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Tutorial:
Conformal learning – prediction with accuracy guarantees

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Agenda

1. Motivation
2. Conformal classification
    1. Derivation + Exercise
    2. Impact of nonconformity functions + Exercise
3. Conformal regression
    1. Derivation
    2. Normalized regression + Exercise
4. TCP and data usage
5. Applications & Generalizations

Why Conformal Learning

- Traditional prediction:
  - Point prediction
  - Accuracy is not guaranteed

ML model

↓

Class 4,
test acc=86%


Insurance


Medicine


Banking

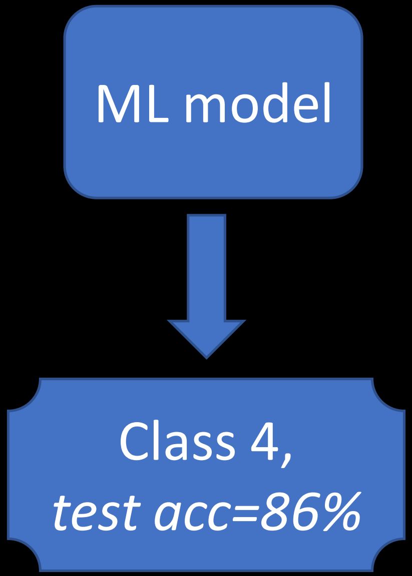
Demo 1: models calibration

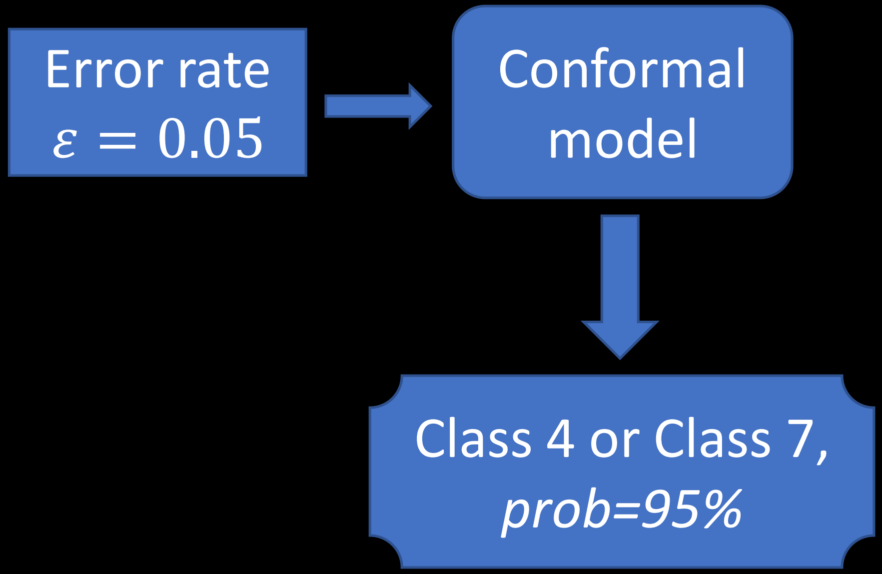
https://github.com/marharyta-aleksandrova/conformal-learning/blob/main/tutorials/Demo_1._Calibration.ipynb

Why Conformal Learning

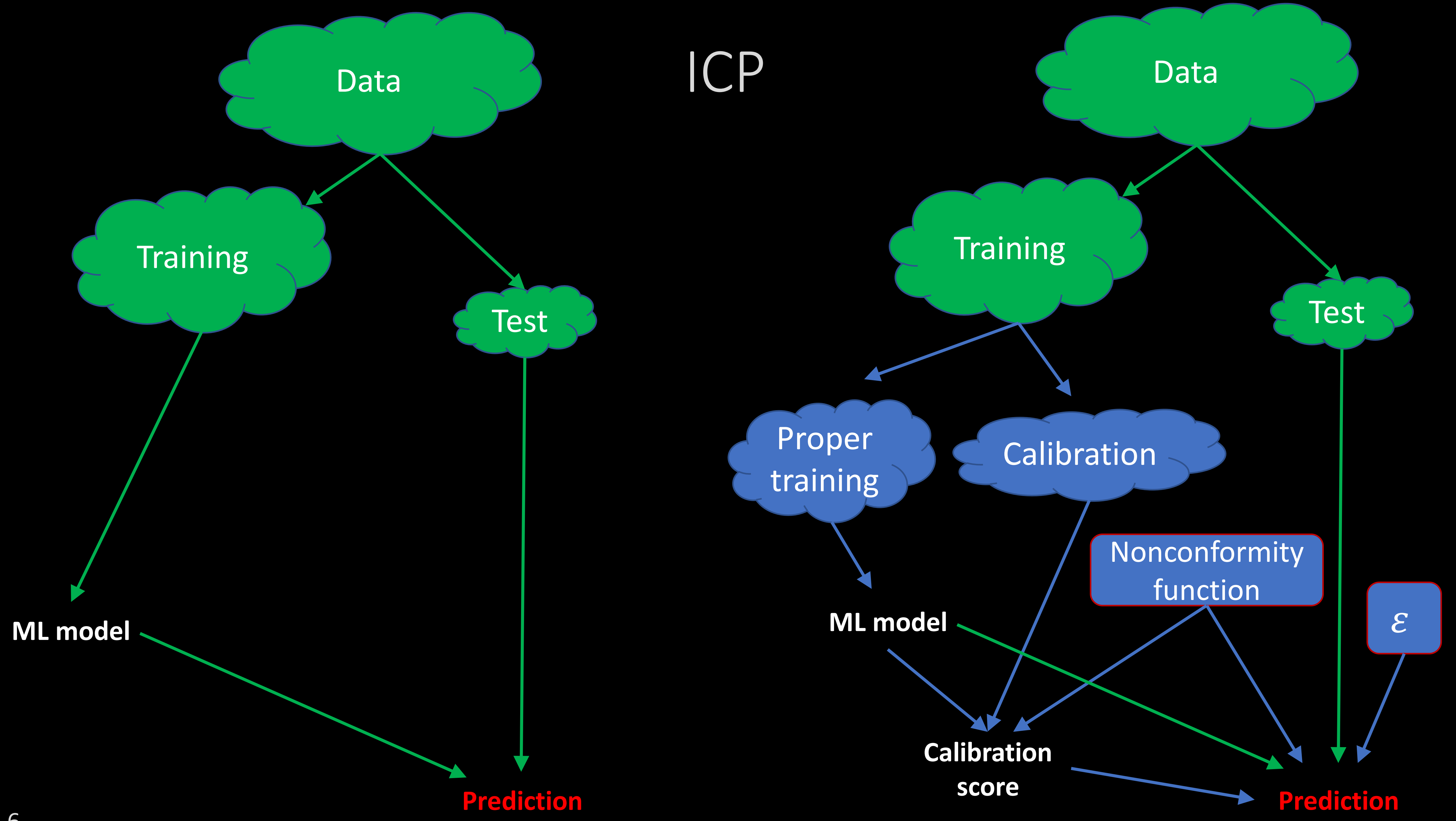
- Traditional prediction:
  - Point prediction
  - Accuracy is not guaranteed

- Conformal prediction:
  - Region prediction
  - Guaranteed accuracy
  - Useful for sensitive applications





ICP


Data
Training
Test
ML model
Prediction
Data
Training
Test
Proper training
Calibration
Nonconformity function
ML model
ε
Calibration score
Prediction

Agenda

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2. **Conformal classification**
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Math revision: Estimating cumulative distribution function from sample

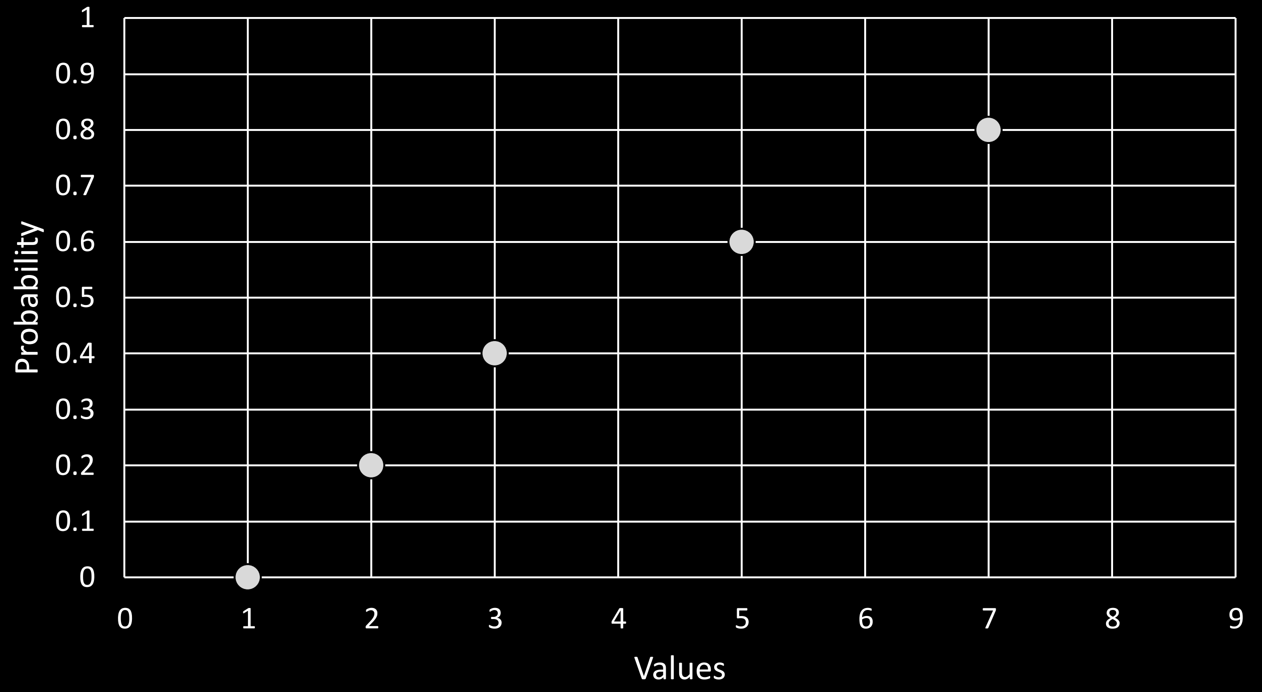
$$F_{f(Z)}(x) = \begin{cases} 0, & x < 1 \\ 0.2, & 1 \le x < 2 \\ 0.4, & 2 \le x < 3 \\ 0.6, & 3 \le x < 5 \\ 0.8, & 5 \le x > 7 \\ 1, & x \ge 7 \end{cases}$$

- Z – random variable
- $f(Z)$ - function of the random variable Z
- From sample estimate cumulative distribution function $f(Z)$:

$$F_{f(Z)}(x) = P(f(Z) \le x)$$

<u>Example:</u> $f(Z)$: 1, 3, 2, 7, 5

- Sorting – $f(Z)$: 1, 2, 3, 5, 7
- $F_{f(Z)}(x)$ is defined as the fraction of the elements

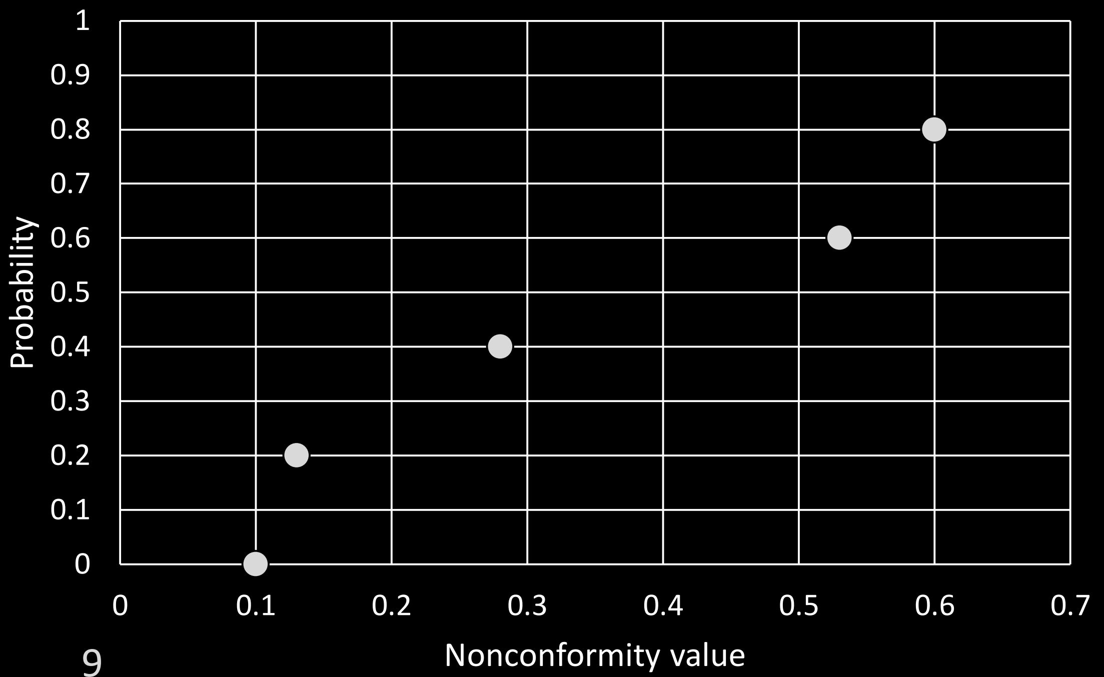


Conformal classification: Example

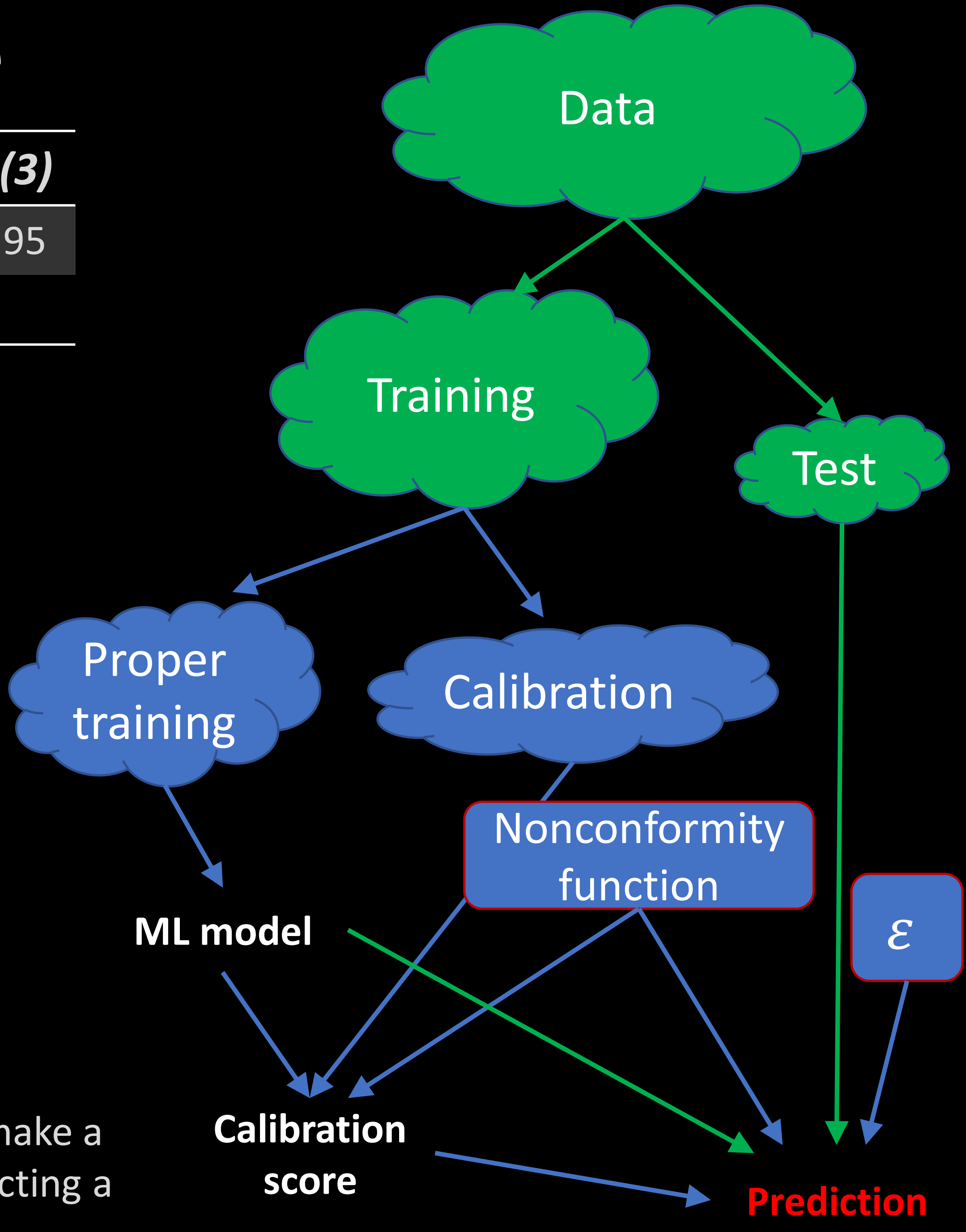
	P(y)	*A = 1-P(y)*
1	0.9	0.1
2	0.87	0.13
3	0.72	0.28
4	0.47	0.53
5	0.40	0.60

	P(1)	*A(1)*	*P(2)*	*A(2)*	*P(3)*	*A(3)*
6	**0.5**	0.5	**0.45**	0.55	**0.05**	0.95
p		0.33		0.17		0

$$p_k^{\tilde{y}} = \frac{\#\left(\alpha_i \geq \alpha_k^{\tilde{y}}\right)}{q+1} < \varepsilon \Rightarrow reject$$



Probability to make a mistake by rejecting a class-label



Demo: Derivation of conformal classification
What about *conformity* functions?

https://github.com/marharyta-aleksandrova/conformal-learning/blob/main/theory/conformal_learning_from_scratch.ipynb

Exercise: Testing conformal classifiers

https://github.com/marharyta-aleksandrova/conformal-learning/blob/main/theory/conformal_learning_from_scratch.ipynb

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Evaluating conformal classifiers

- Validity
  - Empirical error rate
- Efficiency:
  - *avgC* = avg. num. of labels, $\epsilon[0, num\_labels]$, min
  - *oneC* = fraction of singletons, $\epsilon[0,1]$, max
  - *mutlyC* = fraction of predictions with ≥ 1 label, $\epsilon[0,1]$, min
  - *zeroC* = fraction of empty predictions, $\epsilon[0,1]$, min
  - *oneAcc* = fraction of correct singletons , $\epsilon[0,1]$, min

1. {Label1, Label2}
2. {Label5}
3. {Label3}
4. {Label1, Label2, Label5, Label6}

$acc =$
$avgC =$
$oneC =$
$multyC =$
$zeroC =$
$oneArr =$

Evaluating conformal classifiers

- Validity
  - Empirical error rate
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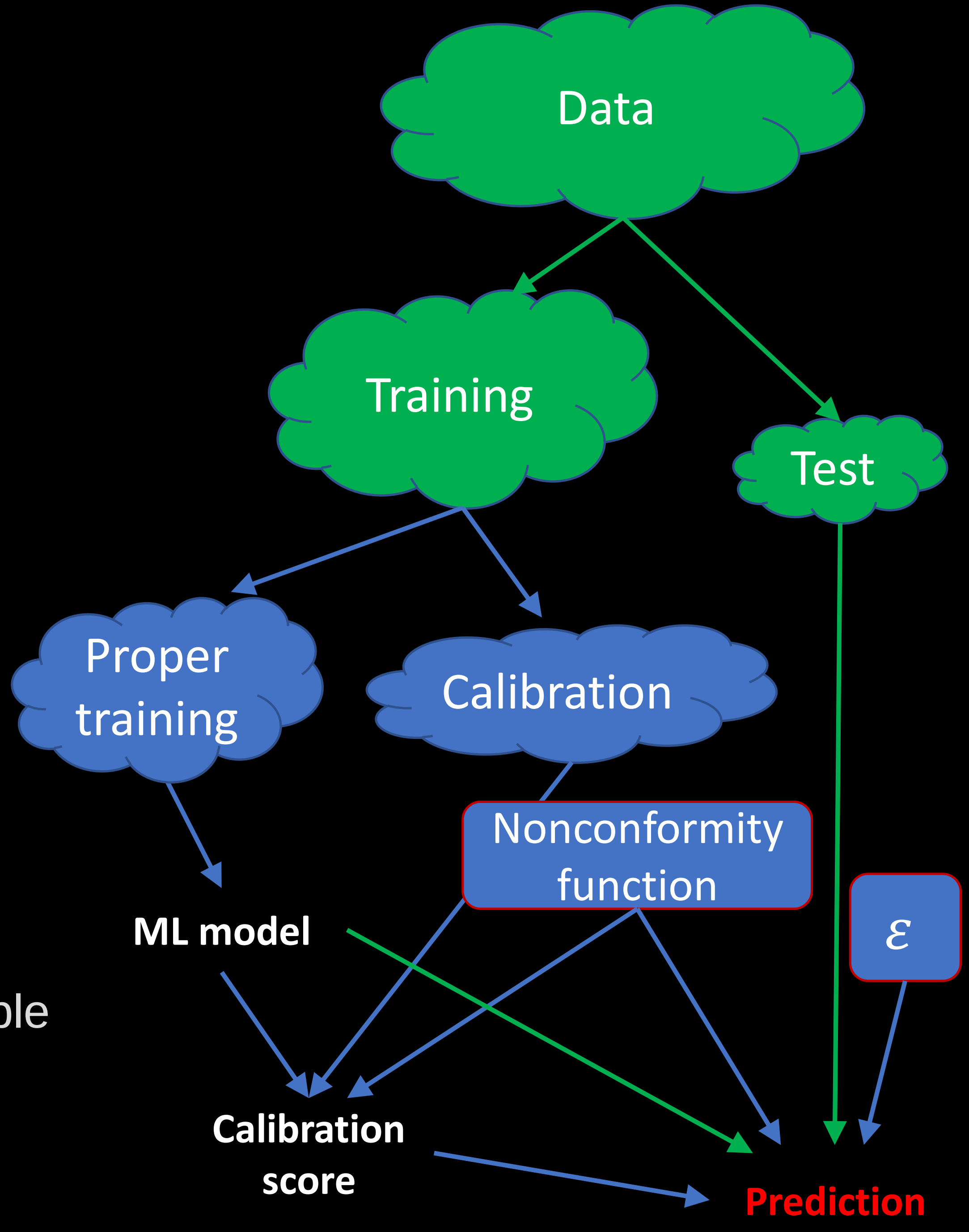
1. {Label1, Label2}
2. {Label5}
3. {Label3}
4. {Label1, Label2, Label5, Label6}

$$acc = \frac{3}{4} = 0.75$$
$$avgC = \frac{2+1+1+4}{4} = \frac{8}{4} = 2$$
$$oneC = \frac{2}{4} = 0.5$$
$$multyC = \frac{2}{4} = 0.5$$
$$zeroC = \frac{0}{4} = 0$$
$$oneArr = \frac{1}{4} = 0.25$$

Non-conformity functions

- Non-conformity function:
  - measure the strangeness of the target pair
  - depend upon the prediction error of an underlying classification or regression model
- Types
  - Model-agnostic
    - Inverse probability
    - Margin – different with the next most possible classifier
  - Model-dependent
    - KNN – distance to neighbors
    - SVM – distance to the separating hyperplane



Non-conformity functions

- Model agnostic
  - Inverse probability
  - Margin

$$A = 1 - p^{\tilde{y}}$$

$$A = \max_{y \neq \tilde{y}} p^{y} - p^{\tilde{y}}$$

	Y=1	*Y=2*	*Y=3*	*Tot*	*Inv_prob*	*Margin*
1	**0.90**	**0.10**	0.00	**1**	**0.10**	**-0.80**
2	0.10	**0.87**	0.03	**1**	**0.90**	**0.77**
3	**0.72**	0.08	**0.20**	**1**	**0.28**	**-0.52**
4	**0.40**	0.39	0.21	**1**	**0.60**	**-0.01**
5	0.45	0.08	**0.47**	**1**	**0.55**	**0.02**

Exercise: Classification – impact of nonconformity functions

https://github.com/marharyta-aleksandrova/conformal-learning/blob/main/tutorials/Exercise_2._Impact_of_nonconformity_functions_classification.ipynb

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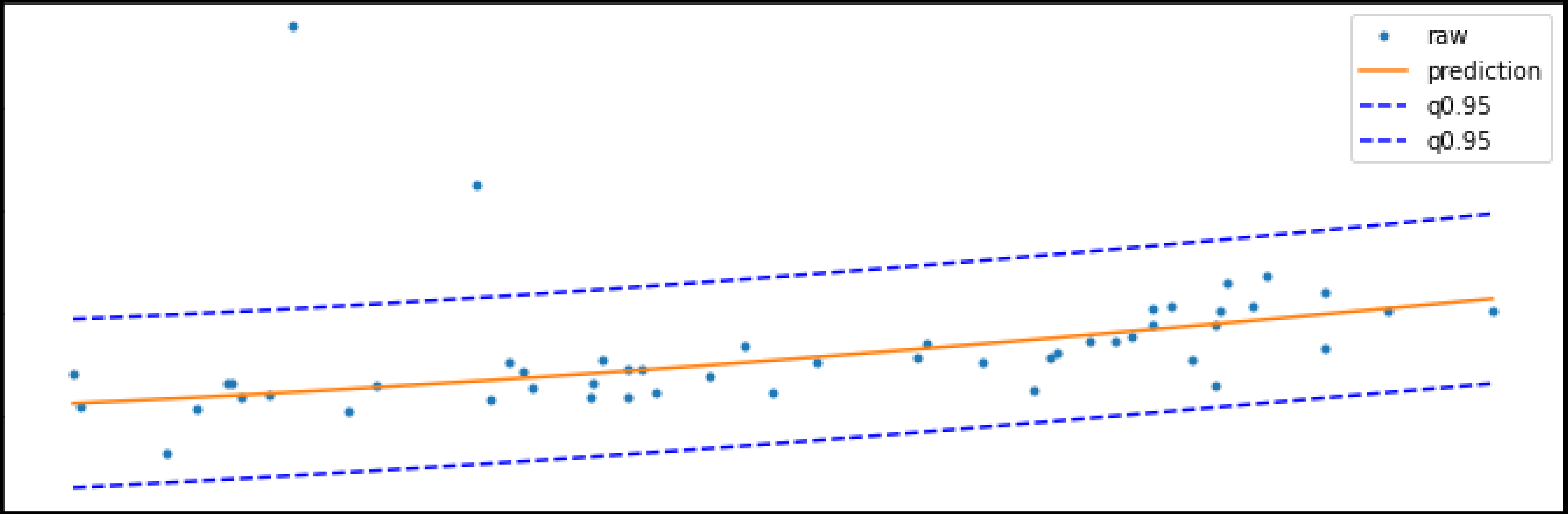
Conformal regression



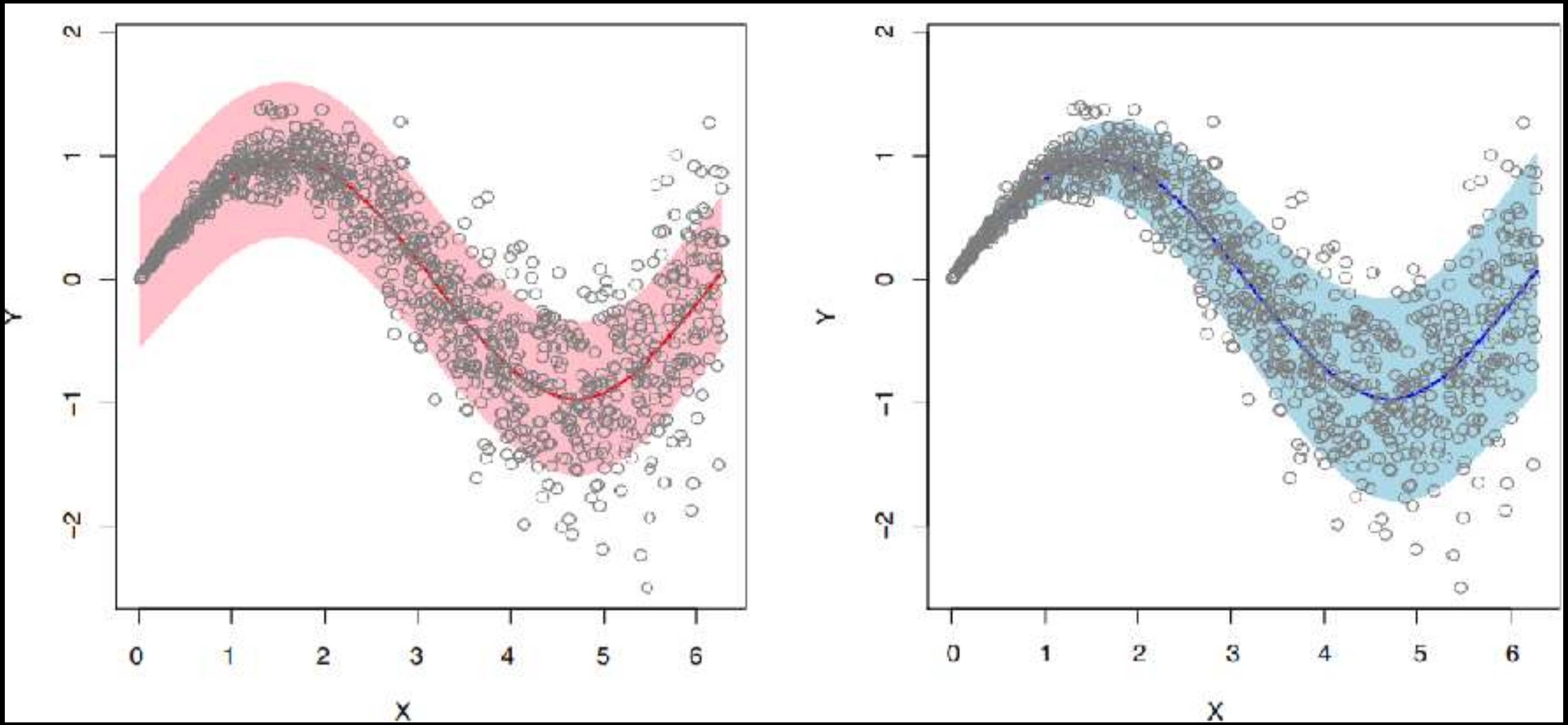
Absolute Error function:

$$A = |y - \tilde{y}|$$

Signed Error function:

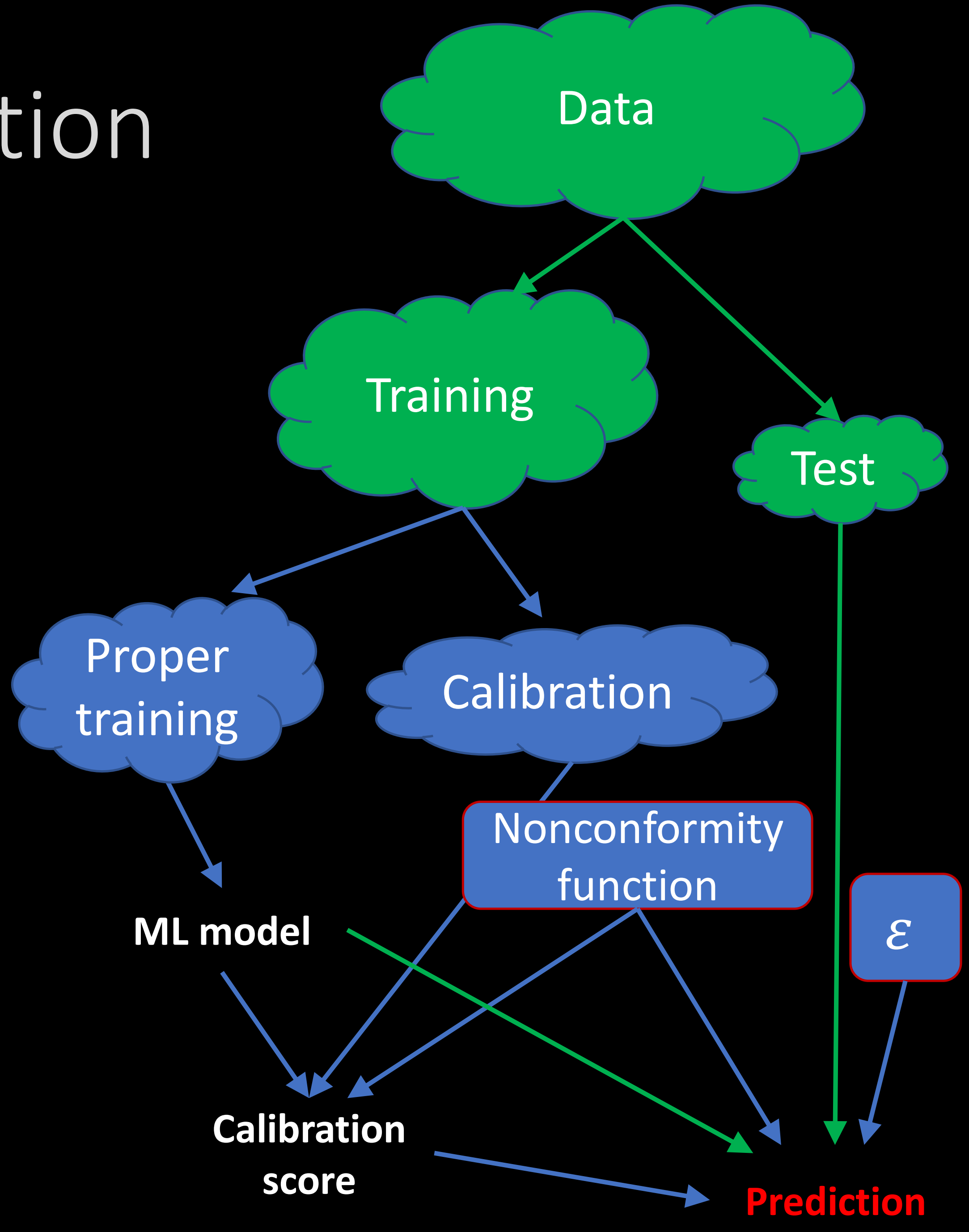
$$A = y - \tilde{y}$$

Conformal regression: size of the prediction interval



Normalized conformal prediction

- One more model is trained to predict errors
- Normalized classification



Exercise: Regression – impact of nonconformity functions

https://github.com/marharyta-aleksandrova/conformal-learning/blob/main/tutorials/Exercise_3._Impact_of_nonconformity_functions_regression.ipynb

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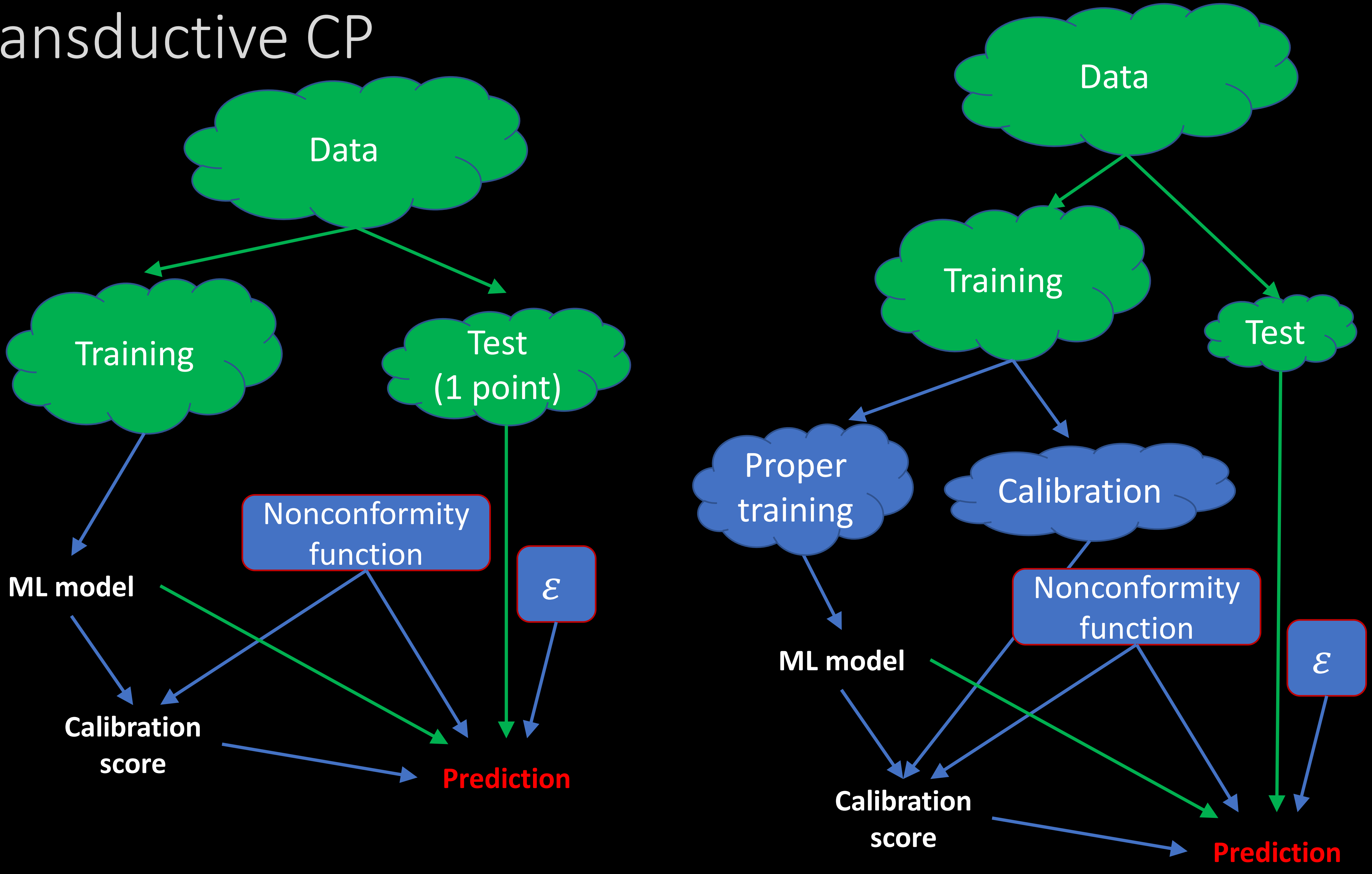
TCP – transductive CP

Model is retrained for every test instance!



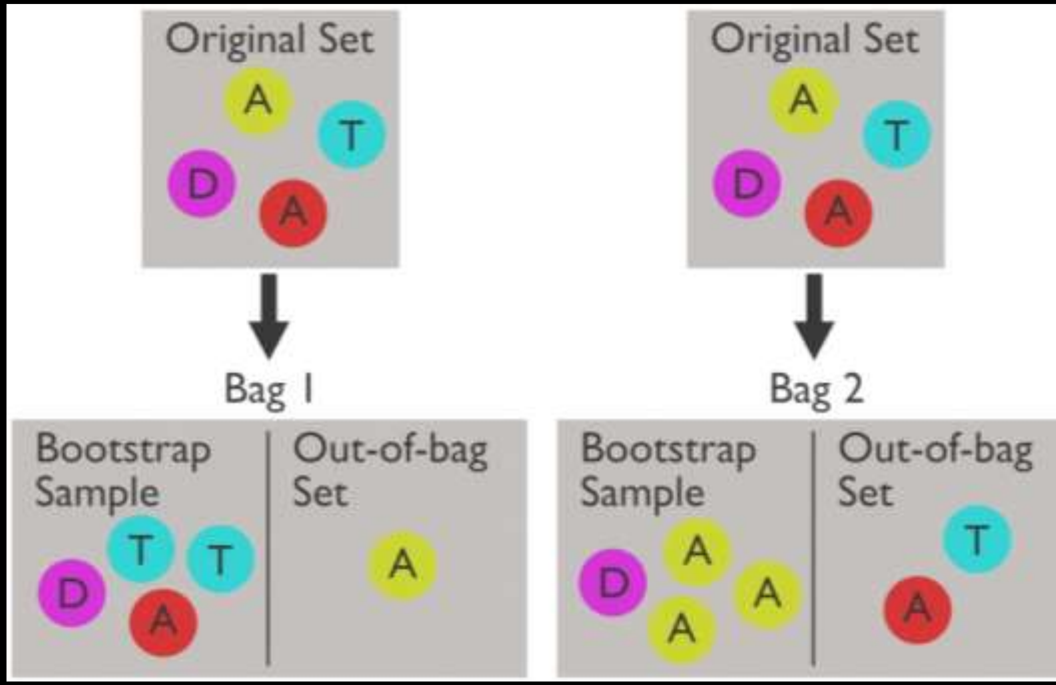
Efficient data usage

Cross-conformal prediction (CCP)

1. Cross-fold validation for conformal prediction
2. Averaging *p*-values

- ➢ Multiple models
- ➢ No validity guarantees

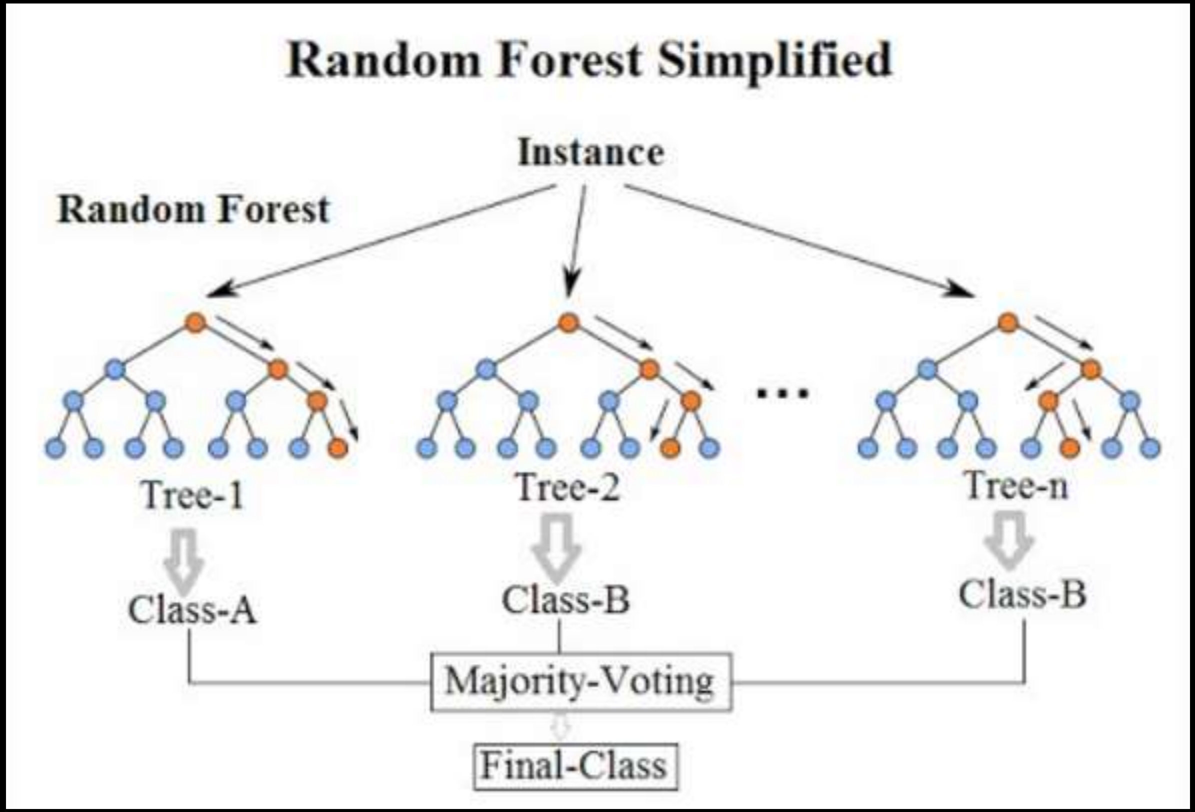
Bootstrap conformal prediction (BCP)

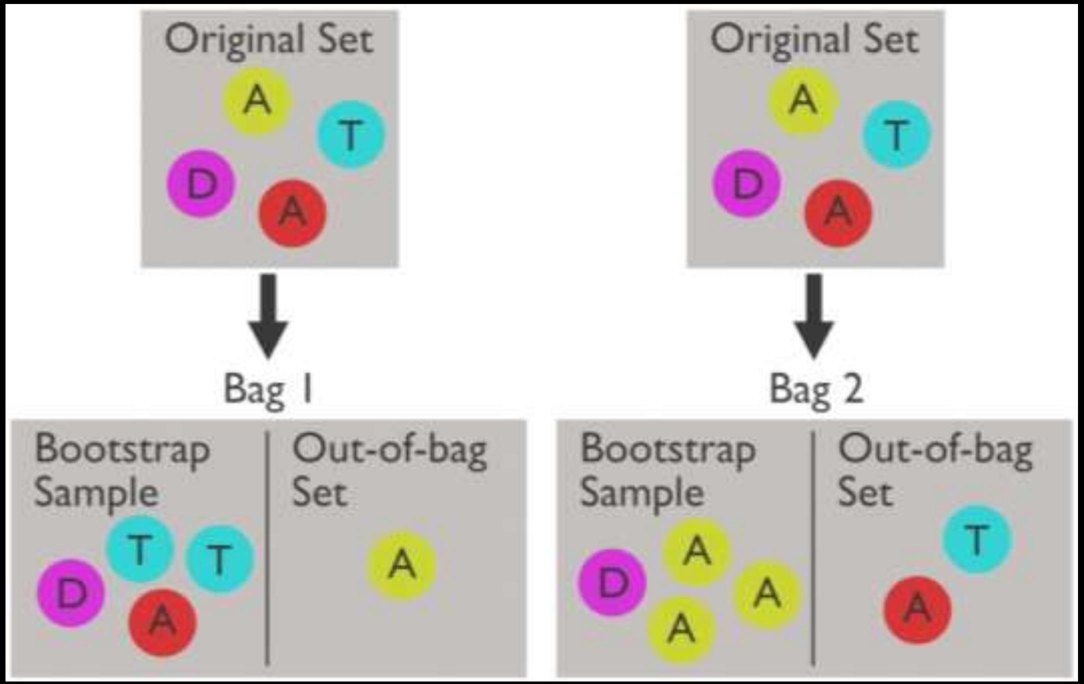


1. Bootstrap replicas (sampling with replacement)
2. *p*-values on out-of-bag + combined

- ➢ Multiple models
- ➢ No validity guarantees

OOB-CP for bagging ensemble models



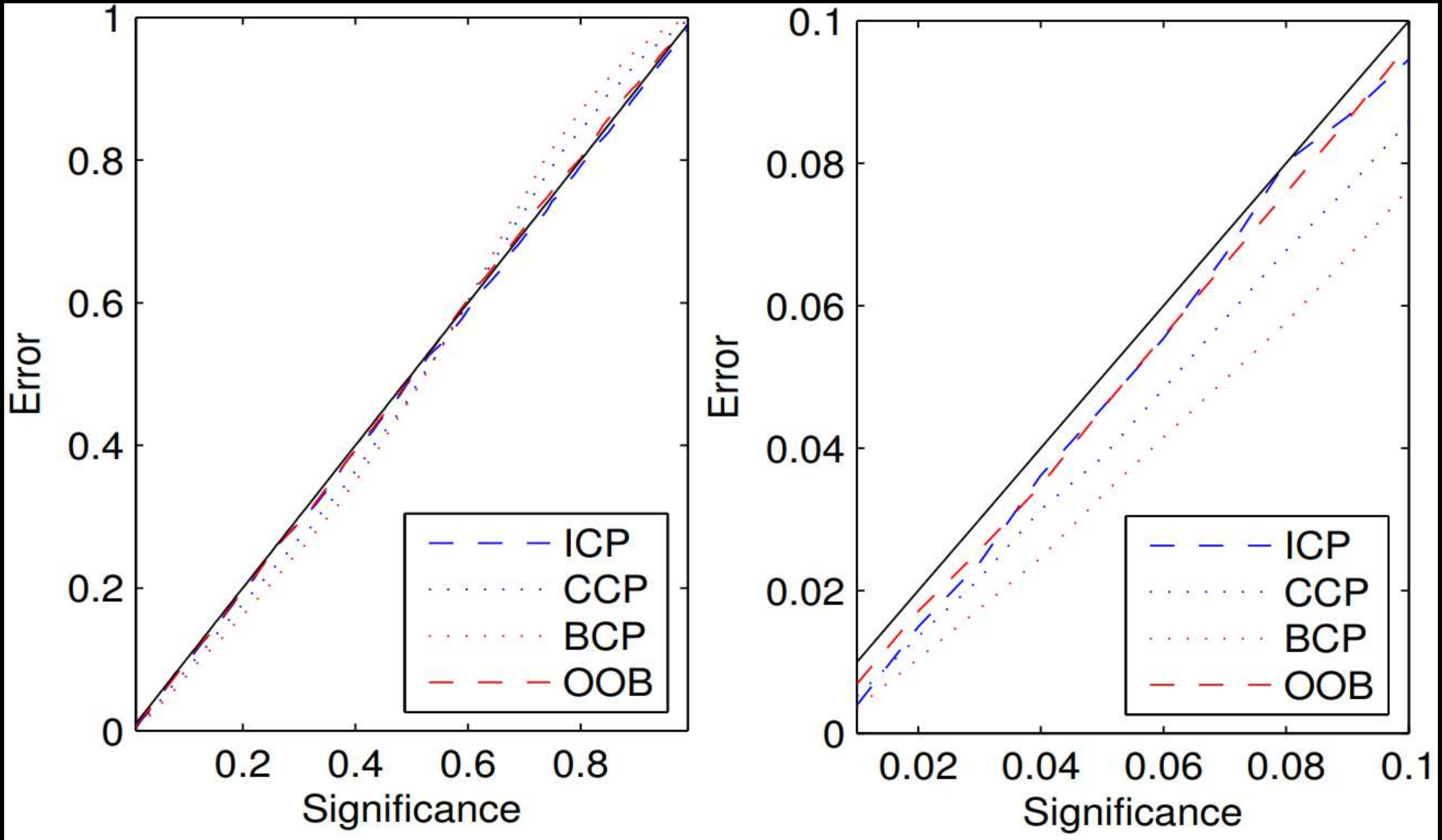


1. Calibration on out-of-bag prediction for training set

✓ Validity is guaranteed

Validity guarantees

Löfström, Tuve, Ulf Johansson, and Henrik Boström. "Effective utilization of data in inductive conformal prediction using ensembles of neural networks." *The 2013 International Joint Conference on Neural Networks (IJCNN)*. IEEE, 2013.



Demo 2: Efficient data usage

https://github.com/marharyta-aleksandrova/conformal-learning/blob/main/tutorials/Demo_2._Efficient_data_usage.ipynb

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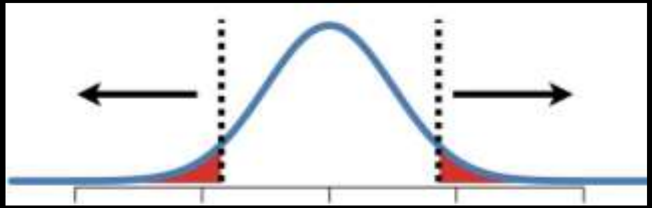
Applications

- Prediction with accuracy guarantees

- Anomaly (outlier) detection

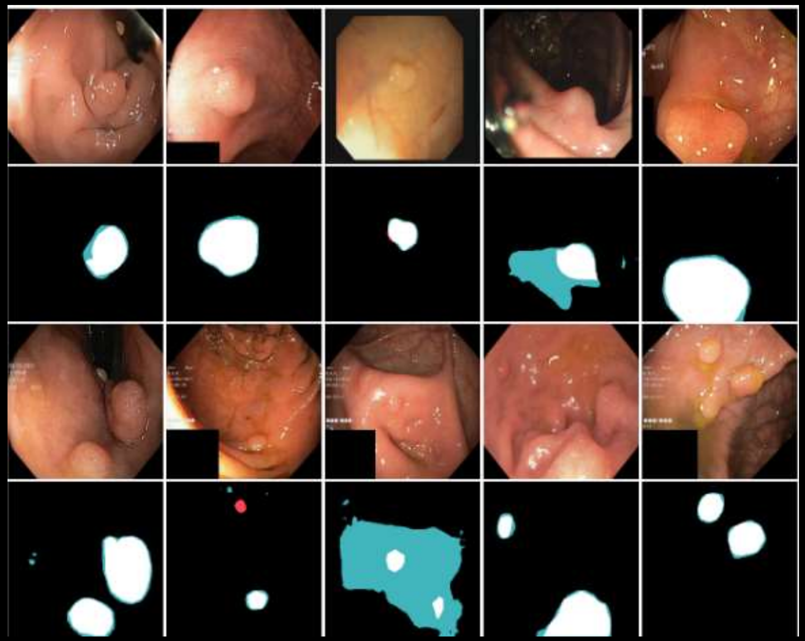


- Statistical tests

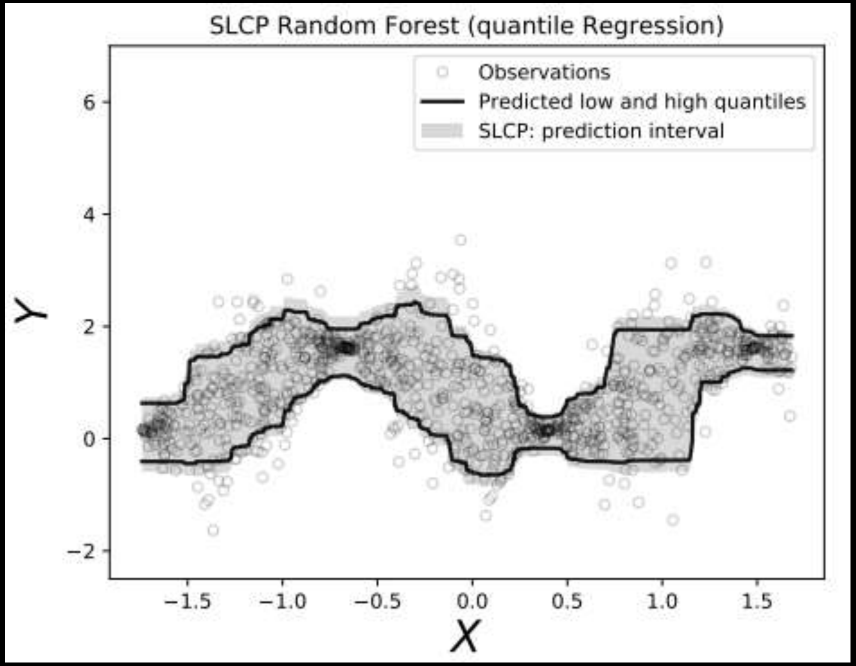
- Causal ML

Generalizations

- Risk controlling prediction sets
  https://github.com/aangelopoulos/rcps
  - Some errors are more expensive than others
  - Can be used for image segmentation



90% of polyp for 90% of images



- Conformalized quantile regression
  Romano, Yaniv, Evan Patterson, and Emmanuel Candes. "Conformalized quantile regression." *Advances in neural information processing systems* 32 (2019).

Resources

- nonconformist library
  https://github.com/donlnz/nonconformist
- Tutorial by Anastasios N. Angelopoulos and Stephen Bates
  https://www.youtube.com/watch?v=nql000Lu_iE
- 2. Vide by Maria Navarro
  https://www.youtube.com/watch?v=r6bhm_A-YcQ&t=9s
- Tutorial by Glenn Shafer and Vladimir Vovk
  https://www.jmlr.org/papers/volume9/shafer08a/shafer08a.pdf
- Conformal learning conference COPA
  https://cml.rhul.ac.uk/copa2021
- Distribution-Free Uncertainty Quantification Workshop at ICML
  https://sites.google.com/berkeley.edu/dfuq21/home?authuser=0
- “Awesome Conformal Prediction” list of resources
  https://github.com/valeman/awesome-conformal-prediction