# Trustworthy Machine Learning

## Conformal Prediction

**Sangdon Park**

POSTECH

# Conformal Prediction

## Vladimir Vovk

FOLLOW

Department of Computer Science, Royal Holloway, University of London
Verified email at rhul.ac.uk - Homepage

Machine Learning  Conformal Prediction  Foundations of Probability  Foundations of Statistics  Mathematical Finance

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| Aggregating strategies<br>V Vovk<br>Proceedings of 3rd Annu. Workshop on Comput. Learning Theory, 371-383 | 956 | 1990 |
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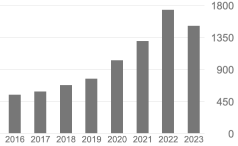

# Conformal Prediction

Vladimir Vovk

## Algorithmic learning in a random world

Authors Vladimir Vovk, Alexander Gammerman, Glenn Shafer

Publication date 2005/3/1

Volume 29

Publisher Springer

Description This book is about conformal prediction, an approach to prediction that originated in machine learning in the late 1990s. The main feature of conformal prediction is the principled treatment of the reliability of predictions. The prediction algorithms described—conformal predictors—are provably valid in the sense that they evaluate the reliability of their own predictions in a way that is neither over-pessimistic nor over-optimistic (the latter being especially dangerous). The approach is still flexible enough to incorporate most of the existing powerful methods of machine learning. The book covers both key conformal predictors and the mathematical analysis of their properties.

Algorithmic Learning in a Random World contains, in addition to proofs of validity, results about the efficiency of conformal predictors. The only assumption required for validity is that of" randomness"(the prediction algorithm is presented with …

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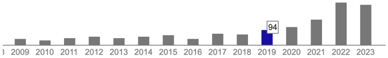


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> ...we are *hedging* the prediction — we are adding to it a statement about how strongly we believe it.
> – Vovk et al., 2005

# Motivation

**Conventional prediction:**

$\hat{y}\Bigg($  $\Bigg) = \widehat{\text{Bulldog}}$

**Conformal prediction:**

$\hat{C}\Bigg($  $\Bigg) = \left\{ \begin{array}{c} \text{Toy terrier} \\ \text{Bulldog} \\ \text{poodle} \end{array} \right\}$

# Motivation

**Conventional prediction:**

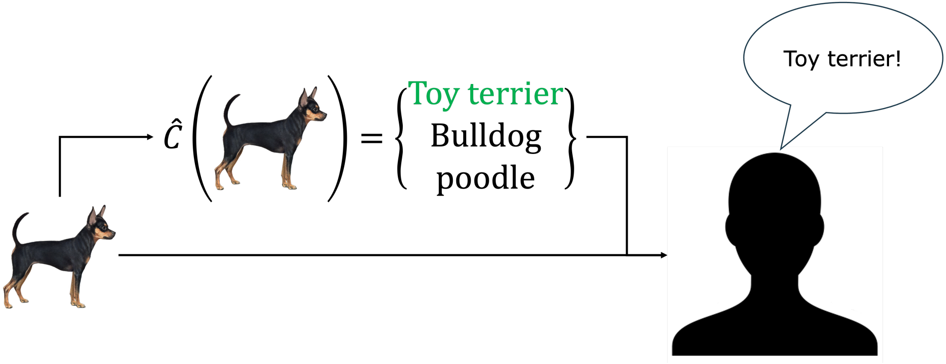
$$f : \mathcal{X} \mapsto \mathcal{Y}$$

**Conformal prediction:**

$$C : \mathcal{X} \mapsto 2^{\mathcal{Y}}$$

- Conventional prediction is a “point” prediction.
- Conformal prediction is a set-valued prediction.
- The set contains “likely-correct” alternative options.
  - The set size measures “uncertainty”!
- Why not confidence prediction? User-friendly?

# Motivation: Decision Making



# Why "Conformal"?

mathoverflow

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PUBLIC

## How is the "conformal prediction" conformal?

Asked 6 years, 5 months ago  Modified 6 months ago  Viewed 2k times

16

+100

Thanks for your interest. The term "conformal prediction" was suggested by Glenn Shafer, and at first I did not like it exactly for the reason that you mention: it has nothing (or very little) to do with conformal mappings in complex analysis. But then I discovered other meanings, even in maths; e.g., Wikipedia has five on its disambiguation page for "conformal":

- Conformal film on a surface (same thickness)
- Conformal fuel tanks on military aircraft
- Conformal coating in electronics
- Conformal hypergraph, in mathematics
- Conformal software, in ASIC Software

So the word did not look taken to me anymore. The expression that we had used before Glenn proposed "conformal prediction" was even worse ("transductive confidence machine").

Thanks to Hengrui Luo for drawing my attention to this question.

As for question (2), the answer depends on which robust predictors you have in mind. The predictors with most similar properties are the ones in classical statistics (such as the standard prediction intervals in linear regression based on Student's t distribution); the main difference is that they are parametric. There is a predictive version of tolerance intervals in nonparametric statistics, but their treatment of objects (x parts of observations (x,y), where y are labels) is limited. Upper bounds on the probability of error given by standard PAC predictors are often too high to be useful.

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answered Apr 13, 2017 at 7:35
Vladimir Vovk

# Conformal (Prediction) Sets

**Definition (conformal set)**

$$C(x) := \{y \in \mathcal{Y} \mid f(x, y) \geq q\}$$

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- We are using more recent notations based on inductive conformal prediction.
  - The notations are from Lei et al. [2018], Vovk et al. [2005], Tibshirani et al. [2019], and their combination.
  - Note that inductive conformal prediction [Papadopoulos et al., 2002] is an efficient variation of full conformal prediction [Vovk et al., 2005].

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  - Note that inductive conformal prediction [Papadopoulos et al., 2002] is an efficient variation of full conformal prediction [Vovk et al., 2005].
- $f : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$: a conformity scoring function
  - Measures how well $(x, y)$ *conforms* to a trained model $f$ (via a proper training set)
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  - Measures how well $(x, y)$ *conforms* to a trained model $f$ (via a proper training set)
  - $f(x, y)$ is a likelihood of $x$ for being $y$
- $q$: A parameter to be chosen by an algorithm.

# Conformity Scoring Functions I

## Conformity scoring functions can be (almost) any model!

**Example (classification)**

$$f(x, y) := f_{\mathsf{cls}}(x, y)$$

- $f_{\mathsf{cls}}$: a classification model, *e.g.*, resnet

# Conformity Scoring Functions II

## Conformity scoring functions can be (almost) any model!

**Example (standard regression in 1-dimension)**

$$f(x, y) := -|\mu(x) - y|$$

- $\mu$: a regressor

# Conformity Scoring Functions III

## Conformity scoring functions can be (almost) any model!

**Example (probabilistic regression)**

$$f(x, y) := \mathcal{N}(y; \mu(x), \sigma^2_{1:d}(x))$$

- *i.e.*, a Gaussian model with a diagonal covariance matrix [Nix and Weigend, 1994])
- $d$: The dimension of $\mathcal{Y}$.
- Implementation: $\mu(x) = f_{\text{mu}}(x)$ and $\ln \sigma^2 = f_{\text{var}}(x)$
  - $f_{\text{mu}}(x)$: a neural network
  - $f_{\text{var}}(x)$: a neural network

# Back to Conformal Sets

## Definition (conformal sets)

$$C(x) := \{y \in \mathcal{Y} \mid f(x, y) \geq q\}$$

- A conformity scoring function $f$ is given.
- $f$ is a target to measure uncertainty.
- How to choose $q$?

# Assumption: Exchangeability

### Assumption

*A sequence of random variables* $X_1, X_2, \ldots$ *is exchangeable if for any permutation* $\sigma$*, the following holds:*

$$\mathbb{P}\left\{X_1 = x_1, X_2 = x_2, \ldots\right\} = \mathbb{P}\left\{X_{\sigma(1)} = x_1, X_{\sigma(2)} = x_2, \ldots\right\}.$$

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- The i.i.d. assumption implies the exchangeability assumption (why?).

# A Goodness Metric: Coverage Guarantee

**Definition (coverage guarantee)**

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

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- The probability is taken over $(X_i, Y_i)$ for $i = 1, \ldots, n+1$.
- $(X_i, Y_i)$ for $i = 1, \ldots, n+1$: the exchangeable samples (thus the i.i.d. samples)

# A Goodness Metric: Coverage Guarantee

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- $\hat{C}$: A conformal set constructed by the training set

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- $(X_i, Y_i)$ for $i = 1, \ldots, n + 1$: the exchangeable samples (thus the i.i.d. samples)
- $\hat{C}$: A conformal set constructed by the training set
- $1 - \alpha \in (0, 1)$: A desired coverage rate

The level $\beta$ quantile of a distribution $F$:

**Definition (quantile)**

$$\text{Quantile}(\beta; F) := \inf\{z \mid \mathbb{P}\{Z \leq z\} \geq \beta\}$$

- $F$: a distribution over the augmented real line, $\mathbb{R} \cup \{\infty\}$
- $Z \sim F$
  - allows multiple instances of the same element

# Quantile

## Quantile of an Empirical Distribution

The level $\beta$ quatile of an empirical distribution of the values $v_{1:n}$:

**Definition (quantile)**

$$\text{Quantile}(\beta; v_{1:n}) := \text{Quantile}\left(\beta; \frac{1}{n}\sum_{i=1}^{n} \delta_{v_i}\right)$$

- $v_{1:n} := \{v_1, \ldots, v_n\}$: an unordered multiset
- $\delta_a$: a $\delta$-distribution (*i.e.*, a point mass at $a$)

# Quantile Lemma

**Lemma (Tibshirani et al. [2019])**

*If* $V_1, \ldots, V_{n+1}$ *are exchangeable random variables, then for any* $\beta \in (0, 1)$*, we have*

$$\mathbb{P}\left\{V_{n+1} \leq \textit{Quantile}(\beta; V_{1:n} \cup \{\infty\})\right\} \geq \beta.$$

- The key lemma for conformal prediction
- Intuition?
- We will see a proof after motivating on this quantile lemma.

# Quantile Algorithm

**Definition (quantile algorithm)**

Given $(X_1, Y_1), \ldots, (X_n, Y_n)$,

$$\hat{q}_{1-\alpha} := \text{Quantile}(1-\alpha, V_{1:n} \cup \{\infty\}),$$

where $V_i := -f(X_i, Y_i)$.

- The implementation is as simple as finding the $k$-th smallest value.

# Coverage Guarantee of the Quantile Algorithm

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

*Assume that* $(X_i, Y_i)$ *for* $i \in \{1, \ldots, n+1\}$ *are exchangeable. For any scoring function* $f$ *and any* $\alpha \in (0,1)$*, denote the conformal set by*

$$\hat{C}(x) := \left\{ y \in \mathcal{Y} \;\middle|\; -f(x,y) \leq \hat{q}_{1-\alpha} \right\}.$$

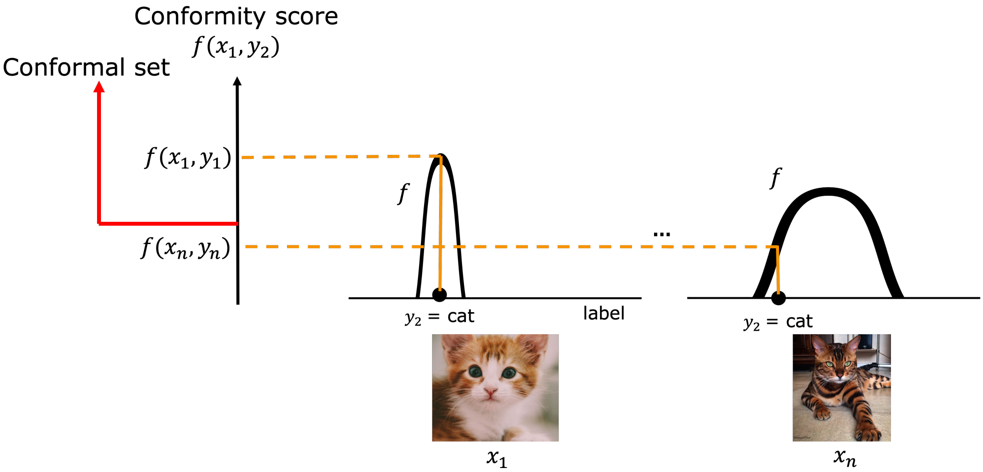
*Then, we have*

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

*where the probability is taken over* $(X_i, Y_i)$.

- This is a marginal coverage guarantee.

# Coverage Guarantee of the Quantile Algorithm: Intuition




- A conformal set contains the most "true scores".

# Coverage Guarantee of the Quantile Algorithm: A Proof Sketch

- Due to the symmetric construction of scores (using the same scoring function $f$), for any permutation $\pi$ we have

$$(Z_1, \dots, Z_{n+1}) \stackrel{d}{=} (Z_{\pi(1)}, \dots, Z_{\pi(n+1)}) \Longrightarrow (V_1, \dots, V_{n+1}) \stackrel{d}{=} (V_{\pi(1)}, \dots, V_{\pi(n+1)})$$

  where $Z_i \coloneqq (X_i, Y_i)$.
- As $(Z_1, \dots, Z_{n+1})$ are exchangeable, so are $(V_1, \dots, V_{n+1})$.
- Use the quantile lemma by letting $\beta = 1 - \alpha$, *i.e.*,

$$\mathbb{P}\Big\{V_{n+1} \leq \text{Quantile}(1-\alpha; V_{1:n} \cup \{\infty\})\Big\} \geq 1 - \alpha.$$

- Observe that

$$Y_{n+1} \in \hat{C}(X_{n+1}) \Longleftrightarrow V_{n+1} \leq \text{Quantile}(1-\alpha, V_{1:n} \cup \{\infty\}).$$

- Thus, we have

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

# Quantile Lemma (Again)

**Lemma (Tibshirani et al. [2019])**

*If* $V_1, \ldots, V_{n+1}$ *are exchangeable random variables, then for any* $\beta \in (0,1)$*, we have*

$$\mathbb{P}\left\{V_{n+1} \leq \mathit{Quantile}(\beta; V_{1:n} \cup \{\infty\})\right\} \geq \beta.$$

- The key lemma for conformal prediction

# Quantile Lemma: A Proof Sketch I

- One fact about quantiles of a discrete distribution $F$ with support points $a_1, \dots, a_k \in \mathbb{R}$:
  - Denote $q := \text{Quantile}(\beta; F)$
  - Reassign the points $a_i$ strictly larger than $q$ to arbitrary values also strictly larger than $q$, yielding a new distribution $\tilde{F}$
  - Still we have $\text{Quantile}(\beta; F) = \text{Quantile}(\beta; \tilde{F})$
- Thus, we have

$$V_{n+1} > \text{Quantile}(\beta; V_{1:n} \cup \{\infty\}) \iff V_{n+1} > \text{Quantile}(\beta; V_{1:n+1}).$$

- This implies

$$\begin{aligned} \mathbb{P}\Big\{V_{n+1} \leq \text{Quantile}(\beta; V_{1:n} \cup \{\infty\})\Big\} &= \mathbb{P}\Big\{V_{n+1} \leq \text{Quantile}(\beta; V_{1:n+1})\Big\} \\ &\geq \frac{\lceil \beta(n+1) \rceil}{n+1} \qquad (1) \\ &\geq \frac{\beta(n+1)}{n+1} = \beta. \end{aligned}$$

# Quantile Lemma: A Proof Sketch II

- Why (1)?
  - By exchangeability, we have for any integer $k \in \{1, \ldots, n+1\}$,

$$\mathbb{P}\left\{V_{n+1} \leq V_{[k]}\right\} \geq \frac{k}{n+1},$$

    where $[k]$ is the $k$-th smallest value of $V_1, \ldots, V_{n+1}$.

# Quantile Lemma: A Proof Sketch III

- Suppose that there is no tie (see Kuchibhotla [2020] for a general proof). We have

$$
\begin{aligned}
\mathbb{P}\left\{V_{n+1} \leq V_{[k]}\right\} &\geq \mathbb{P}\left\{\bigvee_{i=1}^{k} V_{n+1} = V_{[i]}\right\} \\
&= \sum_{i=1}^{k} \mathbb{P}\left\{V_{n+1} = V_{[i]}\right\} \\
&= \sum_{i=1}^{k} \frac{n!}{(n+1)!} \\
&= \frac{k}{n+1}.
\end{aligned} \tag{2}
$$

# Quantile Lemma: A Proof Sketch IV

- Why (2)?
  - ★ For each permutation $\pi$, we have

$$\begin{aligned} \mathbb{P}\{V_1 \le \cdots \le V_{n+1}\} &= \mathbb{P}\{(V_1, \ldots, V_{n+1}) \in A\} \\ &= \mathbb{P}\{(V_{\pi(1)}, \ldots, V_{\pi(n+1)}) \in A\} \\ &= \mathbb{P}\{V_{\pi(1)} \le \cdots \le V_{\pi(n+1)}\} \end{aligned} \tag{3}$$

    where $A \coloneqq \{(x_1, \ldots, x_{n+1}) \mid x_1 \le \cdots \le x_{n+1}\}$ and (3) holds due to the exchangeability assumption.
  - ★ This means that "exchangeability" implies "uniform probability over orders"

# Power of Conformal Prediction

The coverage guarantee is drawn with minimal assumptions.

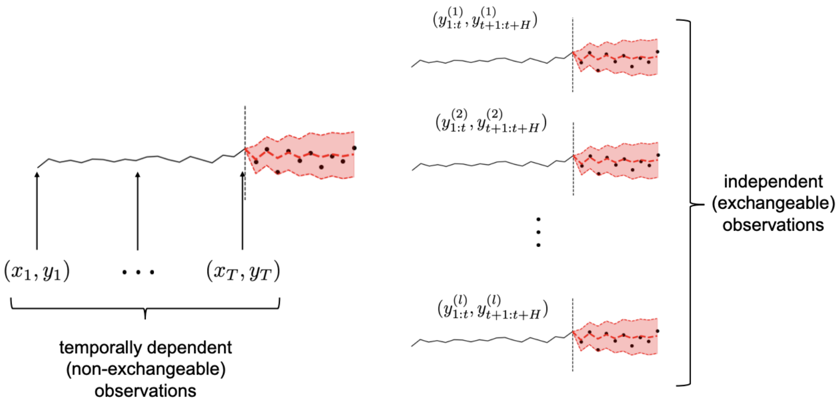
- It does not make assumptions on a distribution except for the exchangeability.
- The guarantee holds for any conformity scoring function.

# Size of Conformal Sets

- Application-dependent issues
  - classification: set size
  - 1-D regression: interval length
  - multi-dimentional regression: *e.g.*, volume
- Larger set: uncertain (*e.g.*, the entire set)
- Smaller set: more certain (*e.g.*, a singleton)
- We will see some analysis in PAC conformal prediction.

# Interesting Variation: Time-series Forecasting

## Conformal Time-series Forecasting [Stankeviciute et al., 2021]




- Conformal prediction for independent time-series data
  - *e.g.*, temperature change for each year

# Conformal Time-series Forecasting I

## Problem

**Setup:**

- $y_{t:t'} \coloneqq (y_t, y_{t+1}, \ldots, y_{t'}) \in \mathbb{R}^d \times \ldots \mathbb{R}^d$: a time-series of $d$-dimensional observation
  - Let $d = 1$
- $H$: a prediction horizon
- $\hat{y}_{t'+1:t'+H}$: predicted future observations (*e.g.*, the output of a RNN)
- $C_{t+h}(y_{1:t})$: a prediction interval at time $t + h$
  - $C_{t+h}(y_{1:t}) \coloneqq [\hat{y}^L_{t+h}, \hat{y}^U_{t+h}]$

# Conformal Time-series Forecasting II

## Problem

**Desired coverage guarantee:**

$$\mathbb{P}\left\{\forall h \in \{1, \ldots, H\},\ y_{t+h} \in C_{t+h}(y_{1:t})\right\} \geq 1 - \alpha$$

- The probability is taken over $y_{1:t+H}$.
- $1 - \alpha$: a desired coverage rate

**Goal:** Find $C_{t+h}$ for all $h \in \{1, \ldots, H\}$.

# Conformal Time-series Forecasting

## Approach

- $\mathcal{D} := \{(y_{1:T}^{(i)}, y_{T+1:T+H}^{(i)})\}_{i=1}^{m}$: a calibration set

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## Approach

- $\mathcal{D} := \{(y^{(i)}_{1:T}, y^{(i)}_{T+1:T+H})\}_{i=1}^{m}$: a calibration set
- Observe that

$$\mathbb{P}\left\{\exists h \in \{1, \dots, H\},\ y_{t+h} \notin C_{t+h}(y_{1:t})\right\} \leq \sum_{h \in \{1,\dots,H\}} \mathbb{P}\{y_{t+h} \notin C_{t+h}(y_{1:t})\} \tag{4}$$

$$\leq \alpha \tag{5}$$

# Conformal Time-series Forecasting

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- $\mathcal{D} := \{(y^{(i)}_{1:T}, y^{(i)}_{T+1:T+H})\}_{i=1}^{m}$: a calibration set
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&\leq \alpha && (5)
\end{aligned}$$

  - (4) holds due to the union bound.

# Conformal Time-series Forecasting

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  - (5) holds if $\mathbb{P}\{y_{t+h} \notin C_{t+h}(y_{1:t})\} \leq \frac{\alpha}{H}$

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$$\leq \alpha \tag{5}$$

  - (4) holds due to the union bound.
  - (5) holds if $\mathbb{P}\{y_{t+h} \notin C_{t+h}(y_{1:t})\} \leq \frac{\alpha}{H}$
- Due to the standard conformal prediction, we can find $C_{t+h}$ such that

$$\mathbb{P}\{y_{t+h} \notin C_{t+h}(y_{1:t})\} \leq \frac{\alpha}{H}.$$

# Conclusion

- Conformal prediction is a powerful tool to construct a prediction set (for measuring uncertainty) with correctness guarantees.
- Conformal prediction has many applications due to its "distribution-free" and "scoring-function-free" nature.
- The original conformal prediction framework can be extended to "conditional" cases (*e.g.*, PAC conformal prediction).

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