

Hands-on Conformal Prediction with PUNCC

Mouhcine MENDIL





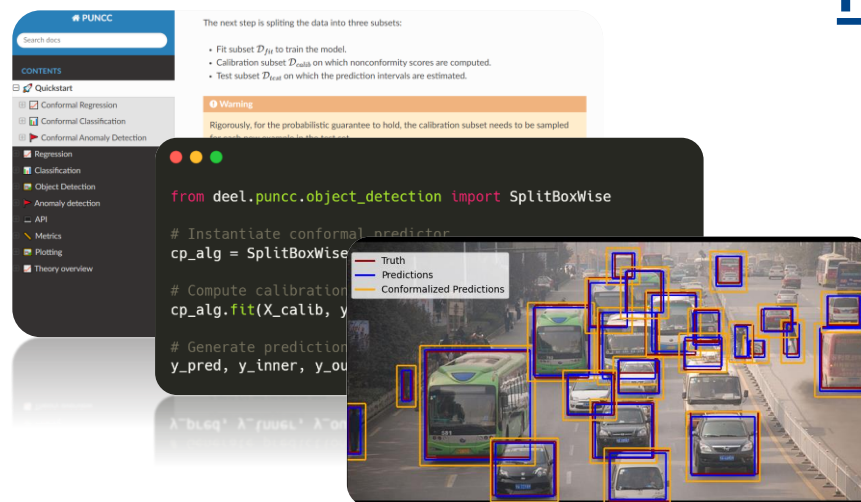
Python 3.8+ License MIT pylint passing tox passing

Puncc (short for Predictive uncertainty calibration and conformalization) is an open-source Python library. It seamlessly integrates a collection of state-of-the-art conformal prediction algorithms and associated techniques for diverse machine learning tasks, including regression, classification and anomaly detection. **Puncc** can be used with any predictive model to provide rigorous uncertainty estimations. Under data exchangeability (or *i.i.d.*), the generated prediction sets are guaranteed to cover the true outputs within a user-defined error α .

Documentation is available [online](https://github.com/deel-ai/puncc).

Table of contents

- [Installation](#)
- [Documentation](#)
- [Tutorials](#)
- [QuickStart](#)
- [Citation](#)
- [Contributing](#)
- [Acknowledgments](#)
- [Creators](#)
- [License](#)



<https://github.com/deel-ai/puncc>

Proceedings of Machine Learning Research 204:1–20, 2023 Conformal and Probabilistic Prediction with Applications

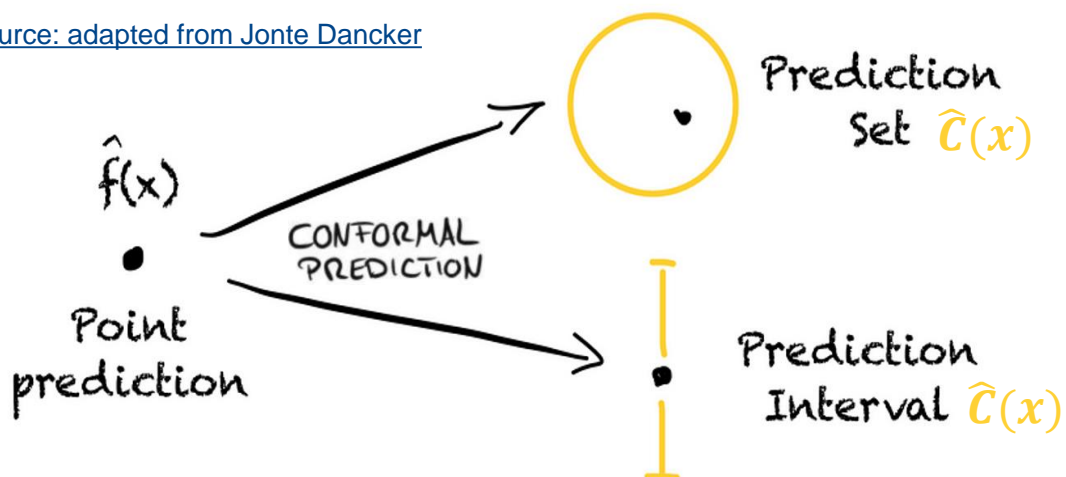
PUNCC: a Python Library for Predictive Uncertainty Calibration and Conformalization

Mouhcine Mendil
IRT Saint Exupéry, Toulouse, France
Luca Mossina
IRT Saint Exupéry, Toulouse, France
David Vigouroux
IRT Saint Exupéry, Toulouse, France

MOUHCINE.MENDIL@IRT-SAINTEXUPERY.COM
LUCA.MOSSINA@IRT-SAINTEXUPERY.COM
DAVID.VIGOUROUX@IRT-SAINTEXUPERY.COM

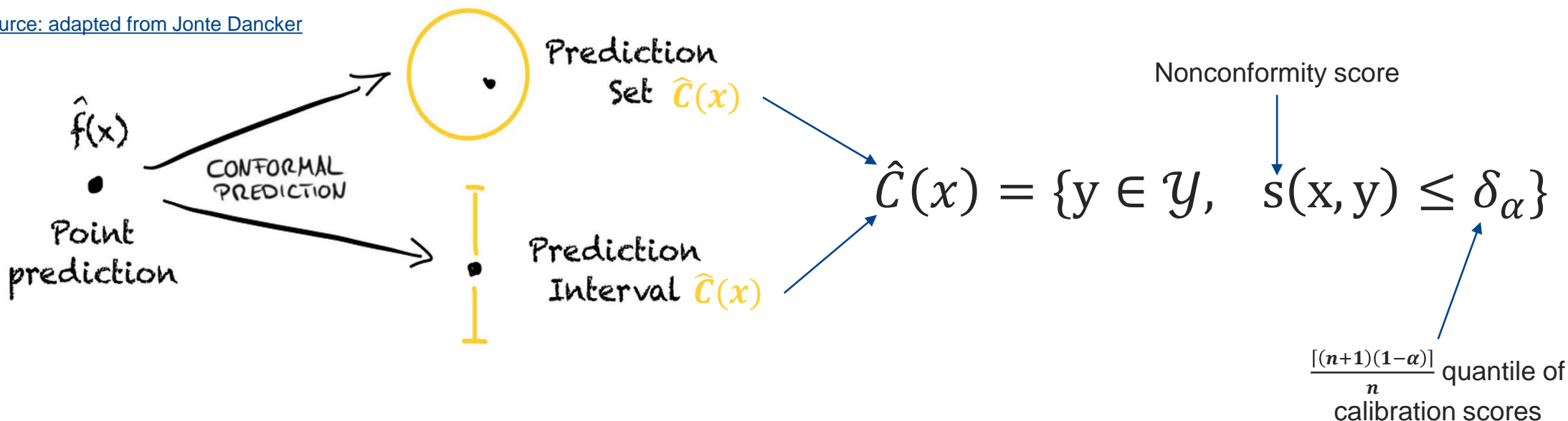
Conformal Prediction: Recap

Source: adapted from Jonte Dancker



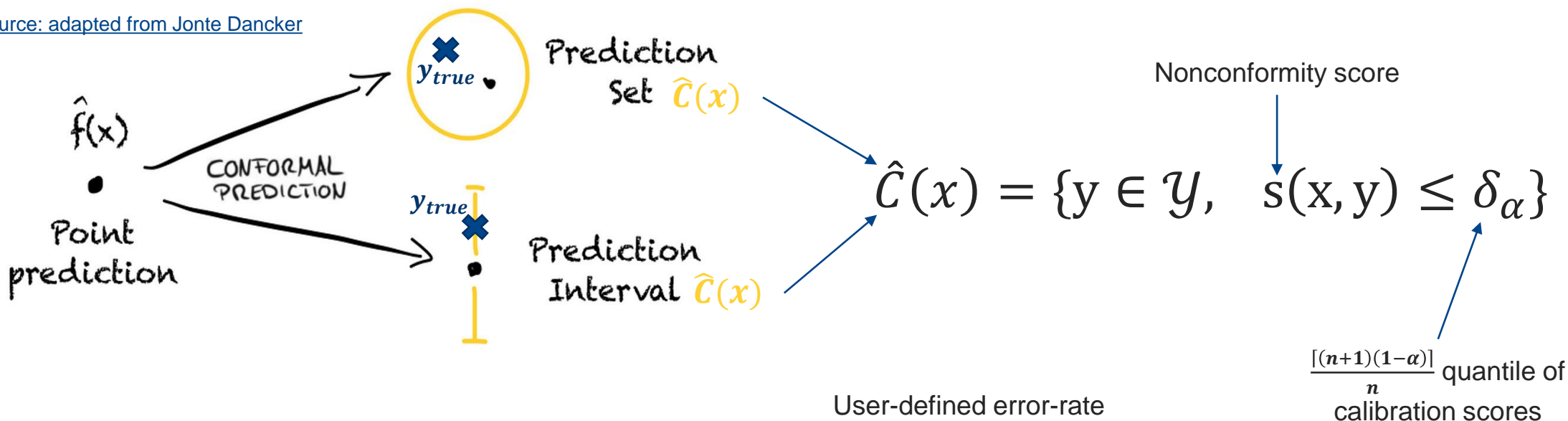
Conformal Prediction: Recap

Source: adapted from Jonte Dancker



Conformal Prediction: Recap

Source: adapted from Jonte Dancker

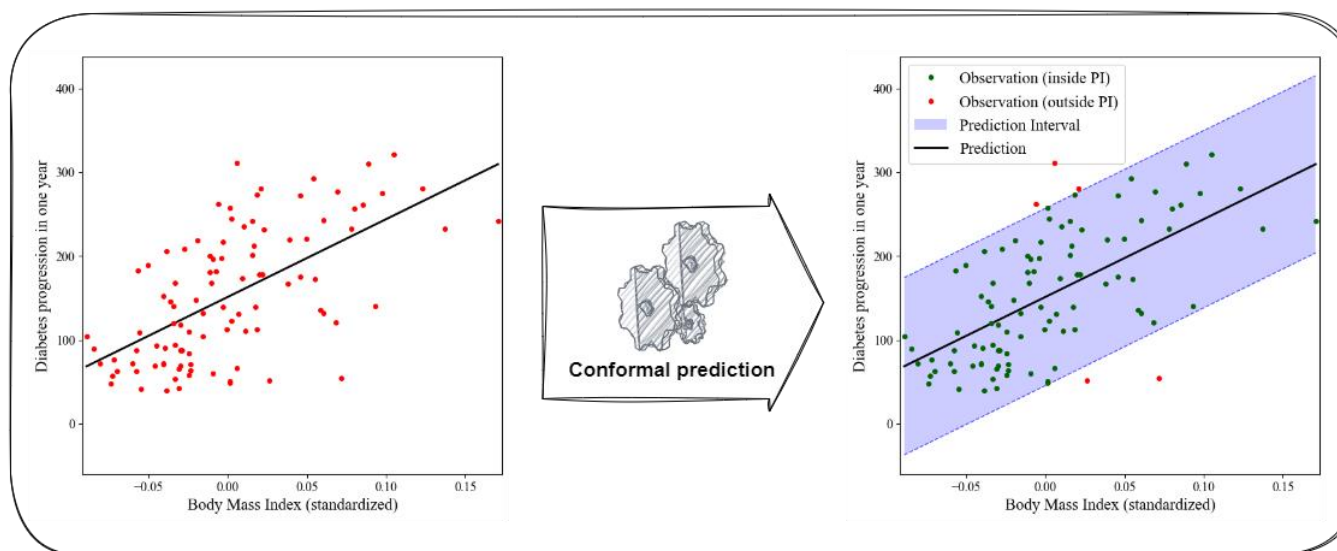
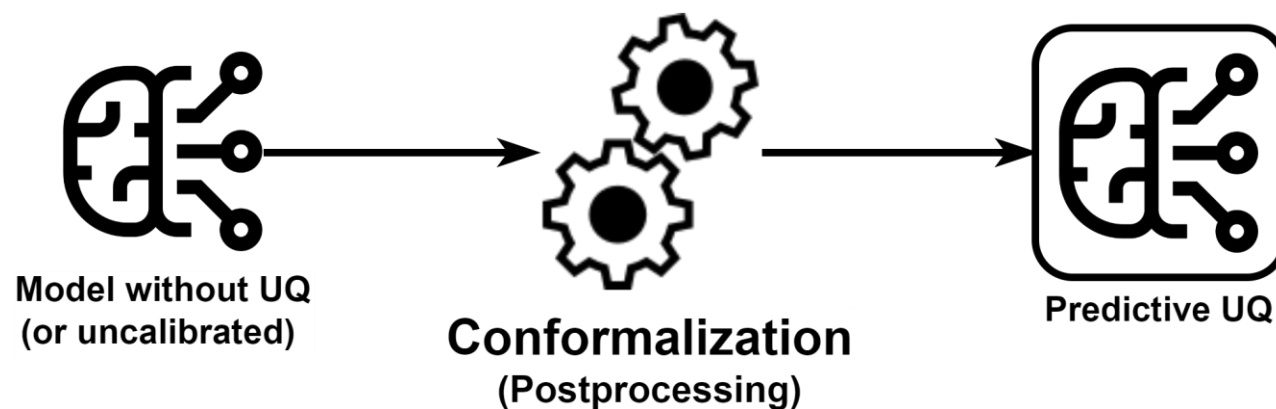


$$P(\mathbf{y}_{true} \in \hat{\mathcal{C}}(x)) \geq 1 - \alpha$$

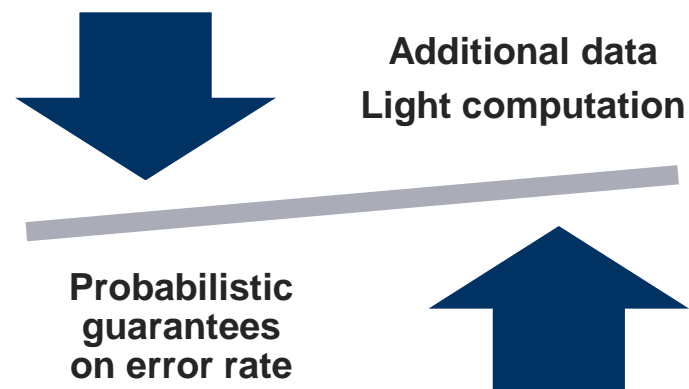
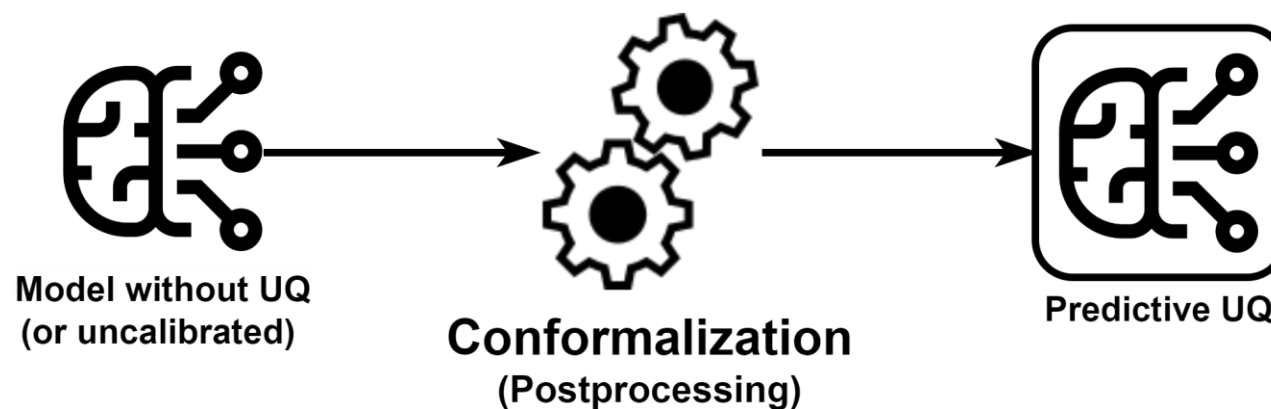
$$\Leftrightarrow P(\mathbf{y}_{true} \notin \hat{\mathcal{C}}(x)) < \alpha$$

If \mathcal{D}_{calib} and (x, y_{true}) are i.i.d

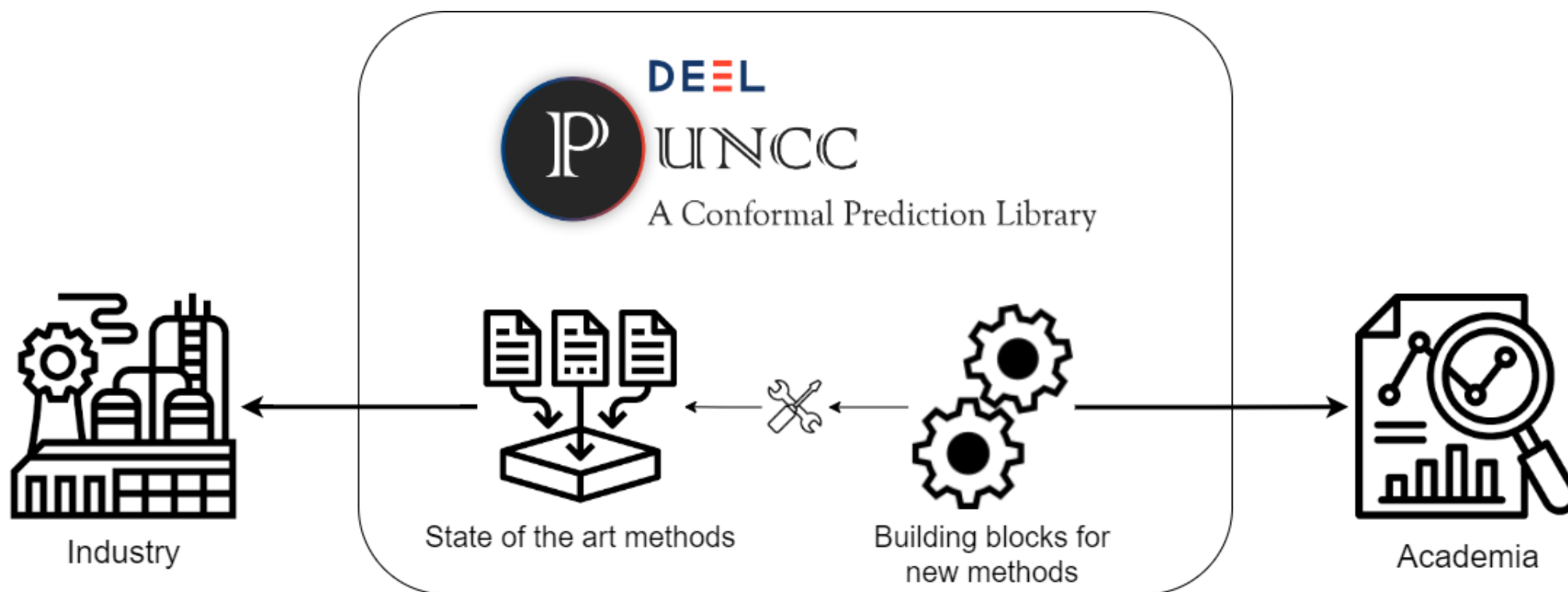
Conformal Prediction: Procedure



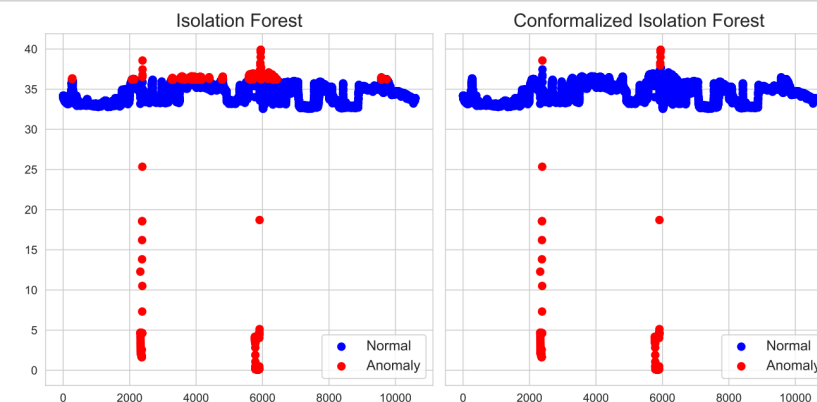
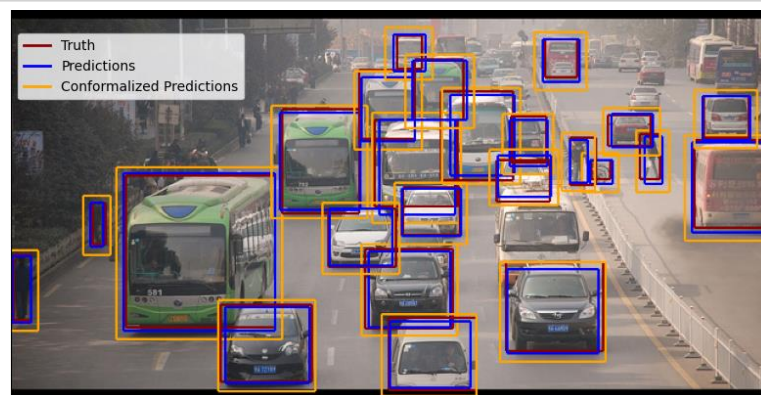
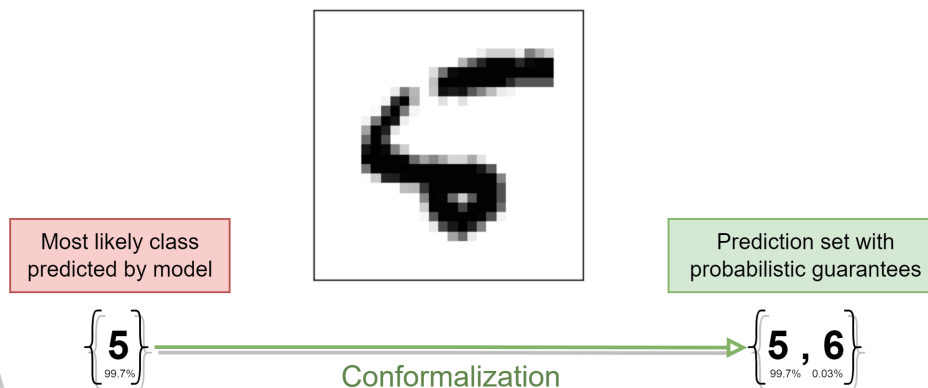
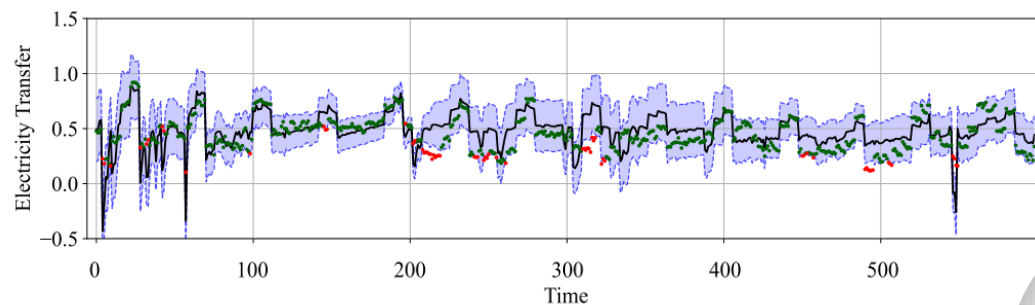
Conformal Prediction: Procedure



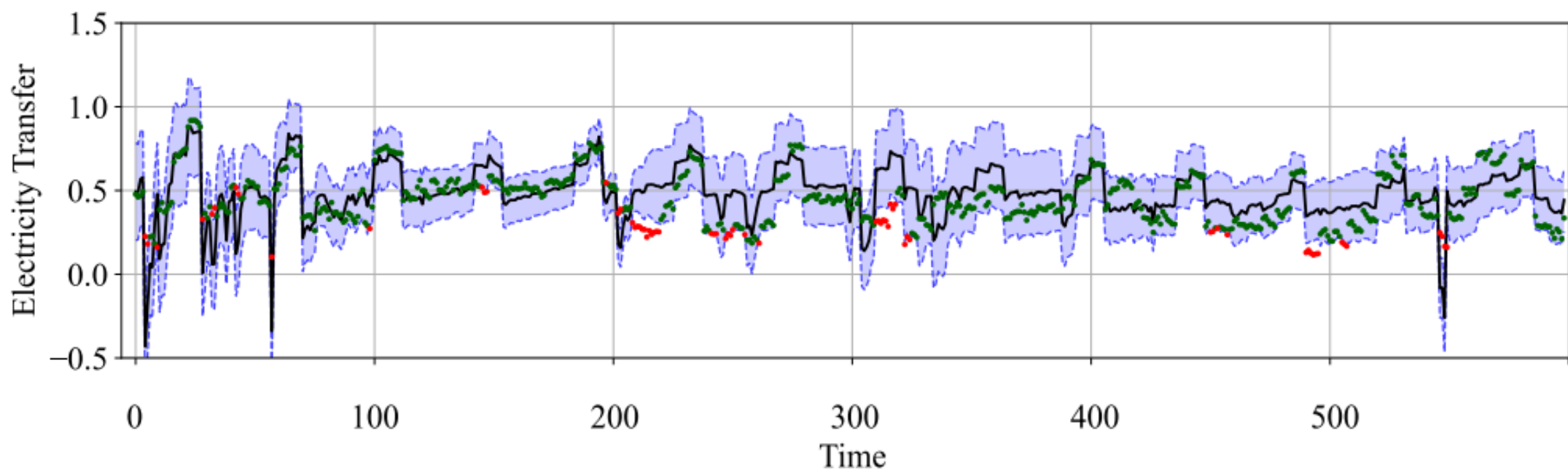
PUNCC Library (Predictive UNcertainty Calibration and Conformalization)



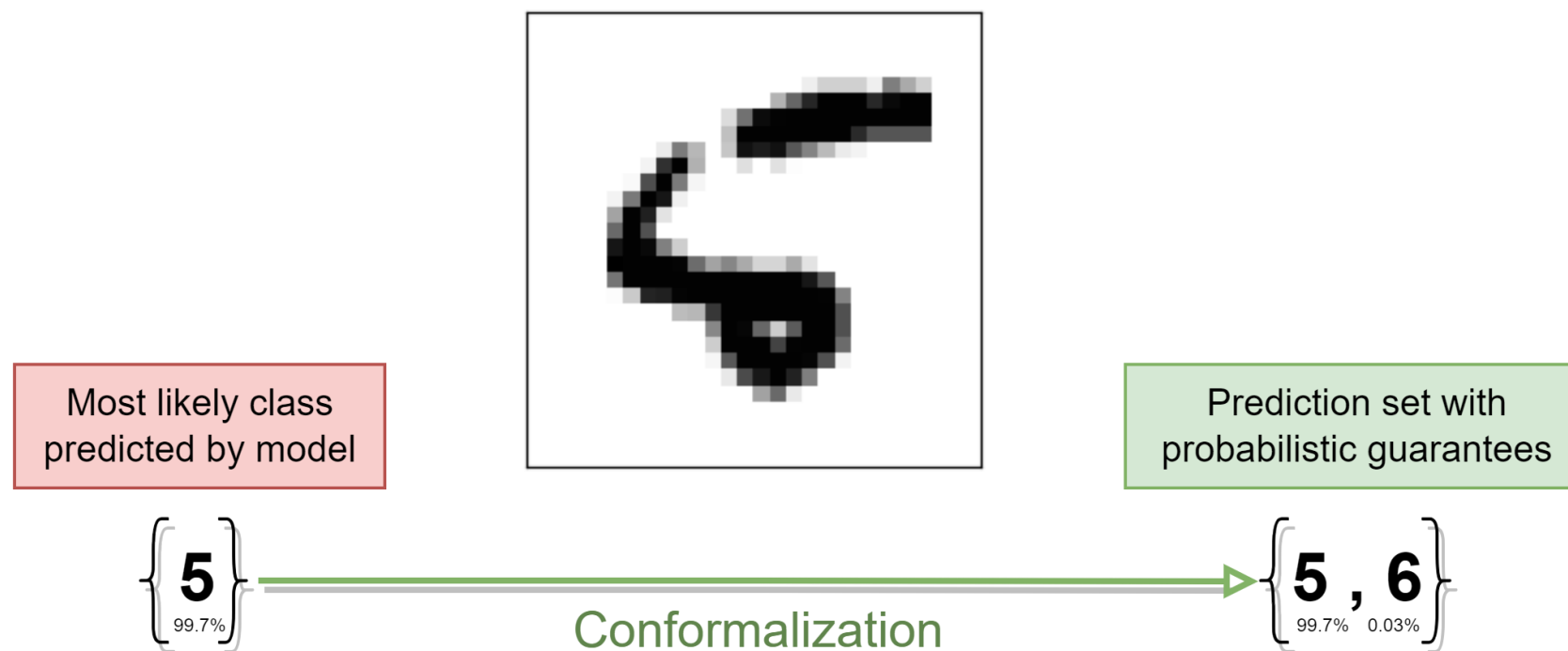
PUNCC for different ML Tasks



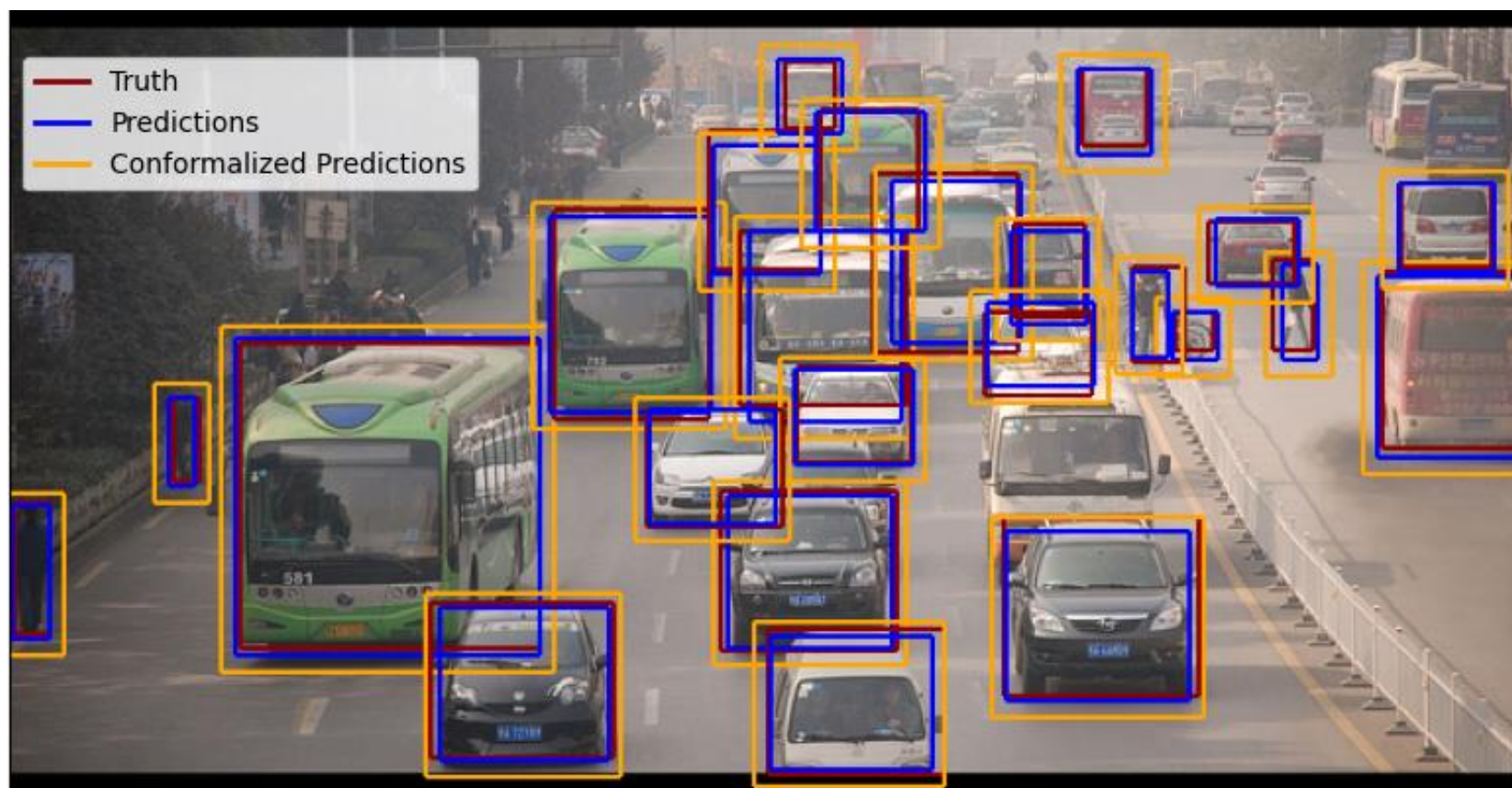
PUNCC: Regression



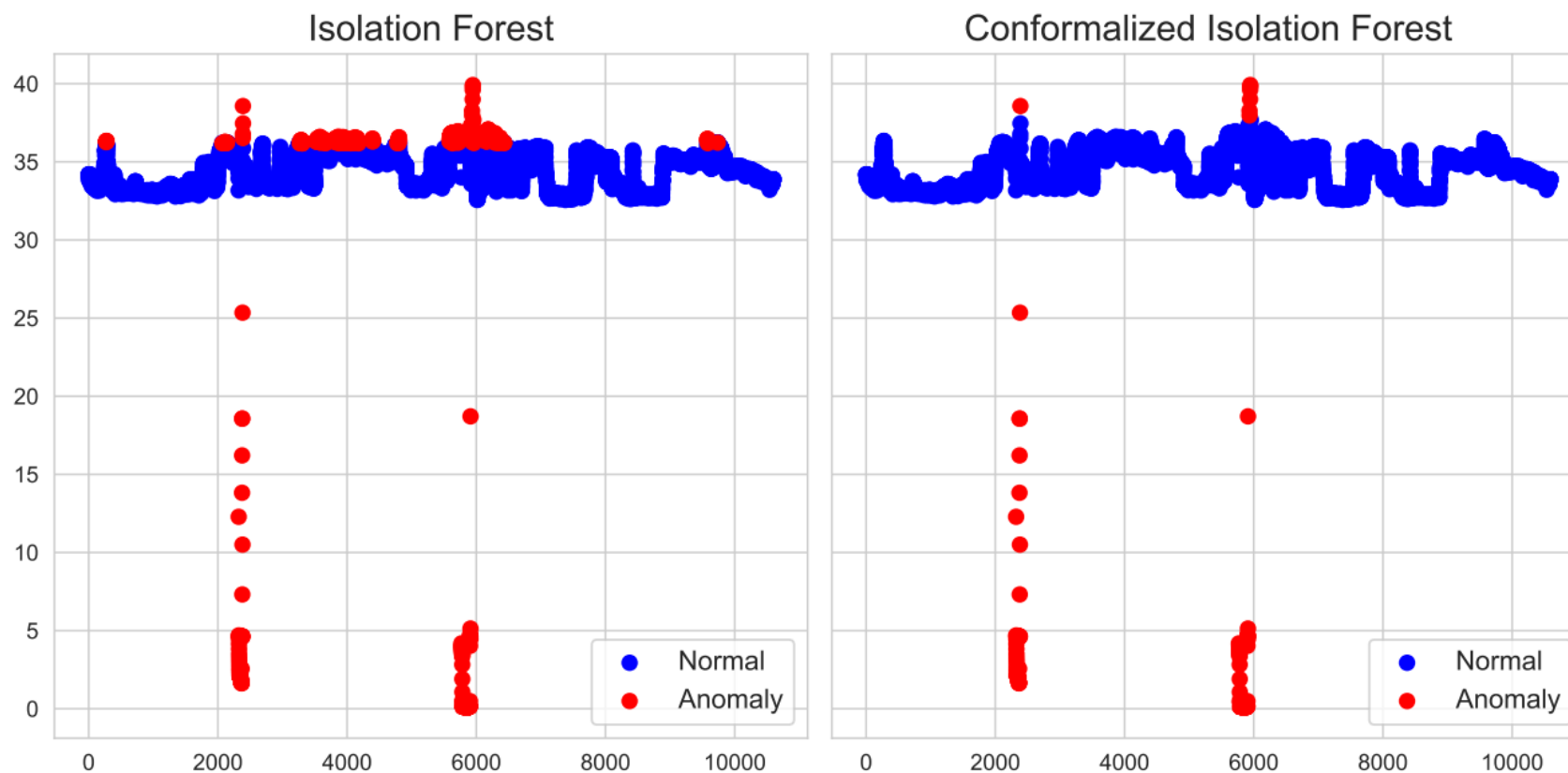
PUNCC: Classification



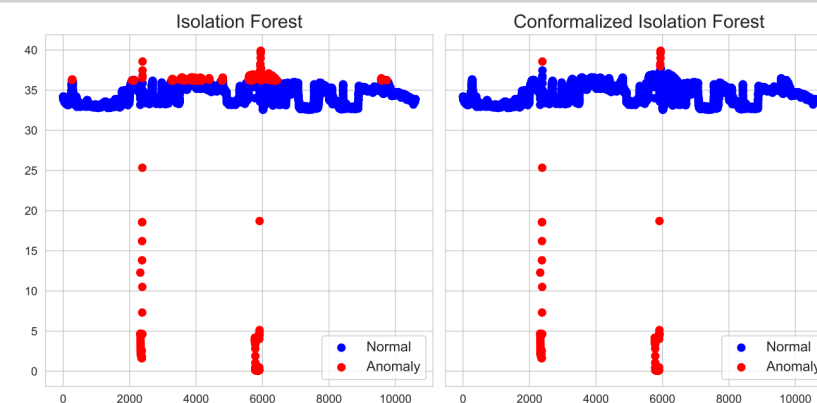
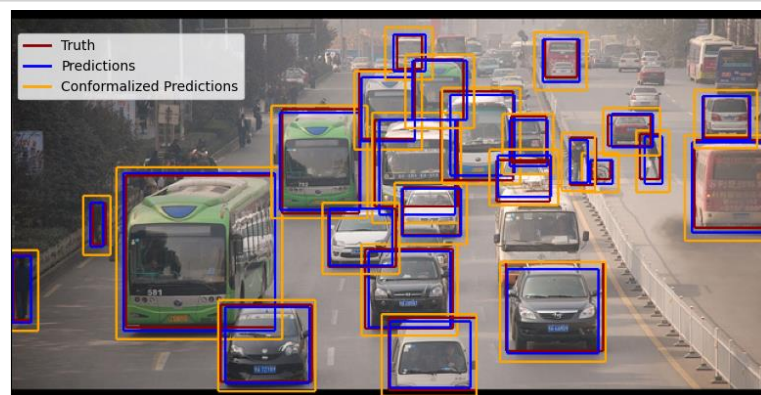
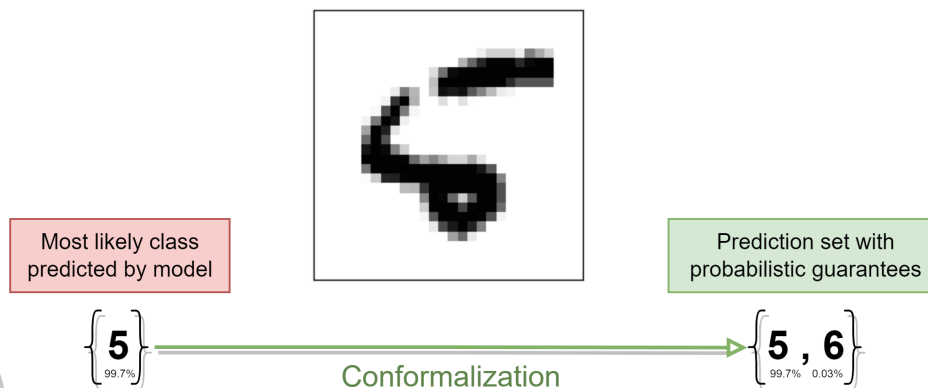
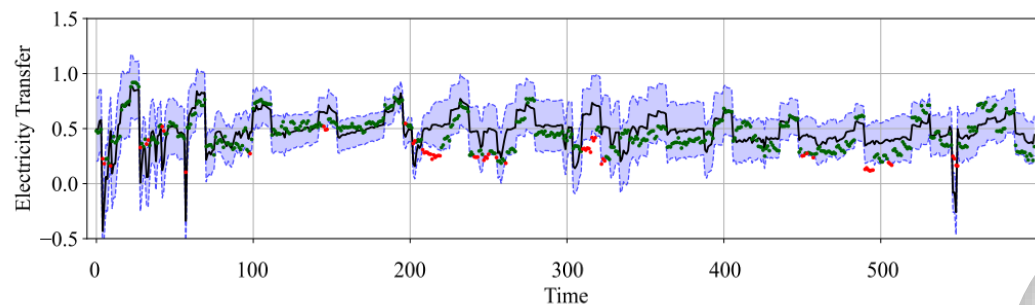
PUNCC: Object Detection



PUNCC: Outlier Detection



PUNCC for different ML Tasks



Conformal Prediction in few lines of code

Conformal Regression

```
from deel.puncc.regression import SplitCP

# Instantiate conformal predictor
cp_alg = SplitCP(Predictor)

# Compute calibration scores
cp_alg.fit(X_calib, y_calib)

# Generate prediction sets
y_pred, y_low, y_high = cp_alg.predict(X_new, alpha=0.1)
```


Conformal Prediction in few lines of code

Conformal Classification

```
from deel.puncc.classification import APS

# Instantiate conformal predictor
cp_alg = APS(Predictor)

# Compute calibration scores
cp_alg.fit(X_calib, y_calib)

# Generate prediction sets
y_pred, set_pred = cp_alg.predict(X_new, alpha=0.1)
```


Conformal Prediction in few lines of code

Conformal Object Detection

```
from deel.puncc.object_detection import SplitBoxWise

# Instantiate conformal predictor
cp_alg = SplitBoxWise(Predictor)

# Compute calibration scores
cp_alg.fit(X_calib, y_calib)

# Generate prediction sets
y_pred, y_inner, y_outer = cp_alg.predict(X_new, alpha=0.1)
```

Interoperability

- ✓ PUNCC supports popular data types and ML libraries and more ...



```

from deel.puncc.api.prediction import BasePredictor
from deel.puncc.classification import APS

# My scikit-learn classifier
sklearn_classifier_model = ...

# Redefine the predict method of your classifier
def MyPredictor(BasePredictor):
    def predict(X):
        return self.model.predict_proba(X)

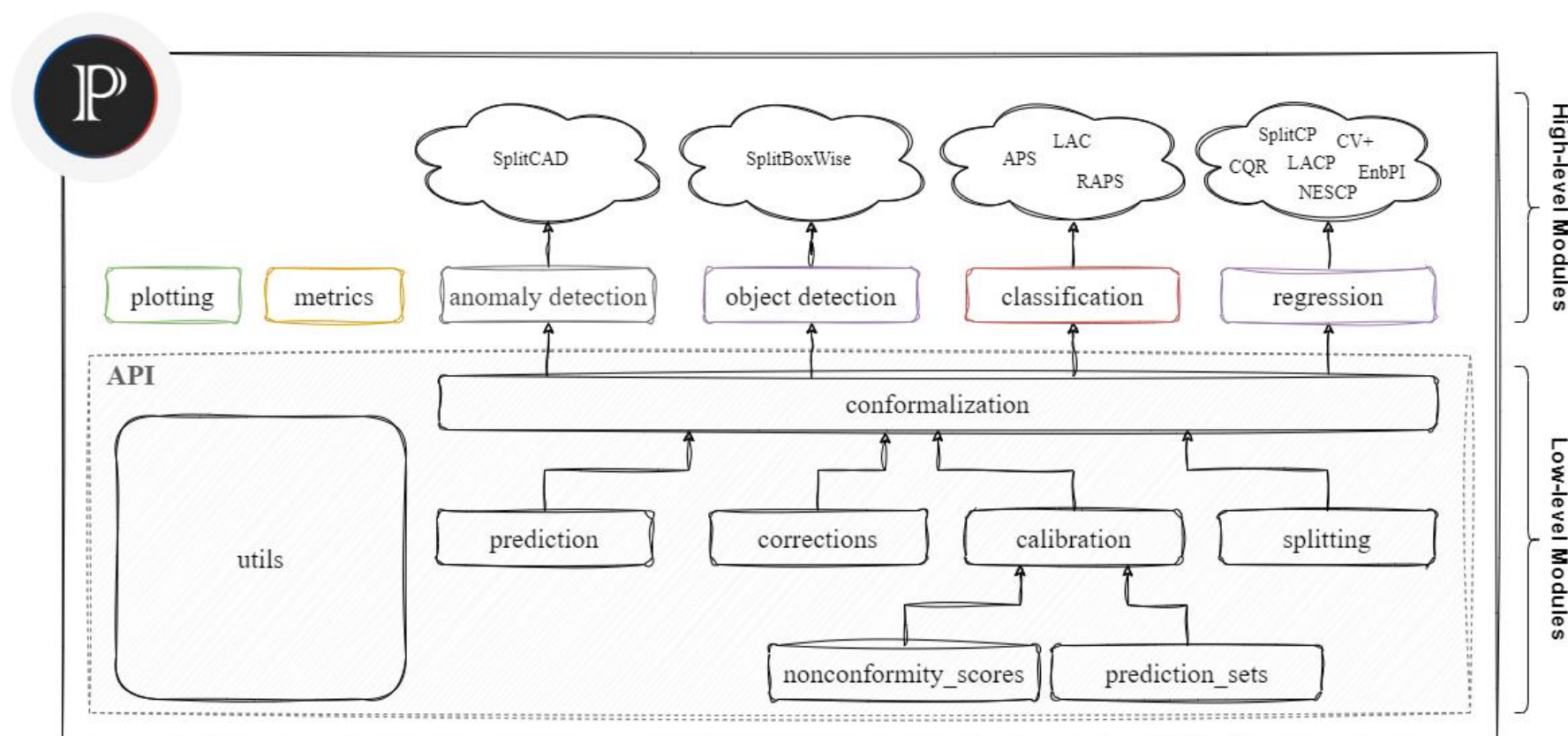
# Wrap scikit-learn classifier to interoperate with puncc
predictor = MyPredictor(sklearn_classifier_model)

# Instantiate the model
cp_alg = APS(predictor)

```

- ✓ Can work on top of UQ models and libraries

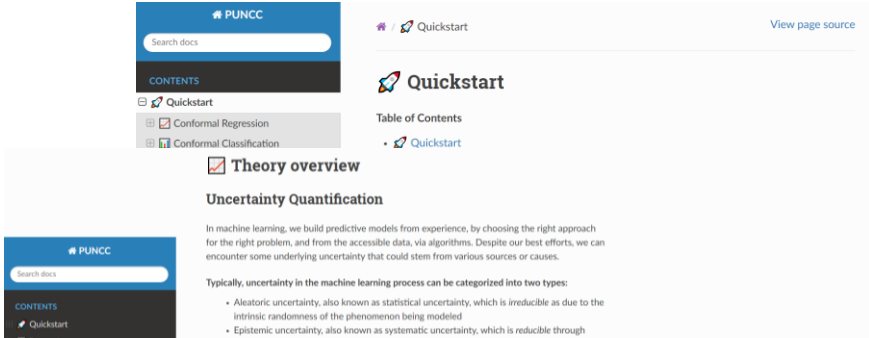
More Flexibility with the API



Low-level API: full customization of CP algorithm (nonconformity scores, cross-validation,)

User Experience

- ✓ Ease of use
- ✓ Documentation and tutorials
- ✓ Scientific rigor
- ✓ Introduction to the theory to help with method selection
- ✓ Tests, CI/CD, ...
- ✓ New features, updates, patches, ...
- ✓ Open to contributions: issues, PRs, ...



The screenshot displays the PUNCC documentation website. The top navigation bar includes a search bar, a 'Quickstart' link, and a 'View page source' link. The main content area is divided into two columns. The left column contains a 'CONTENTS' sidebar with links to 'Quickstart', 'Conformal Regression', and 'Conformal Classification'. The right column shows the 'Quickstart' section, which includes a 'Table of Contents' and a 'Theory overview' section. The 'Theory overview' section discusses 'Uncertainty Quantification' and mentions that uncertainty can be categorized into two types: Aleatoric uncertainty (statistical uncertainty) and Epistemic uncertainty (systematic uncertainty).

Documentation

For comprehensive documentation, we encourage you to visit the [official documentation page](#).

Tutorials

We highly recommend following the introductory tutorials to get familiar with the library and its API.

| Tutorial | Description | Link |
|-----------------------------|--|--|
| Introduction Tutorial | Get started with the basics of <i>puncc</i> . | GITHUB Open in Colab |
| API Tutorial | Learn about <i>puncc</i> 's API. | GITHUB Open in Colab |
| Tutorial on CP with PyTorch | Learn how to use <i>puncc</i> with PyTorch. | GITHUB Open in Colab |
| Conformal Object Detection | Learn to conformalize an object detector. | GITHUB Open in Colab |
| Architecture Overview | Detailed overview of <i>puncc</i> 's architecture. | GITHUB Open in Colab |



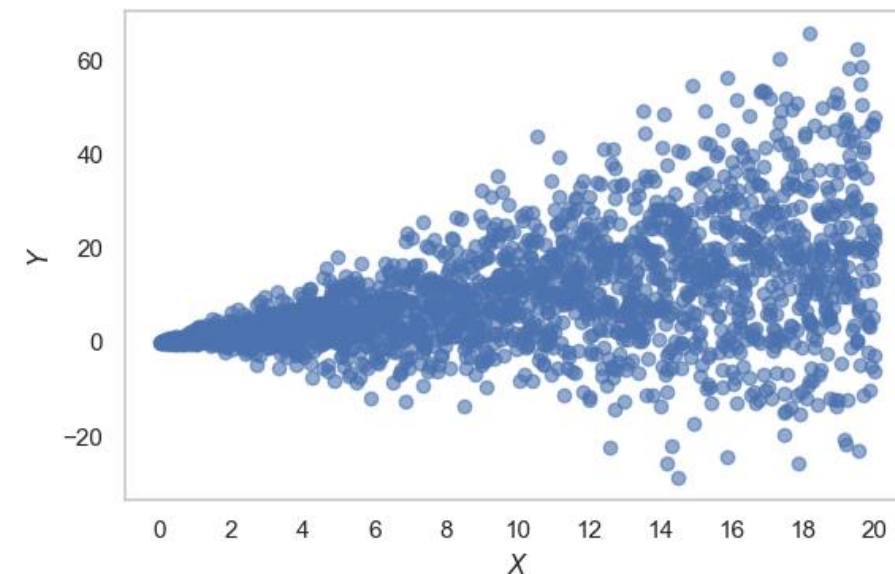
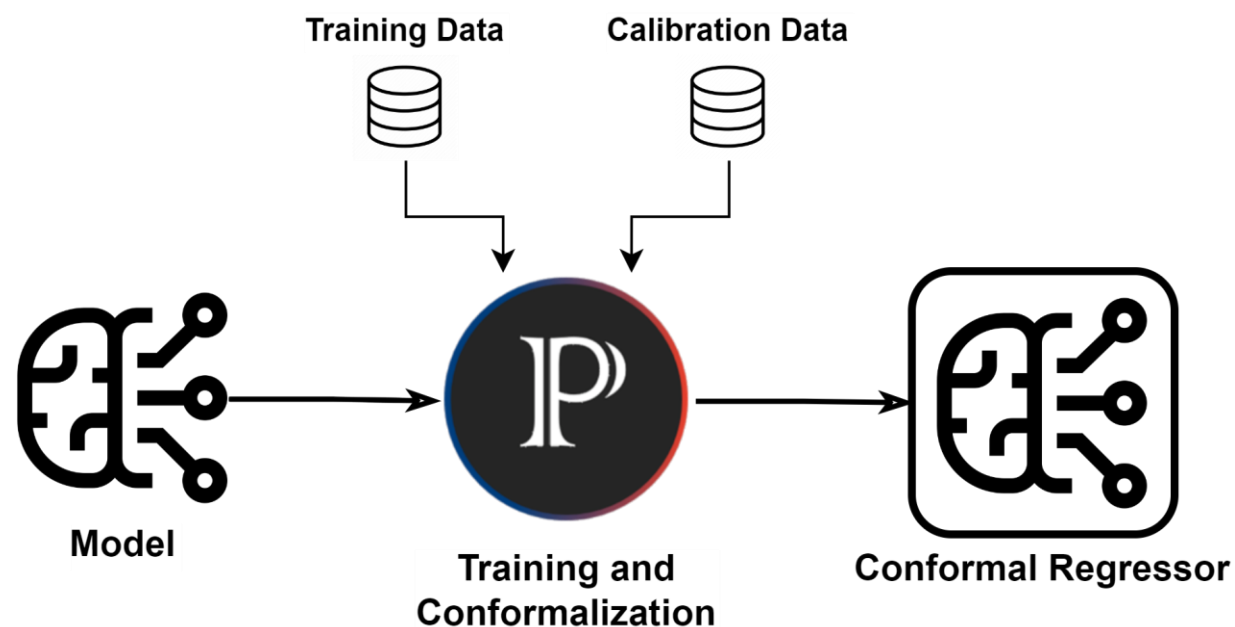
Hands-on Session

<https://github.com/deel-ai/uq-masterclass>



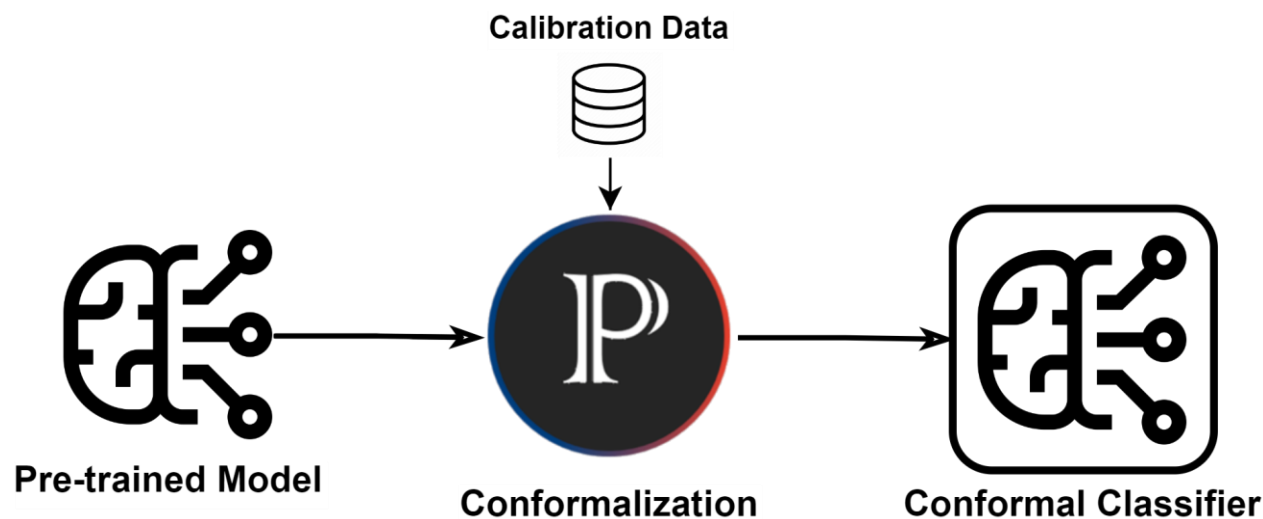
Tutorial on Conformal Regression

- Model to be selected and trained from scratch



Tutorial on Conformal Classification

- Pretrained classifier within existing ML pipeline

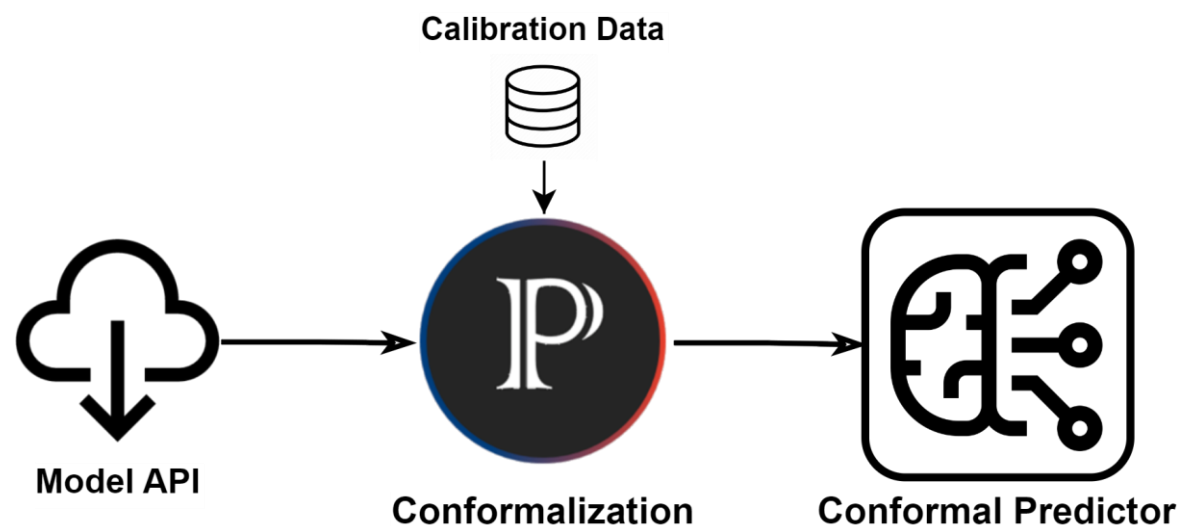


| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 0 | 4 | 1 | 9 | 2 | 1 | 3 | 1 | 4 |
| 3 | 5 | 3 | 6 | 1 | 7 | 2 | 8 | 6 | 9 |
| 4 | 0 | 9 | 1 | 1 | 2 | 4 | 3 | 2 | 7 |
| 3 | 8 | 6 | 9 | 0 | 5 | 6 | 0 | 7 | 6 |
| 1 | 8 | 7 | 9 | 3 | 9 | 8 | 5 | 9 | 3 |
| 3 | 0 | 7 | 4 | 9 | 8 | 0 | 9 | 4 | 1 |
| 4 | 4 | 6 | 0 | 4 | 5 | 6 | 1 | 0 | 0 |
| 1 | 7 | 1 | 6 | 3 | 0 | 2 | 1 | 1 | 7 |
| 9 | 0 | 2 | 6 | 7 | 8 | 3 | 9 | 0 | 4 |
| 6 | 7 | 4 | 6 | 8 | 0 | 7 | 8 | 3 | 1 |

Source: D. Decoste

Tutorial on Conformal Object Detection

- Predictions accessible via API



<https://cocodataset.org/>



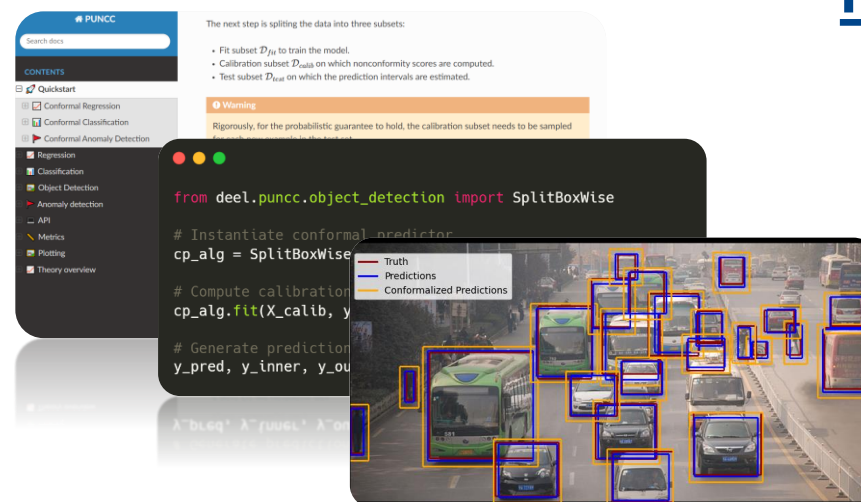
Python 3.8+ License MIT

Puncc (short for Predictive uncertainty calibration and conformalization) is an open-source Python library. It seamlessly integrates a collection of state-of-the-art conformal prediction algorithms and associated techniques for diverse machine learning tasks, including regression, classification and anomaly detection. **Puncc** can be used with any predictive model to provide rigorous uncertainty estimations. Under data exchangeability (or *i.i.d.*), the generated prediction sets are guaranteed to cover the true outputs within a user-defined error α .

Documentation is available [online](https://github.com/deel-ai/puncc).

Table of contents

- [Installation](#)
- [Documentation](#)
- [Tutorials](#)
- [QuickStart](#)
- [Citation](#)
- [Contributing](#)
- [Acknowledgments](#)
- [Creators](#)
- [License](#)



<https://github.com/deel-ai/puncc>

Proceedings of Machine Learning Research 204:1–20, 2023 Conformal and Probabilistic Prediction with Applications

PUNCC: a Python Library for Predictive Uncertainty Calibration and Conformalization

Mouhcine Mendil
IRT Saint Exupéry, Toulouse, France
Luca Mossina
IRT Saint Exupéry, Toulouse, France
David Vigouroux
IRT Saint Exupéry, Toulouse, France

MOUHCINE.MENDIL@IRT-SAINTEXUPERY.COM
LUCA.MOSSINA@IRT-SAINTEXUPERY.COM
DAVID.VIGOUROUX@IRT-SAINTEXUPERY.COM



Thanks for your attention !

