Stable Conformal Prediction Sets

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Abstract

When one observes a sequence of variables \((x_1, y_1), \ldots, (x_n, y_n)\), conformal prediction is a methodology that allows to estimate a confidence set for \(y_{n+1}\) given \(x_{n+1}\) by merely assuming that the distribution of the data is exchangeable. While appealing, the computation of such set turns out to be infeasible in general, e.g., when the unknown variable \(y_{n+1}\) is continuous. In this paper, we combine conformal prediction techniques with algorithmic stability bounds to derive a prediction set computable with a single model fit. We perform some numerical experiments that illustrate the tightness of our estimation when the sample size is sufficiently large.

1 Introduction

In several situations, modern machine learning algorithms can predict an object based on its observed characteristics with impressive accuracy. By nature, these algorithms are often trained on historical datasets sampled from the same distribution and it is important to quantify the uncertainty of their predictions. Conformal prediction is a versatile and simple method introduced in [26, 24] that provides a finite sample and distribution free 100\((1 - \alpha)\)% confidence region on the predicted object based on past observations. It has been applied for designing uncertainty sets in active learning [12], anomaly detection [14, 2], few shot learning [8], time series [5, 27, 6] or to infer the performance guarantee for statistical learning algorithms [13, 4]. We refer to the extensive reviews in [1] for other applications to artificial intelligence.

Despite its nice properties, the computation of conformal prediction sets requires to fit a model on a dataset where the unknown quantity is replaced by a set of candidates. In regression setting where an object can take an uncountable possible value, the set of candidates is infinite. Therefore, in general, computing conformal prediction is infeasible without additional structural assumptions on the underlying model fit. And even so, the calculation costs remain high.

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Contribution. We leverage algorithmic stability to bound the variation of the model w.r.t. changes in the input data. As such, we can provide a tight estimation of the confidence sets without any loss in the coverage guarantee. Our method is computationally efficient since it requires only a single model fit.

Notation. For a nonzero integer $n$, we denote $[n]$ to be the set $\{1, \cdots, n\}$. The dataset of size $n$ is denoted $D_n = (x_i, y_i)_{i \in [n]}$, the row-wise feature matrix $X = [x_1, \cdots, x_n, x_{n+1}]^T$. Given a set $\{u_1, \cdots, u_n\}$, the rank of $u_j$ for $j \in [n]$ is defined as $\text{Rank}(u_j) = \sum_{i=1}^{n} 1_{u_i \leq u_j}$. We denote $u(i)$ the $i$-th order statistics.

2 Conformal Prediction

Conformal prediction [26] is a framework for constructing confidence sets, with the remarkable properties of being distribution free, having a finite sample coverage guarantee, and being able to be adapted to any estimator under mild assumptions. We recall the arguments in [24, 16] to construct a typicalness function based on rank statistics that yields to distribution-free inference methods. The main tool is that the rank of one variable among an exchangeable and identically distributed sequence follows a (sub)-uniform distribution [3].

Lemma 1. Let $U_1, \ldots, U_n, U_{n+1}$ be exchangeable and identically distributed sequence of random variables. Then for any $\alpha \in (0, 1)$, we have

$$\mathbb{P}^{n+1}(\text{Rank}(U_{n+1}) \leq (n + 1)(1 - \alpha)) \geq 1 - \alpha.$$ 

We remind that $y_{n+1}$ is the unknown target variable. We introduce a learning problem with augmented training data $D_{n+1}(z) := D_n \cup \{(x_{n+1}, z)\}$ for $z \in \mathbb{R}$ and with the augmented label $y(z) = (y_1, \cdots, y_n, z)$:

$$\beta(z) \in \arg \min_{\beta \in \mathbb{R}^p} \mathcal{L}(y(z), \Phi(X, \beta)) + \Omega(\beta),$$

where $\Phi$ is a feature map. Given a feature vector $x$, a prediction model can be defined as $\mu_z(x) := \Phi(x, \beta(z))$. For example in case of empirical risk minimization, we have $\mathcal{L}(y(z), \Phi(X, \beta)) = \sum_{i=1}^{n} \ell(y_i, \Phi(x_i, \beta)) + \ell(z, \Phi(x_{n+1}, \beta))$.

Let us define the conformity measure for $D_{n+1}(z)$ as

$$\forall i \in [n], E_i(z) = S(y_i, \mu_z(x_i)) \text{ and } E_{n+1}(z) = S(z, \mu_z(x_{n+1})),$$

where $S$ is a real-valued function e.g., in a linear regression problem, one can take $s(a, b) = |a - b|$. The main idea for constructing a conformal confidence set is to consider the typicalness/conformity of a candidate point $z$ measured as

$$\pi(z) := 1 - \frac{1}{n + 1}\text{Rank}(E_{n+1}(z)).$$
The conformal set gathers the real value \( z \) such that \( \pi(z) \geq \alpha \), if and only if \( E_n(z) \) is ranked no higher than \( \lceil (n+1)(1-\alpha) \rceil \), among \( \{ E_i(z) \}_{i \in [n+1]} \), i.e.,

\[
\Gamma^{(\alpha)}(x_{n+1}) := \{ z \in \mathbb{R} : \pi(z) \geq \alpha \} .
\] (4)

A direct application of Lemma 1 to \( U_i = E_i(y_{n+1}) \) reads \( \mathbb{P}(\pi(y_{n+1}) \leq \alpha) \leq \alpha \), i.e., the random variable \( \pi(y_{n+1}) \) takes small values with small probability and

\[
\mathbb{P}(y_{n+1} \in \Gamma^{(\alpha)}(x_{n+1})) \geq 1 - \alpha .
\]

### 2.1 Computational Limitations and Previous Works

For regression problems where \( y_{n+1} \) lies in a subset of \( \mathbb{R} \), obtaining the conformal set \( \Gamma^{(\alpha)}(x_{n+1}) \) in Equation (4) is computationally challenging. It requires re-fitting the prediction model \( \beta(z) \) for infinitely many candidates \( z \) in order to compute a conformity measure such as \( E_i(z) = |y_i - x_i^\top \beta(z)| \). Except for few examples, the computation of conformal prediction set is infeasible in general.

In Ridge regression, for any \( x \) in \( \mathbb{R}^p \), \( z \mapsto x^\top \beta(z) \) is a linear function of \( z \), implying that \( E_i(z) \) is piecewise linear. Exploiting this fact, an exact conformal set \( \Gamma^{(\alpha)}(x_{n+1}) \) for Ridge regression was efficiently constructed in [20]. Similarly, using the piecewise linearity w.r.t. sparsity level of the Lasso path provided by the Lars algorithm [7], [10] builds a sequence of conformal sets for the Lasso associated to the transition points of the Lars with the observed data \( D_n \). Nevertheless, such procedure breaks the proof technique for the coverage guarantee as the exchangeability of the sequence \( \{ E_i(y_{n+1}) \}_{i \in [n+1]} \) is not necessarily maintained. However, a slight adaptation can fix the previous problem. Indeed using the piecewise linearity in \( z \) of the Lasso solution, [15] proposed a piecewise linear homotopy under mild assumptions, when a single input sample point is perturbed. This finally allows to compute the whole solution path \( z \mapsto \beta(z) \) and successfully provides a conformal set for the Lasso and Elastic Net. Later, [18] proposed an adaptation of approximate the solution path [17], by carefully discretizing the set of candidate restricted into a compact \( [z_{\min}, z_{\max}] \). Assuming the optimization problem in Equation (1) is convex and that the loss function is smooth, this leads to a computational complexity of \( O(1/\sqrt{\epsilon}) \) where \( \epsilon > 0 \) is a prescribed optimization error. A different road is to assume the conformal set \( \Gamma^{(\alpha)}(x_{n+1}) \) in Equation (4) itself is a bounded interval. As such, its endpoints can be estimated by approximating the roots of the function \( z \mapsto \pi(z) - \alpha \). A direct bisection search can then compute a conformal set with a complexity of \( O(\log_2(1/\epsilon_r)) \) [19] where \( \epsilon_r > 0 \) is the tolerance error w.r.t. to exact root.

In this paper, we actually show that a single model fit is enough to tightly approximate the conformal set when the underlying model fitting is stable.
Figure 1: Illustration of the evolution of the conformity function as a function of sample size. The underlying model fit is $\beta(z) \in \arg \min_{\beta \in \mathbb{R}^p} \| y(z) - X\beta \|_1 / (n + 1) + \lambda \| \beta \|^2$ where $y(z) = (y_1, \cdots, y_n, z)$ and we use sklearn synthetic dataset make_regression($n, p = 100, \text{noise} = 1$). We fixed $\hat{z} = 0$ and $\lambda = 0.5$. The set $Z$ is a linear grid in the interval $[y(1), y(n)]$. 

\(\text{(a) } n = 30\) 

\(\text{(b) } n = 90\) 

\(\text{(c) } n = 300\) 

\(\text{(d) } \text{Convergence of the approximation gap } \sup_{z \in Z} \text{Gap}(z, \hat{z}) := \pi_{\text{up}}(z, \hat{z}) - \pi_{\text{lo}}(z, \hat{z})\).
where, we define, for any index \( i \) the conformal prediction set is lower and upper approximated as

\[
\pi
\]

**Corollary 1** (Stable Conformal Sets) \( \Rightarrow \)

3 Approximation via Algorithmic Stability

The Section 2 guarantee that \( \pi(y_{n+1}) \geq \alpha \) with high probability. Since \( y_{n+1} \) is unknown, the conformal set just selects all \( z \) that satisfies the same inequality \( i.e., \Gamma^{(\alpha)}(x_{n+1}) = \{ z : \pi(z) \geq \alpha \} \). This leads to fitting a new model for any \( z \). Here, we take a different strategy. The main remark is that only one element of the dataset changes at a time, then with mild stability assumptions, one can expect that the model prediction will not change drastically. Instead of inverting \( \pi(\cdot) \), we will bound it with quantities independent of the model fit \( \mu_z \) for any \( z \).

**Definition 1** (Algorithmic Stability). A prediction function \( \mu \) is stable if for any observed features \( x_i, i \in [n+1] \), we have

\[
|S(q, \mu_z(x_i)) - S(q, \mu_{\hat{z}}(x_i))| \leq \tau_i \quad \forall z, \hat{z}, q.
\]  

(5)

**Proposition 1.** Assume that the model fit \( \mu \) is stable. Then, we have:

\[
\forall z, \hat{z}, \quad \pi_{\text{lo}}(z, \hat{z}) \leq \pi(z) \leq \pi_{\text{up}}(z, \hat{z}),
\]

with

\[
\pi_{\text{lo}}(z, \hat{z}) := 1 - \frac{1}{n+1} \sum_{i=1}^{n+1} 1_{L_i(z, \hat{z}) \leq U_{n+1}(z, \hat{z})},
\]

\[
\pi_{\text{up}}(z, \hat{z}) := 1 - \frac{1}{n+1} \sum_{i=1}^{n+1} 1_{U_i(z, \hat{z}) \leq L_{n+1}(z, \hat{z})},
\]

where, we define, for any index \( i \) in \([n]\),

\[
L_i(z, \hat{z}) = E_i(\hat{z}) - \tau_i \quad \text{and} \quad L_{n+1}(z, \hat{z}) = S(z, \mu_{\hat{z}}(x_{n+1})) - \tau_{n+1},
\]

\[
U_i(z, \hat{z}) = E_i(\hat{z}) + \tau_i \quad \text{and} \quad U_{n+1}(z, \hat{z}) = S(z, \mu_{\hat{z}}(x_{n+1})) + \tau_{n+1}.
\]

**Proof.** By stability, for any \( q \), we have:

\[
|S(q, \mu_z(x_i)) - S(q, \mu_{\hat{z}}(x_i))| \leq \tau_i.
\]

Applying the previous inequality to \( q = y_i \) for any index \( i \) in \([n+1]\), we have \( L_i(z, \hat{z}) \leq E_i(z) \leq U_i(z, \hat{z}) \) and it holds:

\[
U_i(z, \hat{z}) \leq L_{n+1}(z, \hat{z}) \Rightarrow E_i(z) \leq E_{n+1}(z) \Rightarrow L_i(z, \hat{z}) \leq U_{n+1}(z, \hat{z}).
\]

(6)

Taking the indicator of the corresponding sets, we obtain the result. \( \square \)

**Corollary 1** (Stable Conformal Sets). Under the assumption of Proposition 2, the conformal prediction set is lower and upper approximated as

\[
\Gamma^{(\alpha)}_{\text{lo}}(x_{n+1}) \subset \Gamma^{(\alpha)}(x_{n+1}) \subset \Gamma^{(\alpha)}_{\text{up}}(x_{n+1}),
\]

where \( \Gamma^{(\alpha)}_{\text{lo}}(x_{n+1}) = \{ z : \pi_{\text{lo}}(z, \hat{z}) > \alpha \} \) and \( \Gamma^{(\alpha)}_{\text{up}}(x_{n+1}) = \{ z : \pi_{\text{up}}(z, \hat{z}) > \alpha \} \).
Figure 2: Illustration of the approximation for different values of \( \hat{z} \). We use the same setting as in Figure 1.

**Tighter approximation.** The stable conformal sets require a single model fit \( \mu_z \) for an arbitrary candidate \( \hat{z} \). The approximation gaps are computable as

\[
\max \{ \pi(z) - \pi_{\text{lo}}(z, \hat{z}), \pi_{\text{up}}(z, \hat{z}) - \pi(z) \} \leq \pi_{\text{up}}(z, \hat{z}) - \pi_{\text{lo}}(z, \hat{z}) .
\]

Since the above upper and lower bounds hold for any \( \hat{z} \), tighter approximations are obtained with a batch of candidate \( Z = \hat{z}_1, \ldots, \hat{z}_d \) as

\[
\pi_{\text{up}}(z, Z) = \inf_{z \in Z} \pi_{\text{up}}(z, \hat{z}) \quad \text{and} \quad \pi_{\text{lo}}(z, Z) = \sup_{z \in Z} \pi_{\text{lo}}(z, \hat{z}) .
\]

Another possibility is to build an interpolation of \( z \mapsto \mu_z(\cdot) \) based on query points \( \hat{z}_1, \ldots, \hat{z}_d \). For example let us consider the following linear interpolation

\[
\hat{\mu}_z = \begin{cases} 
\frac{z - z_{\min}}{z_{1} - z_{\min}} \mu_{z_{1}} + \frac{z_{\min} - z}{z_{1} - z_{\min}} \mu_{z_{1+1}} & \text{if } z \leq z_{\min} , \\
\frac{z - z_{\min}}{z_{t-1} - z_{t+1}} \mu_{z_{t-1}} + \frac{z_{t-1} - z}{z_{t} - z_{t+1}} \mu_{z_{t+1}} & \text{if } z \in [z_{t-1}, z_{t+1}] , \\
\frac{z - z_{\min}}{z_{\max} - z_{\min}} \mu_{z_{\max}} + \frac{z_{\max} - z}{z_{\max} - z_{\min}} \mu_{z_{d}} & \text{if } z \geq z_{\max} , 
\end{cases}
\]

Then \( \hat{\mu} \) preserve the stability while providing a better approximation. Indeed

\[
|\mu_z(x_i) - \hat{\mu}_z(x_i)| \leq |\mu_z(x_i) - \alpha_t \mu_{z_{1}}(x_i) - (1 - \alpha_t) \mu_{z_{t+1}}(x_i)| \\
\leq \alpha_t |\mu_z(x_i) - \mu_{z_{1}}(x_i)| + (1 - \alpha_t) |\mu_z(x_i) - \mu_{z_{t+1}}(x_i)| \\
\leq \alpha_t \tau_i + (1 - \alpha_t) \tau_i = \tau_i ,
\]

where \( \alpha_t \in \left\{ \frac{z_{1} - z}{z_{1} - z_{\min}}, \frac{z_{t-1} - z_{t+1}}{z_{t-1} - z_{t+1}}, \frac{z - z_{\min}}{z_{\max} - z_{\min}} \right\} \). An important point is that, by using the stability bound, the coverage guarantee of the interpolated conformal set is preserved without the need of the potential expensive symmetrization proposed in [19]. Such techniques are more relevant when the sample size is small. The upper and lower approximation of the conformity function obtained with the
interpolated model fit along with stability bounds are defined as:
\[ \tilde{\pi}_{lo}(z) = 1 - \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{I}_{L_i(z) \leq U_{n+1}(z)}, \]
\[ \tilde{\pi}_{up}(z) = 1 - \frac{1}{n+1} \sum_{i=1}^{n+1} \mathbb{I}_{U_i(z) \leq L_{n+1}(z)}, \]
where for any index \( i \) in \([n+1]\),
\[ \tilde{L}_i(z) = \tilde{E}_i(z) - \tau_i \quad \text{and} \quad \tilde{U}_i(z) = \tilde{E}_i(z) + \tau_i \]
\[ \tilde{E}_i(z) = S(y_i, \tilde{\mu}_z(x_i)) \quad \text{and} \quad \tilde{E}_{n+1}(z) = S(z, \tilde{\mu}_z(x)) \] .

3.1 Stability Bounds
In this section, we recall some stability bounds. The proof techniques rely on regularity assumptions on the function to be minimized and are relatively standard in optimization [25, Chapter 13]. Stability is a widely used assumption to provide generalization bounds for machine learning algorithms [21, 9]. We specify that here the notion of stability that we ask is related to the variation of the score and not of the loss function in the optimization objective. However, the ideas for establishing the stability bounds are essentially the same and we recall them here for the sake of completeness.

Let us start with the unregularized model where \( \Omega = 0 \) i.e.,
\[ \beta(z) \in \arg \min_{\beta \in \mathbb{R}^p} \mathcal{L}(y(z), \Phi(X, \beta)) = F_z(\Phi(X, \beta)) . \]  
(8)

**Definition 2.** A function \( f \) is \( \lambda \)-strongly convex if for any \( w_0, w \) and \( \alpha \in (0, 1) \)
\[ f(\alpha w_0 + (1-\alpha)w) \leq \alpha f(w_0) + (1-\alpha)f(w) - \frac{\lambda}{2} \alpha (1-\alpha) \|w_0 - w\|^2 . \]  
(9)

**Proposition 2.** Assume that for any \( z \), \( F_z \) is \( \lambda \)-strongly convex and \( \rho \)-Lipschitz. It holds
\[ \|\mu_z(X) - \mu_{z_0}(X)\| \leq \frac{2\rho}{\lambda} . \]

**Proof.** By optimality of \( \beta(z) \), we have
\[ F_z(\Phi(X, \beta(z))) \leq F_z(\Phi(X, \beta)) \quad \forall \beta . \]  
(10)
By strong convexity of \( F_z \), for \( w_0 = \Phi(X, \beta(z_0)) \) and \( w = \Phi(X, \beta(z)) \), it holds
\[ 0 \leq \frac{F_z(\alpha w_0 + (1-\alpha)w) - F_z(w)}{\alpha} \]
\[ \geq F_z(w_0) - F_z(w) - \frac{\lambda}{2} (1-\alpha) \|w_0 - w\|^2 . \]
Since $F_z$ is $\rho$-Lipschitz, we have

$$\frac{\lambda}{2} \|w_0 - w\|^2 \leq F_z(w_0) - F_z(w) \leq \rho \|w - w_0\|.$$

We remind that, $w_0 = \Phi(X, \beta(z_0)) = \mu_{z_0}(X)$ and $w = \Phi(X, \beta(z)) = \mu_z(X)$. Therefore, $\frac{\lambda}{2} \|\mu_z(X) - \mu_{z_0}(X)\| \leq \rho$. \hfill $\square$

The Proposition 2 does not assume that the optimization problem in Equation (8) is convex in the model parameter $\beta$. We can now easily deduce a stability bound according to the Definition 1.

**Corollary 2.** If the score function $S(q, \cdot)$ is $\gamma$-Lipschitz for any $q$, then

$$\tau_i = \frac{2\gamma \rho}{\lambda}, \quad \forall i \in [n+1].$$

When the loss function is not strongly convex, it is known that adding a strongly convex regularization can stabilize the algorithm [25, Chapter 13]. The proof technique is similar to the previous one with the difference that now the bound is on the arg min of the optimization problem and not the predictions of the model. This requires stronger assumptions.

**Proposition 3.** Assume the optimization problem Equation (11) is convex, $\Omega$ is $\lambda$-strongly convex. If the loss $\mathcal{L}$ is convex-$\rho$-Lipschitz, then

$$\|\beta(z) - \beta(z_0)\| \leq \frac{2\rho}{\lambda}.$$

When $\mathcal{L}$ is convex-$\nu$-smooth with $\nu < \lambda$ and $\mathcal{L}(y(z), \mu_z(X)) \leq C$ for any $z$, then

$$\|\beta(z) - \beta(z_0)\| \leq \frac{2\sqrt{2\nu C}}{\lambda - \nu}.$$

These optimization error bounds also implies the following stability bounds.

**Corollary 3.** Assume that the score function $S(q, \cdot)$ is $\gamma$-Lipschitz for any $q$, and the prediction model $\mu_\cdot(x) := \Phi(x, \beta(\cdot))$ satisfies:

$$|\mu_z(x) - \mu_{z_0}(x)| \leq L\Phi|x^\top \beta(z) - x^\top \beta(z_0)| \quad \forall x \in \mathbb{R}^p, \ z, z_0 \in \mathbb{R}.$$

If the loss is $\rho$-Lipschitz, then $\tau_i = \frac{2\gamma \rho L\Phi \|x_i\|}{\lambda}$. If the loss is $\nu$-smooth with $\nu < \lambda$ and bounded by $C$, then $\tau_i = \frac{2\gamma \rho L\Phi \|x_i\| \sqrt{2C}}{\lambda - \nu}$.

Another way to understand such regularized bounds, is to leverage duality. A smoothness assumption in the primal space will translate into a strongly concave assumption in the dual space [11, Theorem 4.2.2, p. 83]. The dual formulation [23, Chapter 31] of Equation (11) reads:

$$\theta(z) \in \arg \max_{\theta \in \mathbb{R}^{n+1}} -\mathcal{L}^*(y(z), -\theta) - \Omega^*(X^\top \theta),$$

\[11\]
where, given a proper, closed and convex function \( f : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\} \), we denoted its Fenchel-Legendre transform as \( f^* : \mathbb{R}^n \to \mathbb{R} \cup \{+\infty\} \) defined by 
\[
\sup_{x \in \text{dom } f} f(x^*) = f^*(x^*) = \sup_{x \in \text{dom } f} f(x^*) - f(x)
\]
with \( \text{dom } f = \{x \in \mathbb{R}^n : f(x) < +\infty\} \).

Let \( P_z \) and \( D_z \) denote the primal and dual objective functions. We have the following classical error bounds for the dual optimization problem. If the loss function \( L \) is \( \nu \)-smooth, then \( L^* \) is \( 1/\nu \)-strongly convex and we have for \( \forall (\beta, \theta) \in \text{dom } P_z \times \text{dom } D_z \)
\[
\|\theta(z) - \theta\|_2^2 \leq 2\nu(D_z(\theta(z)) - D_z(\theta)) \leq 2\nu \text{Gap}_z(\beta, \theta),
\]
where the last inequality follows from weak duality. This readily leads to several possible bounds. If the dual function \( D_z(\cdot) \) is \( \rho^* \)-Lipschitz for any \( z \), then \( \|\theta(z) - \theta\| \leq 2\nu \rho^* \). If the duality gap can be assumed to be bounded by \( C \) for any \( z \in [z_{\min}, z_{\max}] \), then \( \|\theta(z) - \theta\| \leq \sqrt{2\nu C} \). We obtain stability bounds when one uses a the dual solution (the residual) as a conformity score 
\[
S(y(z), \mu_{y_{n+1}}(X)) = |\theta(z)| \text{ where the absolute value is taken coordinate wise.}
\]

4 Numerical Experiments

We conduct all the experiments with a coverage level of 0.9 i.e., \( \alpha = 0.1 \). For comparisons, we run the evaluations on 100 repetitions of examples and display the average of the following performance statistics for different methods: the empirical coverage i.e., the percentage of times the prediction set contains the held-out target \( y_{n+1} \), the length of the confidence intervals, and the execution time. We compare the method we propose \( \text{stabCP} \) with the conformal prediction set computed with an oracle method defined below, with a splitting strategy \( \text{splitCP} \) \([22, 16]\), and finally with an estimation of the \( \alpha \)-level set of the conformity function \( \text{rootCP} \) \([19]\) by root-finding solvers. Note that, when the conformal set is a bounded interval, \( \text{stabCP} \) approximates \( \text{rootCP} \) as in Figure 1 and Figure 2. In all experiments conducted, we observed that the exact conformal prediction set is indeed an interval (although this is often the case, we recall that it might not be in general). For simplicity, we therefore estimated the \( \text{stabCP} \) sets with a root-finding solver as well.

\( \text{oracleCP} \). To define an oracle prediction set as reference, we follow in \([18, 19]\) and assume that the unavailable target variable \( y_{n+1} \) is observed by the algorithm. Hence, we define the oracle scores
\[
\forall i \in [n], \quad E^\text{or}_i = S(y_i, \mu_{y_{n+1}}(x_i)), \quad \text{and} \quad E^\text{or}_{n+1}(z) = S(z, \mu_{y_{n+1}}(x_{n+1})),
\]
Figure 3: Benchmarking conformal sets for the least absolute deviation regression models with a ridge regularization on real datasets. We display the lengths of the confidence sets over 100 random permutation of the data. We denoted $\overline{\text{cov}}$ the average coverage and $\overline{T}$ the average computational time normalized with the average time for computing oracleCP which requires a single model fit on the whole data.
and the oracle conformal set as
\[ \Gamma_{\text{oracle}}^{(\alpha)}(x_{n+1}) := \{ z : \pi_{\text{oracle}}(z) \geq \alpha \} , \]
\[ \pi_{\text{oracle}}(z) = 1 - \frac{1}{n+1} \sum_{i=1}^{n+1} I_{E_{or}^i \leq E_{or}^{n+1}(z)} . \]

splitCP. A popular and classical estimation of conformal prediction set relies on splitting the dataset. The split conformal prediction set introduced in \cite{22}, separates the model fitting and the calibration steps. Let us define
- the training set \( D_{\text{tr}} = \{(x_1, y_1), \ldots, (x_m, y_m)\} \) with \( m < n \),
- the calibration set \( D_{\text{cal}} = \{(x_{m+1}, y_{m+1}), \ldots, (x_n, y_n)\} \).

Then the model is fitted on the training set \( D_{\text{tr}} \) to get \( \mu_{\text{tr}}(\cdot) \) and define the score function on the calibration set \( D_{\text{cal}} \):
\[ \forall i \in [m+1, n], \quad E_{i}^{\text{cal}} = S(y_i, \mu_{\text{tr}}(x_i)), \quad \text{and} \quad E_{n+1}^{\text{cal}}(z) = S(z, \mu_{\text{tr}}(x_{n+1})). \]

Thus, we obtain the split conformal set as
\[ \Gamma_{\text{split}}^{(\alpha)}(x_{n+1}) = \{ z : \pi_{\text{split}}(z) \geq \alpha \} , \]
\[ \pi_{\text{split}}(z) = 1 - \frac{1}{n-m+1} \sum_{i=m+1}^{n+1} I_{E_{i}^{\text{cal}} \leq E_{n+1}^{\text{cal}}(z)} . \]

Discussion. The data splitting approach does not use all the data in the training phase. It is often less statistically efficient, and its interval length can vary greatly depending on the additional randomness of the split. On the contrary, our approach does not use any splitting, provides an approximation of the exact conformal set that is pretty accurate depending on the stability of the model as can be observed on Figure 3. All this requires one and only one data fitting of the underlying learning model. To date, we are not aware of any other method that can obtain a full conformal prediction set with such computational efficiency while ensuring no loss on the coverage guarantee.

However, as can be seen in Figure 4, our proposed method loses precision when the sample size is small. This reflects the difficulty of estimating a reliable confidence set in the absence of algorithmic stability.

Finally, a notorious limitation is that one needs to know explicitly the stability bounds. This can be difficult to estimate for some models. The bounds we presented in Section 3.1 cover a wide range of examples but remain limited when the regression model is not as defined as an arg min of an optimization objective. The splitting strategy remains more flexible. It would be interesting to study fine combinations of data splitting and inclusion of stability bounds to reduce the size of the confidence intervals and their variance.
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