A Glimpse on Conformal prediction

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Agenda

1. **What is CP?**
   - Coverage guarantee
   - LAC, APS
   - Split, CV+, Jackknife+
2. **Experiment**
   - Data
   - Results
3. **Where to start?**
4. **History of CP**
5. **Marginal vs. Conditional Coverage**
   - Group-balanced CP
   - Class-balanced CP
6. **Conformal Change Point Detection**
   - CTM
   - PERMAD Dataset

Heuristic uncertainty → Conformal prediction → Rigourus uncertainty

point prediction → prediction set
with coverage guarantee

prediction interval
without coverage guarantee → prediction interval
with coverage guarantee

uncalibrated probabilistic distribution → well calibrated probabilistic distribution
(Venn predictors)

Coverage guarantee

$$1-\alpha \quad \leq \quad \mathbb{P}\Big(\mathbf{y}_{test} \in \mathbf{C}(\mathbf{x}_{test})\Big) \quad \leq \quad 1-\alpha+\frac{1}{n+1}$$

- **model agnostic**
- **distribution free**
- **finite sample size**
- **minimal assumptions**
  - (exchangeability)

Exchangeability

- Weaker then iid.

$$(X_1, Y_1), \ldots, (X_i, Y_i), \ldots, (X_n, Y_n), (X_{n+1}, Y_{n+1})$$

swap

$$(X_1, Y_1), \ldots, (X_i, Y_i), \ldots, (X_n, Y_n), (X_{n+1}, Y_{n+1})$$

- After swapping the datasets cannot be distinguished

Full Conformal Prediction

- train one model for each label in the label space

$$\forall y \in \mathcal{Y} \quad (X_1, Y_1), \dots, (X_N, Y_N), (X_{n+1}, y) \longrightarrow f^y$$

$$(X_{n+1}, Y_{true})$$ exchangeable to all other points

Conformity scores

$$s_i^y = S\Big((X_i, Y_i), f^y\Big) \quad \text{,for } i = 1, \dots, n$$

$$s_{n+1}^y = S\Big((X_{n+1}, y), f^y\Big)$$

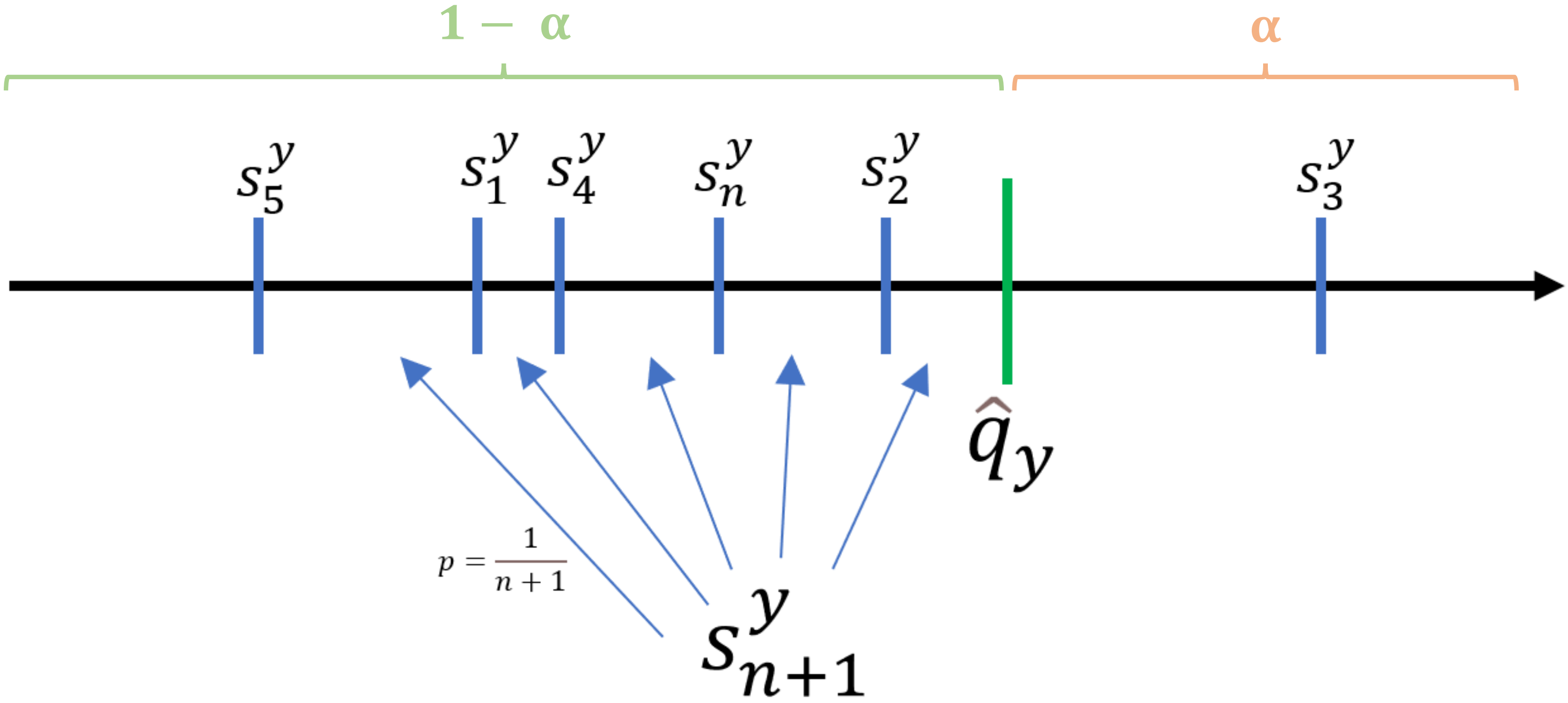
1-alpha quantile

$$\hat{q}^y = \text{Quantile}\left(s_1^y, \dots, s_n^y; \frac{\lceil (1-\alpha)(n+1) \rceil}{n}\right)$$

Prediction set

$$\mathbf{C}(X_{test}) = \left\{ y : s_{n+1}^y \leq \hat{q}^y \right\}$$

1-alpha quantile



Reason: exchangeability of the data

Conformity score

$$s_i = S\Big((X_i, Y_i), \hat{f}\Big)$$

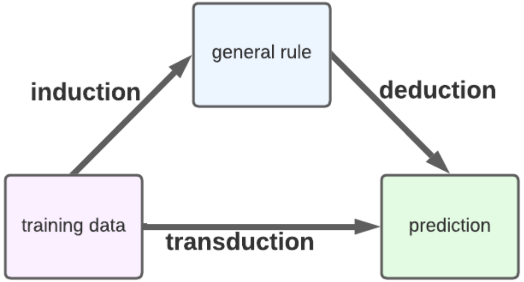
- The higher, the more strange the data point is for the rest of the data
- Can be an arbitrary function
- Coverage guarantee holds for all conformity scores
- BUT! : Informativeness (size of the prediction set) depends on S
- S = Noise function -> Prediction set has size 1-alpha of the label space

Split vs. Full Conformal prediction

Full CP

- transductive
- train one model for each possible label
- start for each prediction from scratch

\+ hight data efficiency
\- high computational effort



Split CP

- inductive
- split data in training
- and calibration set
- only train model once

\- low data efficiency
\+ low computational effort
\+ can be used for pretrained models

Split conformal prediction

Calibration set $$Z_{\text{calib}} = (X_1, Y_1), \ldots, (X_n, Y_n)$$

Conformity score $$s_i = S\Big((X_i, Y_i), \hat{f}\Big)$$

1-alpha Quantile $$\hat{q} := \frac{\lceil (1-\alpha)(n+1) \rceil}{n} \text{ Quantile of: } s_1, \ldots, s_n$$

Prediction set $$\mathbf{C}(X_{test}) = \Big\{ y : s(X_{test}, y) \leq \hat{q} \Big\}$$

[2] Angelopoulos, A. N., & Bates, S. (2021)

Conformal recipe (for split CP)

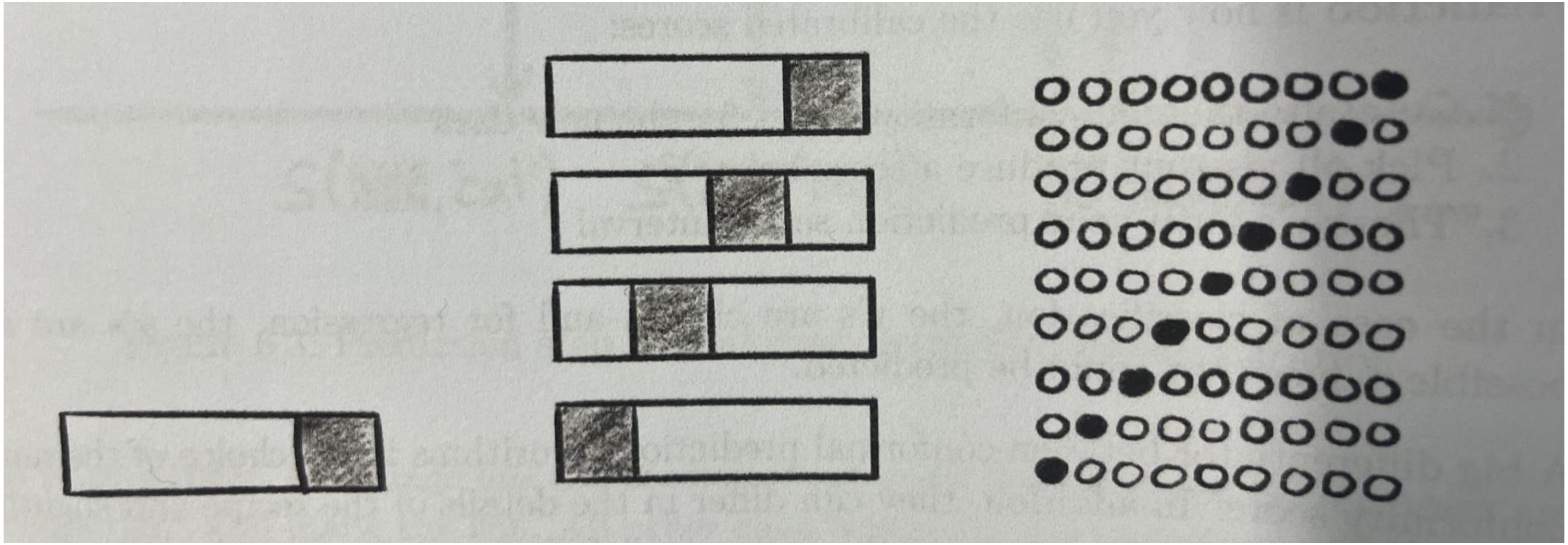
1. Identify a heuristic notion of uncertainty provided by $\hat{f}$
2. Define a score function $S\left(X_i, Y_i; \hat{f}\right)$ based on the heuristic notion of uncertainty.
3. Compute $\hat{q}$ as the $\frac{\lceil(1-\alpha(n+1)\rceil}{n}$ quantile of the calibration scores

$$s_1 = S\left(X_1, Y_1; \hat{f}\right), \ldots, s_n = S\left((X_n, Y_n; \hat{f}\right)$$

4. Calculate the prediction sets for a new data point X_{test} as:

$$\mathbf{C}(X_{test}) = \left\{y : S(X_{test}, y; \hat{f}) \leq \hat{q}\right\}$$

Split, CV+, Jackknife+



Split CV+ Jackknife+

Least Ambiguous set-valued Classifier (lac)

$$s_i = 1 - \hat{f}_{y=y_i}(x_i)$$

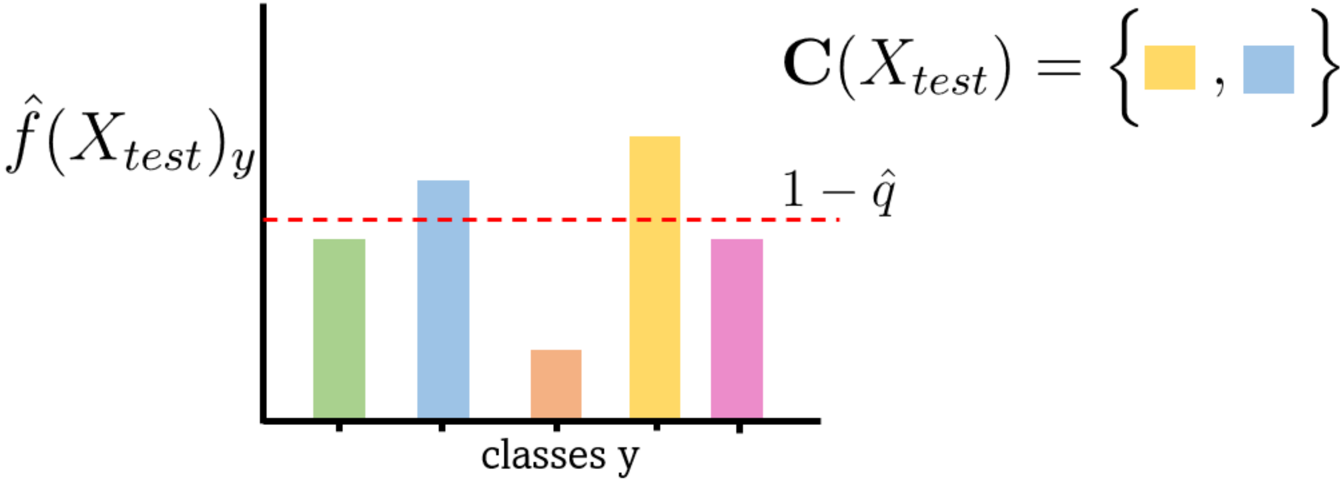
$$\mathbf{C}(X_{test}) = \left\{ y : \hat{f}(X_{test})_y \geq 1 - \hat{q} \right\}$$

- uses only the probability of the true label
- smallest prediction sets (on average)
- lacks adaptivity

[4] Lei, J., & Wasserman, L. (2014)

Least Ambiguous set-valued Classifier (lac)

$$\mathbf{C}(X_{test}) = \left\{ y : \hat{f}(X_{test})_y \geq 1 - \hat{q} \right\}$$



Adaptive prediction scores

$\pi(x)$ Permutation that sorts classes from most to least likely

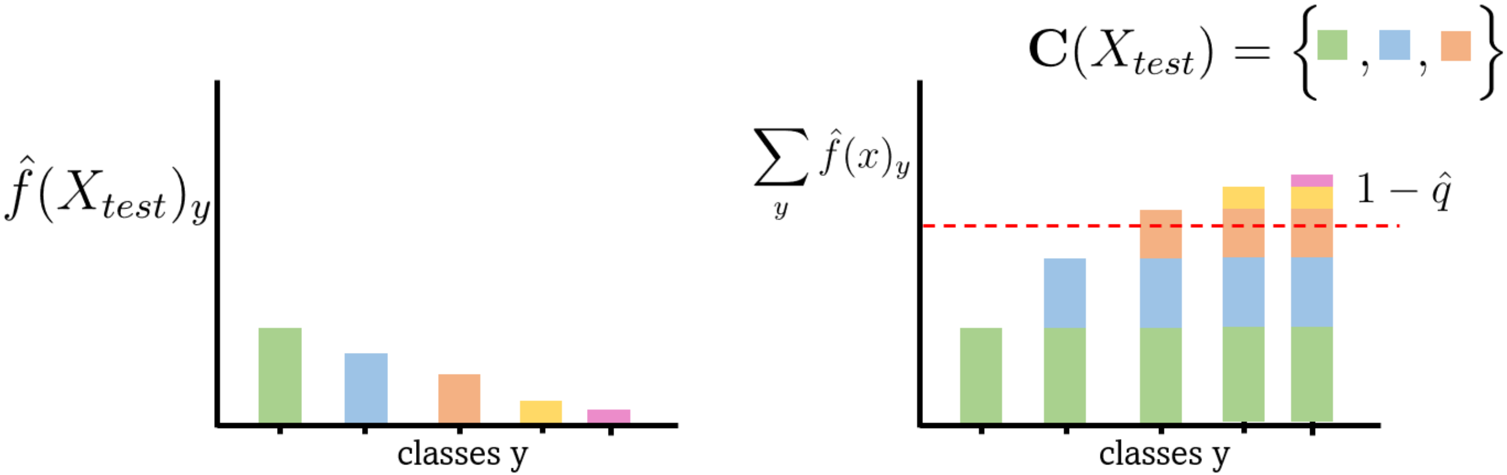
$$s(x, y) = \sum_{j=1}^{c} \hat{f}(x)_{\pi_j(x)} \ , \ \text{where } y = \pi_c(x)$$

- includes the difficulty of a prediction point
- utilizes the scores of all classes, not just the true class
- **more adaptive**

[5] Lei, J. (2014)

Adaptive prediction scores

$$s(x,y)=\sum_{j=1}^{c}\hat{f}(x)_{\pi_j(x)}\ ,\ \text{where } y=\pi_c(x)$$



Adaptive classification with split-conformal calibration (aps)

generalized conditional quantile function for an arbitrary $\tau \in [0,1]$

$$L(x; f, \tau) = \min\{c \in 1, ..., C \ : \ f_{(1)}(x) + f_1(x) + ... + f_c(x) \geq \tau\}$$

$$S(x, u; f, \tau) = \begin{cases} \text{corresponding } y \text{ for the } L(x; f, 1-\alpha) - 1 \text{ largest } f_y(x), & \text{if } u \geq V(x; f, \tau) \\ \text{corresponding } y \text{ for the } L(x; f, 1-\alpha) \text{ largest } f_y(x), & \text{otherwise} \end{cases}$$

$$E(x, y, u; \hat{f}) = \min\{\tau \in [0,1] : y \in S(x, u; f, \tau)\}$$

- works in principle like the other variant
- includes theoretical guarantees and tie-breaking

[3] Romano, Y., Sesia, M., & Candes, E. (2020)

Adaptive classification with split conformal calibration

Algorithm 1 Adaptive classification with split-conformal calibration

1: **Input:** data $\{X_i, Y_i\}_{i=1}^n$, X_{test} , model $\hat{f}$, α
2: X_{train}, $X_{calib} \leftarrow$ train_test_split($\{X_i, Y_i\}_{i=1}^n$)
3: Train $\hat{f}$ on X_{train}
4: Compute $E_i = E(x_i, y_i, u_i; \hat{f})$ for each $x_i, y_i \in X_{calib}$ with function 11
5: Compute $\hat{Q}_{1-\alpha}(\{E_i\}_{i \in X_{calib}})$ as the $\lceil(1-\alpha)(1-|X_{calib}|\rceil$th largest value in E_i
6: **Output** the prediction set:

$$C_{n,\alpha}^{\mathrm{SC}}(x_{test}) = S(x_{test}, u_{test}; \hat{f}, \hat{Q}_{1-\alpha}(\{E_i\}_{i \in X_{calib}}))$$

using the score function S defined in 8.

[3] Romano, Y., Sesia, M., & Candes, E. (2020)

Adaptive classification with CV+

Algorithm 2 Adaptive classification with CV+ calibration

1: **Input:** data $\{X_i, Y_i\}_{i=1}^{n}$, X_{test} , model $\hat{f}$, number of splits $K \leq n$, α
2: Split data into k random distinct subsets $\mathcal{I}_1, \mathcal{I}_2, ..., \mathcal{I}_k$
3: **for** $k \in \{1, ..., k\}$:
4: Train $\hat{f}^{k(i)}$ on $\{X_i, Y_i\}_{i \in \{1,...,n\} \setminus \mathcal{I}_k}$
5: **Output** the prediction set:

$$C_{n,\alpha}^{\mathrm{CV+}}(x_{n+1}) = \Bigg\{ y \in \mathcal{Y} :$$

$$\sum_{n=1}^{n} \mathbf{1}\left[E(x_i, y_i, u_i; \hat{f}^{k(i)}) \leq E(x_{n+1}, y_{n+1}, u_{n+1}; \hat{f}^{k(i)})\right] \leq \lceil (1-\alpha)(1-|n|) \rceil \Bigg\}$$

where $k(i) \in \{1, .., k\}$ denotes the fold containing the ith sample and using the function E defined in 11.

[3] Romano, Y., Sesia, M., & Candes, E. (2020)

Coverage guarantee for CV+

CV+

$$\mathbb{P}\left[Y_{test} \in C_{n,\alpha}^{\mathrm{CV+}}(x_{test})\right] \geq 1 - 2\alpha - \min\left\{\frac{2(1 - 1\backslash K}{n\backslash K + 1}, \frac{1 - K\backslash n}{K + 1}\right\}$$

Jackknife+

Special case of CV+ with k=n

$$\mathbb{P}\left[Y_{test} \in C_{n,\alpha}^{\mathrm{CV+}}(x_{test})\right] \geq 1 - 2\alpha$$

[3] Romano, Y., Sesia, M., & Candes, E. (2020)

Influence of Calibration Set Size

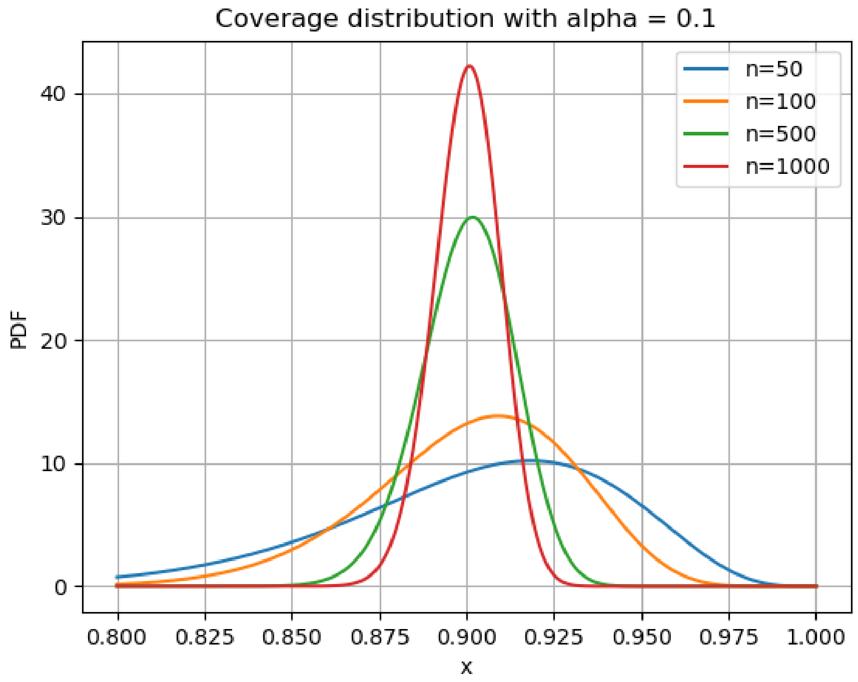
Coverage guarantee holds for coverage of $1 - \alpha$ on **average over the randomness** in the calibration set

ϵ	0.1	0.05	0.01	0.001
$n(\epsilon)$	22	102	9812	244390

Required calibration set size $n(\epsilon)$

for coverage of $1 - 0.9 \pm \epsilon$

with probability $\delta = 0.1$



$$\mathbb{P}\Big(Y_{test} \in C(X_{test}) \mid \{(X_i, Y_i)\}_{i=1}^{y}\Big) \sim Beta(n+1-l, l)\ ,\ l = \lfloor (n+1)\alpha \rfloor$$

[1] Vovk, V. (2012)

Artificial dataset

- 20 features
- 5 classes
- 10.000 datapoints

- 5000 for training/calibration
- (rest) for testing

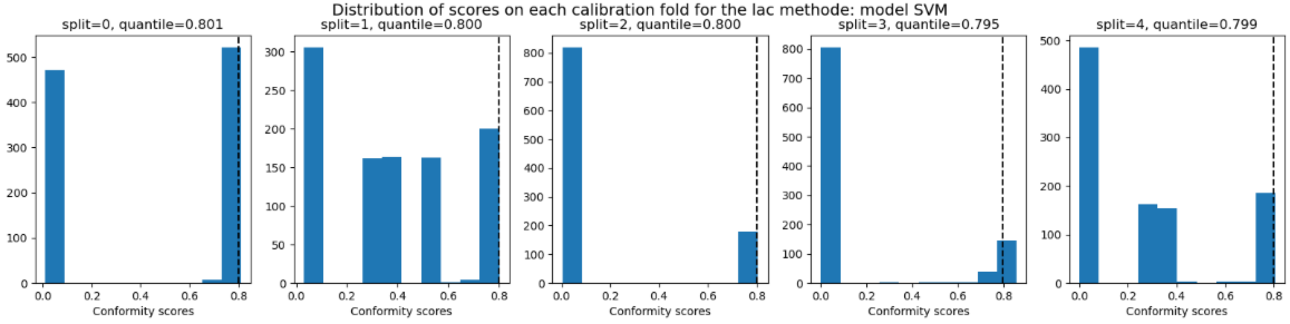
```
def create_artificial_data(n_features, n_classes, sample_size=10000, random_stat=42):
    X, Y = make_classification(
        n_samples=sample_size,
        n_features=n_features,
        n_informative=15,
        n_redundant=2,
        n_repeated=0,
        n_classes=n_classes,
        n_clusters_per_class=1,
        weights=None,
        flip_y=0.001,
        class_sep=1.0,
        hypercube=True,
        shift=0.0,
        scale=2.0,
        shuffle=True,
        random_state=random_stat)
```

Dry Beans dataset

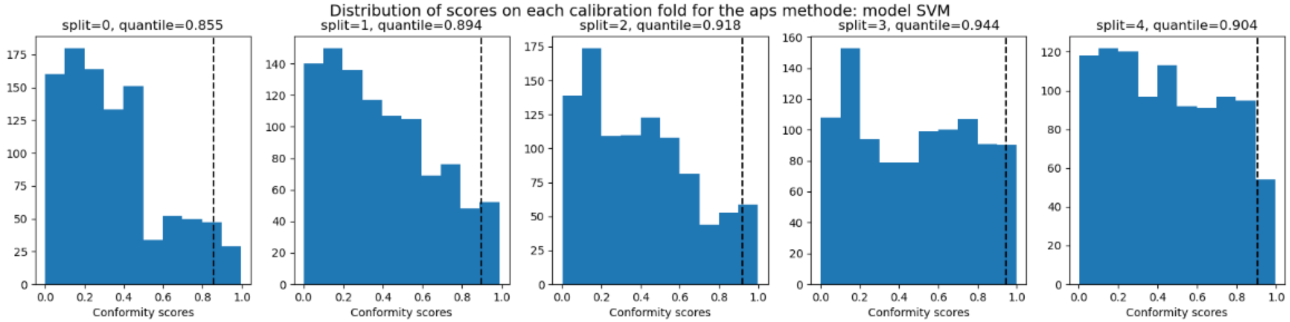
- 13,611 dry beans
- 7 variants (classes)
- 8 features (length, roundness…)

[6] Koklu, M., & Ozkan, I. A. (2020)

Influence of different splits on the conformal scores



(a) least ambiguous set-valued classifier score



(b) adaptive prediction set score

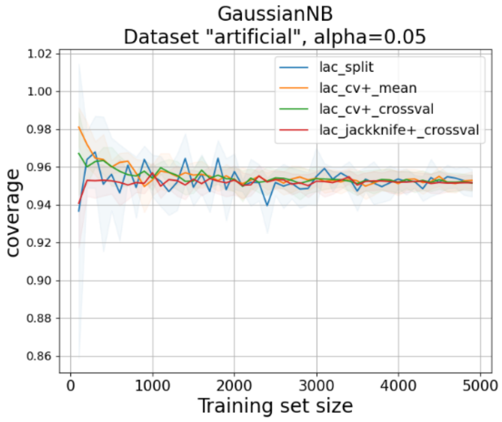
Influence of small datasets on different conformal methods

- **Split** :
  - 20% of the training data as calibration set

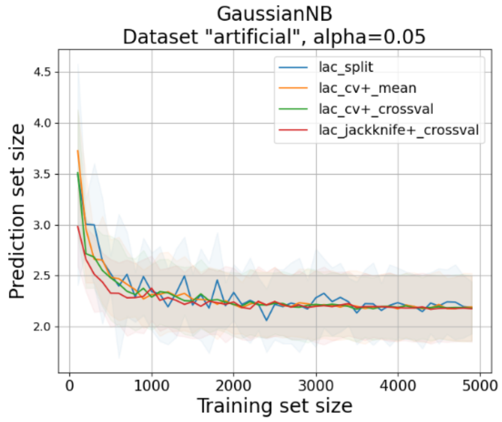
- **CV+** :
  - k=5 splits
  - mean aggregation
  - cross-validation aggregation

- **Jackknife+**
  - like CV+ with k=n

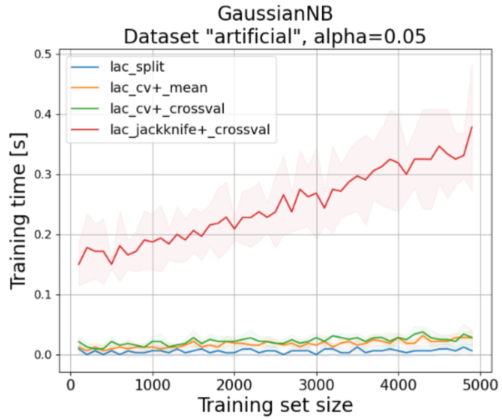
Influence of small datasets on different conformal methods



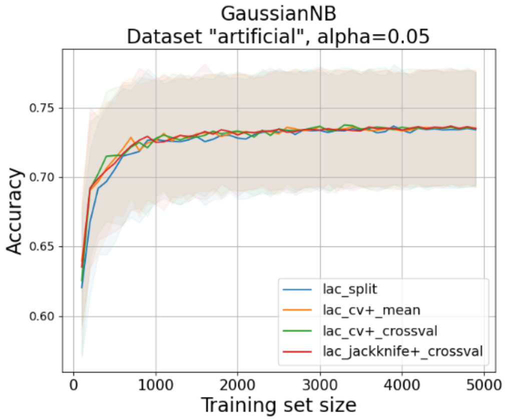
(a) Coverage



(b) Average prediction set size

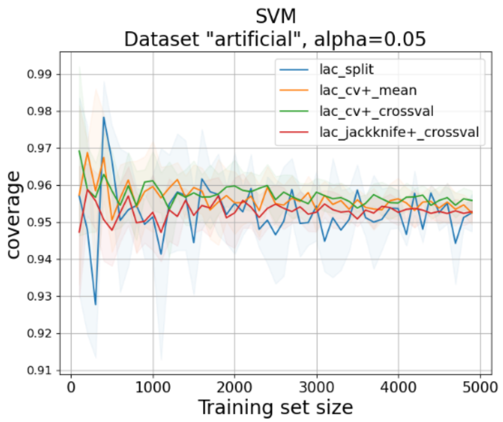


(c) Training time



(d) Accuracy

Influence of small datasets on different conformal methods



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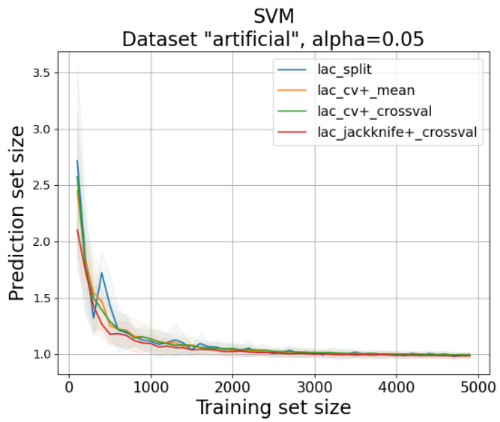
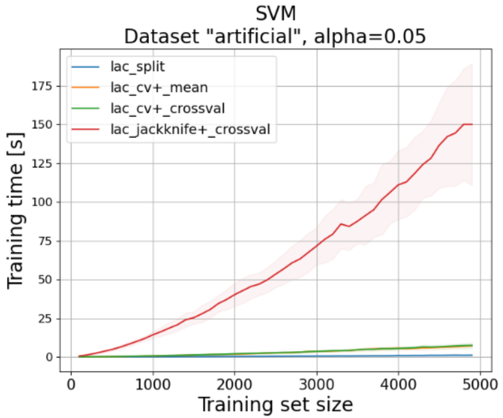


(b) Average prediction set size



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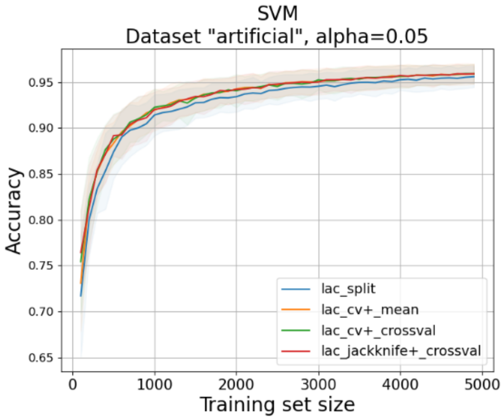

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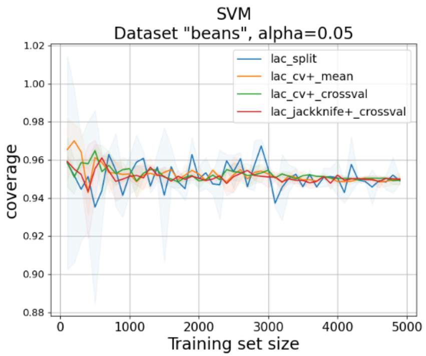

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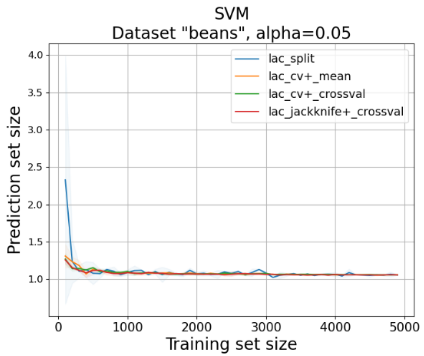
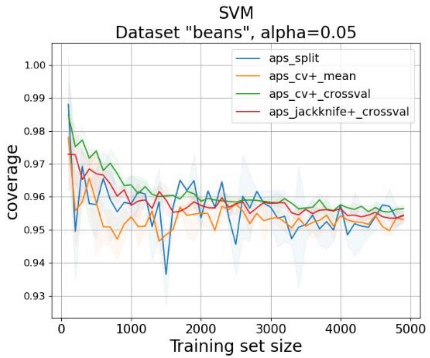


(b) Average prediction set size



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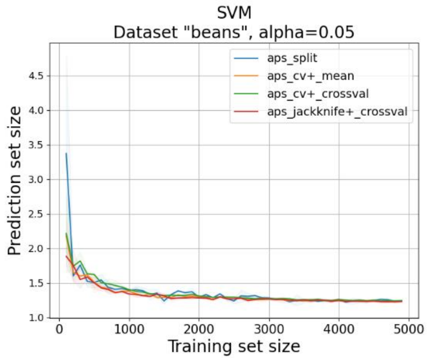
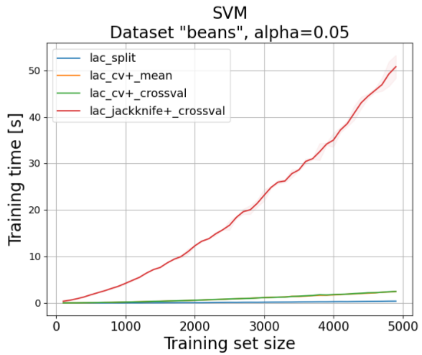


(b) Average prediction set size



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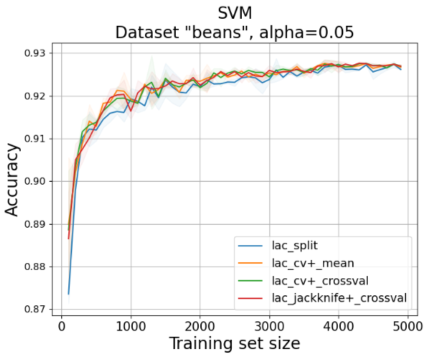
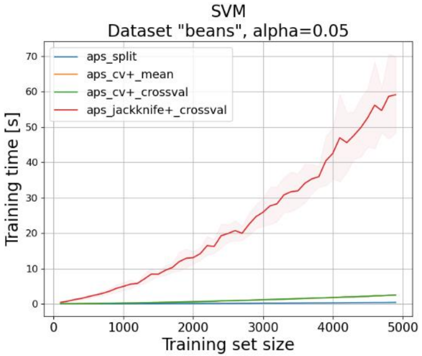


(d) Accuracy



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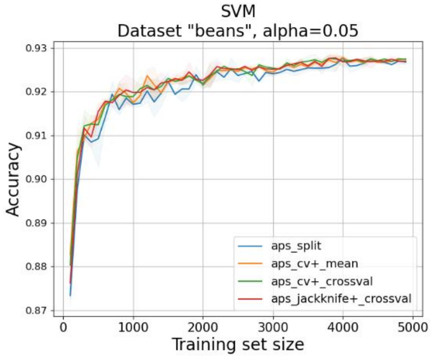
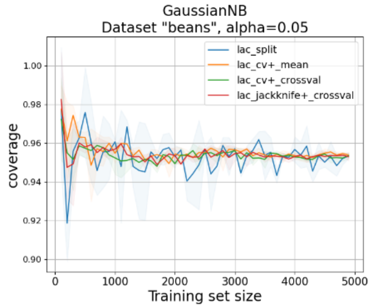


(d) Accuracy

Strange behaviour for aps scores

lac



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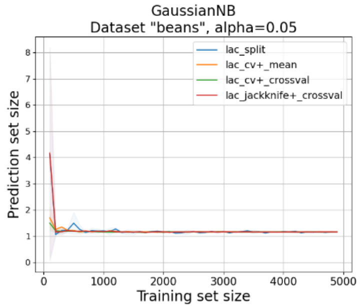
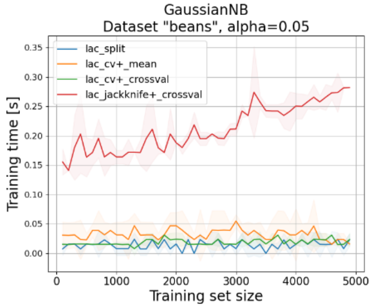


(b) Average prediction set size



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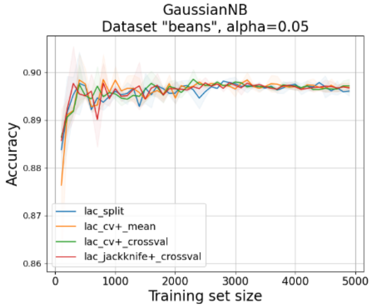
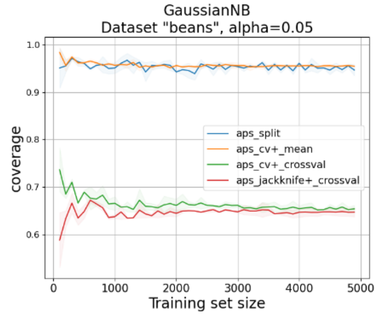


(d) Accuracy

aps



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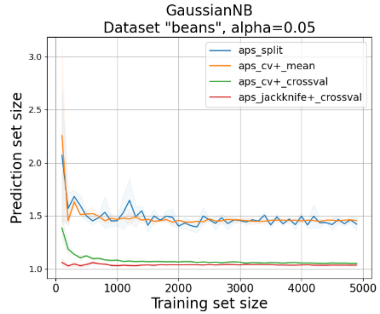
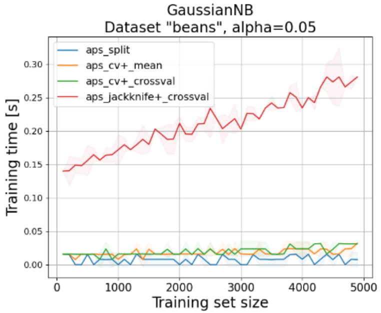
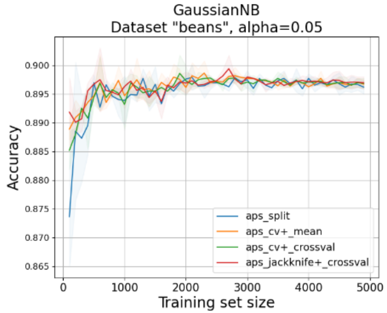


(b) Average prediction set size



(c) Training time



(d) Accuracy

Drawback of Conformal Classifiers

- we must be careful when interpreting conformal classifiers
- make exactly α errors on the long run
- an error is when the correct label is not in the prediction set
- the coverage guarantee only applies apriori, once we have seen a specific prediction, we cannot say that the probability for that prediction to be wrong is α

- Example: two class problem
- Prediction sets containing both classes makes no error
- All errors in singletons
- After observing singleton -> probability of an error is much higher then α

Where to start ?

- **“A gentle introduction to conformal prediction and distribution-free uncertainty quantification”**
  - basic overview and foundations
  - [2] Angelopoulos & Bates
  - video tutorial: Gentle Introduction – Tutorial

- **Awesome Conformal Prediction Git Repo**
  - Valery Manokhin
  - newest stuff
  - Tonnes of papers, tutorials, videos, theses,

- **“Conformal prediction: a unified review of theory and new challenges”**
  - [7] Fontana, Matteo, Gianluca Zeni, and Simone Vantini
  - Contains more the continental approach (after Vovk)

- **Project: A Glimpse on Conformal Prediction**
  - Michel Lutz
  - Conformal-prediction-project-repo

END

Appendix:

- History of CP
- Marginal vs. Conditional Coverage

History of Conformal Prediction - I

1960-1980 Andrei Kolmogorov

- Moscow State University
- randomness, complexity and probability
- algorithmically random sequences, finite Bernulli sequences.
- Vladimir Vovk becomes his

1988 PhD Thesis Vovk

- ‘Predictability of algorithmically random’
- role of finite-sample exchangeability in prediction problems

1996-1999 Vovk, Gammerman, Vapnik

- Royal Holloway University of London
- Develop the Conformal Prediction framework

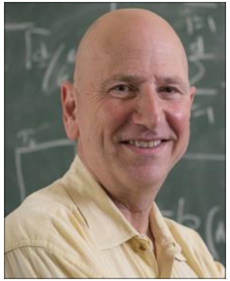
History of Conformal Prediction - III

2014 Sweden

- Ulf Johansson, Henrik Boström & Henrik Linusson
- Jönköping University
- Random forests
- Plenty papers & tutorials
- Venn predictors

2014 Larry Wassermann

- Carnegie Mellon University
- "Ambassadors" for CP in the US
- Class-balanced CP
- Distribution-free predictive inference in regression



2019 Emmanuel Candes

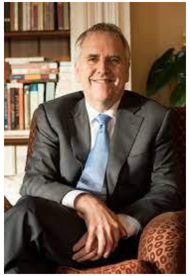
- Stanford University
- Conformalized Quantile Regression
- Plenty papers and fundamental work

History of Conformal Prediction - IV

2020 Adaptive prediction sets
- Romano et al. (Candes group)

2020 Washington Post
- Used CP method to for the U.S. presidential election
- Candes

2021 Michael Jordan
- Anastasios N. Angelopoulos and Stephen Bates
- UC Berkeley
- Large Scale deep learning CP



2021 Conformal Risk Control
- Angelopoulos & Bates

2021 Conformal Outlier Detection
- Bates

History of Conformal Prediction - V

2021 Change point detection
- Vovk

2021 Trak at ICML2021&2022
- Emmanuel Candes

2022 NeurIPS2022
- Emmanuel Candes

2021 Awesome Conformal Prediction
- Git Repo
- Valery Manokhin (PhD Student Vovk)

2022 MAPIE
- Scikit-learn compatible package

2022 CP Beyond Exchangeability
- Candes, Ryan Tibshirani

Marginal vs. conditional coverage

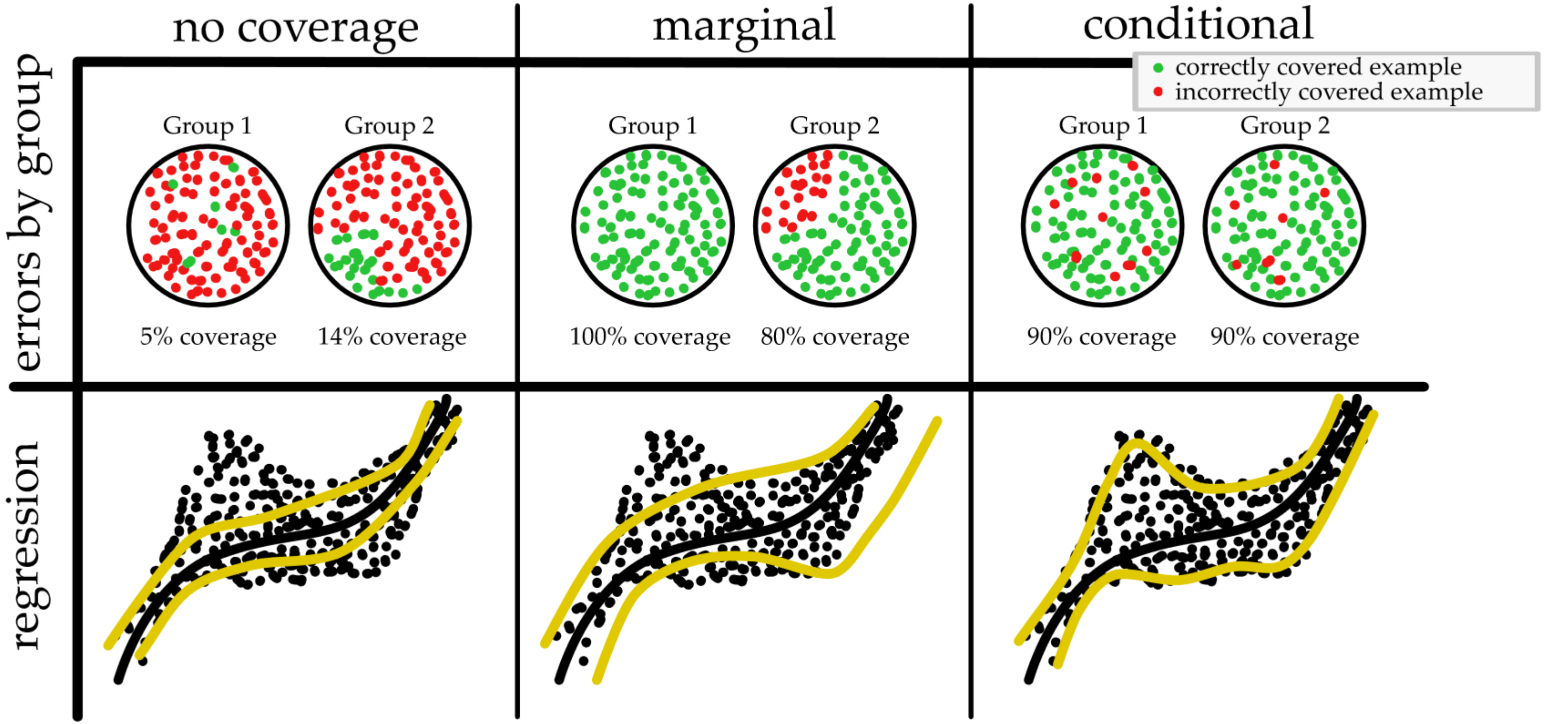
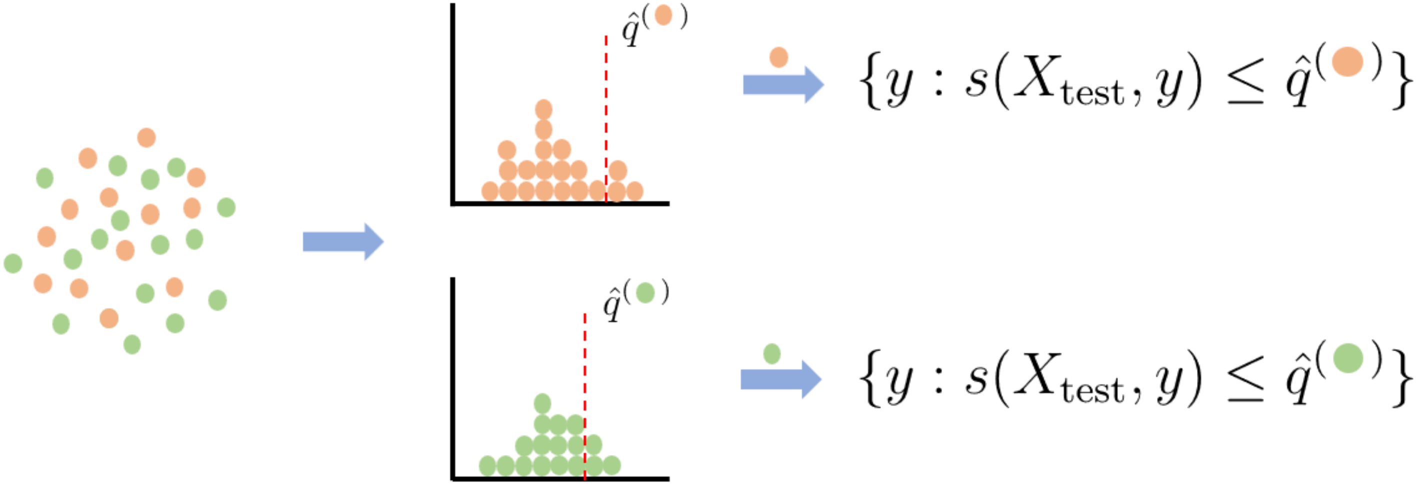


Figure taken from: [2] Angelopoulos, A. N., & Bates

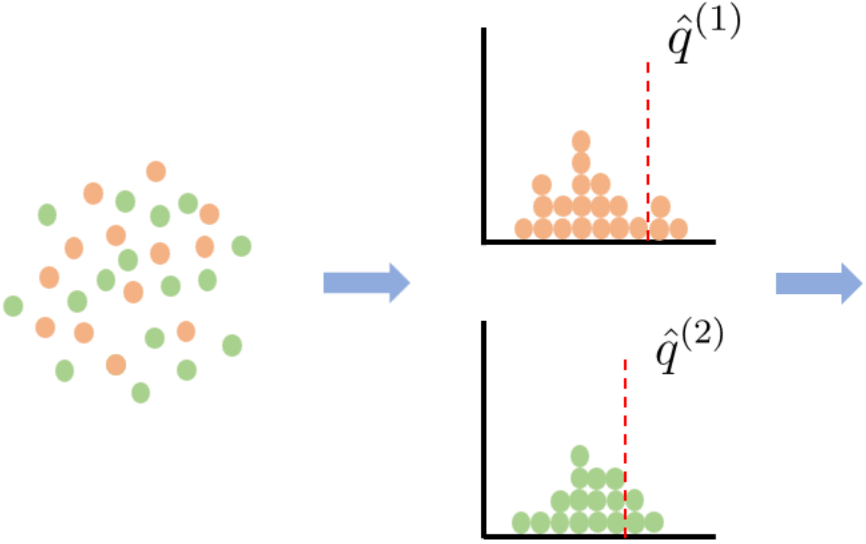
Group-balanced conditional coverage

$$1 - \alpha \leq \mathbb{P}\Big(\mathbf{y}_{test} \in \mathbf{C}(\mathbf{X}_{test}) \mid X_{test} = g_i\Big) \ : \ \forall g \in G$$



Class-balanced conditional coverage

$$1 - \alpha \quad \leq \quad \mathbb{P}\Big(\mathbf{y}_{test} \in \mathbf{C}(\mathbf{X}_{test}) \mid Y_{test} = y\Big)$$



$$\{y : s(X_{\text{test}}, y) \leq \hat{q}^{(\text{y})}\}$$

Additional Experiments – very small datasets

- smallest possible calibration-set size for conformal methods

$$\max(\frac{1}{1-\alpha}, \frac{1}{\alpha})$$

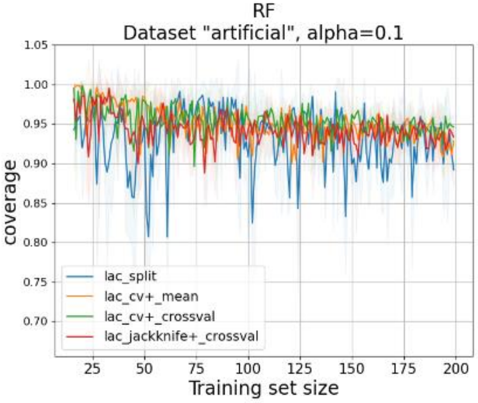
  - necessary for determine the 1-alpha quantile

- smallest training set size $|\mathcal{Y}|$

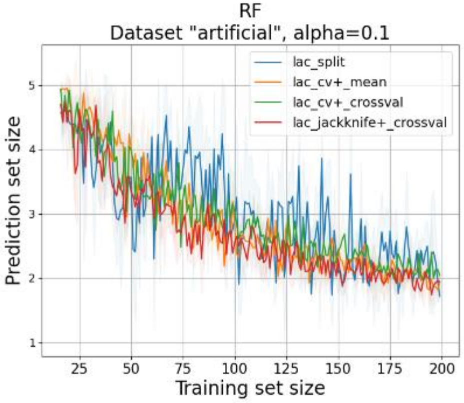
- for 5 classes and alpha=0.1

$$n \geq \frac{1}{1-\alpha} + 1 + |\mathcal{Y}| = 16$$

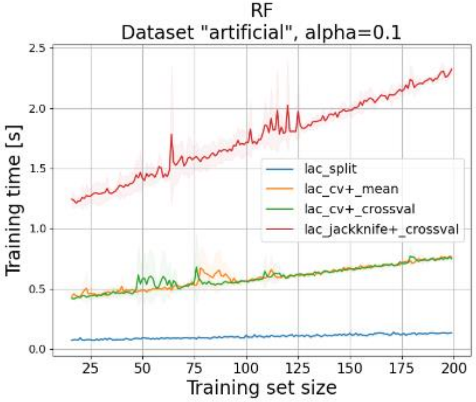
Additional Experiments – very small datasets



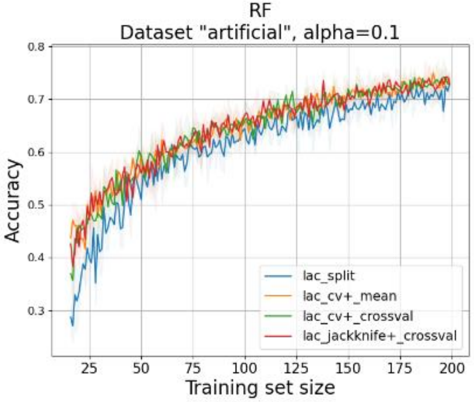
(a) Coverage



(b) Average prediction set size

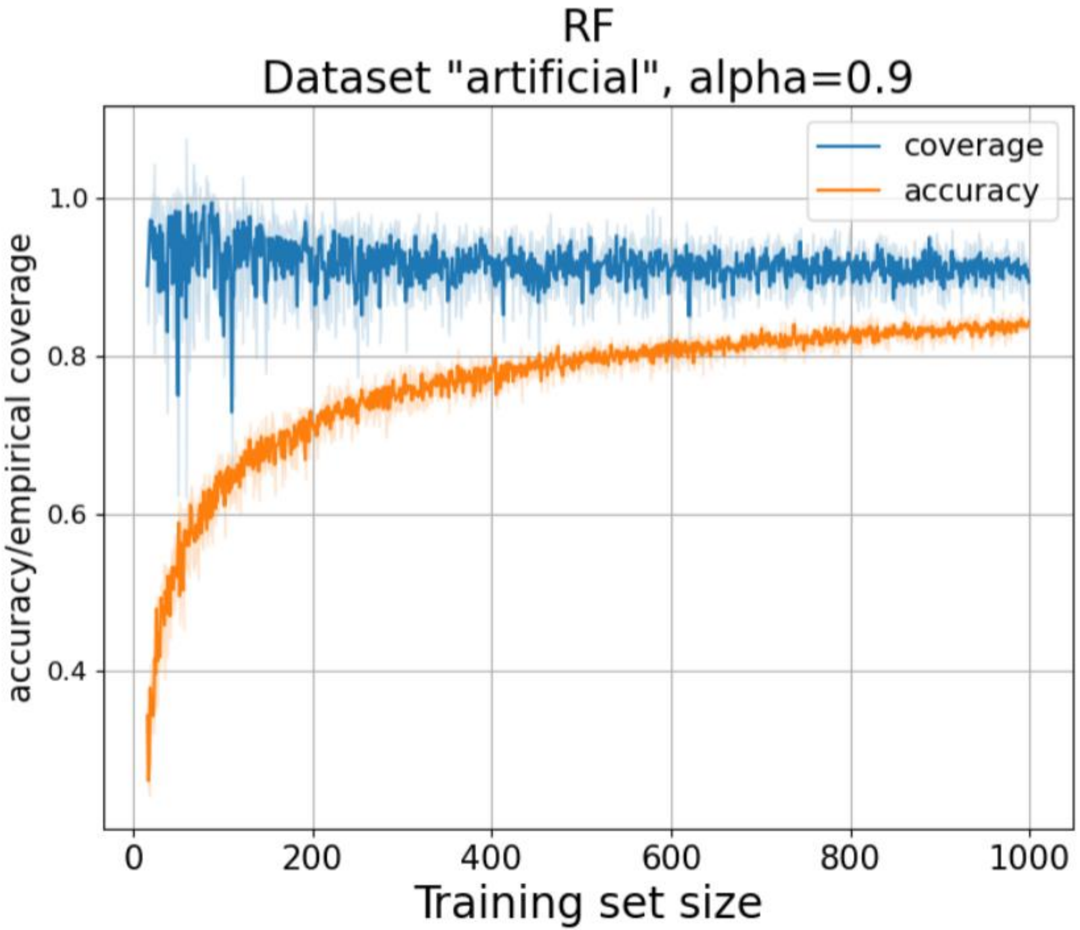


(c) Training time



(d) Accuracy

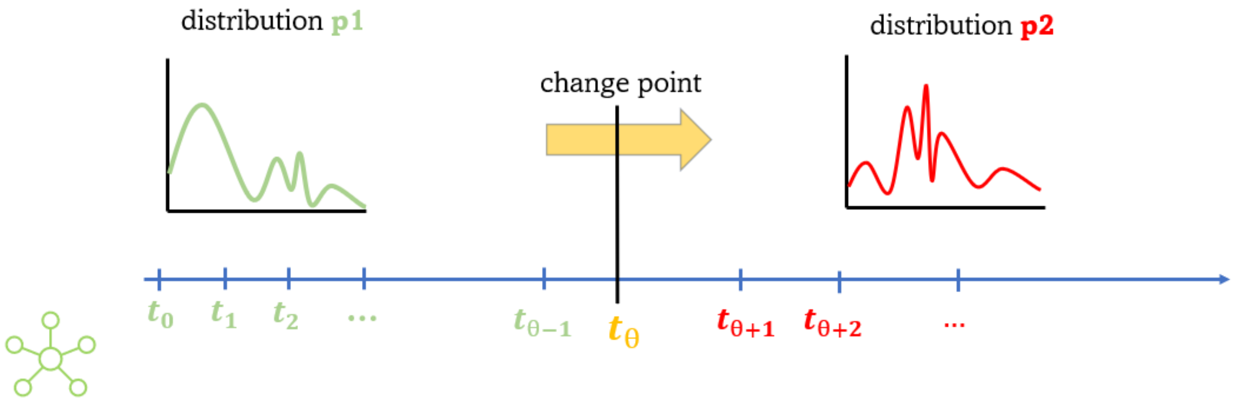
Additional Experiments – direct comparison acc and cov



Conformal Change Point Detection

- Based on Vovks Paper:
  - Retrain or not retrain: conformal test martingales for change-point detection [8] (2021)

Scenario:



t_0 : train model on **p1**

$t_1 - t_{...}$: online evaluation

- calculate CTM M_i at each timepoint

Changepoint detected if:

- M_i > threshold

Conformal Test Martingales CTM

- data sequence: $$(z_1, z_2, \ldots, z_{n+1})$$
- conformity measure: $$s_i = S(z_i)$$
- p-values: $$p_{n+1} = \frac{|\{i|s_i > s_{n+1}\}| + \theta_{n+1}|\{i|s_i = s_{n+1}\}|}{n}$$
- CTM: $$M_{n+1} = F(p_1, p_2, \ldots, p_{n+1})$$

F is a betting martingale function

Betting Martingale

- for all sequences: $p_1, p_2, ..., p_n \ , \ \in [0,1]^n$

$$\int_0^1 F(p_1, ..., p_n, p_{n+1}) du = F(p_1, ..., p_n)$$

- therefore, the following property holds:

$$\mathbb{E}(M_n | S_1, ..., S_{n+1}) = S_{n-1}$$

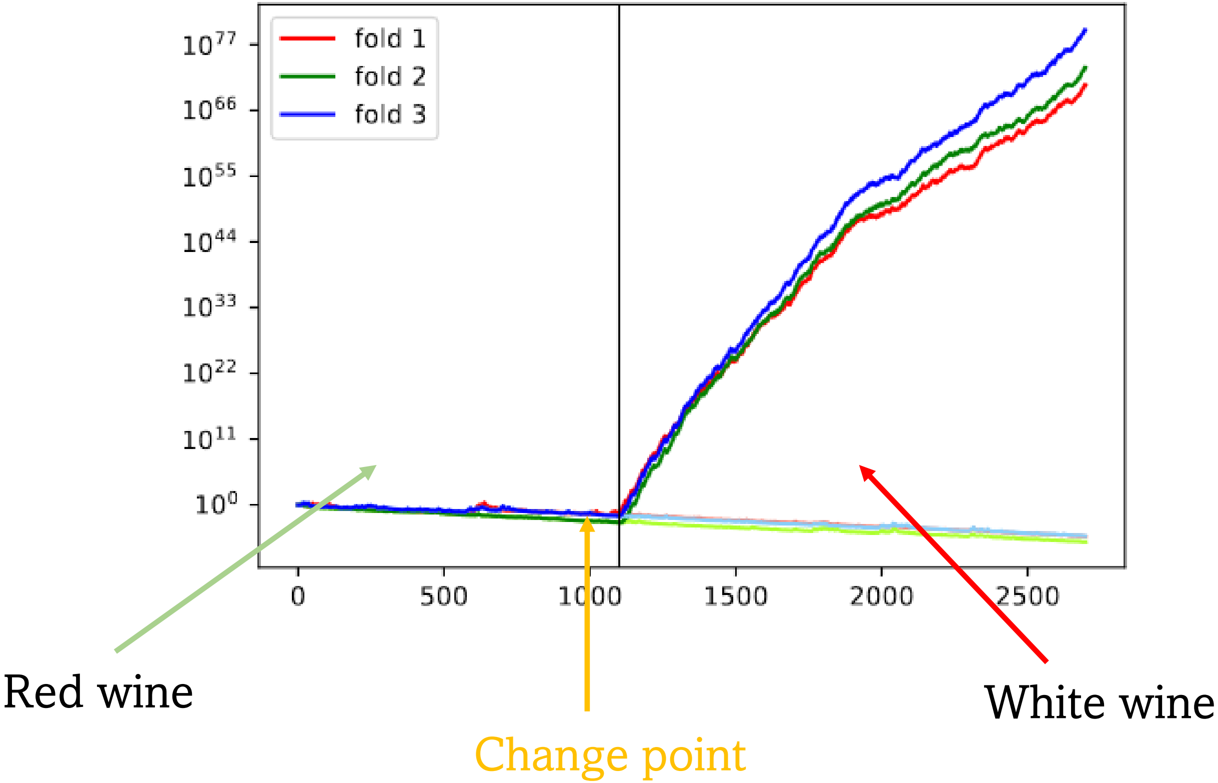
CTM: betting martingale function – Simple Jumper

$$F(p_1, p_2, ..., p_{n+1}) = \int \prod_{i=1}^{n} f_{\epsilon_i}(p_i)\mu(d(\epsilon_1, \epsilon_2, ...))$$

with

$$f_{\epsilon_i}(p) = 1 + \epsilon(p - 0.5)$$

CTM: Vovks results



CTM - properties

- under iid. p-values are uniformly distributed in [0,1]

- Simple Jumper martingales fulfil Ville's inequality:

$$P(\exists i : M_i \geq c) \leq \frac{1}{c}$$

- M_i are equal under iid.
- CTM are equal under iid.
    - **M_i > c with false alarm rate of alpha = 1/c if iid. violated**

CTM: Vovks results

- CTM controls the false alarm rate
  - controlling c

- not as efficient as other methods (CUMSUM, Shiryaev-Roberts procedure)

- Empirically detect change point for clear changepoint and clear to separate distributions after 20-30 datapoints

- best conformity measure function: $$s_i = y_i - \hat{y}_i$$

  - Even better then L1-Norm
  - Possible because real label is available in online setting

PERMAD Dataset

- 41 oncological patients
- total 647 measurements
- different number of measurements per patient (min: 4, max: 46)
- time distributed irregularly and different for each patient
- 91 Features

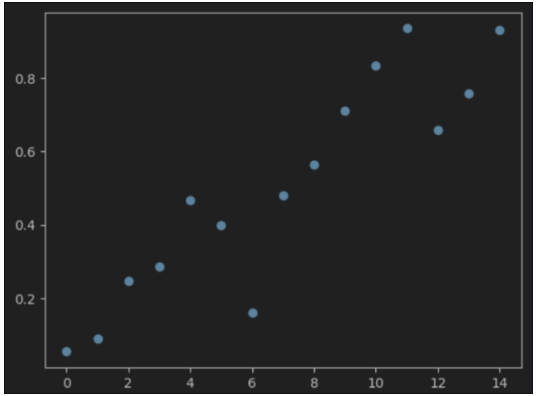
- CT scans at irregular intervals
- progression / non-progression

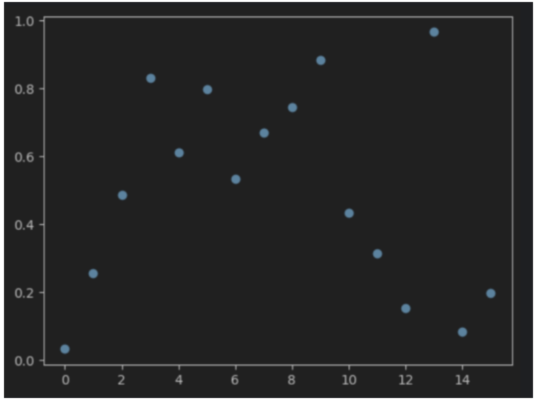
- Task: predict the change-point, from non-progression to progression

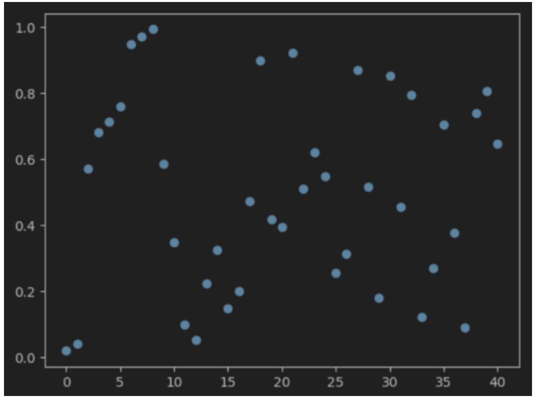
PERMAD Dataset - Idea

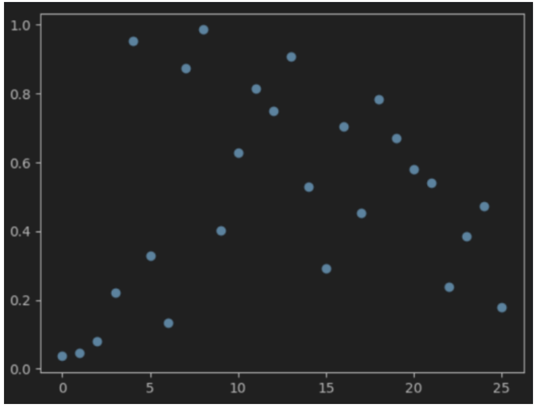
- No ground truth
  - Learn an unsupervised representation of "non-progression" and "progression"
- What is p1 , what p2
  - Solution: fist datapoint of each patient is "non-progression" , last progression
- Model: Autoencoder
- Training: Two AE one in the first one on the last datapoints of all patients
- Non-conformity measure
  - difference between t_0 and t_i (reconstructions / embeddings)
  - use both AEs alone and in combination
  - diff, L1, L2, cross-entropy
- Calculate CTM as search for a method that shows a changepoint

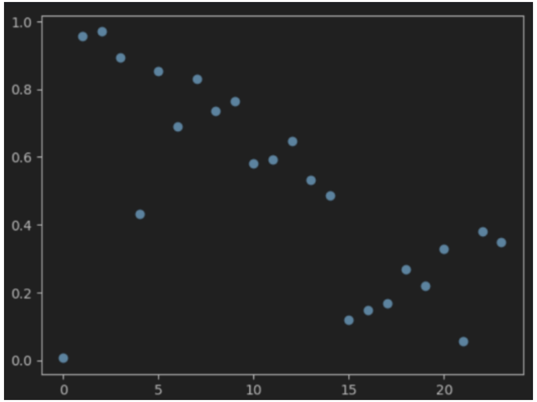
PERMAD Dataset – Results (L1 – embeddings)

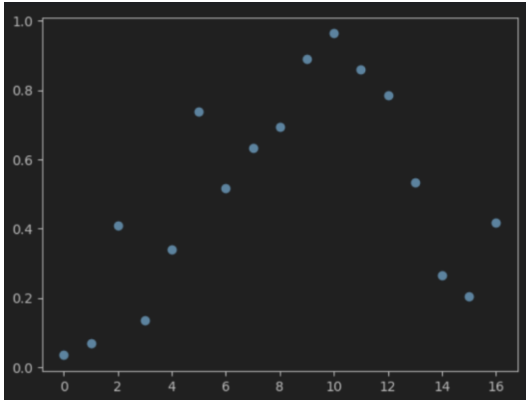




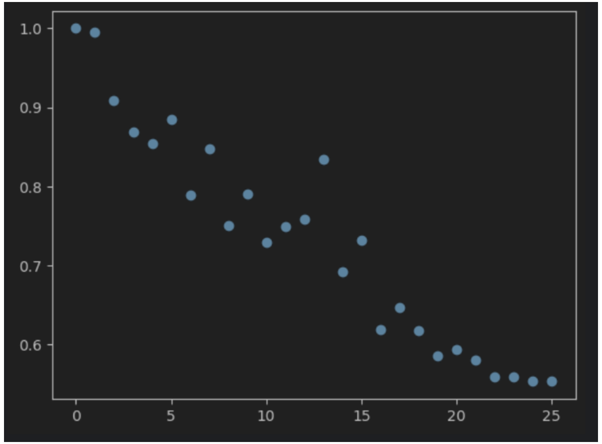


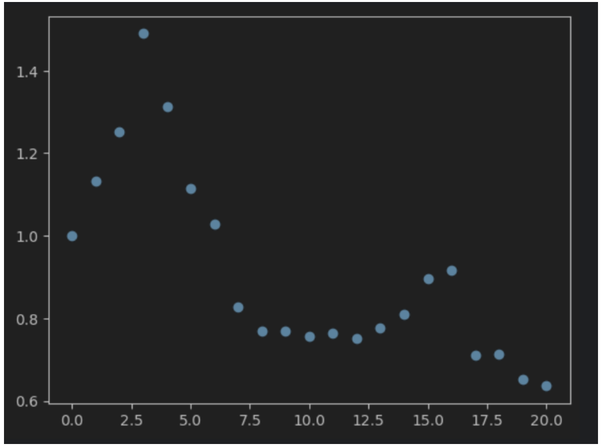


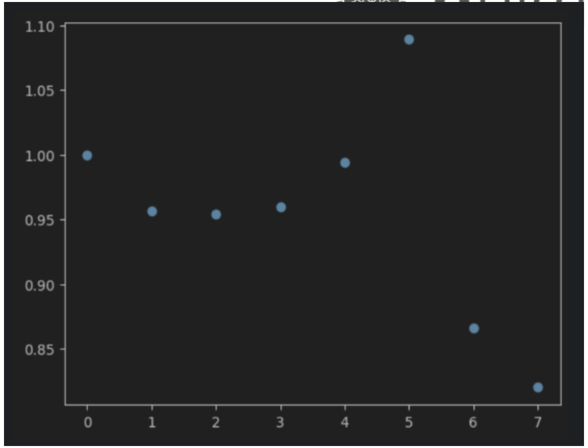


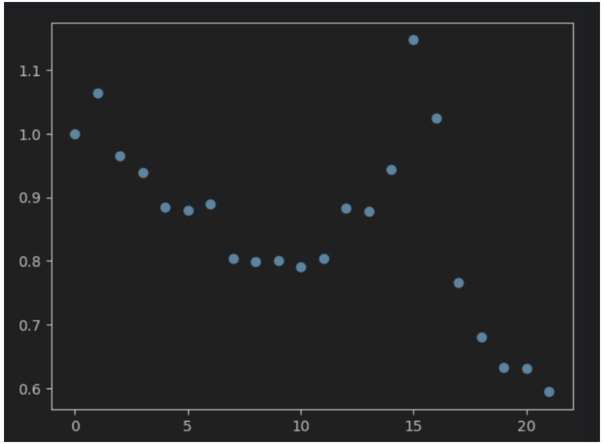


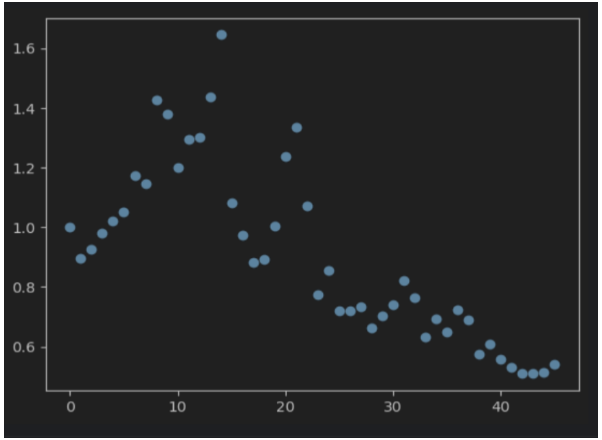
PERMAD Dataset – Results (L2 – embeddings)

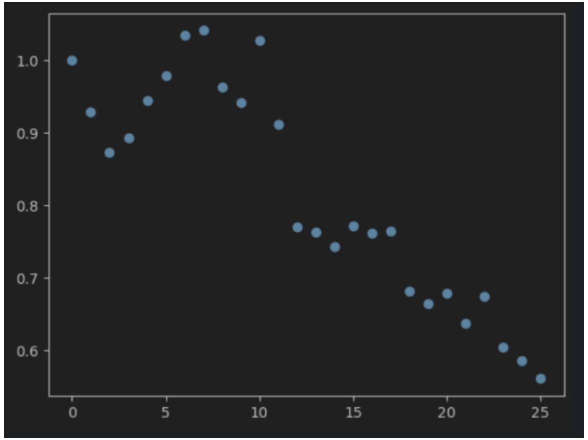




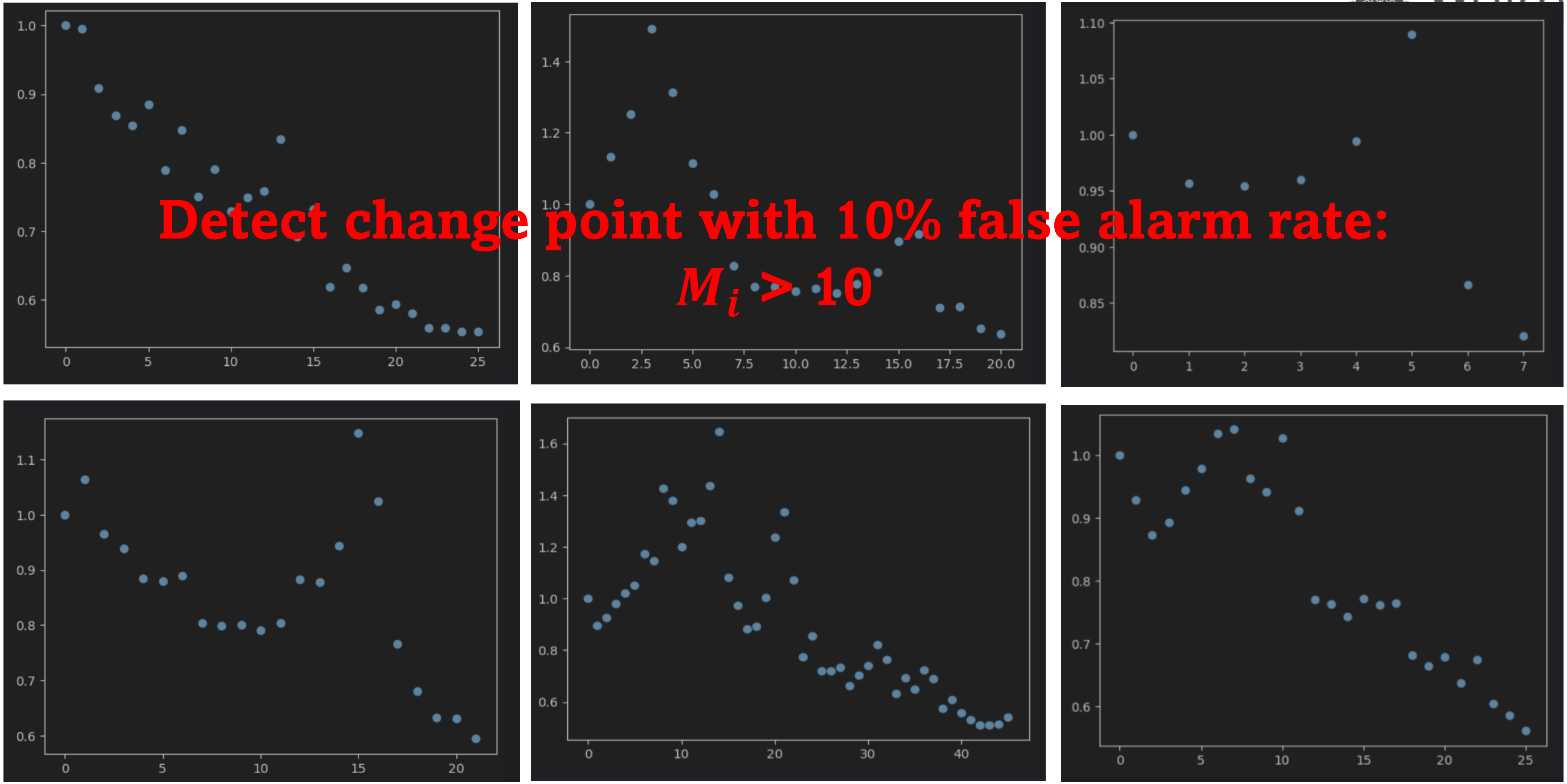








PERMAD Dataset - Results



Detect change point with 10% false alarm rate:

$$M_i > 10$$

PERMAD Dataset - Problems

- CTM and the given task does not match
- No ground truth / no supervised task
- CTM is not efficient (requires in bast case scenarios >20 datapoints of the other distribution)

- Questionable if "non-progression" / "progression" distribution exists ?
- Are intersubject differences bigger then "progression"/ "non-progression"?
- Maybe more than one change point?
  - available features reflect more than just the oncological status
  - Subject: can become sick, co-medication, …
  - smooth transition, not an abrupt change

Quellen

[1] Vovk, V. (2012). Conditional validity of inductive conformal predictors. In Asian conference on machine learning, Vol. -, pp. 475–490. PMLR.

[2] Angelopoulos, A. N., & Bates, S. (2021). A gentle introduction to conformal prediction and distribution-free uncertainty quantification. arXiv preprint arXiv:2107.07511

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[4] Lei, J., & Wasserman, L. (2014). Distribution-free prediction bands for non-parametric regression. Journal of the Royal Statistical Society Series B: Statistical Methodology, 76 (1), 71–96.

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[6] Koklu, M., & Ozkan, I. A. (2020). Multiclass classification of dry beans using computer vision and machine learning techniques. Computers and Electronics in Agriculture, 174, 105507.

[7] Fontana, Matteo, Gianluca Zeni, and Simone Vantini. "Conformal prediction: a unified review of theory and new challenges." Bernoulli 29.1 (2023): 1-23.

[8] Vovk, V., Petej, I., Nouretdinov, I., Ahlberg, E., Carlsson, L., & Gammerman, A. (2021). Retrain or not retrain: Conformal test martingales for change-point detection. In Conformal and Probabilistic Prediction and Applications, pp. 191–210. PMLR.