Sparse Activations as Conformal Predictors

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Conformal prediction (CP)

- Uncertainty quantification framework: strong coverage guarantees, model-agnostic, and distribution-free.
- Given a non-conformity score, CP constructs prediction sets for test instances using calibration data.

Vovk et al., 2005; Angelopoulos and Bates, 2023

Sparse activation functions

- Fenchel-Young losses: framework for sparse activations interpretable as set prediction, such as:
- γ -entmax family: softmax (γ =1) and sparsemax (γ =2); sparse for γ > 1; temperature-controlled sparsity Martins and Astudillo, 2016; Peters et al., 2019; Blondel et al., 2020

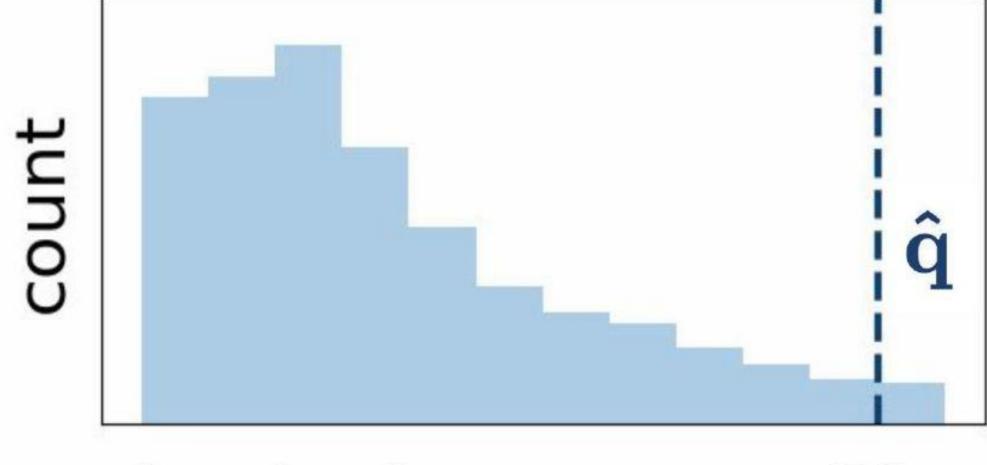
new conformal predictor scaling of sparsemax

temperature generalization

to the

y-entmax

family



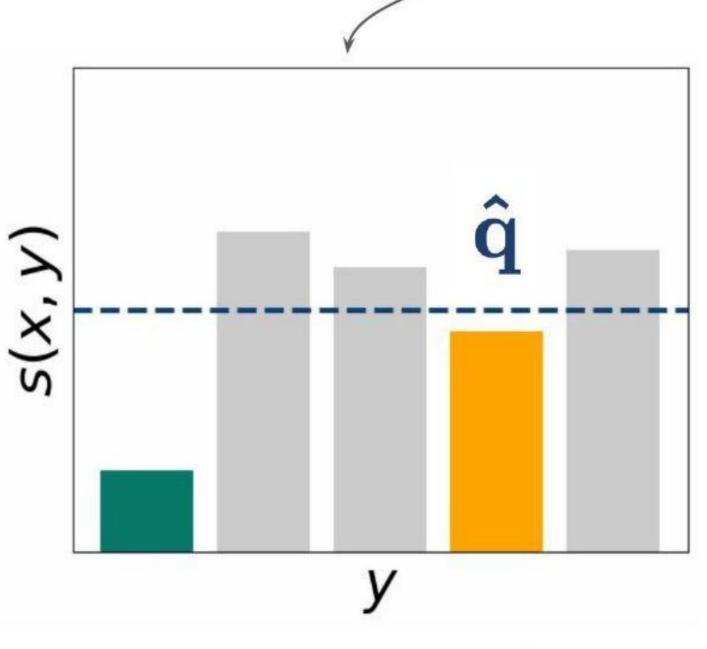
$$s(x, y) = \|\mathbf{z}_{1:k(y)} - z_{k(y)}\mathbf{1}\|_{\frac{1}{v-1}}$$

Calibration

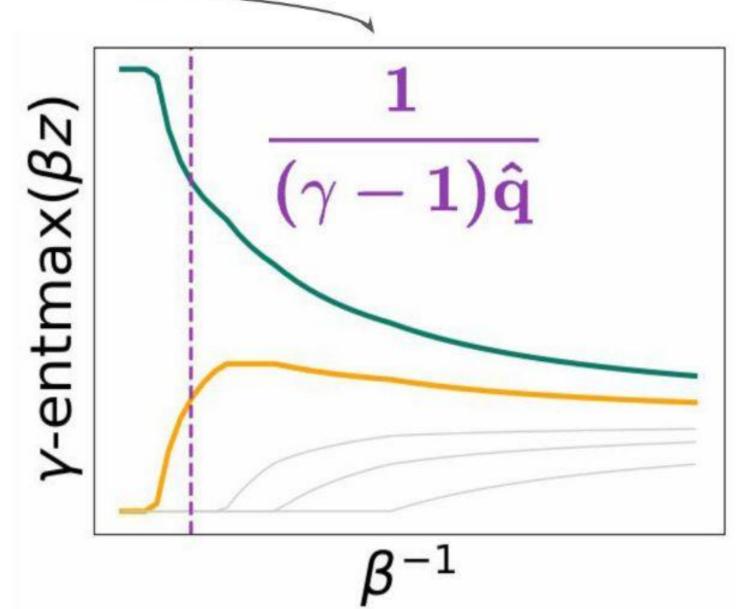
$$\lceil (\mathbf{n} + \mathbf{1})(\mathbf{1} - \alpha) \rceil$$
n
quantile

expanded family of non-conformity scores

> empirical validation on different tasks







Temperature Scaling



Conformalizing entmax

Let
$$z_1 > ... > z_K$$
, support is $j \in S(\beta \mathbf{z}; \gamma) \iff \sum_{k=1}^{j-1} \left[(\gamma - 1)\beta(z_k - z_j) \right]^{\frac{1}{\gamma - 1}} < 1$

Building a conformal predictor, $C_{\alpha}: \mathcal{X} \to 2^{\mathcal{Y}}$, with score:

CIFAR100

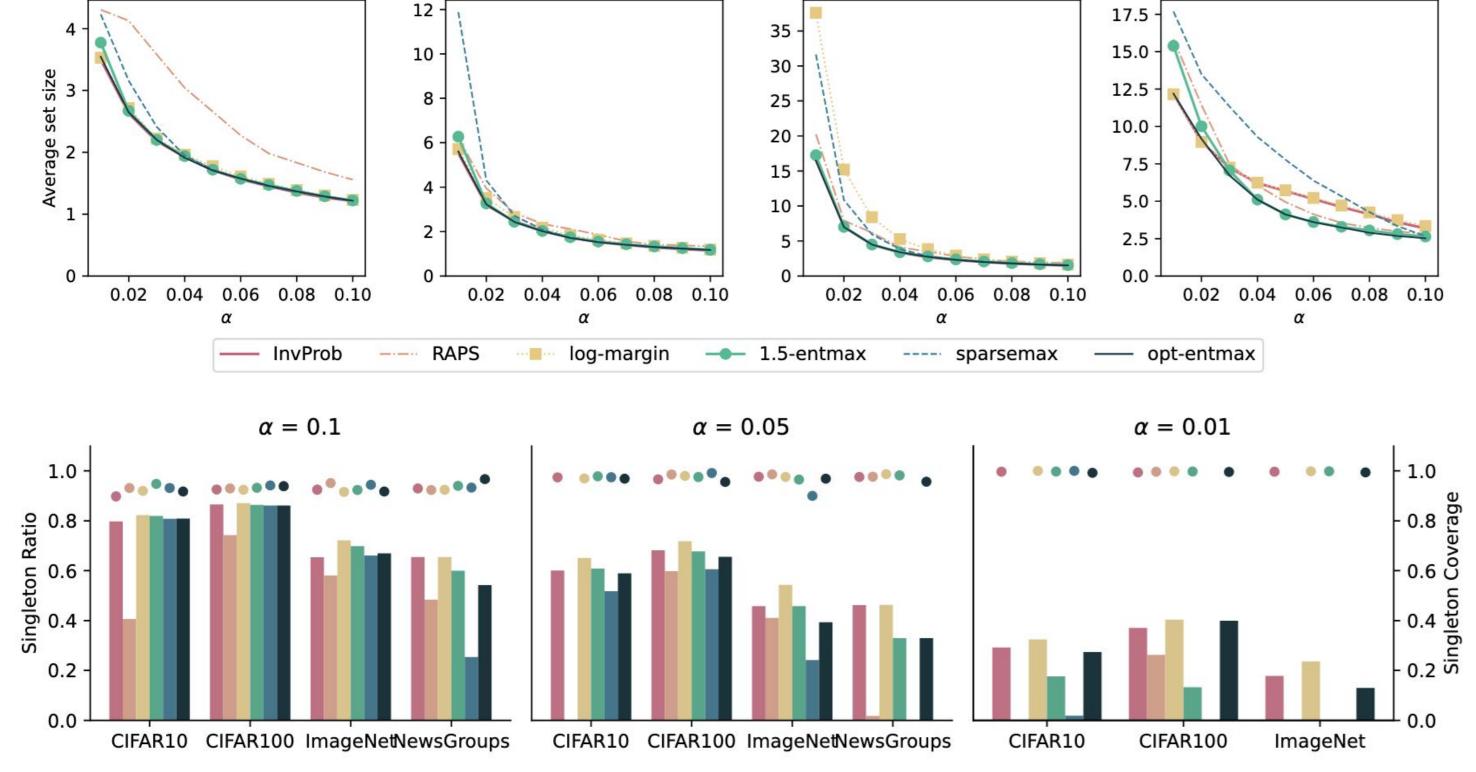
$$s(x, y) = \|\mathbf{z}_{1:k(y)} - z_{k(y)}\mathbf{1}\|_{\delta}$$
, yields: $C_{\alpha}(x) = S(\beta \mathbf{z}; \gamma)$

Interesting findings

- γ can be tuned, yielding method opt-entmax
- limit case (softmax)→ log-odds ratio (log-margin):

$$s(x, y) = \|\mathbf{z}_{1:k(y)} - z_{k(y)}\mathbf{1}\|_{\infty} = z_1 - z_{k(y)} = \log \frac{p_1}{p_{k(y)}}$$

Results



- choice of score is crucial and task-dependent
- new methods (log-margin and opt-entmax):
 - efficiency 🗸
 - adaptiveness 🗸
 - Interpretability 🗸
 - natural calibration assessment

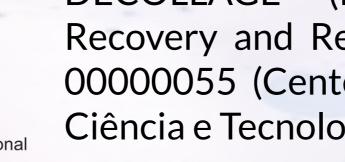






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Acknowledgments: EU's Horizon Europe Research and Innovation Actions (UTTER, 101070631), contract (ERC-2022-CoG DECOLLAGE 101088763), Portuguese Recovery and Resilience Plan through project C645008882-00000055 (Center for Responsible AI), and Fundação para a Ciência e Tecnologia through contract UIDB/50008/2020.

