DEEL
DEpendable & Explainable Learning

# PUNCC:

## Empowering trustworthy AI with reliable predictive uncertainty quantification

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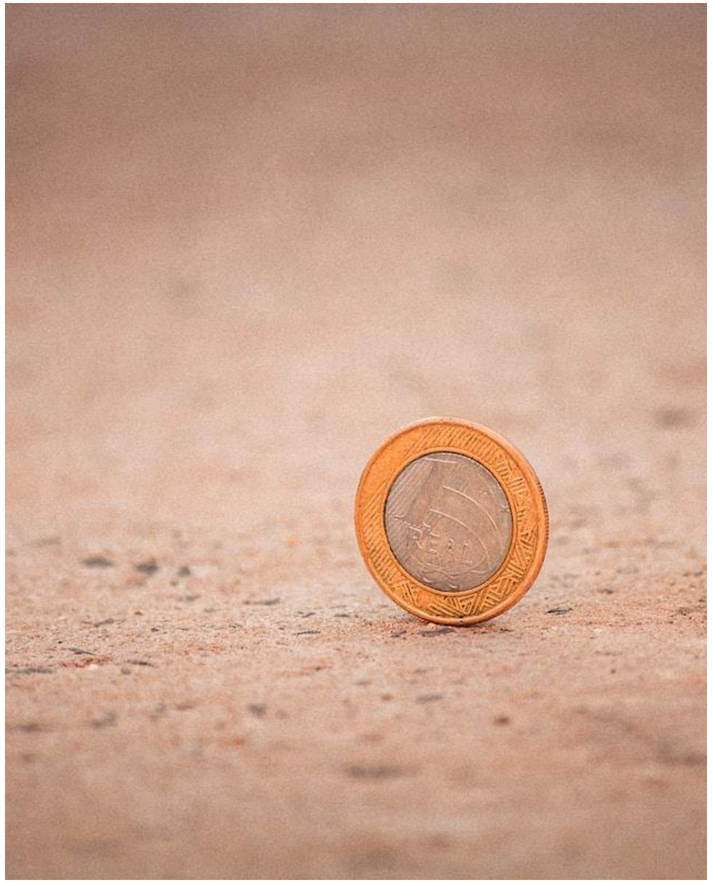
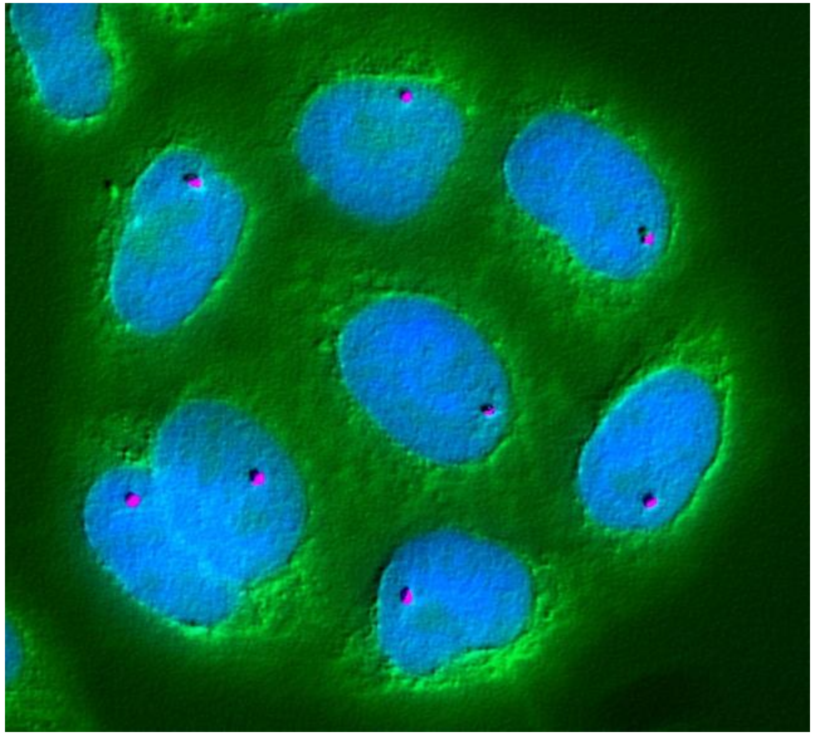
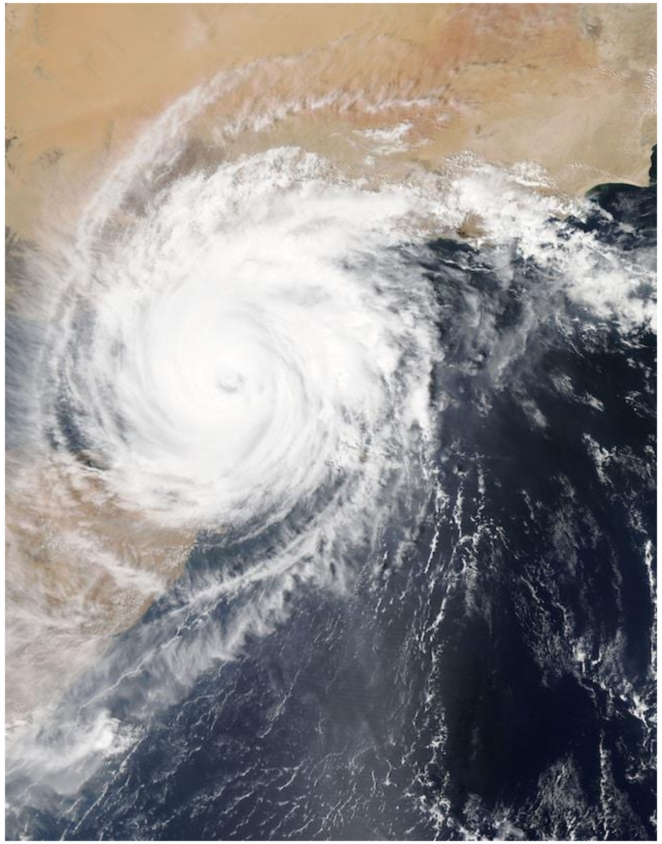
# Uncertainty: A random world







# Predictive Uncertainty


# Epistemic vs Aleatoric Uncertainty


?

# Epistemic vs Aleatoric Uncertainty

HHTTHHTTHTTTHTHTTHHTHTTHH?

12/25 = 0.48 are H

# Epistemic vs Aleatoric Uncertainty

3543 / 5000 = 0.7086
are H

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THHHHHHHHHTHTHHHTTHHHTTHHTHHHHHTHHTHHHHHHHTTHTTTHHTH?

# Epistemic vs Aleatoric Uncertainty


3543 / 5000 = 0.7086
are H

**Epistemic Uncertainty:**

- Unrelated to the phenomenon itself
- Can be reduced with:
  - Additional Observation
  - Noise Reduction
  - Model Complexity

**Aleatoric Uncertainty:**

- Inherent to the phenomenon
- Cannot be reduced

# Uncertainty Quantification

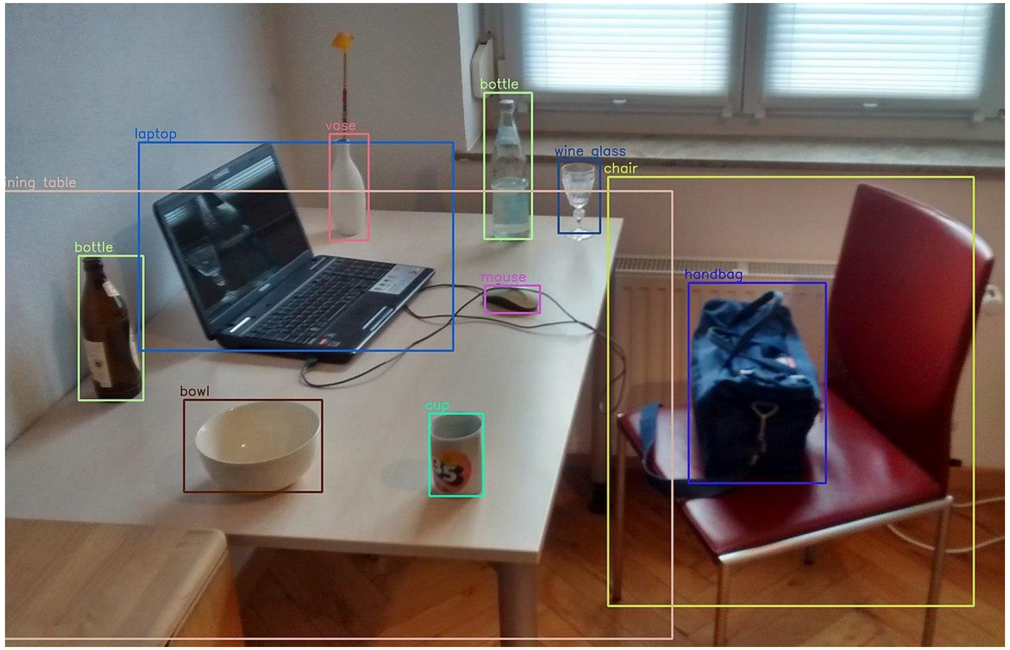
Quantify the uncertainty of a model based on different parameters:

- Number of observations,
- prior knowledge,
- complexity of the model
- …

# Uncertainty Quantification

Classification

Object Detection

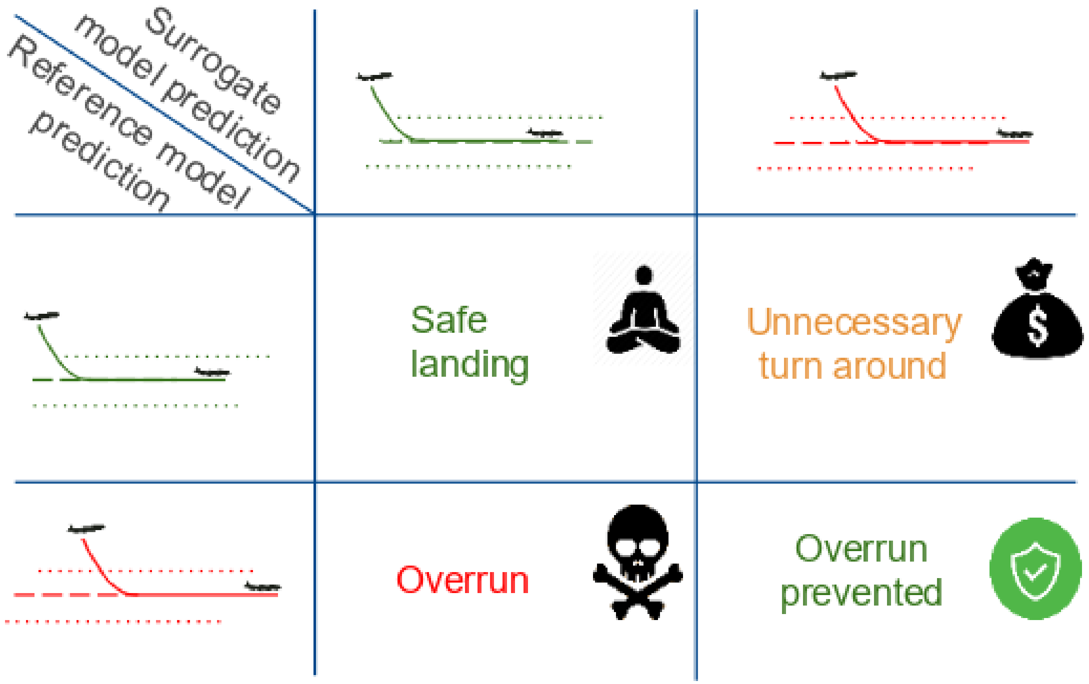


# Why Uncertainty Quantification?

- **Evaluate** the accuracy of the model

- Design **trustworthy** ML components

- Help in the **certification** process of AI-based modules

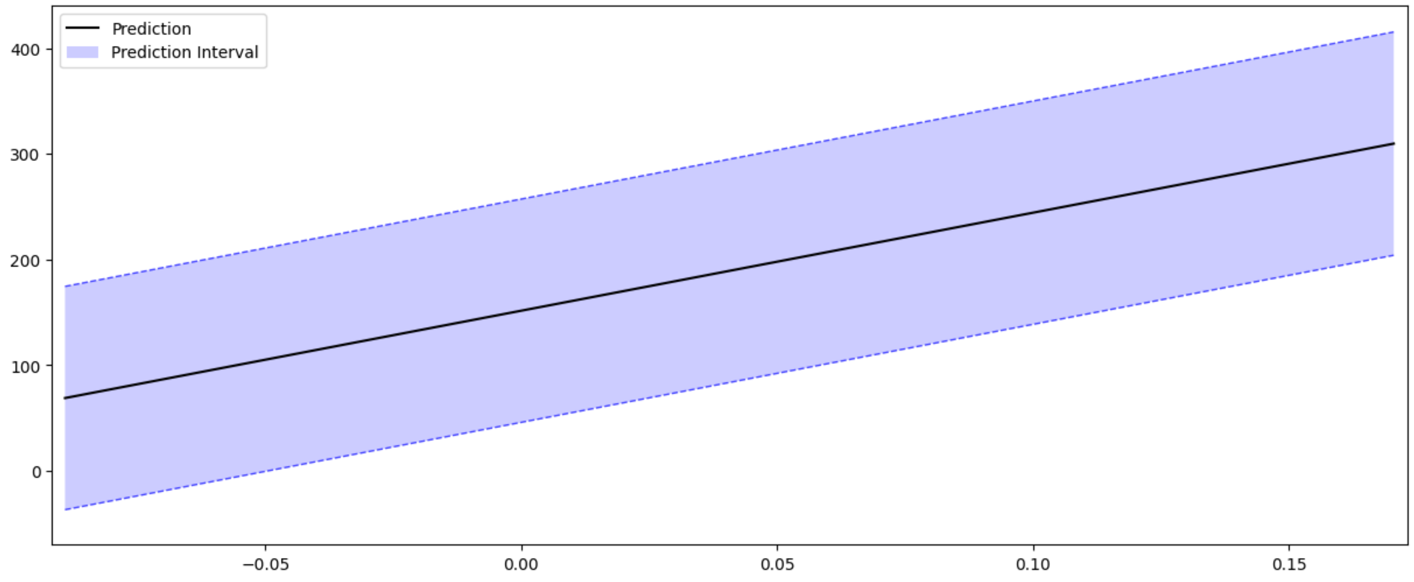


# How to Quantify Uncertainty ?

- Model calibration (e.g. Platt scaling, temperature scaling, …)
- Bayesian Networks
- Model Complexity
- …

# Conformal Prediction

- Model agnostic
- Post-processing
- Finite sample

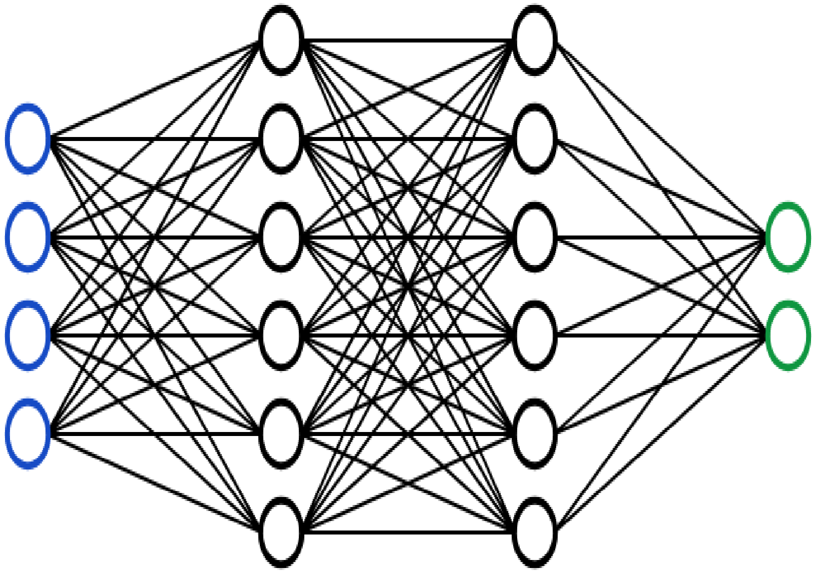



$$P\left(Y_{new} \in \hat{C}(X_{new})\right) \geq 1 - \alpha$$

# Conformal Prediction

Black-box model

Input
$X_{new}$

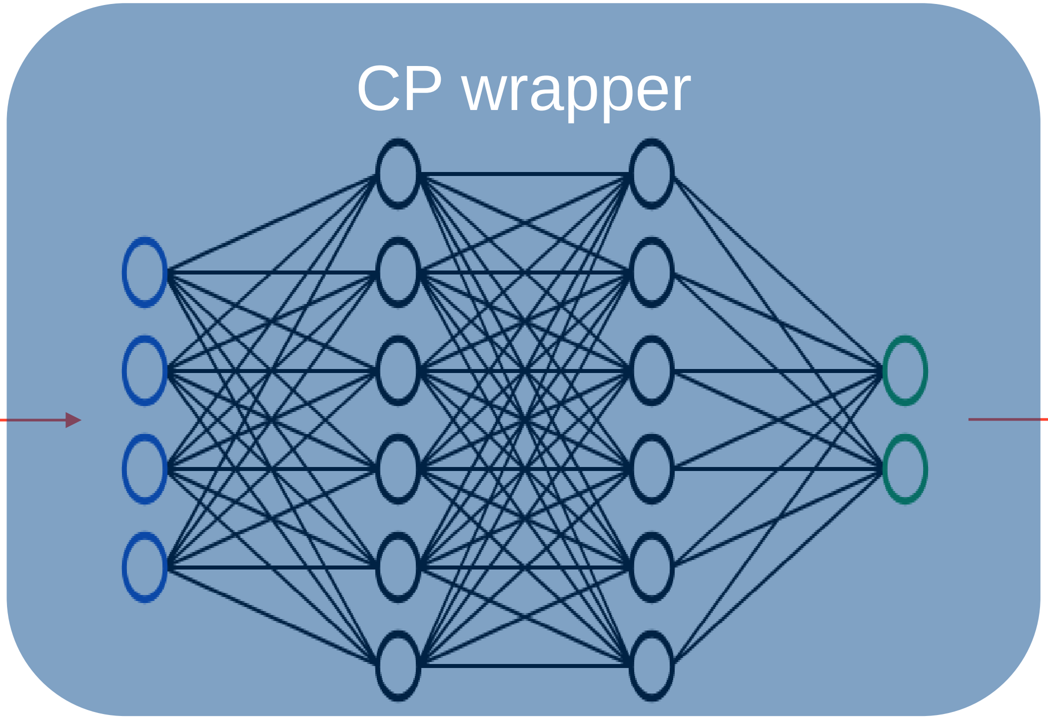


Prediction
$\hat{Y}_{new}$

# Conformal Prediction

User-defined risk level: **α**

Input
$X_{new}$

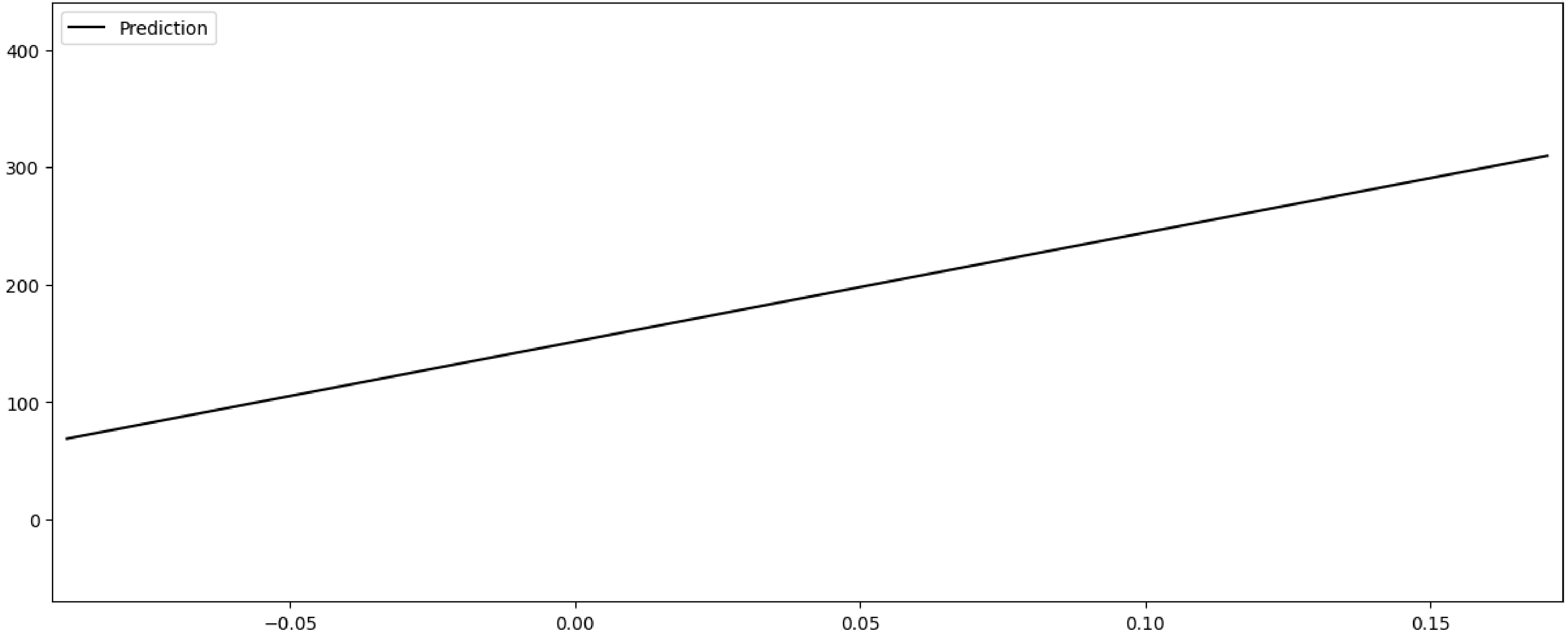



Prediction
$\hat{C}(X_{new})$

Probabilistic Guarantee: $P\left(Y_{new} \in \hat{C}(X_{new})\right) \geq 1 - \alpha$

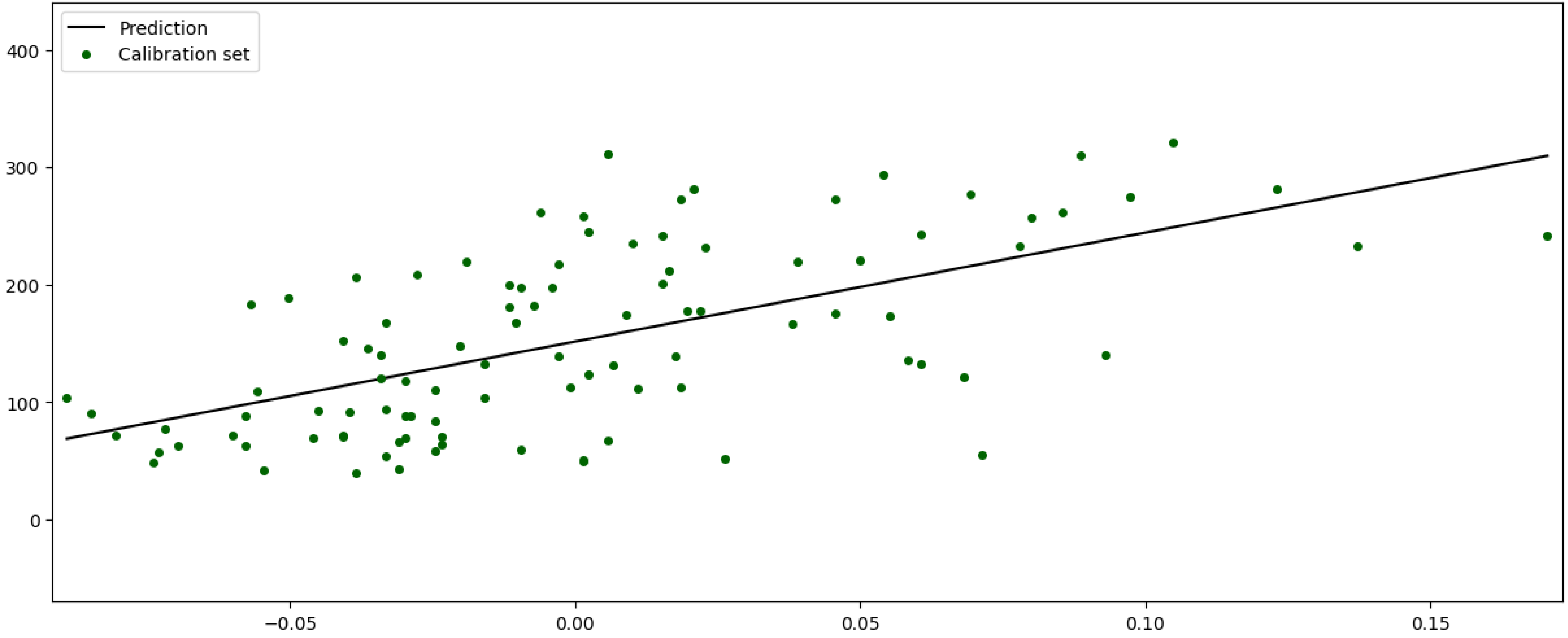
# A statistical approach

We are given a black-box predictor



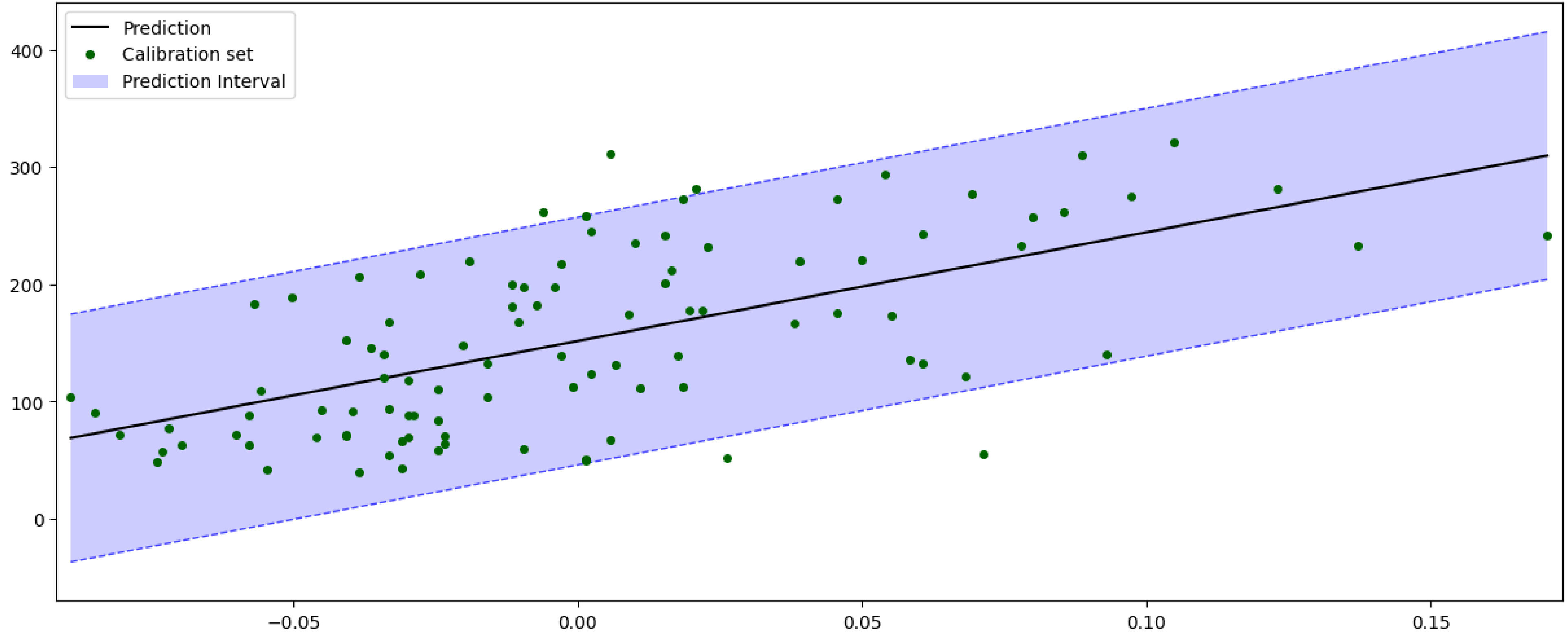
# A statistical approach

Use a representative calibration dataset to measure errors



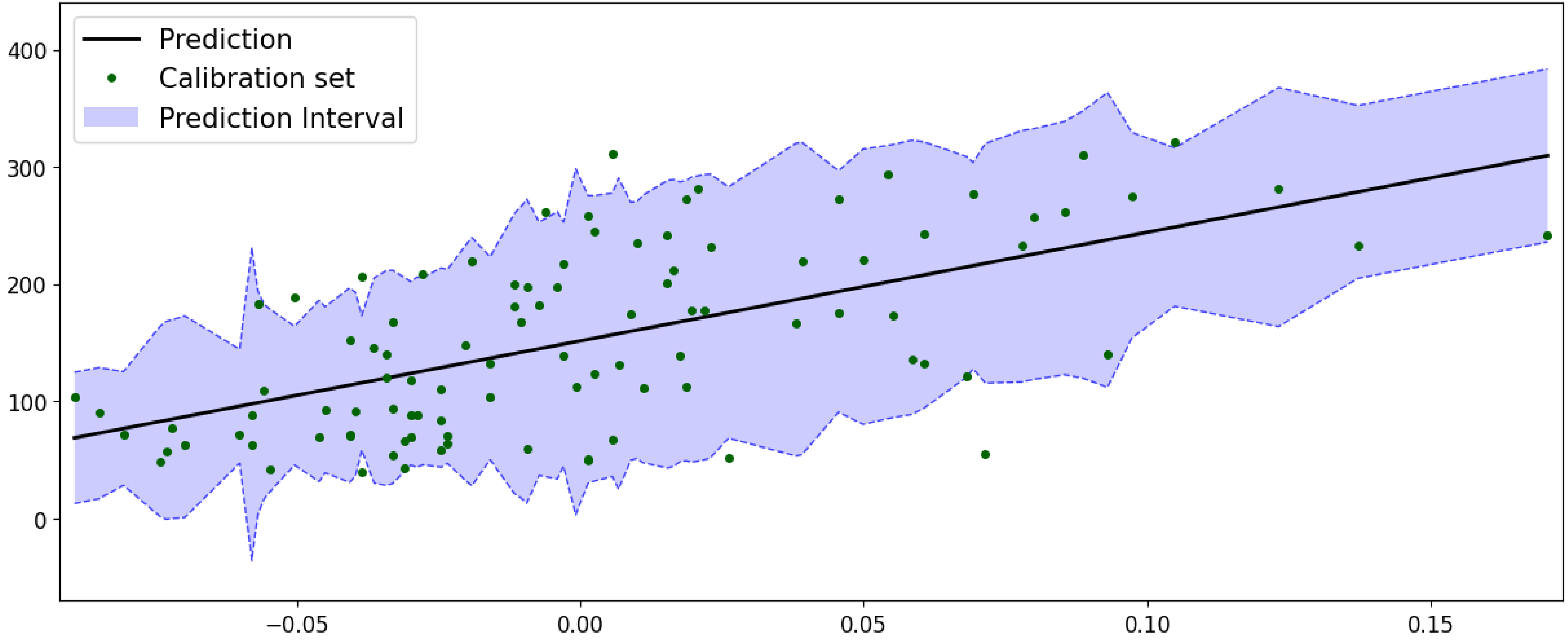
# A statistical approach

Learn prediction intervals with probabilistic guarantees



# A statistical approach

The intervals can be adaptive to heteroskedasticity

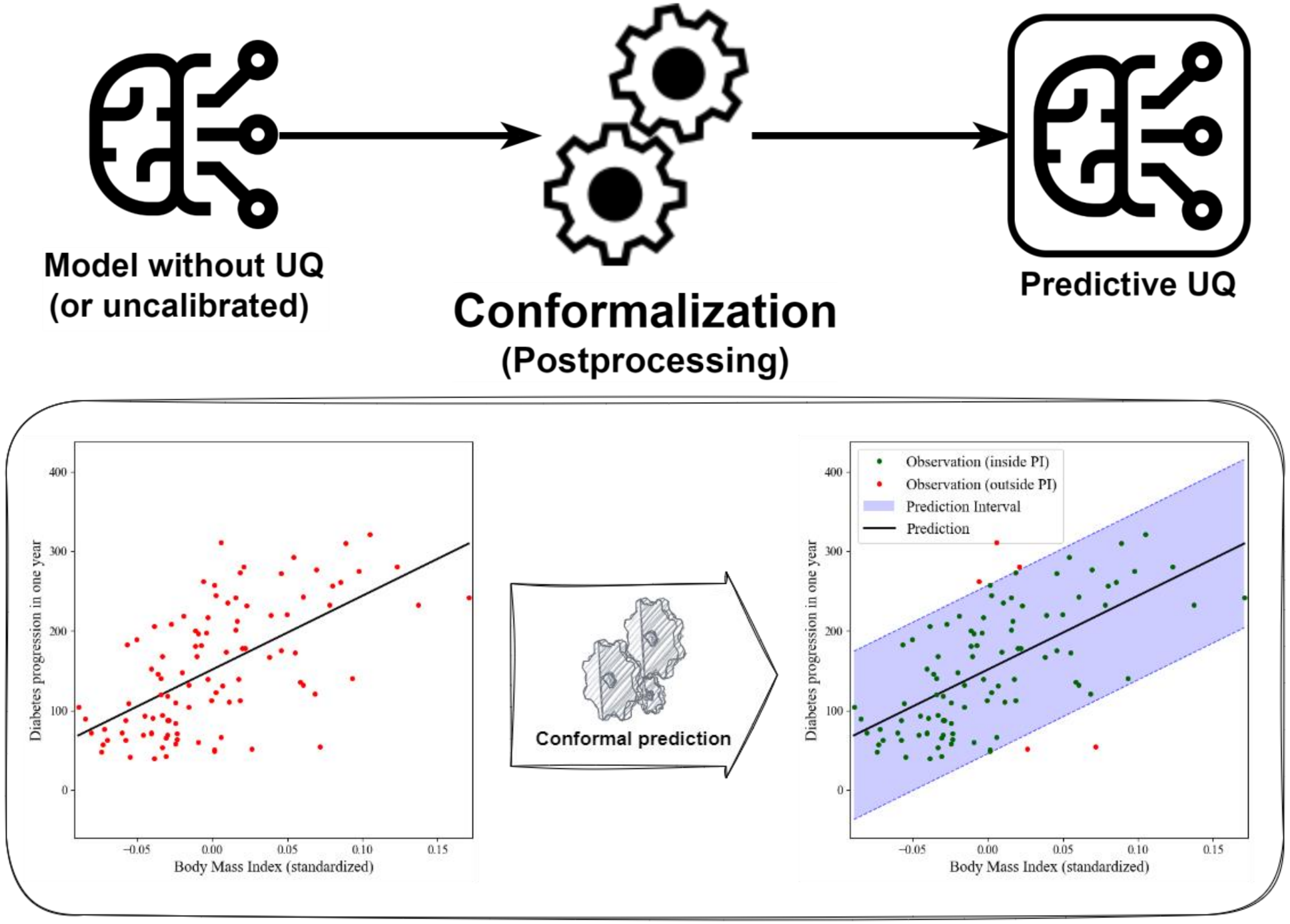


# Beyond Regression and Split-CP

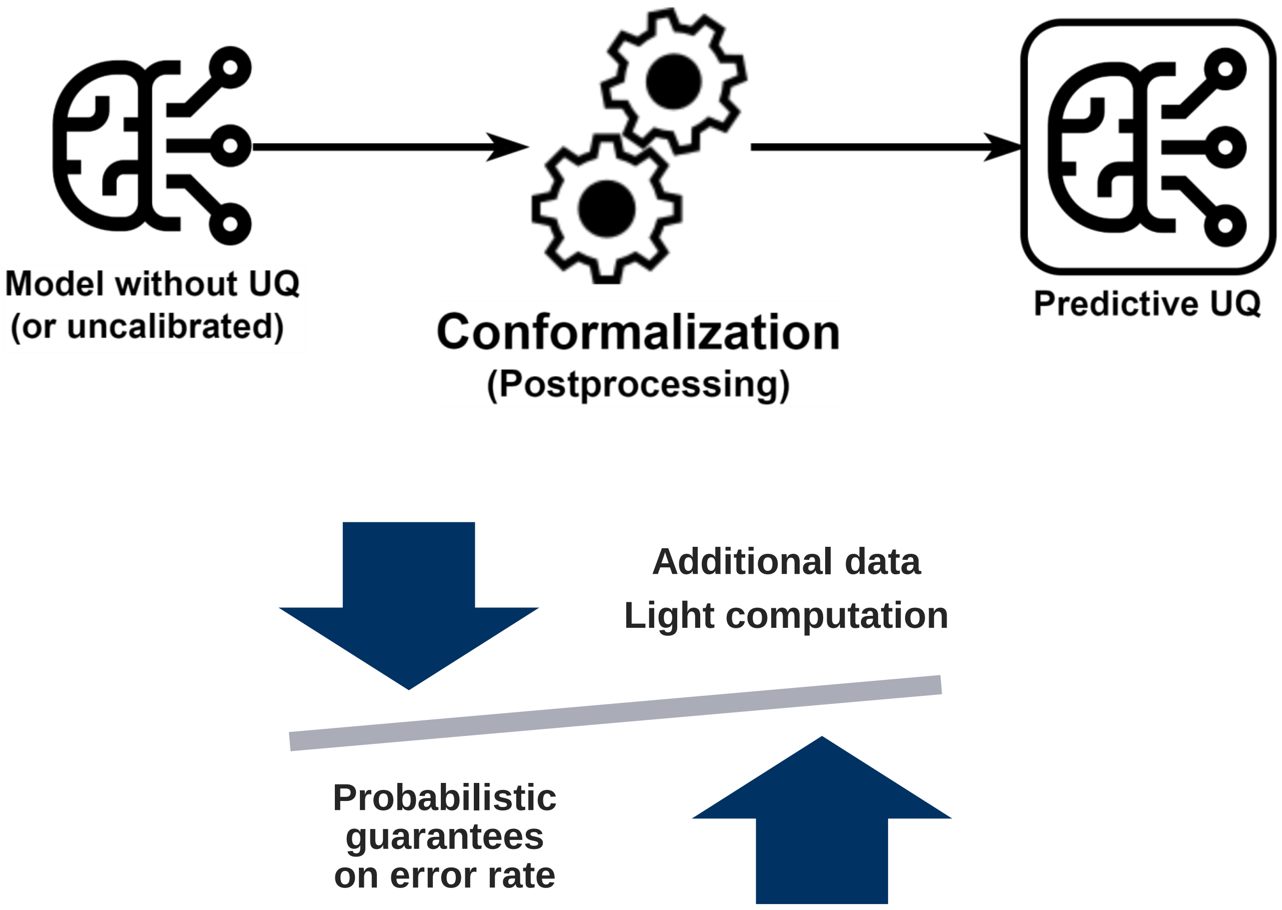
- Regression, Classification, Anomaly Detection, Object Detection,…
- Jacknife+, CV+
- …

# Conformal Prediction in Practice with PUNCC

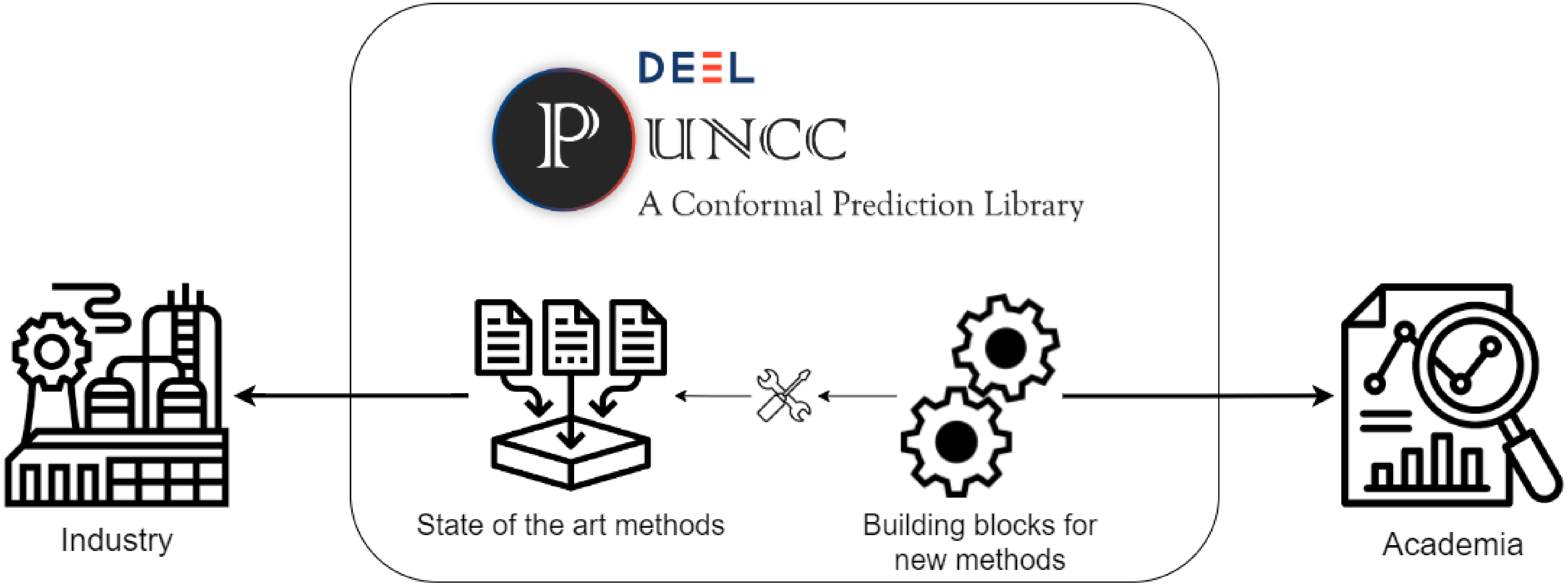
# Conformal Prediction: Procedure



# Conformal Prediction: Procedure



# PUNCC Library (Predictive UNcertainty Calibration and Conformalization)



# PUNCC for different ML Tasks

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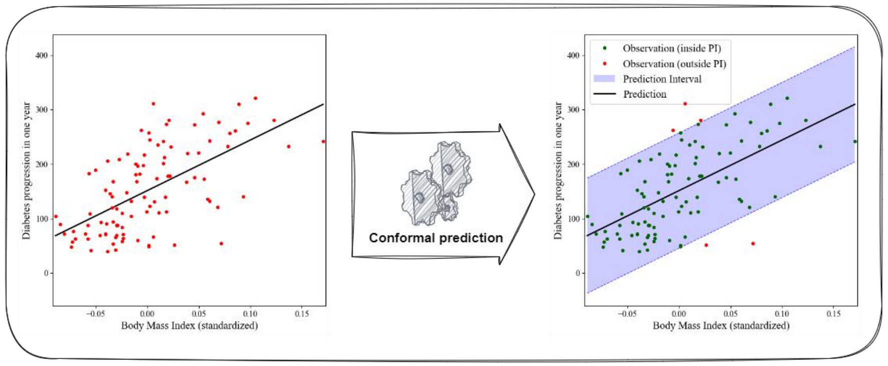
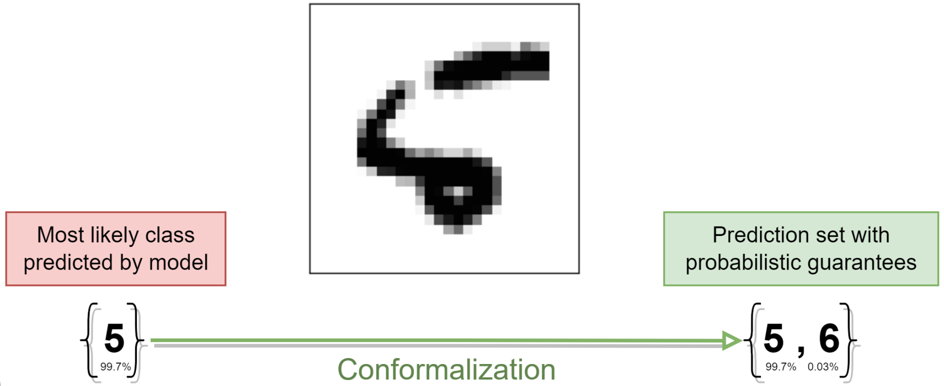
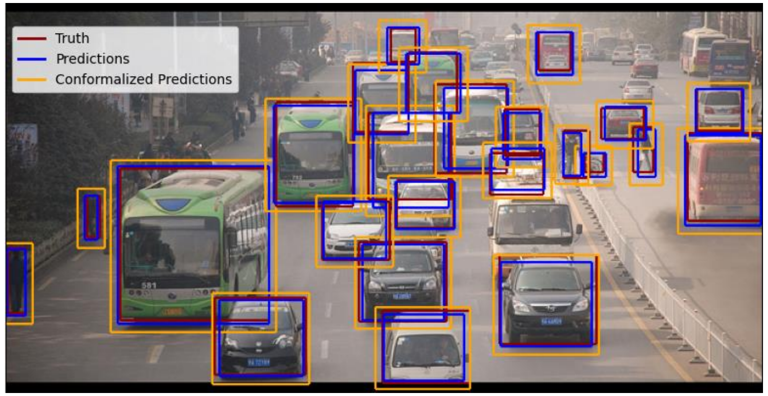
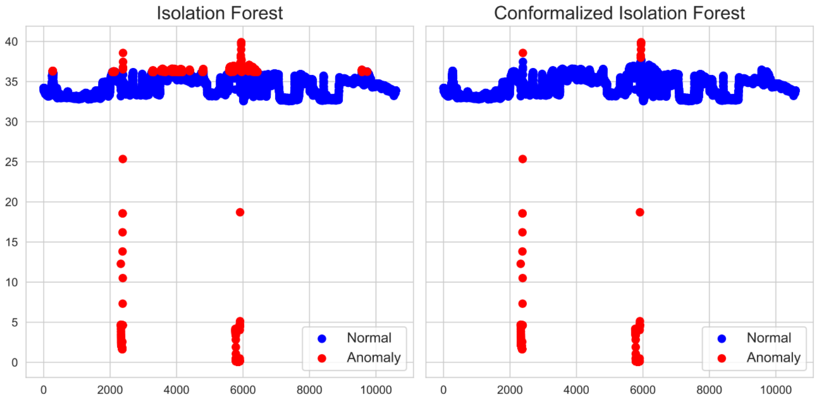
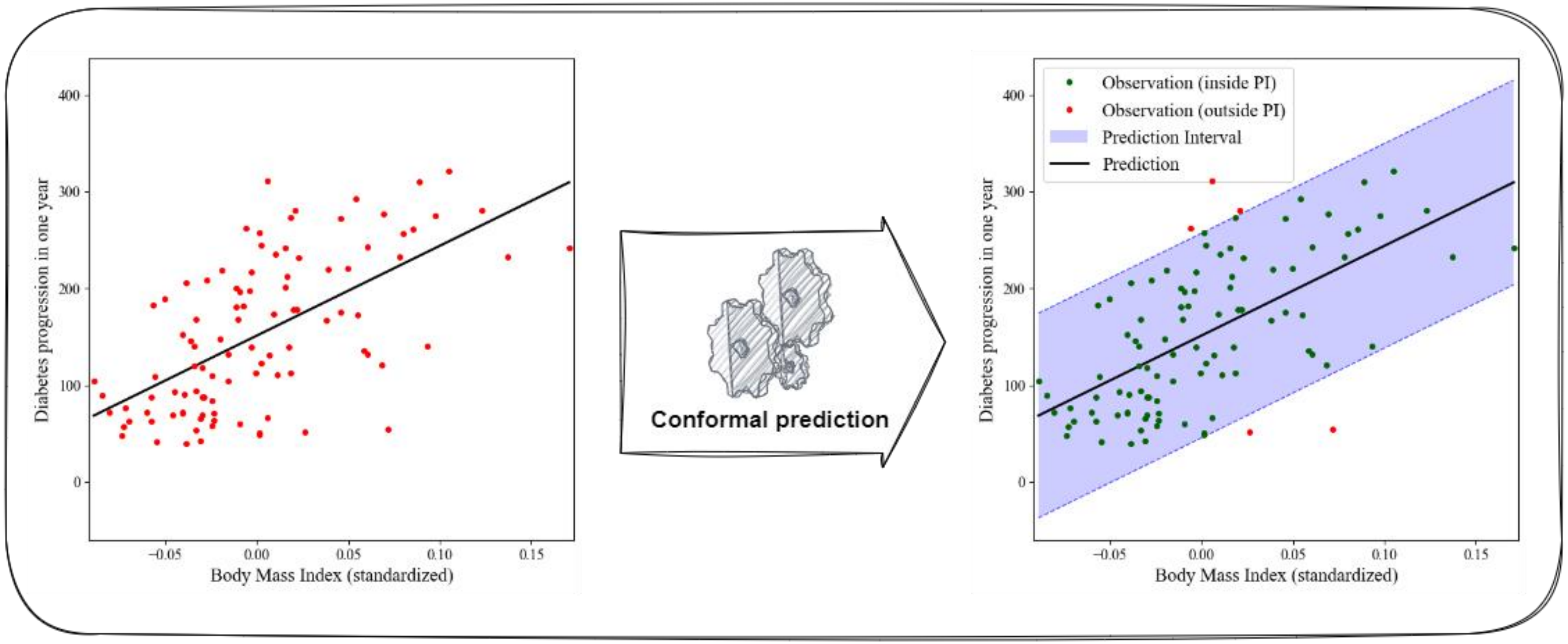


# PUNCC: Regression



# PUNCC: Classification

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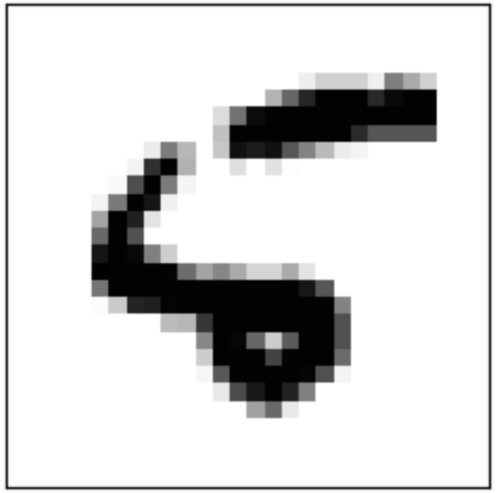

Most likely class predicted by model

{ 5 }
99.7%

Conformalization

Prediction set with probabilistic guarantees

{ 5 , 6 }
99.7% 0.03%

# PUNCC: Object Detection

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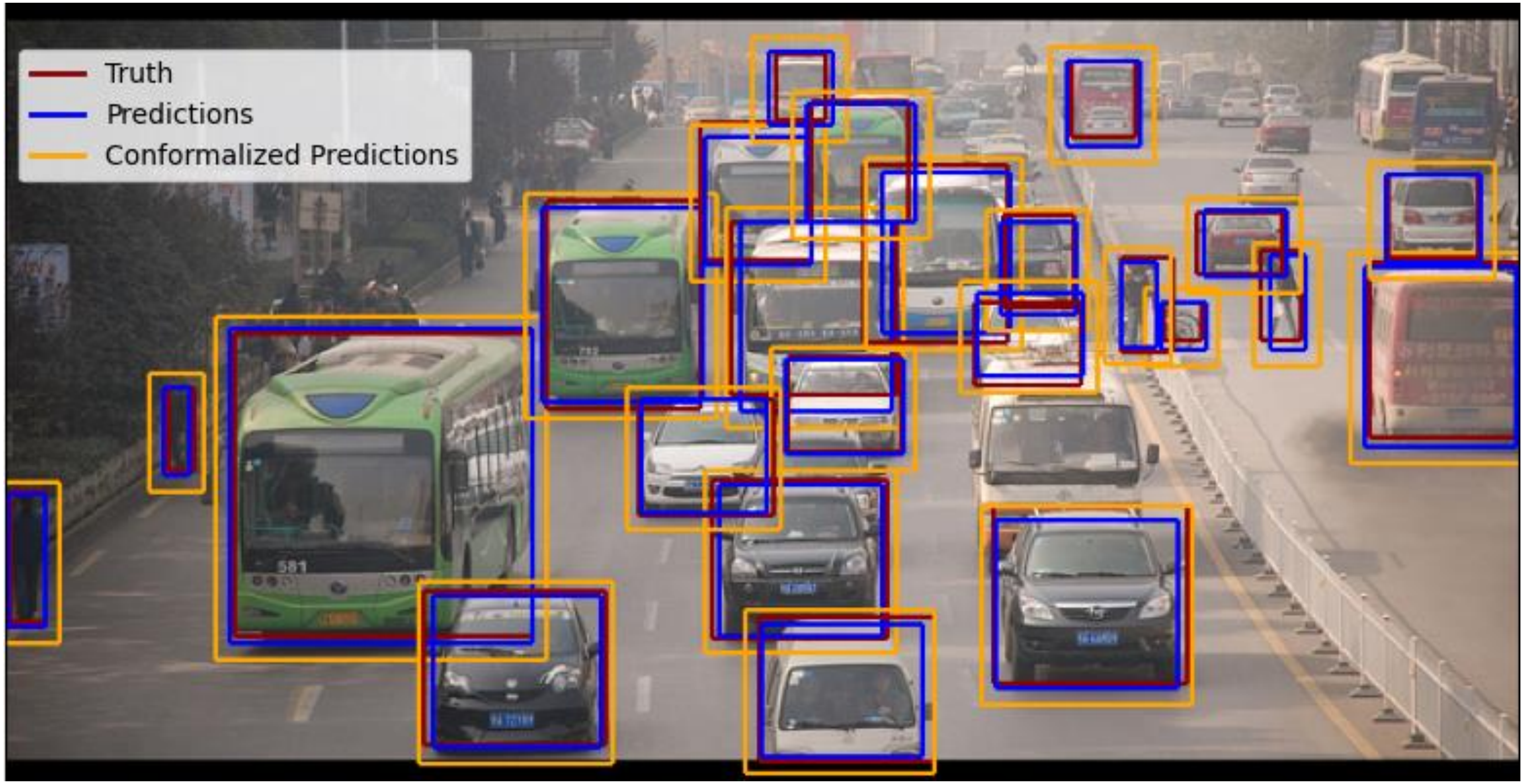
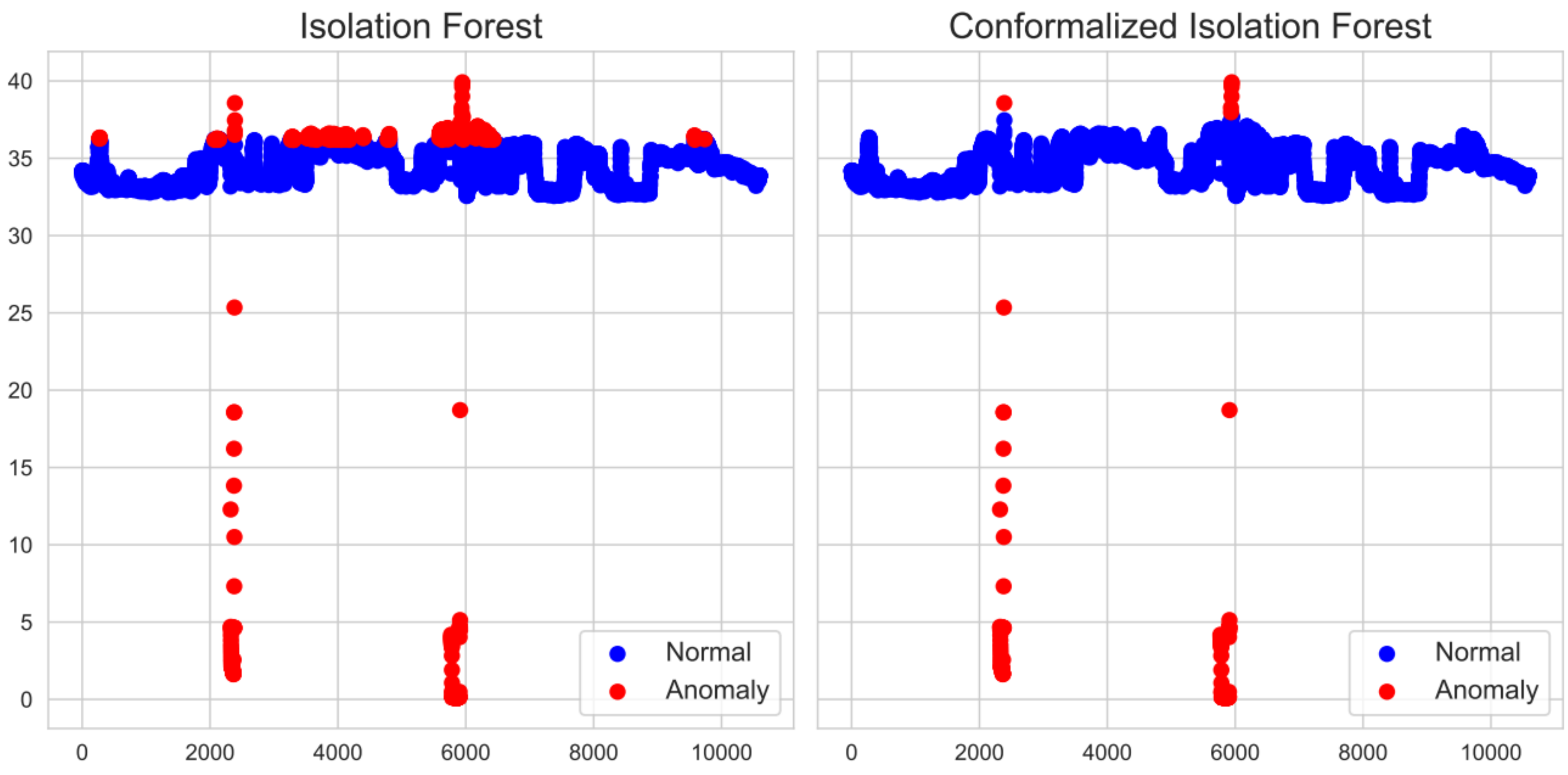
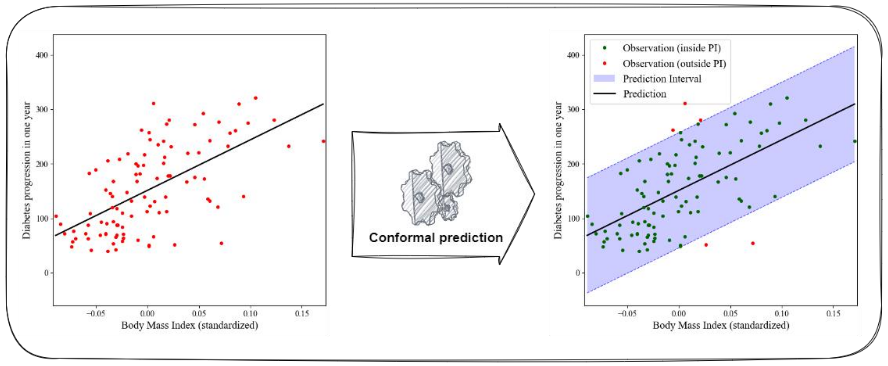
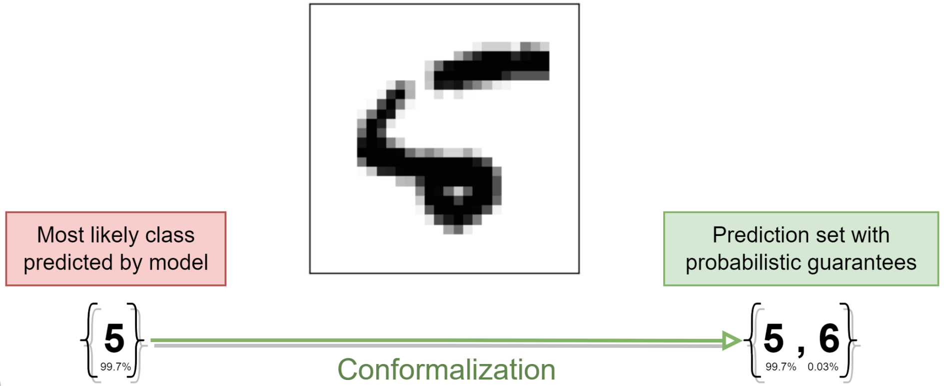


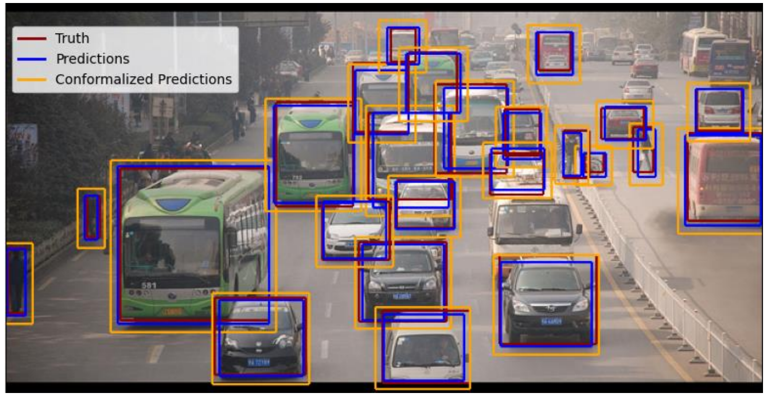
# PUNCC: Anomaly Detection

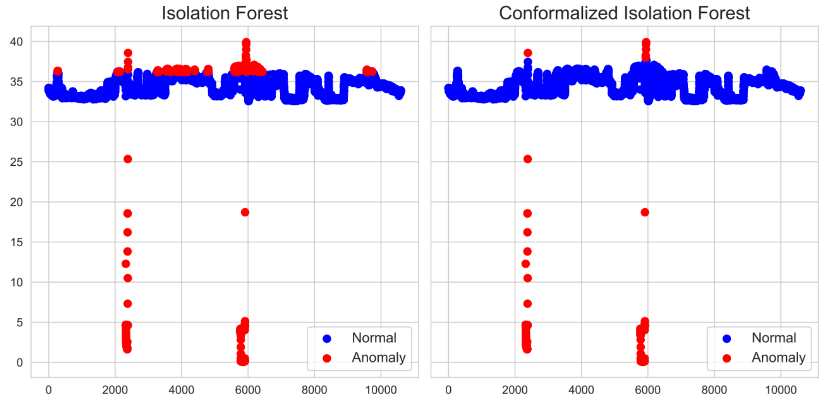


# PUNCC for different ML Tasks



# Conformal Prediction in few lines of code

## Conformal Regression

```python
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

```python
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

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## 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

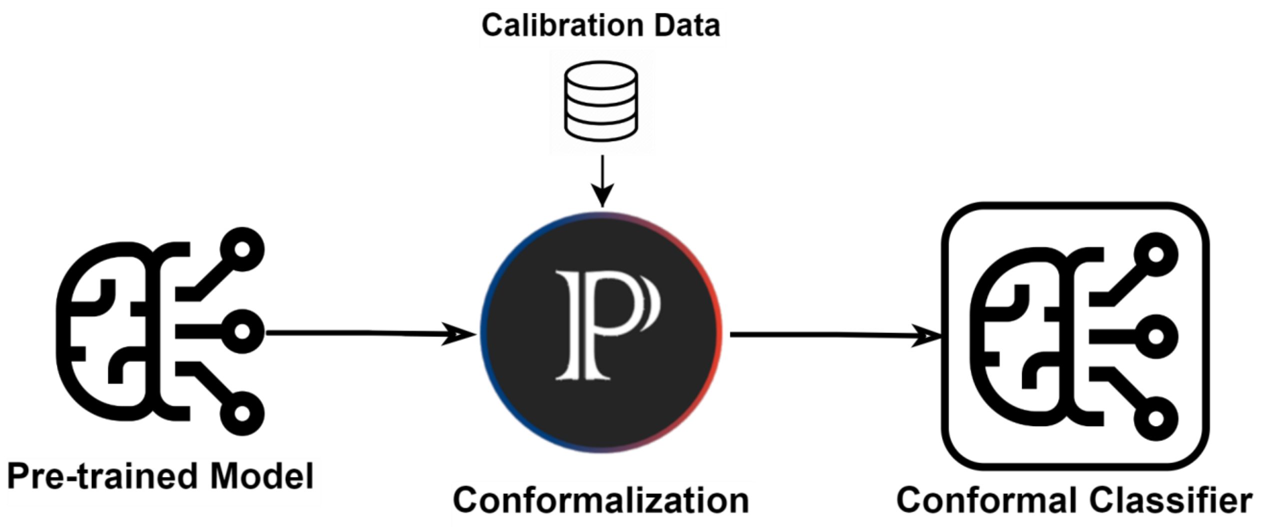
- ❑ PUNCC supports popular data types and ML libraries and more …

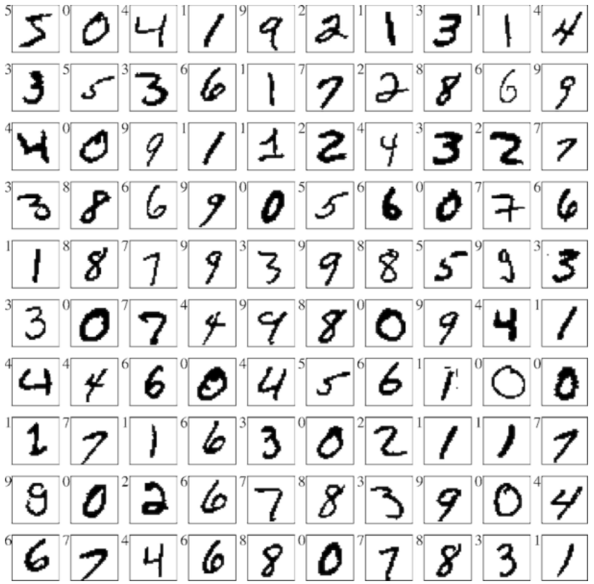
```python
from deel.puncc.api.prediction import BasePredictor
from deel.puncc.classification import APS

# 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

# Demo I: Classification

- ❑ Pretrained classifier within existing ML pipeline

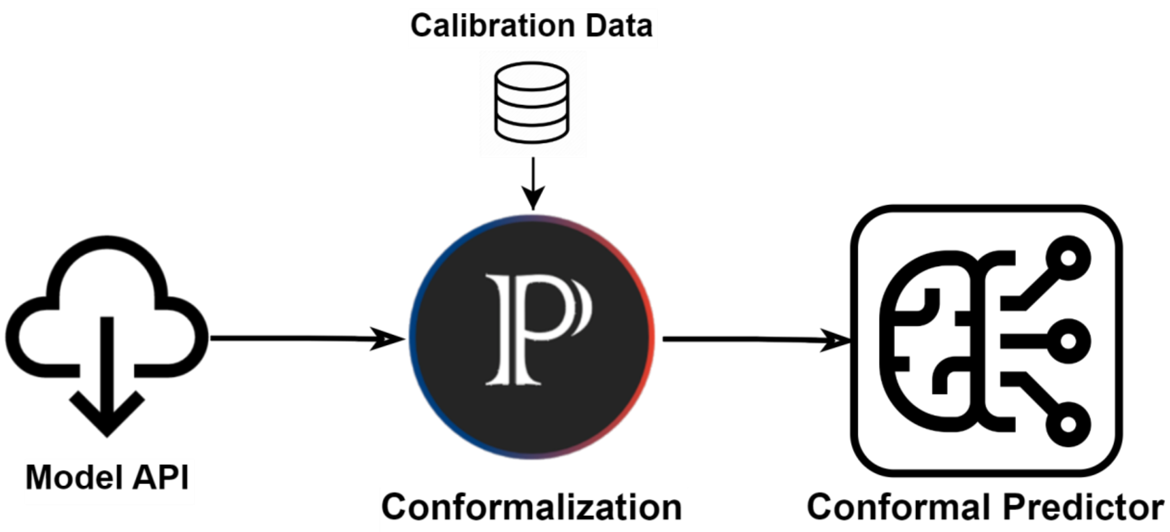


Source: D. Decoste

# Demo II: Object Detection

❑ Predictions accessible via API

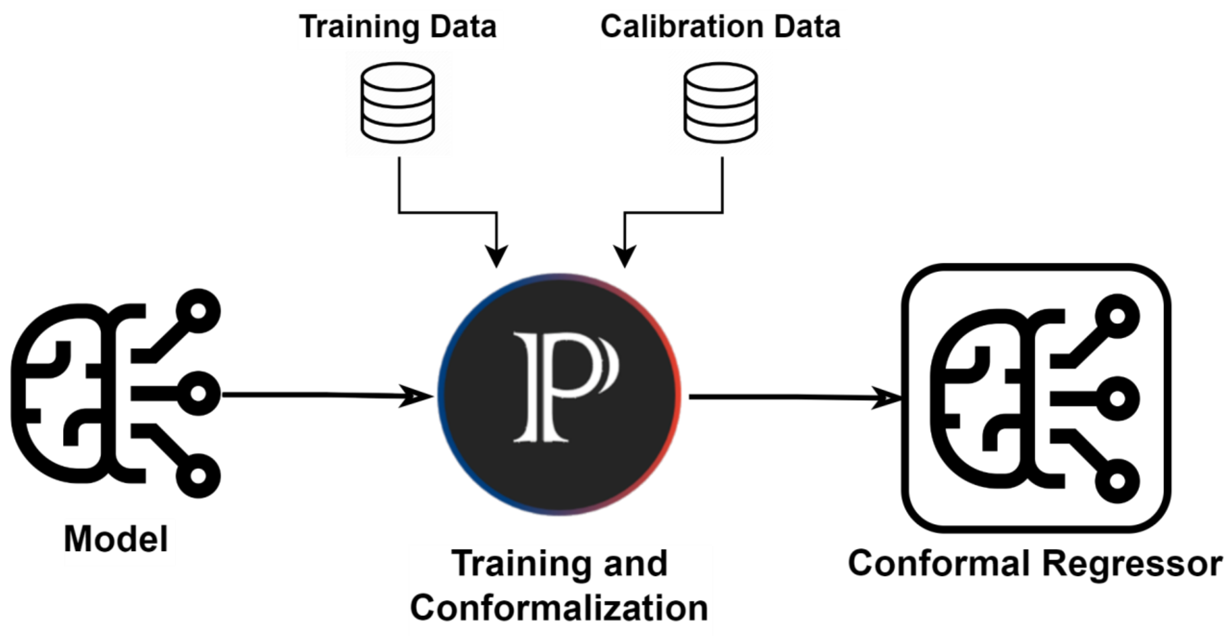




https://cocodataset.org/

# Demo III: Regression

- ❑ Model to be selected and trained from scratch




| | |
|---|---|
| **Number of Instances:** | 442 |
| **Number of Attributes:** | First 10 columns are numeric predictive values |
| **Target:** | Column 11 is a quantitative measure of disease progression one year |
| **Attribute Information:** | • age age in years<br>• sex<br>• bmi body mass index<br>• bp average blood pressure<br>• s1 tc, total serum cholesterol<br>• s2 ldl, low-density lipoproteins<br>• s3 hdl, high-density lipoproteins<br>• s4 tch, total cholesterol / HDL<br>• s5 ltg, possibly log of serum triglycerides level<br>• s6 glu, blood sugar level |

**Source: https://scikit-learn.org**

# PUNCC Project

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- ❑Documentation
- ❑Tutorials
- ❑Tests
- ❑Updates
- ❑Open to contributions

**https://github.com/deel-ai/puncc**

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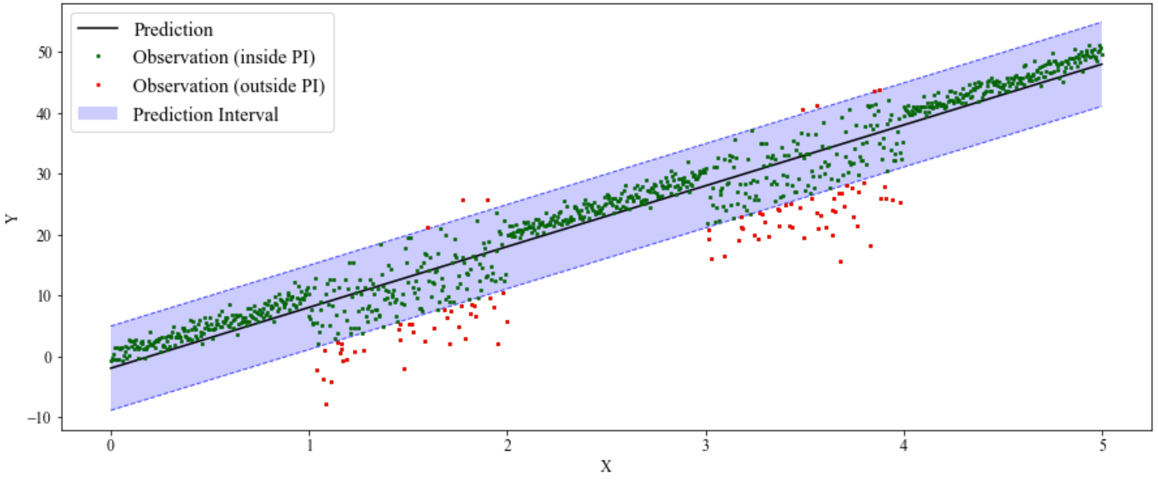
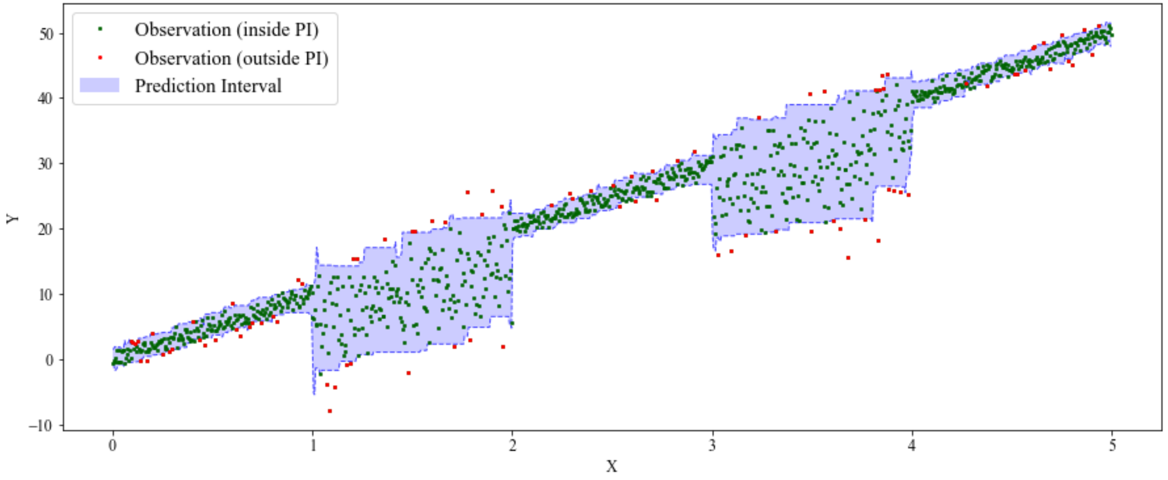
France-Quebec

# Thanks for your attention !

# Conditional Guarantees




90% **marginal** coverage
$P\left(Y_{new} \in \hat{C}(X_{new})\right) \geq 0.9$

90% **conditional** coverage
$\forall x, P\left(Y_{new} \in \hat{C}(X_{new}) \mid X_{new} = x\right) \geq 0.9$

Note that: **conditional** coverage ⇒ **marginal** coverage




11/01/2024