mathcal{X} \to \mathbb{R} \) for \( e \in E \) and \( \varphi_k : \{1, -1\} \times \mathcal{X} \to \mathbb{R} \) for \( k \in [K] \) such that
\[
s(x, y) = \sum_{k=1}^{K} \varphi_k(y_k, x) + \sum_{e=(k, l) \in E} \psi_e(y_k, y_l, x). \tag{14}
\]
Such a score allows us to consider interactions between tasks \( k, l \) while maintaining computational efficiency, and we will show how to construct such a score function both from arbitrary multilabel prediction methods and from those with individual scores as above. When we have a tree-structured score (14), we can use efficient message-passing algorithms [7, 19] to compute the collections (maximum marginals) of scores
\[
S_- := \left\{ \max_{y \in \mathcal{Y}, y_k = -1} s(x, y) \right\}_{k=1}^{K} \quad \text{and} \quad S_+ := \left\{ \max_{y \in \mathcal{Y}, y_k = 1} s(x, y) \right\}_{k=1}^{K} \tag{15}
\]
in time \( O(K) \), from which it is immediate to construct \( \hat{y}_{in} \) and \( \hat{y}_{out} \) as in the conditions (11). We outline the approach in Appendix A.3, as it is not the central theme of this paper, though this efficiency highlights the importance of the tree-structured scores for practicality.

### 3.3 Building tree-structured scores

With the descriptions of the generic multilabel conformalization method in Alg. 2 and that we can efficiently compute predictions using tree-structured scoring functions (14), we now turn to constructing such scoring functions from predictors, which trade between label dependency structure, computational efficiency, and accuracy of the predictive function. We begin with a general case of an arbitrary predictor function, then describe a heuristic graphical model construction when individual label scores are available (as we assume in Alg. 3).
From arbitrary predictions to scores  We begin with the most general case that we have access only to a predictive function $\hat{y}: \mathcal{X} \rightarrow \mathbb{R}^K$. This prediction function is typically the output of some learning algorithm, and in the generality here, may either output real-valued scores $\hat{y}_k(x) \in \mathbb{R}$ or simply output $\hat{y}_k(x) \in \{-1,1\}$, indicating element $k$’s presence.

We compute a regularized scoring function based on a tree-structured graphical model (cf. [19]) as follows. Given a tree $T = ([K], E)$ on the labels $[K]$ and parameters $\alpha \in \mathbb{R}^K$, $\beta \in \mathbb{R}^E$, we define

$$s_{T,\alpha,\beta}(x,y) := \sum_{k=1}^K \alpha_k y_k \hat{y}_k(x) + \sum_{e=(k,l) \in E} \beta_{e} y_k y_l$$  \hspace{1cm} (16)$$

for all $(x, y) \in \mathcal{X} \times \{-1,1\}^K$, where we recall that we allow $\hat{y}_k(x) \in \mathbb{R}$. We will find the tree $T$ assigning the highest (regularized) scores to the true data $(X_i,Y_i)_{i=1}^n$ using efficient dynamic programs reminiscent of the Chow-Liu algorithm [6]. To that end, we use Algorithm 4.

| Algorithm 4: Method to find optimal tree from arbitrary predictor $\hat{y}$. |
|---|
| **Input:** Sample $\{(X_i,Y_i)\}_{i \in \mathcal{I}_1}$, convex regularizers $r_1, r_2 : \mathbb{R} \rightarrow \mathbb{R}$, predictor $\hat{y}: \mathcal{X} \rightarrow \mathbb{R}^K$. |
| **Set** |
| $(\hat{T}, \hat{\alpha}, \hat{\beta}) := \arg \max_{T=[K],E,\alpha,\beta} \left\{ \sum_{i=1}^n s_{T,\alpha,\beta}(X_i,Y_i) - \sum_{k=1}^K r_1(\alpha_k) - \sum_{e \in E} r_2(\beta_e) \right\}$  \hspace{1cm} (17) |
| and return score function $s_{\hat{T},\hat{\alpha},\hat{\beta}}$ of form (16). |

Because the regularizers $r_1, r_2$ decompose along the edges and nodes of the tree, we can implement Alg. 4 using a maximum spanning tree algorithm. Indeed, recall the familiar convex conjugate $r^*(t) := \sup_{\alpha} \{ \alpha t - r(\alpha) \}$ [5]. Then immediately

$$\sup_{\alpha,\beta} \left\{ \sum_{i=1}^n s_{T,\alpha,\beta}(X_i,Y_i) - \sum_{k=1}^K r_1(\alpha_k) - \sum_{e \in E} r_2(\beta_e) \right\}$$

$$= \sum_{k=1}^K r_1^* \left( \sum_{i=1}^n Y_{i,k} \hat{y}_k(X_i) \right) + \sum_{e=(k,l) \in E} r_2^* \left( \sum_{i=1}^n Y_{i,k} Y_{i,l} \right),$$

which decomposes along the edges of the putative tree. As a consequence, we may solve problem (17) by finding the maximum weight spanning tree in a graph with edge weights $r_2^* \left( \sum_{i=1}^n Y_{i,k} Y_{i,l} \right)$ for each edge $(k,l)$, then choosing $\alpha, \beta$ to maximize the objective (17), which is a collection of 1-dimensional convex optimization problems.

From single-task scores to a tree-based probabilistic model  While Algorithm 4 will work regardless of the predictor it is given—which may simply output a vector $\hat{y} \in \{-1,1\}^K$, as in Alg. 3 it is frequently the case that multilabel methods output scores $s_k : \mathcal{X} \rightarrow \mathbb{R}$ for each task. To that end, a natural strategy is to model the distribution of $Y \mid X$ directly via a tree-structured graphical model [21]. Similar to the score in Eq. (14), we define interaction factors $\psi : \{-1,1\}^2 \rightarrow \mathbb{R}^4$ by $\psi(-1,-1) = e_1$, $\psi(1,-1) = e_2$, $\psi(-1,1) = e_3$ and $\psi(1,1) = e_4$.  

the standard basis vectors, and marginal factors $\varphi_k : \{-1, 1\} \times X \to \mathbb{R}^2$ with

$$\varphi_k(y_k, x) := \frac{1}{2} \begin{bmatrix} (y_k - 1) \cdot s_k(x) \\ (y_k + 1) \cdot s_k(x) \end{bmatrix},$$

incorporating information $s_k(x)$ provides on $y_k$. For a tree $T = ([K], E)$, the label model is

$$p_{T,\alpha,\beta}(y \mid x) \propto \exp \left( \sum_{e = (k,l) \in E} \beta_e^T \psi(y_k, y_l) + \sum_{k=1}^K \alpha_k^T \varphi_k(y_k, x) \right),$$

(18)

where $(\alpha, \beta)$ where $\{\eta_\alpha\}_{\alpha \in E \cup [K]}$ is a set of parameters such that, for each edge $e \in E$, $\beta_e \in \mathbb{R}^4$ and $1^T \beta_e = 0$ (for identifiability), while $\alpha_k \in \mathbb{R}^2$ for each label $k \in [K]$. Because we view this as a “bolt-on” approach, applicable to any method providing scores $s_k$, we include only pairwise label interaction factors independent of $x$, allowing singleton factors to depend on the observed feature vector $x$ through the scores $s_k$.

The log-likelihood $\log p_{T,\alpha,\beta}$ is convex in $(\alpha, \beta)$ for any fixed tree $T$, and the Chow-Liu decomposition [6] of the likelihood of a tree $T = ([K], E)$ gives

$$\log p_{T,\alpha,\beta}(y \mid x) = \sum_{k=1}^K \log p_{T,\alpha,\beta}(y_k \mid x) + \sum_{e = (k,l) \in E} \log \frac{p_{T,\alpha,\beta}(y_k, y_l \mid x)}{p_{T,\alpha,\beta}(y_k \mid x) p_{T,\alpha,\beta}(y_l \mid x)},$$

(19)

that is, the sum of the marginal log-likelihoods and pairwise mutual information terms, conditional on $X = x$. Given a sample $(X_i, Y_i)_{i=1}^n$, the goal is to then solve

$$\text{maximize}_{T,\alpha,\beta} L_n(T, \alpha, \beta) := \sum_{i=1}^n \log p_{T,\alpha,\beta}(Y_i \mid X_i).$$

(20)

When there is no conditioning on $x$, the maximal pairwise mutual information terms $\log \frac{p_{T,\alpha,\beta}(y_k, y_l)}{p(y_k)p(y_l)}$ are independent of the tree $T$, allowing Chow and Liu [6] to use a maximum-spanning-tree algorithm to find the tree maximizing the likelihood (20). We heuristically compute empirical conditional mutual informations between each pair $(k, l)$ of tasks, choosing the tree $T$ that maximizes these values to approximate problem (20) in Algorithm 5, using the selected tree $\tilde{T}$ to choose $\alpha, \beta$ maximizing $L_n(\tilde{T}, \alpha, \beta)$. (In the algorithm we superscript $Y$ to make clearer task labels versus observations.)
Algorithm 5: Chow-Liu-type approximate Maximum Likelihood Tree and Scoring Function

Input: Sample \( \{(X^{(i)}, Y^{(i)})\}_{i \in I} \), and \( K \) score functions \( s_k : \mathcal{X} \to \mathbb{R} \).

For each pair \( e = (k, l) \in [K]^2 \):

1. Define the single-edge tree \( T_e = (\{k, l\}, \{e\}) \)
2. Fit model (19) for tree \( T \) via \( (\hat{\alpha}, \hat{\beta}) := \arg\max_{\alpha, \beta} L_n(T_e, \alpha, \beta) \)
3. Estimate empirical mutual information
   \[
   \hat{I}_e := \sum_{i=1}^{n} \log \left( \frac{p_{T_e, \hat{\alpha}, \hat{\beta}}(Y^{(i)}_k, Y^{(i)}_l | X^{(i)})}{p_{T_e, \hat{\alpha}, \hat{\beta}}(Y^{(i)}_k | X^{(i)})p_{T_e, \hat{\alpha}, \hat{\beta}}(Y^{(i)}_l | X^{(i)})} \right)
   \]

Set \( \hat{T} = \text{MAXSPANNINGTREE}(\{\hat{I}_e\}_{e \in [K]^2}) \) and \( (\hat{\alpha}, \hat{\beta}) = \arg\max_{\alpha, \beta} L_n(\hat{T}, \alpha, \beta) \).

Return scoring function

\[
 s_{\hat{T}, \hat{\alpha}, \hat{\beta}}(x, y) := \sum_{e = (k, l) \in E} \hat{\beta}_T \psi(y_k, y_l) + \sum_{k=1}^{K} \hat{\alpha}_T \varphi_k(y_k, x)
\]

The algorithm takes time roughly \( O(nK^2 + K^2 \log(K)) \), as each optimization step solves a concave maximization problem, which is straightforward via a Newton method (or gradient descent). The approach does not guarantee recovery of the correct tree structure even if the model is well-specified, as we neglect any potential information coming from labels other than \( k \) and \( l \) in the estimates \( \hat{I}_e \) for edge \( e = (k, l) \), although we expect the heuristic to return sufficiently reasonable tree structures. In any case, the actual scoring function \( s \) it returns still allows efficient conformalization and valid predictions via Alg. 2, regardless of its accuracy; a more accurate tree will simply allow smaller and more accurate confidence sets (11).

4 Experiments

Our main motivation is to design methods with more robust conditional coverage than the “marginal” split-conformal method (3). Accordingly, the methods we propose in Sections 2 and 3 fit conformalization scores that depend on the features \( x \) and, in some cases, model dependencies among \( y \) variables. Our experiments consequently focus on more robust notions of coverage than the nominal marginal coverage the methods guarantee, and we develop a new evaluation metric for validation and testing of coverage, looking at connected subsets of the space \( \mathcal{X} \) and studying coverage over these. Broadly, we expect our proposed methods to maintain coverage of (nearly) \( 1 - \alpha \) across subsets; as we see presently, the experiments are consistent with this expectation.

Measures beyond marginal coverage Except in simulated experiments, we cannot compute conditional coverage of each instance. Instead, we look at coverage over slabs

\[
 S_{v,a,b} := \left\{ x \in \mathbb{R}^d \mid a \leq v^T x \leq b \right\},
\]
where \( v \in \mathbb{R}^d \) and \( a < b \in \mathbb{R} \), which (as we see presently) allow some calculation of conditional coverage in \( \mathcal{X} \)-space and statistical validity. For a direction \( v \) and threshold \( 0 < \delta \leq 1 \), we then consider the worst coverage over all such slabs containing \( \delta \) mass in \( \{X_i\}_{i=1}^n \), defining

\[
WSC_n(\hat{C}, v) := \inf_{a < b} \left\{ P_n(Y \in \hat{C}(X) \mid a \leq v^T X \leq b) \quad \text{s.t.} \quad P_n(a \leq v^T X \leq b) \geq \delta \right\},
\]

(21)

where \( P_n \) denotes the empirical distribution on \( (X_i, Y_i)_{i=1}^n \). As long as the mapping \( \hat{C} : \mathcal{X} \mapsto \mathcal{Y} \) is constructed independently of \( P_n \), we can show that these quantities concentrate. Indeed, let us temporarily assume that the confidence set has the form \( \hat{C}(x) = \{ y \mid s(x, y) \geq q(x) \} \) for some (arbitrary) scoring \( s : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R} \) and threshold functions \( q \). Let \( V \subset \mathbb{R}^d \); we abuse notation to let \( VC(V) \) be the VC-dimension of the set of halfspaces it induces, where we note that \( VC(V) \leq \min\{d, \log_2 |V|\} \). Then for some numerical constant \( C \), for all \( t > 0 \)

\[
\sup_{v \in V, a \leq b, P_n(X \in S_{v,a,b}) \geq \delta} \left\{ P_n(Y \in \hat{C}(X) \mid X \in S_{v,a,b}) - P(Y \in \hat{C}(X) \mid X \in S_{v,a,b}) \right\} \leq C \sqrt{\frac{VC(V) \log n + t}{\delta n}} \leq C \sqrt{\frac{\min\{d, \log |V|\} \log n + t}{\delta n}}
\]

(22)

with probability at least \( 1 - e^{-t} \). (See Appendix A.4 for a brief derivation of inequality (22) and a few other related inequalities.)

Each of the confidence sets we develop in this paper satisfy \( \hat{C}(x) \supset \{ y \mid s(x, y) \geq q(x) \} \) for some scoring function \( s \) and function \( q \). Thus, if \( \hat{C} : \mathcal{X} \mapsto \mathcal{Y} \) effectively provides conditional coverage at level \( 1 - \alpha \), we should observe that

\[
\inf_{v \in V} WSC_n(\hat{C}, v) \geq 1 - \alpha - O(1) \sqrt{\frac{VC(V) \log n}{\delta n}} \geq 1 - \alpha - O(1) \sqrt{\frac{\min\{d, \log |V|\} \log n}{\delta n}}.
\]

In each of our coming experiments, we draw \( M = 1000 \) samples \( v_j \) uniformly on \( S^{d-1} \), computing the worst-slice coverage (21) for each \( v_j \). In the multiclass case, we expect our conformal quantile classification (CQC, Alg. 1) method to provide larger worst-slab coverage than the standard marginal method (3), while in the multilabel case, we expect that the combination of tree-based scores (Algorithms 4 or 5) with the conformalized quantile inner/outer classification (CQioC, Alg. 2) should provide larger worst-slab coverage than the conformalized direct inner/outer classification (CDioC, Alg. 3). In both cases, we expect that our more sophisticated methods should provide confidence sets of comparable size to the marginal methods. Unlike in the multiclass case, we know of no baseline method for multilabel problems, as the “marginal” method (3) is computationally inefficient when the number of labels grows. For this reason, we focus on the methods in this paper, highlighting the potential advantages of each one while comparing them to an oracle (conditionally perfect) confidence set in simulation.

We present four experiments: two with simulated datasets and two with real datasets (CIFAR-10 [20] and Pascal VOC 2012 [12]), and both in multiclass and multilabel settings. In each experiment, a single trial corresponds to a realized random split of the data between training, validation and calibration sets \( T_1, T_2 \) and \( T_3 \), and in each figure, the red dotted line represents the desired level of coverage \( 1 - \alpha \). Unless otherwise specified, we summarize results via boxplots that display the lower and upper quartiles as the hinges of the box, the median as a bold line, and whiskers that extend to the 5% and 95% quantiles of the statistic of interest (typically coverage or average confidence set size).
4.1 Simulation

4.1.1 More uniform coverage on a multiclass example

Our first experiment is a simulation to allow us to compute the conditional coverage of each sample, studying the performance of our CQC method specifically studies the performance of our CQC method on small sub-populations, a challenge for traditional machine learning models \[10, 13\]. In contrast to the traditional split-conformal algorithm (method (3), cf. \[33\]), we expect the quantile estimator (5) in the CQC method to better account for data heterogeneity, maintaining higher coverage on subsets of the data.

To test this, we generate \( n = 10^5 \) data points \( \{X_i, Y_i\}_{i \in [N]} \) i.i.d. from a Gaussian mixture with one majority group and three minority ones, \( Y \sim \text{Mult}(\pi) \) and \( X | Y = y \sim \mathcal{N}(\mu_y, \Sigma_y) \). \( \text{(23)} \)

where \( \pi = (.7,.1,.1,.1) \) (see Fig. 1). We purposely introduce more confusion for the three minority groups (1, 2 and 3), whereas the majority (0) has a clear linear separation. We choose \( \alpha = 10\% \), the same as the size of the smaller sub-populations, then we apply our CQC method and compare it to both the Marginal (3) and the Oracle (which outputs the smallest conditionally valid \( 1 - \alpha \) confidence set) methods.

The results in Figure 2 are consistent with our expectations. The oracle method dominates, of course, but CQC appears to provide more robust coverage for individual classes than the marginal method. While all methods maintain \( 1 - \alpha \) coverage marginally, the left plot shows that 80% of sampled \( X \) have coverage at least \( 1 - \alpha \) (where \( \alpha = .1 \)) using the CQC method, while the marginal method (3) covers 70% of the time (the “bumps” in plot occur because of the discrete probabilities of observing each class \( y \)). Consequently, the CQC method provides higher coverage on the sub-populations of the data, as it also higher coverage for minority classes (see right plot of Fig. 2).

4.1.2 Improved coverage with graphical models

Our second simulation addresses the multilabel setting, where we have a predictive model outputting scores \( s_k(x) \in \mathbb{R} \) for each task \( k \). We run three methods. First, the direct Inner/Outer method (CDioC), Alg. 3. Second, we use the graphical model score from the likelihood model in Alg. 5 to choose a scoring function \( s_T : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \), which we call the PGM-CQC method; we then either use the CQC method with this scoring function directly,
Figure 2. Simulation results on multiclass problem. Left: X-probability of achieving a given level $t$ of conditional coverage versus coverage $t$, i.e., $t \mapsto P_X(P(Y \in \hat{C}_{\text{Method}}(X) \mid X \geq t))$. The ideal is to observe $t \mapsto 1\{t \leq 1 - \alpha\}$. Right: class-wise coverage $P(Y \in \hat{C}_{\text{Method}}(X) \mid Y = y)$ on the distribution (23) (as in Fig. 1) for each method. Confidence bands and error bars display the range of the statistic over $M = 20$ trials.

Figure 3. Results for simulated multilabel experiment with label distribution (24). Methods are the true oracle confidence set; the conformalized direct inner/outer method (CDioC), Alg. 3; and tree-based methods with implicit confidence sets $\hat{C}_{\text{imp}}$ or explicit inner/outer sets $\hat{C}_{\text{io}}$, labeled ArbiTree and PGM(see description in Sec. 4.1.2). Left: Marginal coverage probability at level $1 - \alpha = 0.8$ for different methods. Right: confidence set sizes of methods.
that is, the implicit confidence set (recall (12)) \( \hat{C}_{\text{imp}}(x) = \{ y \in \mathcal{Y} \mid s_T(x, y) \geq \hat{q}(x) - \hat{Q}_{1-\alpha} \} \) or the explicit \( \hat{C}_{\text{io}} \) set of Eqs. (10)–(11). Finally, we do the same except that we use the arbitrary predictor method (Alg. 4) to construct the score \( s_T \), where we the \( \{ \pm 1 \}^K \) assignment \( \hat{y} \) instead of scores as input predictors, which we term ArbiTree-CQC.

We consider a misspecified logistic regression model, where hidden confounders induce correlation between labels. Because of the dependency structure, we expect the tree-based methods to output smaller and more robust confidence sets the direct CDioC method. Comparing the two score-based methods (CDioC and PGM-CQC) with the scoreless tree method ArbiTree-CQC is perhaps unfair, as the latter uses less information—only signs of predicted labels. Yet we expect the label correlation the ArbiTree-CQC method can leverage to mitigate this disadvantage, at least relative to CDioC.

Our setting follows, where we consider \( K = 5 \) tasks and dimension \( d = 2 \). For each experiment, we choose a tree \( T = ([K], E) \) uniformly at random, where each edge \( e \in E \) has a correlation strength value \( \tau_e \sim \text{Unif}[-5, 5] \), and for every task \( k \) we sample a vector \( \theta_k \sim \text{Unif}(rS^{d-1}) \) with radius \( r = 5 \). For each observation, we draw \( X \sim \text{N}(0, I_d) \) and draw independent uniform hidden variables \( H_e \in \{-1, 1\} \) for each edge \( e \) of the tree. Letting \( E_k \) being the set of edges adjacent to \( k \), we draw \( Y_k \in \{-1, 1\} \) from the logistic model

\[
\mathbb{P}(Y_k = y_k \mid X = x, H = h) \propto \exp\left\{ -y_k \left( 1 + x^T \theta_h + \sum_{e \in E_k} \tau_e h_e \right) \right\}.
\]

We simulate \( n_{\text{total}} = 200,000 \) data points, using \( n_{\text{tr}} = 100,000 \) for training, \( n_{\text{c}} = 40,000 \) for validation, \( n_{\text{c}} = 40,000 \) for calibration, and \( n_{\text{te}} = 20,000 \) for testing.

The methods CDioC and PGM-CQC require per-task scores \( s_k \), so for each method we fit \( K \) separate logistic regressions of \( Y_k \) against \( X \) (leaving the hidden variables \( H \) unobserved) on the training data. We then use the fit parameters \( \hat{\theta}_k \in \mathbb{R}^d \) to define scores \( \hat{s}_k(x) = \hat{\theta}_k^T x \) (for the methods CDioC and PGM-CQC) and the “arbitrary” predictor \( \hat{y}_k(x) = \text{sign}(s_k(x)) \) (for method ArbiTree-CQC). We use a one-layer fully-connected neural network with 16 hidden neurons as the class \( Q \) in the quantile regression step (5) of the methods; no matter our choice of \( Q \), the final conformalization step guarantees (marginal) validity.

Figure 3 and 4 show our results. In Fig. 3, we give the marginal coverage of each method (left plot), including both the implicit \( \hat{C}_{\text{imp}} \) and explicit \( \hat{C}_{\text{io}} \) confidence sets, and the average confidence set sizes for the explicit confidence set \( \hat{C}_{\text{io}} \) in the right plot. We see that the explicit sets \( \hat{C}_{\text{io}} \) in the ArbiTree-CQC and PGM-CQC methods both overcover, and the sizes of \( \hat{C}_{\text{io}} \) for the PGM-CQC and CDioC methods are similar, though the latter has a larger inner and outer sets. On the other hand, the PGM-CQC explicit confidence sets (as they expand (11) the implicit set \( \hat{C}_{\text{imp}} \) provide substantially better coverage than the direct Inner/Outer method CDioC. The confidence sets of the scoreless method ArbiTree-CQC are wider, which is consistent with the limited information available to the method via the predictions \( \hat{y}_k = \text{sign}(s_k) \).

Figure 4 shows our results on the worst-slab coverage measures (21), dovetailing with our expectations that the PGM-CQC and ArbiTree-CQC methods are more robust and feature-adaptive. Each of the \( M = 10^3 \) experiments corresponds to a draw of \( v \sim \text{Unif}(S^{d-1}) \), then evaluating the worst-slab coverage (21) with \( \delta = .2 \). In the left plot, we show the variability across draws of \( v \) for each method, which shows a substantial difference in coverage between the CDioC method and the others. We also perform direct comparisons in the right plot: we draw the same directions \( v \) for each method, and then (for the given \( v \)) evaluate the difference \( \text{WSC}_n(\hat{C}, v) - \text{WSC}_n(\hat{C}', v) \), where \( \hat{C} \) and \( \hat{C}' \) are the confidence sets each method produces,
Figure 4. Distribution of the worst-slab coverage (21) (with $\delta = 20\%$) on mis-specified logistic regression model (24) over $M = 1000$ i.i.d. choices of direction $v \in S^{d-1}$. Left: distribution of $WSC_n(\hat{C}, v)$. Right: distribution of difference $WSC_n(\hat{C}_{\text{Method}_1}, v) - WSC_n(\hat{C}_{\text{Method}_2}, v)$. Method$_2$ is always the CDioC method (Alg. 3), and the other four are ArbiTree-CQC and PGM-CQC with both implicit $\hat{C}_{\text{imp}}$ and explicit $\hat{C}_{\text{io}}$ confidence sets.

respectively. Thus, we see that both tree-based methods always provide better worst-slab coverage, whether we use the implicit confidence sets $\hat{C}_{\text{imp}}$ or the larger direct inner/outer (explicit) confidence sets $\hat{C}_{\text{io}}$, though in the latter case, some of the difference likely comes from the differences in marginal coverage.

4.2 More robust coverage on the CIFAR 10 dataset

In our first real experiment, we study a multiclass image classification problem with the standard CIFAR-10 dataset, which consists of $n = 60,000$ $32 \times 32$ images across 10 classes. We use $n_{\text{tr}} = 50,000$ of them to train the full model, a validation set of size $n_v = 6,000$ for fitting quantile functions and hyperparameter tuning, $n_c = 3,000$ for calibration and the last $n_{\text{te}} = 1,000$ for testing. We train a standard ResNet 50 [14] architecture for 200 epochs, which obtains an accuracy of $92.5 \pm 0.5\%$ on the test set. We use the $d = 256$-dimensional output of the final layer of the ResNet as the inputs $X$ to the quantile estimation.

We then apply the CQC method 1 with $\alpha = 5\%$, and we compare it to the benchmark marginal method (3). We expect the latter to typically output small confidence sets, as the neural network’s accuracy is close to the confidence level $1 - \alpha$; this allows almost (typically) predicting a single label while maintaining marginal coverage. Figure 5 shows this happens precisely. In Figure 6, however, we compare worst-slab coverage (21) over $M = 1000$ draws of $v \overset{\text{iid}}{\sim} \text{Uni}(S^{d-1})$. Here, we see that the CQC method provides slight—but statistically significant—gain in the worst-slab coverage over the marginal method; we expect this more robust coverage from CQC, though in this case the effect is relatively small (about .5–1% better coverage).
Figure 5. Marginal coverage and average confidence set size on CIFAR-10 over $M = 20$ trials.

Figure 6. Worst-slab coverage for CIFAR-10 with $\delta = .1$ over $M = 1000$ draws $r_i \overset{iid}{\sim} \text{Uni}(S^{d-1})$. The dotted line is the desired (marginal) coverage. Left: distribution of worst-slab coverage. Right: distribution of the coverage difference $\text{WSC}_n(\hat{C}_{\text{CQC}}, v) - \text{WSC}_n(\hat{C}_{\text{Marginal}}, v)$. 
Figure 7. Results for PASCAL VOC dataset [12] over $M = 20$ trials. Methods are the conformalized direct inner/outer method (CDioC), Alg. 3; and tree-based methods with implicit confidence sets $\hat{C}_{imp}$ or explicit inner/outer sets $\hat{C}_{io}$, labeled ArbiTree and PGM(see description in Sec. 4.1.2). Left: Marginal coverage probability at level $1 - \alpha = .8$ for different methods. Right: confidence set sizes of methods.

4.3 A multilabel image recognition dataset

Our final set of experiments considers the multilabel image classification problems in the PASCAL VOC 2007 and VOC 2012 datasets [11, 12], which consist of $n_{2012} = 11540$ and $n_{2007} = 9963$ distinct $224 \times 224$ images, where the goal is to predict the presence of entities from $K = 20$ different classes, (e.g. birds, boats, people). We compare the direct inner outer method (CDioC) 3 with the split-conformalized inner/outer method (CQioC) 2, where we use the tree-based score functions that Algorithms 4 and 5 output.

In this problem, we use the $d = 2048$ dimensional output of a ResNet-101 with pretrained weights on the ImageNet dataset [9] as our feature vectors $X$. For each of the $K$ classes, we fit a binary logistic regression model $\hat{\theta}_k \in \mathbb{R}^d$ of $Y_k \in \{\pm 1\}$ against $X$, then use $s_k(x) = \hat{\theta}_k^T x$ as the scores for the PGM-CQC method (Alg. 5). We use $\hat{y}_k(x) = \text{sign}(s_k(x))$ for the ArbiTree-CQC method 4. The F1-score of the fit predictors on held-out data is 0.77, so we do not expect our confidence sets to be uniformly small while maintaining the required level of coverage, in particular for ArbiTree-CQC. We use a validation set of $n_v = 3493$ images to fit the quantile functions (5) as above using a one layer fully-connected neural network with 16 hidden neurons and tree parameters.

The results from Figure 8 are consistent with our hypotheses that the tree-based models should improve robustness of the coverage. Indeed, while all methods ensure marginal coverage at level $\alpha = .8$ (see Fig. 7), Figure 8 shows that worst-case slabs (21) for the tree-based methods have closer to $1 - \alpha$ coverage. In particular, for most random slab directions $v$, the tree-based methods have higher worst-slab coverage than the direct inner/outer method (CDioC, Alg. 3). At the same time, both the CDioC method and PGM-CQC method (using $C_{io}$) provide similarly-sized confidence sets, as the inner set of the PGM-CQC method is
Figure 8. Worst-slab coverage for Pascal-VOC with $\delta = .2$ over $M = 1000$ draws $v \overset{iid}{\sim} \text{Uni}(S_{d-1})$. For tree-structured methods labeled ATree and PGM, we compute the worst-slab coverage using implicit confidence sets $\hat{C}_{\text{imp}}$ and explicit inner/outer sets $\hat{C}_{\text{io}}$ (resp. Imp and IO in this figure). The dotted line is the desired (marginal) coverage. Left: distribution of worst-slab coverage. Right: distribution of the coverage difference $WSC_n(\hat{C}_{\text{Method}}, v) - WSC_n(\hat{C}_{\text{CDioC}}, v)$ for Method $i \in \{\text{ArbiTree-CQC, PGM-CQC}\}$ with implicit $\hat{C}_{\text{imp}}$ or explicit inner/outer $\hat{C}_{\text{io}}$ confidence sets.

typically smaller, as is its outer set. The ArbiTree-CQC method performs poorly on this example: its coverage is at the required level, but the confidence sets are too large and thus essentially uninformative.

5 Conclusions

As long as we have access to a validation set, independent of (or at least exchangeable with) the sets used to fit a predictive model, split conformal methods guarantee marginal validity, which gives great freedom in modeling. It is thus of interest to fit models more adaptive to the signal inputs $x$ at hand—say, by quantile predictions as we have done, or other methods yet to be discovered—that can then in turn be conformalized. As yet we have limited understanding of what “near” conditional coverage might be possible: Barber et al. [1] provide procedures that can guarantee coverage uniformly across subsets of $X$-space as long as those subsets are not too complex, but it appears computationally challenging to fit the models they provide, and our procedures empirically appear to have strong coverage across slabs of the data as in Eq. (21). Our work, then, is a stepping stone toward more uniform notions of validity, and we believe exploring approaches to this—perhaps by distributionally robust optimization [8, 10], perhaps by uniform convergence arguments [1, Sec. 4]—will be both interesting and essential for trusting applications of statistical machine learning.
References

[1] Rina Foygel Barber, Emmanuel J. Candès, Aaditya Ramdas, and Ryan J. Tibshirani. The limits of distribution-free conditional predictive inference. arXiv:1903.04684v2 [math.ST], 2019.

[2] P. L. Bartlett, M. I. Jordan, and J. McAuliffe. Convexity, classification, and risk bounds. *Journal of the American Statistical Association*, 101:138–156, 2006.

[3] Stéphane Boucheron, Olivier Bousquet, and Gábor Lugosi. Theory of classification: a survey of some recent advances. *ESAIM: Probability and Statistics*, 9:323–375, 2005.

[4] Matthew R Boutell, Jiebo Luo, Xipeng Shen, and Christopher M Brown. Learning multi-label scene classification. *Pattern Recognition*, 37(9):1757–1771, 2004.

[5] Stephen Boyd and Lieven Vandenberghe. *Convex Optimization*. Cambridge University Press, 2004.

[6] C. K. Chow and C. N. Liu. Approximating discrete probability distributions with dependence trees. *IEEE Transactions on Information Theory*, 14(3):462–467, 1968.

[7] A. P. Dawid. Applications of a general propagation algorithm for probabilistic expert systems. *Statistics and Computing*, 2(1):25–36, 1992.

[8] Erick Delage and Yinyu Ye. Distributionally robust optimization under moment uncertainty with application to data-driven problems. *Operations Research*, 58(3):595–612, 2010.

[9] J. Deng, W. Dong, R. Socher, L. Li, K. Li, and L. Fei-Fei. ImageNet: a large-scale hierarchical image database. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 248–255, 2009.

[10] John C. Duchi and Hongseok Namkoong. Learning models with uniform performance via distributionally robust optimization. arXiv:1810.08750 [stat.ML], 2018.

[11] M. Everingham, L. Van Gool, C. K. I. Williams, J. Winn, and A. Zisserman. The PASCAL Visual Object Classes Challenge 2007 (VOC2007) Results, 2007. URL http://www.pascal-network.org/challenges/VOC/voc2007/workshop/index.html.

[12] M. Everingham, L. Van Gool, C. K. I. Williams, J. Winn, and A. Zisserman. The PASCAL Visual Object Classes Challenge 2012 (VOC2012) Results, 2012. URL http://www.pascal-network.org/challenges/VOC/voc2012/workshop/index.html.

[13] Tatsunori Hashimoto, Megha Srivastava, Hongseok Namkoong, and Percy Liang. Fairness without demographics in repeated loss minimization. In *Proceedings of the 35th International Conference on Machine Learning*, 2018.

[14] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 770–778, 2016.

[15] Yotam Hechtlinger, Barnabás Póczos, and Larry Wasserman. Cautious deep learning. arXiv:1805.09460 [stat.ML], 2019.

[16] Francisco Herrera, Francisco Charte, Antonio J Rivera, and María J Del Jesus. Multilabel classification. In *Multilabel Classification*, pages 17–31. Springer, 2016.

[17] Armand Joulin, Edouard Grave, Piotr Bojanowski, and Tomas Mikolov. Bag of tricks for efficient text classification. arXiv:1607.01759 [cs.CL], 2016.

[18] Roger Koenker and Gilbert Bassett Jr. Regression quantiles. *Econometrica: Journal of the Econometric Society*, 46(1):33–50, 1978.
[19] Daphne Koller and Nir Friedman. *Probabilistic Graphical Models: Principles and Techniques*. MIT Press, 2009.

[20] Alex Krizhevsky and Geoffrey Hinton. Learning multiple layers of features from tiny images. Technical report, University of Toronto, 2009.

[21] J. Lafferty, A. McCallum, and F. Pereira. Conditional random fields: Probabilistic models for segmenting and labeling sequence data. In *Proceedings of the Eighteenth International Conference on Machine Learning*, pages 282–289, 2001.

[22] Tsung-Yi Lin, Michael Maire, Serge Belongie, James Hays, Pietro Perona, Deva Ramanan, Piotr Dollár, and C. Lawrence Zitnick. Microsoft COCO: Common objects in context. In *Computer Vision – ECCV 2014*, pages 740–755, Cham, 2014. Springer International Publishing.

[23] Huma Lodhi, John Shawe-Taylor, Nello Cristianini, and Christopher J. C. H. Watkins. Text classification using string kernels. *Journal of Machine Learning Research*, 2:419–444, 2002.

[24] Andrew McCallum and Kamal Nigam. Employing EM in pool-based active learning for text classification. In *Machine Learning: Proceedings of the Fifteenth International Conference*, 1998.

[25] Jesse Read, Bernhard Pfahringer, Geoff Holmes, and Eibe Frank. Classifier chains for multi-label classification. *Machine Learning*, 85:333–359, 2011.

[26] Joseph Redmon, Santosh Divvala, Ross Girshick, and Ali Farhadi. You only look once: Unified, real-time object detection. In *Proceedings of the 26th IEEE Conference on Computer Vision and Pattern Recognition*, pages 779–788, 2016.

[27] Yaniv Romano, Evan Patterson, and Emmanuel J. Candès. Conformalized quantile regression. In *Advances in Neural Information Processing Systems 32*, 2019. URL https://arxiv.org/abs/1905.03222.

[28] Mauricio Sadinle, Jing Lei, and Larry Wasserman. Least ambiguous set-valued classifiers with bounded error levels. *Journal of the American Statistical Association*, 114(525):223–234, 2019. doi: 10.1080/01621459.2017.1395341. URL https://doi.org/10.1080/01621459.2017.1395341.

[29] Matteo Sesia and Emmanuel J. Candès. A comparison of some conformal quantile regression methods. *arXiv:1909.05433 [stat.ME]*, 2019.

[30] Mingxing Tan, Ruoming Pang, and Quoc V Le. EfficientDet: Scalable and efficient object detection. *arXiv:1911.09070 [cs.CV]*, 2019.

[31] A. Tewari and P. L. Bartlett. On the consistency of multiclass classification methods. *Journal of Machine Learning Research*, 8:1007–1025, 2007.

[32] Vladimir 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. URL http://proceedings.mlr.press/v25/vovk12.html.

[33] Vladimir Vovk, Alexander Grammerman, and Glenn Shafer. *Algorithmic Learning in a Random World*. Springer, 2005.

[34] Martin J. Wainwright and Michael I. Jordan. Graphical models, exponential families, and variational inference. *Foundations and Trends in Machine Learning*, 1(1–2):1–305, 2008.

[35] Min-Ling Zhang and Zhi-Hua Zhou. Multilabel neural networks with applications to
A Technical proofs and appendices

A.1 Proof of Theorem 3

Our proof adapts arguments similar to those that Sesia and Candès [29] use in the regression setting, repurposing and modifying them for classification. We have that \( \| \hat{s} - s \|_{L^2(P_X)} \overset{p}{\to} 0 \) and \( \| \hat{q}_\alpha^\sigma - q_\alpha^\sigma \|_{L^2(P_X)} \overset{p}{\to} 0 \). We additionally have that

\[
\hat{q} := Q_{1-\alpha}(E^\sigma, \mathcal{I}_3) \overset{p}{\to} 0. \tag{25}
\]

This is item (ii) in the proof of Theorem 1 of Sesia and Candès [29] (see Appendix A of their paper), which proves the convergence (25) of the marginal quantile of the error precisely when \( \hat{q}_\alpha^\sigma \) and \( \hat{s} \) are \( L^2 \)-consistent in probability (when the randomized quantity \( s(x,Y) + \sigma Z \) has a density), as in our Assumption A1.

Recalling that \( \hat{s}, \hat{q} \) tacitly depend on the sample size \( n \), let \( \epsilon > 0 \) be otherwise arbitrary, and define the sets

\[
B_n := \{ x \in \mathcal{X} \mid \| \hat{s}(x, \cdot) - s(x, \cdot) \|_\infty > \epsilon^2 \text{ or } |\hat{q}_\alpha^\sigma(x) - q_\alpha^\sigma(x)| > \epsilon^2 \}.
\]

Then \( B_n \subset \mathcal{X} \) is measurable, and by Markov’s inequality,

\[
P_X(B_n) \leq \frac{\| \hat{s} - s \|_{L^2(P_X)}}{\epsilon} + \frac{\| \hat{q}_\alpha^\sigma - q_\alpha^\sigma \|_{L^2(P_X)}}{\epsilon},
\]

so

\[
P(P_X(B_n) \geq \epsilon) \leq P(\| \hat{s} - s \|_{L^2(P_X)} > \epsilon^2) + P(\| \hat{q}_\alpha^\sigma - q_\alpha^\sigma \|_{L^2(P_X)} > \epsilon^2) \to 0. \tag{26}
\]

Thus, the measure of the sets \( B_n \) tends to zero in probability, i.e., \( P_X(B_n) \overset{p}{\to} 0 \).

Now recall the shorthand (25) that \( \hat{q} = Q_{1-\alpha}(E^\sigma, \mathcal{I}_3) \). Let us consider the event that \( C_{1-\alpha}^\sigma(x, z) \neq C_{1-\alpha}^\sigma(x, z) \). If this is the case, then we must have one of

\[
A_1(x, k, z) := \left\{ \hat{s}(x, k) + \sigma z \geq \hat{q}_\alpha^\sigma(x) - \hat{q} \text{ and } s(x, k) + \sigma z < q_\alpha^\sigma(x) \right\} \quad \text{or} \quad \tag{27}
A_2(x, k, z) := \left\{ \hat{s}(x, k) + \sigma z < \hat{q}_\alpha^\sigma(x) - \hat{q} \text{ and } s(x, k) + \sigma z \geq q_\alpha^\sigma(x) \right\}.
\]

We show that the probability of the set \( A_1 \) is small; showing that the probability of set \( A_2 \) is small is similar. Using the convergence (25), let us assume that \( |\hat{q}| \leq \epsilon \), and suppose that \( x \notin B_n \). Then for \( A_1 \) to occur, we must have both \( s(x, k) + \epsilon + \sigma z \geq q_\alpha^\sigma(x) - 2\epsilon \) and \( s(x, k) + \sigma z < q_\alpha^\sigma(x) \), or

\[
q_\alpha^\sigma(x) - s(x, k) - 3\epsilon \leq \sigma z < q_\alpha^\sigma(x) - s(x, k).
\]

As \( Z \) has a bounded density, we have \( \limsup_{\epsilon \to 0} \sup_{x \in \mathbb{R}} P_Z(a \leq \sigma Z \leq a + 3\epsilon) = 0 \), or (with some notational abuse) \( \limsup_{\epsilon \to 0} \sup_{x \notin B_n} P_Z(A_1(x, k, Z)) = 0 \).
Now, let $F_n = \sigma(\{X_i\}_{i=1}^n, \{Y_i\}_{i=1}^n, \{Z_i\}_{i=1}^n)$ be the $\sigma$-field of the observed sample. Then by the preceding derivation (mutatis mutandis for the set $A_2$ in definition (27)) for any $\eta > 0$, there is an $\epsilon > 0$ (in the definition of $B_n$) such that

$$\sup_{x \in X} \mathbb{P}\left(\hat{C}_{1-\alpha}(x, Z_{n+1}) \neq C_{1-\alpha}(x, Z_{n+1}) \mid F_n\right) 1\{x \notin B_n\} 1\{|\hat{Q}| \leq \epsilon\} \leq \sup_{x \notin B_n} \mathbb{P}(A_1(x, k, Z_{n+1}) \text{ or } A_2(x, k, Z_{n+1}) \mid F_n) 1\{|\hat{Q}| \leq \epsilon\} \leq \eta.$$ 

In particular, by integrating the preceding inequality, we have

$$\mathbb{P}\left(\hat{C}_{1-\alpha}(X_{n+1}, Z_{n+1}) \neq \hat{C}(X_{n+1}, Z_{n+1}), X_{n+1} \notin B_n, |\hat{Q}| \leq \epsilon\right) \leq \eta.$$ 

As $\mathbb{P}(|\hat{Q}| \leq \epsilon) \to 1$ and $\mathbb{P}(X_{n+1} \notin B_n) \to 1$ by the convergence guarantees (25) and (26), we have the theorem.

### A.2 Proof of Theorem 4

We wish to show that $\lim_{\sigma \to 0} \mathbb{P}(C_{1-\alpha}(X, Z) \subset C_{1-\alpha}(X)) = 1$, which, by a union bound over $k \in [K]$, is equivalent to showing

$$\mathbb{P}(s(X, k) + \sigma Z \geq q_{\alpha}(X), s(X, k) < q_{\alpha}(X)) \to 0$$

for all $k \in [K]$. Fix $k \in [K]$, and define the events

$$A := \{s(X, k) < q_{\alpha}(X)\}$$

and

$$B^\sigma := \{s(X, k) + \sigma Z \geq q_{\alpha}(X)\}.$$ 

Now, for any $\delta > 0$, consider $A_\delta := \{s(X, k) \leq q_{\alpha}(X) - \delta\}$. On the event $A_\delta \cap B^\sigma$, it must hold that

$$\delta \leq q_{\alpha}(X) - q_{\alpha}(X) + \sigma Z.$$ 

The following lemma—whose proof we defer to Section A.2.1—shows that the latter can only occur with small probability.

**Lemma A.1.** With probability 1 over $X$, the quantile function satisfies

$$\liminf_{\sigma \to 0} q_{\alpha}(X) \geq q_{\alpha}(X),$$

and hence $\limsup_{\sigma \to 0} \{q_{\alpha}(X) - q_{\alpha}(X) + \sigma Z\} \leq 0$ almost surely.

**Lemma A.1** implies that

$$\mathbb{P}(q_{\alpha}(X) - q_{\alpha}(X) + \sigma Z \geq \delta) \to 0,$$

which, in turn, shows that, for every fixed $\delta > 0$,

$$\mathbb{P}(A_\delta \cap B^\sigma) \to 0.$$
To conclude the proof, fix $\epsilon > 0$. The event $A_\delta$ increases to $A$ when $\delta \to 0$, so there exists $\delta > 0$ so that

$$P(A \setminus A_\delta) \leq \epsilon.$$ 

Finally,

$$\limsup_{\sigma \to 0} P(A \cap B^\sigma) \leq P(A \setminus A_\delta) + \limsup_{\sigma \to 0} P(A_\delta \cap B^\sigma) \leq \epsilon,$$

as $\limsup_{\sigma \to 0} P(A_\delta \cap B^\sigma) = 0$. We conclude the proof by sending $\epsilon \to 0$.

### A.2.1 Proof of Lemma A.1

Fix $x \in X$. Let $F_{\sigma,x}$ and $F_x$ be the respective cumulative distribution functions of $s^\sigma(x, Y, Z)$ and $s(x, Y)$ conditionally on $X = x$, and define the (left-continuous) inverse CDFs

$$F_{\sigma,x}^{-1}(u) = \inf\{t \in \mathbb{R} : u \leq F_{\sigma,x}(t)\} \quad \text{and} \quad F_x^{-1}(u) = \inf\{t \in \mathbb{R} : u \leq F_x(t)\}.$$

We use a standard lemma about the convergence of inverse CDFs, though for lack of a proper reference, we include a proof in Section A.2.2.

**Lemma A.2.** Let $(F_n)_{n \geq 1}$ be a sequence of cumulative distribution functions converging weakly to $F$, with inverses $F_n^{-1}$ and $F^{-1}$. Then for each $u \in (0,1)$,

$$F^{-1}(u) \leq \liminf_{n \to \infty} F_n^{-1}(u) \leq \limsup_{n \to \infty} F_n^{-1}(u) \leq F^{-1}(u^+). \quad (28)$$

As $F_{\sigma,x}$ converges weakly to $F_x$ as $\sigma \to 0$, Lemma A.2 implies that

$$F_x^{-1}(\alpha) \leq \liminf_{\sigma \to 0} F_{\sigma,x}^{-1}(\alpha).$$

But observe that $q^\sigma_{\alpha}(x) = F_{\sigma,x}^{-1}(\alpha)$ and $q_\alpha(x) = F_x^{-1}(\alpha)$, so that we have the desired result $q_\alpha(x) \leq \liminf_{\sigma \to 0} q^\sigma_{\alpha}(x)$.

### A.2.2 Proof of Lemma A.2

We prove only the first inequality, as the last inequality is similar. Fix $u \in (0,1)$ and $\epsilon > 0$. $F$ is right-continuous and non-decreasing, so its set of continuity points is dense in $\mathbb{R}$; thus, there exists a continuity point $w$ of $F$ such that $w < F^{-1}(u) \leq w + \epsilon$.

Since $w < F^{-1}(u)$, it must hold that $F(w) < u$, by definition of $F^{-1}$. As $w$ is a continuity point of $F$, $\lim_{n \to \infty} F_n(w) = F(w) < u$, which means that $F_n(w) < u$ for large enough $n$, or equivalently, that $w < F_n^{-1}(u)$. We can thus conclude that

$$\liminf_{n \to \infty} F_n^{-1}(u) \geq w \geq F^{-1}(u) - \epsilon.$$

Taking $\epsilon \to 0$ proves the first inequality.

### A.3 Efficient computation of maximal marginals for condition (11)

We describe a more or less standard dynamic programming approach to efficiently compute the maximum marginals (15) (i.e. maximal values of a tree-structured score $s : Y = \{-1, 1\}^K \to \mathbb{R}$), referring to standard references on max-product message passing [7, 34, 19] for more. Let
$T = ([K], E)$ be a tree with nodes $[K]$ and undirected edges $E$, though we also let $\text{edges}(T)$ and $\text{nodes}(T)$ denote the edges and nodes of the tree $T$. Assume

$$s(y) = \sum_{k=1}^{K} \varphi_k(y_k) + \sum_{e=(k,l) \in E} \psi_e(y_k, y_l).$$

To compute the maximum marginals $\max_{y \in Y} \{s(y) \mid y_k = \hat{y}_k\}$, we perform two message passing steps on the tree: an upward and downward pass. Choose a node $r$ arbitrarily to be the root of $T$, and let $T_{\text{down}}$ be the directed tree whose edges are $E$ with $r$ as its root (which is evidently unique); let $T_{\text{up}}$ be the directed tree with all edges reversed from $T_{\text{down}}$.

A maximum marginal message passing algorithm then computes a single downward and a single upward pass through each tree, each in topological order of the tree. The downward messages $m_{l \rightarrow k} : \{-1,1\} \rightarrow \mathbb{R}$ are defined for $\hat{y} \in \{-1,1\}$ by

$$m_{l \rightarrow k}(\hat{y}) = \max_{y_i \in \{-1,1\}} \left\{ \varphi_l(y_l) + \psi_{l,k}(y_l, \hat{y}) + \sum_{e:(i \rightarrow l) \in \text{edges}(T_{\text{down}})} m_{i \rightarrow l}(y_i) \right\},$$

while the upward pass is defined similarly except that $T_{\text{up}}$ replaces $T_{\text{down}}$. After a single downward and upward pass through the tree, which takes time $O(K)$, the invariant of message passing on the tree [19, Ch. 13.3] then guarantees that for each $k \in [K]$,

$$\max_{y \in Y} \{s(y) \mid y_k = \hat{y}_k\} = \varphi_k(\hat{y}_k) + \sum_{e=(l,k) \in T} m_{l \rightarrow k}(\hat{y}_k), \tag{29}$$

where we note that there exists exactly one message to $k$ (whether from the downward or upward pass) from each node $l$ neighboring $k$ in $T$.

We can evidently then compute all of these maximal values (the sets $S_k$ in Eq. (15)) simultaneously in time of the order of the number of edges in the tree $T$, or $O(K)$, as each message $m_{l \rightarrow k}$ can appear in at most one of the maxima (29), and there are $2K$ messages.

### A.4 Concentration of coverage quantities

We sketch a derivation of inequality (22); see also [1, Theorem 5] for related arguments.

We begin with a technical lemma that is the basis for our result. In the lemma, we abuse notation briefly, and let $\mathcal{F} \subset \mathcal{Z} \rightarrow \{0,1\}$ be a collection of functions with VC-dimension $d$. We define $Pf = \int f(z) dP(z)$ and $P_n f = \frac{1}{n} \sum_{i=1}^{n} f(Z_i)$, as is standard.

**Lemma A.3** (Relative concentration bounds, e.g. [3], Theorem 5.1). Let $\text{VC}(\mathcal{F}) \leq d$. There is a numerical constant $C$ such that for any $t > 0$, with probability at least $1 - e^{-t}$,

$$\sup_{f \in \mathcal{F}} \left\{ |Pf - P_n f| - C \sqrt{\min \{Pf, P_n f\} \frac{d \log n + t}{n}} \right\} \leq C \frac{d \log n + t}{n}.$$

**Proof** By Boucheron et al. [3, Thm. 5.1] for $t > 0$, with probability at least $1 - e^{-t}$ we have

$$\sup_{f \in \mathcal{F}} \frac{Pf - P_n f}{\sqrt{Pf}} \leq C \sqrt{\frac{d \log n + t}{n}}$$

and

$$\sup_{f \in \mathcal{F}} \frac{P_n f - Pf}{\sqrt{P_n f}} \leq C \sqrt{\frac{d \log n + t}{n}}.$$
Let \( \varepsilon_n = C \sqrt{(d \log n + t)/n} \) for shorthand. Then the second inequality is equivalent to the statement that for all \( f \in \mathcal{F} \),

\[
P_n f - P f \leq \frac{1}{2\eta} P_n f + \frac{\eta \varepsilon_n^2}{2} \quad \text{for all } \eta > 0.
\]

Rearranging the preceding display, we have

\[
\left(1 - \frac{1}{2\eta}\right) (P_n f - P f) \leq \frac{1}{2\eta} P f + \frac{\eta \varepsilon_n^2}{2}.
\]

If \( \sqrt{P f} \geq \varepsilon_n \), we set \( \eta = \sqrt{P f}/\varepsilon_n \) and obtain

\[
\frac{1}{2} (P_n f - P f) \leq \frac{1}{2} (P f + \varepsilon_n^2) \leq \frac{1}{2} (\sqrt{P f} \varepsilon_n + \varepsilon_n^2).
\]

In either case,

\[
P_n f - P f \leq C \left[ \sqrt{P f \frac{d \log n + t}{n}} + \frac{d \log n + t}{n} \right].
\]

A symmetric argument replacing each \( P_n \) with \( P \) (and vice versa) gives the lemma.

We can now demonstrate inequality (22). Let \( V \subset \mathbb{R}^d \) and \( \mathcal{V} := \{ \{ x \in \mathbb{R}^d \mid v^T x \leq 0 \} \}_{v \in \mathcal{V}} \) the collection of halfspaces it induces. The collection \( S = \{ S_{v,a,b} \}_{v \in \mathcal{V}, a < b} \) of slabs has VC-dimension \( \text{VC}(S) \leq O(1) \text{VC}(\mathcal{V}) \). Let \( f : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \) and \( c : S \to \mathbb{R} \) be arbitrary functions. If for \( S \subset \mathcal{X} \) we define \( S^+ := \{ (x,y) \mid x \in S, f(x,y) \geq c(S) \} \) and the collection \( S^+ := \{ S^+ \mid S \in S \} \), then \( \text{VC}(S^+) \leq \text{VC}(S) + 1 \) [1, Lemma 5]. As a consequence, for the conformal sets inequality (22) specifies, for any \( t > 0 \) we have with probability at least 1 \( - e^{-t} \) that

\[
\left| P_n(Y \in \hat{C}(X), X \in S_{v,a,b}) - P(Y \in \hat{C}(X), X \in S_{v,a,b}) \right| \leq O(1) \left[ \sqrt{\min\{P(Y \in \hat{C}(X), X \in S_{v,a,b}), P_n(Y \in \hat{C}(X), X \in S_{v,a,b})\} \frac{\text{VC}(\mathcal{V}) \log n + t}{n} + \frac{\text{VC}(\mathcal{V}) \log n + t}{n}} \right]
\]

simultaneously for all \( v \in V, a < b \in \mathbb{R} \), and similarly

\[
\left| P_n(X \in S_{v,a,b}) - P(X \in S_{v,a,b}) \right| \leq O(1) \left[ \sqrt{\min\{P(X \in S_{v,a,b}), P_n(X \in S_{v,a,b})\} \frac{\text{VC}(\mathcal{V}) \log n + t}{n} + \frac{\text{VC}(\mathcal{V}) \log n + t}{n}} \right].
\]

Now, we use the following simple observation. For any \( \varepsilon \) and nonnegative \( \alpha, \beta, \gamma \) with \( \alpha \leq \gamma \) and \( 2|\varepsilon| \leq \gamma \),

\[
\left| \frac{\alpha}{\gamma + \varepsilon} - \frac{\beta}{\gamma} \right| \leq \frac{|\alpha - \beta|}{\gamma} + \frac{|\alpha|}{\gamma} \frac{2|\varepsilon|}{\gamma^2 + \gamma \varepsilon} \leq \frac{|\alpha - \beta|}{\gamma} + \frac{2|\varepsilon|}{\gamma}.
\]

Thus, as soon as \( \delta \geq \frac{\text{VC}(\mathcal{V}) \log n + t}{\min n} \), we have with probability at least 1 \( - e^{-t} \) that

\[
\left| P_n(Y \in \hat{C}(X) \mid X \in S_{v,a,b}) - P(Y \in \hat{C}(X) \mid X \in S_{v,a,b}) \right| = \left| \frac{P_n(Y \in \hat{C}(X), X \in S_{v,a,b})}{P_n(X \in S_{v,a,b})} - \frac{P(Y \in \hat{C}(X), X \in S_{v,a,b})}{P(X \in S_{v,a,b})} \right| \leq O(1) \left[ \sqrt{\frac{\text{VC}(\mathcal{V}) \log n + t}{\delta n}} + \frac{\text{VC}(\mathcal{V}) \log n + t}{\delta n} \right]
\]
simultaneously for all $v \in V, a < b \in \mathbb{R}$, where we substitute $\gamma = P(X \in S_{v,a,b})$, $\alpha = P(Y \in \hat{C}(X), X \in S_{v,a,b})$, $\beta = P_n(Y \in \hat{C}(X), X \in S_{v,a,b})$, and $\varepsilon = (P_n - P)(X \in S_{v,a,b})$. Note that if $\frac{\text{VC}(V) \log n + t}{\delta n} \geq 1$, the bound is vacuous in any case.