Epistemic Uncertainty in Conformal Scores: A Unified Approach

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Presented by Mian Wei

Uncertainty

What is uncertainty? and why do we care?

[1] source: https://medium.com/data-science/how-confidence-and-prediction-intervals-work-4592019576d8

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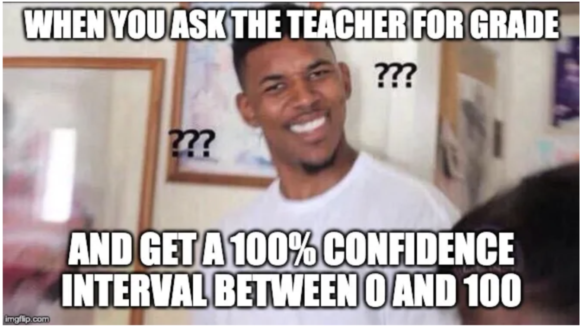

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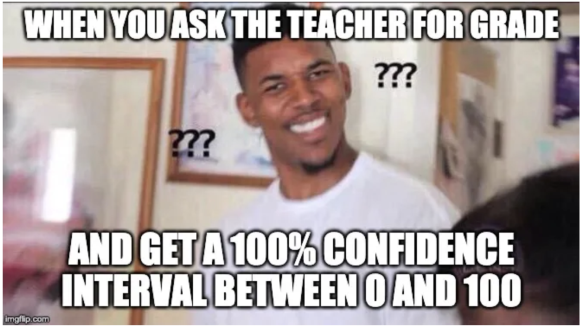

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- 100% confidence: GOOD!
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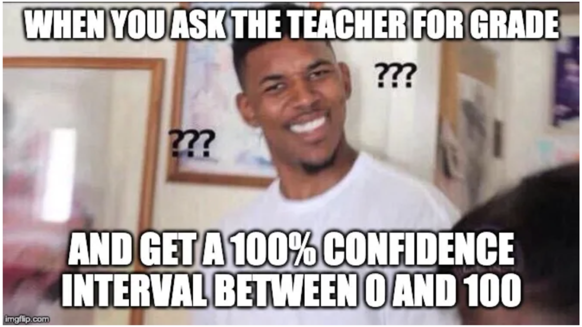

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- 100% confidence: GOOD!
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- $\implies$ Less confident but still high
- $\implies$ Band as tight as possible

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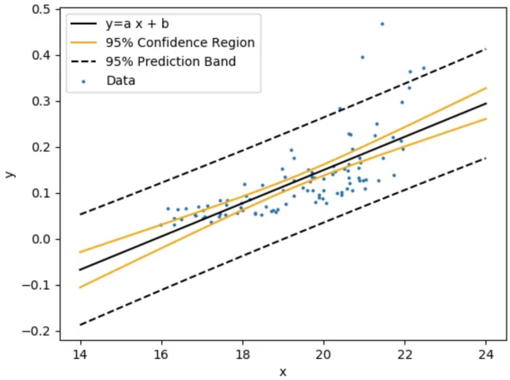
Confidence Interval v.s. Prediction Interval



[2]

"What is the average blood pressure?" v.s. "What might the next patient's blood pressure be?"

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Conformal Prediction

Assumption: The data points $(x_1, y_1), \ldots, (x_n, y_n)$ are **exchangeable**.
Decide:

- A predictive model $\hat{f}(x)$ (e.g., regression)

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- Compute the empirical quantile $q_{1-\alpha}$ of the scores;
- Construct the prediction interval for a new input x_{n+1} as:

$$\widehat{C}(x_{n+1}) = \left[\hat{f}(x_{n+1}) - q_{1-\alpha},\ \hat{f}(x_{n+1}) + q_{1-\alpha}\right]$$

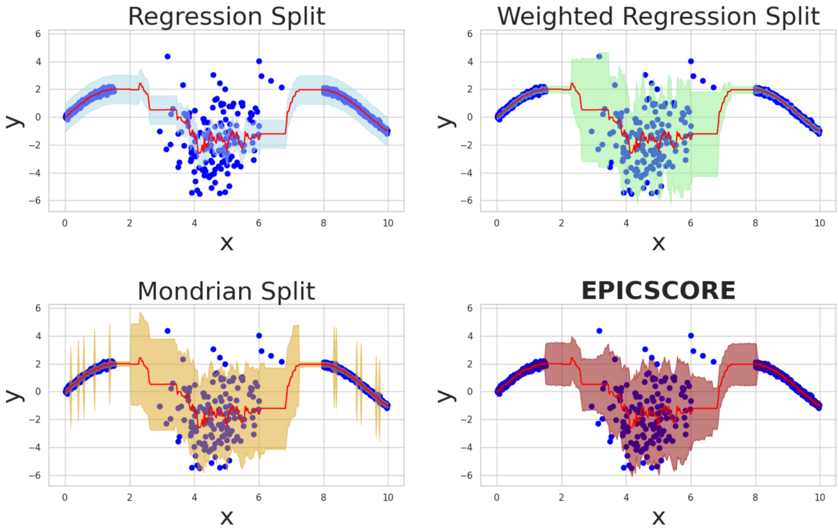
Aleatoric and Epistemic Uncertainty

Aleatoric Uncertainty: inherent in the data, irreducible
Epistemic Uncertainty: due to lack of knowledge (model or data), reducible

For Conformal Prediction

- Aleatoric Uncertainty: noisy data $\rightarrow$ wider interval, naturally captured
- Epistemic Uncertainty: not captured
  - Model: predefined. *"Is this model confident here?"*
  - Data: In regions with no training data, may still produce confident-looking intervals

Aleatoric and Epistemic Uncertainty



Motivation & Novelty

Goal: integrate epistemic uncertainty into the conformal prediction framework.

Two main directions:

- Redesign the conformal score, e.g., weighted regression split:

$$s(x, y) = \frac{|y - \hat{y}|}{\hat{\sigma}(x)}$$

- Adapt cutoffs locally, e.g., Mondrian conformal regression, partition the feature space into bins

For this paper:

- Uses Bayesian modeling to capture epistemic uncertainty;
- Model-agnostic — works with any Bayesian model;
- Can be layered on any conformal score;
- Marginal and asymptotic conditional coverage.

EPICSCORE

Input:

- Dataset $D = \{(X_i, Y_i)\}_{i=1}^{n}$, where $X_i \in \mathcal{X}$ and $Y_i \in \mathcal{Y}$.
- A conformal score function $s(x, y)$.
- Nominal level $\alpha \in (0, 1)$.
- A new test point X_{n+1}.

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Step I: Fit Conformal Scores

1. Split D into:
   - Training set D_{train}
   - Calibration set D_{cal}
2. Use D_{train} to fit a base predictive model, and construct the initial conformal score function $s(x, y)$.

Step II: Fit the Predictive Function

1. Split the calibration set D_{cal} into:
    - $D_{\text{cal},1}$ – for fitting the predictive distribution
    - $D_{\text{cal},2}$ – for computing the quantile cutoff

EPICSCORE

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2. Transform $D_{\text{cal},1}$ into score data:

$$D = \{(X, S) \mid S = s(X, Y),\ (X, Y) \in D_{\text{cal},1}\}$$

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3. Use Bayesian models to estimate the predictive cumulative distribution function (CDF):

$$F(s \mid x, D) = \int F(s \mid x, \theta) f(\theta \mid D)\, d\theta$$

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Modeling choices for $F(s \mid x, D)$:

- Gaussian Processes (GPs)
- Bayesian Additive Regression Trees (BART)
- Mixture Density Networks with MC-Dropout

Step III Procedure:

1. Compute EPICSCORE for all elements of $D_{\text{cal},2}$ by:

$$s'(x, y) = F(s(x, y) \mid x, D)$$

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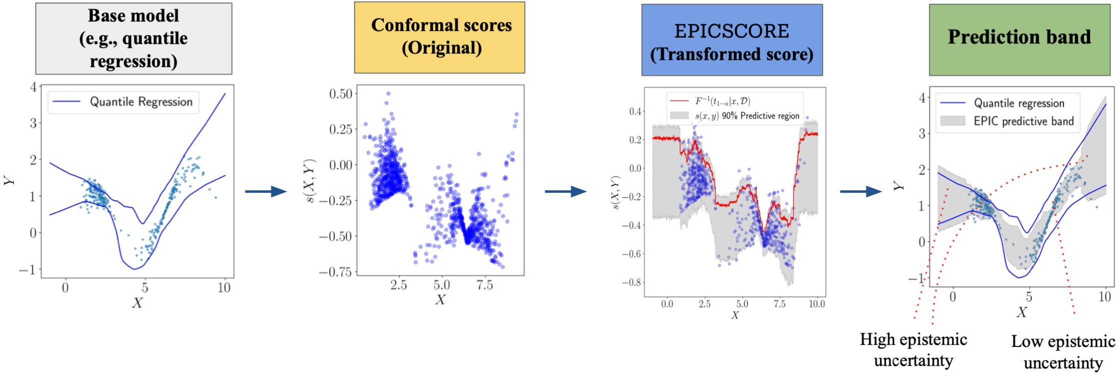
2. Compute the $(1 - \alpha)$ empirical quantile $t_{1-\alpha}$ of the conformal scores
3. Define the prediction region for a new input X_{n+1}:

$$\mathcal{R}_{\text{EPIC}}(X_{n+1}) = \{y : s'(X_{n+1}, y) \leq t_{1-\alpha}\}$$

or equivalently, using the original score s:

$$\mathcal{R}_{\text{EPIC}}(X_{n+1}) = \{y : s(X_{n+1}, y) \leq F^{-1}(t_{1-\alpha} \mid X_{n+1}, D)\}$$

Intuition Behind



"Uncertainty of uncertainty"

Special Cases

Case 1: Regression

- Original score

$$s(x, y) = |y - g(x)|$$

- EPICSCORE:

$$s'(x, y) = F(s(x, y) \mid x, D)$$

- Prediction interval:

$$g(x) \pm F^{-1}(t_{1-\alpha} \mid x, D)$$

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Case 2: Quantile Regression (CQR)

- Original score:

$$s(x, y) = \max\{q_{\alpha_1}(x) - y,\ y - q_{\alpha_2}(x)\}$$

- Prediction interval:

$$[q_{\alpha_1}(x) - F^{-1},\ q_{\alpha_2}(x) + F^{-1}]$$

Special Cases

Case 3: Classification

- Negative softmax score or APS-style score:

$$s(x, y) = -\hat{P}(y \mid x) \quad \text{or} \quad \sum_{y' : \hat{P}(y'|x) > \hat{P}(y|x)} \hat{P}(y'|x)$$

- EPICSCORE:

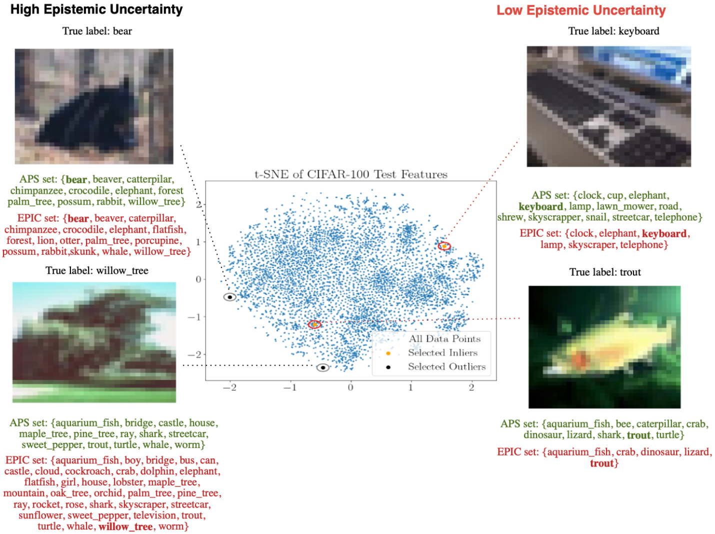
$$s'(x, y) = \sum_{y' : s(x, y') \leq s(x, y)} P(y' \mid x, D)$$

  Where $P(y' \mid x, D)$ is the Bayesian predictive class probability.

- Prediction Set:

$$\mathcal{C}(x) = \{y : s'(x, y) \leq t_{1-\alpha}\}$$

Classification



Theory

Theorem (Marginal Coverage)

Assuming that the data are independent and identically distributed (i.i.d.), the confidence region constructed by `EPICSCORE` *satisfies marginal coverage, that is,*

$$\mathbb{P}(Y \in R_{EPIC}(\mathbf{X})) \geq 1 - \alpha.$$

Moreover, if the fitted scores follow a continuous joint distribution, the upper bound also holds:

$$\mathbb{P}(Y \in R_{EPIC}(\mathbf{X})) \leq 1 - \alpha + \frac{1}{1 + |\mathcal{D}_{cal,2}|}.$$

Theory

Assumption 1. For any $\varepsilon > 0$, we assume uniform convergence in probability over the randomness in D:

$$\lim_{|D|\to\infty} \mathbb{P}\left(\sup_{s,\mathbf{x}} |F(s \mid \mathbf{x}, D) - F(s \mid \mathbf{x}, \theta^*)| > \varepsilon\right) = 0.$$

Theorem (Asymptotic Conditional Coverage)

Under Assumption 1, and assuming that the data are independent and identically distributed (i.i.d.), the confidence region constructed by `EPICSCORE` *satisfies the asymptotic conditional coverage condition, that is:*

$$\lim_{|\mathcal{D}_{cal}|\to\infty} \mathbb{P}(Y \in R_{EPIC}(\mathbf{X}) \mid \mathbf{X} = \mathbf{x}) = 1 - \alpha.$$

Experiments

Setup

- 13 datasets
- 40% training, 40% calibration, 20% test, averaged over 50 random splits
- AISL (Average Interval Score Loss)

Models for the predictive distribution

- **Bayesian Additive Regression Trees (BART)** [CGM12]: sum of regression trees,

$$s(Y, X) \mid X, \boldsymbol{\theta} \sim \phi\left(\sum_{i=1}^{m} G_i(X, T_i, M_i), \sigma\right),$$

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- **Gaussian Processes (GP)** [WR06]: score follows the form $s(Y, \mathbf{x}) = f(\mathbf{x}) + \varepsilon$, with $\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$, and $f(\mathbf{x}) \sim GP(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$ is a Gaussian process.

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- **Mixture Density Networks with Monte Carlo Dropout (MDN-MC)** [Bis94, GG16]: weighted sum of Gaussian components,

$$f(s(y, \mathbf{x}) \mid \mathbf{x}) = \sum_{k=1}^{K} \pi_k(\mathbf{x}) \mathcal{N}(s(y, \mathbf{x}) \mid \mu_k(\mathbf{x}), \sigma_k^2(\mathbf{x})),$$

Experiments

Quantile-Regression baselines

- **CQR** [RPC19]: Conformalized quantile regression with fixed cutoff.
- **CQR-r** [SC20]: Scaled version of CQR to adapt to interval width.
- **UACQR-P, UACQR-S** [RFBW24]: Ensemble-based corrections to capture epistemic uncertainty.

Regression Baselines

- **Regression Split** [LW14]: Classic conformal method using residuals.
- **Weighted Regression Split** [LGR+18]: Adjusts cutoff using predicted residual scale.
- **Mondrian Conformal Regression** [BJ20]: Builds local bins to improve conditional coverage.

Table 1: Quantile regression AISL values for each method and dataset. The table reports the mean across 50 runs, with twice the standard deviation in brackets. Bold values indicate the best-performing method within a 95% confidence interval. EPICSCORE demonstrates strong performance across most datasets and consistently ranks among the top methods.

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)**

Experiments

Table 2: Regression AISL values for each method and dataset. The reported values represent the average across 50 runs, with two times the standard deviation in parentheses. Bolded values highlight the method with superior performance within a 95% confidence interval. `EPICSCORE` demonstrates competitive or superior performance compared to other methods.

Dataset	EPIC-BART	EPIC-GP	EPIC-MDN	Mondrian	Reg-split	Weighted
airfoil	**19.747 (0.767)**	**20.287 (0.686)**	**19.823 (0.675)**	21.532 (0.919)	21.201 (0.98)	**20.276 (0.819)**
bike $\times(10^1)$	**36.381 (0.463)**	41.448 (0.575)	**37.041 (0.452)**	38.190 (0.403)	43.918 (0.567)	37.773 (0.468)
concrete	**52.098 (2.237)**	**52.998 (2.359)**	**51.648 (2.185)**	61.915 (2.815)	**54.902 (2.634)**	58.399 (3.165)
cycle	**19.418 (0.211)**	**19.522 (0.221)**	**19.436 (0.213)**	**19.403 (0.226)**	**19.73 (0.208)**	**19.49 (0.207)**
electric	**0.048 (<0.001)**	0.049 (<0.001)	**0.048 (<0.001)**	0.05 (<0.001)	0.05 (0.001)	**0.048 (<0.001)**
homes $\times(10^5)$	5.921 (0.0716)	6.192 (0.0689)	**5.546 (0.0545)**	5.710 (0.053)	7.569 (0.098)	5.860 (0.056)
meps19	86.039 (2.421)	87.086 (2.405)	**75.061 (1.807)**	79.192 (1.821)	109.83 (2.695)	92.433 (3.259)
protein	18.885 (0.054)	18.772 (0.065)	17.735 (0.055)	**17.586 (0.051)**	19.423 (0.055)	18.314 (0.065)
star $\times(10^1)$	**105.616 (1.255)**	**106.112 (0.998)**	**106.368 (1.173)**	109.346 (1.119)	**105.250 (1.038)**	129.492 (1.657)
superconductivity	54.895 (0.364)	59.16 (0.449)	**53.406 (0.365)**	58.065 (0.313)	68.183 (0.418)	54.981 (0.345)
WEC $\times(10^5)$	1.437 (0.010)	1.435 (0.011)	**1.283 (0.009)**	**1.294 (0.009)**	1.620 (0.009)	1.410 (0.009)
winered	**3.152 (0.07)**	**3.171 (0.064)**	**3.101 (0.062)**	3.262 (0.069)	**3.214 (0.063)**	3.415 (0.067)
winewhite	**3.104 (0.027)**	3.187 (0.029)	**3.129 (0.029)**	**3.087 (0.023)**	3.181 (0.028)	3.189 (0.033)

Accommodation

Is it worth reading? Yes.

- Introduces **EPICSCORE** — a model-agnostic method that integrates epistemic uncertainty into conformal prediction
- Captures the *uncertainty of uncertainty* using Bayesian modeling
- Provides theoretical guarantees for both marginal and conditional coverage
- Includes extensive experiments and implementation details (code available on GitHub)

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