Epistemic Uncertainty in Conformal Scores: A Unified Approach

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Context

Introduction

- Focus shift: point predictions to prediction uncertainty.
- Conformal Prediction: predictive regions with finite-sample marginal validity under mild i.i.d. assumptions (Vovk et al. 2005, Shafer & Vovk 2008).
- Main ingredient: conformal score $s(\mathbf{x}, y)$.
- Choice of conformity score is critical: influences the shape and informativeness of predictive regions (Angelopoulos & Bates 2021).
- Standard CP: mostly capture **aleatoric uncertainty**.
- Another source of uncertainty: **epistemic uncertainty** (Hüllermeier & Waegeman 2021).
- CP with narrow predictive intervals in regions with few training data.

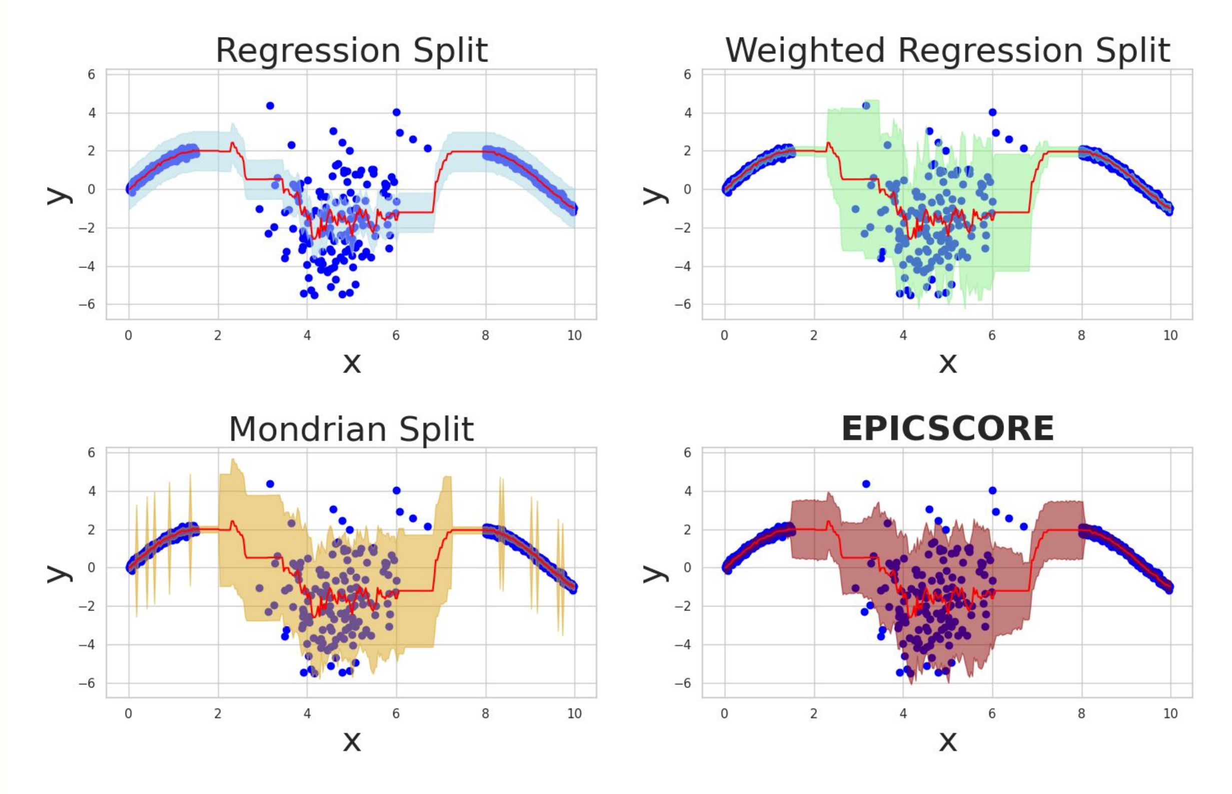


Figure 1: A comparison of predictive intervals from standard split-conformal regression and our proposed EPICSCORE approach.

Existing approaches

- Few strategies focus on integrating epistemic uncertainty.
- Existing approaches (e.g., Rosselini et al. 2024, Cocheteux et al. 2025) restricted to specific conformal scores (quantilic or regression).
- Our approach:
  - Integrate epistemic uncertainty on **any** conformal score;
  - Leverage Bayesian approaches to model epistemic uncertainty of $s(\mathbf{X}, Y)$;
  - Maintains marginal coverage guarantees (achieves asymp conditional);
  - **Enhance** rather than **replace** the conformal score;

Our approach

Review of split-CP

- Partitions data into $\mathcal{D}_{\text{train}}$ and $\mathcal{D}_{\text{calib}}$.
- Fit nonconformity score $s(\mathbf{X}, Y)$ on $\mathcal{D}_{\text{train}}$.
- Compute $t_{1-\alpha}$ using the calibration set:

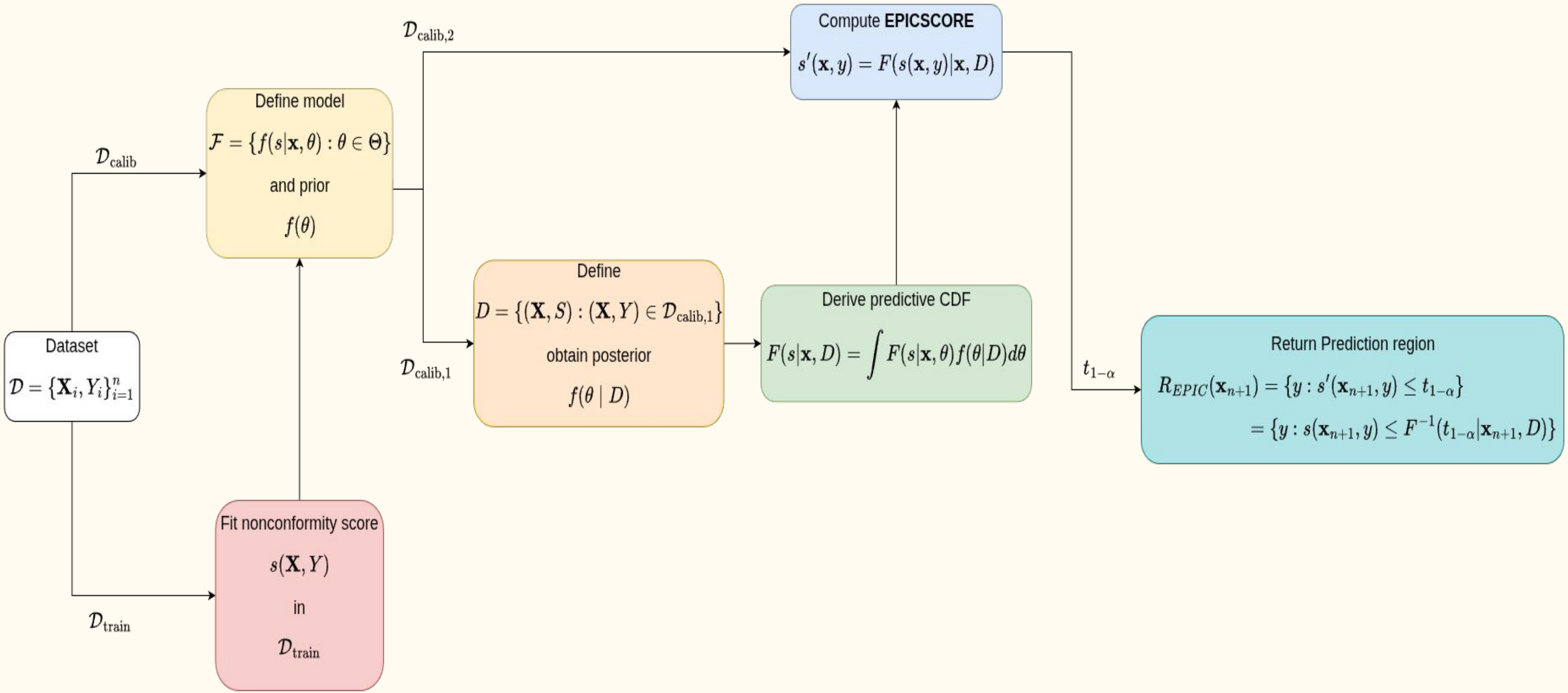
$$t_{1-\alpha} = \text{Quantile}_{1-\alpha}\{s(\mathbf{X}_i, Y_i) : (\mathbf{X}_i, Y_i) \in \mathcal{D}_{\text{calib}}\}.$$

- Prediction set for a new X_{n+1} :

$$R(\mathbf{X}_{n+1}) = \{y : s(\mathbf{X}_{n+1}, y) \leq t_{1-\alpha}\}.$$

- Marginal coverage guarantee $\mathbb{P}(Y_{n+1} \in R(\mathbf{X}_{n+1})) \geq 1 - \alpha.$

EPICSCORE



Compute **EPICSCORE**
$s'(\mathbf{x}, y) = F(s(\mathbf{x}, y)|\mathbf{x}, D)$
$\mathcal{D}_{\text{calib},2}$
Define model
$\mathcal{F} = \{f(s|\mathbf{x}, \theta) : \theta \in \Theta\}$
and prior
$f(\theta)$
$\mathcal{D}_{\text{calib}}$
Define
$D = \{(\mathbf{X}, S) : (\mathbf{X}, Y) \in \mathcal{D}_{\text{calib},1}\}$
obtain posterior
$f(\theta \mid D)$
Derive predictive CDF
$F(s|\mathbf{x}, D) = \int F(s|\mathbf{x}, \theta) f(\theta|D) d\theta$
Dataset
$\mathcal{D} = \{\mathbf{X}_i, Y_i\}_{i=1}^n$
$\mathcal{D}_{\text{calib},1}$
$t_{1-\alpha}$
Return Prediction region
$R_{EPIC}(\mathbf{x}_{n+1}) = \{y : s'(\mathbf{x}_{n+1}, y) \leq t_{1-\alpha}\}$
$= \{y : s(\mathbf{x}_{n+1}, y) \leq F^{-1}(t_{1-\alpha}|\mathbf{x}_{n+1}, D)\}$
Fit nonconformity score
$s(\mathbf{X}, Y)$
in
$\mathcal{D}_{\text{train}}$
$\mathcal{D}_{\text{train}}$

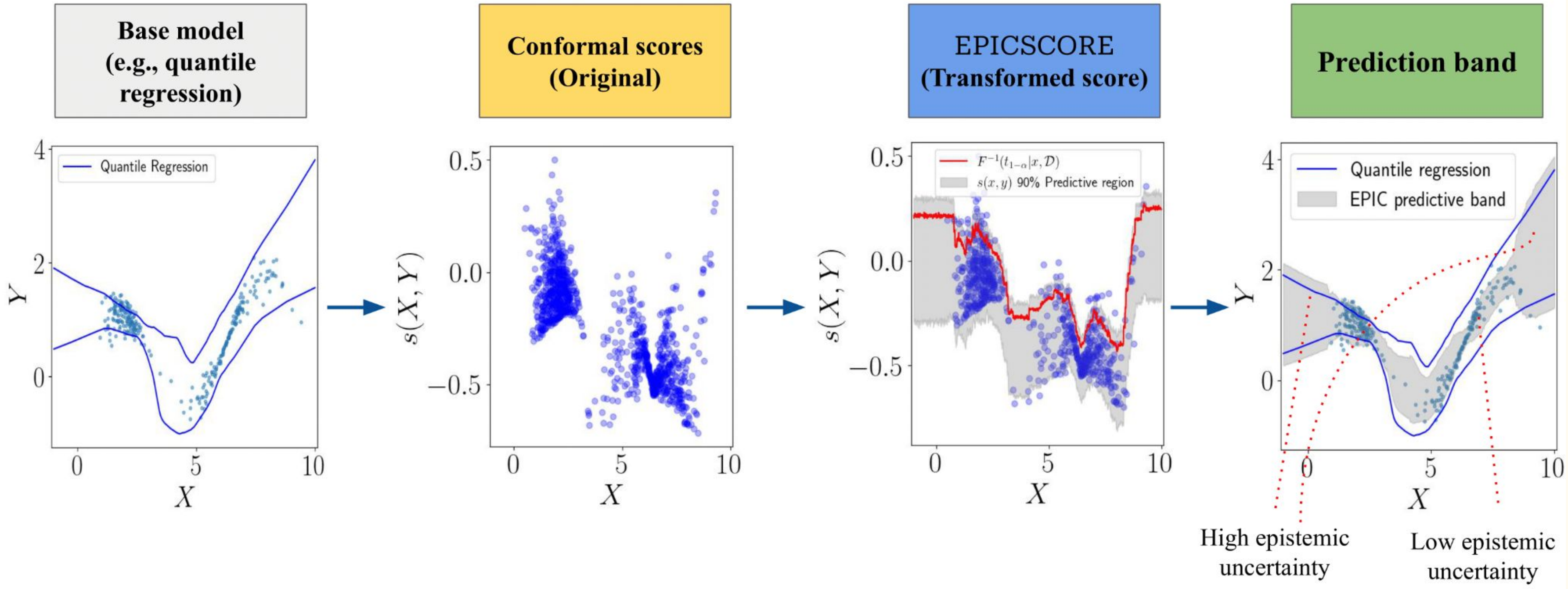


Figure 2: EPICSCORE illustration scheme

Theoretical guarantees and some details

- Marginal Coverage guarantee (**Theorem 1**).
- Asymp. conditional coverage if predictive distribution converges (**Theorem 2**).
- Practical model choices for predictive distribution:
  - BART (Chipman et al. 2012);
  - Gaussian Process (Williams & Rassmussen 2006);
  - Mixture Density Network with MC-Dropout (Bishop 1994, Gal & Gharamani 2016)

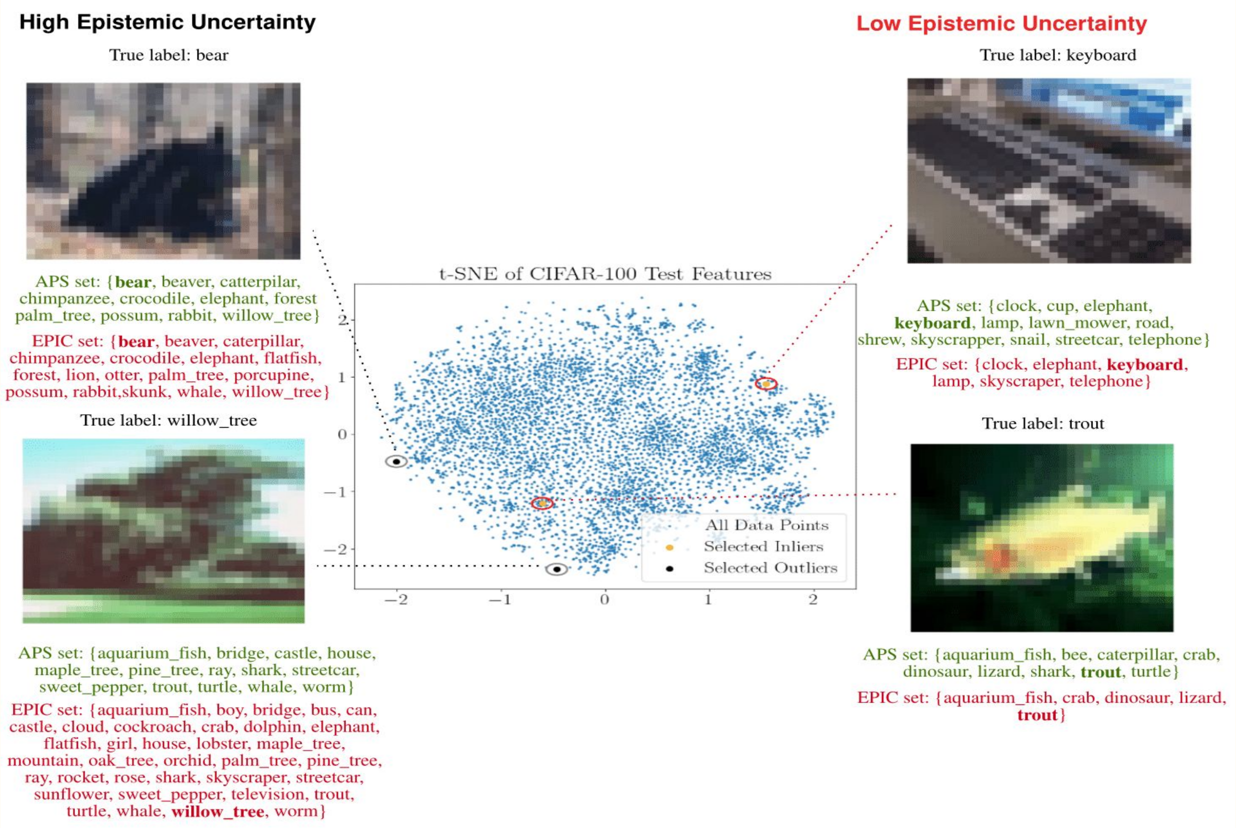
Applications

Real data comparisons

- Comparisons over 13 real datasets
- 6 different metrics, with highlight for two:
  - Average Interval Score Loss
  - Outlier to inlier interval ratio
- Comparing in regression and quantile regression contexts

Dataset	EPIC-BART	EPIC-GP	EPIC-MDN	CQR	CQR-r	UACQR-P	UACQR-S
airfoil	19.361 (0.234)	19.704 (0.27)	**18.799 (0.29)**	20.521 (0.234)	20.535 (0.236)	23.021 (0.337)	20.188 (0.3)
bike $\times(10^1)$	44.722 (0.297)	47.818 (0.320)	**43.858 (0.326)**	45.628 (0.256)	45.638 (0.258)	53.413 (0.376)	**43.815 (0.385)**
concrete	**42.765 (0.723)**	45.276 (0.764)	44.442 (0.8)	46.882 (0.681)	46.896 (0.683)	52.789 (1.097)	47.324 (1.349)
cycle	34.435 (0.142)	35.054 (0.131)	**34.077 (0.129)**	39.218 (0.134)	39.408 (0.136)	43.775 (0.181)	35.346 (0.197)
electric	0.099 (< 0.001)	0.096 (< 0.001)	**0.082 (< 0.001)**	0.102 (0.001)	0.102 (0.001)	0.111 (0.001)	0.097 (< 0.001)
homes $\times(10^5)$	7.739 (0.066)	8.098 (0.072)	**7.225 (0.049)**	8.360 (0.075)	8.433 (0.078)	11.427 (0.131)	8.544 (0.107)
meps19	**65.085 (1.469)**	**64.907 (1.56)**	**64.3 (1.528)**	**64.239 (1.56)**	**64.239 (1.56)**	71.015 (1.763)	**63.737 (1.461)**
protein	17.687 (0.019)	18.096 (0.037)	**17.417 (0.019)**	17.7 (0.015)	17.7 (0.016)	18.149 (0.015)	17.691 (0.015)
star $\times(10^1)$	**98.466 (0.768)**	**98.033 (0.750)**	**98.725 (0.754)**	**97.770 (0.725)**	**97.791 (0.724)**	99.782 (0.647)	99.809 (0.968)
superconductivity	74.37 (0.222)	80.278 (0.266)	**70.212 (0.196)**	75.496 (0.219)	75.508 (0.218)	87.929 (0.513)	73.971 (0.404)
WEC $\times(10^5)$	2.925 (0.009)	2.665 (0.012)	**2.374 (0.010)**	3.138 (0.009)	3.142 (0.009)	3.517 (0.010)	3.046 (0.010)
winered	**3.007 (0.058)**	**3.009 (0.059)**	**2.977 (0.05)**	**2.979 (0.069)**	**2.978 (0.069)**	3.059 (0.069)	**2.999 (0.063)**
winewhite	3.334 (0.03)	3.327 (0.034)	**3.219 (0.03)**	3.316 (0.036)	3.315 (0.036)	3.378 (0.038)	**3.2 (0.036)**

Application to image data



Final Remarks

Final remarks

- EPICSCORE: new conformal score incorporating epistemic uncertainty into **any** predictive region.
- Preserves marginal coverage and achieves asymptotic conditional coverage.
- Good empirical results.
- Approach flexible to different problems (classification, regression, etc.).
- Future works:
  - Extend EPICSCORE to settings with distribution shift.
  - Circumvent splitting of calibration set.

Thank you!

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Poster session 1 - Today!

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