MODEL-AGNOSTIC PREDICTIVE UNCERTAINTY FOR EARTH OBSERVATION APPLICATIONS

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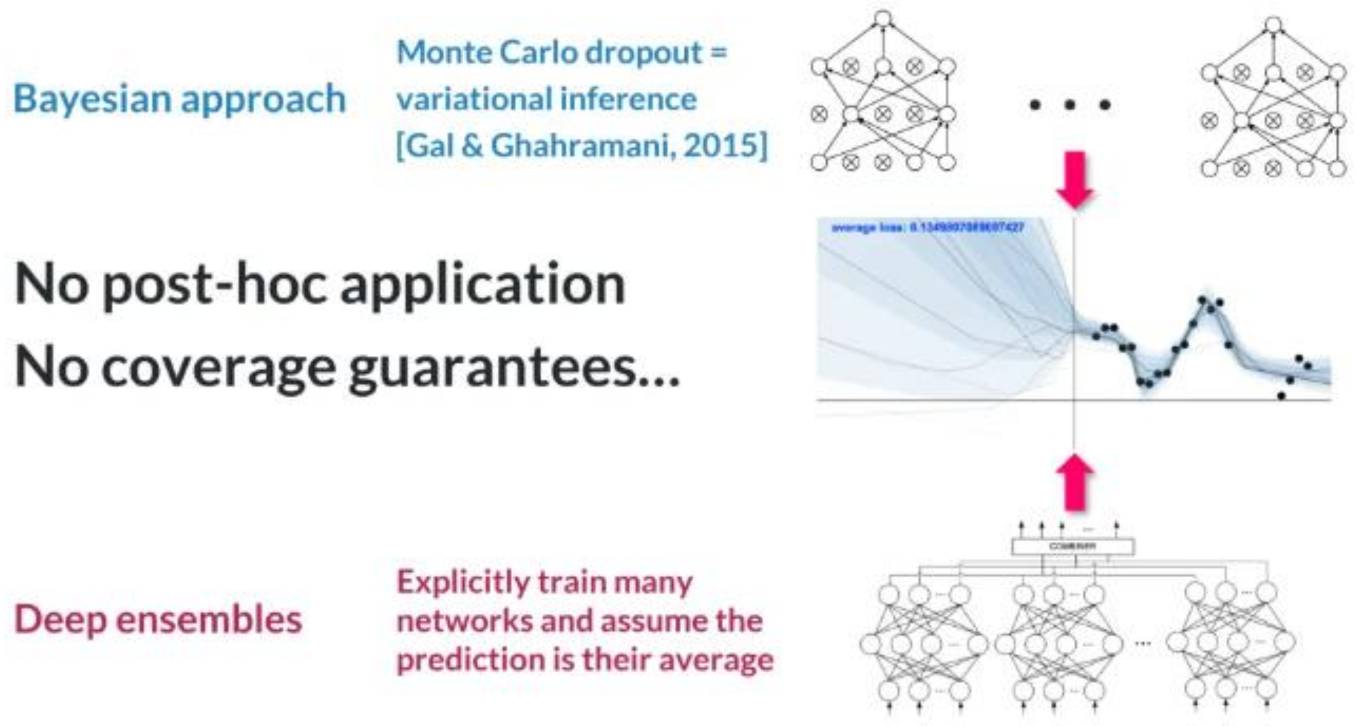
Motivation: (How much) can we Trust an AI Prediction?

*How can we systematically **quantify** the **uncertainty** of predictions in **AI** while ensuring reliable **theoretical guarantees** and **independently** of the underlying **model architecture**?*



Uncertainty quantification blog post - van der Schaar Lab

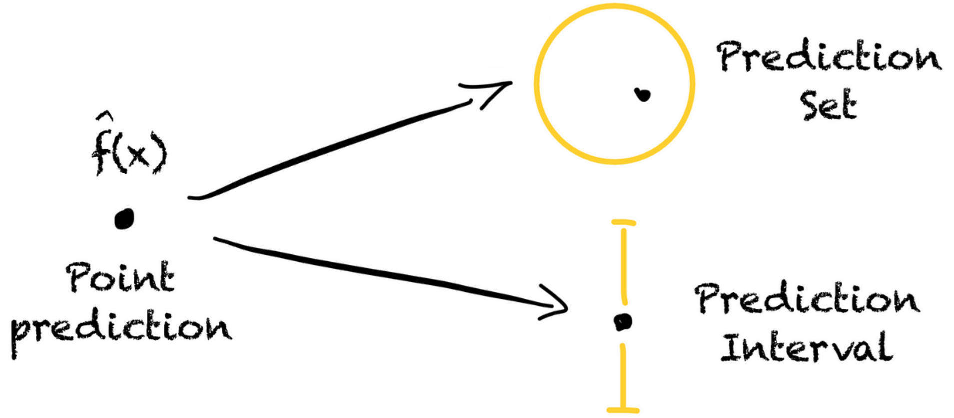
Conformal Prediction: Definition

Theorem: Full Conformal Prediction

If (X_i, Y_i) for $i = 1, \dots, n$ is an exchangeable sequence (ordering of observations/data is irrelevant), then for a new exchangeable pair (X_{n+1}, Y_{n+1}):

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

Ground truth Y_{n+1} is contained in the predicted set $C(X_{n+1})$ at chosen significance level α



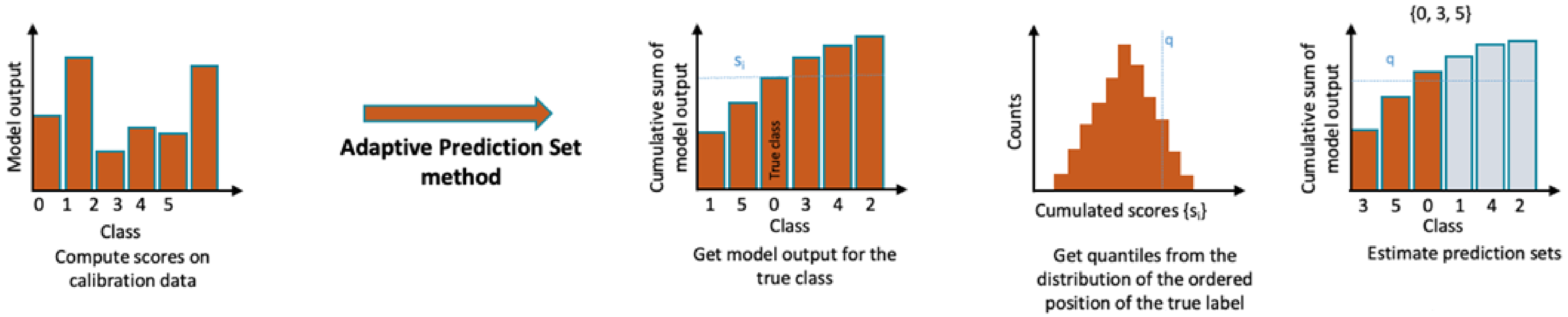
All You Need Is Conformal Prediction, Towards Data Science

CP Methodologies: Adaptive Predictive Sets

- With **non-conformity scores *s*** (e.g. 1-softmax) construct sets as $\mathrm{C}(x) = \{y : s(x,y) \leq \hat{q}\}$, this is the Least Ambiguous Classifier (**LAC**) split conformal method.
- However in Adaptive Predictive Sets (**APS**) our non-conformity score **cumulatively** adds classes until the true class threshold $\hat{q}$, **more uncertain** predictions lead to **larger sets**.

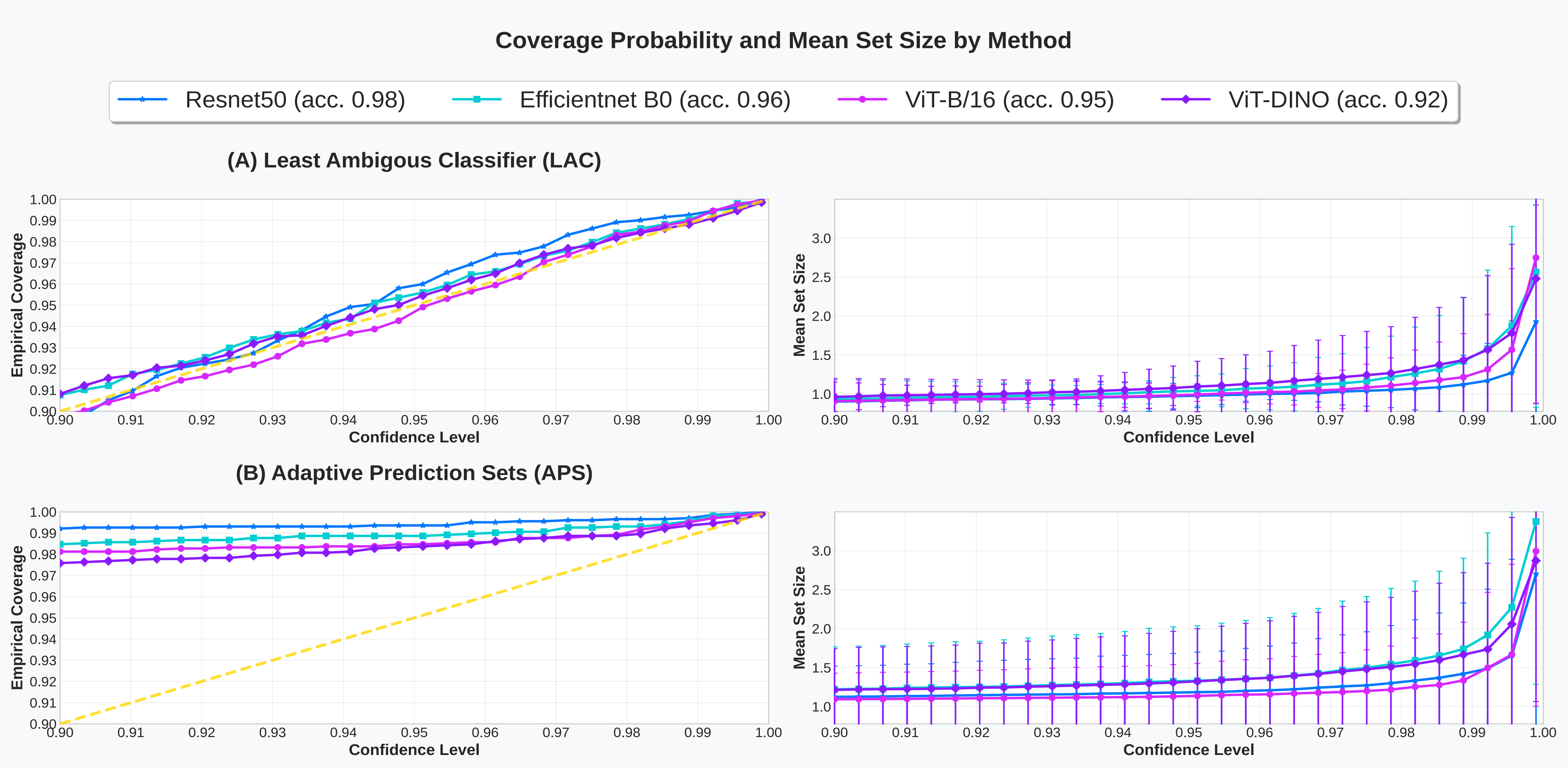
$$\mathcal{C}(x) = \{\pi_1(x), \ldots, \pi_k(x)\}, \text{ where } k = \sup \left\{ k' : \sum_{j=1}^{k'} \hat{f}(x)_{\pi_j(x)} < \hat{q} \right\}$$

- However this can lead to very large prediction sets, to overcome this Regularized Adaptive Prediction Sets (**RAPS**) introduces a **penalization term $\boldsymbol{\lambda}$**, $\mathrm{C}(x) = \{y : s(x,y) \leq \hat{q} + \lambda g(k)\}$



https://mapie.readthedocs.io

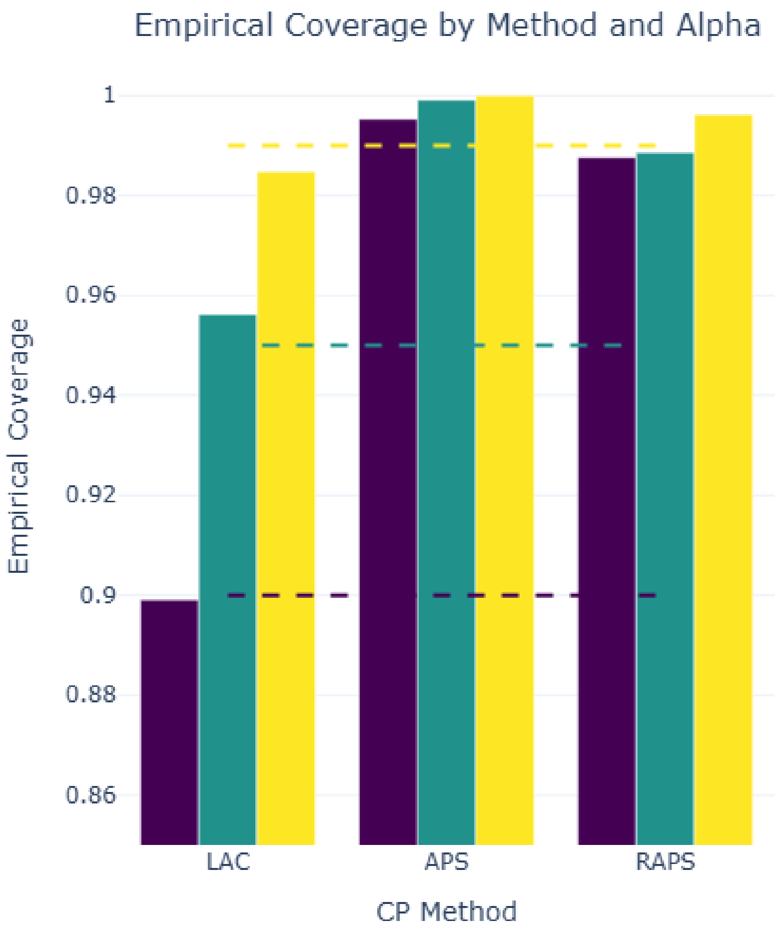
Results I: LAC and APS to CNNs and ViTs on EuroSAT

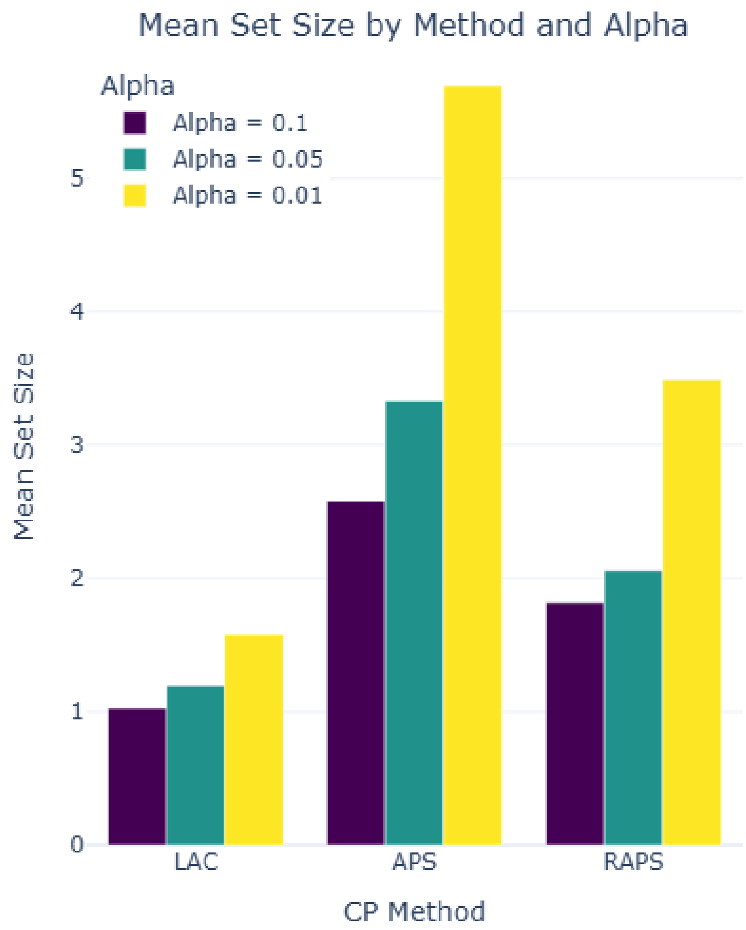


- **Empirical coverage** across varying confidence levels is shown (left), alongside the corresponding **mean set sizes** with associated variances (right).

Results II: CP methods with Resnet50, UC Merced Dataset

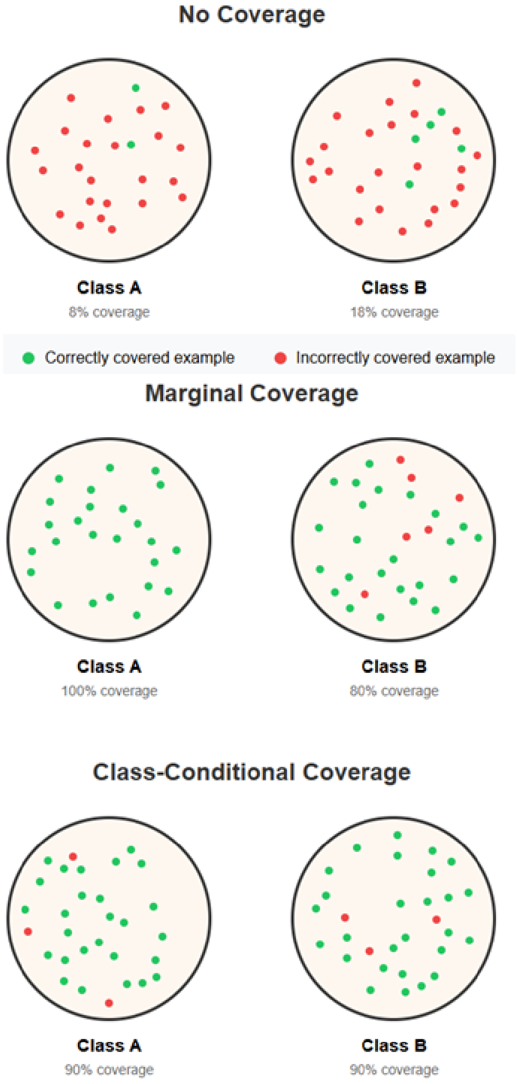
Alpha	CP Method	Predicted Set Sizes 0	1	2	3	4+
0.01	LAC	0	598	315	115	22
	APS	0	319	94	70	567
	RAPS	0	261	113	65	611
0.05	LAC	14	823	205	8	0
	APS	0	547	83	57	363
	RAPS	0	451	90	504	5
0.10	LAC	54	914	82	0	0
	APS	0	621	95	60	274
	RAPS	0	575	93	382	0

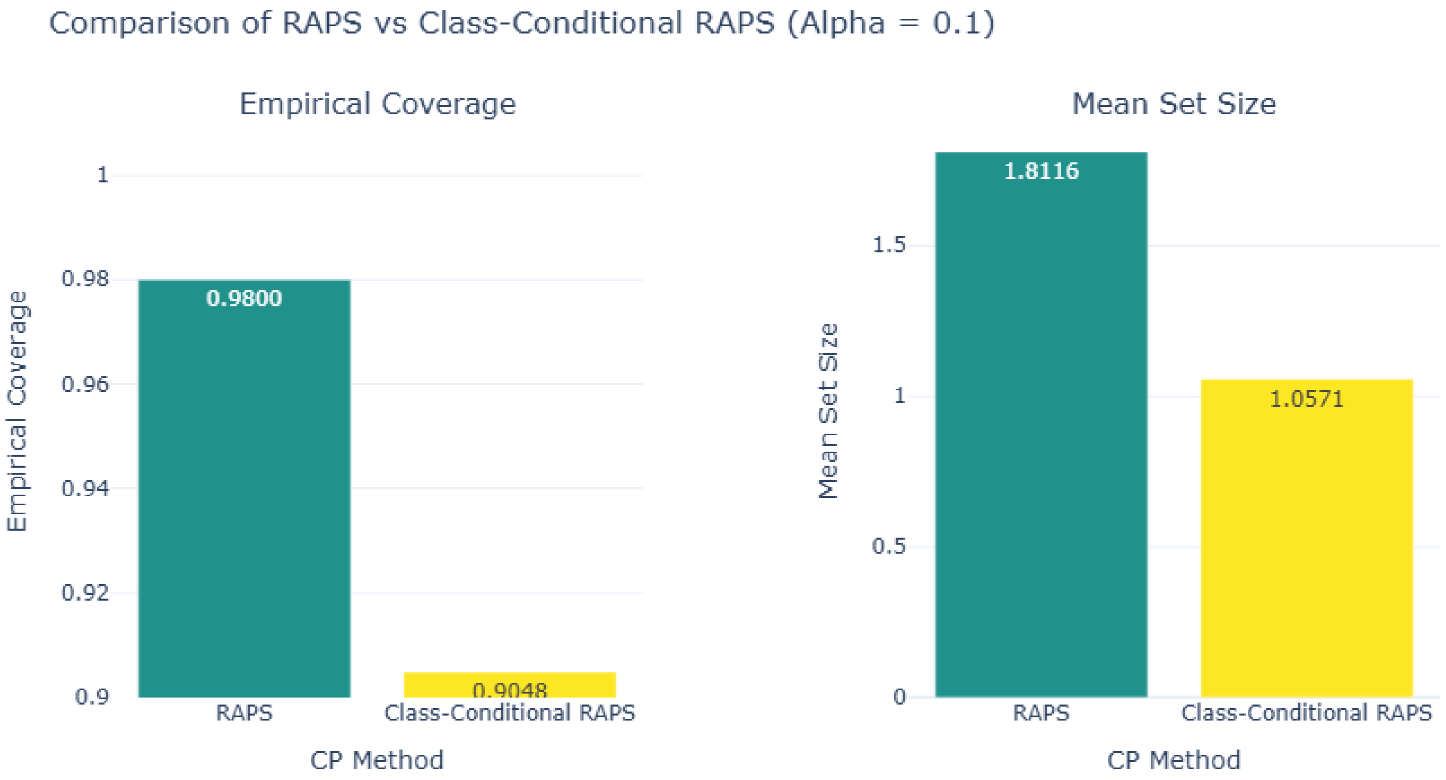




- **LAC can produce empty sets**, using **APS** overly satisfies coverage and **produces large sets** (uninformative), **RAPS** regularization **optimizes** the **trade-off coverage ↔ set size.**

Results III: CP methods with Resnet on UC Merced Dataset





- **CC-RAPS** evaluates **each class against its own class-specific threshold**, only including it if its score exceeds its corresponding threshold. Resulting in **more precise prediction sets.**

Discussion

We analyzed **multiple Split CP methods across** various **architectures** and **datasets:**

- **Class-Conditional RAPS allows the most precise prediction sets,** without losing theoretical guarantees.
- All models verify CP, with **ResNet50 demonstrating most consistent and efficient behavior**, while ViTs show higher variance despite competitive accuracy.

CP proves to be a **versatile, rigorous framework** applicable to **black-box algorithms** for **UQ** in **practical EO cases.**

EuroSAT dataset

References

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Imprint

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