Assumption-free uncertainty quantification for black box models

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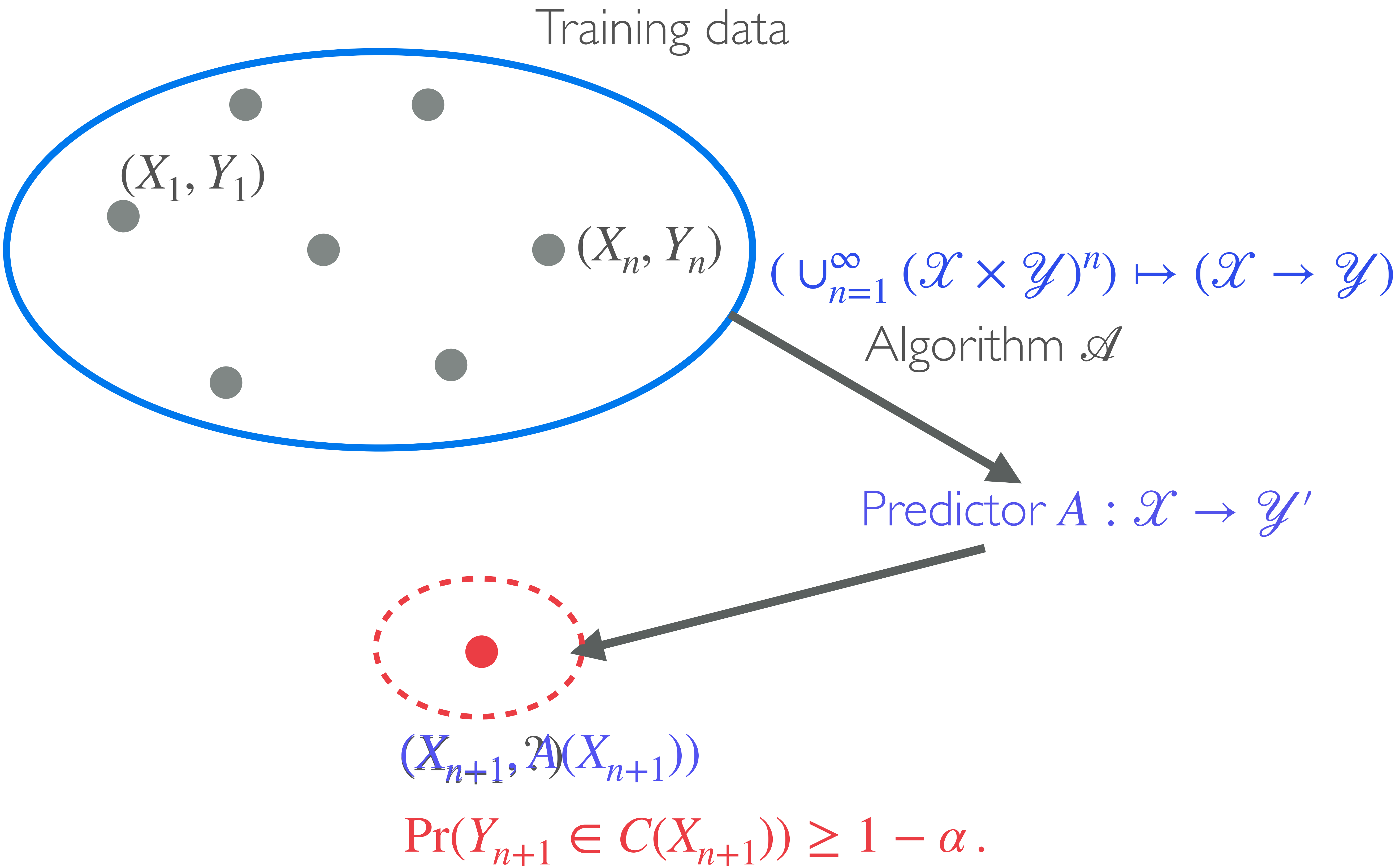
Outline

1. ***What does "predictive inference" mean?***
2. Methods for assumption-free predictive inference
3. Empirical observations
4. Generalizations
5. Open problems + summary

Prediction vs "Predictive Inference"



Why "Predictive Inference"?

Why do we want $\Pr(Y_{n+1} \in C(X_{n+1})) \geq 1 - \alpha$?

eg: time taken to airport (Y) at some time of day (X)

A "mean" prediction of 80mins is not useful because 80 +/- 5 mins is very different from 80 +/- 40 mins.

To make real-world decisions based on predictions, we need to quantify uncertainty of those predictions.

Prediction interval vs Confidence interval

Predictor (prediction algorithm)

$$(\cup_{n=1}^{\infty} (\mathscr{X} \times \mathscr{Y})^n) \mapsto (\mathscr{X} \to \mathscr{Y}')$$

Prediction interval (or set)

$\Pr(Y_{n+1} \in C(X_{n+1})) \geq 1 - \alpha\,.$ vol$(C_n) \geq q_{1-\alpha}(P_{Y|X=X_{n+1}})\,.$

Estimator (estimation algorithm)

$$(\cup_{n=1}^{\infty} (\mathscr{X} \times \mathscr{Y})^n) \mapsto \Theta$$

Confidence interval (or set)

$\Pr(\theta \in C_n) \geq 1 - \alpha\,.$ Often, vol$(C_n) \to 0$ as $n \to \infty\,.$

Need to assume a model relating Y to X.
θ is a subset of model parameters.
eg: assume $Y = X\theta +$ noise.

"Assumption-free" Predictive Inference

Given data $D_n \equiv (X_1, Y_1), \ldots, (X_n, Y_n) \sim P_X \times P_{Y|X} \equiv P_{XY}$,

any algorithm $\mathscr{A} : (\cup_{n=1}^{\infty} (\mathscr{X} \times \mathscr{Y})^n) \mapsto (\mathscr{X} \to \mathscr{Y}')$,

and $X_{n+1} \sim P_X$, produce a set $C(X_{n+1}) \equiv C_{\mathscr{A}, D_n}(X_{n+1})$ s.t.

for all P_{XY}, algorithms $\mathscr{A}$, $\Pr(Y_{n+1} \in C(X_{n+1})) \geq 1 - \alpha$.

Remarks

(a) *don't need iid data, just exchangeable*

(b) *algorithm optional, assumed permutation-invariant*

(c) *trivial without size/efficiency requirement*

(d) *probability is over all training, test data, algorithm*

(e) *not conditional on* X_{n+1}

Vovk, Shafer, and others, 2000-19

Conditional coverage is impossible without assumptions

We will achieve $\Pr(Y_{n+1} \in C(X_{n+1})) \geq 1 - \alpha$.

Not $\forall x$, $\Pr(Y_{n+1} \in C(X_{n+1}) \mid X_{n+1} = x) \geq 1 - \alpha$.

In fact, one can prove that assumption-free conditional inference is impossible.
(the expected volume of the set must be infinite)

Balasubramanian, Ho and Vovk '14

Lei, Wasserman, Rinaldo, Tibshirani '18

BaCaRaTi'19

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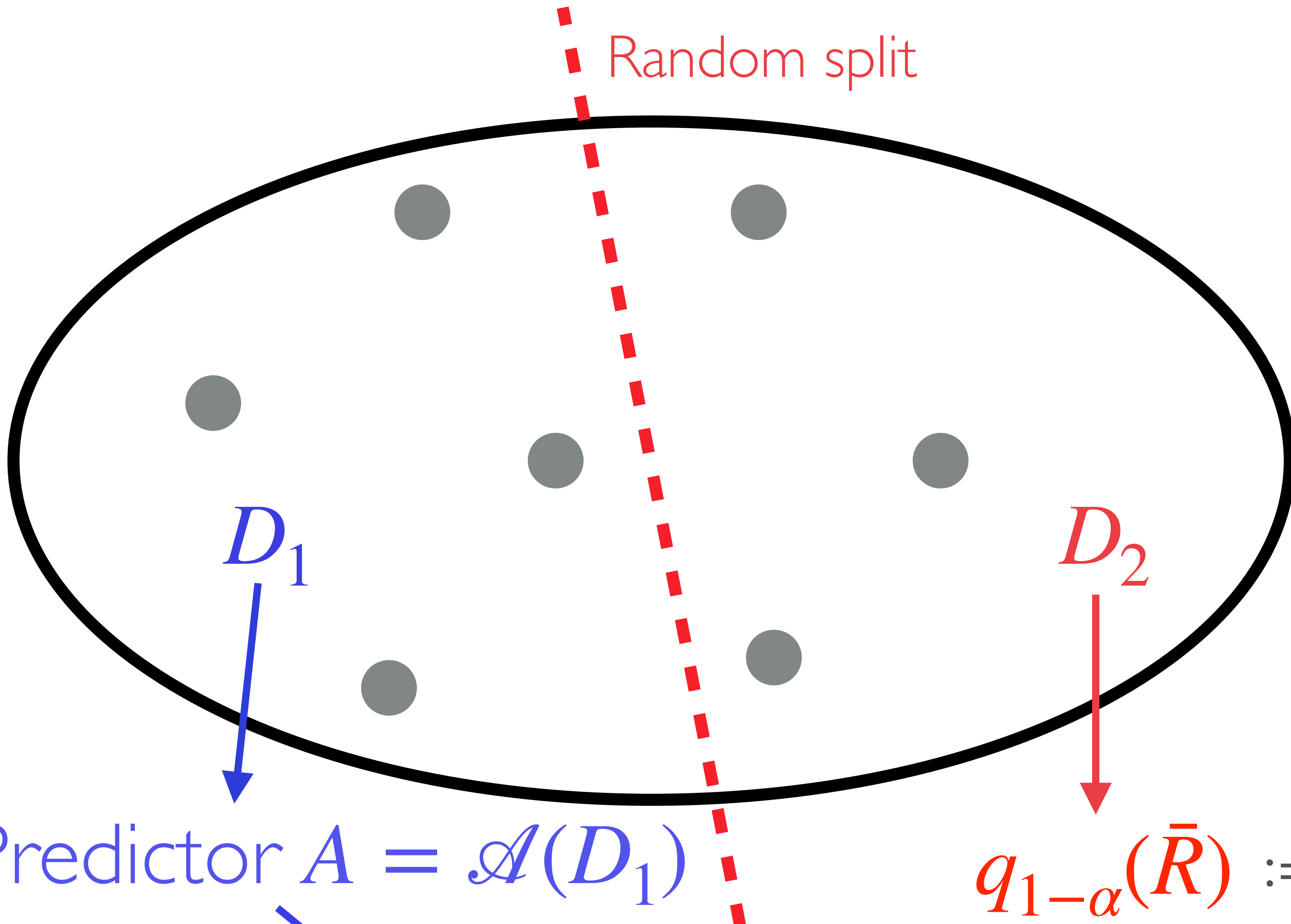
Split/"Inductive" Conformal Prediction

Training data



Hold-out scores $R_i \equiv R_A(X_i, Y_i)$

eg: residual $R_i := |Y_i - A(X_i)|$

Let $\bar{R} = \{R_i\}_{i \in D_2}$

$R_{n+1} = |Y_{n+1} - A(X_{n+1})|$

$R_1, \ldots, R_{n_2}, R_{n+1}$ exchangeable

$\implies$ rank(R_{n+1}) is uniform ★

Predictor $A = \mathscr{A}(D_1)$

$q_{1-\alpha}(\bar{R})$ $:= \lceil (1-\alpha)(n_2+1) \rceil$ ranked element of $\bar{R}$

w.h.p. $R_{n+1} \equiv |Y_{n+1} - A(X_{n+1})| \leq q_{1-\alpha}(\bar{R})$

$\implies$ w.h.p. $Y_{n+1} \in \{y : |y - A(X_{n+1})| \leq q_{1-\alpha}(\bar{R})\}$

$C(X_{n+1}) := [A(X_{n+1}) \pm q_{1-\alpha}(\bar{R})]$ $\equiv \{y : |y - A(X_{n+1})| \leq q_{1-\alpha}(\bar{R})\}$

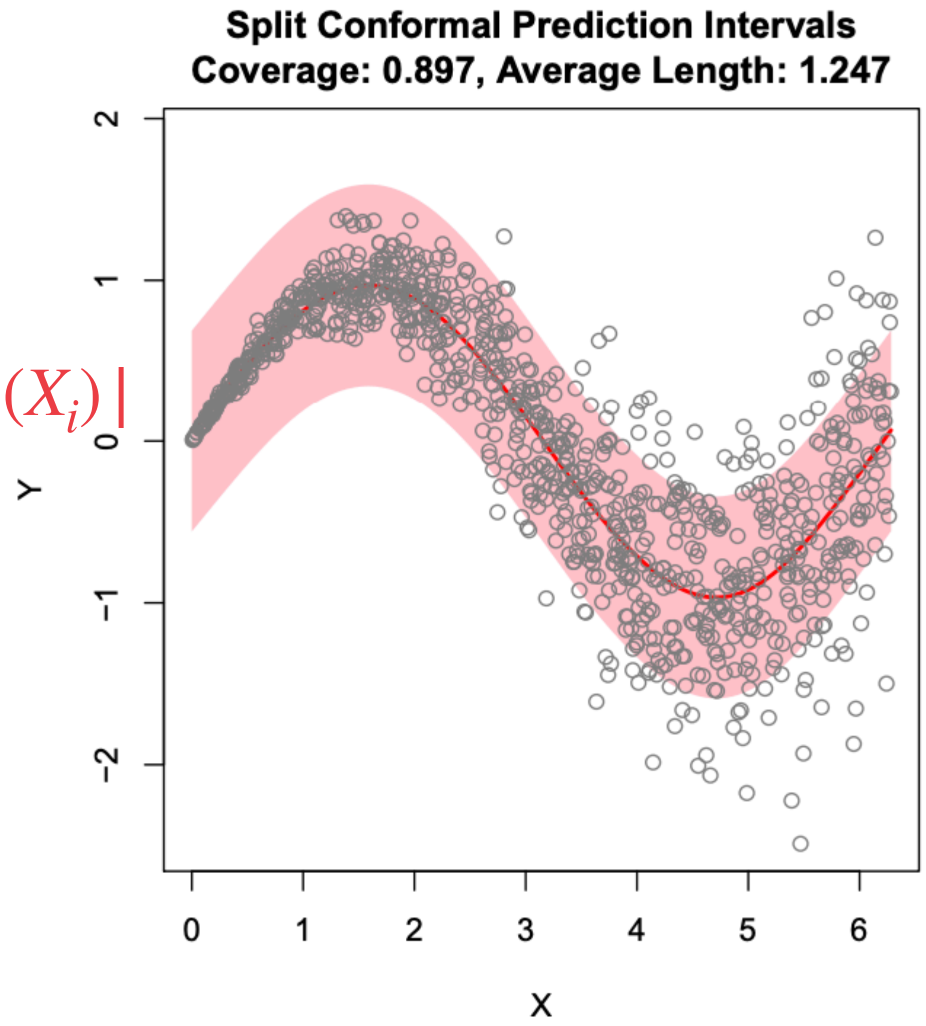
$\Pr(Y_{n+1} \in C(X_{n+1})) \geq 1 - \alpha$.

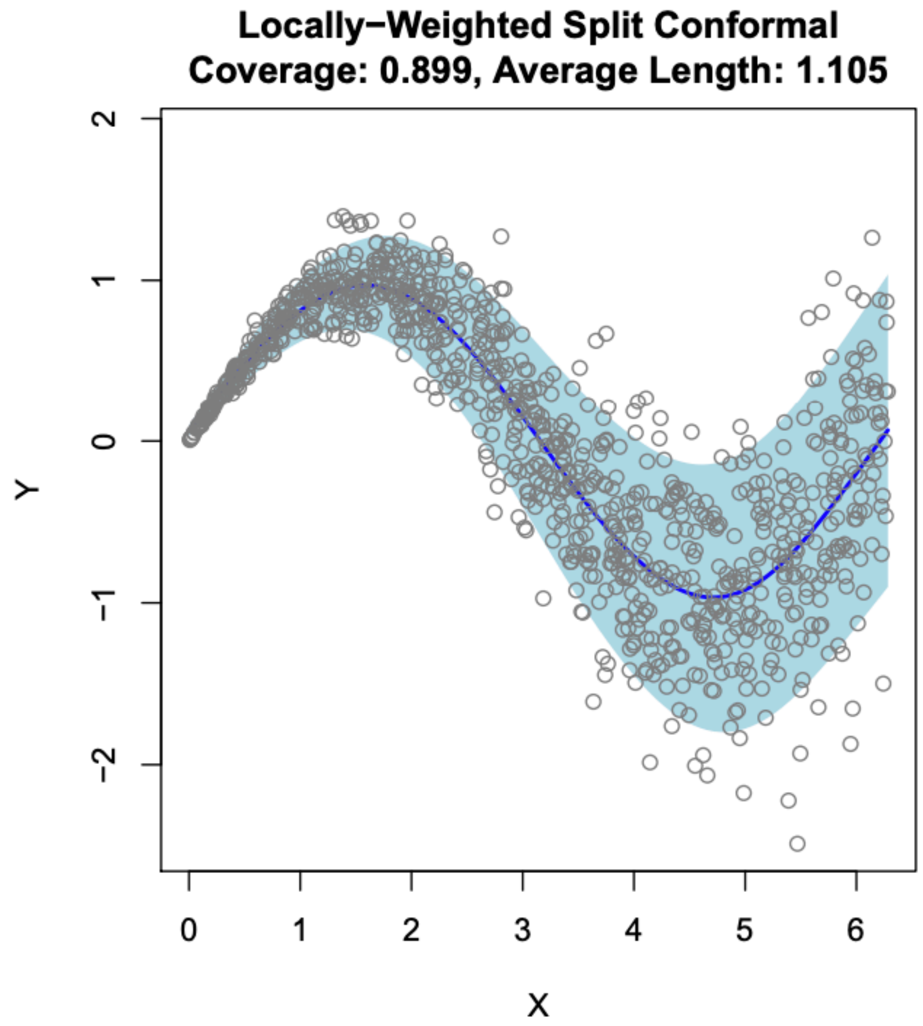
$\leq^* 1 - \alpha + \frac{1}{n_2 + 1}$.

Papadopoulos, Proedrou, Vovk, Gammerman '02
Lei, Wasserman, Rinaldo, Tibshirani '18

LWRT'18

$R_i := |Y_i - A(X_i)|$





$$R_i := \frac{|Y_i - A(X_i)|}{\sigma(X_i)}$$

Classifier $A : \mathscr{X} \to \Delta(\mathscr{Y})$ or $\mathbb{R}^{\mathscr{Y}}$

$$R_i := \sum_{k=1}^{K} [A(X_i)]_k \, \mathbf{1}_{[A(X_i)]_k > [A(X_i)]_{Y_i}}$$

or $R_i :=$ rank(Y_i) in $A(X_i)$