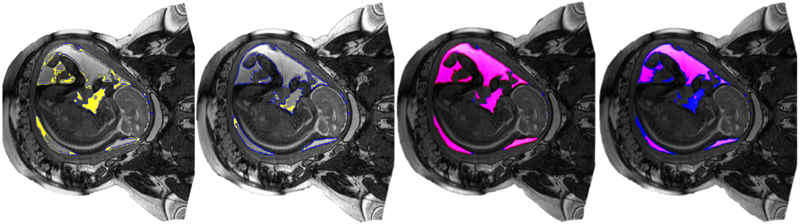
Split Conformal Prediction for Dependent Data

Paulo Orenstein

June 15th, 2022

IMPA



Joint work with Roberto Imbuzeiro Oliveira, Thiago Ramos, João Vitor Romano and others

Agenda

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- Extending split CP to dependent data: new results
- In practice: effect of dependency is negligible
- Conclusion: further directions

Video with blue solid.

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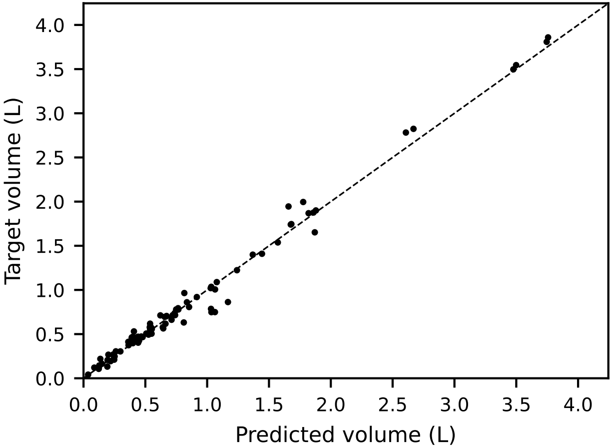
- How: segment each layer in the MRI using U-Net, count voxel size for volume
- Results: $\sim$ 92% Dice accuracy in under 5 seconds

Video with estimates.

Results


4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Target volume (L)
0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0
Predicted volume (L)

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  - "I'm 90% sure the true AF volume is between 2.72L and 2.88L"
  - "I'm 90% sure the true AF volume is between 1.90 and 3.70L"
- How can we provide valid predictive intervals for black-box prediction methods?

Given data $\{(X_i, y_i)\}_{i=1}^n$ to train any prediction method $\hat{\mu}$ and any level $\alpha \in (0, 1)$, can we construct a prediction set $C_{1-\alpha}(x)$ such that, for a new point (X_{n+1}, y_{n+1}),

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(For us, X_i is an MRI exam, y_i is the fluid volume, $\hat{\mu}$ is a U-Net, C is a rule specifying a volume interval for X_i.)

Conformal Prediction

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*Vovk, Gammerman, and Shafer. "Algorithmic learning in a random world", Springer (2005).

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[†] Angelopoulos and Bates, "A Gentle Introduction to Conformal Prediction", arXiv (2021).

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- We will consider the most popular incarnation: split CP[‡]

[‡] Lei, G'Sell, Rinaldo, Tibshirani, and Wasserman, "Distribution-free predictive inference for regression", JASA (2018).

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- We will consider the most popular incarnation: split CP
- Important assumption: data $(X_i, y_i)_{i=1}^n$ is exchangeable (which is implied by iid)

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Proof sketch: since data is exchangeable, $\hat{s}_j$ are also exchangeable. Consider the $1-\alpha$ quantile of $\{\hat{s}_j\}_{j \in I_{\text{cal}}} \cup \{\hat{s}_k\}$; the probability of $\hat{s}_k$ being bigger than the quantile must be bigger than $1-\alpha$.

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So: $\mathbb{P}[\hat{s}_k \leq \hat{q}_{(1+1/n_{\text{cal}})(1-\alpha)}(\{\hat{s}_j\}_{j \in I_{\text{cal}}})] = \mathbb{P}[\hat{s}_k \leq \hat{q}_{(1-\alpha)}(\{\hat{s}_j\}_{j \in I_{\text{cal}}} \cup \{\infty\})] \geq 1-\alpha.$ □

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Empirical coverage

Conditional coverage

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If the data $\{(X_i, y_i)\}_{i=1}^n$ is iid, then for any $\varepsilon > 0$ there exists $c_\varepsilon > 0$ such that

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Thus, split CP can guarantee coverage even if conditioned on some events.

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- Simple to implement, computationally cheap
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  - conditional likelihood: $\hat{s}_{\text{tr}}(x, y) = -\log \hat{p}(y|x)$
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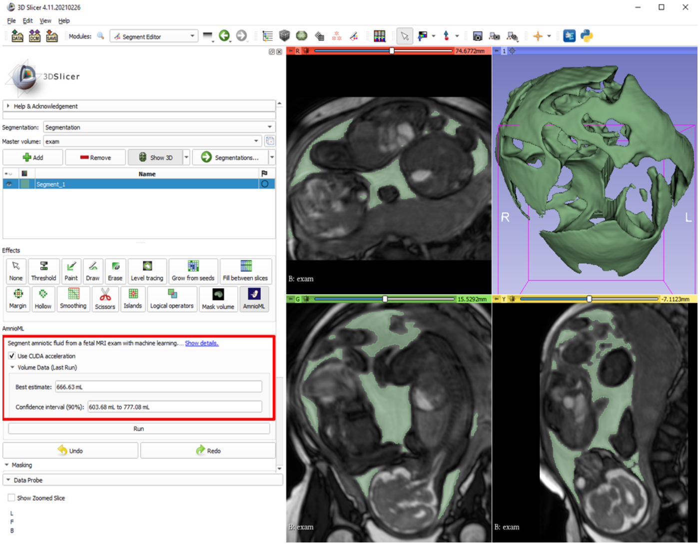
- Many more generalizations: e.g., prediction masks*

*Bates, Angelopoulos, Lei, Malik, and Jordan, "Distribution-free, risk-controlling prediction sets"

Results: Split CP



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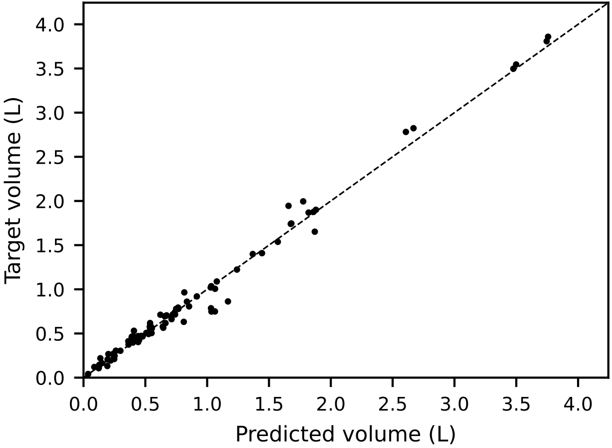

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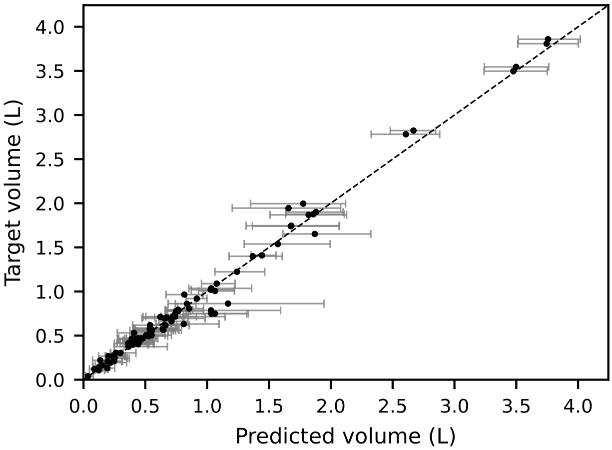

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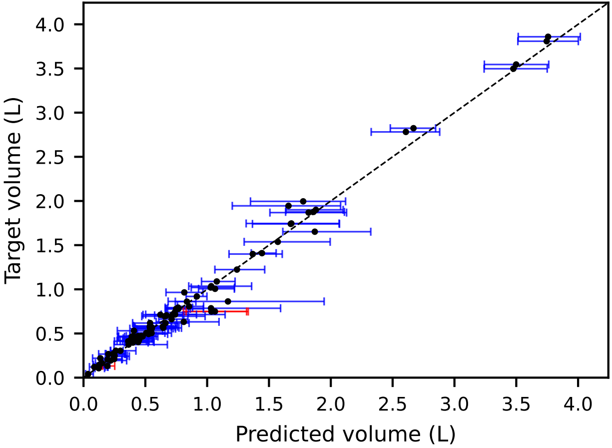

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(For us, some exams came from the same mother at different stages in the pregnancy.)

Dealing with Dependence

- Recent interest in independent data with distributional drift*

*Barber, Candès, Ramdas and Tibshirani. "Conformal prediction beyond exchangeability", arXiv (2022).

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- Our work[†]: rebuild split conformal prediction without exchangeability

[†]Oliveira, O., Ramos, Romano, "Split Conformal Prediction for Dependent Data", arXiv (2022).

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- Recent interest in independent data with distributional drift
- Our work: rebuild split conformal prediction without exchangeability
- Intuition: see how data CDF concentrates when exchangeability is replaced by looser conditions:

$$\mathbb{P}[y_k \in C_{1-\alpha+\eta}(X_k)] \geq 1-\alpha, \text{ so } \mathbb{P}[y_k \in C_{1-\alpha}(X_k)] \geq 1-\alpha-\eta,$$

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- Tools: concentration inequalities and decoupling properties

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- Examples: Markov chains, renewal processes, AR(1)

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- Assumptions on data:
  - Stationarity: $(Z_t, \ldots, Z_m) \stackrel{d}{=} (Z_{t+k}, \ldots, Z_{t+m+k})$
  - β-mixing: $\beta(a) = \|\mathbb{P}_{-\infty:0,a:\infty} - \mathbb{P}_{-\infty:0} \otimes \mathbb{P}_{a:\infty}\|_{TV} \xrightarrow{a \to \infty} 0$
- Data is time-invariant and asymptotically independent
- Examples: Markov chains, renewal processes, AR(1)
- Main theoretical tool: Blocking technique*

*Yu, "Rates of Convergence of Empirical Processes of Stationary Mixing Sequences", Annals of Probability (1994)

Main Theoretical Results

Marginal coverage

Empirical coverage

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Suppose that $\{(X_i, y_i)\}_{i=1}^{n}$ is stationary β-mixing. Given $\alpha \in (0,1)$ and $\delta_{\text{cal}} > 0$, for $k \in I_{\text{test}}$,

$$\mathbb{P}[y_k \in C_{1-\alpha}(X_k)] \geq 1 - \alpha - \eta,$$

with $\eta = \varepsilon_{\text{cal}} + \varepsilon_{\text{tr}} + \delta_{\text{cal}}$, where $\varepsilon_{\text{tr}} = \beta(k - n_{\text{tr}})$.

Empirical coverage

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Empirical coverage

Suppose that $\{(X_i, y_i)\}_{i=1}^n$ is stationary β-mixing. Given $\alpha \in (0,1)$ and $\delta_{\text{cal}} > 0$, $\delta_{\text{test}} > 0$:

$$\mathbb{P}\left[\frac{1}{n_{\text{test}}} \sum_{k \in I_{\text{test}}} \mathbb{I}_{[y_k \in C_{1-\alpha}(X_k)]} \geq 1 - \alpha - \eta\right] \geq 1 - \delta_{\text{cal}} - \delta_{\text{test}},$$

with $\eta = \varepsilon_{\text{cal}} + \varepsilon_{\text{test}}$.

The Details

- $F_{\text{cal}} = \left\{(a, m, r) \in \mathbb{N}_+^3 : 2ma = n_{\text{cal}} - r + 1, \delta_{cal} > 4(m-1)\beta(a) + \beta(r)\right\}$
- $F_{\text{test}} = \left\{(a, m, s) \in \mathbb{N}_+^3 : 2ma = n_{\text{test}} - s, \delta_{test} > 4(m-1)\beta(a) + \beta(n_{\text{cal}})\right\}$
- $\tilde{\sigma}(a) = \sqrt{1/4 + (2/a)\sum_{j=1}^{a-1}(a-j)\beta(j)}$
- $\varepsilon_{\text{cal}} = \inf_{(a,m,r)\in F_{\text{cal}}} \left\{\tilde{\sigma}(a)\sqrt{\frac{4}{n_{\text{cal}}-r+1}\log\left(\frac{4}{\delta_{\text{cal}}-4(m-1)\beta(a)-\beta(r)}\right)} + \frac{1}{3m}\log\left(\frac{4}{\delta_{\text{cal}}-4(m-1)\beta(a)-\beta(r)}\right) + \frac{r-1}{n_{\text{cal}}}\right\}$
- $\varepsilon_{\text{test}} = \inf_{(a,m,s)\in F_{\text{test}}} \left\{\tilde{\sigma}(a)\sqrt{\frac{4}{n_{\text{test}}}\log\left(\frac{4}{\delta_{\text{test}}-4(m-1)\beta(a)-\beta(n_{\text{cal}})}\right)} + \frac{1}{3m}\log\left(\frac{4}{\delta_{\text{test}}-4(m-1)\beta(a)-\beta(n_{\text{cal}})}\right) + \frac{s}{n_{\text{test}}}\right\}$

Conditional Theoretical Results

Marginal coverage, conditional version

Empirical coverage, conditional version

Conditional Theoretical Results

Marginal coverage, conditional version

Suppose that $\{(X_i, y_i)\}_{i=1}^{n}$ is stationary β-mixing. Given $\alpha \in (0,1)$ and $\delta_{\text{cal}} > 0$, for any $k \in I_{\text{test}}$ and $K \in \mathcal{K}$ (with $\text{VC}(\mathcal{K}) = d, \mathbb{P}[X_k \in K] > \gamma$),

$$\mathbb{P}[y_k \in C_{1-\alpha}(X_k; K) \mid X_k \in K] \geq 1 - \alpha - \eta,$$

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Empirical coverage, conditional version

Conditional Theoretical Results

Marginal coverage, conditional version

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Empirical coverage, conditional version

Suppose that $\{(X_i, y_i)\}_{i=1}^n$ is stationary β-mixing. Given $\alpha \in (0,1)$ and $\delta_{\text{cal}} > 0$, $\delta_{\text{test}} > 0$ and $K \in \mathcal{K}$:

$$\mathbb{P}\left[\inf_{K \in \mathcal{K}} \frac{1}{n_{\text{test}}(K)} \sum_{k \in I_{\text{test}}(K)} \mathbb{I}_{[y_k \in C_{1-\alpha}(X_k; K)]} \geq 1 - \alpha - \eta\right] \geq 1 - \delta_{\text{cal}} - \delta_{\text{test}},$$

with $\eta = \varepsilon_{\text{cal}} + \varepsilon_{\text{test}}$.

The Details

- $G_{\text{cal}} = \left\{(a, m, r) \in \mathbb{N}_+^3 : 2ma = n_{\text{cal}} - r + 1, \delta_{cal} > 16(m-1)\beta(a) + \beta(r)\right\}$

- $G_{\text{test}} = \left\{(a, m, s) \in \mathbb{N}_+^3 : 2ma = n_{\text{test}} - s, \delta_{test} > 8(m-1)\beta(a) + \beta(n_{\text{cal}})\right\}$

- $\varepsilon_{\text{cal}} = \inf_{(a,m,r)\in G_{\text{cal}}} \left\{ \frac{1}{\gamma} \left(4\sqrt{\frac{\log(2(m+1)^d)}{m}} + \frac{2(r-1)}{n_{\text{cal}}} + 2\sqrt{\frac{1}{2m} \log\left(\frac{16}{\delta_{\text{cal}} - 16(m-1)\beta(a) - \beta(r)}\right)}\right)\right\}$

- $\varepsilon_{\text{test}} = \inf_{(a,m,s)\in G_{\text{test}}} \left\{ \frac{1}{\gamma} \left(4\sqrt{\frac{\log(2(m+1)^d)}{m}} + \frac{2s}{n_{\text{test}}} + 2\sqrt{\frac{1}{2m} \log\left(\frac{8}{\delta_{\text{test}} - 8(m-1)\beta(a) - \beta(n_{\text{cal}})}\right)}\right)\right\}$

Application: Autoregressive Process

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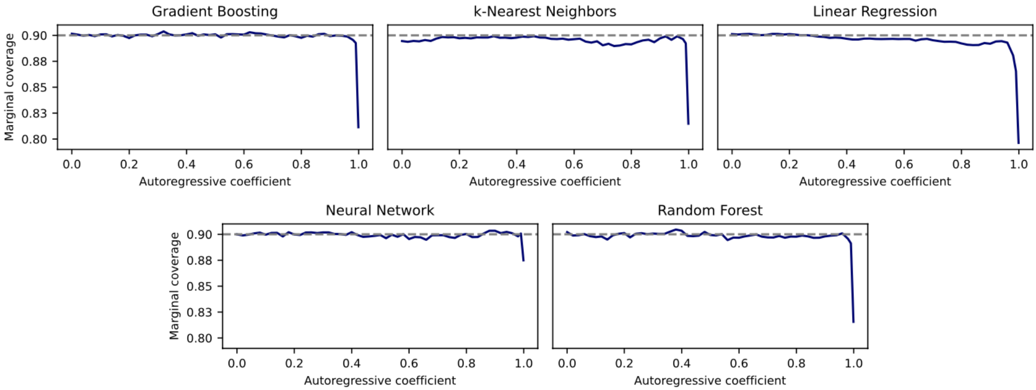

Application: Finance

- Time series with EUR/USD spot exchange rate; predictions with boosting

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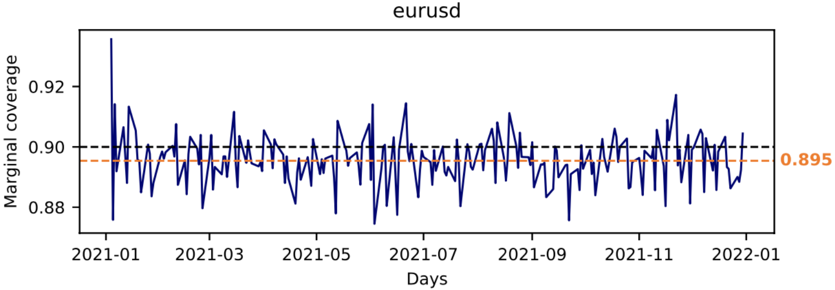

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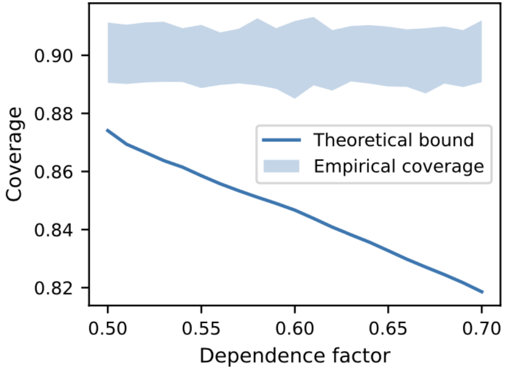

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- Uncertainty quantification is crucial for the deployment of ML systems.
- Conformal prediction is a set of tools that yield marginal, empirical and conditional coverage.
- It traditionally requires little beyond exchangeability; we show it works even for dependent data.
- Our results can be extended beyond stationarity and to non-split CP (e.g., rank-one-out, risk-controlling prediction sets).
- There is much more theory and algorithms to be developed on top of it.

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