Statistical Learning: Anytime Valid Conformal prediction

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Introduction and Motivation

- Continuation of previous semester's work on conformal prediction
- Focus on advanced methods for uncertainty quantification
- Conformal prediction produces prediction sets with guaranteed coverage probability
- Classical approach: conformal predictors based on p-values
- This work explores an alternative: conformal e-prediction (using e-values)

Introduction and Motivation

- Limitations of p-values:
  - Susceptible to misuse (e.g., p-hacking)
  - Selective reporting and inflated Type I error
  - Dependence on fixed sampling schemes
- Advantages of e-values:
  - Valid under flexible or unknown sampling schemes
  - Allow data-dependent (post-hoc) choice of significance level
  - Can be combined across experiments (via multiplication)
  - Remain valid under sequential data collection (anytime validity)
- Key idea:
  - E-values can be constructed as supermartingales
  - Useful for adaptive procedures, online learning, and sequential experiments

Definitions

We begin with a sample space Ω equipped with a σ-algebra $\mathcal{F}$, and the set $\mathcal{M}$ of all probability measures on $(\Omega, \mathcal{F})$, whose elements are the distributions.

We assume that our data $X = (X_1, \dots, X_n)$ are described by some distribution $P_0 \in \mathcal{M}$.

Definition

An *e-variable* E for $\mathcal{P}$ is a $[0, \infty]$-valued random variable satisfying

$$\mathbb{E}_P[E] \leq 1 \quad \text{for all } P \in \mathcal{P}.$$

An e-variable E is *exact* if

$$\mathbb{E}_P[E] = 1 \quad \text{for all } P \in \mathcal{P}.$$

Definition

A *p-variable* P for $\mathcal{P}$ is a $[0, \infty)$-valued random variable satisfying

$$P(P \leq \alpha) \leq \alpha \quad \text{for all } \alpha \in (0, 1) \text{ and all } P \in \mathcal{P}.$$

A p-variable P is *exact* if

$$P(P \leq \alpha) = \alpha \quad \text{for all } \alpha \in (0, 1) \text{ and all } P \in \mathcal{P}.$$

E-values and P-values

E-variables and p-variables are random variables, while e-values and p-values refer to their realized values after observing the data.

[Markov's inequality for e-values] Let E be an e-variable for $\mathcal{P}$. Then

$$P\left(E \geq \frac{1}{\alpha}\right) \leq \alpha \quad \text{for all } P \in \mathcal{P} \text{ and } \alpha \in (0,1]. \tag{1}$$

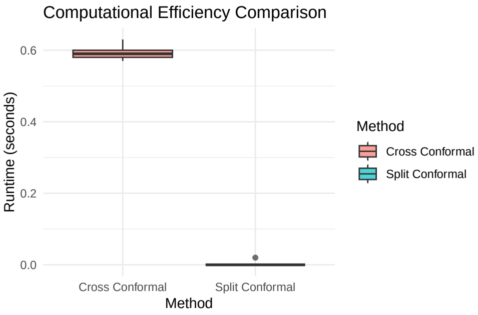
Hence, $1/E$ is a p-variable, $(\alpha E) \wedge 1$ is a level-α test, and $1_{\{E \geq 1/\alpha\}}$ is a level-α binary test. This allows for the construction of conformal sets. Conformal e-prediction refers to conformal prediction methods based on e-variables.

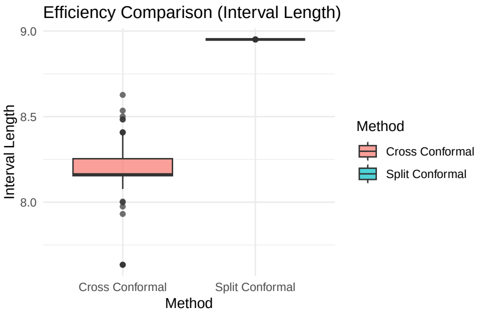
Conformal e-Prediction Setup

- Training data: $z_i = (x_i, y_i)$ for $i = 1, \dots, n$
- Goal: predict label y for a new object x
- Assign a score function:
  - $f(z_1, \dots, z_n, x, y)$ measures plausibility of label y
- Data space:
  - Objects: $\mathcal{X}$, labels: $\mathcal{Y}$
  - Observations: $\mathcal{Z} = \mathcal{X} \times \mathcal{Y}$
- Nonconformity *e*-measure:
  - Maps sequences $(z_1, \dots, z_m)$ to scores $(\alpha_1, \dots, \alpha_m)$
  - Permutation invariant
  - Average constraint: $\frac{1}{m} \sum_{i=1}^{m} \alpha_i \leq 1$
- Conformal *e*-predictor:
  - $f(z_1, \dots, z_n, x, y) = \alpha_{n+1}$
  - Gives a score for each possible label

Split and Cross Conformal e-Prediction

- Key components:
  - Summary space Σ
  - Nonconformity map: $A : \mathcal{Z}^+ \to \Sigma$
  - Normalization: $N : \Sigma^+ \to [0, \infty)^+$ (ensures average ≤ 1)
- Split conformal:
  - Split data into training and calibration sets
  - Compute summaries for calibration and test candidate
  - Normalize to obtain conformal e-values α_y
  - Predictor: $f(z_1, \ldots, z_n, x, y) = \alpha_y$
  - Computationally efficient under suitable A and N
- Cross-conformal:
  - Split data into K folds
  - Train/calibrate across all folds
  - Average fold-wise e-values
  - Improves predictive efficiency compared to split method


Computational Efficiency Comparison
Runtime (seconds)
0.6
0.4
0.2
0.0
Cross Conformal
Split Conformal
Method
Method
Cross Conformal
Split Conformal


Efficiency Comparison (Interval Length)
Interval Length
9.0
8.5
8.0
Cross Conformal
Split Conformal
Method
Method
Cross Conformal
Split Conformal

Batch Anytime-Valid Conformal Prediction

- Data arrive sequentially in batches with possible distribution shifts.
- Goal: construct prediction sets $\hat{C}_t$ with global guarantee

$$\mathbb{P}\left(\forall t \geq 1,\ S_{t,n_t+1} \in \hat{C}_t\right) \geq 1 - \alpha.$$

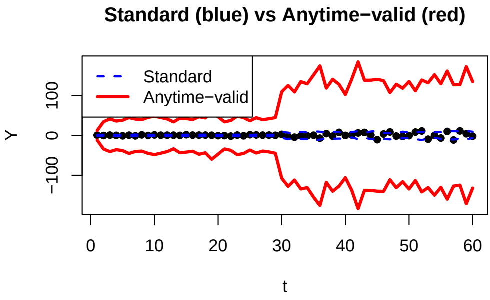
- Standard conformal prediction ensures per-batch coverage, but **fails** to guarantee validity over time.
- Solution: use **test supermartingales** and **Ville's inequality**.

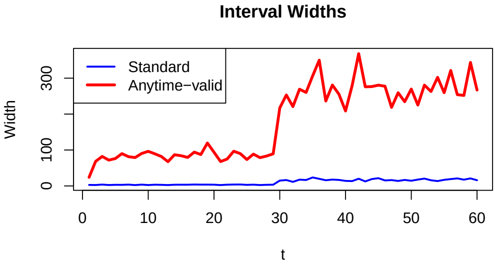
Theorem (Ville's Inequality)

Let $\{M_t\}_{t\geq 0}$ be a nonnegative supermartingale. Then, for any $\alpha \in (0,1)$,

$$\mathbb{P}\left(\forall t \geq 0,\ M_t < \frac{1}{\alpha}\right) \geq 1 - \alpha.$$

- Construct e-values $E_s = \frac{S_s^{n_s+1}}{\frac{1}{n_s+1}\sum_{j=1}^{n_s+1} S_s^j}$ and martingale $M_t = \prod_{s=1}^{t} E_s$.
- Define $\hat{C}_t$ via constraint $M_t < 1/\alpha \Rightarrow$ anytime-valid coverage.


Standard (blue) vs Anytime−valid (red)
Standard
Anytime−valid
Y
100
0
−100
0
10
20
30
40
50
60
t


Interval Widths
Standard
Anytime−valid
Width
300
100
0
0
10
20
30
40
50
60
t

Data-Dependent Conformal Prediction via E-values

- Classical conformal prediction fixes $\alpha \Rightarrow$ guarantees $1-\alpha$ coverage but **no control on set size**.
- Idea: allow α to be **data-dependent** ($\tilde{\alpha}$).

Definition

We say that a nonnegative random variable P is a post-hoc p-variable if

$$\sup_{\tilde{\alpha}} \frac{\mathbb{P}(P \leq \tilde{\alpha} \mid \tilde{\alpha})}{\tilde{\alpha}} \leq 1,$$

where the supremum is over every random variable $\tilde{\alpha} > 0$.

Theorem

P is a post-hoc p-variable if and only if

$$\mathbb{E}\left[\frac{1}{P}\right] \leq 1.$$

Data-Dependent Conformal Prediction via E-values

- Using e-values:

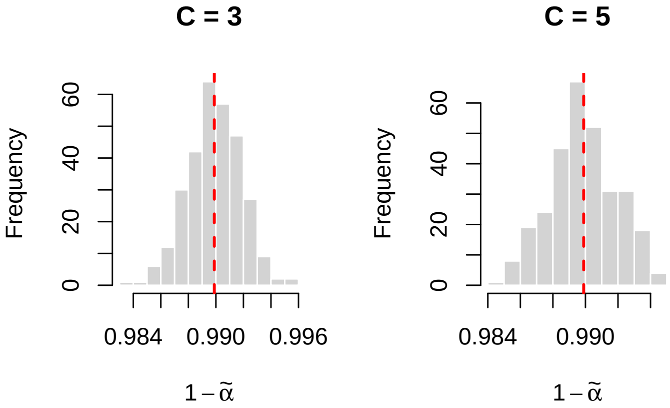
$$E = \frac{S(X_{n+1}, Y_{n+1})}{\frac{1}{n+1}\sum_{i=1}^{n+1} S(X_i, Y_i)}$$

gives adaptive validity via $P = 1/E$.

- Guarantee (data-dependent coverage):

$$\mathbb{E}\left(\frac{\mathbb{P}(Y_{n+1} \notin \hat{C}_n^{\tilde{\alpha}} \mid \tilde{\alpha})}{\tilde{\alpha}}\right) \leq 1.$$

- Enables:
  - Adaptive choice of $\tilde{\alpha}$
  - Control of set size (e.g. enforce $|\hat{C}_n^{\alpha}| \leq C$)



C = 3
Frequency
0
20
40
60
0.984
0.990
0.996
1 – α̃
C = 5
Frequency
0
20
40
60
0.984
0.990
1 – α̃

Monte Carlo Conformal E-Prediction

- Setting: each input X_i has multiple labels $Y_i^{(j)}$, $j = 1, \ldots, m$ (e.g. multiple experts).
- Data are **not exchangeable** $\Rightarrow$ standard conformal prediction fails.
- Idea: use all labels via **e-values** instead of selecting one.
- For each expert:

$$E_j = \frac{S_{n+1}}{\frac{1}{n+1}\left(\sum_{i=1}^{n} S_i^{(j)} + S_{n+1}\right)}$$

- Average preserves validity:

$$\bar{E} = \frac{1}{m}\sum_{j=1}^{m} E_j \quad \text{is an e-variable.}$$

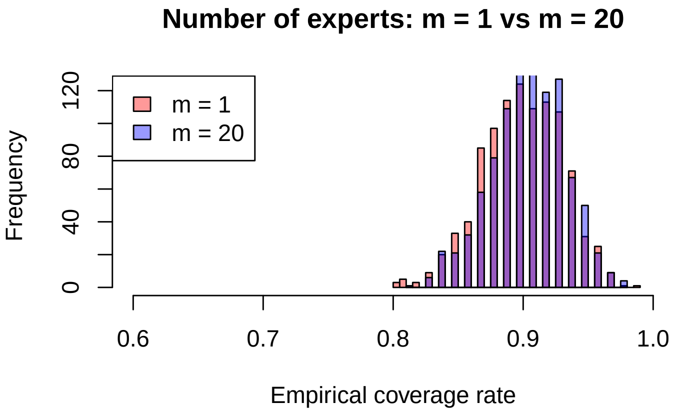
- Conformal set:

$$\hat{C}_n(x) = \{y : \bar{E} < 1/\alpha\}$$

- Guarantee:

$$\mathbb{P}(Y_{n+1} \in \hat{C}_n(X_{n+1})) \geq 1 - \alpha$$

- Key advantage: uses all experts $\Rightarrow$ reduces variability while maintaining $1 - \alpha$ coverage.


Number of experts: m = 1 vs m = 20
m = 1
m = 20
Frequency
0
40
80
120
0.6
0.7
0.8
0.9
1.0
Empirical coverage rate

AI use

I used Generative AI in my report

- to generate parts of the code for experiments and visualization
- for checking grammatical errors

References

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