Tutorial on Conformal Predictive Distributions

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Contents of the tutorial

- **Conformal Predictive Distributions** (Vovk et al., 2017) are a novel approach to estimating the probability distribution of a continuous variable that depends on a number of features.
- CPDs probabilities correspond to long-term relative frequencies (within statistical fluctuation) under minimal assumptions.
  - CPDs require only that the data be generated independently by an unknown but fixed distribution.
  - No assumption on the type of distribution
  - No need of a prior
- Outline of the tutorial
  - Motivation, context
  - Predictive Distribution, Conformal Predictive Distribution
  - KRRPM
  - Evaluation of PD and real-life examples

The roots of prior-free predictive distributions

- Suppose data $\mathcal{D}$ is generated by a known distribution with unknown parameter θ, which we want to estimate.
- Bayesian statistics can provide a distribution for the parameter
  - Estimating a probability distribution comes naturally to Bayesian methods
    $$p(\theta|\mathcal{D}) \propto p(\theta)p(\mathcal{D}|\theta)$$
  - but you have to specify a prior $p(\theta)$.
- Frequentist statistics provides Confidence Intervals
  - Given $\alpha \in [0, 1]$ coverage probability, we compute an interval
    $$L(\mathcal{D}, \alpha), U(\mathcal{D}, \alpha)$$
    that contains the actual θ a fraction α of the time.
- $p(\theta|\mathcal{D})$ does not make sense in a strict frequentist framework.
- But frequentists recognized that predictive distributions would be useful!

Prior-free posterior distributions

- "The Holy Grail of parametric statistics" (Efron, 2010)
- Early attempts to arrive at prior-free posterior distributions can be traced back to Fisher's fiducial approach in the 1930s.
  - Not completely formalized; controversial; referred to as "Fisher's biggest blunder".
- There is now a resurgence of interest in the topic.
- Conformal Predictive Distributions are part of this trend.

Predictive Distributions: our setting

- Unrestricted randomness, i.i.d. data
  - $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ generated independently by fixed, but unknown $P(X, Y)$
- Intuitively, we seek an $F(y, x)$ that has the properties of a Cumulative Distribution Function in y.

$$F(y, x, \mathcal{D}) = P\{Y \leq y | X = x)$$

As long as $(x_i, y_i) \sim P(X, Y)$, the intervals $(-\infty, y)$ contain y_i with relative frequency $F(y, x_i)$

A property of CDF

- Let $F_X()$ be the (Cumulative) Distribution Function of the Random Variable X.

$$F_X(x) = P\{X \leq x\}$$

- The RV that is obtained by evaluating the F_X on the RV X is uniformly distributed.

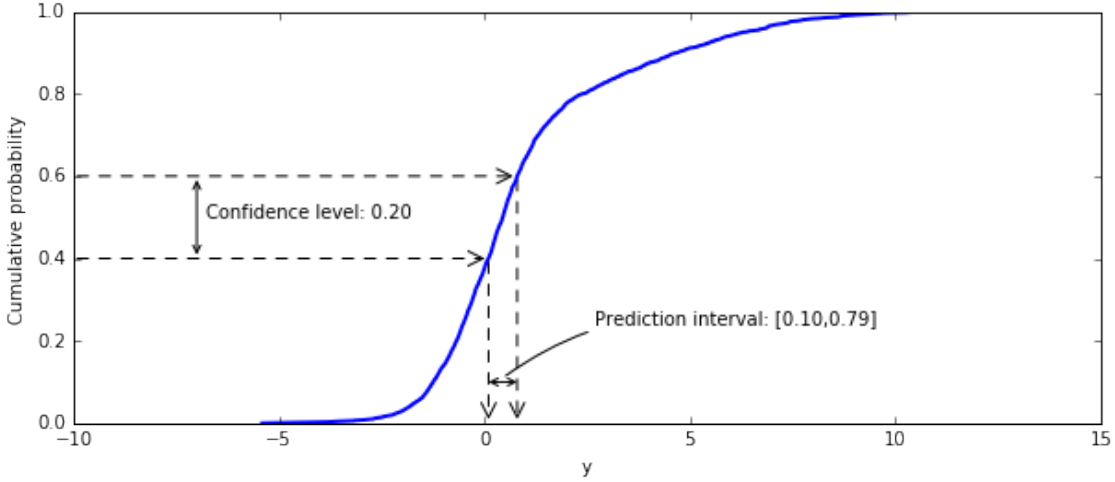
$$F_X(X) \sim U(0,1)$$

Predictive Distributions

- Suppose we have observations $z_1, \ldots, z_n$ from a set $\mathbf{Z} = \mathbf{X} \times \mathbb{R}$ and a test object $x_{n+1} \in \mathbf{X}$
- Let's call Predictive Distribution a function $Q(z_1, \ldots, z_n, (x_{n+1}, y))$ that
  - for any choice of training sequence $z_1, \ldots, z_n$ and any choice of test object x_{n+1} has the following properties of a CDF:
    - $Q(z_1, \ldots, z_n, (x_{n+1}, y))$ is monotonically increasing in y
    - $\lim_{y \to -\infty} Q(z_1, \ldots, z_n, (x_{n+1}, y)) = 0$
    - $\lim_{y \to +\infty} Q(z_1, \ldots, z_n, (x_{n+1}, y)) = 1$.
  - for any joint probability distribution P on $\mathbf{Z}$,
    - $Q(z_1, \ldots, z_n, z_{n+1}) \sim U$ when $(z_1, \ldots, z_{n+1}) \sim P^{n+1}$.
- This definition omits some technicalities to keep things simple.

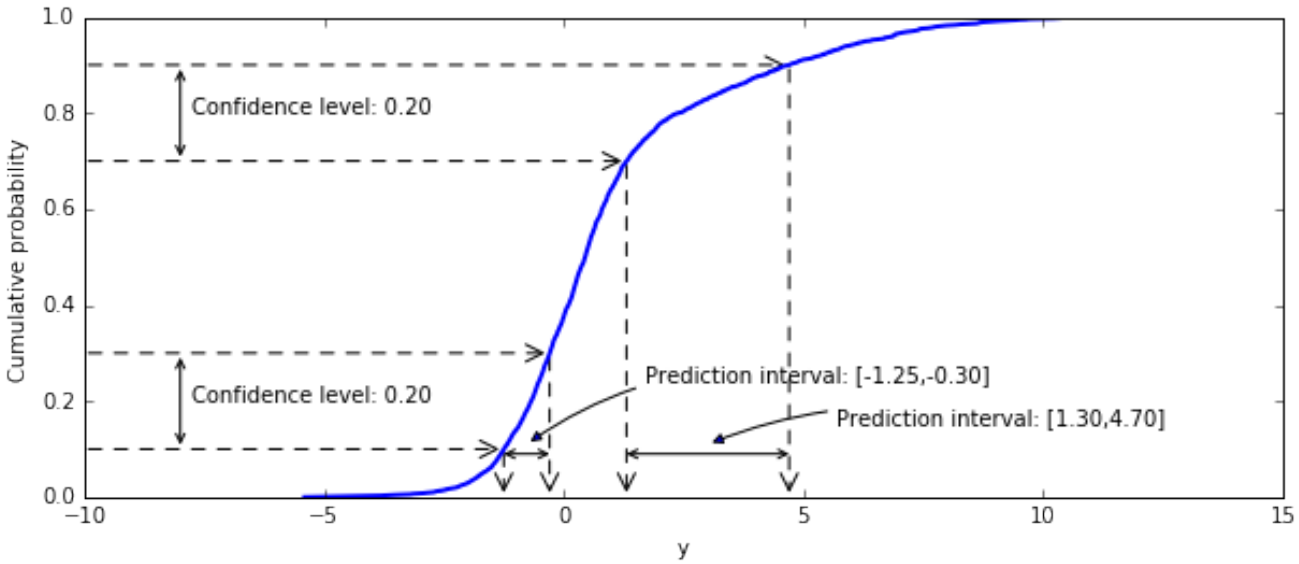
Predictive Distributions

- The "uniformity" property confers the ability to produce prediction intervals with **guaranteed coverage**
- Guaranteed coverage is the key property of predictive distributions
  - We can choose a confidence level α and we can read, off the predictive distribution, intervals of y in which the actual value falls with rate α (barring statistical fluctuation).



Predictive Distribution Interpretation

- Note that one can choose different prediction intervals for a given confidence level.



- One can choose the narrowest
  - i.e. where the slope of the predictive distribution is largest
- Or one around the median (previous slide)

An aside: Why CDF?

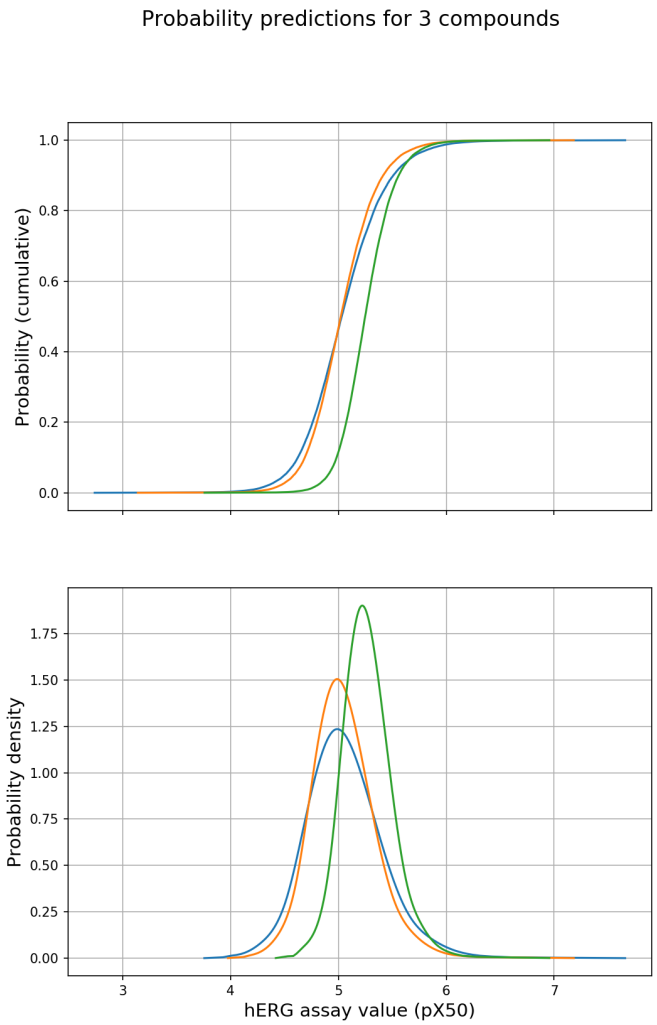
- The ECDF is guaranteed to converge to CDF for i.i.d. data (Glivenko-Cantelli theorem)
- The ECDF converges fast to the CDF (Dvoretzky–Kiefer–Wolfowitz inequality)
- To obtain a PDF you have to solve an ill-posed (unstable) problem:

$$\int h(x-t)f(t)dt = F(t) \qquad \text{where } h(x) \text{ is the step function}$$

  - stable: a small variation in the right-side $F(x)$ results in a small change in the solution $f(x)$

An aside: Why CDF?

- Pros
  - Computing an ECDF from data is straightforward.
  - You can read probabilities easily off the chart.
- Cons
  - Perceptually challenging to evaluate density
  - You can't find the mode immediately.



Conformal Predictive Distributions

- It is possible to obtain Predictive Distributions by using a variant of Conformal Prediction for Regression.
- We define as conformity measure a function

$$A(z_1, \ldots, z_{n+1})$$

invariant w.r.t. permutations of the first n arguments.

- Given (x_{n+1}, y), we compute conformity scores α_i^y as:

$$\begin{aligned} \alpha_i^y &:= A(z_1, \ldots, z_{i-1}, z_{i+1}, \ldots, z_n, (x_{n+1}, y), z_i), \qquad i = 1, \ldots, n, \\ \alpha_{n+1}^y &:= A(z_1, \ldots, z_n, (x_{n+1}, y)). \end{aligned}$$

- Subject to some conditions on $A()$, the predictive distribution is then

$$Q(z_1, \ldots, z_n, (x_{n+1}, y)) := \frac{1}{n+1}\left(\left|\left\{i = 1, \ldots, n+1 \mid \alpha_i^y < \alpha_{n+1}^y\right\}\right|\right)$$

Requirements on the conformity measure

- Q() can be viewed as the estimate of probability under i.i.d. of drawing an observation with a smaller value of the CM than the hypothetical observation (x_{n+1}, y).
  It is as if we were testing the null hypothesis of i.i.d. using α as test statistic and computing the p-value Q().

- In contrast to CP, not all functions with the specified invariance property are conformity measures that result in valid predictive distributions.

- For the resulting Q() to have the properties of CDF, the conformity measure must be such that:
  - $\alpha^y_{n+1} - \alpha^y_i$ is a monotonically increasing function of $y \in \mathbb{R}$
  - $\lim_{y \to \pm\infty}(\alpha^y_{n+1} - \alpha^y_i) = \pm\infty$

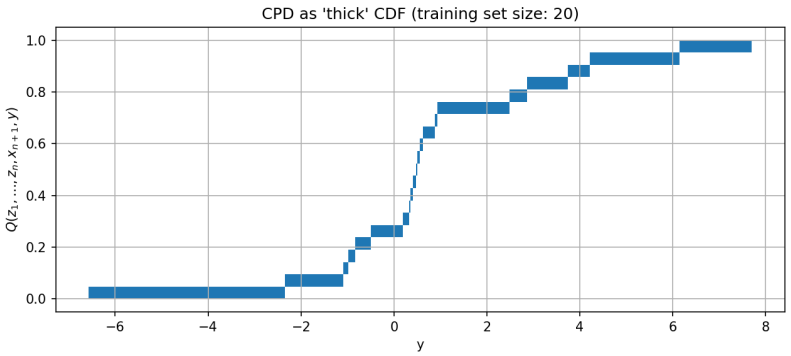
- A simple example is the $y - \hat{y}_{n+1}$ where $\hat{y}_{n+1}$ is the estimate obtained with K nearest neighbours regression.

Some details

- The definition was simplified for the sake of clarity.
- The properly defined CPD has a randomness element

$$Q(z_1, \ldots, z_n, (x_{n+1}, y)) := \frac{1}{n+1}\left(\left|\left\{i = 1, \ldots, n+1 \mid \alpha_i^y < \alpha_{n+1}^y\right\}\right|\right) + \frac{\tau}{n+1}\left(\left|\left\{i = 1, \ldots, n+1 \mid \alpha_i^y = \alpha_{n+1}^y\right\}\right|\right)$$

  where $\tau \sim U(0,1)$
- Informally, it's a "thick" distribution function, but the thickness is $\frac{1}{n+1}$, so it matters little as soon as you have a reasonably sized training set



Kernel Ridge Regression Predictive Machine

- Let's use Kernel Ridge Regression

$$\hat{y}_{n+1} := k'(K + aI)^{-1} Y$$

where $k_i = \mathcal{K}(x_i, x_{n+1})$, $K_{i,j} := \mathcal{K}(x_i, x_j)$, $i, j = 1, \ldots, n$.
Unfortunately, $y - \hat{y}_{n+1}$ is not a proper conformity measure. It fails to produce a strictly increasing function in y for high-leverage objects.

- Another possibility is to include the test object with the hypothetical label in the training set of the KRR.

$$\hat{\bar{y}}_{n+1} := \bar{k}'(\bar{K} + aI)^{-1} \bar{Y}$$

where $\bar{k}_i = \mathcal{K}(x_i, x_{n+1})$, $\bar{K}_{i,j} := \mathcal{K}(x_i, x_j)$, $\bar{y}_i = y_i$, $i, j = 1, \ldots, n+1$.
This too fails to guarantee a strictly increasing function in y.

Kernel Ridge Regression Predictive Machine

- A conformity measure is obtained as:

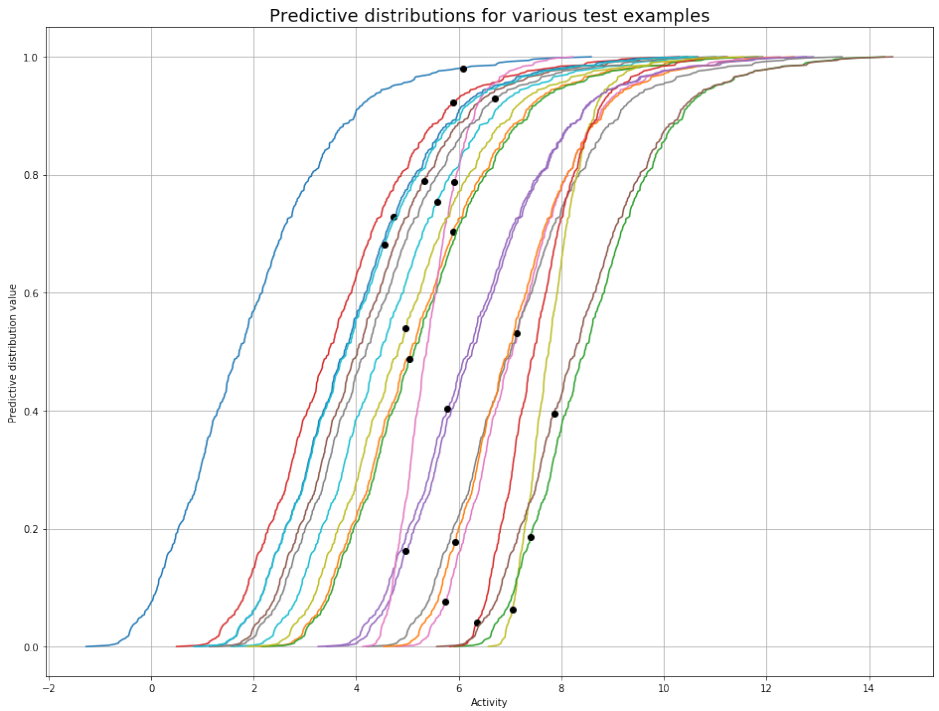
$$\frac{y_{n+1} - \hat{\bar{y}}_{n+1}}{\sqrt{1 - \bar{h}_{n+1}}}$$

  where $\bar{h}_{n+1}$ is the element $\bar{H}_{n+1,n+1}$ of the hat matrix $\bar{H} := (\bar{K} + aI)^{-1}\bar{K}$

- There exists an explicit form of the resulting KRRPM.
  It can be implemented in a way that avoids recomputing from scratch the hat matrix for every test object.

Application of KRRPM to Chemoinformatics

- Data set from a study on an enzyme
  - 1368 compounds
  - 68 features (PhysChem properties)
- Training set: 1000 observations, randomly sampled
- KRRPM using Laplace kernel



Desirable properties of PD

- **Validity**
  The predicted probabilities correspond to the long-term relative frequencies
- **Specificity** (a.k.a. Sharpness)
  The intervals for a given probability are as narrow as possible
- You can always make a valid predictive distribution: just output for all test objects the same PD, the ECDF of the label. But this would be a terrible forecast as it would have no specificity.
- CPDs guarantee validity under i.i.d.
  One can concentrate on improving specificity

Evaluating Predictive Distributions

- For probabilistic predictions, there are some established "scores"
  - Brier loss: $\frac{1}{n}\sum_{i=1}^{n}(p_i - o_i)^2$
  - Log loss: $\frac{1}{n}\sum_{i=1}^{n}(o_i \log p_i + (1 - o_i)\log(1 - p_i))$
- These apply to tasks in which predictions must assign probabilities to a set of mutually exclusive **discrete** outcomes.
- They can be used on predictive distributions but they do not evaluate the PDs in their entirety.
- There are metrics and diagnostic tools for PDs
  - PIT, CRPS
  - Validity plot, Interval boxplots

Assessing validity

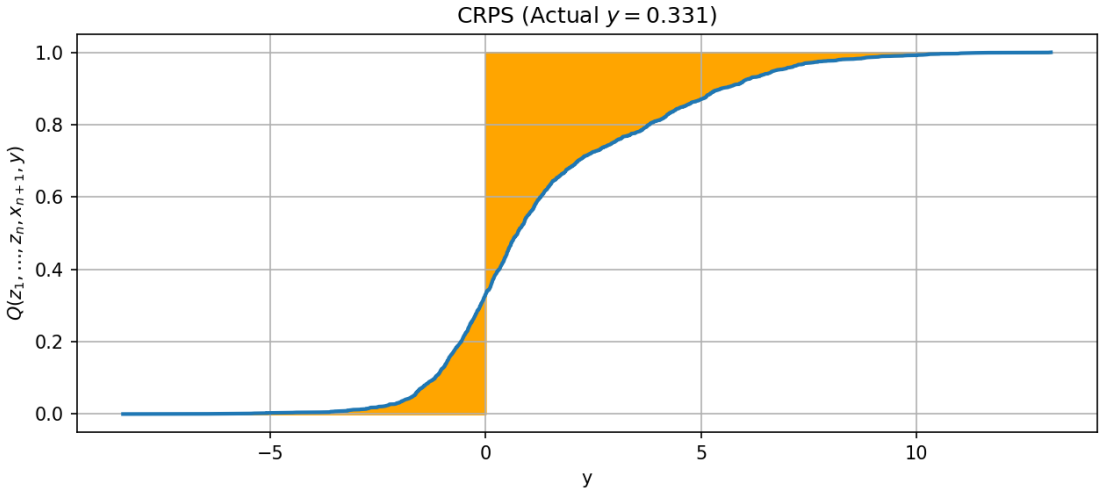
- Probability Integral Transform (PIT): evaluate $F_i()$ on the actual label y_i
- If the predictions $F_i(y)$ are ideal, $F_i(y_i)$ are variates from a $U(0,1)$ distribution.
- The PIT can be used to check validity.
- The histogram of the PIT should be as flat as possible.
- Perhaps better, the ECDF of the PIT should be as close as possible to the (0,0)-(1,1) diagonal
  - Kolmogorov-Smirnov statistic and K-S test

Continuous Ranked Probability Score (CRPS)

- The quadratic measure of discrepancy between the forecast CDF $F(y, x)$ and the "ideal forecast CDF" given the scalar observation y

$$\mathrm{CRPS}(F, x, y) = \int_{\mathbb{R}} [F(t, x) - \mathbb{I}(t \geq y)]^2 \, dt$$

where $\mathbb{I}()$ is the indicator function.

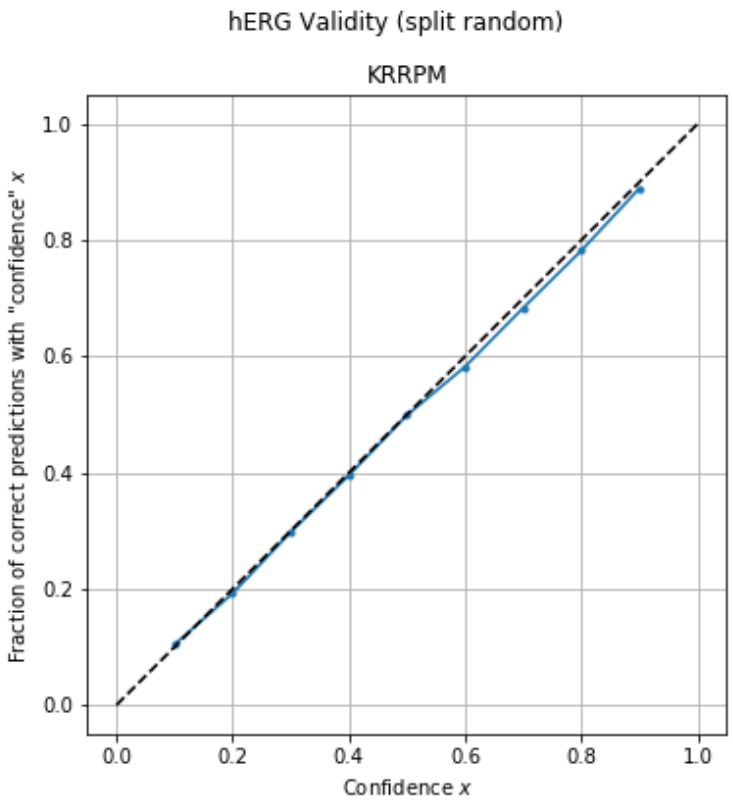


- For a number of predictions, one takes the average:

$$\overline{\mathrm{CRPS}}(F) = \frac{1}{n} \sum_{i=1}^{n} \mathrm{CRPS}(F, x_i, y_i)$$

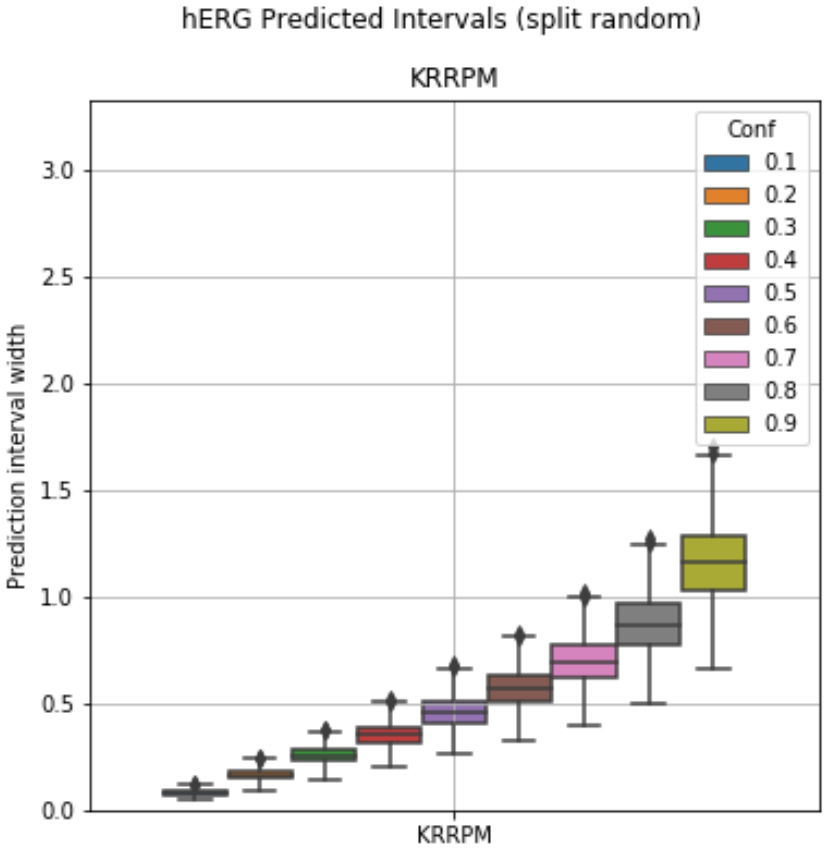
Practical diagnostic tools: Validity plot

- Validity plot: actual coverage vs. confidence
- For all the confidence values of interest (e.g. $0.1, 0.2, \ldots, 0.9$)
  - compute the intervals for the objects in the validation set
  - compute the relative frequency of "interval contains actual label"
- The relative frequency should be close to the confidence

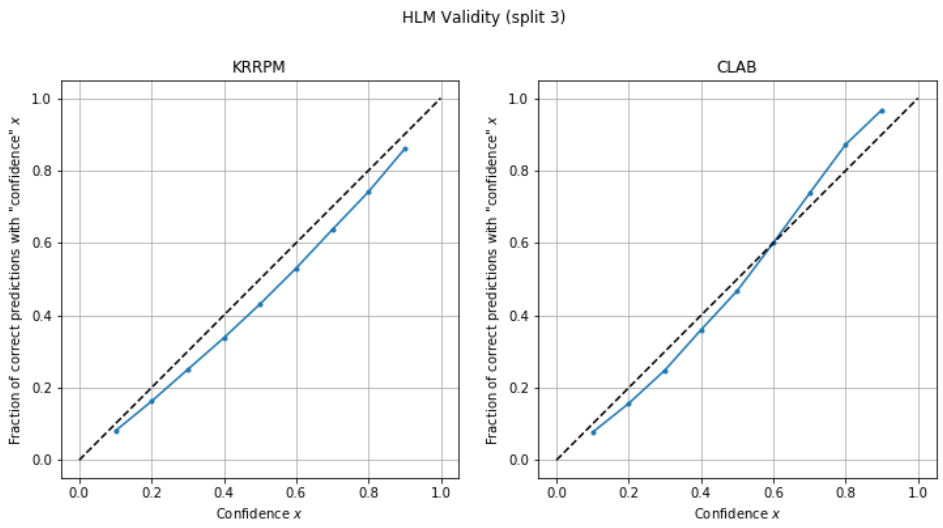


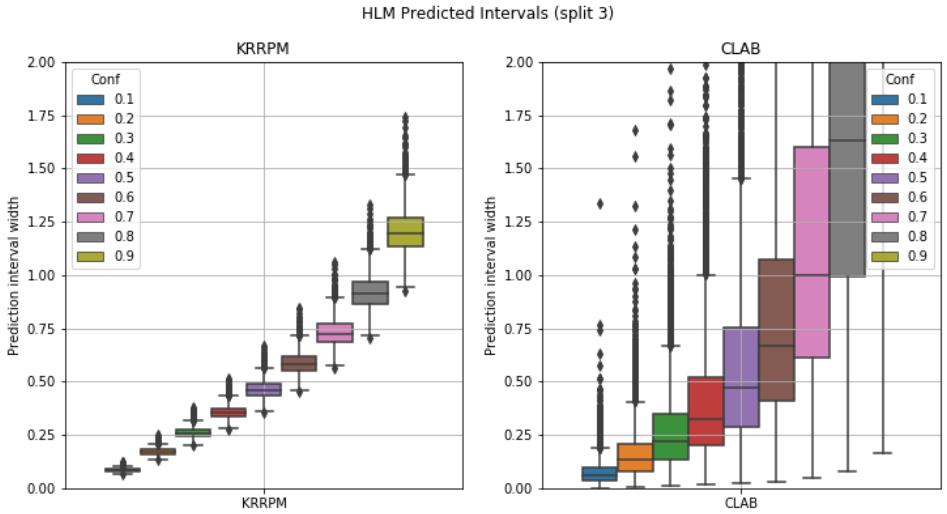
Practical diagnostic tools: Interval boxplots

- Descriptive statistics of the intervals
- The narrower the intervals, the more useful the predictions.



A real-life comparison





Observations

- The validity guarantee rests on the i.i.d. assumption.
  - $\{(x_1, y_1), \ldots, (x_n, y_n)\} \sim P^n(X, Y)$, where $(x_i, y_i) \sim P(X, Y)$
  - It is a minimal assumption of regularity
  - But it can be violated very easily in practice!
    - $P(X, Y) = P(X)\, P(Y|X)$
    - $P(X)$ varies: covariate shift
    - $P(Y|X)$ varies: in high-dimensional spaces, one visits just a small portion
- You should not assess validity and efficiency separately.
  - There is a trade-off between the two

Summary

- Conformal Predictive Distributions offer a prior-free, non-parametric way to estimate the distribution of random variable Y for an object x, based on previous data $(x_1, y_1), \ldots, (x_n, y_n)$.
- CPDs have a validity guarantee under a minimal assumption of test and training data being i.i.d.
  - CPD require only that the data be generated independently by an unknown but fixed distribution.
- KRRPM uses the flexible and regularized method of Kernel Ridge Regression to generate Conformal Predictive Distributions.

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