Model-Free Predictive Inference
DSO 621

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Introduction

Problem setup

Assumption:

$$(X_i, Y_i) \overset{\text{iid}}{\sim} P_{X,Y}$$

The joint distribution $P_{X,Y}$ is unknown.

- $X \in \mathbb{R}^p$ explanatory variables
- $Y \in \mathbb{R}$ response variable

Data: $\{(X_i, Y_i)\}_{i=1}^n$.

Goal: predict Y_{n+1} given X_{n+1}, **accounting for uncertainty**.

Prediction sets

Assumption:

$$(X_i, Y_i) \overset{\text{iid}}{\sim} P_{X,Y}$$

Fix $\alpha \in (0,1)$ and construct a prediction rule $\hat{C}_\alpha$ such that

$$\hat{C}_\alpha(X) \subseteq \mathbb{R}$$

and

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

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In regression problems, we may want $\hat{C}_\alpha(X)$ to be an interval.

Example (regression)

X: Facebook page features, Y: number of comments

Test: X_{n+1}. What could Y_{n+1} be?

Example (classification)

X: Image, Y: label

Test point: 

What digit is this? Probably 5 or 6.

Review of classical linear regression

Suppose

- X_i are fixed,
- $Y_i = X_i^\top \beta + \varepsilon_i$, where $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$.

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Data: $\mathbb{X} \in \mathbb{R}^{n \times p}, \mathbb{Y} \in \mathbb{R}^n$. Least-squares estimate of β:

$$\hat{\beta} = (\mathbb{X}^\top \mathbb{X})^{-1} \mathbb{X}^\top \mathbb{Y} \sim \mathcal{N}(\beta, \sigma^2 (\mathbb{X}^\top \mathbb{X})^{-1})$$

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Predictions:

$$\hat{Y}_{n+1} = X_{n+1}^\top \hat{\beta} \sim \mathcal{N}(X_{n+1}^\top \beta, \sigma^2 X_{n+1}^\top (\mathbb{X}^\top \mathbb{X})^{-1} X_{n+1})$$

Review of classical linear regression (continued)

Predictions:

$$\hat{Y}_{n+1} = X_{n+1}^{\top}\hat{\beta}$$

Review of classical linear regression (continued)

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$$\begin{aligned}\hat{Y}_{n+1} &= X_{n+1}^\top \hat{\beta} \\ &= X_{n+1}^\top \beta + \sigma \sqrt{X_{n+1}^\top (\mathbb{X}^\top \mathbb{X})^{-1} X_{n+1}} \cdot \mathcal{N}(0,1)\end{aligned}$$

Review of classical linear regression (continued)

Predictions:

$$\begin{aligned}
\hat{Y}_{n+1} &= X_{n+1}^\top \hat{\beta} \\
&= X_{n+1}^\top \beta + \sigma \sqrt{X_{n+1}^\top (\mathbb{X}^\top \mathbb{X})^{-1} X_{n+1}} \cdot \mathcal{N}(0,1) \\
&= Y_{n+1} - \sigma \cdot \mathcal{N}(0,1) + \sigma \sqrt{X_{n+1}^\top (\mathbb{X}^\top \mathbb{X})^{-1} X_{n+1}} \cdot \mathcal{N}(0,1)
\end{aligned}$$

Review of classical linear regression (continued)

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&= Y_{n+1} + \sigma \sqrt{1 + X_{n+1}^\top (\mathbb{X}^\top \mathbb{X})^{-1} X_{n+1}} \cdot \mathcal{N}(0,1).
\end{aligned}
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Review of classical linear regression (continued)

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Recall that

$$(n-p-1)\hat{\sigma}^2 = \mathrm{RSS} \sim \sigma^2 \cdot \chi^2_{n-p-1}$$

Review of classical linear regression (continued)

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Recall that

$$(n-p-1)\hat{\sigma}^2 = \mathrm{RSS} \sim \sigma^2 \cdot \chi^2_{n-p-1}$$

Therefore,

$$\sigma = \frac{\hat{\sigma}}{\sqrt{\chi^2_{n-p-1}/(n-p-1)}}.$$

Review of classical linear regression (continued)

Replace σ with $\hat{\sigma}$ into formula for prediction:

$$
\begin{aligned}
\hat{Y}_{n+1} &= Y_{n+1} + \sigma\sqrt{1 + X_{n+1}^\top(\mathbb{X}^\top\mathbb{X})^{-1}X_{n+1}} \cdot \mathcal{N}(0,1) \\
&= Y_{n+1} + \hat{\sigma}\sqrt{1 + X_{n+1}^\top(\mathbb{X}^\top\mathbb{X})^{-1}X_{n+1}} \cdot \frac{\mathcal{N}(0,1)}{\sqrt{\chi^2_{n-p-1}/(n-p-1)}} \\
&= Y_{n+1} + \hat{\sigma}\sqrt{1 + X_{n+1}^\top(\mathbb{X}^\top\mathbb{X})^{-1}X_{n+1}} \cdot t_{n-p-1}
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\end{aligned}$$

Prediction interval $(1-\alpha)$ for Y_{n+1}:

$$\hat{C}_\alpha(X_{n+1}) = \hat{Y}_{n+1} \pm \hat{\sigma}\sqrt{1 + X_{n+1}^\top(\mathbb{X}^\top\mathbb{X})^{-1}X_{n+1}} \cdot t_{n-p-1}^{(\alpha/2)}.$$

Review of classical linear regression (continued)

The prediction interval

$$\hat{C}_\alpha(X_{n+1}) = \hat{Y}_{n+1} \pm \hat{\sigma}\sqrt{1 + X_{n+1}^\top(\mathbb{X}^\top\mathbb{X})^{-1}X_{n+1}} \cdot t_{n-p-1}^{(\alpha/2)}.$$

satisfies:

$$\mathbb{P}\left[Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \mid \mathbb{X}, X_{n+1}\right] = 1 - \alpha.$$

Model-free predictive inference

$$(X_i, Y_i) \overset{\text{iid}}{\sim} P_{X,Y}$$

Much more general problem:

- $P(Y \mid X)$ could be anything (completely unknown)
- Prediction rule $\hat{Y}$ is a machine learning black box
  (e.g., neural network, random forests, Bayesian trees, ...)

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We need some leverage:

- X is random
- Prediction coverage will not be conditional on X

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

Exchangeability

Exchangeable random variables

We say that $Z_1, Z_2, \ldots, Z_n$ are exchangeable if and only if, for any permutation σ of $\{1, \ldots, n\}$,

$$p(Z_1, Z_2, \ldots, Z_n) = p(Z_{\sigma(1)}, Z_{\sigma(2)}, \ldots, Z_{\sigma(n)}).$$

For example, $Z_1, Z_2, \ldots, Z_n$ are exchangeable if they are i.i.d.

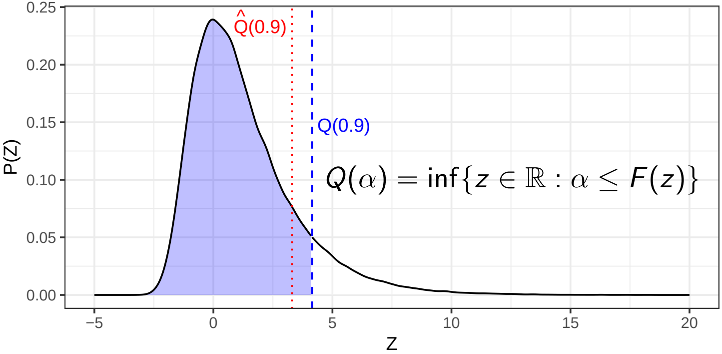
Prediction without covariates

Suppose we have

$$Z_i \overset{\text{exch.}}{\sim} P_Z, \qquad Z \in \mathbb{R}$$

and we want to use the first n data points to construct a one-sided prediction interval $\hat{C}_\alpha = (-\infty, \hat{U}_{1-\alpha}]$ such that

$$\mathbb{P}\left[Z_{n+1} \leq \hat{U}_{1-\alpha}\right] \geq 1 - \alpha.$$



Empirical quantiles

Empirical CDF and quantile function:

$$\hat{F}_n(z) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}\left[Z_i \leq z\right], \qquad \hat{Q}_n(\alpha) = Z_{(\lceil \alpha n \rceil)}$$

Lemma

Suppose $Z_1, \ldots, Z_n$ are exchangeable random variables. For any $\alpha \in \{0, 1\}$,

$$\mathbb{P}\left[Z_n \leq \hat{Q}_n(\alpha)\right] \geq \alpha.$$

Moreover, if $Z_1, \ldots, Z_n\}$ are a.s. distinct,

$$\mathbb{P}\left[Z_n \leq \hat{Q}_n(\alpha)\right] \leq \alpha + \frac{1}{n}.$$

Proof (a)

Notation:

$$\hat{F}_n(z) := \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}\left[Z_i \le z\right], \qquad \hat{Q}_n(\alpha) := Z_{(\lceil \alpha n \rceil)}.$$

Claim:

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Proof:

$$\mathbb{P}\left[Z_n \le \hat{Q}_n(\alpha)\right]$$

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&\ge \alpha.
\end{aligned}$$

Proof (b)

Notation:

$$\hat{F}_n^{-}(z) := \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}\left[Z_i < z\right], \qquad \hat{R}_n(\alpha) := Z_{(\lfloor \alpha n \rfloor + 1)}.$$

Claim: if $Z_1, \ldots, Z_n\}$ are a.s. distinct,

$$\mathbb{P}\left[Z_n \leq \hat{Q}_n(\alpha)\right] \leq \alpha + \frac{1}{n}.$$

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&\leq \alpha + \frac{1}{n}.
\end{aligned}$$

Inflation of quantiles

Lemma

Suppose $Z_1, \ldots, Z_{n+1}$ are exchangeable random variables.
For any $\alpha \in \{0, 1\}$, define α_n as:

$$\alpha_n = \left(1 + \frac{1}{n}\right)\alpha.$$

Then,

$$\mathbb{P}\left[Z_{n+1} \leq \hat{Q}_n(\alpha_n)\right] \leq \alpha.$$

Moreover, if $\{Z_1, \ldots, Z_{n+1}\}$ are a.s. distinct,

$$\mathbb{P}\left[Z_n \leq \hat{Q}_n(\alpha_n)\right] \leq \alpha + \frac{1}{n+1}.$$

Proof (a)

Notation:

$$\hat{F}_n(z) := \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}\left[Z_i \le z\right], \qquad \hat{Q}_n(\alpha) := Z_{(\lceil \alpha n \rceil)},$$

$$\hat{F}_{n+1}(z) := \frac{1}{n+1}\sum_{i=1}^{n+1} \mathbb{1}\left[Z_i \le z\right], \qquad \hat{Q}_{n+1}(\alpha) := Z_{(\lceil \alpha (n+1) \rceil)}.$$

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Proof:

$$\mathbb{P}\left[Z_{n+1} \leq \hat{Q}_n(\alpha_n)\right] = \mathbb{P}\left[Z_{n+1} \leq \hat{Q}_n\left((1+1/n)\alpha\right)\right]$$

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&\ge \alpha.
\end{aligned}$$

Proof (b)

Notation:

$$\hat{F}_n^-(z) := \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}\left[Z_i < z\right], \qquad \hat{R}_n(\alpha) := Z_{(\lfloor \alpha n \rfloor + 1)}.$$

Claim: if $Z_1, \ldots, Z_{n+1}\}$ are a.s. distinct,

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\end{aligned}$$

One-sided prediction interval without covariates

Suppose $Z_1, \dots, Z_{n+1}$ are exchangeable random variables.
For any $\alpha \in \{0, 1\}$, define $\hat{C}_\alpha$ as

$$\hat{C}_\alpha = (-\infty, \hat{Q}_n(\alpha_n)].$$

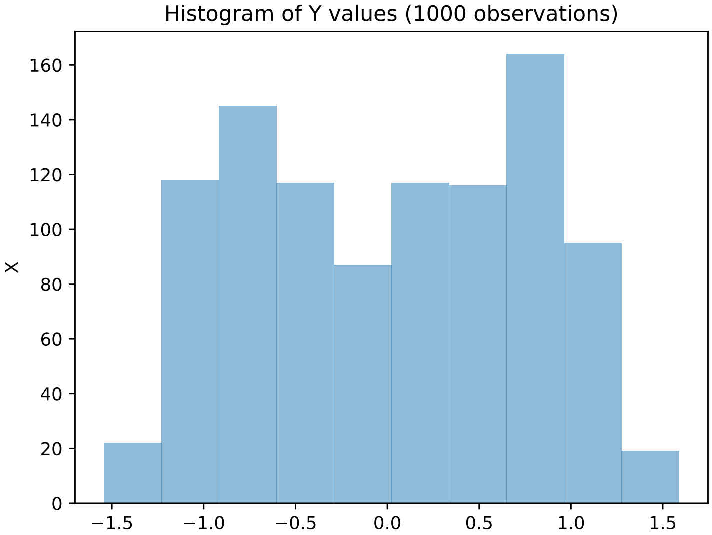
Then,

$$\alpha \leq \mathbb{P}\left[Z_{n+1} \in \hat{C}_\alpha\right] \leq \alpha + \frac{1}{n}.$$

Split Conformal Prediction

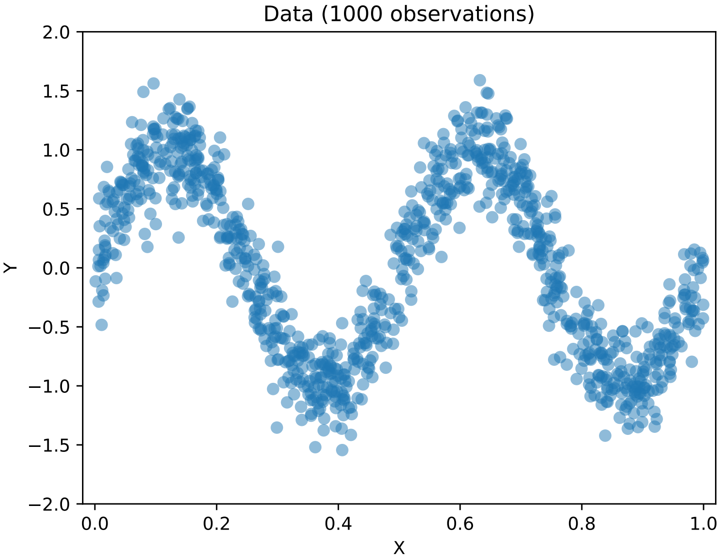
Prediction with covariates

We would like to predict a variable Y...



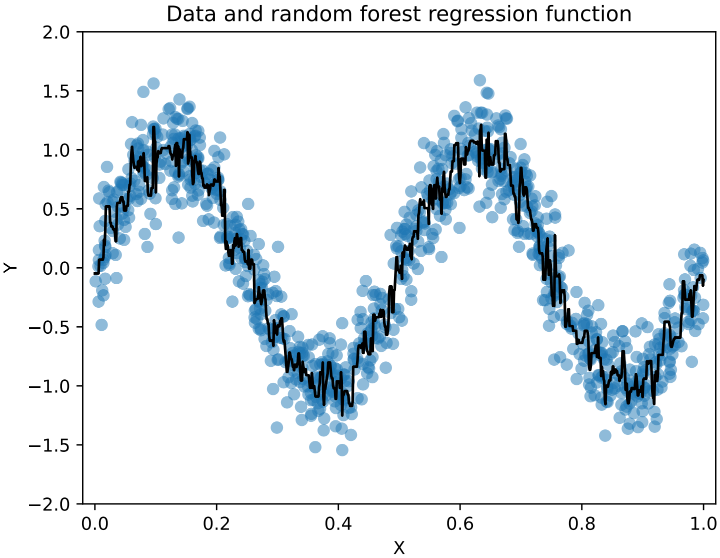
Prediction with covariates

We would like to predict a variable Y... **using some covariates** X.



Machine-learning prediction

Lots of machine-learning algorithms. But how confident are we?



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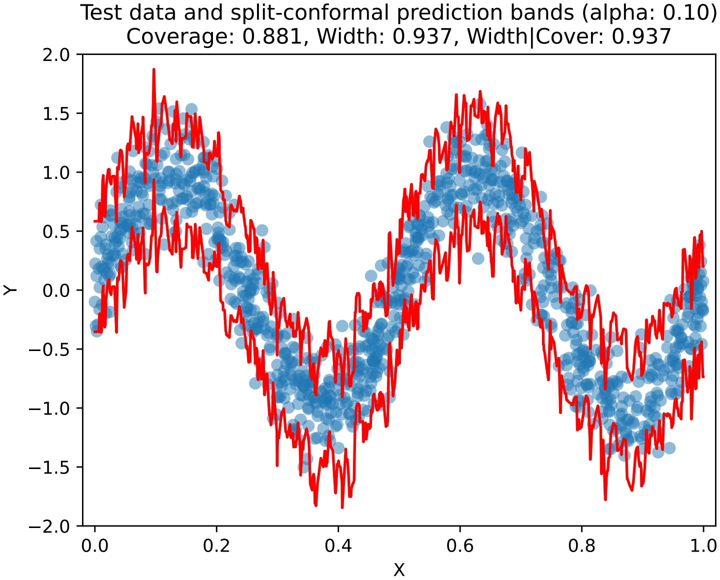

Conformal prediction

Key ideas:

1. Use ML to project project the problem into 1 dimension.
2. Apply the empirical quantile lemmas presented earlier.
3. Some kind of data hold-out is needed to ensure exchangeability with the test data.

This is a general recipe, many different variations are possible.

Split-conformal prediction

Algorithm 1: Split-conformal prediction

Input: Data $\{(X_i, Y_i)\}_{i=1}^n$, test point X_{n+1}, $\alpha \in (0,1)$
black-box model $\mathcal{B}$, level $\alpha \in (0,1)$

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Output:

$\hat{C}_\alpha(X_{n+1}) = [\hat{f}(X_{n+1}) - \hat{Q}_n(Z_{\mathcal{I}_2}, \beta_n), \hat{f}(X_{n+1}) + \hat{Q}_n(Z_{\mathcal{I}_2}, \beta_n)]$

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Why does this work?

$$Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \quad \Longleftrightarrow \quad Z_{n+1} \leq \hat{Q}_n(Z_{\mathcal{I}_2}, \beta_n).$$

Marginal coverage of split-conformal prediction

Theorem ([Vovk et al., 2005, Lei et al., 2018])

Suppose $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ *are exchangeable. Then, the split-conformal prediction intervals* $\hat{C}_\alpha$ *satisfy*

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

Moreover, if the residuals $\{Z_{n/2+1}, \ldots, Z_{n+1}\}$ *are a.s. distinct,*

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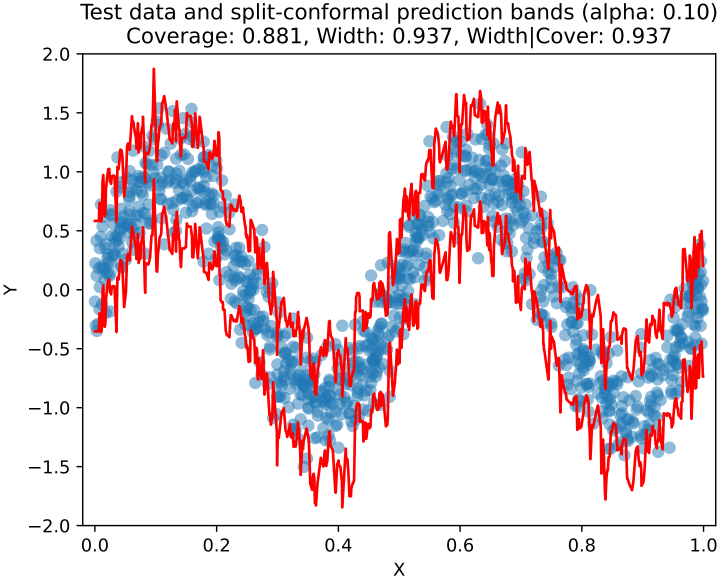
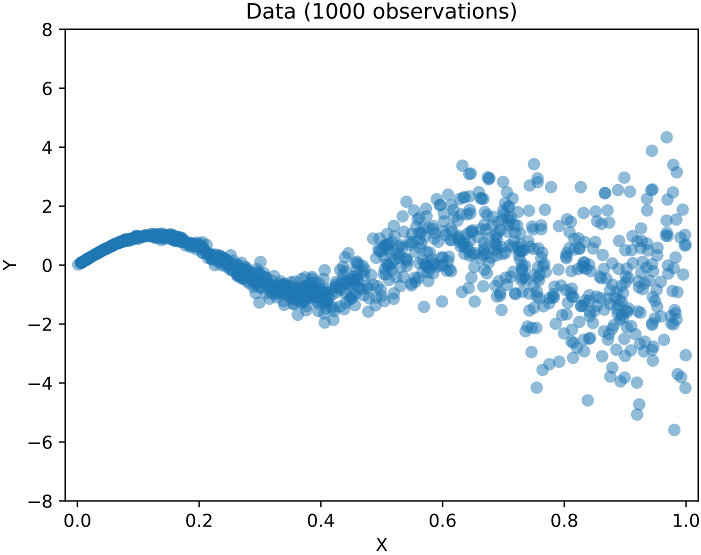
Split-conformal prediction bands



Heteroscedasticity

Suppose now Y heteroscedastic.



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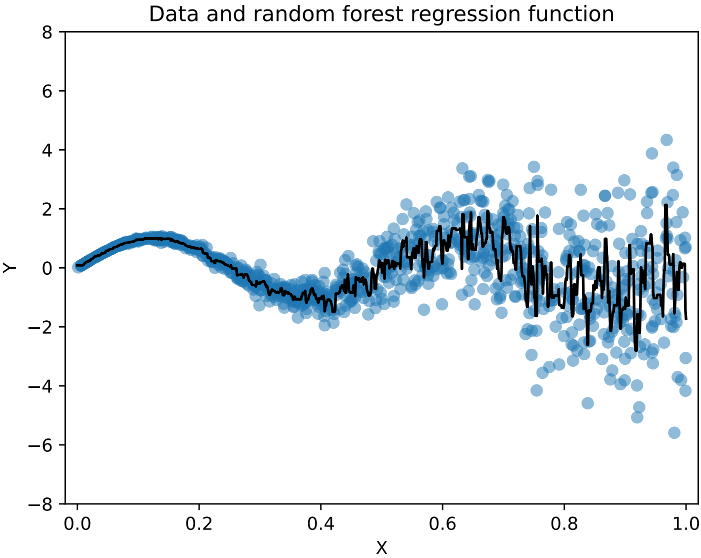

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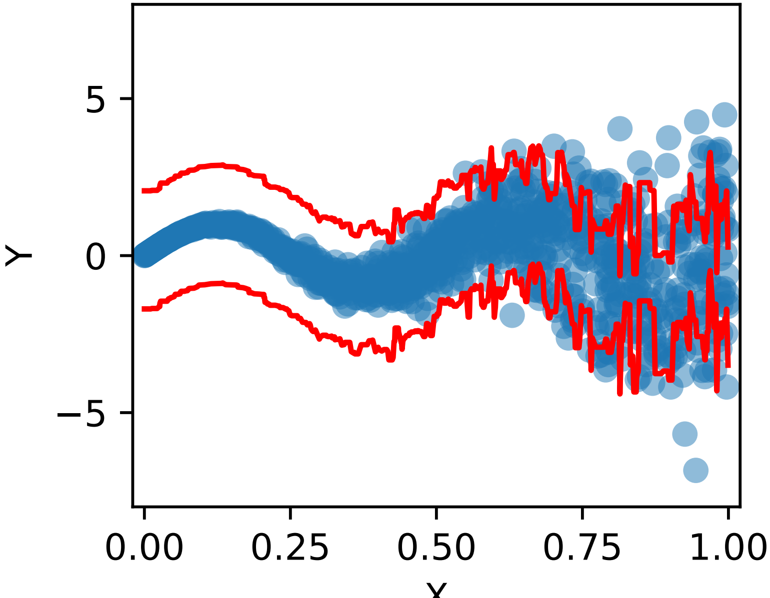

Conditional quantiles

The goal of quantile regression is to estimate conditional quantiles of $Y \mid X$ instead of the conditional mean, $\mathbb{E}[Y \mid X]$.

$$q_\alpha(x) = \inf\{y \in \mathbb{R} : F(y \mid X = x) \geq \alpha\}$$

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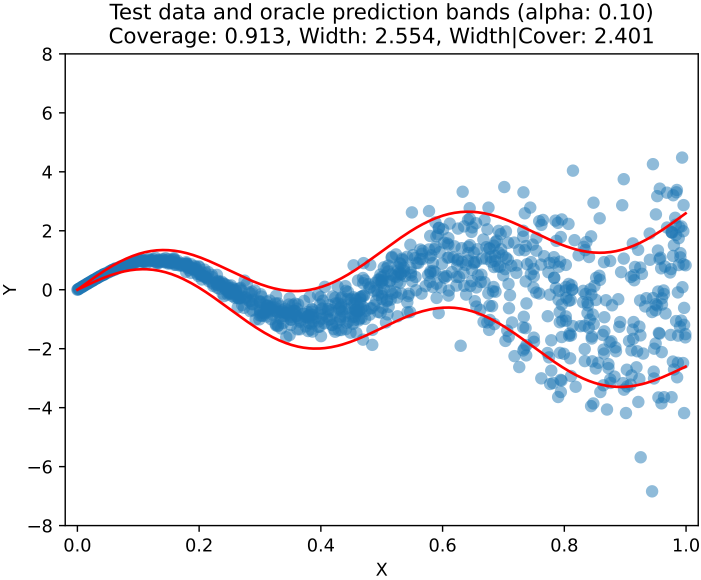
An oracle that knows $P(Y \mid X)$ would predict as follows:

$$C_\alpha^{\text{oracle}}(Y_{n+1} \mid X_{n+1} = x) = [q_{\alpha/2}(x), q_{1-\alpha/2}(x)].$$

Oracle predictions



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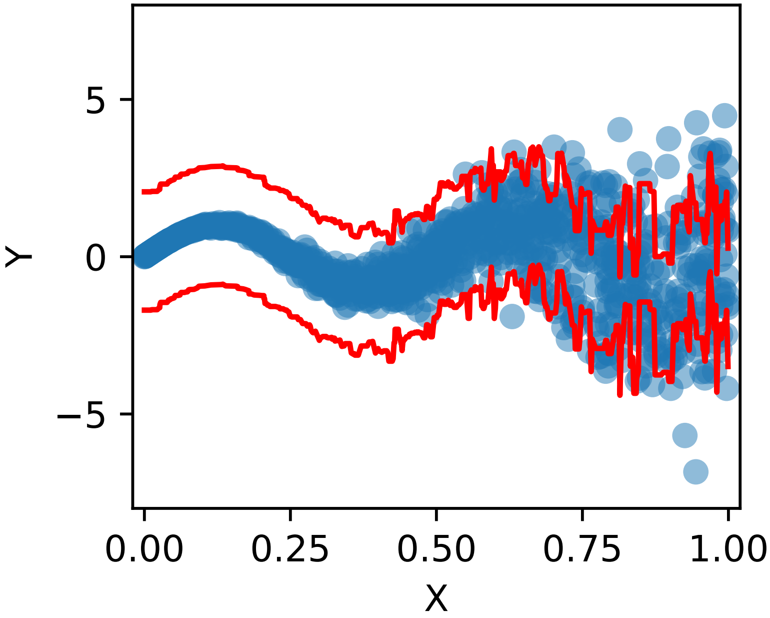
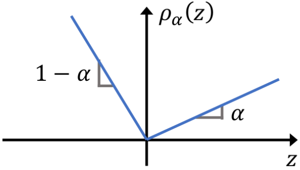


Quantile regression

Quantile regression:

$$\hat{\theta}_\alpha = \arg\min_\theta \frac{1}{n} \sum_{i=1}^{n} \rho_\alpha \left(Y_i, f_\theta(X_i) \right)$$

$$\rho_\alpha(y, \hat{y}) := \begin{cases} \alpha(y - \hat{y}) & \text{if } y - \hat{y} > 0, \\ (1-\alpha)(\hat{y} - y) & \text{otherwise} \end{cases}$$



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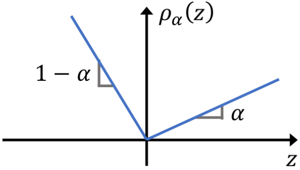

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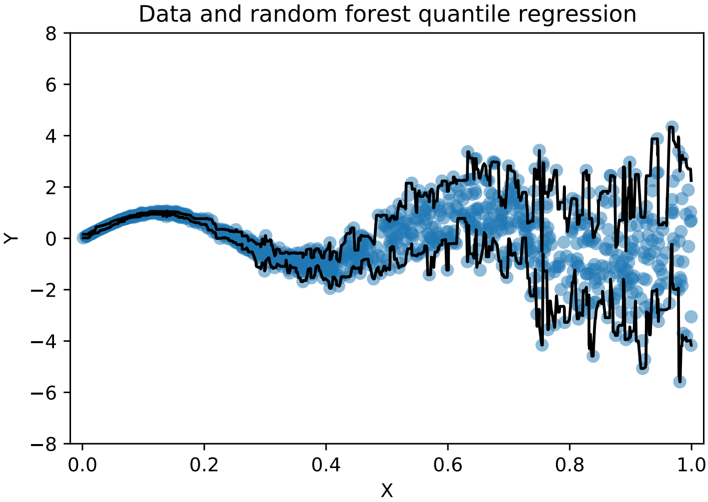
Key idea: Leibniz integral rule

$$q_\alpha(x) = \arg\min_{f(x)} \mathbb{E}\left[\rho_\alpha(Y, f(x))\right]$$

Quantile regression in action

We can fit conditional quantiles, but without guarantees.



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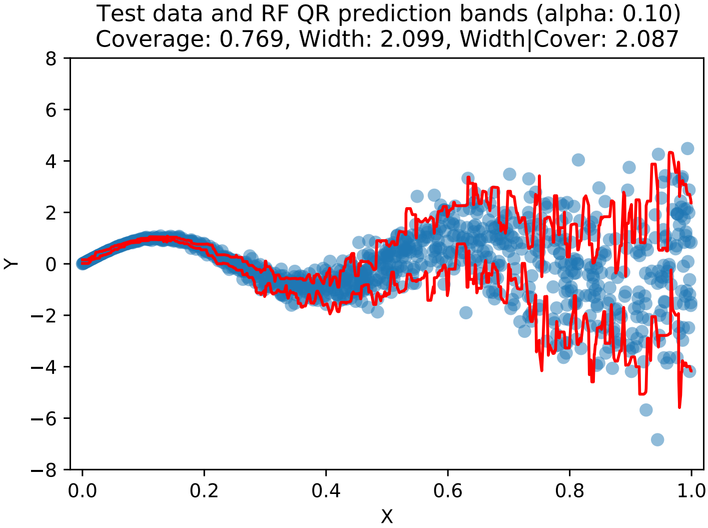

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$$= \begin{cases} Y_i - \hat{q}_{1-\alpha/2}(X_i) & \text{if } Y_i > \hat{q}_{1-\alpha/2}(X_i), \\ \hat{q}_{\alpha/2}(X_i) - Y_i & \text{if } Y_i < \hat{q}_{\alpha/2}(X_i), \\ \max\left\{ Y_i - \hat{q}_{1-\alpha/2}(X_i), \hat{q}_{\alpha/2}(X_i) - Y_i \right\} & \text{otherwise.} \end{cases}$$

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Compact notation (equivalent):

$$Z_i = \max\left\{ Y_i - \hat{q}_{1-\alpha/2}(X_i), \hat{q}_{\alpha/2}(X_i) - Y_i \right\}.$$

Split-conformal + quantile regression

Algorithm 2: Split-conformal quantile regression

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Why does this work? Same story as before.

$$Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \iff Z_{n+1} \leq \hat{Q}_n(Z_{\mathcal{I}_2}, \beta_n).$$

Marginal coverage of split-conformal prediction

Theorem ([Romano et al., 2019b])

Suppose $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ *are exchangeable. Then, the split-conformal QR prediction intervals* $\hat{C}_\alpha$ *satisfy*

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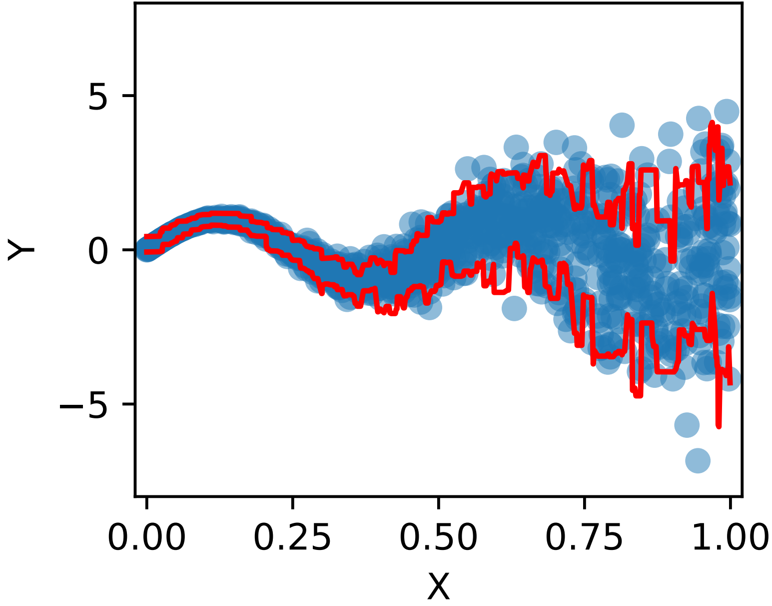
Conformal quantile regression



Efficiency of conformal quantile regression

Theorem ([Sesia and Candès, 2020])

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(A3) Assume that the probability density of the conformity scores is bounded away from zero in an open neighborhood of zero.

Then,

$$\mathcal{L}\left(\hat{C}_\alpha(X_{n+1}) \triangle C_\alpha^{\text{oracle}}(X_{n+1})\right) = o_{\mathbb{P}}(1),$$

where $\mathcal{L}$ *is the Lebesgue measure and* $A \triangle B = (A \setminus B) \cup (B \setminus A)$.

Asymptotic conditional coverage

Definition (Asymptotic conditional coverage)

We say that a sequence $\hat{C}_n$ of random prediction bands has asymptotic conditional coverage at the level $1-\alpha$ if there exists a sequence of random sets $\Lambda_n \subseteq \mathbb{R}^d$ such that

$$\mathbb{P}\left[X \in \Lambda_n\right] = 1 - o_{\mathbb{P}}(1)$$

and

$$\sup_{x \in \Lambda_n} \left| \mathbb{P}\left[Y \in \hat{C}_n(x) \mid X = x \right] - (1-\alpha) \right| = o_{\mathbb{P}}(1).$$

Asymptotic conditional coverage for CQR (under consistency and regularity assumptions) follows immediately from previous theorem.

Approximate finite-sample conditional coverage?

Is it possible to achieve finite-sample conditional coverage?

$$\mathbb{P}\left[Y_{n+1} \in \hat{C}_n^{?}(x) \mid X_{n+1} = x\right] \geq 1 - \alpha, \qquad \forall x$$

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No.

Proposition ([Vovk, 2012, Lei et al., 2013])

Suppose $\hat{C}_n$ satisfies conditional coverage at level α. Then,

$$\mathbb{E}\left[\mathcal{L}(\hat{C}_n(X_{n+1})\right] = +\infty$$

unless

$$\mathbb{P}\left[X_{n+1} = x\right] > 0.$$

Finite-sample conditional coverage?

Is approximate finite-sample conditional coverage possible?
Fix $\delta \in (0,1)$. Can we obtain the following in a non-trivial way?

$$\mathbb{P}\left[Y_{n+1} \in \hat{C}_n^{?}(x) \mid X_{n+1} \in \mathcal{X}\right] \geq 1 - \alpha,$$
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$$1 - \alpha\delta$$

However, this is extremely conservative.

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However, this is extremely conservative.

Sadly, [Foygel Barber et al., 2020] prove this is also the best way.

Coverage conditional on a discrete variable [Romano et al., 2019a]

Suppose $X_i = (X_{i,1}, X_{i,2}) \in \mathbb{R} \times \{0,1\}$.
It's easy to obtain coverage conditional on the discrete variable.

$$\mathbb{P}\left[Y_{n+1} \in \hat{C}_n^?(x) \mid X_{n+1} \in \mathbb{R} \times \{k\}\right] \geq 1 - \alpha, \qquad \forall k \in \{0,1\}$$

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Compute quantiles of conformity scores separately for each class.
For $k \in \{0,1\}$, we will use

$$\mathcal{I}_{2,k} = \{ i \in \mathcal{I}_2 : X_{i,2} = k \},$$
$$\hat{Q}_{\beta_{|\mathcal{I}_{2,k}|}}(\mathcal{I}_{2,k}, k, W\beta_{|\mathcal{I}_{2,k}|}).$$

The predictions will use the $\hat{Q}$ corresponding to the k in $X_{n+1,2}$.

Relaxed conditional coverage [Foygel Barber et al., 2020]

Similar idea can also be used with continuous variables, conditioning on a ball around a certain point.
However, this will greatly reduce the effective sample size.

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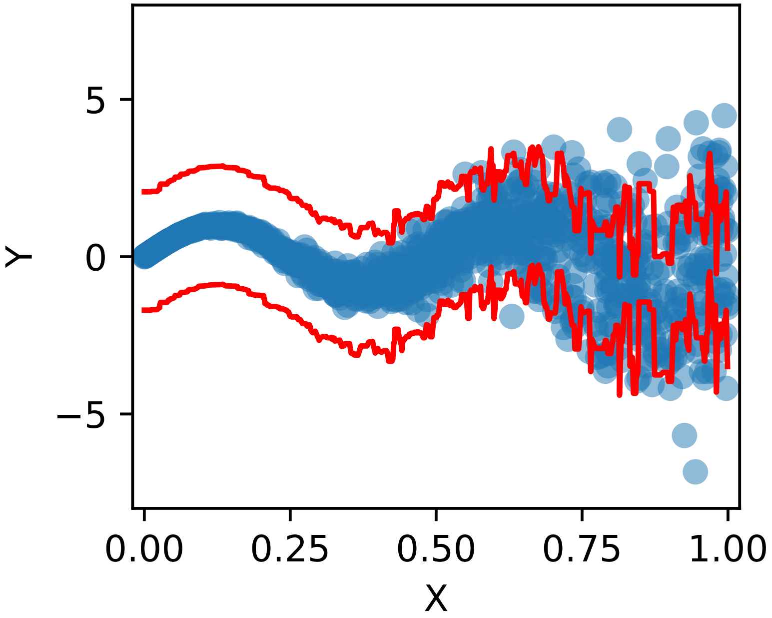
However, this will greatly reduce the effective sample size.

In the end, we typically settle for marginal coverage in theory, but we can design the algorithm carefully to seek good conditional coverage in practice.

CQR can improve conditional coverage in practice



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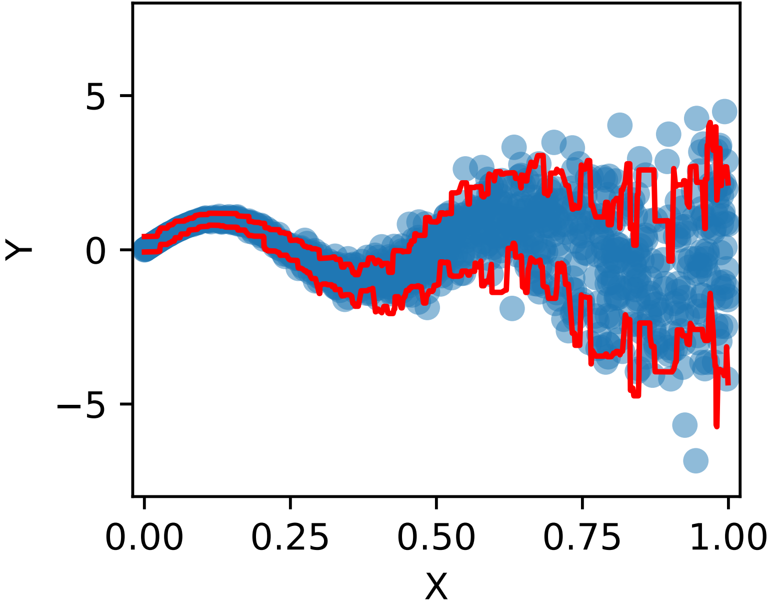

Worst-slab coverage [Cauchois et al., 2020]

How can we measure conditional coverage?

Fix a vector $v \in \mathbb{R}^p$ and two scalars $a < b$. Then, define

$$S_{v,a,b} = \{x \in \mathbb{R}^p : a \leq v^T x \leq b\}$$

For any fixed prediction set $\hat{\mathcal{C}}$ and $\delta \in (0,1)$, define

$$\mathrm{WSC}(\hat{\mathcal{C}}; \delta) = \inf_{v \in \mathbb{R}^p,\ a<b \in \mathbb{R}} \left\{ \mathbb{P}[Y \in \hat{\mathcal{C}}(X) \mid X \in S_{v,a,b}] \text{ s.t. } \mathbb{P}[X \in S_{v,a,b}] \geq 1-\delta \right\}.$$

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Can be approximated by estimating v^*, a^*, b^* on hold-out data. [Romano et al., 2020]

Split Conformal Classification

The classification problem

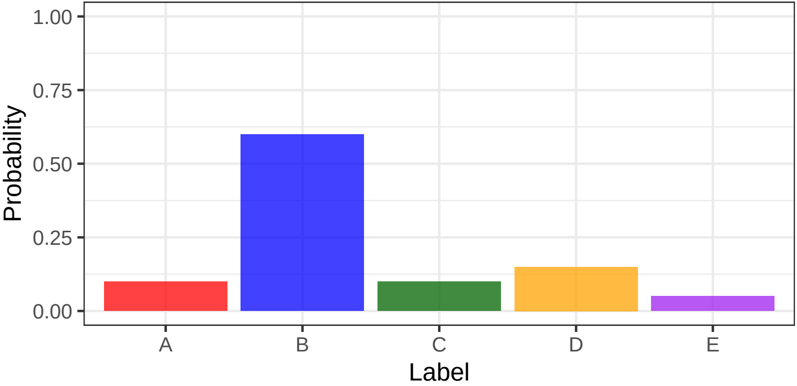
Suppose $Y_i \in \{1, 2, \ldots, C\}$ is a *categorical* variable.
We still want

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

The previous residuals (or conformity scores) no longer make sense.

The classification oracle [Romano et al., 2020]

For any $x \in \mathbb{R}^p$, set $\pi_y(x) = \mathbb{P}[Y = y \mid X = x]$ for each $y \in \mathcal{Y}$.



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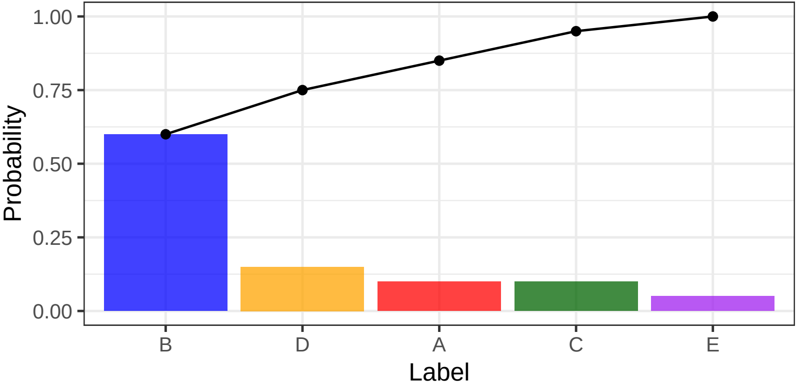

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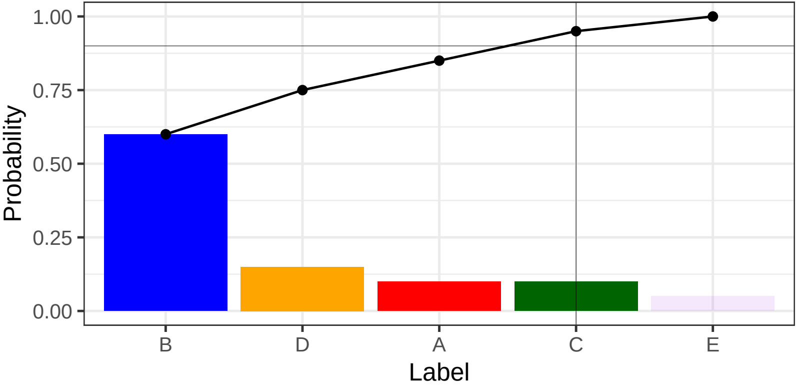

The conservative classification oracle [Romano et al., 2020]

For any $x \in \mathbb{R}^p$, set $\pi_y(x) = \mathbb{P}[Y = y \mid X = x]$ for each $y \in \mathcal{Y}$.

For $\tau \in [0, 1]$, define the *generalized conditional quantile* function

$$L(x; \pi, \tau) = \\ \min\{c \in \{1, \ldots, C\} \ : \ \pi_{(1)}(x) + \pi_{(2)}(x) + \ldots + \pi_{(c)}(x) \geq \tau\},$$

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The (conservative) oracle prediction set is:

$$C^{\text{oracle+}}(x) = \{\text{`}y\text{' indices of the } L(x; \pi, 1-\alpha) \text{ largest } \pi_y(x)\}.$$

The classification oracle

Define a function $\mathcal{S}$ with input x, $u \in [0,1]$, π, and τ:

$$\mathcal{S}(x,u;\pi,\tau) =$$
$$\begin{cases} \text{`}y\text{' indices of the } L(x;\pi,\tau)-1 \text{ largest } \pi_y(x), & \text{if } u \leq V(x;\pi,\tau), \\ \text{`}y\text{' indices of the } L(x;\pi,\tau) \text{ largest } \pi_y(x), & \text{otherwise,} \end{cases}$$

where

$$V(x;\pi,\tau) = \frac{1}{\pi_{(L(x;\pi,\tau))}(x)} \left[\sum_{c=1}^{L(x;\pi,\tau)} \pi_{(c)}(x) - \tau \right].$$

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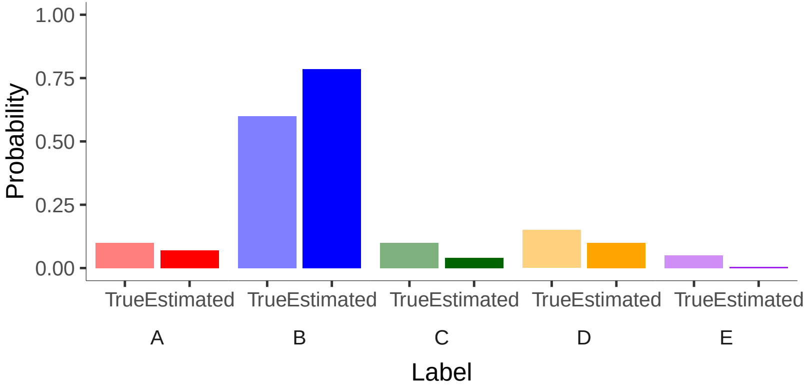
Then, the (tight) oracle would draw $U \sim \mathrm{Unif}(0,1)$ and predict:

$$C^{\mathrm{oracle}}(x) = \mathcal{S}(x,U;\pi,1-\alpha).$$

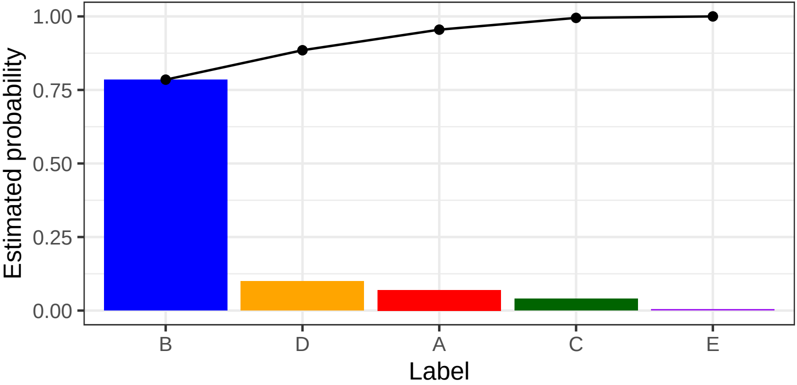
Black-box classification

We can use a black-box classifier compute an estimate $\hat{\pi}$ of π.



Plug-in prediction rule

Plug the probability estimates into the oracle decision rule.



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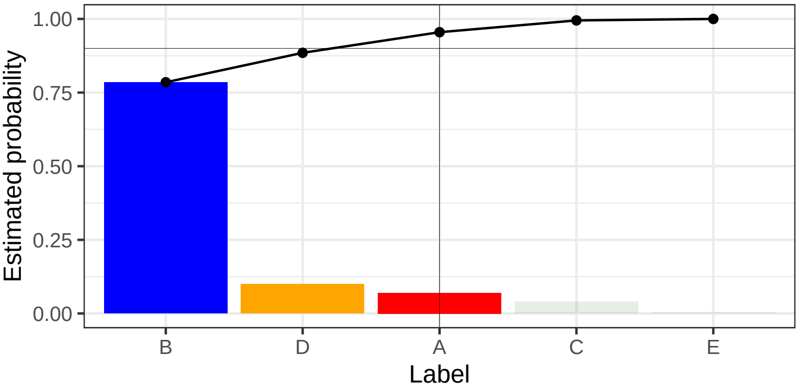

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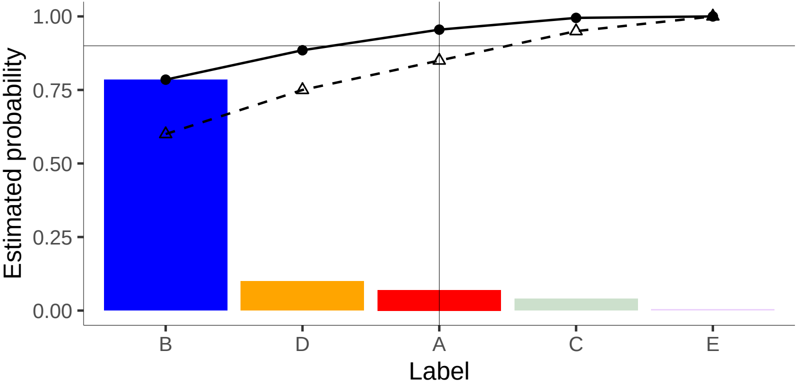

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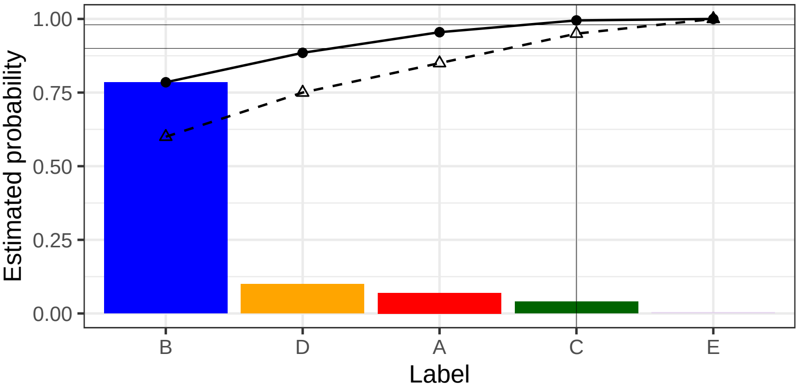
The probability estimates are often overconfident.
Therefore, we need to be more conservative.



Generalized inverse quantile conformity scores

Define a *generalized inverse quantile* conformity score function $\mathcal{Z}$ with input $x, y, u, \hat{\pi}$,

$$\mathcal{Z}(x, y, u; \hat{\pi}) = \min \{\tau \in [0, 1] : y \in \mathcal{S}(x, u; \hat{\pi}, \tau)\},$$

Interpretation:

how far do we need to go before y is classified correctly?

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Split-conformal classification

Algorithm 3: Split-conformal classification

1: **Input**: Data $\{(X_i, Y_i)\}_{i=1}^{n}$, test point X_{n+1}, $\alpha \in (0,1)$
2: black-box model $\mathcal{B}$, level $\alpha \in (0,1)$

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Output: $\hat{C}_\alpha(X_{n+1}) = \mathcal{S}(X_{n+1}, U_{n+1}; \hat{\pi}, \hat{Q}_n(Z_{\mathcal{I}_2}, \beta_n))$

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Why does this work?

$$Y_{n+1} \in \hat{C}_\alpha(X_{n+1}) \quad \Longleftrightarrow \quad Z_{n+1} \leq \hat{Q}_n(Z_{\mathcal{I}_2}, \beta_n).$$

Marginal coverage of split-conformal classification

Theorem (Romano, S., and Candès, 2020)

Suppose $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ are exchangeable. Then, the split-conformal classification sets $\hat{C}_\alpha$ satisfy

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

Moreover, under some additional smoothness assumption,

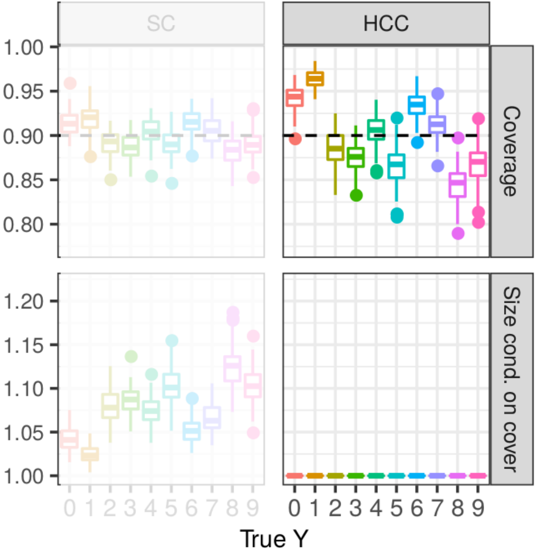
$$\mathbb{P}\left[Y_{n+1} \in \hat{C}_\alpha(X_{n+1})\right] \leq 1 - \alpha + \frac{2}{n}.$$

Tmp

$$\mathbb{P}\left[Y_{n+1} \in \hat{C}_{\alpha}(x) \mid X_{n+1} = x\right] \geq 1 - \alpha.$$

Performance on MNIST data

Handwritten digit classification. Some digits are harder.



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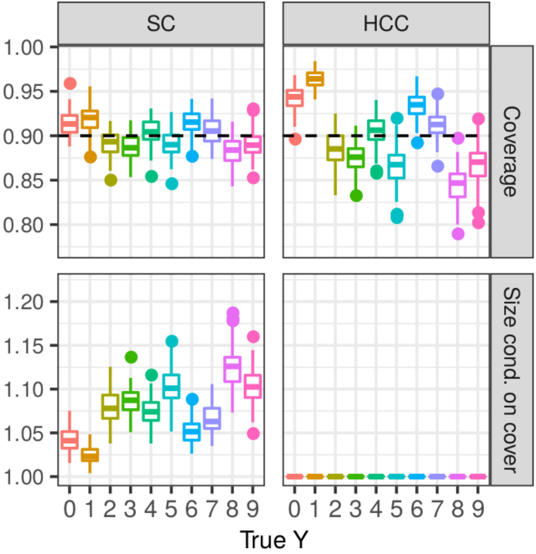

Alternative conformal hold-out methods

Full conformal

Split conformal uses only $n/2$ samples to fit the black-box model. Can we do better?

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1. For each possible value y of Y, define an augmented data set:

$$\mathcal{D}_y = \{(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, y)\}$$

2. Fit the black-box model on the new data. $\mathcal{B} : \mathcal{D}_y \to \hat{f}_y$

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3. Compute residuals (or conformity scores) on all points in $\mathcal{D}_y$:

$$\begin{aligned} Z_{y,i} &= |Y_i - \hat{f}_y(X_i)|, \quad i \in \{1, \ldots, n\}, \\ Z_{y,n+1} &= |y - \hat{f}_y(X_{n+1})|. \end{aligned}$$

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4. Rank $Z_{y,n+1}$ among $\{Z_{y,i}\}_{i=1}^{n+1}$.

Full conformal (continued)

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$$R_y = \sum_{i=1}^{n+1} \mathbb{1}\left[Z_{y,i} \leq Z_{y,n+1}\right]$$

Full conformal (continued)

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$$R_y = \sum_{i=1}^{n+1} \mathbb{1}\left[Z_{y,i} \leq Z_{y,n+1}\right] = 1 + \sum_{i=1}^{n} \mathbb{1}\left[Z_{y,i} \leq Z_{y,n+1}\right]$$

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5. Include y in $\hat{C}_\alpha^{\text{full}}$ if $R_y \leq \lceil (1-\alpha)(n+1) \rceil$.

Full conformal (continued)

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5. Include y in $\hat{C}_\alpha^{\text{full}}$ if $R_y \leq \lceil (1-\alpha)(n+1) \rceil$.

Finally, the prediction set is

$$\hat{C}_\alpha^{\text{full}}(X_{n+1}) = \left\{ y \in \mathbb{R} : R_y \leq \lceil (1-\alpha)(n+1) \rceil \right\}.$$

Full conformal (continued)

4. Rank $Z_{y,n+1}$ among $\{Z_{y,i}\}_{i=1}^{n+1}$

$$R_y = \sum_{i=1}^{n+1} \mathbb{1}\left[Z_{y,i} \leq Z_{y,n+1}\right] = 1 + \sum_{i=1}^{n} \mathbb{1}\left[Z_{y,i} \leq Z_{y,n+1}\right]$$

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Of course, we could also use full-conformal with different scores (e.g., quantile regression or classification).

Marginal coverage of full-conformal prediction

Theorem ([Vovk et al., 2005, Lei et al., 2018])

Suppose $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ *are exchangeable. Then, the full-conformal prediction intervals* $\hat{C}_\alpha$ *satisfy*

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

Moreover, if the residuals $\{Z_{n/2+1}, \ldots, Z_{n+1}\}$ *are a.s. distinct,*

$$\mathbb{P}\left[Y_{n+1} \in \hat{C}_\alpha(X_{n+1})\right] \leq 1 - \alpha + \frac{1}{n+1}.$$

Full-conformal is expensive

Full-conformal prediction is often prohibitively expensive.

It requires re-fitting the black-box model for every new X_{n+1} and every possible value of y.

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Can we do something in between full and split conformal?

Cross-validation+ [Barber et al., 2019]

Or perhaps we could call this *CV-conformal*.

Very similar to cross-conformal inference. [Vovk, 2015]

1. Divide the data points into K folds

$$\begin{aligned}
\mathcal{I}_1 &= \left\{1, \ldots, \frac{n}{K}\right\}, \\
\mathcal{I}_2 &= \left\{\frac{n}{K} + 1, \ldots, 2\frac{n}{K}\right\}, \\
&\ldots \\
\mathcal{I}_K &= \left\{(K-1)\frac{n}{K} + 1, \ldots, n\right\},
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$$\ldots$$
$$\mathcal{I}_K = \left\{(K-1)\frac{n}{K} + 1, \ldots, n\right\},$$

2. Train the black-box model on each $\mathcal{I}_k$ and evaluate the conformity scores on $\{1, \ldots, n\} \setminus \mathcal{I}_k$.

Cross-validation+ (continued)

Define a *conformity score function*:

$$\mathcal{Z}(x, y, \hat{f}) = |y - \hat{f}(x)|$$

Denote by $\hat{f}_k$ the black-box model trained on $\mathcal{I}_k$.

Denote by $k(i)$ the fold to which point i belongs, $\forall i \in \{1, \ldots, n\}$. Then, we will compute

$$Z_i = \mathcal{Z}(X_i, Y_i, \hat{f}_{k(i)}).$$

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The prediction set at level α for X_{n+1} will be:

$$\hat{C}_\alpha^{\text{cv}+} = \left\{ y : \sum_{i=1}^{n} \mathbb{1}\left[Z_i < \mathcal{Z}(X_{n+1}, y, \hat{f}_{k(i)}) \right] \leq (1-\alpha)(n+1) \right\}$$

Closed-form cross-validation+

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is equivalent to

$$\hat{C}_\alpha^{\text{cv}+} = \left[\hat{Q}^-_{\alpha,n}\left(\hat{f}_{k(i)}(X_{n+1}) - Z_i \right), \hat{Q}^+_{\alpha,n}\left(\hat{f}_{k(i)}(X_{n+1}) + Z_i \right) \right],$$

where

$$\hat{Q}^-_{\alpha,n}(\tilde{Z}) = \tilde{Z}_{\lfloor \alpha(n+1) \rfloor}, \qquad \hat{Q}^+_{\alpha,n}(\tilde{Z}) = \tilde{Z}_{\lceil (1-\alpha)(n+1) \rceil}.$$

Closed-form cross-validation+ (continued)

Suppose

$$Y_{n+1} \notin \left\{ y : \sum_{i=1}^{n} \mathbb{1}\left[Z_i < \mathcal{Z}(X_{n+1}, y, \hat{f}_{k(i)}) \right] \leq (1-\alpha)(n+1) \right\}.$$

That means, for at least $(1-\alpha)(n+1)$ values of i,

$$\begin{aligned} \mathcal{Z}(X_{n+1}, Y_{n+1}, \hat{f}_{k(i)}) &> Z_i \\ |Y_{n+1} - \hat{f}_{k(i)}(X_{n+1})| &> |Y_i - \hat{f}_{k(i)}(X_i)| \end{aligned}$$

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Marginal coverage of CV+

Theorem ([Barber et al., 2019])

Suppose $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ *are exchangeable. Then, the CV+ prediction intervals* $\hat{C}_\alpha^{cv+}$ *satisfy*

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Why 2α? It's pessimistic. Coverage often above $1 - \alpha$ in practice.

Coverage is almost exact if the base algorithm is “stable” [Barber et al., 2019].

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[Steinberger and Leeb, 2018] proves a related method is "valid conditional on data set" if the base algorithm is "stable".

Proof for CV+ (setup)

Augmented data: imagine we have access to $m = n/K$ test points

$$(X_{n+1}, Y_{n+1}, U_{n+1}), \dots, (X_{n+m}, Y_{n+m}, U_{n+m}),$$

which we put in the extra fold $\mathcal{I}_{K+1}$.

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Tournament (with teams) interpretation: i “won” against j.

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We will show that that $Y_{n+1} \in \hat{C}_\alpha^{\text{cv+}}$ if and only if

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Proof for CV+ (strategy)

Define the set of *outstanding players*

$$\mathcal{S}(A) = \left\{ i \in \{1, \ldots, n+m\} : \sum_{i=1}^{n+m} A_{n+1,i} > (1-\alpha)(n+1) \right\}$$

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Strategy: prove that

- all players equally likely to be outstanding (exchangeability)
- only so many players can be outstanding (basic logic)

Proof for CV+ (exchangeability)

Let Π be a $(n+m) \times (n+m)$ permutation matrix **that does not mix players assigned to different teams**, such that

$$(\Pi A \Pi^\top)_{ij} = A_{i',j'}$$

We can prove that $A \stackrel{d}{=} \Pi A \Pi^\top$.

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Clearly, $A_{\sigma(i)\sigma(j)} = 0 = A_{i,j}$ if $k(i) = k(j)$.

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OK, so we have $A \stackrel{d}{=} \Pi A \Pi^\top$.

Suppose Π is such that $\sigma(n+1) = j$, for any $j \in \{1, \dots, n+m\}$. Then,

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$$\mathbb{P}\left[(n+1) \in \mathcal{S}(A)\right] = \frac{1}{n+m} \sum_{i=1}^{n+m} \mathbb{P}\left[j \in \mathcal{S}(A)\right] = \frac{\mathbb{E}\left[|\mathcal{S}(A)|\right]}{n+m}.$$

Proof for CV+ (logic)

How large can $|\mathcal{S}(A)|$ be? Remember we defined

$$A_{ij} = \begin{cases} 0, & \text{if } k(i) = k(j), \\ \mathbb{1}\left[\mathcal{Z}(X_j, Y_j, \tilde{f}_{k(i),k(j)}) < \mathcal{Z}(X_i, Y_i, \tilde{f}_{k(i),k(j)})\right], & \text{if } k(i) \neq k(j), \end{cases}$$

Think of A_{ij} as indicating whether i wins a game against j, within a tournament with $n + m$ participant.

Note that i and j do not play each other if $k(i) = k(j)$.

Proof for CV+ (logic)

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$\mathcal{S}(A)$ is the set of players that win at least $(1 - \alpha)(n + 1)$ games.

Proof for CV+ (logic)

If $i \in \mathcal{S}(A)$, it lost at most $\alpha(n+1)+1$ games.

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$$\frac{s(s-1)}{2} \leq s(\alpha(n+1)+1) + \sum_{k=1}^{k} \frac{s_k(s_k-1)}{2}.$$

Therefore,

$$|\mathcal{S}(A)| = s \leq 2\alpha(n+1) + m - 2.$$

Proof for CV+ (wrapping up)

Putting everything together:

$$\mathbb{P}\left[(n+1) \in \mathcal{S}(A)\right] = \frac{\mathbb{E}\left[|\mathcal{S}(A)|\right]}{n+m}.$$

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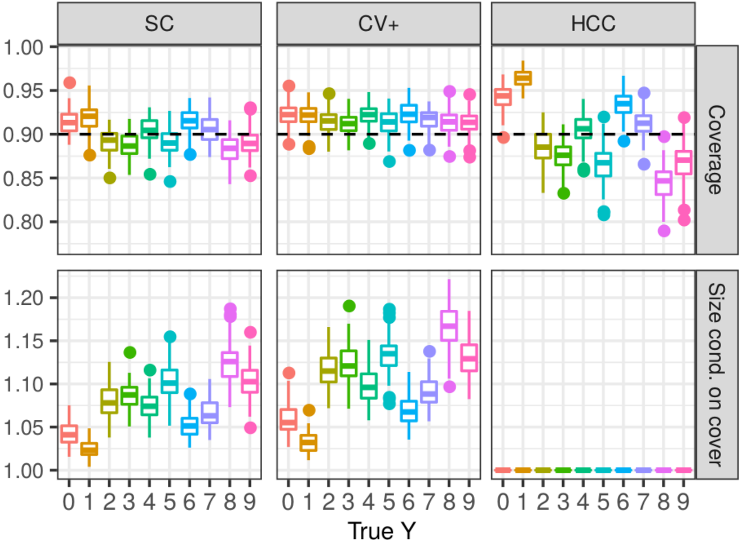
Therefore,

$$\begin{aligned}
\mathbb{P}\left[(n+1) \in \mathcal{S}(A)\right] &\leq \frac{2\alpha(n+1) + m - 2}{n+m} \\
&= \frac{2\alpha(n+m) + 2\alpha(1-m) + m - 2}{n+m} \\
&= 2\alpha + \frac{(m-1)(1-2\alpha) - 1}{n+m} \\
&\leq 2\alpha + \frac{1 - K/n}{K+1}.
\end{aligned}$$

Performance of CV+ on MNIST data



Slightly too conservative here, but often gives shorter intervals.

Other hold-out methods

Ensemble learning with bootstrap involves hold-out data.
A variation of CV+ can be obtained in that setting.

[Kim et al., 2020]

Some open research problems

Choosing conformity scores

Which conformity scores should we use?

Lots of options (e.g., residuals, distances from QR bands, . . .).

Several alternatives were proposed for CQR.

There was a natural choice for classification.

Work in progress.

Outlier detection

Outlier detection is closely related to prediction.

What's an efficient way of doing it with a conformal approach?

Work in progress.

Training black-box models

Conformal is a wrapper around black-box prediction algorithms.

However, there is only so much we can do if the black-box is bad.

Can we use some of these ideas to train better tuned black-box algorithms?

Work in progress.

Prediction in low signal-to-noise problems

In some problems, there is a lot of noise in $P(Y \mid X)$.

We may be able to learn something about $P(Y \mid X)$ without trying to predict individual observations.

Limited exchangeability

What if it is not the case that all data points are exchangeable?

What can we do under weaker exchangeability assumptions?

Measuring feature importance

The work of [Lei et al., 2018] connects prediction and variable importance measurement.

However, it focuses on variables that affect $\mathbb{E}[Y \mid X]$.

We may be interested in detecting that some feature affects the spread of Y.

Software

Python

- CQR `https://sites.google.com/view/cqr/home`
- Conformal classification `https://github.com/msesia/arc`
- Other methods `https://github.com/donlnz/nonconformist`

R

- https://github.com/ryantibs/conformal

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