Conformal prediction with localization

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Abstract

We propose a new method called localized conformal prediction, where we can perform conformal inference using only a local region around a new test sample to construct its confidence interval. Localized conformal inference is a natural extension to conformal inference to the setting where we want to perform conformal inference adaptively. We prove that our proposal can also have assumption-free and finite sample coverage guarantees, and we compare the behaviors of localized conformal inference and conformal inference in simulations.

To our knowledge, this is the first work that generalizes the method of conformal prediction to the case where we can break the data exchangeability, so as to give the test sample a special role.

1 Introduction

Let \( Z_i := (X_i, Y_i) \in \mathbb{R}^p \times \mathbb{R} \) for \( i = 1, \ldots, n \) be i.i.d regression data from some distribution \( \mathcal{P} \). Let \( Z_{n+1} = (X_{n+1}, Y_{n+1}) \) be a new test sample with its response \( Y_{n+1} \) unobserved. Given a nominal coverage level \( \alpha \), we are interested in constructing confidence intervals (CI) \( \hat{C}(x) \), indexed by \( x \in \mathbb{R}^p \), such that

\[
P(\hat{Y}_{n+1} \in \hat{C}(X_{n+1})) \geq \alpha, \quad \forall \mathcal{P}.
\]

The conformal inference is a framework for constructing \( \hat{C}(x) \) satisfying eq. (1), assuming only that \( Z_{n+1} \) also comes from \( \mathcal{P} \) \cite{Vovk2005, Shafer2008, Vovk2009, Lei2014, Lei2018}.

Conformal inference constructs CI based on a score function \( V : \mathbb{R}^p \times \mathbb{R} \rightarrow [0, \infty) \). The score function measures how unlikely a sample is from distribution \( \mathcal{P} \), and is constructed in a way such that \( V_i = V(Z_i) \) are exchangeable with each other for \( i = 1, \ldots, n + 1 \). By exchangeability, we know \( \mathbb{P} \{ V_{n+1} \leq Q(\alpha; V_{1:n} \cup \{ \infty \}) \} \geq \alpha, \quad \forall \mathcal{P} \).

\[
P \{ V_{n+1} \leq Q(\alpha; V_{1:n} \cup \{ \infty \}) \} \geq \alpha, \quad \forall \mathcal{P}.
\]

where \( Q(\alpha; V_{1:n} \cup \{ \infty \}) \) is the level \( \alpha \) quantile of the empirical distribution of \( \{ V_1, \ldots, V_n, \infty \} \). Although the construction of \( V \) can also be data-dependent, for illustration purposes, let’s first consider a data-independent \( V(x, y) = |y - \mu(x)| \) where \( \mu(x) \) is a fixed prediction function for the response \( y \in \mathbb{R} \) at \( x \in \mathbb{R}^p \).

To decide whether any value \( y \) is included in \( \hat{C}(X_{n+1}) \), conformal inference tests the null hypothesis that \( Y_{n+1} = y \) based on eq. (2), and includes \( y \) in \( \hat{C}(X_{n+1}) \) if \( V(z_{n+1}) \leq Q(\alpha; V_{1:n} \cup \infty) \), where \( z_{n+1} = (X_{n+1}, y) \).

While it is good to have an almost assumption-free CI, the conformal inference CI for \( V_{n+1} \) treats all training samples equally, regardless their distance to \( X_{n+1} \). However, in some cases, we may want to emphasize more a local region around \( X_{n+1} \). Such a localized approach is especially desirable when the distribution of \( V(Z_{n+1}) \) is heterogeneous across different values for \( X_{n+1} \). Consider the example \( Y_i = X_i + \varepsilon_i \) with \( \varepsilon_i | X_i \sim \frac{|X_i|}{|X_i|+1} N(0,1) \), and \( X_i \sim Unif(-2,2) \) for \( i = 1, 2, \ldots, n + 1 \). We construct the CI for \( Y_{n+1} \) by applying conformal inference to the score function \( V(x, y) = |x - y| \). Figure 1 shows the conformal confidence band using 1000 training samples (blue curves) and the underlying true confidence band (black curves) at level \( \alpha = .95 \). The conformal confidence band lacks heterogeneity because it has treated all training samples equally for all test sample observations.

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In this paper, we propose a novel approach to build CI using localized conformal inference, which allows for decision rules that may depend on $X_{n+1}$. The main idea is to introduce a localizer around $X_{n+1}$, and up-weight samples close to $X_{n+1}$ according to the localizer. For example, consider a localizer

$$H(X_i) = \begin{cases} 1 & \text{if } X_i \text{ is among the 100 nearest neighbors of } X_{n+1} \\ 0 & \text{otherwise} \end{cases}.$$ 

We include the response value $y$ in $\hat{C}(X_{n+1})$ if and only if $V(z_{n+1})$ is smaller than the $\tilde{\alpha}$ quantile of a weighted empirical distribution, where we assign weight $\frac{H(X_i)}{\sum_{j=1}^{n} H(X_j)}$ to $Y_i$ for $i = 1, \ldots, n$ and weight $\frac{H(X_{n+1})}{\sum_{j=1}^{n+1} H(X_j)}$ to $\infty$. We show that we can choose $\tilde{\alpha}$ strategically such that we have finite sample coverage as described in eq. (1). In Figure 1, the red curve is the confidence band using the localized conformal inference with the nearest neighbor localizer $H$ that we have just described. We can see that it does capture the heterogeneity of the underlying truth much better than the conformal confidence band. Performing conformal inference while emphasizing the special role of $X_{n+1}$ is an interesting problem, and to our knowledge, this is the first method providing a theoretical guarantee.

The paper is organized as follows. In Section 2, we give a brief summary of some related work in applying conformal inference to achieve local coverage. In Section 3, we introduce the idea of localized conformal prediction, focusing on the case where we have a fixed score function with i.i.d generated training and test samples. We provide simulation results comparing localized conformal inference and the conformal inference in Section 4.

Although in practice, a fixed score function is often desired to make the method computationally feasible, the idea of localized conformal inference can also work with a data-dependent score function. The assumption of i.i.d data can also be relaxed to the case where there can be potential covariate shift. In Section 5, we give details about how to apply the idea of localized conformal prediction with data-dependent score functions and in the case of covariate shift, we also relate localized conformal inference to the notation of local coverage in this section. Finally, in Section 6, we describe the main theoretical results, including the finite sample coverage validity of the proposed methods.
2 Related work

One possible perspective for capturing the local structure of $V(Z_{n+1})$ at different $X_{n+1}$ is to consider the conditional coverage validity (Vovk 2012, Lei & Wasserman 2014):

$$\Pr \{Y_{n+1} \in \hat{C}(x_0) | X_{n+1} = x_0 \} \geq \alpha \quad \text{for all } \mathcal{P}. \quad (3)$$

However, let $\mathcal{N}(\mathcal{P})$ denote a set of non-atom points for $\mathcal{P}$, it is impossible to achieve the finite sample conditional validity without letting $\hat{C}(x)$ have infinite length for all $x \in \mathcal{N}(\mathcal{P})$ (Vovk 2012, Lei & Wasserman 2014, Barber et al. 2019):

**Proposition 2.1.** For any $x_0 \in \mathcal{N}(\mathcal{P})$, if the conditional validity in eq. (3) is satisfied, we have $E[|\hat{C}(x_0)|] = \infty$.

Approaches have then been proposed to construct CIs with approximate conditional coverage validity or local coverage validity.

One such approach that can lead to heterogeneous CI with a finite sample (marginal) coverage guarantee is described in Vovk (2012), Lei & Wasserman (2014) and Barber et al. (2019), which partitions the feature space into $K$ finite subsets and applies conformal inference to each of the subsets:

$$\Pr \{Y_{n+1} \in \hat{C}(X_{n+1}) | X_{n+1} \in \mathcal{X}_k \} \geq \alpha, \forall k = 1, 2, \ldots, K.$$ 

for some fixed partition $\cup_{k=1}^{K} \mathcal{X}_k = \mathbb{R}^p$.

This approach requires to fix $\cup_{k=1}^{K} \mathcal{X}_k$ before looking at the test sample $X_{n+1}$. In particular, with $\cup_{k=1}^{K} \mathcal{X}_k$ being a fixed partition, we can have less than ideal performance for $X_{n+1}$ close to the boundary of $\mathcal{X}_k$.

Another approach is to reweight the empirical distribution of $\{X_1, \ldots, X_n, X_{n+1}\}$ with $m$ different Gaussian kernels centered at a set of fixed points $\{x_i \in \mathbb{R}^p, i = 1, \ldots, m\}$, and correspondingly, construct $m$ different confidence intervals $\hat{C}(X_{n+1}, x_i), i = 1, \ldots, m$ for $Y_{n+1}$. The final CI $\hat{C}(X_{n+1}) = \bigcup_{i=1}^{m} \hat{C}(X_{n+1}, x_i)$ is the union of all constructed CIs (Barber et al. 2019). Similar to the previous approach, it is not ideal to have fixed $\{x_i \in \mathbb{R}^p, i = 1, \ldots, m\}$, and the action of taking the union may lead to unnecessarily wide CIs.

3 Localized conformal inference with fixed score function $V(.)$

We start with the setting where the score function $V(.)$ is fixed. For example, $V(x, y) = |y - \mu(x)|$ where $\mu(x)$ is a fixed prediction function for the response $y \in \mathbb{R}$ at $x \in \mathbb{R}^p$. In practice, this can correspond to the cases where

1. We perform sample splitting, using one fold of the data to train $V(.)$ and the other fold to perform conformal inference.
2. We have learned $V(.)$ from previous data, but want to apply it to a new data set.

Let the localizer function $H(x_1, x_2, X) \in [0, 1]$ for $x_1, x_2 \in \mathbb{R}^p$ be a function that may depend on the set $X = \{X_1, \ldots, X_{n+1}\}$, and always satisfies $H(x, x, X) = 1$ for all $x \in \mathbb{R}^p$. For the convenience of notation, we define $H_i(\cdot) := H(X_i, X)$ be the localizer centered at $X_i$, and $H_{i,j} := H_i(X_j) = H(X_i, X_j, X)$. For any distribution $\mathcal{F}$ on $\mathbb{R}$, define its level $\alpha$ quantile as

$$Q(\alpha; \mathcal{F}) = \inf \{t : \Pr \{T \leq t | T \sim \mathcal{F} \} \geq \alpha\}$$

Let $\delta_v$ be a point mass at $v, v_{1:n} := \sum_{i=1}^{n} \delta_{v_i}$ be the empirical distribution of $\{v_1, \ldots, v_n\}$, and $v_{1:n} \cup v_{n+1} := \sum_{i=1}^{n+1} \delta_v$ be the empirical distribution of $\{v_1, \ldots, v_n, v_{n+1}\}$.

The biggest difference between conformal inference and localized conformal inference is that, instead of using the level $\alpha$ quantile of the empirical distribution, we consider the level $\hat{\alpha}$ quantile of the weighted empirical distribution, with weight proportional to $H_{n+1,i}$ for sample $X_i$. The weights allow us to emphasize more the samples close to $X_{n+1}$. Let $p_{i,j}^H := \frac{H_{i,j}}{\sum_{k=1}^{m} H_{i,k}}$ for $i, j = 1, \ldots, n + 1$, and define $\tilde{F}_i := \sum_{j=1}^{n+1} p_{i,j}^H \delta_{v_j}$
as the weighted empirical distribution of \( \{V_1, \ldots, V_n, V_{n+1}\} \) using the localizer centered at \( X_i \), for \( i = 1, \ldots, n+1 \). Let \( \tilde{F} = \sum_{i=1}^{n} p^H_{i,n+1} \delta_{v_i} + p^H_{i+1, n+1} \delta_{\infty} \) be the distribution replacing \( V_{n+1} \) with \( \infty \) in \( \tilde{F}_{n+1} \). We show that \( \tilde{\alpha} \) can be strategically chosen to guarantee the finite sample coverage.

**Corollary 3.1.** Let \( Z_1, \ldots, Z_{n+1} \overset{i.i.d.}{\sim} \mathcal{P} \), and \( V(.) \) be a fixed function. For any \( \tilde{\alpha} \), let \( v_i^* = Q(\tilde{\alpha}; \tilde{F}), i = 1, 2, \ldots, n+1 \). If \( \tilde{\alpha} \) satisfies

\[
\sum_{i=1}^{n+1} \frac{1}{n+1} 1_{V_i \leq v_i^*} \geq \alpha. \tag{G1}
\]

then \( \Pr \{ V_{n+1} \leq Q(\tilde{\alpha}; \tilde{F}_{n+1}) \} \geq \alpha \), and equivalently,

\[
\Pr \{ V_{n+1} \leq Q(\tilde{\alpha}; \tilde{F}) \} \geq \alpha.
\]

Corollary 3.1 is a special case of Lemma 6.3. Here, we provide some intuition for why such an \( \tilde{\alpha} \) can guarantee a level \( \alpha \) coverage. Conformal inference relies on the exchangeability of data. However, when weighting samples based on a localizer, we can break the exchangeability in the training and test samples. Corollary 3.1 suggests a way of picking \( \tilde{\alpha} \) that restores some underlying exchangeability, by considering not only the weighted samples based on the localizer around \( X_{n+1} \), but also localizers around each of the trainings samples \( X_1, \ldots, X_n \). This restoration of exchangeability is essential for the proof.

It is obvious that for \( V_{n+1} = V(X_{n+1}, y) \) and any given \( y \), \( v_i^* \) is non-decreasing in \( \tilde{\alpha} \). Thus, \( \tilde{\alpha} \) satisfies eq. (G1) if any smaller value satisfies it. In practice, we would like to pick a small \( \tilde{\alpha} \) in order to construct a short CI. Based on Corollary 3.1 to obtain an interval \( \tilde{C}(X_{n+1}) \) for \( Y_{n+1} \), for every possible response value \( y \), we let \( \tilde{\alpha}(y) \) be the smallest value for \( \tilde{\alpha} \) such that eq. (G1) holds with \( V_{n+1} = V(X_{n+1}, y) \), and include \( y \) in \( \tilde{C}(X_{n+1}) \) if \( V(X_{n+1}, y) \leq Q(\tilde{\alpha}(y); \tilde{F}) \).

Such an algorithm is too computationally expensive to carry out in practice. We instead provide Corollary 3.2, which is a special case of Lemma 6.6 and is the foundation of a practical procedure. How do we interpret Corollary 3.2? Instead of finding the smallest value of \( \tilde{\alpha}(y) \) that makes eq. (G1) hold for each individual \( y \), we find \( \tilde{\alpha} \) that makes eq. (G1) hold for all \( y \) simultaneously. It turns out that for every \( \tilde{\alpha} \) with \( \tilde{\alpha}^*: = Q(\tilde{\alpha}; \tilde{F}) < \infty \) (otherwise, the constructed CI is \([0, \infty)\), and the coverage requirement is satisfied), we need only to check two cases: (1) eq. (G1) holds for all \( V(X_{n+1}, y) \leq Q(\tilde{\alpha}; \tilde{F}) \) if and only if it holds at \( V(X_{n+1}, y) = 0 \), and (2) eq. (G1) holds for all \( V(X_{n+1}, y) > Q(\tilde{\alpha}; \tilde{F}) \) if it holds when \( v_i^* = Q(\tilde{\alpha}; \sum_{j=1}^{n} p_{i,j}^H \delta_{v_j} + p_{i,n+1}^H \delta_{\infty}) \) in eq. (G1) for \( i = 1, \ldots, n \). Rigorous arguments can be found in the proof of Lemma 6.6.

**Corollary 3.2.** Let \( Z_1, \ldots, Z_{n+1} \overset{i.i.d.}{\sim} \mathcal{P} \), and \( V(.) \) be a fixed function. For any \( \tilde{\alpha} \), let \( \tilde{v}_1 = Q(\tilde{\alpha}; \sum_{j=1}^{n} p_{1,j}^H \delta_{v_j} + p_{1,n+1}^H \delta_{\infty}), \tilde{v}_2 = Q(\tilde{\alpha}; \sum_{j=1}^{n} p_{i,j}^H \delta_{v_j} + p_{i,n+1}^H \delta_{\infty}) \). If \( \tilde{v}_* = \infty \) or if

\[
\sum_{i=1}^{n} \frac{1}{n+1} 1_{V_i \leq v_1^*} \geq \alpha \quad \text{and} \quad \sum_{i=1}^{n} \frac{1}{n+1} 1_{V_i \leq v_2^*} + \frac{1}{n+1} \geq \alpha. \tag{G2}
\]

then we have \( \Pr \{ V_{n+1} \leq Q(\tilde{\alpha}; \tilde{F}) \} \geq \alpha \).

In Corollary 3.2 \( \tilde{\alpha} \) satisfies eq. (G1) if any smaller value satisfies it. Based on Corollary 3.2 we can use Algorithm 1 to construct the CI for \( Y_{n+1} \), which first constructs the CI for \( V_{n+1} \) by doing a grid search over values of \( \tilde{\alpha} \) to find a small value satisfying eq. (G1).

**Algorithm 1** Localized conformal inference with fixed score function

1. Using grid search for \( \tilde{\alpha} \) in \((0, 1)\), find the smallest value such that either eq. (G2) holds or \( Q(\tilde{\alpha}; \tilde{F}) = \infty \).

2. Return the CI \( \tilde{C}(X_{n+1}) = \{ y : V(X_{n+1}, y) \leq Q(\tilde{\alpha}; \tilde{F}) \} \).

Note that \( \tilde{\alpha} \) and \( \tilde{F} \) do not depend on \( y \), and typically, it is easy to invert \( V(x, y) \leq Q(\tilde{\alpha}; \tilde{F}) \) for any given \( x \). As a direct application of Corollary 3.2, Algorithm 1 will have the finite sample coverage guarantee.
**Theorem 3.3.** Let $Z_1, \ldots, Z_{n+1} \overset{i.i.d.}{\sim} P$, and $V(.)$ be a fixed function. Let $\tilde{C}(X_{n+1}) := \{ y : V(X_{n+1}, y) \leq Q(\hat{\alpha}, \tilde{F}) \}$ as described in Algorithm 1. Then we have $\mathbb{P}\{ y \in \tilde{C}(X_{n+1}) \} \geq \alpha$.

Usual conformal inference is a special case of the localized conformal inference when $H_{i,j} = 1$, $\forall i, j = 1, \ldots, n + 1$.

**Proposition 3.4.** Let $H_{i,j} = 1$, $\forall i, j = 1, \ldots, n + 1$, and let $\tilde{\alpha} = \alpha$. Then, either $\tilde{v}^\ast = \infty$ or eq. (G2) holds, and Corollary 3.2 recovers the result that $\mathbb{P}\{ V_{n+1} \leq Q(\alpha; V_{1:n} \cup \{ \infty \}) \} \geq \alpha$.

*Proof.* When $H_{i,j} = 1$ and $\tilde{\alpha} = \alpha$, we know $\tilde{v}^\ast = Q(\alpha; V_{1:n} \cup \{ \infty \})$. Let $v_{1}^\ast = Q(\alpha; V_{1:n} \cup \{ \tilde{v}^\ast \})$ and $v_{2}^\ast = Q(\alpha; V_{1:n} \cup \{ 0 \}, \forall i = 1, \ldots, n$. Without loss of generality, suppose $V_1 \leq V_2 \leq \ldots \leq V_n$ and $\tilde{v}^\ast = V_{(n+1)\alpha}$.

We show that we must have $\tilde{v}^\ast = \infty$ or eq. (G2). If $\tilde{v}^\ast < \infty$, then, we have $\lceil (n+1)\alpha \rceil \leq n$, and

1. If $v_{1}^\ast = v < \tilde{v}^\ast$, then, $\tilde{v}^\ast$ and $\{ V_{1:(n+1)\alpha}, V_{(n+1)\alpha+1}, \ldots, V_n \}$ are both greater than $v$. Thus, $v$ is at most $\left[ \frac{(n+1)\alpha - 1}{n+1} \right] < \alpha$ quantile of the empirical distribution $V_{1:n} \cup \{ \tilde{v}^\ast \}$, which is a contradiction. On the other hand, by definition of $\tilde{v}^\ast$, we know

$$
\sum_{i=1}^{n} \frac{1}{n+1} I_{V_i \leq \tilde{v}^\ast} + \frac{1}{n+1} I_{\infty \leq \tilde{v}^\ast} = \sum_{i=1}^{n} \frac{1}{n+1} I_{V_i \leq \tilde{v}^\ast} \geq \alpha.
$$

Hence, $\sum_{i=1}^{n} \frac{1}{n+1} I_{V_i \leq v_{1}^\ast} \geq \alpha$.

2. It is easy to check that $v_{2}^\ast = Q(\left[ \alpha - \frac{1}{n+1} \right] + \frac{n^2}{n+1}; V_{1:n})$. Hence, $v_{2}^\ast$ is the $\lceil \left[ \alpha - \frac{1}{n+1} \right] + \frac{n^2}{n+1} \rceil$ smallest value in $\{ V_1, \ldots, V_n \}$. Consequently, we have

$$
\sum_{i=1}^{n} \frac{1}{n+1} I_{V_i \leq v_{2}^\ast} + \frac{1}{n+1} = \left[ \frac{\alpha - \frac{1}{n+1}}{1} + \frac{n^2}{n+1} \right] + 1 \geq \frac{\alpha(n+1)}{n+1}.
$$

Combine them together, we know that $\tilde{\alpha} = \alpha$ leads to $\tilde{v}^\ast = \infty$ or eq. (G2), and Corollary 3.2 recovers the result that $\mathbb{P}\{ V_{n+1} \leq Q(\alpha; V_{1:n} \cup \{ \infty \}) \} \geq \alpha$.

Two questions the reader may want to ask are: (1) how tight is the coverage of the localized conformal prediction CI, and (2) what happens if we simply let $\tilde{\alpha} = \alpha$ without tuning it based on eq. (G2)? The answer to both of these will depend on the localizer $H$.

In Corollary 3.1, if we choose $\tilde{\alpha}$ to be the smallest value satisfying eq. (G1), the coverage may not be exactly $\alpha$ because we may not be able to select $\tilde{\alpha}$ such that $\sum_{i=1}^{n+1} \frac{1}{n+1} I_{V_i \leq v_{1}^\ast} = \alpha$ exactly. However, Corollary 3.5 says that if we take a random decision rule to get rid of the rounding issue in Corollary 3.1, then the resulting randomized decision rule will be tight.

**Corollary 3.5.** In the setting of Corollary 3.1, for any $\alpha \in (0, 1)$, let $\tilde{\alpha}_1$ be the smallest value of $\tilde{\alpha}$ such that $\sum_{i=1}^{n+1} \frac{1}{n+1} I_{V_i \leq v_{1}^\ast} \geq \alpha$, and let $\tilde{\alpha}_2$ be the largest of $\tilde{\alpha}$ such that $\sum_{i=1}^{n+1} \frac{1}{n+1} I_{V_i \leq v_{2}^\ast} < \alpha$. Let $\alpha_1, \alpha_2$ be the values of $\sum_{i=1}^{n+1} \frac{1}{n+1} I_{V_i \leq v_{1}^\ast}$ attained at $\tilde{\alpha}_1, \tilde{\alpha}_2$, and let $\tilde{\alpha} = \{ \begin{array}{ll} \tilde{\alpha}_1 & \text{w.p. } \frac{\alpha_1 - \alpha_2}{\alpha_1 - \alpha} \\ \tilde{\alpha}_2 & \text{w.p. } \frac{\alpha - \alpha_2}{\alpha_1 - \alpha} \end{array}$. Then, we have

$$
\mathbb{P}\{ V_{n+1} \leq Q(\tilde{\alpha}; \tilde{F}) \} = \alpha.
$$

Corollary 3.5 is a special case of the more general result Lemma 6.5.

For the second question, we provide Example 3.6 and Example 3.7 here, which show that letting $\tilde{\alpha} = \alpha$ may lead to both over-coverge and under-coverge.
Example 3.6. Let $\alpha \in (0, 1)$, let $P_X$ be any jointly continuous density for feature $x$, and consider the localizer $H(x_1, x_2) = \exp(-\frac{|x_1 - x_2|}{\sigma})$. For any $1 > \epsilon > \alpha$, we can always choose $\alpha$ to be small enough such that with probability at least $\epsilon$, we have $\sum_{i=1}^{n} H(X_{n+1}, X_i) < \frac{1}{\alpha}$ when $X_1, \ldots, X_{n+1}$ are independently generated from $P_X$. Then, with probability at least $\epsilon$, we will have $Q(\alpha; \hat{F}) = \infty > V_{n+1}$. Hence, the achieved coverage is at least $\epsilon > \alpha$.

Example 3.7. We consider an intuitive approach that practitioners may want to perform in practice: Let $H_{i,j} = 1_{|X_i - X_j| \leq h}$ for some fixed distance $h$ and let $\hat{\alpha} = \alpha \in (0, 1)$. Consider the following distribution:

$$X_i = \begin{cases} -1 & \text{w.p. } \frac{1-\alpha}{2-\alpha} \\ 0 & \text{w.p. } \frac{2(1-\alpha)}{2-\alpha} \\ 1 & \text{w.p. } \frac{1-\alpha}{2-\alpha} \end{cases}$$

and $Y_i = X_i + \epsilon_i$ with $\epsilon_i|X_i \sim \text{Uniform}([-2|X_i|, 2|X_i|])$. Let $V(x, y) = |y - x|$. Then $V_i \sim \text{Uniform}(0, 2|X_i|)$. Suppose we set $h = 1.5$, and consider the asymptotic case when $n \to \infty$: If $X_{n+1} = 1$, we know that the method considers only training samples at 1 and at 0, with asymptotic proportions $(1 - \alpha)$ and $\alpha$ respectively. Then $Q(\alpha; \hat{F}) \to 0$ at $X_{n+1} = 1$ and $P(V_{n+1} \leq Q(\alpha; \hat{F})|X_{n+1} = 1) \to 0$. Similarly, we have $P(V_{n+1} \leq Q(\alpha; \hat{F})|X_{n+1} = -1) \to 0$. Thus, the achieved coverage is asymptotically $1 - \frac{2(1-\alpha)}{2-\alpha}$, and we have an under-coverage of

$$\alpha - (1 - \frac{2(1-\alpha)}{2-\alpha}) = \alpha \frac{1-\alpha}{2-\alpha}, \forall \alpha \in [0, 1].$$

3.1 Choice of $H$

The choice of $H$ will greatly influence how localized our algorithm is. Suppose that we have a data set $D_0$ which is generated according to $P$ and is independent of $Z = \{Z_1, \ldots, Z_n, Z_{n+1}\}$. We consider two types of localizers and will tune them using $D_0$:

1. Distance based localizer

$$H_h(x_1, x_2, X) = 1_{|\frac{1}{h} \sum_{i=1}^{n+1} \delta(x_i - x_1)| \leq 1}.$$ 

2. Nearest-neighbor based localizer

$$H_h(x_1, x_2, X) = 1_{|x_1 - x_2| \leq Q(\frac{h}{h} \sum_{i=1}^{n+1} \delta(x_i - x_1))}.$$ 

Remark 3.8. In high-dimension where $p$ is large, instead of applying the localizer to the raw feature $x$, we usually will prefer to use a low dimensional function $t: \mathbb{R}^p \to \mathbb{R}^K$, and apply $H$ to $t(x)$. How to find a good $t$ is non-trivial and is beyond the scope of this paper, and here we simply let $t(x) = x_j$ where $j$ is the direction that leads to the largest mutual information between the scores and feature $j$ using $D_0$.

The parameter $h$ governs the degree of localization: the smaller $h$ is, the more localized the final result will be. Let $\mathcal{X}$ be a subset of $D_0$. We suggest to pick $h$ such that in $\mathcal{X}$: (1) the average length for CI is small, (2) the average variance of lengths of CIs conditional on $x$ is small, and (3) the coverage is at least $\alpha$ for the constructed CI in $\mathcal{X}$.

We consider the subset $\mathcal{X}$ instead of every sample in $D_0$ because, for the distance based localizer, it is okay if we have a small portion of samples with $\infty$-length CI. In this case, we can compare choices of $h$ based on those points with finite length CIs by considering a subset of samples. Exact steps that we use can be found in Appendix [A].

4 Empirical study with fixed $V(.)$

We compare the localized conformal inference band (LCB) and conformal inference band (CB) under different settings in this section.
Example 4.1 (Simulation A). Let \( X_i \sim N(0,1) \) and \( Y_i = X_i + \epsilon_i \) for \( i = 1, \ldots, n+1 \). We use the fixed score function \( V(X_i, Y_i) = |Y_i - X_i| \) to do inference for both the conformal and localized conformal approaches. For localized conformal inference, we consider the distance based localizer \( H^1_h(X_j, X_i) = 1_{|X_j - X_i| \leq h} \) and the nearest-neighbor based localizer \( H^2_h(X_j, X_i) = 1_{|X_j - X_i| \leq Q(h \sum_{k=1}^{n+1} \frac{1}{n} \delta_{X_k - X_i})} \) for \( h \) nearest neighbors. We try three different values \( h_1, h_2 \) and \( h_3 \) of the tuning parameter \( h \). For \( H^1_h \), we let \( h_1 = 0.1, h_2 = 1 \) and \( h_3 = \hat{h}_1 \), and for \( H^2_h \), we let \( h_1 = 40, h_2 = 500 \) and \( h_3 = \hat{h}_2 \), where \( \hat{h}_1 \) and \( \hat{h}_2 \) are automatically chosen using another \( i.i.d \) generated data set with \( n \) samples according to Appendix B.

For each of the following noise generating mechanisms, we let \( n = 500 \) and repeat the experiment 1000 times: (a) \( \epsilon_i \overset{i.i.d.}{\sim} N(0,1) \), (b) \( \epsilon_i \mid X_i \overset{i.i.d.}{\sim} \frac{1}{2|X_i|+1} N(0,1) \), and (c) \( \epsilon_i \mid X_i \overset{d}{\sim} \frac{|X_i|}{|X_i|+1} N(0,1) \). Table 1 shows the achieved coverage for \( \alpha = .80 \) and \( \alpha = .95 \). We can see that both conformal prediction and localized conformal prediction with different localizers have achieved the desired coverage. Figure 2 shows the constructed confidence bands across 1000 repetitions using different methods at \( \alpha = .95 \).

As \( h \) increases, the localized conformal bands become more similar to the conformal bands. Comparing results for localized conformal inference with \( h = h_1 \) and \( h = h_2 \), we see that small \( h \) reveals more local structure. Using the automatic tuning procedure, we have successfully chosen large \( h \) when the underlying distribution of \( V(X_{n+1}) \) is homogeneous and small \( h \) when it is heterogeneous across different values of \( X_{n+1} \).

Example 4.2 (Simulation B). Let \( Y_i = X_i^T \beta + \epsilon_i \), with \( \beta = (\underbrace{1, \ldots, 1, 0, \ldots, 0}_{3}, \underbrace{0, \ldots, 0}_{p-3})^T \), \( X_{i,j} \sim \text{Unif}[-3,3] \) for \( i = 1, \ldots, n+1 \) and \( j = 1, \ldots, p \), and we consider two cases of error distribution: (a) \( \epsilon_i \overset{i.i.d.}{\sim} N(0,1) \), and (b) \( \epsilon_i \mid X_i \sim \begin{cases} .5N(0,1) & |X_{i,p}| \leq 1 \\ 2N(0,1) & |X_{i,p}| > 1 \end{cases} \). We let \( V(x,y) = |y - \mu(x)| \), where \( \mu(x) \) is the prediction model \( \mu(x) \) trained using cross-validation lasso regression on a data set \( D_0 \) of size \( n = 500 \). We use an independent set \( D_3 \) of size \( n = 500 \) to perform the conformal inference and localized conformal inference. For localized conformal inference, we use both the distance based localizer \( H^1_h \) and the nearest-neighbor based localizer \( H^2_h \) with the tuning parameter \( h \) automatically chosen as described in Appendix B using \( D_0 \). We perform 1000 experiments for \( p = 3 \) and \( p = 500 \). We see that all three constructions have controlled the coverage in Table 2. In Figure 3, we plot the constructed CIs at \( \alpha = .95 \) for \( V_i \) using different methods and the true values of \( V_i \) across 1000 repetitions.
Figure 2: Simulation A: Confidence bands constructed using 1000 repetitions with targeted level at $\alpha = .95$. The black, blue, red and green dots respectively represent (1) the true responses for the test samples (response), (2) the conformal confidence bands (CB), (3) the localized conformal confidence bands with distance localizer $H^1_\text{LCB1}$, and (4) the localized conformal confidence bands with nearest-neighbor based localizer $H^2_\text{LCB2}$. The red dots close to the top and bottom within each plot represent samples whose CIs based on LCB1 have infinite length (both the CB and the LCB2 do not have infinite length CI by construction).
Figure 3: Simulation B: Confidence bands constructed using 1000 repetitions with targeted level at $\alpha = .95$. The black, blue, red and green dots respectively represent (1) actual $V_i$ for the test samples (error), (2) the conformal inference (CB) for $V_i$, (3) the localized conformal inference for $V_i$ with distance based localizer $H^1_h$ (LCB1), and (4) the localized conformal inference with nearest-neighbor based localizer $H^2_h$ (LCB2).
5 Extensions

In this part, we draw a connection between the method of localized conformal and the notion of local coverage. We also consider two extensions of the localized conformal inference. One is to allow the score function to be data-dependent (but the exchangeability requirement is still needed), another is to relax the assumption that the training data and the test data are independently and identically generated from \( \mathcal{P} \) to the setting where there can be covariate-shift.

5.1 Relation to local coverage

In [Barber et al. (2019a)], the authors suggest to consider the following type of local coverage: let \( x_0 \in \mathbb{R}^p \) and \( P_{X_0} \) be a distribution concentrated at \( x_0 \), with \( \frac{dP_{X_0}(x)}{dx} \propto \frac{dP_{X}(x)}{dx} K(\frac{x-x_0}{h}) \) and \( K(\cdot) \) being the Gaussian kernel with bandwidth \( h \), we would like \( \hat{C}(x_0) \) such that

\[
\mathbb{P}\{\hat{Y}_{n+1} \in \hat{C}(x_0)\} \geq \alpha, \quad \hat{X}_{n+1} \sim P_{X_0}^{\hat{X}_{n+1}}, \hat{Y}_{n+1} \sim P_{Y|X}
\]

(4)

The proposal discussed in [Barber et al. (2019a)] considers the situation where we want eq. (4) to hold for a set of fixed values for \( x_0 \), and different values of \( x_0 \) can lead to different constructed CIs for a new observation \( X_{n+1} \) (see section 2).

With the score function \( V(\cdot) \) fixed, localized conformal inference provide a simple way to construct a unique \( \hat{C}(X_{n+1}) \) for every test sample such that the type local coverage requirement defined in eq.(4) is satisfied.

Let \( H(x_1, x_2, X) = H(x_1, x_2) \) to be a data-independent localizer and define the localized distribution \( P_{X_0}^{\hat{X}_{n}}(\cdot) \) around \( x_0 \) as \( \frac{dP_{X_0}(x)}{dx} \propto \frac{dP_{X}(x)}{dx} H(x_0, x) \), and \( \hat{F} \) is defined with the localizer \( H(X_{n+1},.\)).

Theorem 5.1. Let \( Z_1, \ldots, Z_n \overset{i.i.d.}{\sim} \mathcal{P} \) and \( V(\cdot) \) to be fixed. Let \( \hat{C}(X_{n+1}) := \{y: V(X_{n+1}, y) \leq Q(\alpha, \hat{F})\} \). Conditional on \( X_{n+1} \), let

\[
\hat{X}_{n+1}|X_{n+1} \sim P_{X}^{\hat{X}_{n+1}} \quad \text{and} \quad \hat{Y}_{n+1}|\hat{X}_{n+1} \sim P_{Y|X}.
\]

Then, we have \( \mathbb{P}\{\hat{Y}_{n+1} \in \hat{C}(X_{n+1})|X_{n+1} = x_0\} \geq \alpha \) for all \( x_0 \).

The proof of Theorem 5.1 is given in Appendix A. The confidence interval \( \hat{C}(X_{n+1}) \) is indexed by \( X_{n+1} \), and when the training set does not change, we will have a unique confidence interval for every realization of \( X_{n+1} \). Note that local coverage statement of \( \hat{C}(X_{n+1}) \) here is not sufficient for the marginal coverage defined in eq.(4), nor is it necessary for the later (see Section 3).

5.2 Localized conformal inference with data-dependent score function

In this section, we consider a more general case where the score function can have some data dependency but still leads to exchangeability. Let \( Z = \{Z_1, \ldots, Z_n, Z_{n+1}\} \) be the set of training and test samples, the score function can depend on the set \( Z \) but not their ordering, and have the form \( V(\cdot, Z) \). To accommodate for this more general case and distinguish it from the case with fixed score function, we introduce some new notations for convenience: Define

\[
V_{i}^{z_{n+1}} := V(Z_i, Z)|_{Z_{n+1} = z_{n+1}}, \forall i = 1, \ldots, n + 1.
\]

\[
\hat{F}_{i}^{z_{n+1}} := \sum_{j=1}^{n+1} P_{i,j}^{H}|_{V_{i}^{z_{n+1}}} \delta_{V_{j, \hat{X}_{i}^{z_{n+1}}}}, \forall i = 1, \ldots, n + 1.
\]

\[
\hat{F}^{z_{n+1}} := \sum_{j=1}^{n} P_{n+1,j}^{H}|_{V_{j, \hat{X}_{n+1}}^{z_{n+1}}} + P_{n+1,n+1}^{H}\delta_{\infty} \mid_{Z_{n+1} = z_{n+1}}.
\]

as the realizations of \( V(Z_i, Z) \) and the weighted distribution \( \hat{F}_{i}, \hat{F} \) at \( Z_{n+1} = z_{n+1} \). For example, \( V_{n+1}^{z_{n+1}} = V(z_{n+1}, \{Z_1, \ldots, Z_n, z_{n+1}\}) \) and \( V_{i}^{z_{n+1}} = V(Z_i, \{Z_1, \ldots, Z_n, z_{n+1}\}) \) for \( i = 1, \ldots, n \). We will always use
V and F with the superscript to represent that data-dependency is allowed, and use the ones without superscript to represent that the score function is fixed.

Corollary 5.2 and Corollary 5.5 are extensions of Corollary 3.1 and 3.5 to settings when the score function is data dependent, and are applications of Lemma 6.3 and Lemma 6.5.

**Corollary 5.2.** Let $Z_1, \ldots, Z_{n+1} \overset{i.i.d.}{\sim} \mathcal{P}$. For any $\hat{\alpha}$, define $v_i^\alpha = Q(\hat{\alpha}; \hat{F}_i^{Z_{n+1}})$, $i = 1, 2, \ldots, n + 1$. If $\hat{\alpha}$ satisfies

$$
\sum_{i=1}^{n+1} \frac{1}{n+1} \mathbb{1}_{V_{i}^{Z_{n+1}} \leq v_i^\alpha} \geq \alpha
$$

Then $\mathbb{P} \left\{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{F}_n^{Z_{n+1}}) \right\} \geq \alpha$, and equivalently,

$$
\mathbb{P} \left\{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{F}_n^{Z_{n+1}}) \right\} \geq \alpha.
$$

**Remark 5.3.** When $H_{i,j} = 1$, $\forall i, j = 1, \ldots, n+1$, we have $\hat{F}_n^{Z_{n+1}} = V_{1:n}^{Z_{n+1}} \cup \{\infty\}$, and $v_i^\alpha = Q(\hat{\alpha}; V_{1:n}^{Z_{n+1}})$, $\forall i = 1, \ldots, n + 1$. Since eq. (5) holds for if and only if $v_i^\alpha \geq Q(\alpha; V_{1:n}^{Z_{n+1}})$. We recovered the conformal inference result [Vovk et al. 2005] that

$$
\mathbb{P} \left\{ V_{n+1}^{Z_{n+1}} \leq Q(\alpha; V_{1:n}^{Z_{n+1}} \cup \{\infty\}) \right\} \geq \alpha.
$$

Based on Corollary 5.2, we can construct the CI by checking if we should include $y$ in $\hat{C}(X_{n+1})$ for every possible value $y$.

**Theorem 5.4.** In the setting of Corollary 5.2, let $z_{n+1} = (X_{n+1}, y)$, and let $\hat{\alpha}(y)$ be values indexed by $y$. Let $\hat{C}(X_{n+1}) := \{ y : V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}(y); \hat{F}_n^{Z_{n+1}}) \}$. If $\hat{\alpha}(y)$ satisfies eq. (5) at $Z_{n+1} = z_{n+1}$, we have

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

Same as in the setting with fixed score function, Corollary 5.5 says that if we take a random decision rule to get rid of the rounding issue in Corollary 5.2, then the resulting randomized decision rule will be tight.

**Corollary 5.5.** In the setting of Corollary 5.2, for any $\alpha \in (0, 1)$, let $\hat{\alpha}_1$ be the smallest value of $\hat{\alpha}$ such that

$$
\sum_{i=1}^{n+1} \frac{1}{n+1} \mathbb{1}_{V_{i}^{Z_{n+1}} \leq v_i^\alpha} \geq \alpha,
$$

and let $\hat{\alpha}_2$ be the largest of $\hat{\alpha}$ such that

$$
\sum_{i=1}^{n+1} \frac{1}{n+1} \mathbb{1}_{V_{i}^{Z_{n+1}} \leq v_i^\alpha} < \alpha.
$$

Let $\alpha_1, \alpha_2$ be the values of $\sum_{i=1}^{n+1} \frac{1}{n+1} \mathbb{1}_{V_{i}^{Z_{n+1}} \leq v_i^\alpha}$, attained at $\hat{\alpha}_1, \hat{\alpha}_2$, and let $\hat{\alpha} = \begin{cases} \hat{\alpha}_1 & \text{w.p. } \frac{\alpha_2 - \alpha}{\alpha_2 - \alpha_1} \\ \hat{\alpha}_2 & \text{w.p. } \frac{\alpha - \alpha_1}{\alpha_2 - \alpha_1} \end{cases}$. Then, we have

$$
\mathbb{P} \left\{ V_{n+1} \leq Q(\hat{\alpha}; \hat{F}) \right\} = \alpha.
$$

In all of our empirical study, we have only carried out localized conformal inference with fixed score function. This is because the general recipe described in Theorem 5.4 is too computationally expensive: for every $y$, we need to retrain our prediction model to get $V_{n+1}(x)$ and then re-calculate $v_i^\alpha$ and $\hat{\alpha}(y).$ Similar problems are encountered by the conformal inference for data dependent score function $V(., Z)$, and sample-splitting is often used to reduce the computation [Papadopoulos et al. 2002, Lei et al. 2015]. We include the general setting here for the sake of completeness and show that the idea of localized conformal inference can be extended to the regime where the idea of conformal prediction also works.

### 5.3 Covariate shift

When there is potential covariate-shift, we assume the training and test data can be generated from different distributions in their feature space [Shimodaira 2000, Sugiyama & Müller 2005, Sugiyama et al. 2007, Quionero-Candela et al. 2009]:

$$
Z_{n+1} \sim \hat{P} = \hat{P}_X \times P_{Y|X}, \ Z_i \overset{i.i.d.}{\sim} P = P_X \times P_{Y|X}, i = 1, \ldots, n.
$$
The distribution of $Y|X$ is still assumed to be the same for the training and test samples. The work of Barber et al. (2019) extends conformal inference to this setting. Assuming that $\hat{P}_X$ is absolutely continuous with respect to $P_X$, with known $w(x) = \frac{d\hat{P}_X}{dP_X}$, we can perform conformal inference using weighted exchangeability.

**Proposition 5.6** (Barber et al. (2019)). Let $p_i = \frac{w(X_i)}{\sum_{i=1}^{n} w(X_i)}$. For any $\alpha$, we have

$$P(V_{n+1}^{Z_n+1} \leq Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i^{z_{n+1}}} + p_{n+1} \delta_{\infty})) \geq \alpha.$$  

Knowing the density ratio function $w(x)$, we can generalize localized conformal inference to take into consideration the covariate shift in a straightforward manner: both Theorem 6.4 and Theorem 6.7 consider this general case. More concretely, to accommodate to the covariate shift, we need only to consider a weighted evaluation equations in Corollary 3.5/Algorithm 1 (fixed score function) and Theorem 5.4 (data-dependent score function):

1. In Corollary 3.5/Algorithm 1, we change eq. (G2) into

$$\sum_{i=1}^{n} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} 1_{V_i \leq v_1^*} \geq \alpha,$$

$$\sum_{i=1}^{n} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} 1_{V_i \leq v_2^*} \geq \alpha.$$  

2. Theorem 5.4, we change eq. (5) into

$$\sum_{i=1}^{n+1} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} 1_{V_i^{z_{n+1}} \leq v_i^*} \geq \alpha.$$  

Under the covariate shift, localized conformal inference may help to limit the influence of samples with extremely large weight $w(X_i)$. If $\hat{P}_X$ and $P_X$ are not close to each other, the (weighted) conformal prediction may construct a CI strongly influenced by a few samples with extremely large $w(X_i)$, even though $X_{n+1}$ can be far from those $X_i$.

To illustrate this, let $Y_i = X_i + \epsilon_i$, with $\epsilon_i \sim N(0,1)$ for $i = 1, \ldots, n+1$, and $X_i \sim N(0,1)$ for $i = 1, \ldots, n$, $X_{n+1} \sim N(3,1)$. Consider the score function $V(x, y) = |y-x|$ and let the training sample size be $n = 500$. We compare weighted conformal inference and localized conformal inference. For localized conformal inference, we use a nearest-neighbor based localizer:

$$H(x_1, x_2, X) = w(x_2) 1_{\{|w(x_2) - w(x_1)| \leq Q(\alpha; \sum_{i=1}^{n} \delta_{w(X_i)-w(x_1)})\}}$$

We let $h = 450$ to limit the influence of the training samples with extreme weights on $X_{n+1}$ far away from them.

In this section, we provide theories for the more general case where there may be covariate-shift.

**Assumption 6.1.** The samples are independently generated and the distributions of the training samples and the test sample can be different due to covariance-shift:

$$Z_{n+1} \sim \hat{P}_X \times P_{Y|X}, \quad Z_i \sim P = P_X \times P_{Y|X}, \quad \forall i = 1, 2, \ldots, n.$$  

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Then we have $P$.

Assumption 6.2. $\tilde{P}_X$ is absolute continuous with respect to $P_X$, with $w(x) = \frac{d\tilde{P}_X(x)}{dP_X(x)}$.

We consider $w(x)$ to be known and when $w(x) = 1$, $\forall x \in \mathbb{R}^p$, we return to the i.i.d data setting.

Lemma 6.3. Suppose Assumptions 6.1 - 6.2 hold. For any $\tilde{\alpha}$, define $v_i^\ast = Q(\tilde{\alpha}; \mathcal{F}_{Z_{n+1}}^i)$, $i = 1, \ldots, n + 1$. If

$$\sum_{i=1}^{n+1} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{I}_{V_i Z_{n+1} \leq v_i^\ast} \geq \alpha$$

Then $P(V_{n+1}^{Z_{n+1}} \leq Q(\tilde{\alpha}; \mathcal{F}_{Z_{n+1}})) \geq \alpha$, and equivalently,

$$P(V_{n+1}^{Z_{n+1}} \leq Q(\tilde{\alpha}; \mathcal{F}_{Z_{n+1}})) \geq \alpha.$$

Theorem 6.4 is a direct result of Lemma 6.3.

Theorem 6.4. In the setting of Lemma 6.3, let $z_{n+1} = (X_{n+1}, y)$, and $\tilde{\alpha}(y)$ be any value that satisfies eq. (G1w) when $V_{n+1} = V(z_{n+1})$. Let $\tilde{C}(X_{n+1}) := \{ y : V_{n+1}^{Z_{n+1}} \leq Q(\tilde{\alpha}(y); \mathcal{F}_{Z_{n+1}}) \}$. Then $P(y \in \tilde{C}(X_{n+1})) \geq \alpha$.

Lemma 6.5 provides a way to choose $\tilde{\alpha}$ with guaranteed coverage, by considering localizers centered at each of the sample to restore exchangeability. The coverage of Lemma 6.3 is not exact because we may not be able to find $\tilde{\alpha}$ to make eq. (G1w) take equal sign. Lemma 6.5 says that if we take a random decision rule to get rid of the rounding issue, we can have an algorithm with tight coverage.

Lemma 6.5. In the setting of Lemma 6.3, for any $\alpha \in (0, 1)$, let $\tilde{\alpha}_1$ be the smallest value of $\tilde{\alpha}$ such that

$$\sum_{i=1}^{n+1} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{I}_{V_i Z_{n+1} \leq v_i^\ast} \geq \alpha,$$

and $\tilde{\alpha}_2$ be the largest value of $\tilde{\alpha}$ such that

$$\sum_{i=1}^{n+1} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{I}_{V_i Z_{n+1} \leq v_i^\ast} < \alpha.$$

Let $\tilde{\alpha}_1$ and $\tilde{\alpha}_2$ be the values of

$$\sum_{i=1}^{n+1} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{I}_{V_i Z_{n+1} \leq v_i^\ast}$$

attained at $\tilde{\alpha}_1$, $\tilde{\alpha}_2$, and let $\tilde{\alpha} = \left\{ \begin{array}{ll} \tilde{\alpha}_1 & w.p. \frac{\alpha - \alpha_2}{\alpha_1 - \alpha_2} \\ \tilde{\alpha}_2 & w.p. \frac{\alpha - \alpha_1}{\alpha_1 - \alpha_2} \end{array} \right.$.

Then we have $P\left\{ V_{n+1}^{Z_{n+1}} \leq Q(\tilde{\alpha}; \mathcal{F}_{Z_{n+1}}) \right\} = \alpha$.

When the score function is fixed, we can come up with a decision rule that does not depend on $y$. 
Lemma 6.6. Suppose Assumption 6.1 - 6.2 hold. Let \( V(.) \) to be a fixed function. For any \( \tilde{\alpha} \), define \( \bar{\nu}^* = Q(\tilde{\alpha}; \bar{F}) \) and \( \nu_{11}^* = Q(\tilde{\alpha}; \sum_{j=1}^{n} p_{i,j}^H \delta_{v_j} + p_{i,n+1}^H \delta_{v^*}) \), \( \nu_{12}^* = Q(\tilde{\alpha}; \sum_{j=1}^{n} p_{i,j}^H \delta_{v_j} + p_{i,n+1}^H \delta_{v^*}) \). If \( \bar{\nu}^* = \infty \) or if

\[
\begin{align*}
\sum_{i=1}^{n} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} I_{V_i \leq v_{11}^*} &\geq \alpha, \\
\sum_{i=1}^{n} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} I_{V_i \leq v_{12}^*} + \frac{w(X_{n+1})}{\sum_{j=1}^{n+1} w(X_j)} &\geq \alpha.
\end{align*}
\]

Then we have \( P(V_{n+1} \leq Q(\tilde{\alpha}; \bar{F}) \geq \alpha \).

Theorem 6.7 is a direct application of Lemma 6.6.

Theorem 6.7. In the setting of Lemma 6.6, let \( z_{n+1} = (X_{n+1}, y) \) and \( \bar{C}(X_{n+1}) := \{ y : V(z_{n+1}) \leq Q(\tilde{\alpha}; \bar{F}) \} \). If \( \bar{\nu}^* = \infty \) or if eq. (G2w) holds, then we have \( P(Y_{n+1} \in \bar{C}(X_{n+1})) \geq \alpha \).

7 Discussion

In this paper, we have described a new way perform conformal inference with localization. This localized conformal inference approach is data adaptive, and have finite sample coverage guarantee without distributional assumptions on \( Y|X \). An interesting future direction would be to apply the idea of localized conformal prediction under the presence of outliers. Conformal inference has been used in classification problems for outlier detection (Hechtlinger et al. 2018, Guan & Tibshirani 2019). Localized conformal inference with distance-based localizer seems to be an useful framework for making prediction in the presence of outliers, both within regression and classification problems if we can find a proper localizer. Compared with most other outlier detection approaches (Hodge & Austin 2004, Chandola et al. 2009), it can use information from the response, since the degree of localization will depend on the distribution of prediction errors.

A Proofs

Lemma A.1 and Lemma A.2 will be most important components for the proofs of Lemma 6.3, Lemma 6.5 and Lemma 6.6.

Lemma A.1. For any \( \alpha \) and sequence \( \{V_1, \ldots, V_{n+1}\} \), we have

\[
V_{n+1} \leq Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{V_{n+1}}) \Leftrightarrow V_{n+1} \leq Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{\infty}),
\]

where \( \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{V_{n+1}} \) and \( \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{\infty} \) are some weighted empirical distributions with weights \( p_i \geq 0 \) and \( \sum_{i=1}^{n+1} p_i = 1 \).

Proof. By definition, we know

\[
V_{n+1} \leq Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{V_{n+1}}) \Rightarrow V_{n+1} \leq Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{\infty}).
\]

To show that Lemma A.1 holds, we only need to show that

\[
V_{n+1} > Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{V_{n+1}}) \Rightarrow V_{n+1} > Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{\infty}).
\]

Without loss of generality, we assume \( 0 = V_0 \leq V_1 \leq V_2 \leq \ldots \leq V_n \), and consider the case where \( V_{n+1} > Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{V_{n+1}}) \).
In this case, we must have $\sum_{i=1}^{n} p_i \geq \alpha$, and the empirical lower $\alpha$ quantile is the smallest index $i$ such that $\sum_{j=1}^{i} p_j \geq \alpha$. Let $i^* \leq n$ be this index. Since $V_{n+1} > V_i$ and $\sum_{j=1}^{i} p_j \geq \alpha$, by definition, we know

\[
\sum_{i=1}^{n} \mathbb{1}_{V_i \leq V_i^*} \geq \alpha \iff Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{\infty}) \leq V_i^* \\
\Rightarrow V_{n+1} > Q(\alpha; \sum_{i=1}^{n} p_i \delta_{V_i} + p_{n+1} \delta_{\infty}).
\]

\[\square\]

**Lemma A.2.** For any event \(\mathcal{T} := \{\{Z_i, i = 1, \ldots, n + 1\} = \{z_i := (x_i, y_i), i = 1, \ldots, n + 1\}\},\)

we have

\[
\mathbb{P}\{V_{n+1}^{Z_{n+1}} \leq Q(\tilde{\alpha}; \sum_{i=1}^{n+1} p_{n+1,i} \delta_{V_{n+1}^{z_{n+1}}})|\mathcal{T}\} = \mathbb{E}\left\{\sum_{i=1}^{n+1} \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)} \mathbb{1}_{v_i \leq v_i^*}|\mathcal{T}\right\},
\]

where $v_i = V(z_i, (z_1, \ldots, z_n, z_{n+1}))$, $v_i^* = Q(\tilde{\alpha}; \sum_{j=1}^{n+1} p_{n+1,j} \delta_{V_{n+1}^{z_{n+1}}})$ for $i = 1, 2, \ldots, n+1$, and $\tilde{\alpha} = \tilde{\alpha}(Z)$ can be dependent on the data through the set $Z$ where $Z = \{Z_1, \ldots, Z_{n+1}\}$. The expectation on the right-hand-side is taken over the randomness of $\tilde{\alpha}$ conditional on $\mathcal{T}$.

**Proof.** Let $\sigma$ be a permutation of numbers $1, 2, \ldots, n + 1$. We know that

\[
P(\sigma_{n+1} = i|\mathcal{T}) = \frac{w(x_i)\#\{\sigma: \sigma_{n+1} = i\}}{\sum_{j=1}^{n+1} w(x_j)\#\{\sigma: \sigma_{n+1} = j\}} = \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)}.\]

Also, since the function $V(., Z) = V(.)$ and the localizer $H(., X) = H(., .)$ have fixed function forms conditional on $\mathcal{T}$, and $\tilde{\alpha}$ (can be random) is independent of the data conditional $\mathcal{T}$, we also have

\[
\mathbb{P}\{V_{n+1}^{Z_{n+1}} \leq Q(\tilde{\alpha}; \sum_{i=1}^{n+1} p_{n+1,i} \delta_{V_{n+1}^{z_{n+1}}})|\mathcal{T}, \tilde{\alpha}\} \\
= \sum_{i=1}^{n+1} P(\sigma_{n+1} = i|\mathcal{T}) \mathbb{1}_{\{V_{n+1} \leq v_{n+1}^*(\sigma)|\mathcal{T}, \sigma_{n+1} = i\}} \\
= \sum_{i=1}^{n+1} \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)} \mathbb{1}_{\{v_i \leq v_{n+1}^*(\sigma)|\mathcal{T}, \sigma_{n+1} = i\}}
\]

where $v_{n+1}^*(\sigma) = Q(\tilde{\alpha}; \sum_{j=1}^{n} p_{n+1,j} \delta_{V_{n+1}^{z_{n+1}}})$ is the realization of $v_i^*$ with data permutation $\sigma$ conditional on $\mathcal{T}$ and $\tilde{\alpha}$:

\[
v_{n+1}^*(\sigma) = Q(\tilde{\alpha}; \sum_{k=1}^{n+1} p_{n+1,k} H(x_{\sigma_k}, x_{\sigma_k}) \delta_{V_{n+1}^{z_{n+1}}})
\]

With a slight abuse of notation, we let $v_i^*$ corresponds to the case where $\sigma_i = i$. We immediately observe that

\[
v_i^*(\sigma) = v_{\sigma_i}^*
\]

Consequently, we have

\[
\mathbb{P}\{V_{n+1}^* \leq v_{n+1}^*|\mathcal{T}, \tilde{\alpha}\} = \sum_{i=1}^{n+1} \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)} \mathbb{1}_{\{v_i \leq v_{n+1}^*\}}.
\]

Marginalize over $\tilde{\alpha}|\mathcal{T}$, we have

\[
\mathbb{P}\{V_{n+1}^* \leq v_{n+1}^*|\mathcal{T}\} = \mathbb{E}\left\{\sum_{i=1}^{n+1} \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)} \mathbb{1}_{\{v_i \leq v_{n+1}^*\}}|\mathcal{T}\right\}
\]

\[\square\]
A.1 Proof of Lemma 6.3

Define
\[ \mathcal{T} := \{ (Z_i, i = 1, \ldots, n + 1) = (z_i := (x_i, y_i), i = 1, \ldots, n + 1) \} . \]

When we choose \( \hat{\alpha} \) such that eq. (G1) is satisfied, this decision rule does not depend on the ordering of data conditional on \( \mathcal{T} \): for any permutation \( \sigma \) of numbers \( 1, 2, \ldots, n + 1 \), we have
\[
\sum_{i=1}^{n+1} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{I}_{v_i^{n+1} \leq v_i^*} | \mathcal{T}, \sigma = \sum_{i=1}^{n+1} \frac{w(x_{\sigma_i})}{\sum_{j=1}^{n+1} w(x_{j})} \mathbb{I}_{v_{\sigma_i} \leq v_{\sigma_i}^*} = \sum_{i=1}^{n+1} \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)} \mathbb{I}_{v_i \leq v_i^*} .
\]

Since \( V(\cdot, Z) \) and \( H(\cdot, \cdot, X) \) are fixed functions conditional on \( \mathcal{T} \) (see the arguments for eq. (6) in Lemma A.2). Hence, apply Lemma A.2 we have
\[
\mathbb{P} \{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{\mathcal{F}}_{n+1}^{Z_{n+1}}) | \mathcal{T} \} = \mathbb{E} \left\{ \sum_{i=1}^{n+1} \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)} \mathbb{I}_{v_i \leq v_i^*} | \mathcal{T} \right\} \geq \alpha .
\]

Marginalize over \( \mathcal{T} \), we have
\[
\mathbb{P} \{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{\mathcal{F}}_{n+1}^{Z_{n+1}}) \} \geq \alpha .
\]
By Lemma A.1 equivalently, we also have
\[
\mathbb{P} \{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{\mathcal{F}}_{n+1}^{Z_{n+1}}) \} \geq \alpha .
\]

A.2 Proof of Lemma 6.5

Define
\[ \mathcal{T} := \{ (Z_i, i = 1, \ldots, n + 1) = (z_i := (x_i, y_i), i = 1, \ldots, n + 1) \} . \]

Following the same argument as used for \( \hat{\alpha} \) in the proof of Lemma 6.3, we know that both \( \hat{\alpha}_1, \hat{\alpha}_2 \) and \( \alpha_1 \), \( \alpha_2 \) are fixed conditional on \( \mathcal{T} \). As a result, when \( \hat{\alpha} = \left\{ \hat{\alpha}_1 \text{ w.p. } \frac{\alpha_1 - \alpha_2}{\alpha_1 - \alpha_2}, \hat{\alpha}_2 \text{ w.p. } \frac{\alpha_1 - \alpha_2}{\alpha_1 - \alpha_2} \right\} \), we know that \( \hat{\alpha} \) is independent of the data conditional on \( \mathcal{T} \). Apply Lemma A.2 we have
\[
\mathbb{P} \{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{\mathcal{F}}_{n+1}^{Z_{n+1}}) | \mathcal{T} \} = \mathbb{E} \left\{ \sum_{i=1}^{n+1} \frac{w(x_i)}{\sum_{j=1}^{n+1} w(x_j)} \mathbb{I}_{v_i \leq v_i^*} | \mathcal{T} \right\} = \frac{\alpha_1 - \alpha_2}{\alpha_1 - \alpha_2} + \frac{\alpha_1 - \alpha}{\alpha_1 - \alpha_2} = \alpha .
\]

Marginalize over \( \mathcal{T} \), we have
\[
\mathbb{P} \{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{\mathcal{F}}_{n+1}^{Z_{n+1}}) \} = \alpha .
\]
By Lemma A.1 equivalently, we have
\[
\mathbb{P} \{ V_{n+1}^{Z_{n+1}} \leq Q(\hat{\alpha}; \hat{\mathcal{F}}_{n+1}^{Z_{n+1}}) \} = \alpha .
\]

A.3 Proof of Lemma 6.6

For any \( \hat{\alpha} \) and \( Z_{n+1} = (X_{n+1}, y) \), let \( u_i^* = Q(\hat{\alpha}; \sum_{j=1}^{n} p_{i,j}^H \delta_{V_j} + p_{i,n+1}^H \delta_{V_{n+1}}), \forall i = 1, 2, \ldots, n + 1 \), and
\[ \hat{\alpha}(y) := \sum_{i=1}^{n+1} \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{I}_{v_i \leq v_i^*} \quad \text{for } v_i^* \text{ evaluated at } Z_{n+1} = (X_{n+1}; y) . \]

Apply Lemma A.2 let \( \mathcal{T}(y) = \{ (Z_i, i = 1, \ldots, n + 1) = (z_i := (x_i, y_i), i = 1, \ldots, n + 1) \} \), where \( z_i = (x_i, y_i) \) for \( i = 1, \ldots, n \) and \( z_{n+1} = (x_{n+1}, y) \), we have
\[
\mathbb{P} \{ V_{n+1} \leq Q(\hat{\alpha}; \sum_{j=1}^{n} p_{n+1,j}^H \delta_{V_j} + p_{n+1,n+1}^H \delta_{\infty}) | \cup_{y \in \mathcal{T}} \mathcal{T}(y) \} .
\]
\[
\geq \min_y \mathbb{P}\{V_{n+1} \leq Q(\hat{\alpha}; \sum_{j=1}^n p_{n+1,j}^H \delta V_j + p_{n+1,n+1}^H \delta_{\infty})|T(y)\}
= \min_y \{\hat{\alpha}(y)|T(y)\}. \tag{7}
\]

If we can show that we are choosing \( \hat{\alpha} \) such that \( \min_y \hat{\alpha}(y) \geq \alpha \), then we can prove Lemma \[6.6\] by marginalizing over \( z_i \) for \( i = 1, \ldots, n \) and \( x_{n+1} \). Also, notice that when \( \bar{v}^* = \infty \), any coverage requirement will be satisfied, hence, we need only to consider the case when \( \bar{v}^* < \infty \).

The key observations which we use to prove it are that, for any \( \bar{v} \), \( y \) only influences \( v_i^* \) through \( V_{n+1} \).

- \( v_i^* \) is non-decreasing as \( V_{n+1} \) increases. Thus, \( \sum_{i=1}^n \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{1}_{V_i \leq v_i^*} \) is non-decreasing as \( V_{n+1} \) increases.

- \( \bar{v}^* = v_{n+1}^* \) if \( V_{n+1} > \bar{v}^* \). If \( \bar{v}^* = \infty \), we have \( \bar{v}^* = v_{n+1}^* \). Otherwise, the quantile \( Q(\hat{\alpha}; \hat{F}) \) takes value in \( \{V_1, \ldots, V_n\} \), and suppose it is the \( (i^*)^{th} \) (\( \leq n \)) smallest value in \( \{V_1, \ldots, V_n\} \). Without loss of generality, suppose \( V_1 \leq V_2 \leq \ldots \leq V_n \). By definition, \( i^* \) is the smallest number such that

\[
\sum_{i=1}^{i^*} \frac{p_{n+1,j}^H \delta V_j}{\sum_{j=1}^{n+1} p_{n+1,j}^H \delta V_j} \geq \hat{\alpha}.
\]

On the one hand, according to the definition of \( Q(\hat{\alpha}; \hat{F}) \), we have \( Q(\hat{\alpha}; \hat{F}) \leq V_{i^*} \). Hence, \( v_{n+1}^* \geq \bar{v}^* \). On the other hand, we always have \( Q(\alpha; \hat{F}) \geq Q(\alpha, \sum_{j=1}^{n+1} p_{n+1,j}^H \delta V_j) \). Consequently, we have \( \bar{v}^* = v_{n+1}^* \).

Hence, when \( \bar{v}^* < \infty \), we consider two cases:

1. If \( \bar{v}^* < V_{n+1} \), use the fact that \( v_i^* \) is non-decreasing in \( V_{n+1} \) and \( v_{n+1}^* = \bar{v}^* \), we have

\[
\inf_{\bar{v}^* < V_{n+1} \leq \infty} \hat{\alpha}(y) = \inf_{V_{n+1} > \bar{v}^*} \left\{ \sum_{i=1}^n \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{1}_{V_i \leq v_i^*} \right\}
\geq \sum_{i=1}^n \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{1}_{V_i \leq v_{i^*}^*}.
\]

2. If \( V_{n+1} \leq \bar{v}^* \), again by the non-decreasing nature of \( \sum_{i=1}^n \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{1}_{V_i \leq v_i^*} \), we have

\[
\inf_{V_{n+1} \leq \bar{v}^* < \infty} \hat{\alpha}(y) = \sum_{i=1}^n \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{1}_{V_i \leq v_{i^*}^*} + \frac{w(X_{n+1})}{\sum_{j=1}^{n+1} w(X_j)}.
\]

Combine them together, when \( \bar{v}^* < \infty \), we have

\[
\inf_y \hat{\alpha}(y) \geq \min\left( \sum_{i=1}^n \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{1}_{V_i \leq v_{i^*}^*}, \sum_{i=1}^n \frac{w(X_i)}{\sum_{j=1}^{n+1} w(X_j)} \mathbb{1}_{V_i \leq v_{i^*}^*} + \frac{w(X_{n+1})}{\sum_{j=1}^{n+1} w(X_j)} \right).
\]

Hence, if \( \hat{\alpha} \) leads to \( \bar{v}^* = \infty \) or makes eq.\ref{G21} hold, we have

\[
\mathbb{P}\{V_{n+1} \leq Q(\hat{\alpha}; \hat{F})|\cup_{y \in \mathcal{Y}} T(y)\} \geq \alpha.
\]

Marginalizing over \( z_i \) for \( i = 1, \ldots, n \) and \( x_{n+1} \), we have

\[
\mathbb{P}\{V_{n+1} \leq Q(\hat{\alpha}; \hat{F})\} \geq \alpha.
\]
A.4 Proof of Theorem 5.1

Proof. Conditional on $X_{n+1} = x_0$, define $\hat{p}(x) = \frac{H(x_0,x)}{\sum_{j=1}^{n} H(x_0,X_j) + H(x_0,X_{n+1})}$ and let

$$\tilde{C}(X_{n+1},x_0) := \{ y : V(\tilde{X}_{n+1}, y) \leq Q(\alpha; \sum_{i=1}^{n} \hat{p}(X_i)\delta_{V_i} + \hat{p}(X_{n+1})\delta_{\infty}) \}.$$ 

As a direct application of Proposition 5.6, we have

$$\mathbb{P}\{\tilde{Y}_{n+1} \in \tilde{C}(X_{n+1},x_0)\} \geq \alpha.$$ 

Since the $H(x_0, x_0) \geq H(x_0, \tilde{X}_{n+1})$, define $p(x) = \frac{H(x_0,x)}{\sum_{j=1}^{n} H(x_0,X_j) + H(x_0,x_0)}$, we have

$$Q(\alpha; \sum_{i=1}^{n} \hat{p}(X_i)\delta_{V_i} + \hat{p}(X_{n+1})\delta_{\infty}) \leq Q(\alpha; \sum_{i=1}^{n} p(X_i)\delta_{V_i} + p(x_0)\delta_{\infty}).$$

Hence, let $\tilde{C}(x_0) := \{ y : V(\tilde{X}_{n+1}, y) \leq Q(\alpha; \sum_{i=1}^{n} p(X_i)\delta_{V_i} + p(x_0)\delta_{\infty}) \}$, we have

$$\mathbb{P}\{\tilde{Y}_{n+1} \in \tilde{C}(x_0)\} \geq \alpha.$$ 

The above is true for all $x_0 \in \mathbb{R}^p$, thus, we have $\mathbb{P}\{\tilde{Y}_{n+1} \in \tilde{C}(X_{n+1})|X_{n+1} = x_0\} \geq \alpha$ for all $x_0$. \qed

B Choice of $H$

We consider two types of localizers in this paper:

1. Distance based localizer: We let $H_h(x_1, x_2, X) = 1_{[|x_1 - x_2| \leq 1]}$.

2. Nearest-neighbor based localizer: $H_h(x_1, x_2, X) = 1_{[x_1 - x_2] \leq Q(\frac{1}{\pi h}; \sum_{i=1}^{n} \delta_{X_i - x_1})}$.

In practice, we can pick $h$ beforehand based on a date set $D_0$ that is independent of $Z = \{Z_1, \ldots, Z_n, Z_{n+1}\}$, with $Z_i^0 \overset{i.i.d.}{\sim} \mathcal{P}$ for $Z_i^0 = (X_i^0, Y_i^0) \in D_0$, $i = 1, \ldots, m$. Let $X^0 = \{X_0^0, \ldots, X_m^0\}$.

Define the score for sample $Z_i^0$ as $V_i^0 = V(Z_i^0)$ if $V(.)$ is also independent of $D_0$. If $V(.)$ is trained using $D_0$, we suggest to let $V_i^0$ be its score from cross-validation using $D_0$. For example, suppose $V(z) = |y - \hat{\mu}(z)|$, where $\hat{\mu}(.)$ is the prediction function trained using $D_0$, we can let

$$V_i^0 = |Y_i^0 - \hat{\mu}(X_i^0)|$$

where $\hat{\mu}(X_i^0)$ is the trained prediction function with a subset in $D_0 \setminus \{Z_i^0\}$.

Now, based on the discussion in section 3, let $h_1 < h_2 < \ldots < h_L$, we use the following steps to choose $h$ from $h_l$, $1 \leq l \leq L$ automatically using $D_0$. To reduce the computational complexity, we simply let $\tilde{\alpha} = \alpha$ in Algorithm 1.

1. Let $\hat{v}_{i,l}^*$ be the realization of $\hat{v}^*$ at $\tilde{\alpha} = \alpha$, with test sample $Z_i^0$ and training samples $D_0 \setminus \{Z_i^0\}$, and with parameter $h_l$ for the localizer $H$: $\hat{v}_{i,l}^* = Q(\alpha; \sum_{j \neq i} p_{i,j}^l \delta_{V_j^0} + p_{i,i}^l \delta_{\infty})$, here $p_{i,j}^l = \frac{H_{h_l}(X_i^0, X_j^0, X_0^0)}{H_{h_l}(X_i^0, X_j^0, X_{n+1})}.$

2. As $h$ becomes smaller, the percent of $\hat{v}_{i,l}^*$ being $\infty$ may becomes higher for $i = 1, \ldots, m$ (note that if $\hat{v}_{i,l}^* = \infty$, then, for $l_2 < l_1$, $\hat{v}_{i,l_2}^* = \infty$). We consider only those $h_l$ that result in less than $(1 - \omega)$ percent of $\infty$, and let $\mathcal{X} \in D_0$ be the intersection of samples with finite $\hat{v}_{i,l}^*$ for all $h_l$ we consider.

3. Let $s_l = \frac{\sum_{i=1}^{m} \hat{v}_{i,l}^* 1_{X_i^0 \in \mathcal{X}}}{\sum_{i=1}^{m} 1_{X_i^0 \in \mathcal{X}}}$ be an estimate of average CI length in $\mathcal{X}$ using $h_l$.

4. Let $\gamma_l = \frac{1 - \alpha}{\sum_{i=1}^{m} 1_{X_i^0 \in \mathcal{X}}}$, $\gamma_l \in 1$ be a measure of degree of empirical under-coverage. (if the empirical coverage for samples in $\mathcal{X}$ is at least $\alpha$ using $h_l$, $\gamma_l = 1$; otherwise, $\gamma_l > 1$.)
5. We estimate the average standard deviation with Bootstrap: for each sample \( X_i^0 \) and \( h = h_l \), let \( \tilde{v}_{i,l}^{b,*} \), \( b = 1, \ldots, B \), be the value \( \tilde{v}^* \) with test sample \( X_i^0 \) and \( (n - 1) \) training samples \( Z_{j}^0 \) bootstrapped from \( D_0 \) with their corresponding score values \( V_{j}^0 \). Let \( \sigma_{i,l} \) be the estimated standard deviation using those \( \tilde{v}_{i,l}^{b,*} \) with finite values for \( b = 1, \ldots, B \), and let \( \bar{\sigma}_l \) be the average standard deviation of \( \sigma_{i,l} \) across \( i = 1, \ldots, m \).

6. Choose \( h \) as

\[
\hat{h} = \arg \min_{h \in \{h_1, \ldots, h_L\}} (\gamma_l \times (s_l + \sigma_l)).
\]

By default, we let \( \omega = .9 \) and \( B = 20 \). In high-dimension where \( p \) is large, instead of applying the localizer to the raw feature \( x \), we usually will prefer to use a low dimensional function \( t : \mathbb{R}^p \to \mathbb{R}^K \), and apply \( H \) to \( t(x) \). How to find a good \( t \) is non-trivial and beyond the scope of this paper, and here we simply let \( t(x) = x_j \) where \( j \) is the direction that leads to the largest mutual information between \( V_{i}^0 \) and \( X_{i,j}^0 \), \( i = 1, \ldots, m \).

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