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Part of Capgemini Invent

COPA 2023- The 12th Symposium on Conformal and Probabilistic Prediction with Applications

Flexible and Systematic Uncertainty Estimation with Conformal Prediction via the MAPIE library

2023/09/15

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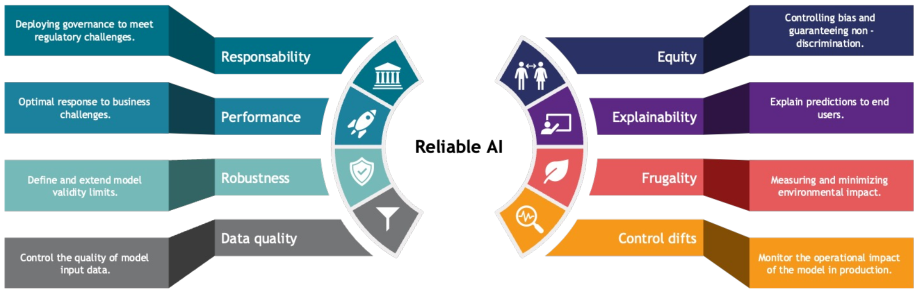
Part 1

MAPIE

To the origins of MAPIE



Our motivations for developping MAPIE

- Uncertainty quantification (UQ) for model predictions is of crucial importance for developing and deploying reliable artificial intelligence (AI) systems:
  - **to better understand the predictive power** of their model.
  - **to assess the validity** of model predictions on new data points.
  - **to help risk management** when making business decisions based on AI system predictions.
  - **to assess the compliance of the AI system** with the regulation.
  - **to be more transparent and trustworthy** for people impacted by the decisions made from AI.
  - ...

MAPIE - Model Agnostic Prediction Interval Estimator

scikit-learn-contrib / **MAPIE** Public

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- Since 2021, we are developing the MAPIE library based on conformal prediction framework [1-2].
- **MAPIE** is an open-source Python library hosted on scikit-learn-contrib project that allows you to:

  1) easily **compute conformal prediction intervals/sets** with controlled marginal coverage rate for regression [3,4,8], classification (binary and multi-class) [5-7] and time series [9].

  2) easily **control risks** (such as coverage, recall or any other non-monotone risk) for more complex tasks (multi-label classification, semantic segmentation, …) [10-12].

  3) easily **wrap any model** (*scikit-learn, tensorflow, pytorch*, ...).

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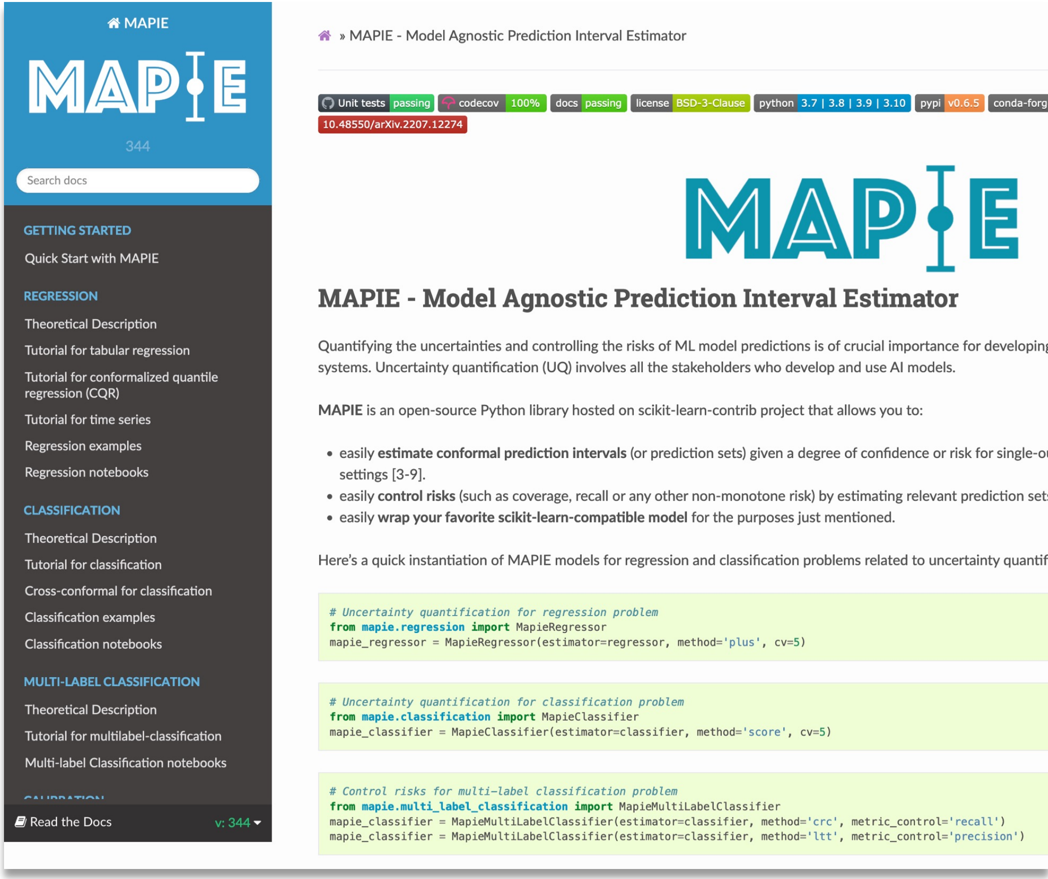
Part 2

MAPIE

How does it work?



MAPIE

344

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» MAPIE - Model Agnostic Prediction Interval Estimator

Unit tests passing | codecov 100% | docs passing | license BSD-3-Clause | python 3.7 | 3.8 | 3.9 | 3.10 | pypi v0.6.5 | conda-forg

10.48550/arXiv.2207.12274

MAPIE

MAPIE - Model Agnostic Prediction Interval Estimator

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- easily **estimate conformal prediction intervals** (or prediction sets) given a degree of confidence or risk for single-o settings [3-9].
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- easily **wrap your favorite scikit-learn-compatible model** for the purposes just mentioned.

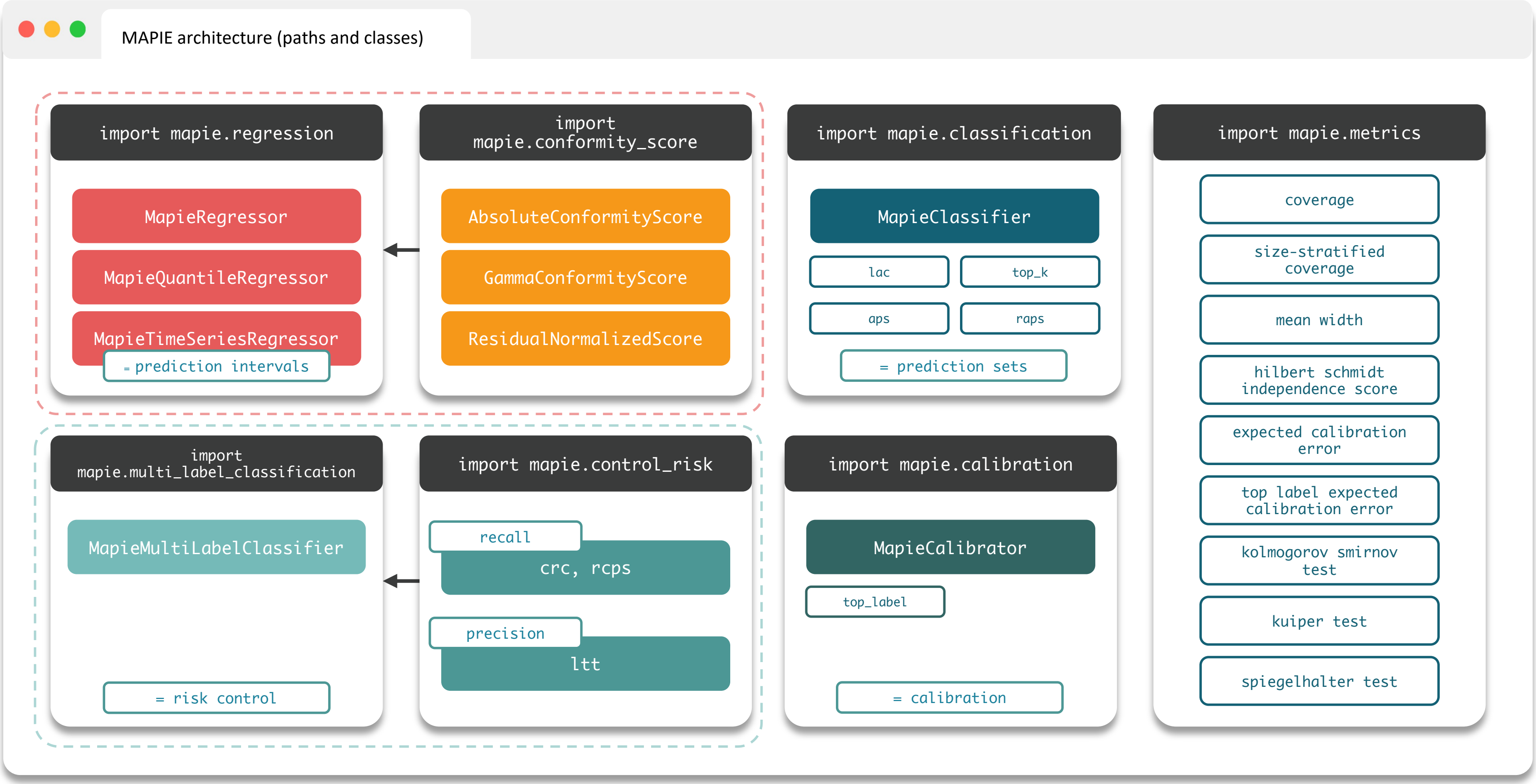
Here's a quick instantiation of MAPIE models for regression and classification problems related to uncertainty quantif

```
# Uncertainty quantification for regression problem
from mapie.regression import MapieRegressor
mapie_regressor = MapieRegressor(estimator=regressor, method='plus', cv=5)
```

```
# Uncertainty quantification for classification problem
from mapie.classification import MapieClassifier
mapie_classifier = MapieClassifier(estimator=classifier, method='score', cv=5)
```

```
# Control risks for multi-label classification problem
from mapie.multi_label_classification import MapieMultiLabelClassifier
mapie_classifier = MapieMultiLabelClassifier(estimator=classifier, method='crc', metric_control='recall')
mapie_classifier = MapieMultiLabelClassifier(estimator=classifier, method='ltt', metric_control='precision')
```

Software architecture of MAPIE



⚡ Quick start with MAPIE

quickstart.py

```
# installation via `pip`
$ pip install mapie
```

MAPIE in practice

1. Identify a (pre-trained) model.
2. Wrap it with the MAPIE class.
3. Fit the new model to calibration data.
4. Predict the target on the test data to obtain the prediction intervals/sets.

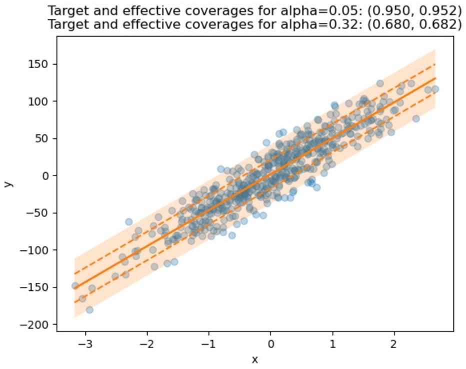
Easy to use, yet powerful! 🔥

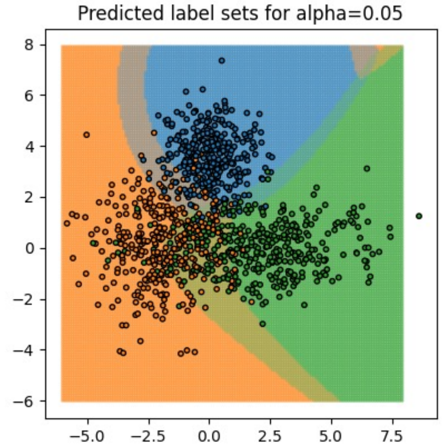
MAPIE for regression (pre-fit / split-conformal)

code.py

```
import numpy as np
from sklearn.linear_model import LinearRegression
from sklearn.datasets import make_regression
from sklearn.model_selection import train_test_split

from mapie.regression import MapieRegressor


X, y = make_regression(n_samples=500, n_features=1)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5)
X_train, X_calib, y_train, y_calib = train_test_split(X_train, y_train, test_size=0.5)

regressor = LinearRegression().fit(X_train, y_train)

mapie_regressor = MapieRegressor(estimator=regressor, method='plus', cv='prefit')

mapie_regressor = mapie_regressor.fit(X_calib, y_calib)
y_pred, y_pis = mapie_regressor.predict(X_test, alpha=[0.05, 0.32])
```

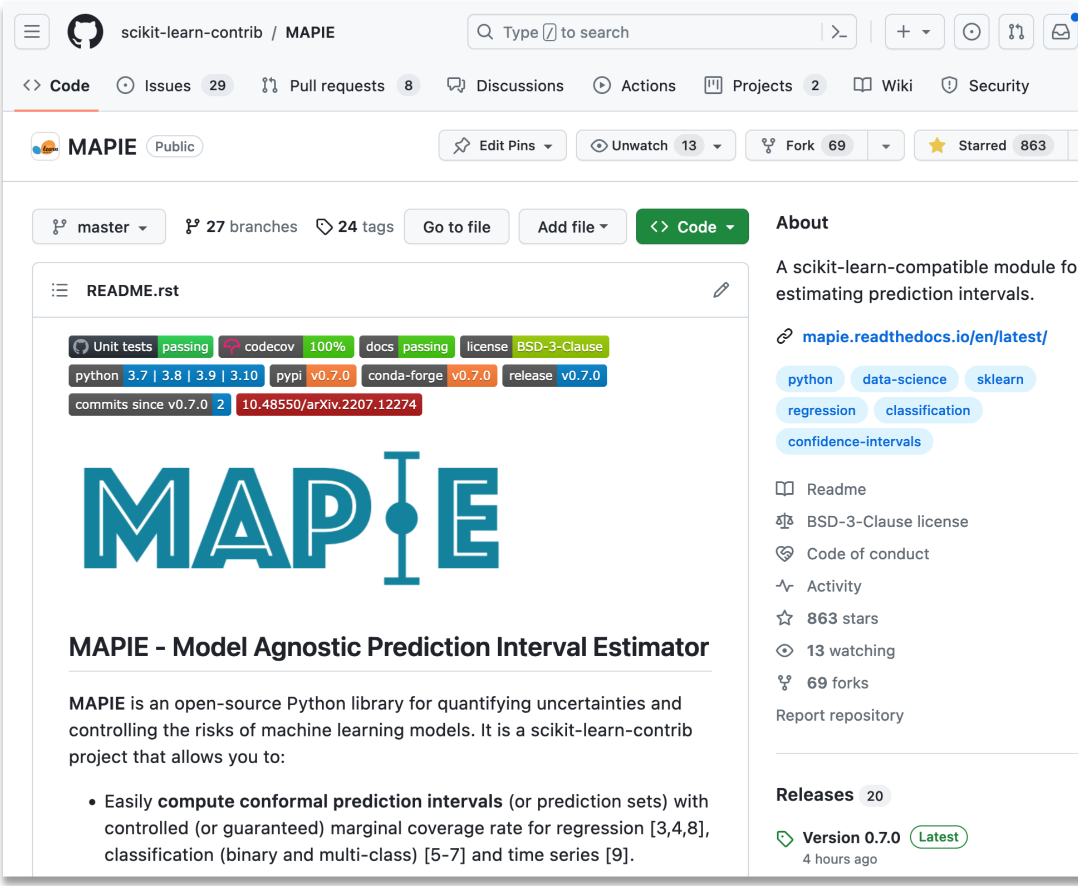
1 2 3 4





Part 3

How to contribute?



Focus on a MAPIE contribution to the ConformityScore module

A new family of non-conformity scores “**p-Normalized residual non-conformity score**“.

- <u>Motivations for its integration into MAPIE:</u>
    - **Theoretical demonstration**: "Global marginal coverage guarantee" for cross-conformal methods.
    - **Practical interest**: Useful where the uncertainty is of the order of magnitude of the prediction (heteroskedasticity).
    - **Advantages**: Model agnostic.
- <u>In practice:</u> implementation of a new class, GammaConformityScore (special case when p=2).

Assumption	Induced non-conformity score	Induced limits of the prediction interval
$Y = \mu(x) + \sigma(x)\epsilon$ $\sigma(x) \propto \lvert\mu(x)\rvert^{p/2}$	$s(x,y) = \left\lvert\frac{y - \hat{\mu}(x)}{\hat{\mu}(x)^{p/2}}\right\rvert$	$\hat{y}^{\pm}_{bound} = \hat{\mu}(X_{n+1}) \pm \hat{q}^{\pm}_{n,\alpha} \lvert\hat{\mu}(X_{n+1})\rvert^{p/2}$

n calibration samples ; α level of risk ; x features ; y target ; s non-conformity score function ; $\hat{\mu}$ estimated model ; $\hat{y}$ prediction ; $\hat{s}$ estimated non-conformity score ; $\hat{q}^{\pm}_{n,\alpha}$ upper and lower quantiles ; $\hat{Q}^{\pm}_{n,\alpha}$ upper and lower quantile estimators ; (X_{n+1}, Y_{n+1}) test data ; $\hat{C}_{n,\alpha}(X_{n+1})$ prediction interval

Theoretical results on p-normalized residual non-conformity scores

Theorem 1 (Global marginal coverage guarantee) *We state that, for any signed loss score function $f(\hat{y}, y)$ monotonically increasing on $\hat{y}$ and monotonically decreasing on y (the higher the absolute value, the more atypical the point), for any conformal prediction methods in Table 3.1, the prediction interval satisfies the marginal coverage:*

$$P\{Y_{n+1} \in \hat{C}_{n,\alpha}(X_{n+1})\} \gtrsim 1 - \alpha$$

Method	**Theoretical coverage**	**Training cost**	**Evaluation cost**
Naïve	No guarantee	1	n_{test}
Split	$\geq 1-\alpha$	1	n_{test}
Jackknife	No guarantee	n	n_{test}
Jackknife+	$\geq 1-2\alpha$	n	$n \times n_{\text{test}}$
Jackknife-minmax	$\geq 1-\alpha$	n	$n \times n_{\text{test}}$
CV	No guarantee	K	n_{test}
CV+	$\geq 1-2\alpha$	K	$K \times n_{\text{test}}$
CV-minmax	$\geq 1-\alpha$	K	$K \times n_{\text{test}}$
Jackknife-aB+	$\geq 1-2\alpha$	K	$K \times n_{\text{test}}$
Jackknife-aB-minmax	$\geq 1-\alpha$	K	$K \times n_{\text{test}}$

Table 1: Theoretical marginal coverage and reminder of the training cost and the evaluation cost for conformal prediction methods (Foygel Barber et al., 2021).

n calibration samples ; α level of risk ; x features ; y target
(X_{n+1}, Y_{n+1}) test data ; $\hat{C}_{n,\alpha}(X_{n+1})$ prediction interval

Expanding the available family of non-conformity scores for regression

Non-conformity scores for MapieRegressor

MapieRegressor | **AbsoluteConformityScore**

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

$$\hat{y}^{\pm}_{bound} = \hat{\mu}(X_{n+1}) \pm \hat{q}^{\pm}_{n,\alpha}$$

MapieRegressor | **GammaConformityScore**

Proposed in the paper.

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

$$\hat{y}^{\pm}_{bound} = \hat{\mu}(X_{n+1}) \pm \hat{q}^{\pm}_{n,\alpha}\, |\hat{\mu}(X_{n+1})|$$

Release 0.4.0

MapieRegressor | **ResidualNormalizedScore**

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

$$\hat{y}^{\pm}_{bound} = \hat{\mu}(X_{n+1}) \pm \hat{q}^{\pm}_{n,\alpha}\, |\hat{\sigma}(X_{n+1})|$$

MapieQuantileRegressor

$$s(x,y) = \max(y - \hat{Q}^{+}_{n,\alpha}(x), \hat{Q}^{-}_{n,1-\alpha}(x) - y)$$

$$\hat{y}^{\pm}_{bound} = \hat{Q}^{\pm}_{n,\alpha}(X_{n+1}) + \hat{q}^{\pm}_{n,\alpha}$$

quantile of the non-conformity scores

quantile regressor

n calibration samples ; α level of risk ; x features ; y target ; s non-conformity score function ; $\hat{\mu}$ estimated model ; $\hat{y}$ prediction ; $\hat{s}$ estimated non-conformity score ; $\hat{q}^{\pm}_{n,\alpha}$ upper and lower quantiles ; $\hat{Q}^{\pm}_{n,\alpha}$ upper and lower quantile estimators ; (X_{n+1}, Y_{n+1}) test data ; $\hat{C}_{n,\alpha}(X_{n+1})$ prediction interval

How to expand non-conformity scores in MAPIE?

ConformityScore template in MAPIE

```python
class ConformityScore(metaclass=ABCMeta):
    """...

    def __init__(...

    @abstractmethod
    def get_signed_conformity_scores(...

    @abstractmethod
    def get_estimation_distribution(...

    def check_consistency(...

    def get_conformity_scores(...

    @staticmethod
    def get_quantile(...

    def get_bounds(...
```

ConformityScore interface needs
to implement two abstact methods.

GammaConformityScore class in MAPIE implementing ConformityScore

```python
class GammaConformityScore(ConformityScore):
    def __init__(self) -> None:
        super().__init__(sym=False, consistency_check=False, eps=EPSILON)

    def get_signed_conformity_scores(
        self, X: ArrayLike, y: ArrayLike, y_pred: ArrayLike
    ) -> NDArray:
        self._check_observed_data(y)
        self._check_predicted_data(y_pred)
        return np.divide(np.subtract(y, y_pred), y_pred)

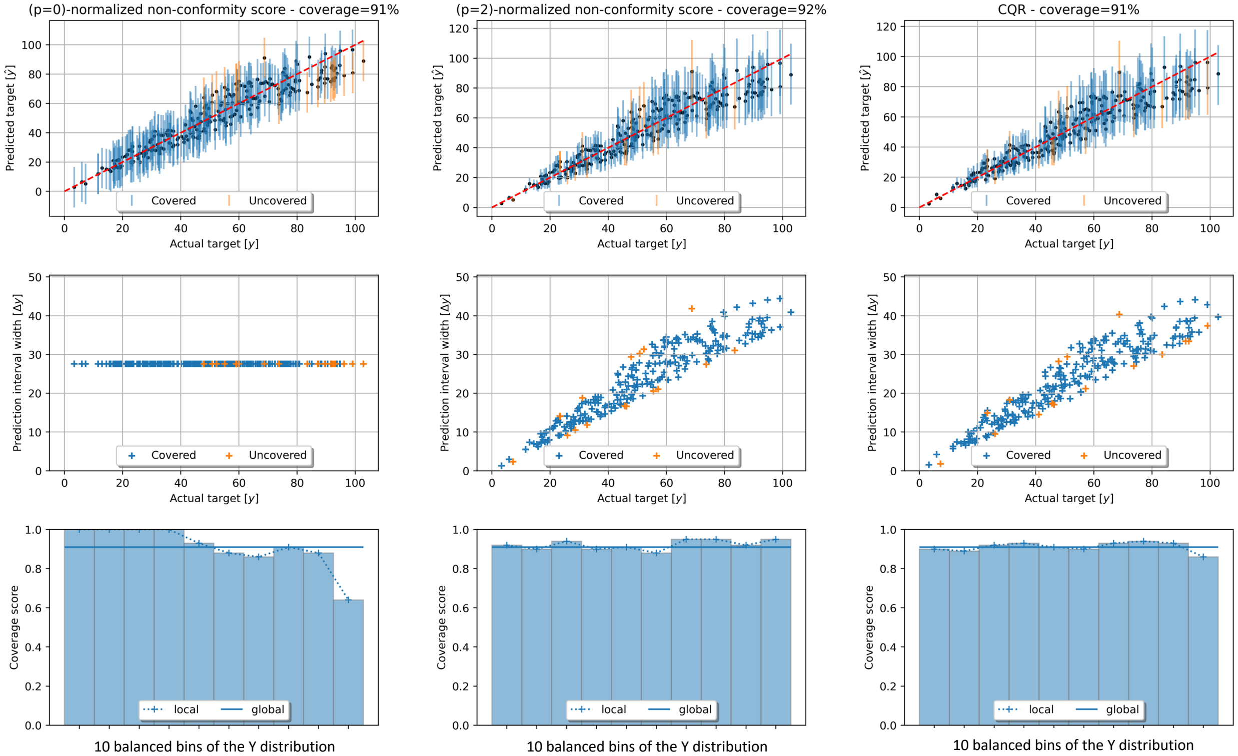
    def get_estimation_distribution(
        self,
        X: ArrayLike,
        y_pred: ArrayLike,
        conformity_scores: ArrayLike
    ) -> NDArray:
        self._check_predicted_data(y_pred)
        return np.multiply(y_pred, np.add(1, conformity_scores))
```

GammaConformityScore class implements
the two abstract methods.

Comparison of non-conformity scores on heteroskedastic dataset

MapieRegressor | MapieRegressor | MapieQuantileRegressor

AbsoluteConformityScore | GammaConformityScore



Empirical coverage computed with respect to 10 balanced bins of the Y distribution.

Assumption

$$Y = \mu(x) + \sigma(x)\epsilon$$
$$\sigma(x) \propto |\mu(x)|$$

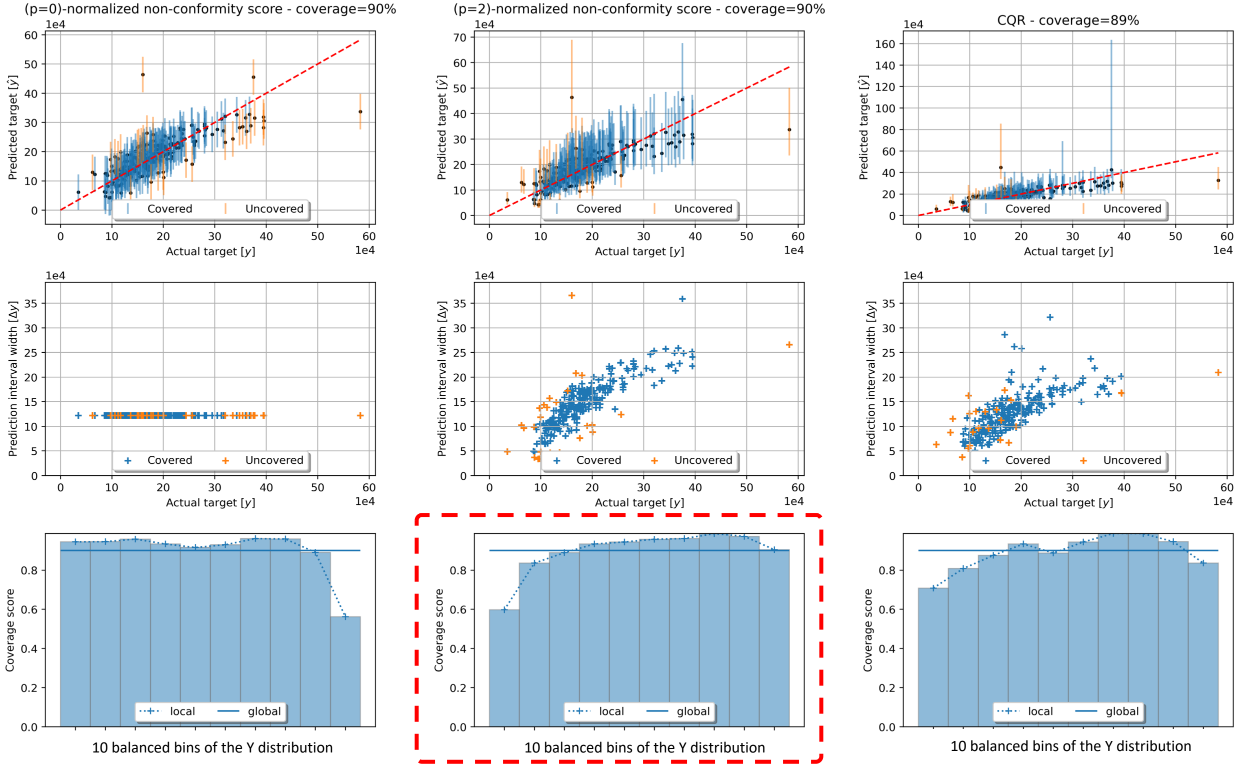
- Absolute score is not adaptive (constant prediction interval width).
- Gamma score and CQR methods are more adaptive.
- **Advantage**: GammaScore is model agnostic whereas CQR requires a quantile regressor.

Comparison of non-conformity scores on House Price dataset

MapieRegressor | AbsoluteConformityScore

MapieRegressor | GammaConformityScore

MapieQuantileRegressor



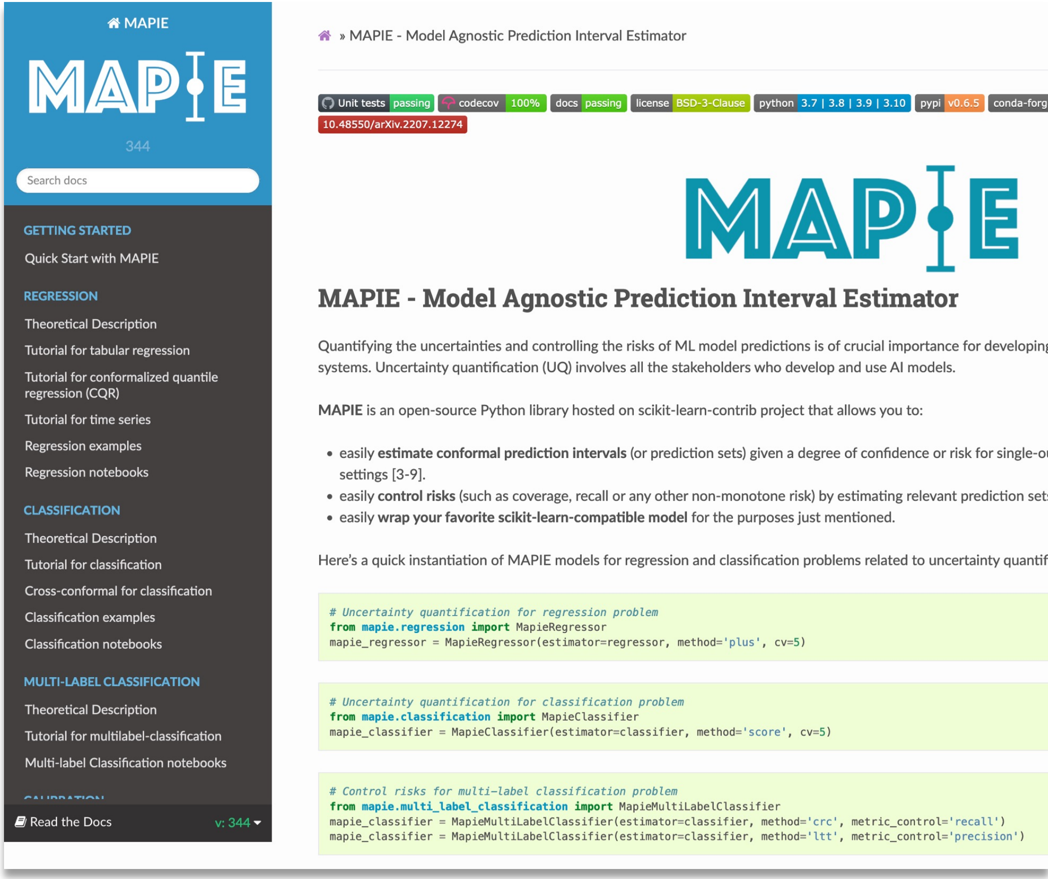
Empirical coverage computed with respect to 10 balanced bins of the price (Y) distribution.

- Gamma score gives better coverage for high prices
- Efficiency balance can be done with the p-normalised score.
- In this application, decision maker is more focused on high prices than in low prices.
- **Limitations**: prior motivated by business, well-designed for this data dispersion.

Partie 4

MAPIE

Wrap Up: the evolution of the open-source library



MAPIE

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GETTING STARTED

Quick Start with MAPIE

REGRESSION

Theoretical Description

Tutorial for tabular regression

Tutorial for conformalized quantile regression (CQR)

Tutorial for time series

Regression examples

Regression notebooks

CLASSIFICATION

Theoretical Description

Tutorial for classification

Cross-conformal for classification

Classification examples

Classification notebooks

MULTI-LABEL CLASSIFICATION

Theoretical Description

Tutorial for multilabel-classification

Multi-label Classification notebooks

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Unit tests passing | codecov 100% | docs passing | license BSD-3-Clause | python 3.7 | 3.8 | 3.9 | 3.10 | pypi v0.6.5 | conda-forg

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mapie_classifier = MapieMultiLabelClassifier(estimator=classifier, method='ltt', metric_control='precision')
```

What can you find in MAPIE?

Summary table of algorithms implemented in MAPIE

Task	Feature	Algorithm	Reference
PI/PS	MapieRegressor MapieClassifier	**Jackknife/CV+**	Rina Foygel Barber, Emmanuel J. Candès, Aaditya Ramdas, and Ryan J. Tibshirani. “Predictive inference with the jackknife+.” Ann. Statist., 49(1):486–507, (2021).
		Jackknife/CV+ ab	Kim, Byol, Chen Xu, and Rina Barber. “Predictive inference is free with the jackknife+-after-bootstrap.” Advances in NeurIPS 33 (2020): 4138-4149.
Prediction intervals (PI)	AbsoluteConformityScore GammaConformityScore ResidualNormalizedScore	**Absolute Score**	Vovk, Vladimir, Alexander Gammerman, and Glenn Shafer. Algorithmic Learning in a Random World. Springer Nature, 2005
		Gamma Score	Cordier, Thibault, Vincent Blot, Louis Lacombe, Thomas Morzadec, Arnaud Capitaine, Nicolas Brunel “Flexible and Systematic Uncertainty Estimation with Conformal Prediction via the MAPIE library”, COPA (2023)
		Normalized Score	Papadopoulos, Harris, Proedrou, Kostas, Vovk, Volodya, and Gammerman, Alex. "Inductive confidence machines for regression". In Machine Learning: ECML (2002).
	MapieTimeSeriesRegressor	**EnbPI**	Xu, Chen, and Yao Xie. “Conformal prediction interval for dynamic time-series.” International Conference on Machine Learning. PMLR, (2021).
	MapieQuantileRegressor	**CQR**	Romano, Yaniv, Evan Patterson, and Emmanuel Candes. “Conformalized quantile regression.” Advances in neural information processing systems 32 (2019).
Prediction sets (PS)	MapieClassifier	**LAC / LABEL**	Sadinle, Mauricio, Jing Lei, and Larry Wasserman. “Least ambiguous set-valued classifiers with bounded error levels.” Journal of the American Statistical Association 114.525 (2019): 223-234.
		APS	Romano, Yaniv, Matteo Sesia, and Emmanuel Candès. “Classification with valid and adaptive coverage.” Advances in NeurIPS 33 (2020): 3581-3591.
		Top-K	Angelopoulos, Anastasios, et al. “Uncertainty sets for image classifiers using conformal prediction.” International Conference on Learning Representations (2021).
		RAPS	Angelopoulos, Anastasios, et al. “Uncertainty sets for image classifiers using conformal prediction.” International Conference on Learning Representations (2021).
Control Risks (CR)	MapieMultiLabelClassifier	**RCPS**	Bates, Stephen, et al. “Distribution-free, risk-controlling prediction sets.” Journal of the ACM (JACM) 68.6 (2021): 1-34.
		CRC	Angelopoulos, Anastasios N., Stephen, Bates, Adam, Fisch, Lihua, Lei, and Tal, Schuster. “Conformal Risk Control.” (2022).
		LTT	Angelopoulos, Anastasios N., Stephen, Bates, Emmanuel J. Candès, et al. “Learn Then Test: Calibrating Predictive Algorithms to Achieve Risk Control.” (2022).
Calib.	MapieCalibrator	**Top-label**	Gupta, Chirag, and Aaditya K. Ramdas. “Top-label calibration and multiclass-to-binary reductions.” arXiv preprint arXiv:2107.08353 (2021).

What can you find in the release 0.7.0 of MAPIE?

Summary table of algorithms implemented in MAPIE

Release 0.7.0

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	MapieQuantileRegressor	CQR	Romano, Yaniv, Evan Patterson, and Emmanuel Candes. “Conformalized quantile regression.” Advances in neural information processing systems 32 (2019).
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		APS	Romano, Yaniv, Matteo Sesia, and Emmanuel Candès. “Classification with valid and adaptive coverage.” Advances in NeurIPS 33 (2020): 3581-3591.
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		CRC	Angelopoulos, Anastasios N., Stephen, Bates, Adam, Fisch, Lihua, Lei, and Tal, Schuster. “Conformal Risk Control.” (2022).
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Calib.	MapieCalibrator	Top-label	Gupta, Chirag, and Aaditya K. Ramdas. “Top-label calibration and multiclass-to-binary reductions.” arXiv preprint arXiv:2107.08353 (2021).

What do you want to do in MAPIE 0.8.0?

- **General assembly form** (afternoon of the 17th November 2023)
    - Discuss about next prioritized contributions of MAPIE 0.8.0
        - Binary Classification (Mondrian, Venn ABERS, ...)
        - Time Series (ACI, ...)
        - Distribution Shift
        - ...
- **Call for MAPIE contributions, examples and applications**
    - Integrate your notebooks in the example gallery of MAPIE
    - ...

Join us!

MAPIE - general assembly

https://forms.office.com/e/xwrd5Q7UaT

References

[1] Vovk, Vladimir, Alexander Gammerman, and Glenn Shafer. Algorithmic Learning in a Random World. Springer Nature, 2022.

[2] Angelopoulos, Anastasios N., and Stephen Bates. “Conformal prediction: A gentle introduction.” Foundations and Trends® in Machine Learning 16.4 (2023): 494-591.

[3] Rina Foygel Barber, Emmanuel J. Candès, Aaditya Ramdas, and Ryan J. Tibshirani. “Predictive inference with the jackknife+.” Ann. Statist., 49(1):486–507, (2021).

[4] Kim, Byol, Chen Xu, and Rina Barber. “Predictive inference is free with the jackknife+-after-bootstrap.” Advances in Neural Information Processing Systems 33 (2020): 4138-4149.

[5] Sadinle, Mauricio, Jing Lei, and Larry Wasserman. “Least ambiguous set-valued classifiers with bounded error levels.” Journal of the American Statistical Association 114.525 (2019): 223-234.

[6] Romano, Yaniv, Matteo Sesia, and Emmanuel Candès. “Classification with valid and adaptive coverage.” Advances in Neural Information Processing Systems 33 (2020): 3581-3591.

[7] Angelopoulos, Anastasios, et al. “Uncertainty sets for image classifiers using conformal prediction.” International Conference on Learning Representations (2021).

[8] Romano, Yaniv, Evan Patterson, and Emmanuel Candès. “Conformalized quantile regression.” Advances in neural information processing systems 32 (2019).

[9] Xu, Chen, and Yao Xie. “Conformal prediction interval for dynamic time-series.” International Conference on Machine Learning. PMLR, (2021).

[10] Bates, Stephen, et al. “Distribution-free, risk-controlling prediction sets.” Journal of the ACM (JACM) 68.6 (2021): 1-34.

[11] Angelopoulos, Anastasios N., Stephen, Bates, Adam, Fisch, Lihua, Lei, and Tal, Schuster. “Conformal Risk Control.” (2022).

[12] Angelopoulos, Anastasios N., Stephen, Bates, Emmanuel J. Candès, et al. “Learn Then Test: Calibrating Predictive Algorithms to Achieve Risk Control.” (2022).

[13] Gupta, Chirag, and Aaditya K. Ramdas. “Top-label calibration and multiclass-to-binary reductions.” arXiv preprint arXiv:2107.08353 (2021).

MAPIE