Conformal Inference Methods in Deep Learning

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Introduction:
Why conformal inference?

General setup for supervised learning

Assumption:

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

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: fit a model that can predict Y_{n+1} given X_{n+1}.

This class: how to **account for predictive uncertainty**?

Example (classification)

X: Image, Y: label

Test point: 

What digit is this? Probably 5 or 6.

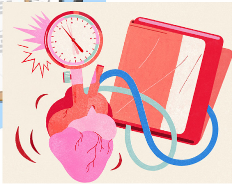
Example (regression)

X: Facebook page features, Y: number of comments

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

Example (regression)

X: Clinical history, genetic data, demographics. Y: blood pressure



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

Quantifying uncertainty via prediction sets

Instead of a point prediction, output a set of likely outcomes. E.g.,

- The digit is either a 5 or a 6.
- The blood pressure will be between 120-129 mmHg.

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Fix $\alpha \in (0, 1)$ and construct a prediction rule $\hat{C}_\alpha$ s.t. the set

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

has *marginal coverage* at level $1 - \alpha$:

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

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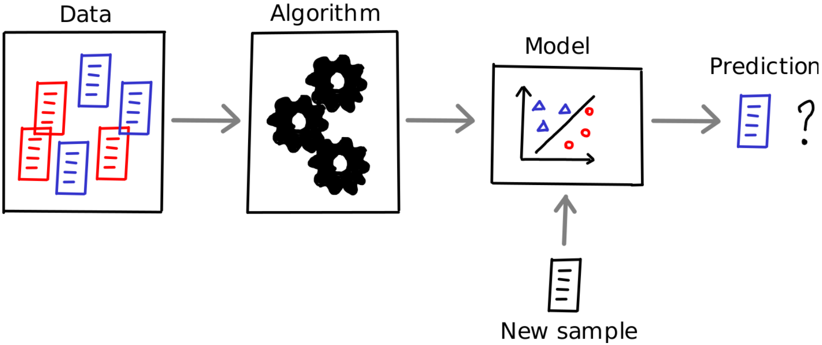
In regression problems, we may want $\hat{C}_\alpha(X)$ to be an interval.
In classification problems, it will be a discrete set.

The model-free predictive inference framework

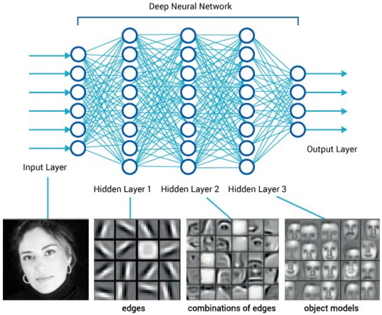
Data-generating model: $(X_i, Y_i) \stackrel{\text{iid}}{\sim} P_{X,Y}$.

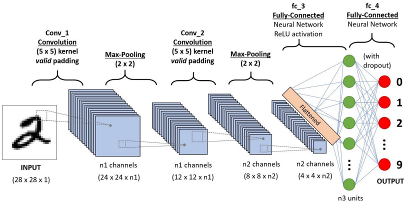


Challenges:

1. $P(Y \mid X)$ could be anything (completely unknown)
2. The prediction model may be a machine learning black box (e.g., neural network, random forests, Bayesian trees, ...)

Successes of deep learning models





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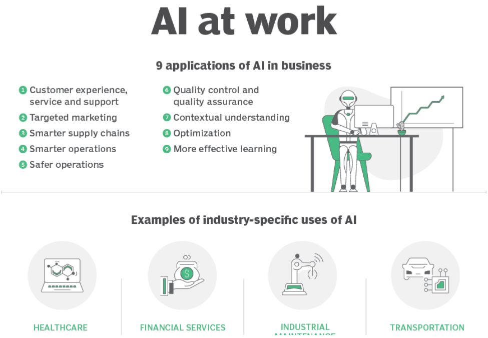

forbes.com

AI Models To Boost Lending And How Your Business Could Benefit From Them

Peter Shubenok

6-8 minutes

Peter Shubenok is the Founder and CEO at RNDpoint, a leading provider of lending platforms for Banks and MFIs.

What could possibly go wrong with machine learning?

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New research indicates that AI may be more prone to making mistakes than humans in image-based medical diagnoses because of the features they use for analysis.

theguardian.com

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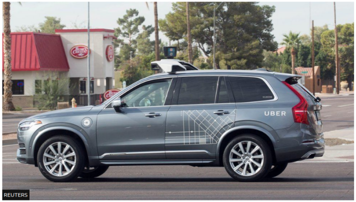

The self-driving Volvo hit a pedestrian at 39mph, despite the presence of a safety driver

Uncertainty and confidence in machine learning

Published in Towards Data Science

Michel Kana, Ph.D

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Uncertainty in Deep Learning. How To Measure?

A hands-on tutorial on Bayesian estimation of epistemic and aleatoric uncertainty with Keras. Towards a social acceptance of AI.

> My Deep Learning Model Says: “sorry, I don’t know the answer”. That can be absolutely OK.

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Second opinion needed: communicating uncertainty in medical machine learning

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Daniel Ackerman | MIT News Office

November 20, 2020

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In the News

Emmanuel Candès Keynotes NeurIPS 2022

Faculty Director, Emmanuel Candès, is giving a keynote address at the upcoming Neural Information Processing System (NeurIPS) conference on Tuesday, November 29, 2022

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Conformal Prediction in 2022

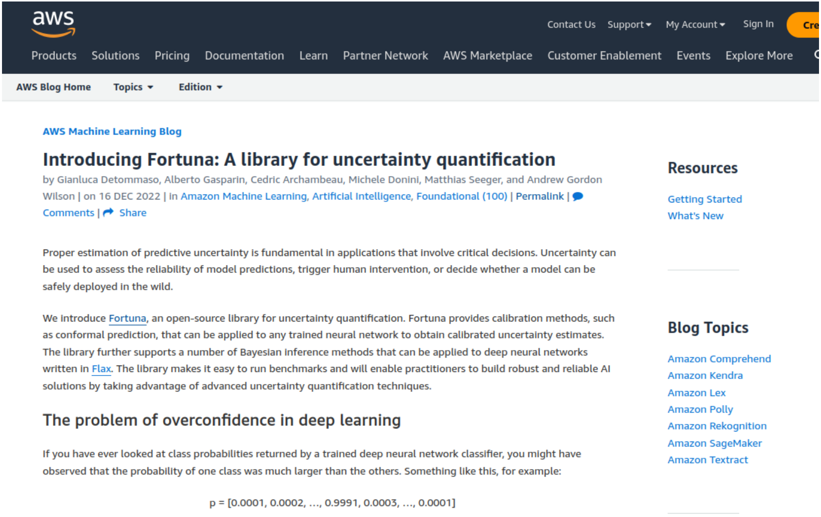
Emmanuel Candes

Moderator: Alekh Agarwal

Hall H

[Abstract]

. . . both within and beyond academia



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Introducing Fortuna: A library for uncertainty quantification

by Gianluca Detommaso, Alberto Gasparin, Cedric Archambeau, Michele Donini, Matthias Seeger, and Andrew Gordon Wilson | on 16 DEC 2022 | in Amazon Machine Learning, Artificial Intelligence, Foundational (100) | Permalink | Comments | Share

Proper estimation of predictive uncertainty is fundamental in applications that involve critical decisions. Uncertainty can be used to assess the reliability of model predictions, trigger human intervention, or decide whether a model can be safely deployed in the wild.

We introduce Fortuna, an open-source library for uncertainty quantification. Fortuna provides calibration methods, such as conformal prediction, that can be applied to any trained neural network to obtain calibrated uncertainty estimates. The library further supports a number of Bayesian inference methods that can be applied to deep neural networks written in Flax. The library makes it easy to run benchmarks and will enable practitioners to build robust and reliable AI solutions by taking advantage of advanced uncertainty quantification techniques.

The problem of overconfidence in deep learning

If you have ever looked at class probabilities returned by a trained deep neural network classifier, you might have observed that the probability of one class was much larger than the others. Something like this, for example:

p = [0.0001, 0.0002, …, 0.9991, 0.0003, …, 0.0001]

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Chapter 1:
Review of linear regression

Review of classical linear regression

Linear regression model:

- 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)

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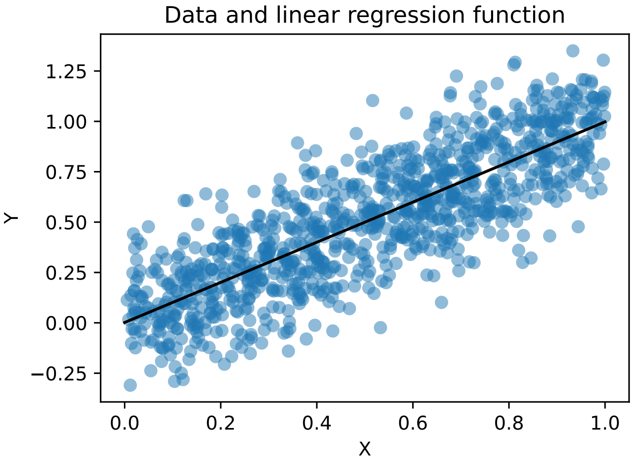

Review of classical linear regression (continued)

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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)

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&= 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}
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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).
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Review of classical linear regression (continued)

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Recall that

$$
\hat{\sigma}^2 = \frac{\text{RSS}}{(n-p-1)} \sim \sigma^2 \cdot \frac{\chi^2_{n-p-1}}{n-p-1},
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Review of classical linear regression (continued)

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

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:

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

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

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

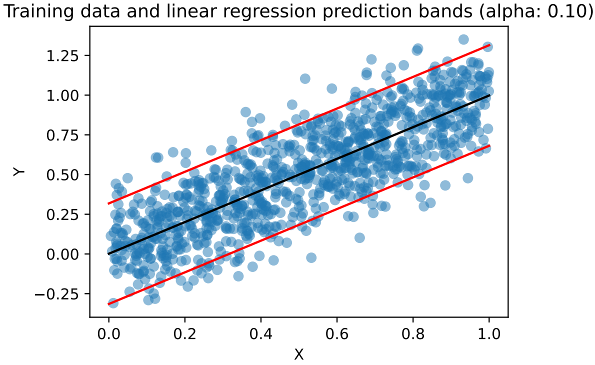
Review of classical linear regression (continued)

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 *conditional coverage*:

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



Review of classical linear regression (continued)

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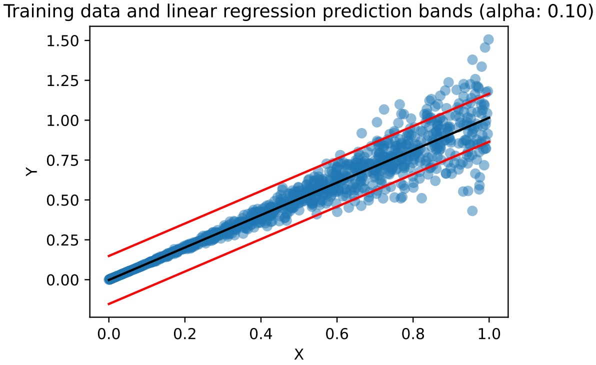

Review of classical linear regression (continued)

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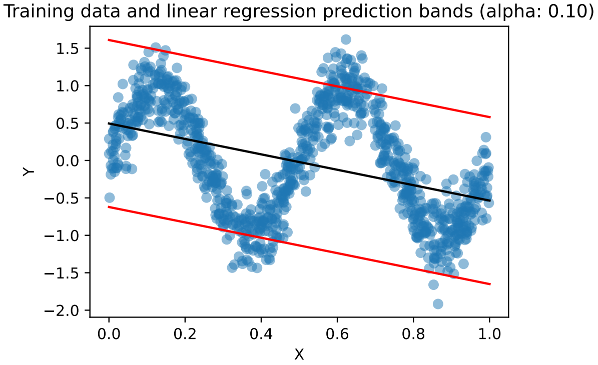


Model-free predictive inference

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

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, ...)

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, ...)

We need some leverage:

- The data are random
- The test point is random
- Coverage will only be *marginal* (not conditional on X_{n+1}):

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

Chapter 2:
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.

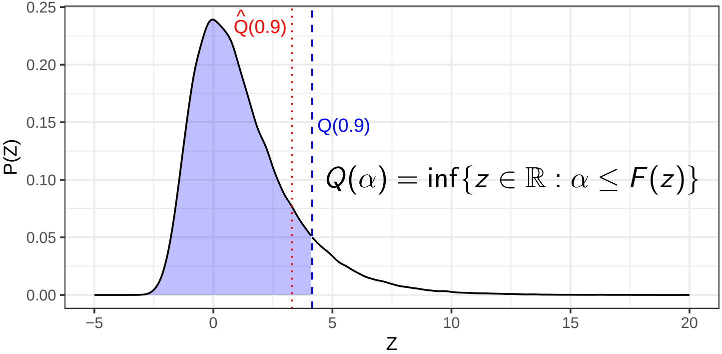
Prediction without covariates

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 (1)

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

See whiteboard.

Ref: [Romano et al., 2019b]

Inflation of quantiles

Lemma (2)

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

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

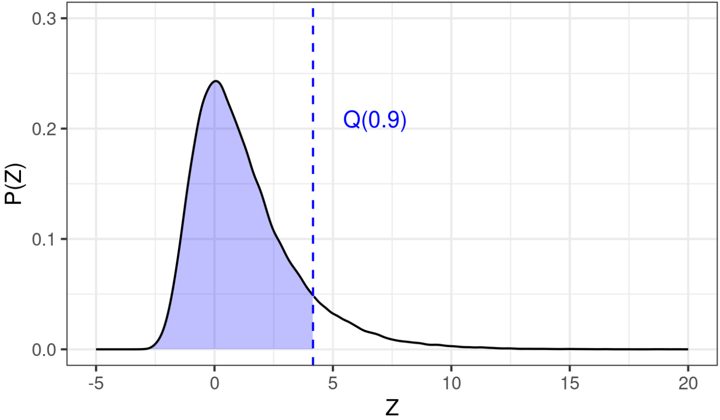
Then,

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

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

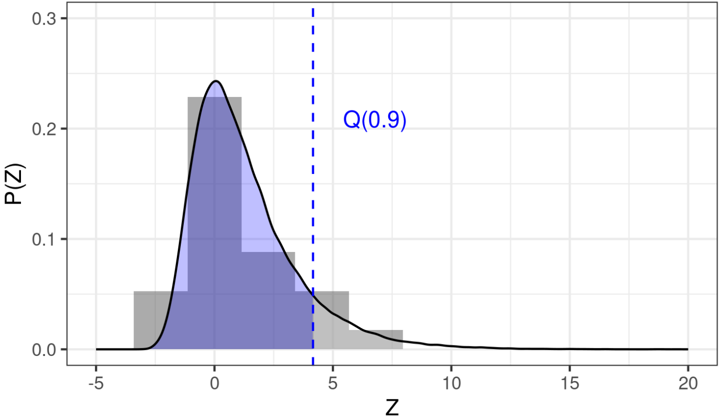
$$\mathbb{P}\left[Z_{n+1} \leq \hat{Q}_n(\alpha_n)\right] \leq \alpha + \frac{1}{n}.$$

Inflation of quantiles (intuition)



Inflation of quantiles (intuition)

Data set of size 50



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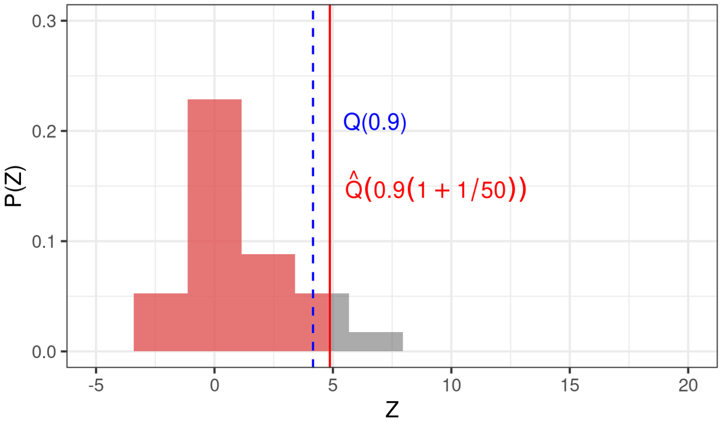


Proof

See whiteboard.

Ref: [Romano et al., 2019b]

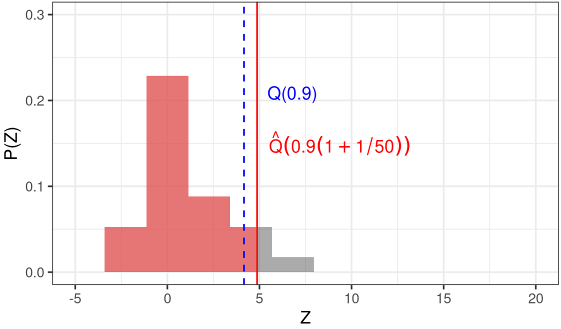
One-sided prediction interval without covariates

Suppose $Z_1, \ldots, Z_{n+1}$ 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,

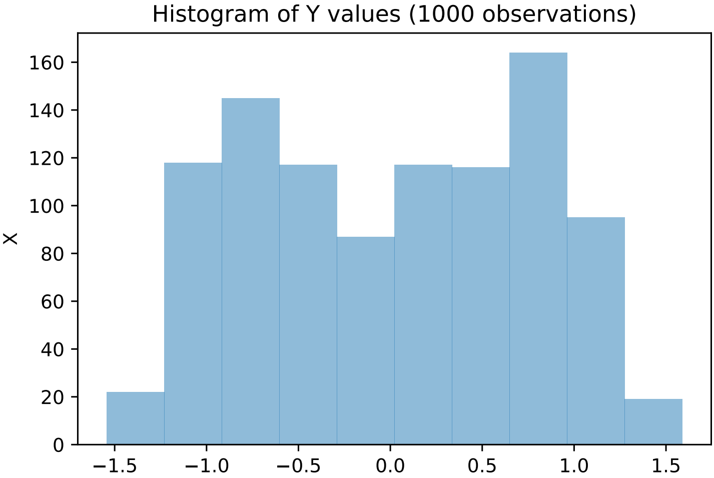
$$\alpha \leq \mathbb{P}\left[Z_{n+1} \in \hat{C}_\alpha\right] \leq \alpha + \frac{1}{n}.$$



Chapter 3:
Split Conformal Prediction

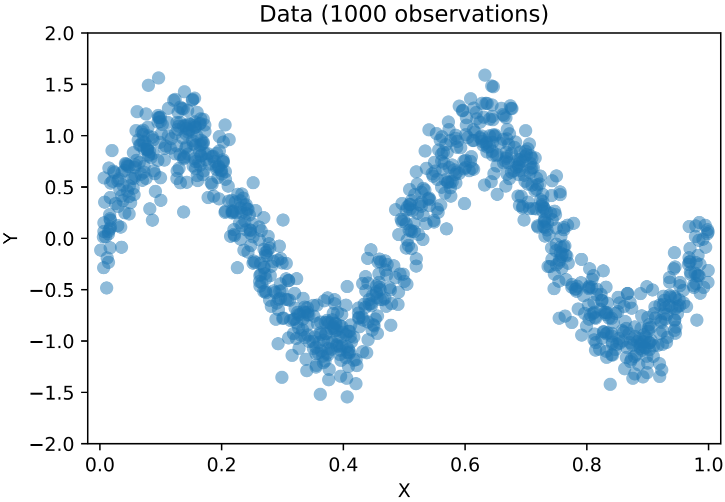
Prediction with covariates

We would like to predict a variable Y...



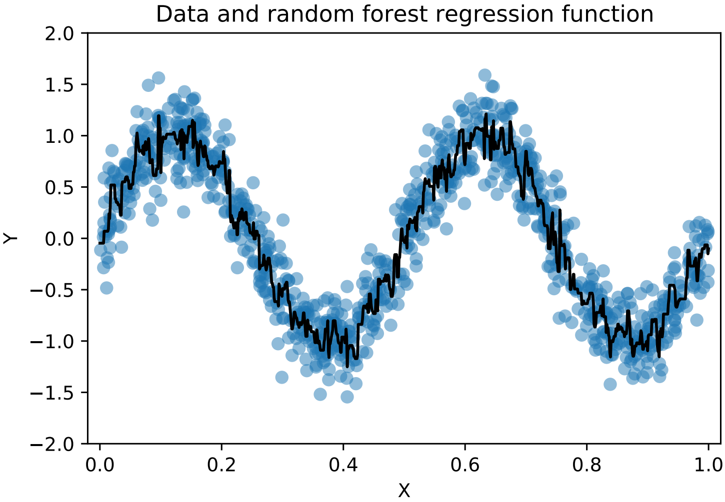
Prediction with covariates

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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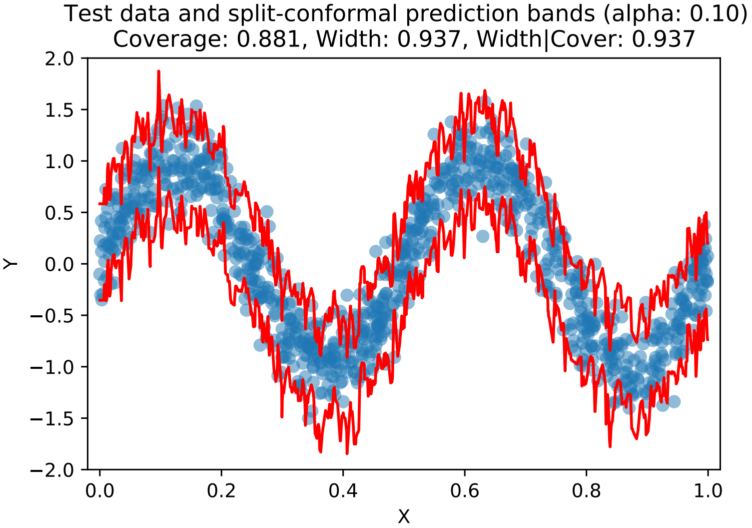

Conformal prediction

Key ideas:

1. Use ML to project project the problem into 1 dimension (evaluate residuals).
2. Apply the empirical quantile lemmas presented earlier to predict the (absolute) residual of the test point.
3. Some kind of data hold-out is needed to ensure exchangeability with the test data (avoid overfitting).

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

Split-conformal prediction

Algorithm 1: Split-conformal prediction

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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7: **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])

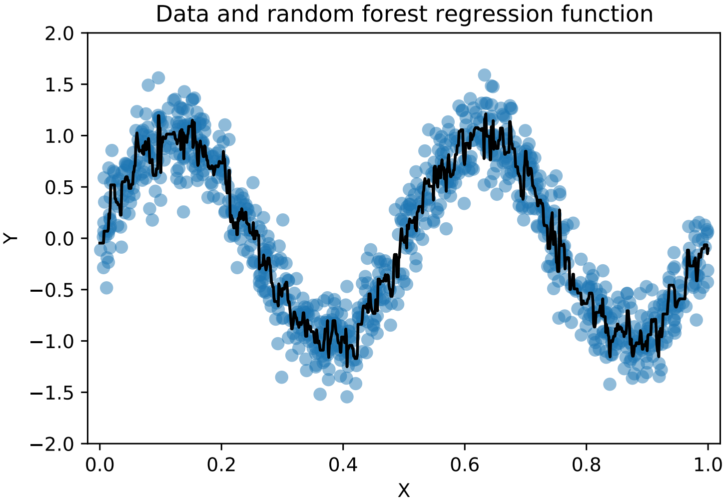
Suppose $(X_1, Y_1), (X_2, Y_2), \dots, (X_{n+1}, Y_{n+1})$ *are exchangeable. Then, the split-conformal prediction intervals* $\hat{C}_\alpha$ *satisfy*

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

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

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

Split-conformal prediction bands



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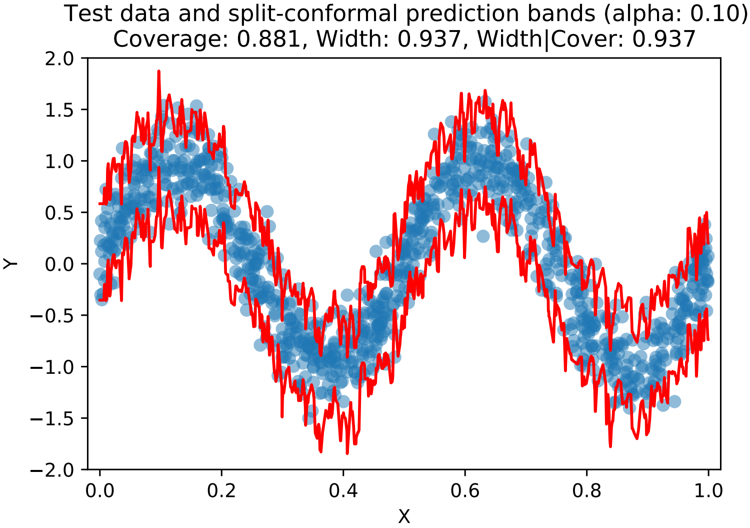
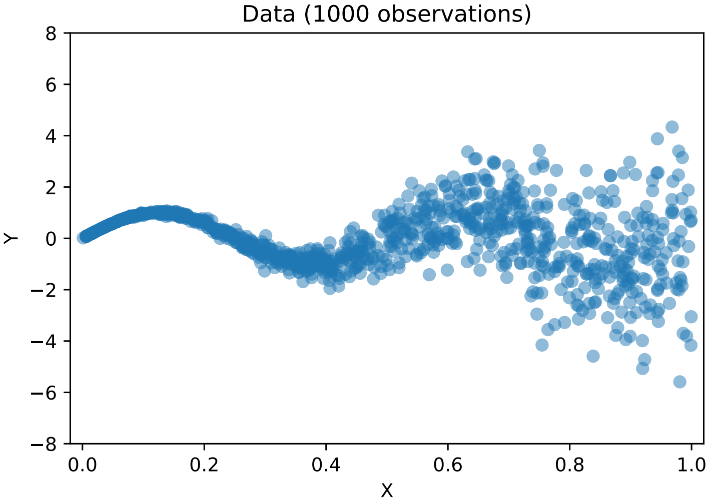


Chapter 4:
Conformalized Quantile Regression

Heteroscedasticity

Suppose now Y heteroscedastic.



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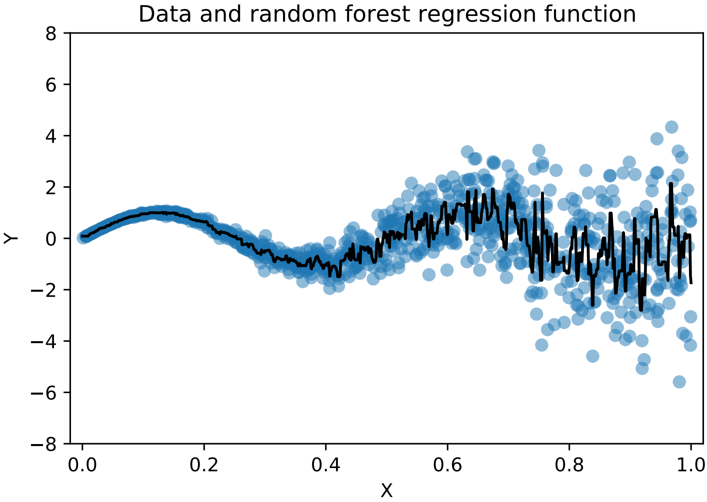

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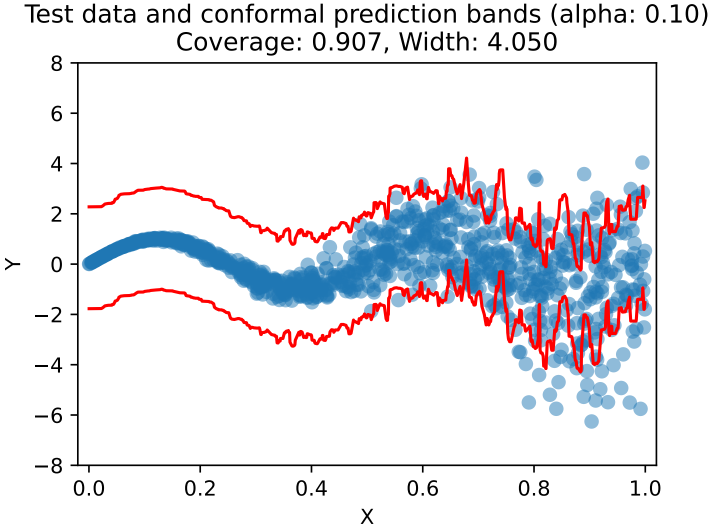

Conditional quantiles

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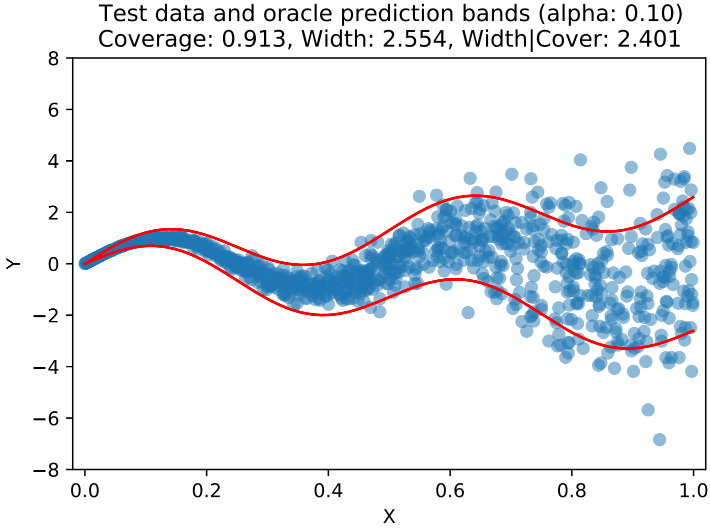
An oracle that knows $P(Y \mid X)$ would predict as follows:

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

Oracle predictions



Quantile regression

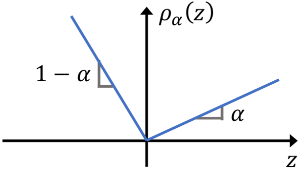
Goal: estimate a function $\hat{q}_\alpha(x)$,

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

Fit the parameters θ_α by minimizing the "pinball" loss:

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

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



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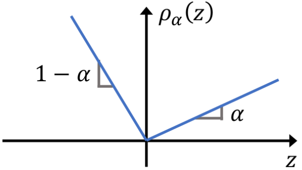

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Key idea: Leibniz integral rule

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

Multiple deep quantile regression models

Goal: estimate two functions, $\hat{q}_{\alpha_{\text{lower}}}(x)$ and $\hat{q}_{\alpha_{\text{upper}}}(x)$,

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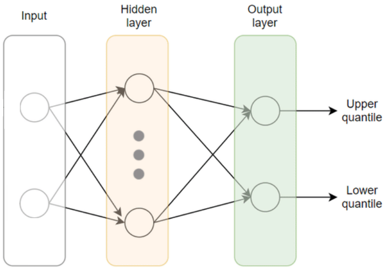

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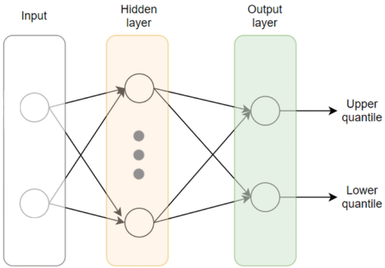

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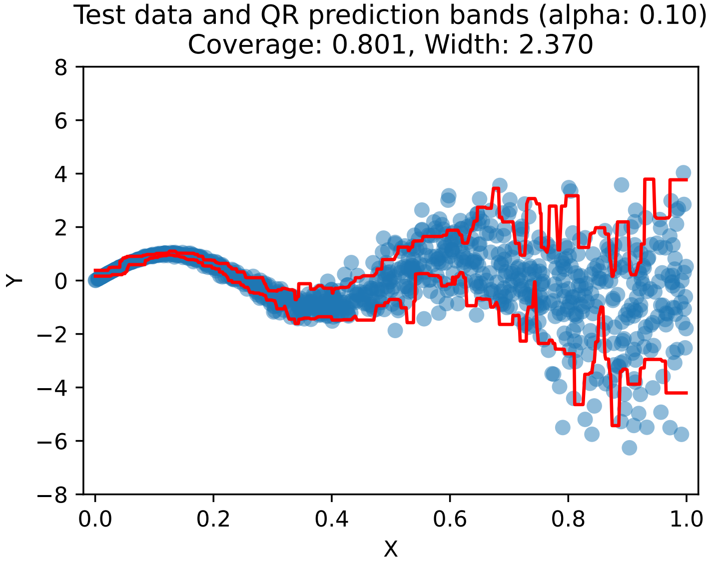
Beware of *quantile crossing*.

E.g., swap $\hat{q}_{\alpha_{\text{lower}}}(x)$ and $\hat{q}_{\alpha_{\text{upper}}}(x)$ if necessary.

Quantile regression in action

We can fit conditional quantiles, but without guarantees.



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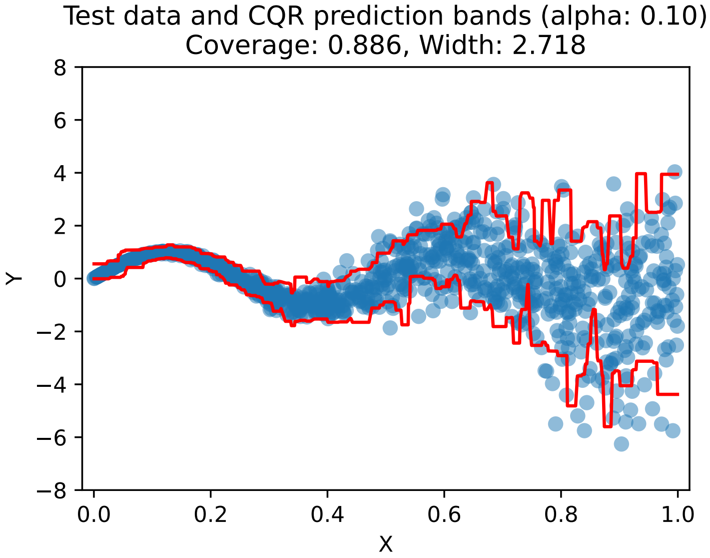

Generalized residuals for quantile regression

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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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\end{aligned}
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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

Input: Data $\{(X_i, Y_i)\}_{i=1}^{n}$, test point X_{n+1}, $\alpha \in (0, 1)$
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5: Evaluate residuals (*conformity scores*) on $\mathcal{I}_2$:

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Why does this work? Same story as before.

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

Marginal coverage of split-conformal prediction

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

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

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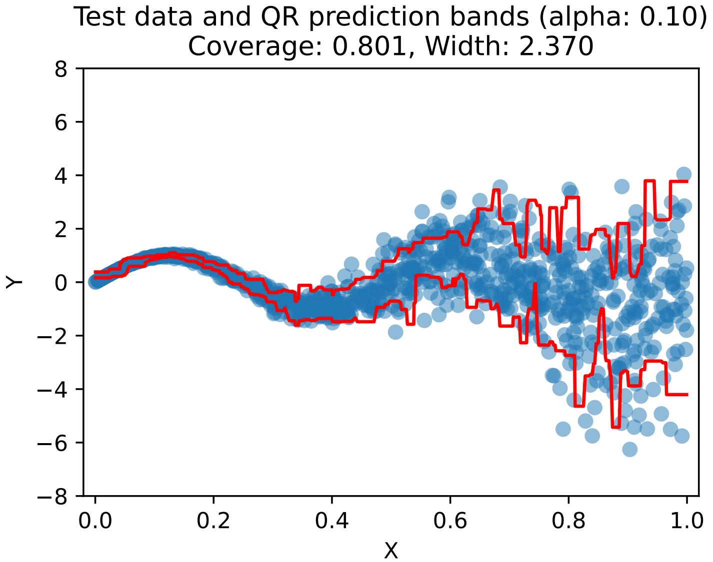
Conformal quantile regression



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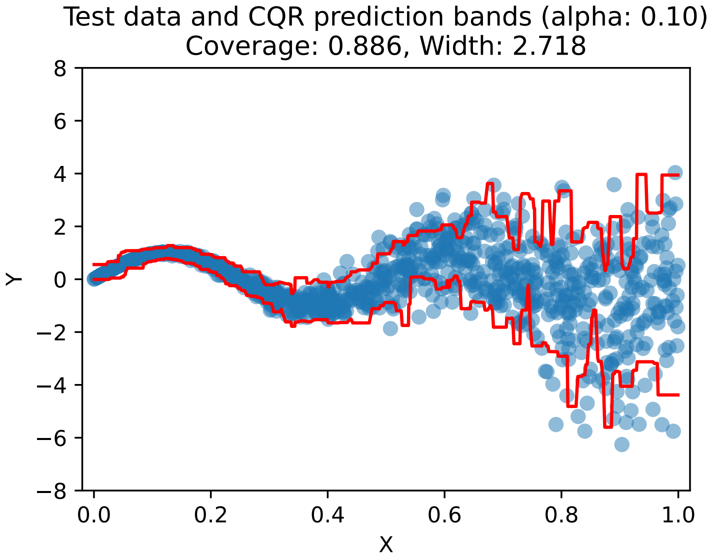

Computer session I

Chapter 5:
Beyond marginal coverage

Efficiency of conformal quantile regression

Theorem ([Sesia and Candès, 2020])

(A1) Assume $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ *are i.i.d.*

Efficiency of conformal quantile regression

Theorem ([Sesia and Candès, 2020])

(A1) Assume $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ *are i.i.d.*

(A2) Assume that

$$\mathbb{P}\left[\mathbb{E}\left[\left(\hat{q}_{\alpha/2}(X) - q_{\alpha/2}(X)\right)^2 \mid \hat{q}_{\alpha/2}, \hat{q}_{1-\alpha/2}\right] \leq \eta_n\right] \geq 1 - \rho_n,$$

$$\mathbb{P}\left[\mathbb{E}\left[\left(\hat{q}_{1-\alpha/2}(X) - q_{1-\alpha/2}(X)\right)^2 \mid \hat{q}_{\alpha/2}, \hat{q}_{1-\alpha/2}\right] \leq \eta_n\right] \geq 1 - \rho_n,$$

for some sequences $\eta_n = o(1)$ *and* $\rho_n = o(1)$*, as* $n \to \infty$*.*

Efficiency of conformal quantile regression

Theorem ([Sesia and Candès, 2020])

(A1) Assume $(X_1, Y_1), (X_2, Y_2), \ldots, (X_{n+1}, Y_{n+1})$ *are i.i.d.*

(A2) Assume that

$$\mathbb{P}\left[\mathbb{E}\left[\left(\hat{q}_{\alpha/2}(X) - q_{\alpha/2}(X)\right)^2 \mid \hat{q}_{\alpha/2}, \hat{q}_{1-\alpha/2}\right] \leq \eta_n\right] \geq 1 - \rho_n,$$
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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 $k \in \{0, 1\}$, use only the data in

$$\mathcal{I}_{2,k} = \{i \in \mathcal{I}_2 : X_{i,2} = k\},$$

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

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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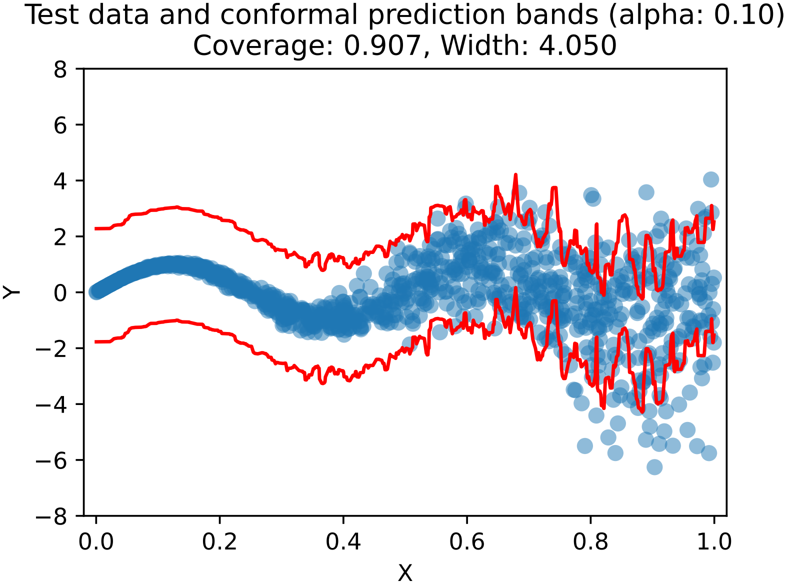
However, this will greatly reduce the effective sample size.

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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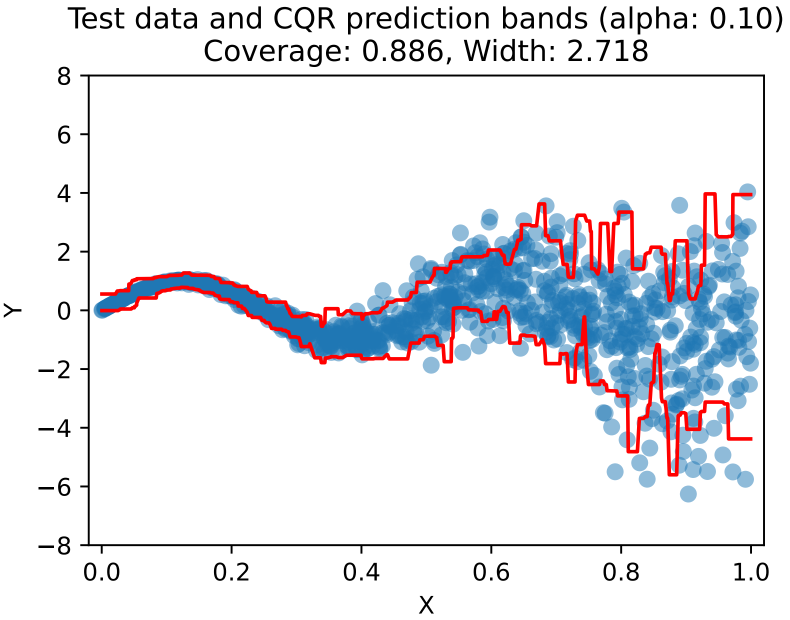

Worst-slab coverage [Cauchois et al., 2020]

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]

Chapter 6:
Split Conformal Classification

The classification problem

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

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

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

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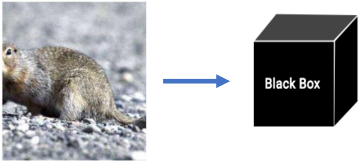
$C($$) = \{5, 6\}$

Uncertainty estimation via calibrated prediction sets



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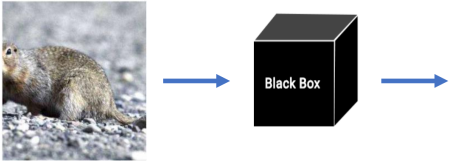

{Marmot, Fox Squirrel, Mink, Weasel}

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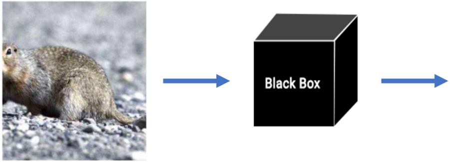

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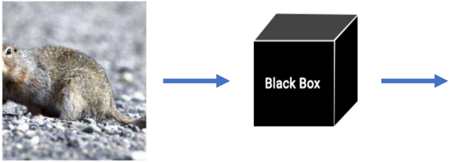

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Ideal goal: prediction sets with conditional coverage.

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

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Unfortunately, this is impossible to achieve in finite samples without very strong assumptions. [Barber et al. (2021)]

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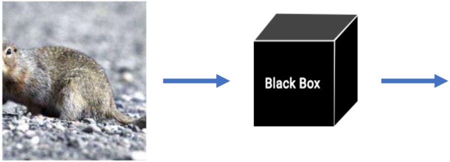

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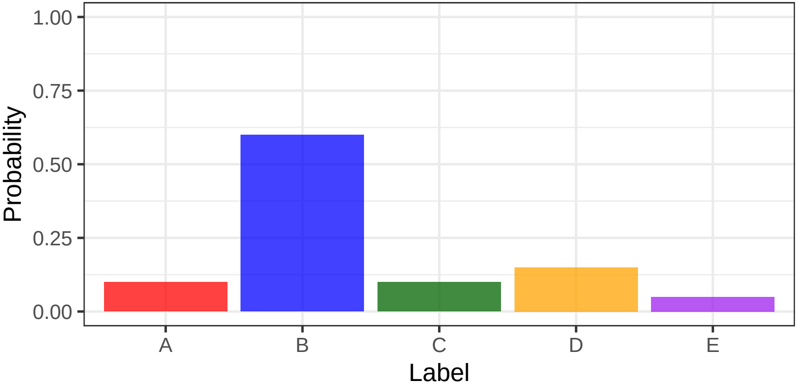
Practical goal: prediction sets with marginal coverage.

$$\mathbb{P}\left[Y_{n+1} \in \hat{\mathcal{C}}_n(X_{n+1}) \mid X_{n+1}\right] \geq 1 - \alpha \quad (\text{e.g.,} = 90\%)$$

Prediction sets for classification: the ideal approach

Conditional class probabilities (oracle):

$$\pi_y(x) = \mathbb{P}[Y = y \mid X = x]$$



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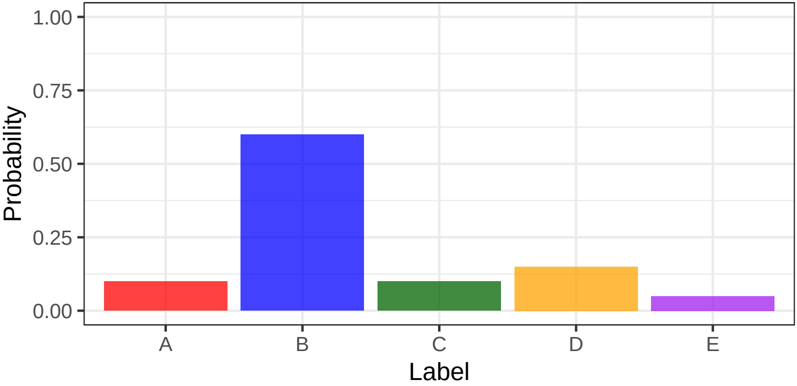

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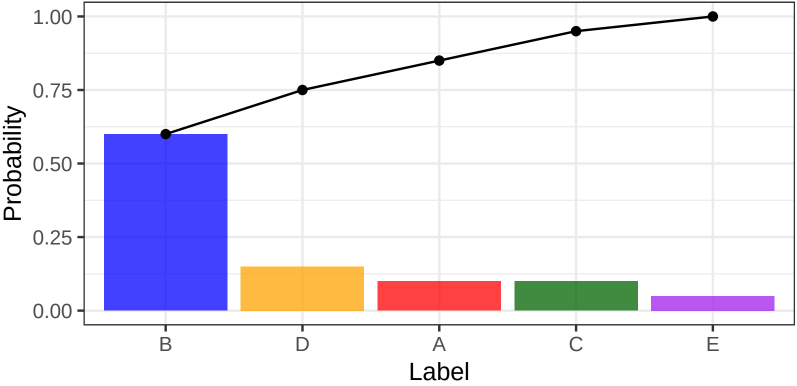

Step 1: sort the classes by their probability and compute the CDF.

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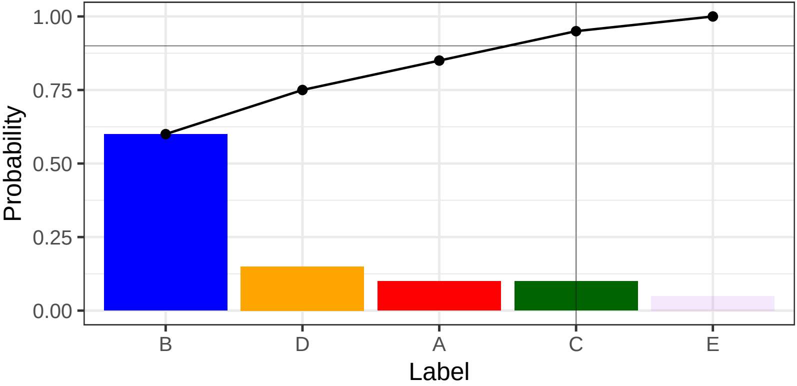
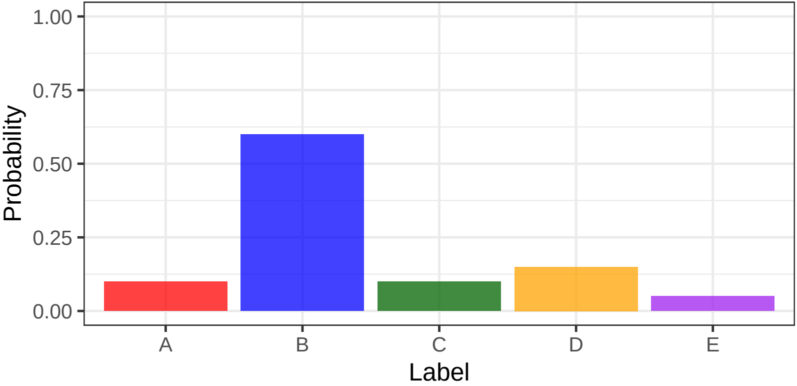


Step 2: find where the CDF crosses above the $1 - \alpha$ level.

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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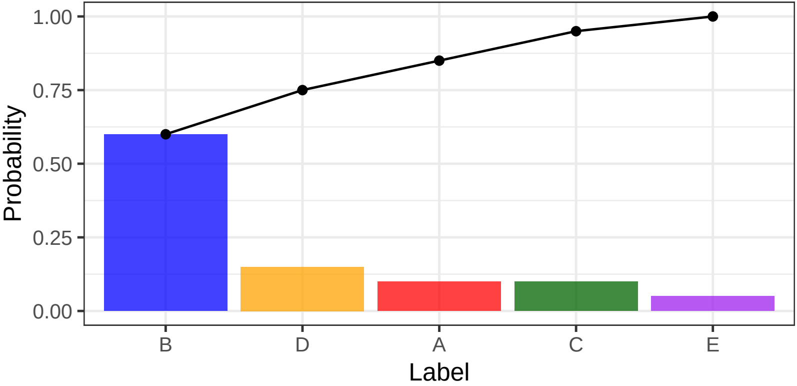

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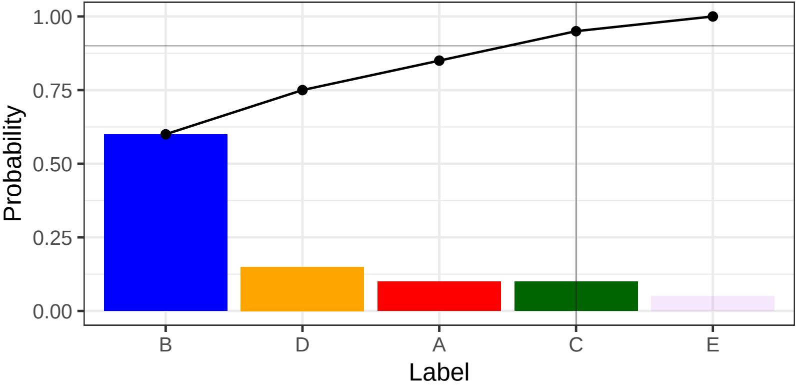

The conservative classification oracle [Romano et al., 2020]

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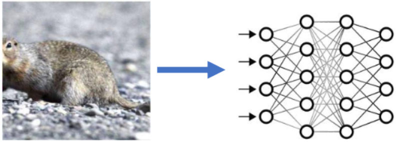
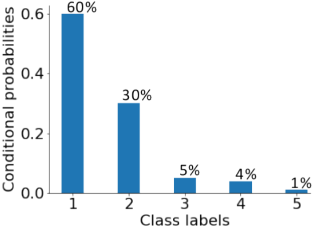
Then, the (tight) oracle would draw $U \sim \mathrm{Unif}(0,1)$ and predict:

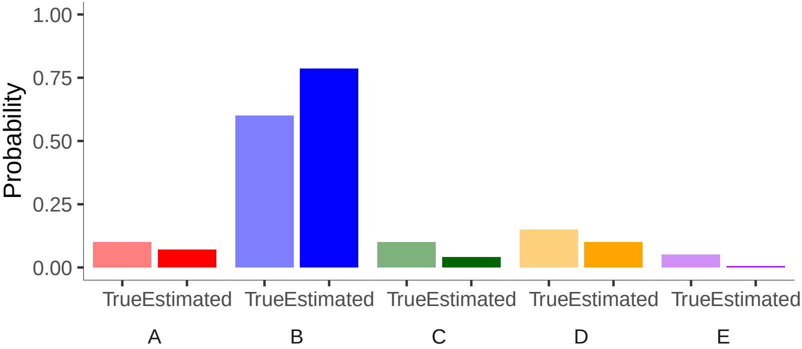
$$C^{\text{oracle}}(x) = \mathcal{S}(x,U;\pi,1-\alpha).$$

Machine learning classification models

In practice, we use probability estimates that may not be accurate.

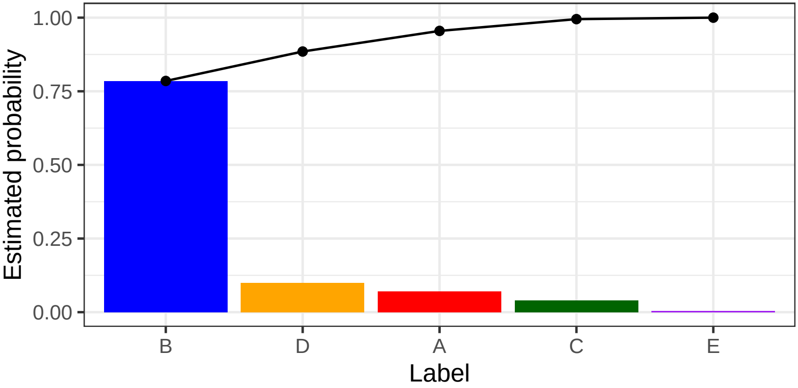






Plug-in prediction sets will often fail

Plug the estimated probabilities into the oracle prediction rule.



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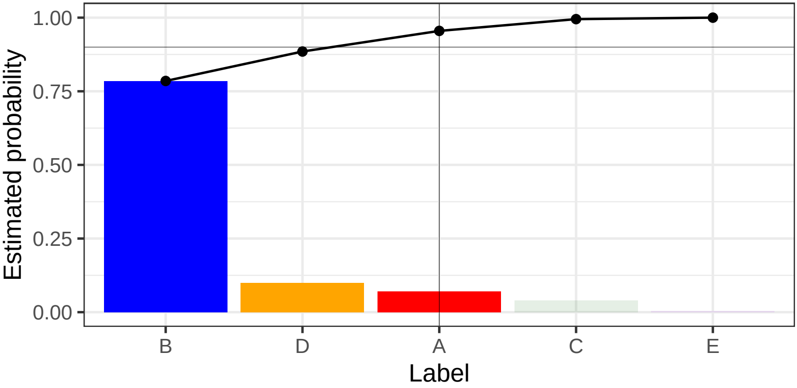

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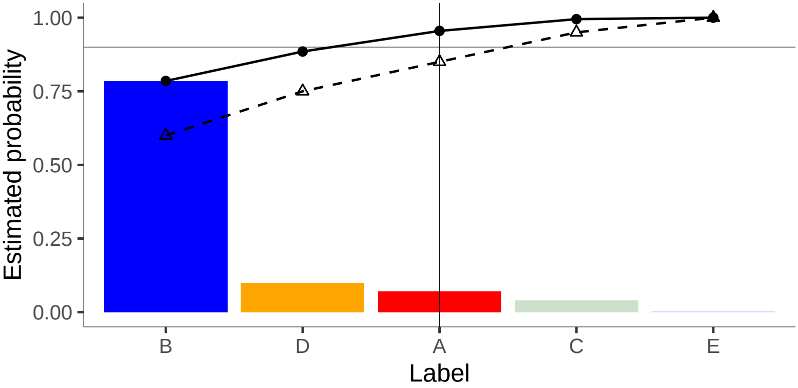

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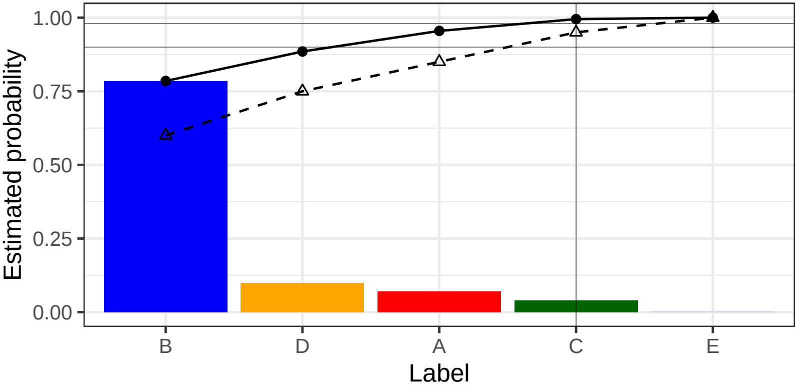
The probability estimates are often overconfident.
This tends to lead to under-coverage.

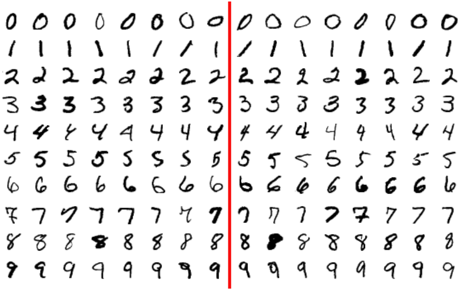


Split-conformal inference

Full data set

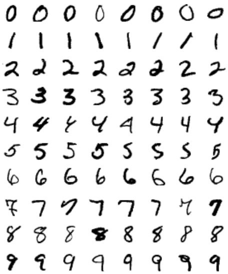
Split-conformal inference

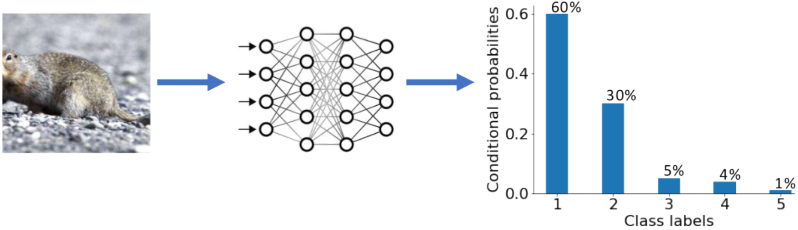
(1) Randomly split the data into two subsets



Split-conformal inference

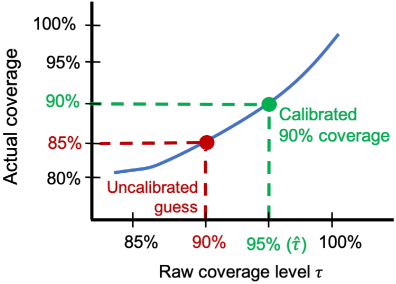
(2) Learn a model using training data





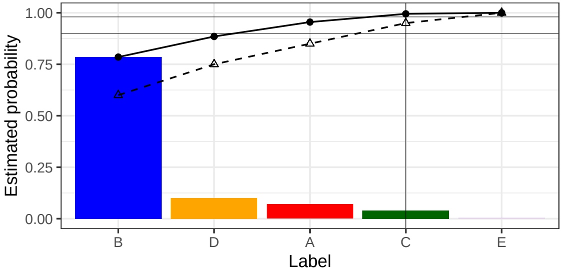
Split-conformal inference

(3) Make prediction sets and evaluate coverage on calibration data



Calibration via conformity scores

How far in τ (above $1-\alpha$) before Y_i is classified correctly?



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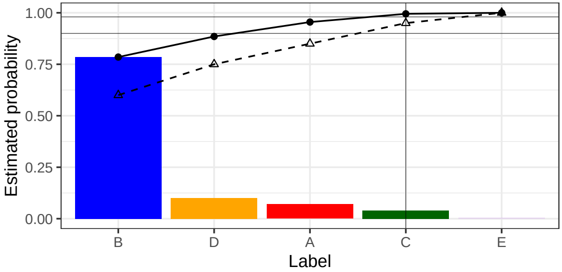

Evaluate conformity scores for all n calibration data points:

$$W_i = \min \left\{ \tau \in [0,1] : Y_i \in \mathcal{S}(X_i; \hat{\pi}, \tau) \right\},$$

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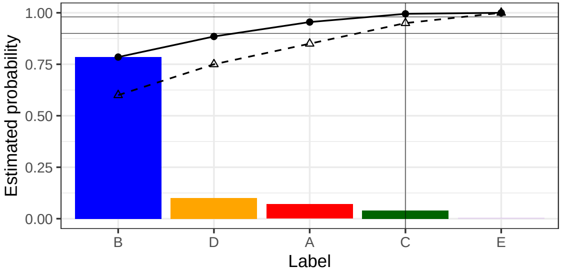

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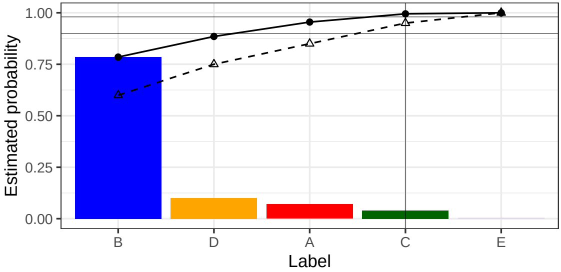
Compute

$$\hat{Q}_n(W_{\mathcal{I}_{\mathrm{cal}}}, \beta_n) = W_{(\lceil n\beta_n \rceil)}, \qquad \beta_n = (1-\alpha)(1+1/n)$$

Calibration via conformity scores

How far in τ (above $1-\alpha$) before Y_i is classified correctly?



Evaluate conformity scores for all n calibration data points:

$$W_i = \min\left\{\tau \in [0,1] : Y_i \in \mathcal{S}(X_i; \hat{\pi}, \tau)\right\},$$

Compute

$$\hat{Q}_n(W_{\mathcal{I}_{\text{cal}}}, \beta_n) = W_{(\lceil n\beta_n \rceil)}, \qquad \beta_n = (1-\alpha)(1+1/n)$$

Predict

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

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

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,

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

Computer session II

Chapter 7:
Full conformal inference

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

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

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

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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 $R_y \leq \lceil (1-\alpha)(n+1) \rceil$.

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Finally, the prediction set is

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

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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,*

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

Limitations of full-conformal inference

1. Overfitting may reduce power, since all in-sample residuals may become equal to zero.

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1. Overfitting may reduce power, since all in-sample residuals may become equal to zero.
2. Re-training the model for each new test point (and possible value of Y_{n+1}) is often prohibitively expensive.

Can we do something in between full and split conformal?

Chapter 8:
Cross-validation+

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

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

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$$\mathcal{I}_K = \left\{(K-1)\frac{n}{K} + 1, \ldots, n\right\},$$

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,

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

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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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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

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

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

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Note that $\tilde{f}_{k,K+1} = \hat{f}_k$.

Define the matrix $A \in \{0,1\}^{(n+m)\times(n+m)}$ as:

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

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

Proof for CV+ (setup)

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

$$\sum_{i=1}^{n+m} A_{n+1,i} > (1-\alpha)(n+1)$$

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$$\sum_{i=1}^{n+m} A_{n+1,i} > (1-\alpha)(n+1)$$

Recall that $Y_{n+1} \notin \hat{C}_\alpha^{\text{cv+}}$ if and only if

$$\begin{aligned}\beta_n &= (1-\alpha)(n+1) \\ &\geq \sum_{i=1}^{n} \mathbb{1}\left[Z_i < \mathcal{Z}(X_{n+1}, Y_{n+1}, \hat{f}_{k(i)})\right]\end{aligned}$$

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&= \sum_{i=1}^{n} A_{n+1,i} = \sum_{i=1}^{n+m} A_{n+1,i}.
\end{aligned}$$

Proof for CV+ (strategy)

Define the set of *outstanding players*

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

We know $Y_{n+1} \notin \hat{C}_{\alpha}^{\text{cv+}}$ if and only if $(n+1) \in \mathcal{S}(A)$.

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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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&= A_{i,j}.
\end{aligned}$$

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

Proof for CV+ (exchangeability)

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

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

$$(n+1) \in \mathcal{S}(A) \quad \Leftrightarrow \quad j \in \mathcal{S}(\Pi A \Pi^\top).$$

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All players are equally likely to be outstanding!

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All players are equally likely to be outstanding!

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

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 $k(i) = k(j)$.

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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 $k(i) = k(j)$.

$\mathcal{S}(A)$ 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.

Let $s = |\mathcal{S}(A)|$ and $s_k = |\mathcal{S}(A) \cap \mathcal{I}_k|$ ($\#$ outstanding players in k).

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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:

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

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

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Putting everything together:

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

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

Therefore,

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

Computer session III

To learn more

References and resources

github.com/valeman/awesome-conformal-prediction

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Some areas on which I've worked recently.

Skewed data

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Testing for outliers with conformal p-values.

- [Bates et al., 2023]
- [Liang et al., 2022]
- [Bashari et al., 2023]

NESS session on Tuesday morning

NESS Symposium 2023

Event Schedule

<	Sat Jun 03	Sun Jun 04	Mon Jun 05	Tue Jun 06	>

sesia

Displaying agenda in event timezone (6:14 PM EDT)

9:50 AM

Recent Developments of Conformal Inference

9:50 AM – 11:30 AM

CDS 1101

Invited Session

This session will consist four speakers from academia who are experts in conformal inference.

Session Chair/Organizer

G

Guanyu Hu

Speakers

Matteo Sesia
Assistant Professor of Data Sciences and Operations
University of Southern California

Yinchu Zhu
Brandeis University

Adam Fisch
MIT

Stephen Bates
Postdoctoral researcher
UC Berkeley

4 Subsessions

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