

EFFICIENT CREDAL PREDICTION THROUGH DECALIBRATION

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006 Paper under double-blind review

ABSTRACT

011 A reliable representation of uncertainty is essential for the application of mod-
 012 ern machine learning methods in safety-critical settings. In this regard, the use
 013 of credal sets (i.e., convex sets of probability distributions) has recently been pro-
 014 posed as a suitable approach to representing epistemic uncertainty. However, as
 015 with other approaches to epistemic uncertainty, training credal predictors is com-
 016 putationally complex and usually involves (re-)training an ensemble of models.
 017 The resulting computational complexity prevents their adoption for complex mod-
 018 els such as foundation models and multi-modal systems. To address this problem,
 019 we propose an efficient method for credal prediction that is grounded in the notion
 020 of relative likelihood and inspired by techniques for the calibration of probabilistic
 021 classifiers. For each class label, our method predicts a range of plausible proba-
 022 bilities in the form of an interval. To produce the lower and upper bounds of
 023 these intervals, we propose a technique that we refer to as decalibration. **Exten-**
 024 **sive experiments show that our method yields credal sets with strong performance**
 025 **across diverse tasks, including coverage–efficiency evaluation, out-of-distribution**
 026 **detection, and in-context learning.** Notably, we demonstrate credal prediction on
 027 models such as TabPFN and CLIP—architectures for which the construction of
 028 credal sets was previously infeasible.

1 INTRODUCTION

031 Modern machine learning (ML) is increasingly deployed in domains where decisions carry real con-
 032 sequences, from energy systems (Miele et al., 2023) and weather forecasting (Bulte et al., 2025)
 033 to healthcare (Löhr et al., 2024). In such domains, we need models that not only make accurate
 034 predictions, but also express what they do *not* know. A useful starting point is the distinction be-
 035 between *aleatoric* and *epistemic* uncertainty (Hüllermeier & Waegeman, 2021). Aleatoric uncertainty
 036 reflects irreducible randomness in the data. Epistemic uncertainty reflects limited knowledge and, in
 037 principle, can be reduced with more or better information. While standard probabilistic predictors
 038 capture the former, representing the latter typically requires higher-order formalism.

039 Credal sets, i.e., (convex) sets of probability distributions, offer such a view. Instead of committing
 040 to a single predictive distribution, a credal predictor returns a set of plausible distributions, thereby
 041 making epistemic uncertainty explicit (Levi, 1978; Walley, 1991). Credal methods have appealing
 042 semantics but can be computationally demanding: many pipelines rely on ensembles or approximate
 043 posteriors to explore the space of plausible models, which is difficult to justify for large and complex
 044 models such as foundation models, CLIP (Radford et al., 2021) or TabPFN (Hollmann et al., 2022).

045 We take a different route. Building on a likelihood-based notion of plausibility (Löhr et al., 2025), we
 046 construct credal predictions *from a single trained model by decalibration*: we systematically perturb
 047 the model’s logits so that the resulting probabilities move away from the maximum-likelihood fit
 048 while staying within a prescribed relative-likelihood budget. For each class, this procedure yields
 049 a plausible probability interval; their product forms a credal set that reflects epistemic uncertainty
 050 without retraining (cf. Figure 1). Intuitively, calibration adjusts probabilities to be more correct,
 051 whereas decalibration explores how far they can be pushed and still remain supported by the data.

052 In this light, our **contributions** are as follows. ① A model-agnostic, post-hoc method for credal
 053 prediction via *decalibration*, logit perturbations that produce class-wise plausible probability in-
 054 tervals under a relative-likelihood budget, yielding credal sets with the clear semantics “reachable

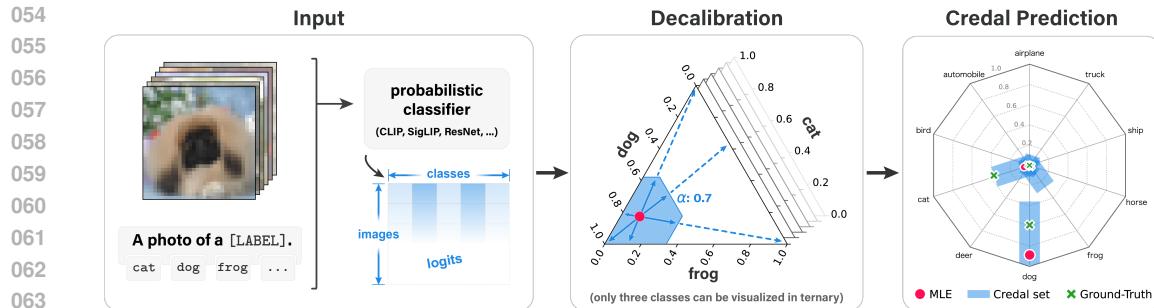


Figure 1: Overview of Efficient Credal Prediction through Decalibration. Given a probabilistic classifier (maximum likelihood estimate), our method *decalibrates* the predicted distributions by their logits. The resulting *credal set* contains the *ground-truth distribution*, as visualized in the *credal spider plot* (see Appendix C for an explanation). Note that we only show the decalibration of three classes for visualization purposes—in practice, all classes are decalibrated.

without sacrificing more than a chosen fraction of training likelihood.” The procedure requires *no retraining* and only logits, enabling use with large pretrained models. ② Theoretically, we show the relative-likelihood feasibility set induced by logit shifts is convex (and compact on an identifiability hyperplane); that upper class-wise bounds arise from a single convex optimization; and that in a one-dimensional, class-specific shift the plausible interval endpoints solve two convex programs with monotone probabilities, implying nested credal sets as the likelihood budget tightens. ③ Empirically, across benchmarks our credal sets achieve favorable coverage–efficiency trade-offs and competitive out-of-distribution detection while reducing computational cost by orders of magnitude. The method enables credal prediction for previously out-of-reach models such as TabPFN and CLIP, and we introduce *credal spider plots* to visualize interval-based sets beyond three classes.

2 CREDAL PREDICTION BASED ON PLAUSIBLE INTERVALS

We assume a supervised classification setting, where \mathcal{X} denotes the instance space, and $\mathcal{Y} = \{1, \dots, K\}$ the finite set of class labels. Further, we assume that the learner has access to (i.i.d.) training data $\mathcal{D}_{\text{train}} = \{(\mathbf{x}^{(n)}, y^{(n)})\}_{n=1}^N \subset \mathcal{X} \times \Delta_K$. In this paper, we consider hypotheses of the form $h : \mathcal{X} \rightarrow \Delta_K$, mapping instances $\mathbf{x} \in \mathcal{X}$ to probability distributions over \mathcal{Y} ; by Δ_K we denote the set of all probability distributions on the label space \mathcal{Y} . Our primary concern is *predictive uncertainty*, i.e., the uncertainty about the predicted label \hat{y}_q at a query point $\mathbf{x}_q \in \mathcal{X}$. While probabilistic predictors $\mathcal{X} \rightarrow \Delta_K$, $\mathbf{x}_q \mapsto h(\mathbf{x}_q) = p(\cdot \mid \mathbf{x}_q, h)$ do account for aleatoric uncertainty, they do not represent *epistemic uncertainty* about the predicted probability $p(\cdot \mid \mathbf{x}_q, h)$. To make this uncertainty explicit, we move from point predictions in Δ_K to sets and consider an uncertainty-aware, set-valued predictor $H : \mathcal{X} \rightarrow \mathcal{K}(\Delta_K)$, where $\mathcal{K}(\Delta_K)$ denotes a suitable family of subsets of the simplex (e.g., nonempty closed convex sets). In this view, the prediction at \mathbf{x}_q is no longer a single vector $h(\mathbf{x}_q) \in \Delta_K$, but a set $H(\mathbf{x}_q) = \mathcal{Q}_{\mathbf{x}_q} \subseteq \Delta_K$, which we refer to as a *credal prediction*.

Credal sets have emerged as a compelling representation of (epistemic) uncertainty in contemporary machine learning research, yet there is no consensus on how to *construct* them in a principled and scalable way. We aim for a construction that is (i) statistically well-founded, (ii) semantically transparent, and (iii) computationally feasible for modern large models. Many existing pipelines either rely on Bayesian posteriors (Caprio et al., 2024a), thus inheriting prior sensitivity and computational burden, or on ad-hoc ensembling and heuristics that offer weak interpretability (Wang et al., 2025a). In contrast, following Löhr et al. (2025), we adopt a *likelihood-based* notion of plausibility that is prior-free, data-driven, and well established in statistical inference. Concretely, relative (normalized) likelihood provides a scalar measure of model plausibility: a model is considered plausible at level $\alpha \in (0, 1]$ if its likelihood is at least an α -fraction of the maximum likelihood in the model class. This yields an α -indexed family of *plausibility regions* in parameter space, whose images in prediction space induce (class-wise) *plausible probability intervals*. These intervals serve as the *inputs* that generate a credal set in the simplex.

With respect to our desiderata (i)–(iii), Löhr et al. (2025) already address (i) and (ii): the likelihood ratio supplies a prior-free, data-driven evidential scale that is standard in statistics, and normalizing by the maximum likelihood yields nested, interpretable α -cuts. This viewpoint is well established, likelihood ratios underpin classical confidence regions and tests and admit a clear calibration narrative (e.g., Wilks, 1938; Cox & Hinkley, 1979; Royall, 2017; Edwards, 2018), thereby providing both principledness and transparency. What remains largely open is (iii): *computational feasibility*. For modern large models (foundation models, large language models, and multi-modal systems), retraining ensembles or running costly Bayesian pipelines is often prohibitive. This work aims to close this gap by deriving efficient credal predictions while retaining the likelihood-based semantics. We first fix notation and briefly recall the (relative) likelihood-based construction.

Let $L : \mathcal{H} \rightarrow [0, \infty)$ denote the (empirical) likelihood of a hypothesis on $\mathcal{D}_{\text{train}}$, and let

$$\gamma(h) := \frac{L(h)}{\sup_{h \in \mathcal{H}} L(h)} \in [0, 1].$$

Thus $\gamma(h)$ is the *relative likelihood* (likelihood ratio) of h with respect to a maximum-likelihood solution: $\gamma(h) = 1$ for any MLE (if it exists) and decreases as the fit worsens; equivalently, $\log \gamma(h)$ is the log-likelihood gap, and $-2 \log \gamma(h)$ is the usual likelihood-ratio statistic.

For $\alpha \in (0, 1]$, define the *plausible model set* (viz. relative-likelihood α -cut)

$$\mathcal{C}_\alpha := \{h \in \mathcal{H} : \gamma(h) \geq \alpha\}.$$

Given $\mathbf{x} \in \mathcal{X}$, the predictive image of \mathcal{C}_α is $\mathcal{Q}_{\mathbf{x}, \alpha} := \{p(\cdot | \mathbf{x}, h) : h \in \mathcal{C}_\alpha\} \subseteq \Delta_K$. A convenient class-wise summary of $\mathcal{Q}_{\mathbf{x}, \alpha}$ is given by the marginal extrema

$$\underline{p}_k(\mathbf{x}) := \inf_{h \in \mathcal{C}_\alpha} p_k(\mathbf{x}, h), \quad \bar{p}_k(\mathbf{x}) := \sup_{h \in \mathcal{C}_\alpha} p_k(\mathbf{x}, h), \quad k = 1, \dots, K. \quad (1)$$

We then define the *box credal set* at \mathbf{x} as

$$\square_{\mathbf{x}, \alpha} := \left\{ p \in \Delta_K : \underline{p}_k(\mathbf{x}) \leq p_k \leq \bar{p}_k(\mathbf{x}) \quad \forall k \right\}. \quad (2)$$

By construction, $\mathcal{Q}_{\mathbf{x}, \alpha} \subseteq \square_{\mathbf{x}, \alpha}$; thus, the box is a tractable outer approximation that preserves all classwise extrema. We state a simple, yet illustrative monotonicity property:

Proposition 2.1. *If $0 < \alpha_2 \leq \alpha_1 \leq 1$, then $\mathcal{C}_{\alpha_1} \subseteq \mathcal{C}_{\alpha_2}$ and $\mathcal{Q}_{\mathbf{x}, \alpha_1} \subseteq \mathcal{Q}_{\mathbf{x}, \alpha_2}$. Thus, for all k ,*

$$\underline{p}_k(\mathbf{x}; \alpha_1) \geq \underline{p}_k(\mathbf{x}; \alpha_2) \quad \text{and} \quad \bar{p}_k(\mathbf{x}; \alpha_1) \leq \bar{p}_k(\mathbf{x}; \alpha_2).$$

If a maximum-likelihood estimator $h^{\text{ML}} \in \mathcal{H}$ exists, then $\mathcal{Q}_{\mathbf{x}, 1} = \{p_k(\mathbf{x}, h^{\text{ML}})\}$ and $[\underline{p}_k(\mathbf{x}; 1), \bar{p}_k(\mathbf{x}; 1)] = \{p_k(\mathbf{x}, h^{\text{ML}})\}$. As $\alpha \downarrow 0$, $\mathcal{Q}_{\mathbf{x}, \alpha} \rightarrow \{h(\mathbf{x}) : L(h) > 0\}$, and the intervals expand accordingly to the coordinatewise infima/suprema over that limit set.

Proposition 2.1 shows that increasing the plausibility threshold α yields nested prediction sets and monotonically tighter classwise intervals. This monotonicity underpins the so-called *coverage–efficiency* trade-off used in our evaluation: larger α typically lowers coverage but improves efficiency (smaller sets), allowing α to be tuned to the desired operating point. In this vein, it is natural to evaluate set-valued predictions along two axes, *coverage* and *efficiency*.

Coverage. Given a set-valued predictor H , coverage is the probability that the ground-truth conditional distribution $p^*(\cdot | \mathbf{x})$ is contained in the predicted set:

$$C(H) = \mathbb{E}[\mathbf{1}\{p^*(\cdot | \mathbf{x}) \in H(\mathbf{x})\}], \quad (3)$$

where the expectation is over the marginal of \mathbf{x} on \mathcal{X} .

Efficiency. To reward informative (i.e., small) sets, we use the complement of the average interval width across classes (positively oriented: higher is better):

$$E(H) = 1 - \mathbb{E}\left[\frac{1}{K} \sum_{k=1}^K (\bar{p}_k(\mathbf{x}) - \underline{p}_k(\mathbf{x}))\right]. \quad (4)$$

Pragmatically, constructing relative-likelihood α -cuts by training ensembles to hit prescribed likelihood ratios is principled, but computationally heavy, and hypotheses tend to cluster near the MLE unless $\alpha \approx 1$, which is a poor fit for modern large models. To overcome this limitation, we propose an efficient method for credal prediction that is grounded in the notion of relative likelihood and inspired by techniques for the calibration of probabilistic classifiers, which we will call *decalibration*.

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3 EFFICIENT CREDAL PREDICTION THROUGH DECALIBRATION

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 164 We propose *decalibration* as a single-model route to plausibility: starting from the maximum-
 165 likelihood predictor h^{ML} , we deliberately distort predicted probabilities, thereby moving from bet-
 166 ter predictions (high likelihood) to worse ones (lower likelihood). However, to keep predictions
 167 plausible, we make sure to remain within a prescribed relative-likelihood budget $\alpha \in (0, 1]$. The
 168 probabilities reachable under this budget induce, for any query \mathbf{x} , classwise plausible intervals and
 169 hence a box credal set, without retraining or ensembling. Broadly speaking, we answer the follow-
 170 ing question: to what extent can we decrease or increase the predicted probabilities for a specific
 171 class before reaching a state where predictions become unfeasible (have relative likelihood $< \alpha$)?
 172

 173 Thus, the idea is to keep the likelihood semantics but make the search cheap: rather than training
 174 many “plausible” models, we start from the MLE and deliberately push its probabilities toward less
 175 likely configurations, while enforcing a global relative-likelihood budget α , as illustrated in Figure 1.
 176 This turns the classical likelihood-ratio view (“models within an LR ball are plausible”) into a post-
 177 hoc exploration of the model’s output space. As the budget is imposed on the training likelihood,
 178 any probability vector we produce is still supported by the data up to the chosen evidence level.
 179

 180 Operationally, we implement the exploration with simple, low-dimensional transforms of the MLE’s
 181 logits, expressive enough to traverse a wide range of alternative class probabilities yet requiring nei-
 182 ther retraining nor access to the backbone’s gradients. Compared to ensembles that approximate the
 183 same plausibility region by re-optimizing parameters, decalibration is orders of magnitude faster and
 184 model-agnostic, i.e., it works on top of any pretrained classifier. It is particularly suited to inference-
 185 only or API-gated systems, foundation models, LLMs, and multimodal encoders, where parameters
 186 are frozen or proprietary and retraining, fine-tuning, or ensembling is impractical or disallowed. At
 187 the same time, the outputs inherit clear interpretation, “probabilities reachable without losing more
 188 than an α -fraction of likelihood”, and the resulting intervals are nested as α increases.
 189

 190 Among many possible post-hoc maps on probabilities, we instantiate decalibration with a simple
 191 yet expressive family that operates on *logits*: we add a global bias vector $c \in \mathbb{R}^K$ to every ex-
 192 ample’s logits (both train and test) and then apply softmax. This choice is model-agnostic (no
 193 retraining or gradients), preserves the learned representation, and induces a concave change in training
 194 log-likelihood, which in turn makes the α -plausible set convex. Intuitively, c effects controlled
 195 *odds tilts* between classes; its softmax invariance under $c \mapsto c + t\mathbf{1}$ yields a natural identifiability
 196 hyperplane and keeps optimization well posed as we shall demonstrate now. Formally, consider a
 197 predictor that produces logits $z^{(n)} \in \mathbb{R}^K$ on the training set and logits $z(\mathbf{x}) \in \mathbb{R}^K$ for any test point
 198 \mathbf{x} . Let $c = (c_1, \dots, c_K)^\top \in \mathbb{R}^K$ and define, for each training point n and each class j ,
 199

$$p_j^{(n)}(c) = \frac{\exp(z_j^{(n)} + c_j)}{\sum_{\ell=1}^K \exp(z_\ell^{(n)} + c_\ell)}, \quad p_j(\mathbf{x}; c) = \frac{\exp(z_j(\mathbf{x}) + c_j)}{\sum_{\ell=1}^K \exp(z_\ell(\mathbf{x}) + c_\ell)}.$$

 200 Set $\Delta\ell(c) = \sum_{n=1}^N (\log p_{y^{(n)}}^{(n)}(c) - \log p_{y^{(n)}}^{(n)}(0))$ and $F(\alpha) = \{c \in \mathbb{R}^K : \Delta\ell(c) \geq \log \alpha\}$.
 201 Further, note that $\Delta\ell(c + t\mathbf{1}) = \Delta\ell(c)$ and $p_j(\mathbf{x}; c + t\mathbf{1}) = p_j(\mathbf{x}; c)$ for all $t \in \mathbb{R}$.
 202

 203 Concretely, this decalibration procedure fixes the family and its feasibility region $F(\alpha)$; what fol-
 204 lows establishes the key structural properties that make the method tractable: smooth concavity of
 205 $\Delta\ell$, convexity/compactness of the feasible set, and a convex-optimization characterization of the
 206 upper credal bound (Proposition 3.1). We then specialize to the one-dimensional slice $c = t\mathbf{e}_k$,
 207 yielding endpoint formulas and simple convex programs for the scalar case (Corollary 3.1).
 208

 209 **Proposition 3.1.** *Let $H := \{c \in \mathbb{R}^K : \mathbf{1}^\top c = 0\}$ be the identifiability hyperplane. Then:*

 210 (a) $\Delta\ell$ is C^∞ and concave on \mathbb{R}^K , with $\nabla\Delta\ell(c) = \sum_{n=1}^N (\mathbf{e}_{y^{(n)}} - p^{(n)}(c))$ and

$$\nabla^2\Delta\ell(c) = - \sum_{n=1}^N \left(\text{Diag}(p^{(n)}(c)) - p^{(n)}(c) p^{(n)}(c)^\top \right) \preceq 0.$$

 211 Moreover, $\Delta\ell$ is strictly concave on H provided at least two classes appear in \mathcal{D} , namely,
 212 $N_j > 0$ for at least two j , where $N_j = \#\{n : y^{(n)} = j\}$. Consequently, $F(\alpha)$ is convex
 213 and translation-invariant along $\text{span}\{\mathbf{1}\}$. The section $F_H(\alpha) := F(\alpha) \cap H$ is nonempty
 214 and compact whenever at least two classes appear.
 215

216 (b) For each fixed \mathbf{x} and k , the map $c \mapsto \log p_k(\mathbf{x}; c) = (z_k(\mathbf{x}) + c_k) - \log \sum_{\ell=1}^K e^{z_\ell(\mathbf{x}) + c_\ell}$ is
 217 C^∞ and concave on \mathbb{R}^K with $\nabla \log p_k(\mathbf{x}; c) = \mathbf{e}_k - p(\mathbf{x}; c)$ and

219
$$\nabla^2 \log p_k(\mathbf{x}; c) = -\left(\text{Diag}(p(\mathbf{x}; c)) - p(\mathbf{x}; c) p(\mathbf{x}; c)^\top\right) \preceq 0.$$

 220

221 In particular, $c_k \mapsto p_k(\mathbf{x}; c)$ is strictly increasing (holding c_j , $j \neq k$, fixed), and $c_j \mapsto$
 222 $p_k(\mathbf{x}; c)$ is strictly decreasing for $j \neq k$.

223 (c) The upper credal bound is the value of the convex optimization problem

225
$$\bar{p}_k(\mathbf{x}) = \sup_{c \in F(\alpha)} p_k(\mathbf{x}; c) = \sup_{c \in F(\alpha)} \exp(\log p_k(\mathbf{x}; c)) = \exp\left(\sup_{c \in F(\alpha)} \log p_k(\mathbf{x}; c)\right),$$

 226

227 and the inner problem $\sup_{c \in F(\alpha)} \log p_k(\mathbf{x}; c)$ is a concave maximization, i.e., a convex
 228 optimization. An optimizer always exists on $F_H(\alpha)$, and is unique modulo addition of
 229 constants along $\text{span}\{\mathbf{1}\}$.

230 (d) The lower credal bound $\underline{p}_k(\mathbf{x}) = \inf_{c \in F(\alpha)} p_k(\mathbf{x}; c)$ is, in general, not a convex optimiza-
 231 tion problem. Nevertheless, when $F_H(\alpha)$ is compact, a minimizer exists and is attained at
 232 an extreme point of the convex set $F_H(\alpha)$.

233 We prove Proposition 3.1 in Appendix A. Proposition 3.1 (a) guarantees that the likelihood-based
 234 feasibility region is a well-posed convex set (compact on the hyperplane H), so optimization over it
 235 is stable. Moreover, (b) shows the test objective inherits the same curvature structure as the training
 236 likelihood. Together these yield (c): the *upper* credal bound is the value of a single convex program
 237 with a unique optimizer on H , while (d) clarifies that the *lower* bound is generally nonconvex and
 238 lives on the boundary/extreme points of $F_H(\alpha)$. Practically, we compute upper bounds reliably by
 239 convex solvers, and treat lower bounds via boundary exploration or by adopting tractable 1-D slices.

240 It is also natural to restrict to class-specific biases $c = t \mathbf{e}_k$. On this one-dimensional slice the fea-
 241 sibility set becomes an interval and the class- k probability is monotone in t , allowing exact bounds
 242 via interval endpoints, which we show in the following.

243 **Corollary 3.1.** Now restrict to shifts of the form $c = t \mathbf{e}_k$, $t \in \mathbb{R}$ and define

244
$$\Delta\ell_k(t) := \Delta\ell(t \mathbf{e}_k), \quad F_k(\alpha) := \{t \in \mathbb{R} : \Delta\ell_k(t) \geq \log \alpha\} = \{t : t \mathbf{e}_k \in F(\alpha)\}.$$

245 Then the following hold:

246 (a) $\Delta\ell_k$ is C^2 and strictly concave on \mathbb{R} . Consequently $F_k(\alpha)$ is a nonempty interval; if
 247 $0 < N_k < N$, it is compact $[t_k^-, t_k^+]$, otherwise it is a closed (possibly half-infinite) interval.

248 (b) For every fixed \mathbf{x} , the map $t \mapsto p_k(\mathbf{x}; t \mathbf{e}_k)$ is strictly increasing on \mathbb{R} .

249 (c) With $t_k^- = \inf F_k(\alpha)$ and $t_k^+ = \sup F_k(\alpha)$,

250
$$\underline{p}_k(\mathbf{x}) = p_k(\mathbf{x}; t_k^- \mathbf{e}_k), \quad \bar{p}_k(\mathbf{x}) = p_k(\mathbf{x}; t_k^+ \mathbf{e}_k).$$

251 (d) The endpoints t_k^-, t_k^+ solve the convex programs

252
$$\min_{t \in \mathbb{R}} t \text{ s.t. } -\Delta\ell_k(t) \leq -\log \alpha, \quad \min_{t \in \mathbb{R}} (-t) \text{ s.t. } -\Delta\ell_k(t) \leq -\log \alpha.$$

253 We prove Corollary 3.1 in Appendix A. Algorithmically, the scalar case reduces computing
 254 $(\underline{p}_k(\mathbf{x}), \bar{p}_k(\mathbf{x}))$ to finding the two endpoints t_k^- and t_k^+ of the feasible interval, e.g., by bisection
 255 on $\Delta\ell_k(t) = \log \alpha$; the bounds are then $p_k(\mathbf{x}; t_k^- \mathbf{e}_k)$ and $p_k(\mathbf{x}; t_k^+ \mathbf{e}_k)$. Throughout the empirical
 256 evaluation, we focus on the one-dimensional setting, which admits convexity of the lower and upper
 257 probability bounds. We defer details about the practical computation of the bounds to Appendix B.

258 4 EMPIRICAL RESULTS

259 In this section, we empirically evaluate our proposed method with the following **research objectives**
 260 in mind. First, we assess the quality of the uncertainty representation by standard metrics and show

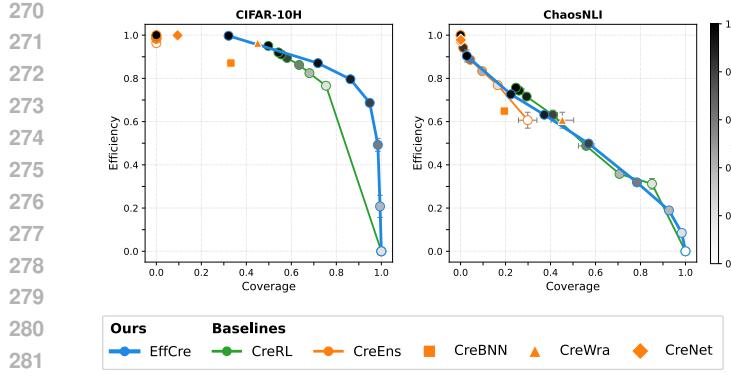


Figure 2: Coverage versus Efficiency. Comparison on CIFAR-10 and CHAOSNLI. The plot highlights the Pareto trade-off: higher coverage often requires lower efficiency, while EffCre consistently advances the Pareto front over baselines.

its strong performance compared to baselines in Section 4.1. Second, we evaluate the method on common downstream tasks and emphasize the competitive performance—while far more efficient—when compared to baselines in Section 4.2. Third, we highlight the distinctive advantage of our method that it can construct uncertainty representations for large architectures such as TabPFN or CLIP, where retraining is infeasible in Sections 4.3 and 4.4.

Thus, we present scenarios where our method (EffCre, see Appendix B for implementation details) newly enables the construction of uncertainty representations and, where possible, we compare it to the following suitable baselines, which represent the current state-of-the-art in credal prediction: Credal Wrapper (CreWra) (Wang et al., 2025a), Credal Ensembling (CreEns) (Nguyen et al., 2025), Credal Bayesian Neural Networks (CreBNN) (Caprio et al., 2024a), Credal Interval Net (CreNet) (Wang et al., 2025b), and Credal Relative Likelihood (CreRL) (Löhr et al., 2025). The code for all experiments is published in a Github repository¹ and the detailed experimental setup can be found in Appendix D.

4.1 COVERAGE VERSUS EFFICIENCY

We compare our method to the baselines in terms of coverage (3) and efficiency (4). Ideally, a credal predictor generates sets of a small size (high efficiency) that cover the ground-truth conditional distribution (high coverage). Moreover, because the relative importance of coverage and efficiency may vary across applications, methods that allow to trade-off one against the other, depending on the setting, are favored.

Setup. We train a multilayer perceptron (MLP) on the embeddings of CHAOSNLI and a ResNet18 (He et al., 2016) on CIFAR-10 (Krizhevsky et al., 2009) (Schmarje et al., 2022). The models are trained with regular labels and evaluated against ground-truth distributions. Such ground-truth distributions are derived from multiple annotator labels, available through CIFAR-10H (Peterson et al., 2019) for the CIFAR-10 test set, while CHAOSNLI provides them directly.

Results. We present results for coverage versus the efficiency in Figure 2. The CIFAR-10 dataset shows that our method Pareto dominates CreRL in the high coverage region, while performing similarly in the medium coverage region. In addition, EffCre Pareto dominates the CreBNN, CreWra, CreNet baselines. For the CHAOSNLI dataset our method performs similarly to CreRL in the high coverage region and similar to CreEns in the low coverage region. Whereas the aforementioned baselines can only traverse the low coverage *or* high coverage regions, our method can traverse both regions, allowing a user to specify almost any coverage or efficiency value. Furthermore, our method dominates CreBNN with $\alpha = 0.95$, whereas it performs similarly to CreNet and CreWra, again with the caveat that these methods are restricted to the low coverage region. For results on an additional dataset, we refer to Appendix E.1. Lastly, note that, while in Section 2, we assume $\alpha > 0$, in the coverage and efficiency experiments we explicitly use $\alpha = 0$ as a verification that our method

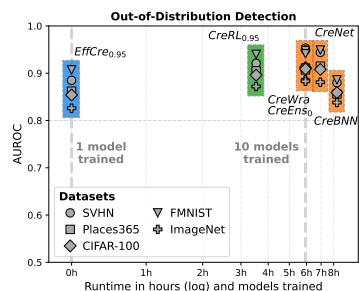


Figure 3: Out-of-Distribution Detection. Performance (AUROC, based on epistemic uncertainty) as a function of required number of models and training time (in hours).

¹<https://anonymous.4open.science/r/efficient-credal-prediction/>.

324 produces sufficiently diverse sets. Broadly speaking, if our method is not able to generate dense
 325 credal sets for $\alpha = 0$, we cannot expect it to reliably reach the edges of the plausible probability
 326 intervals.

328 4.2 OUT-OF-DISTRIBUTION DETECTION

330 Besides coverage and efficiency, out-of-distribution detection is a commonly used proxy to evaluate
 331 the quality of credal predictions. Modern machine learning systems should be able to detect whether
 332 the data they receive is in-distribution (ID) or out-of-distribution (OOD) as strong performance on
 333 this task is an indication of a good epistemic uncertainty representation. So far, many approaches
 334 have been unable to provide epistemic uncertainty representation due to prohibitive computational
 335 costs; our method directly addresses this. To demonstrate this, we analyze the trade-off between the
 336 training time and performance, in terms of AUROC, for our method and compare it to baselines.

337 **Setup.** We train a ResNet18 on CIFAR-10, which serves as the ID data and introduce it to several
 338 other datasets that serve as the OOD data. Epistemic uncertainty is quantified based on a commonly-
 339 used measure from [Abellán et al. \(2006\)](#),

$$340 \quad \text{EU}(\mathcal{Q}_x) := \bar{S}(\mathcal{Q}_x) - \underline{S}(\mathcal{Q}_x), \quad (5)$$

341 where $\bar{S}(\mathcal{Q}_x) = \sup_{p(\cdot|x) \in \mathcal{Q}_x} S(p(\cdot|x))$, and $\underline{S}(\mathcal{Q}_x)$ defined analogously, are the upper and lower
 342 Shannon entropy², respectively.

343 **Results.** We report the OOD detection results alongside training time in Figure 3 and provide
 344 additional results and hyperparameter ablations in Appendix F.1. Since any approach requires at
 345 least one trained model (e.g., an MLE predictor), our method EffCre comes with no extra training
 346 cost, as it can be applied post-hoc in a highly efficient manner. Although the baselines achieve
 347 slightly higher AUROC scores on the OOD task, they rely on ensembles of models, which demand
 348 a substantial number of members (e.g., 10 models) and therefore significantly increase training
 349 time. While CreWra, CreEns, CreNet, and CreBNN require full training of each ensemble member,
 350 CreRL is slightly more efficient due to its early-stopping criterion. However, our approach EffCre
 351 is substantially more efficient compared to all baselines, enabling the application even to large-scale
 352 models.

354 4.3 IN-CONTEXT LEARNING WITH TABPFN

356 To highlight the ability of our method to be applied
 357 in a *post-hoc* manner, requiring only logits, we apply
 358 it to a foundation model for tabular data. TabPFN
 359 ([Hollmann et al., 2025](#)) is a prior-fitted transformer,
 360 trained on a large number of synthetic datasets. It
 361 uses in-context learning, based on all training data
 362 and additional exemplary instances, to make predic-
 363 tions, while not requiring any gradient-based chang-
 364 ing of its weights. Therefore, the baselines used in
 365 the experiments in Sections 4.1 and 4.2 cannot be ap-
 366 plied as they require training (an ensemble), which,
 367 besides being challenging due to computational cost,
 368 also requires the *original* training data, which we do
 369 not have access to.

370 **Setup Coverage Versus Efficiency.** To illustrate
 371 the proper uncertainty representation generated by
 372 using our method on top of TabPFN, we compute
 373 the coverage and efficiency of the predicted credal
 374 sets by applying it to all multi-class datasets³ from
 375 the TABARENA benchmark ([Erickson et al., 2025](#)).
 376 Since these datasets do not provide ground-truth

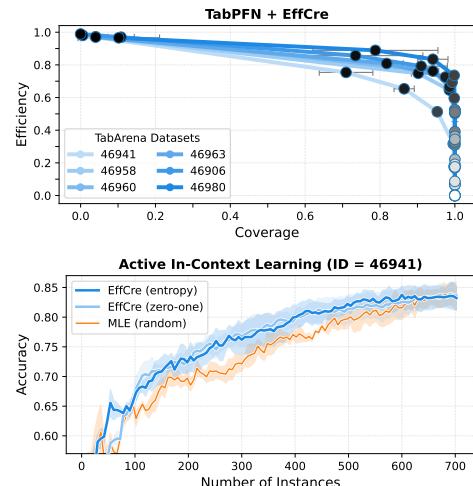


Figure 4: EffCre used with TabPFN.
Top: Coverage versus efficiency performance all multi-class TABARENA datasets.
Bottom: Active In-Context Learning performance versus the random baseline.

²Shannon entropy: $S(p(\cdot|x)) = -\sum_{k=1}^K p_k(\mathbf{x}) \log p_k(\mathbf{x})$ with $0 \log 0 = 0$ by definition.

³The datasets included in TabArena v0.1. This collection may be subject to change.

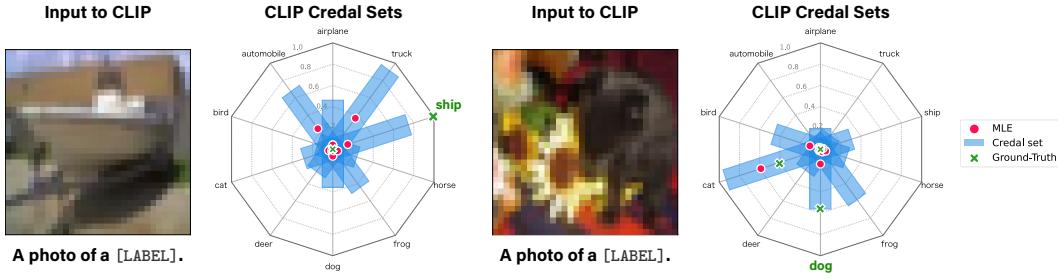


Figure 5: Credal Prediction with CLIP. Examples from CIFAR-10H with high epistemic uncertainty (left) and high aleatoric uncertainty (right) as predicted by applying our method on CLIP.

conditional distributions, we propose a simple way to create *semi-synthetic ground-truth distributions* to allow evaluation by coverage and efficiency. Details about this experiment and the process of creating such distributions can be found in Appendix E.3 and Appendix D.5, respectively.

Results Coverage Versus Efficiency. We show the coverage and efficiency results in Figure 4, confirming that uncertainty representations obtained by applying our method to TabPFN provide small sets that often include the ground-truth distribution.

In addition, we perform active in-context learning, which has become an important task in the context of foundation models since labeling represents the limiting factor to leveraging pre-trained models effectively. Ideally, a model—equipped with a reliable (epistemic) uncertainty representation—is able to sample informative instances, which, when used for in-context learning, improve the performance more than a random sample of instances would.

Setup Active Learning. Specifically, we quantify epistemic uncertainty using (5) and additionally use a measure based on zero-one-loss, which has been shown to perform well on similar tasks (Hofman et al., 2024). Concretely,

$$\text{EU}(\mathcal{Q}_x) = \max_{p(\cdot|x), p'(\cdot|x) \in \mathcal{Q}_x} \max_k p_k(x) - p_{\arg \max_k p'_k(x)}(x). \quad (6)$$

We perform this task for a number of TABARENA datasets using $\alpha = 0.8$. For more details regarding the experimental setup and additional results, we refer to Appendix E.3.

Results Active Learning. We present the results in Figure 4. This highlights the ability of our method to represent its epistemic uncertainty well, in order to sample the most informative instances accordingly. An ablation on α in the active in-context learning setting can be found in Appendix F.2.

4.4 ZERO-SHOT CLASSIFICATION WITH CLIP-BASED MODELS

We demonstrate the flexibility of our method by creating credal sets for vision-language models (VLMs), including CLIP (Radford et al., 2021), SigLIP (Zhai et al., 2023), SigLIP-2 (Tschanen et al., 2025), and BiomedCLIP (Zhang et al., 2024).

Setup Coverage Versus Efficiency. To demonstrate the proper uncertainty representation generated by using our method on top of CLIP-based models—something that is computationally prohibitive for the baselines—we compute the coverage and efficiency of the predicted credal sets by applying it to CIFAR-10, using CIFAR-10H as ground-truth distributions. Therefore, we turn the models into zero-shot classifiers by reformulating the label set into natural-language templates and comparing the resulting text embeddings with image embeddings (see Appendix D.6 for details and performance results).

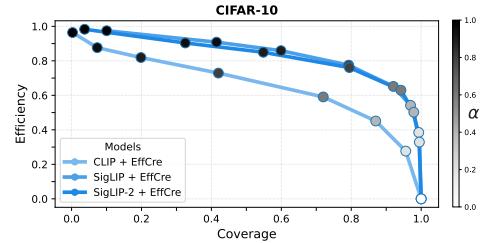


Figure 6: EffCre used with CLIP-based models. We demonstrate the performance of EffCre by applying it to CLIP, SigLIP, and SigLIP-2 without retraining—something that can't be done by the baselines.

432 **Results Coverage Versus Efficiency.** Figure 6 shows performance on the coverage-efficiency trade-
 433 off, with our method performing well, being able to reach regions with high coverage and high
 434 efficiency for CLIP, SigLIP, and SigLIP-2.

435 To further highlight the usefulness of our method, we compare the predicted credal sets to human
 436 uncertainty patterns. To visualize credal sets beyond three classes, we propose *credal spider plots*
 437 where each axis corresponds to a class and intervals mark upper and lower probabilities (see Ap-
 438 pendix C for a detailed guide). Profiles such as MLE predictions or ground-truth distributions can
 439 be overlaid for direct comparison.

440 **Setup Qualitative Evaluation.** For the visual evaluation, we apply our method on top of CLIP-
 441 based models and predict credal sets for CIFAR-10 while using CIFAR-10H to reference ground-truth
 442 distributions. We sort and present instances from CIFAR-10-H’s test split based on the aleatoric and
 443 epistemic uncertainties represented by the predicted credal sets of the CLIP-based models.

444 **Results Qualitative Evaluation.** Figure 5 presents two instances from CIFAR-10-H’s test split: the
 445 left image is misclassified by the MLE due to the unusual context of the ship being out of water in a dock.
 446 Our method reflects the resulting epistemic uncertainty with plausible intervals across all
 447 classes and higher probability intervals for class ship, truck, and automobile. The right image shows
 448 an animal in an ambiguous pose: the ground-truth distribution splits mass between dog and cat,
 449 representing aleatoric uncertainty. Our method represents this uncertainty well, covering the true
 450 distribution even though the MLE misclassifies the image as cat. Additional multilingual examples
 451 and further results are shown in Appendix E.4.

456 5 RELATED WORK

457 Credal sets originate in imprecise-probability literature (Levi, 1978; Walley, 1991). In machine
 458 learning, credal sets offer an appealing way to represent epistemic uncertainty, motivating work on
 459 (credal) uncertainty quantification (Hüllermeier et al., 2022; Sale et al., 2023; Hofman et al., 2024;
 460 Chau et al., 2025a), calibration (Jürgens et al., 2025; Chau et al., 2025b), self-supervision (Lienen
 461 & Hüllermeier, 2021), and learning theory (Caprio et al., 2024b). A consensus on construction has
 462 not emerged, current practice spans a variety of designs that trade theoretical guarantees against
 463 practicality in different ways. Some methods use conformal prediction to obtain credal sets with
 464 finite-sample validity guarantees (Javanmardi et al., 2024). Others form sets by aggregating multiple
 465 predictors, whether standard deep ensembles (Wang et al., 2025a; Nguyen et al., 2025), interval-
 466 head networks trained with tailored losses (Wang et al., 2025b), or Bayesian ensembles built from
 467 posterior samples (Caprio et al., 2024a). Recently, Löhr et al. (2025) adopted a relative-likelihood
 468 criterion (Birnbaum, 1962; Antonucci et al., 2012; Senge et al., 2014) to form credal sets in machine
 469 learning settings.

470 Ensemble training underpins much of the prior work, but for large model architectures, retraining—
 471 even once—is rarely feasible. This, in turn, has led to lightweight alternatives for representing
 472 uncertainty. One line of work focuses on single forward pass methods to estimate uncertainty (van
 473 Amersfoort et al., 2020; Mukhoti et al., 2023), e.g., via distance-based features (Liu et al., 2020)
 474 or evidential Dirichlet heads (Sensoy et al., 2018; Amini et al., 2020), though recently evidential
 475 variants were criticized (Bengs et al., 2023; Jürgens et al., 2024). In contrast, approximate Bayesian
 476 inference techniques such as Laplace approximations (Daxberger et al., 2021; Weber et al., 2025)
 477 and variational last-layer or sub-ensemble approaches (Valdenegro-Toro, 2019; Kristiadi et al., 2020;
 478 Harrison et al., 2024) reduce cost by training only limited parts of the network. Similarly, others
 479 compress ensembles by sharing parameters (Durasov et al., 2021; Laurent et al., 2023) or by distill-
 480 ing ensemble knowledge into a single model (Malinin et al., 2020; Penso et al., 2022). Another line
 481 of work focuses on large models such as diffusion or language models and explores low-rank adap-
 482 tation to efficiently build ensembles for uncertainty quantification (Berry et al., 2024; Yang et al.,
 483 2024; Wang et al., 2024). Yet, computationally efficient methods for credal prediction remain absent
 484 from the literature.

486

6 DISCUSSION

488 We presented a post-hoc, model-agnostic method for credal prediction that captures epistemic un-
 489 certainty as class-wise *plausible probability intervals* derived from relative likelihood. The key idea,
 490 *decalibration*, perturbs a trained model’s logits under a global likelihood-ratio budget, thereby ex-
 491 ploring less-likely yet still plausible predictions without retraining. We formally analyze decalibra-
 492 tion and show that the logit-shift feasibility set is convex (compact on an identifiability hyperplane).
 493 In the one-logit (class-specific) case, each interval endpoint is obtained by solving a small convex
 494 program, readily handled by off-the-shelf optimizers. Empirically, our method matches or surpasses
 495 baselines on coverage–efficiency and is competitive for OOD detection, while cutting computation
 496 by orders of magnitude. Because it is post-hoc and needs only logits, we apply it to large pretrained
 497 models—including TabPFN and CLIP—for which ensemble retraining is impractical.
 498

499 **Limitations and Future Work.** We primarily deploy the one-logit (class-specific) variant of our
 500 logit-shift family. The fully coupled case remains open; upper bounds still reduce to a convex
 501 program, whereas lower bounds are non-convex. Developing reliable relaxations, certificates, or
 502 approximation schemes, and clarifying their statistical trade-offs, is a promising direction. Open-
 503 vocabulary, multimodal models such as CLIP raise additional challenges. Because the label set is
 504 chosen at inference time, uncertainty should reflect not only prediction but also label selection and
 505 prompt choice. Designing credal formalisms and evaluation protocols for this setting is an important
 506 avenue for future work.
 507

508 **Reproducibility Statement.** We are committed to ensuring the reproducibility of our results. To
 509 this end, we provide our **code** in the following Github repo <https://anonymous.4open.science/r/efficient-credal-prediction/>. The **theoretical results** in Section 3 are
 510 accompanied by proofs in Appendix A and, where necessary, the assumptions have been discussed.
 511 The full **experimental setup**, used to produce the results presented in Section 4 and Appendices E
 512 and F, is provided in Appendix D. In particular, we discuss details about **datasets**, including the
 513 transformation performed on the input to models and the creation of (semi-synthetic) ground truth
 514 distributions in Appendices D.2 and D.5. The **models** we use, and our implementation of them, are
 515 discussed in detail in Appendix D.1. We elaborate on the implementation of all **baselines** in Ap-
 516 pendix D.3 and details regarding the practical implementation of **our method**, that are not discussed
 517 in the main paper, are provided in Appendix B.
 518

519

REFERENCES

520 Joaquín Abellán, George J. Klir, and Serafín Moral. Disaggregated total uncertainty measure for
 521 credal sets. *Int. J. Gen. Syst.*, 35(1):29–44, 2006.

522 Alexander Amini, Wilko Schwarting, Ava Soleimany, and Daniela Rus. Deep evidential regression.
 523 In Hugo Larochelle, Marc’Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan-Tien
 524 Lin (eds.), *Advances in Neural Information Processing Systems 33: Annual Conference on Neural
 525 Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020.

526 Alessandro Antonucci, Marco E. G. V. Cattaneo, and Giorgio Corani. Likelihood-based robust clas-
 527 sification with bayesian networks. In Salvatore Greco, Bernadette Bouchon-Meunier, Giulianella
 528 Coletti, Mario Fedrizzi, Benedetto Matarazzo, and Ronald R. Yager (eds.), *Advances in Computa-
 529 tional Intelligence - 14th International Conference on Information Processing and Management
 530 of Uncertainty in Knowledge-Based Systems, IPMU 2012, Catania, Italy, July 9-13, 2012, Pro-
 531 ceedings, Part III*, volume 299 of *Communications in Computer and Information Science*, pp.
 532 491–500. Springer, 2012.

533 Viktor Bengs, Eyke Hüllermeier, and Willem Waegeman. On second-order scoring rules for epis-
 534 temic uncertainty quantification. In Andreas Krause, Emma Brunskill, Kyunghyun Cho, Barbara
 535 Engelhardt, Sivan Sabato, and Jonathan Scarlett (eds.), *International Conference on Machine
 536 Learning, ICML 2023, 23-29 July 2023, Honolulu, Hawaii, USA*, volume 202 of *Proceedings of
 537 Machine Learning Research*, pp. 2078–2091. PMLR, 2023.

538 Lucas Berry, Axel Brando, and David Meger. Shedding light on large generative networks: Es-
 539 timating epistemic uncertainty in diffusion models. In *Conference on Uncertainty in Artificial
 Intelligence*, 2024.

540 Allan Birnbaum. On the foundations of statistical inference. *Journal of the American Statistical
541 Association*, 57(298):269–306, 1962.
542

543 Bernd Bischl, Giuseppe Casalicchio, Taniya Das, Matthias Feurer, Sebastian Fischer, Pieter Gijs-
544 bers, Subhaditya Mukherjee, Andreas C Müller, László Németh, Luis Oala, Lennart Purucker,
545 Sahithya Ravi, Jan N van Rijn, Prabhant Singh, Joaquin Vanschoren, Jos van der Velde, and Mar-
546 cel Wever. Openml: Insights from 10 years and more than a thousand papers. *Patterns*, 6(7):
547 101317, 2025.

548 Christopher Bülte, Nina Horat, Julian Quinting, and Sebastian Lerch. Uncertainty quantification for
549 data-driven weather models. *Artificial Intelligence for the Earth Systems*, 2025.
550

551 Michele Caprio, Souradeep Dutta, Kuk Jin Jang, Vivian Lin, Radoslav Ivanov, Oleg Sokolsky, and
552 Insup Lee. Credal bayesian deep learning. *Trans. Mach. Learn. Res.*, 2024, 2024a.

553 Michele Caprio, Maryam Sultana, Eleni Elia, and Fabio Cuzzolin. Credal learning theory. In Amir
554 Globersons, Lester Mackey, Danielle Belgrave, Angela Fan, Ulrich Paquet, Jakub M. Tomczak,
555 and Cheng Zhang (eds.), *Advances in Neural Information Processing Systems 38: Annual Con-
556 ference on Neural Information Processing Systems 2024, NeurIPS 2024, Vancouver, BC, Canada,
557 December 10 - 15, 2024*, 2024b.

558

559 Siu Lun Chau, Michele Caprio, and Krikamol Muandet. Integral imprecise probability metrics.
560 *arXiv preprint arXiv:2505.16156*, 2025a.

561 Siu Lun Chau, Antonin Schrab, Arthur Gretton, Dino Sejdinovic, and Krikamol Muandet. Credal
562 two-sample tests of epistemic uncertainty. In Yingzhen Li, Stephan Mandt, Shipra Agrawal,
563 and Mohammad Emtiyaz Khan (eds.), *International Conference on Artificial Intelligence and
564 Statistics, AISTATS 2025, Mai Khao, Thailand, 3-5 May 2025*, volume 258 of *Proceedings of
565 Machine Learning Research*, pp. 127–135. PMLR, 2025b.

566

567 David Roxbee Cox and David Victor Hinkley. *Theoretical statistics*. CRC Press, 1979.

568

569 Erik A. Daxberger, Agustinus Kristiadi, Alexander Immer, Runa Eschenhagen, Matthias Bauer, and
570 Philipp Hennig. Laplace redux - effortless bayesian deep learning. In Marc’Aurelio Ranzato,
571 Alina Beygelzimer, Yann N. Dauphin, Percy Liang, and Jennifer Wortman Vaughan (eds.), *Ad-
572 vances in Neural Information Processing Systems 34: Annual Conference on Neural Information
573 Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual*, pp. 20089–20103, 2021.

574

575 Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale
576 hierarchical image database. In *2009 IEEE Computer Society Conference on Computer Vision
577 and Pattern Recognition (CVPR 2009), 20-25 June 2009, Miami, Florida, USA*, pp. 248–255.
IEEE Computer Society, 2009.

578

579 Nikita Durasov, Timur M. Bagautdinov, Pierre Baqué, and Pascal Fua. Maskensembles for uncer-
580 tainty estimation. In *IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2021,
581 virtual, June 19-25, 2021*, pp. 13539–13548. Computer Vision Foundation / IEEE, 2021.

582

583 Anthony William Fairbank Edwards. Likelihood. In *The New Palgrave Dictionary of Economics*,
584 pp. 7857–7860. Springer, 2018.

585

586 Nick Erickson, Lennart Purucker, Andrej Tschalzev, David Holzmüller, Prateek Mutalik Desai,
587 David Salinas, and Frank Hutter. Tabarena: A living benchmark for machine learning on tab-
588 ular data. *CoRR*, abs/2506.16791, 2025.

589

590 James Harrison, John Willes, and Jasper Snoek. Variational bayesian last layers. In *The Twelfth
591 International Conference on Learning Representations, ICLR 2024, Vienna, Austria, May 7-11,
592 2024*. OpenReview.net, 2024.

593

594 Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recog-
595 nition. In *2016 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2016, Las
596 Vegas, NV, USA, June 27-30, 2016*, pp. 770–778. IEEE Computer Society, 2016.

594 Paul Hofman, Yusuf Sale, and Eyke Hüllermeier. Quantifying aleatoric and epistemic uncertainty:
 595 A credal approach. In *ICML 2024 Workshop on Structured Probabilistic Inference & Generative*
 596 *Modeling*, 2024.

597

598 Noah Hollmann, Samuel Müller, Katharina Eggensperger, and Frank Hutter. Tabpfn: A transformer
 599 that solves small tabular classification problems in a second. *arXiv preprint arXiv:2207.01848*,
 600 2022.

601

602 Noah Hollmann, Samuel Müller, Lennart Purucker, Arjun Krishnakumar, Max Körfer, Shi Bin Hoo,
 603 Robin Tibor Schirrmeister, and Frank Hutter. Accurate predictions on small data with a tabular
 604 foundation model. *Nat.*, 637(8044):319–326, 2025.

605

606 Eyke Hüllermeier and Willem Waegeman. Aleatoric and epistemic uncertainty in machine learning:
 607 An introduction to concepts and methods. *Machine learning*, 110(3):457–506, 2021.

608

609 Eyke Hüllermeier, Sébastien Destercke, and Mohammad Hossein Shaker. Quantification of credal
 610 uncertainty in machine learning: A critical analysis and empirical comparison. In James Cussens
 611 and Kun Zhang (eds.), *Uncertainty in Artificial Intelligence, Proceedings of the Thirty-Eighth*
 612 *Conference on Uncertainty in Artificial Intelligence, UAI 2022, 1-5 August 2022, Eindhoven, The*
 613 *Netherlands*, volume 180 of *Proceedings of Machine Learning Research*, pp. 548–557. PMLR,
 2022.

614

615 Alireza Javanmardi, David Stutz, and Eyke Hüllermeier. Conformalized credal set predictors. In
 616 Amir Globersons, Lester Mackey, Danielle Belgrave, Angela Fan, Ulrich Paquet, Jakub M. Tom-
 617 czak, and Cheng Zhang (eds.), *Advances in Neural Information Processing Systems 38: An-*
 618 *nual Conference on Neural Information Processing Systems 2024, NeurIPS 2024, Vancouver, BC,*
 619 *Canada, December 10 - 15, 2024*, 2024.

620

621 Mira Jürgens, Nis Meinert, Viktor Bengs, Eyke Hüllermeier, and Willem Waegeman. Is epistemic
 622 uncertainty faithfully represented by evidential deep learning methods? In *Forty-first Interna-*
 623 *tional Conference on Machine Learning, ICML 2024, Vienna, Austria, July 21-27, 2024*. Open-
 624 Review.net, 2024.

625

626 Mira Jürgens, Thomas Mortier, Eyke Hüllermeier, Viktor Bengs, and Willem Waegeman. A calibra-
 627 tion test for evaluating set-based epistemic uncertainty representations. *CoRR*, abs/2502.16299,
 2025.

628

629 Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In Yoshua Bengio
 630 and Yann LeCun (eds.), *3rd International Conference on Learning Representations, ICLR 2015,*
 631 *San Diego, CA, USA, May 7-9, 2015, Conference Track Proceedings*, 2015.

632

633 Agustinus Kristiadi, Matthias Hein, and Philipp Hennig. Being bayesian, even just a bit, fixes
 634 overconfidence in relu networks. In *Proceedings of the 37th International Conference on Machine*
 635 *Learning, ICML 2020, 13-18 July 2020, Virtual Event*, volume 119 of *Proceedings of Machine*
 636 *Learning Research*, pp. 5436–5446. PMLR, 2020.

637

638 Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images.
 639 2009.

640

641 Olivier Laurent, Adrien Lafage, Enzo Tartaglione, Geoffrey Daniel, Jean-Marc Martinez, Andrei
 642 Bursuc, and Gianni Franchi. Packed ensembles for efficient uncertainty estimation. In *The*
 643 *Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda,*
 644 *May 1-5, 2023*. OpenReview.net, 2023.

645

646 Isaac Levi. On indeterminate probabilities. In *Foundations and Applications of Decision Theory:*
 647 *Volume I Theoretical Foundations*, pp. 233–261. Springer, 1978.

648

649 Yucen Lily Li, Daohan Lu, Polina Kirichenko, Shikai Qiu, Tim G. J. Rudner, C. Bayan Bruss,
 650 and Andrew Gordon Wilson. Out-of-distribution detection methods answer the wrong questions.
 651 *CoRR*, abs/2507.01831, 2025.

648 Julian Lienen and Eyke Hüllermeier. Credal self-supervised learning. In Marc'Aurelio Ranzato,
 649 Alina Beygelzimer, Yann N. Dauphin, Percy Liang, and Jennifer Wortman Vaughan (eds.), *Ad-*
 650 *vances in Neural Information Processing Systems 34: Annual Conference on Neural Information*
 651 *Processing Systems 2021, NeurIPS 2021, December 6-14, 2021, virtual*, pp. 14370–14382, 2021.

652 Jeremiah Z. Liu, Zi Lin, Shreyas Padhy, Dustin Tran, Tania Bedrax-Weiss, and Balaji Lakshmi-
 653 narayanan. Simple and principled uncertainty estimation with deterministic deep learning via
 654 distance awareness. In Hugo Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina
 655 Balcan, and Hsuan-Tien Lin (eds.), *Advances in Neural Information Processing Systems 33: An-*
 656 *nual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12,*
 657 *2020, virtual*, 2020.

658 Timo Löhr, Michael Ingrisch, and Eyke Hüllermeier. Towards aleatoric and epistemic uncertainty in
 659 medical image classification. In *International Conference on Artificial Intelligence in Medicine*,
 660 pp. 145–155. Springer, 2024.

662 Timo Löhr, Paul Hofman, Felix Mohr, and Eyke Hüllermeier. Credal prediction based on relative
 663 likelihood. *CoRR*, abs/2505.22332, 2025.

664 Ilya Loshchilov and Frank Hutter. SGDR: stochastic gradient descent with warm restarts. In *5th*
 665 *International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26,*
 666 *2017, Conference Track Proceedings*. OpenReview.net, 2017.

668 Andrey Malinin, Bruno Mloedeniec, and Mark J. F. Gales. Ensemble distribution distillation. In
 669 *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia,*
 670 *April 26-30, 2020*. OpenReview.net, 2020.

671 Valentin Margraf, Marcel Wever, Sandra Gilhuber, Gabriel Marques Tavares, Thomas Seidl, and
 672 Eyke Hüllermeier. Alpbench: A benchmark for active learning pipelines on tabular data. *CoRR*,
 673 abs/2406.17322, 2024.

674 Eric Stefan Miele, Nicole Ludwig, and Alessandro Corsini. Multi-horizon wind power forecasting
 675 using multi-modal spatio-temporal neural networks. *Energies*, 16(8):3522, 2023.

677 Jishnu Mukhoti, Andreas Kirsch, Joost van Amersfoort, Philip H. S. Torr, and Yarin Gal. Deep
 678 deterministic uncertainty: A new simple baseline. In *IEEE/CVF Conference on Computer Vision*
 679 *and Pattern Recognition, CVPR 2023, Vancouver, BC, Canada, June 17-24, 2023*, pp. 24384–
 680 24394. IEEE, 2023.

681 Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bissacco, Bo Wu, and Andrew Y. Ng. Reading
 682 digits in natural images with unsupervised feature learning. In *NIPS Workshop on Deep Learning*
 683 *and Unsupervised Feature Learning 2011*, 2011.

684 Vu-Linh Nguyen, Sébastien Destercke, and Eyke Hüllermeier. Epistemic uncertainty sampling. In
 685 Petra Kralj Novak, Tomislav Smuc, and Saso Dzeroski (eds.), *Discovery Science - 22nd Interna-*
 686 *tional Conference, DS 2019, Split, Croatia, October 28-30, 2019, Proceedings*, volume 11828 of
 687 *Lecture Notes in Computer Science*, pp. 72–86. Springer, 2019.

689 Vu-Linh Nguyen, Haifei Zhang, and Sébastien Destercke. Credal ensembling in multi-class classi-
 690 fication. *Machine Learning*, 114(1):19, 2025.

691 Yixin Nie, Xiang Zhou, and Mohit Bansal. What can we learn from collective human opinions on
 692 natural language inference data? In Bonnie Webber, Trevor Cohn, Yulan He, and Yang Liu (eds.),
 693 *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing,*
 694 *EMNLP 2020, Online, November 16-20, 2020*, pp. 9131–9143. Association for Computational
 695 Linguistics, 2020.

696 Rafal Obuchowicz, Mariusz Oszust, and Adam Piórkowski. Interobserver variability in quality
 697 assessment of magnetic resonance images. *BMC Medical Imaging*, 20(1):109, 2020.

699 F. Pedregosa, G. Varoquaux, A. Gramfort, V. Michel, B. Thirion, O. Grisel, M. Blondel, P. Pretten-
 700 hofer, R. Weiss, V. Dubourg, J. Vanderplas, A. Passos, D. Cournapeau, M. Brucher, M. Perrot, and
 701 E. Duchesnay. Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*,
 12:2825–2830, 2011.

702 Coby Penso, Idan Achituv, and Ethan Fetaya. Functional ensemble distillation. In Sanmi Koyejo,
 703 S. Mohamed, A. Agarwal, Danielle Belgrave, K. Cho, and A. Oh (eds.), *Advances in Neural In-*
 704 *formation Processing Systems 35: Annual Conference on Neural Information Processing Systems*
 705 *2022, NeurIPS 2022, New Orleans, LA, USA, November 28 - December 9, 2022*, 2022.

706 Joshua C. Peterson, Ruairidh M. Battleday, Thomas L. Griffiths, and Olga Russakovsky. Human
 707 uncertainty makes classification more robust. In *2019 IEEE/CVF International Conference on*
 708 *Computer Vision, ICCV 2019, Seoul, Korea (South), October 27 - November 2, 2019*, pp. 9616–
 709 9625. IEEE, 2019.

710 Alec Radford, Jong Wook Kim, Chris Hallacy, Aditya Ramesh, Gabriel Goh, Sandhini Agar-
 711 wal, Girish Sastry, Amanda Askell, Pamela Mishkin, Jack Clark, Gretchen Krueger, and Ilya
 712 Sutskever. Learning transferable visual models from natural language supervision. In *Proce-*
 713 *edings of the 38th International Conference on Machine Learning, ICML 2021, 18-24 July 2021,*
 714 *Virtual Event*, volume 139 of *Proceedings of Machine Learning Research*, pp. 8748–8763. PMLR,
 715 2021.

716 Richard Royall. *Statistical evidence: a likelihood paradigm*. Routledge, 2017.

717 Yusuf Sale, Michele Caprio, and Eyke Hüllermeier. Is the volume of a credal set a good measure for
 718 epistemic uncertainty? In *Uncertainty in Artificial Intelligence*, pp. 1795–1804. PMLR, 2023.

719 Lars Schmarje, Vasco Grossmann, Claudius Zelenka, Sabine Dippel, Rainer Kiko, Mariusz Oszust,
 720 Matti Pastell, Jenny Stracke, Anna Valros, Nina Volkmann, and Reinhard Koch. Is one annotation
 721 enough? - A data-centric image classification benchmark for noisy and ambiguous label estima-
 722 tion. In Sanmi Koyejo, S. Mohamed, A. Agarwal, Danielle Belgrave, K. Cho, and A. Oh (eds.),
 723 *Advances in Neural Information Processing Systems 35: Annual Conference on Neural Infor-*
 724 *mation Processing Systems 2022, NeurIPS 2022, New Orleans, LA, USA, November 28 - December*
 725 *9, 2022*, 2022.

726 Robin Senge, Stefan Bösner, Krzysztof Dembczynski, Jörg Haasenritter, Oliver Hirsch, Norbert
 727 Donner-Banzhoff, and Eyke Hüllermeier. Reliable classification: Learning classifiers that distin-
 728 guish aleatoric and epistemic uncertainty. *Inf. Sci.*, 255:16–29, 2014.

729 Murat Sensoy, Lance M. Kaplan, and Melih Kandemir. Evidential deep learning to quantify clas-
 730 sification uncertainty. In Samy Bengio, Hanna M. Wallach, Hugo Larochelle, Kristen Grauman,
 731 Nicolò Cesa-Bianchi, and Roman Garnett (eds.), *Advances in Neural Information Processing*
 732 *Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018,*
 733 *December 3-8, 2018, Montréal, Canada*, pp. 3183–3193, 2018.

734 Michael Tschannen, Alexey Gritsenko, Xiao Wang, Muhammad Ferjad Naeem, Ibrahim Alabdul-
 735 mohsin, Nikhil Parthasarathy, Talfan Evans, Lucas Beyer, Ye Xia, Basil Mustafa, Olivier Hénaff,
 736 Jeremiah Harmsen, Andreas Steiner, and Xiaohua Zhai. SigLIP 2: Multilingual vision-language
 737 encoders with improved semantic understanding, localization, and dense features. *preprint*
 738 *arXiv:2502.14786*, 2025.

739 Matias Valdenegro-Toro. Deep sub-ensembles for fast uncertainty estimation in image classifica-
 740 tion. *CoRR*, abs/1910.08168, 2019.

741 Joost van Amersfoort, Lewis Smith, Yee Whye Teh, and Yarin Gal. Uncertainty estimation using
 742 a single deep deterministic neural network. In *Proceedings of the 37th International Conference*
 743 *on Machine Learning, ICML 2020, 13-18 July 2020, Virtual Event*, volume 119 of *Proceedings*
 744 *of Machine Learning Research*, pp. 9690–9700. PMLR, 2020.

745 Pauli Virtanen, Ralf Gommers, Travis E. Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau,
 746 Evgeni Burovski, Pearu Peterson, Warren Weckesser, Jonathan Bright, Stéfan J. van der
 747 Walt, Matthew Brett, Joshua Wilson, K. Jarrod Millman, Nikolay Mayorov, Andrew R. J. Nel-
 748 son, Eric Jones, Robert Kern, Eric Larson, C J Carey, İlhan Polat, Yu Feng, Eric W. Moore,
 749 Jake VanderPlas, Denis Laxalde, Josef Perktold, Robert Cimrman, Ian Henriksen, E. A. Quintero,
 750 Charles R. Harris, Anne M. Archibald, Antônio H. Ribeiro, Fabian Pedregosa, Paul van Mul-
 751 bregt, and SciPy 1.0 Contributors. SciPy 1.0: Fundamental Algorithms for Scientific Computing
 752 in Python. *Nature Methods*, 17:261–272, 2020. doi: 10.1038/s41592-019-0686-2.

756 Peter Walley. Statistical reasoning with imprecise probabilities. 1991.
 757

758 Kaizheng Wang, Fabio Cuzzolin, Keivan Shariatmadar, David Moens, and Hans Hallez. Credal
 759 wrapper of model averaging for uncertainty estimation in classification. In *The Thirteenth In-*
 760 *ternational Conference on Learning Representations, ICLR 2025, Singapore, April 24-28, 2025*.
 761 OpenReview.net, 2025a.

762 Kaizheng Wang, Keivan Shariatmadar, Shireen Kudukkil Manchingal, Fabio Cuzzolin, David
 763 Moens, and Hans Hallez. Creinns: Credal-set interval neural networks for uncertainty estima-
 764 tion in classification tasks. *Neural Networks*, 185:107198, 2025b.

765 Yibin Wang, Haizhou Shi, Ligong Han, Dimitris N. Metaxas, and Hao Wang. Blob: Bayesian
 766 low-rank adaptation by backpropagation for large language models. In Amir Globersons, Lester
 767 Mackey, Danielle Belgrave, Angela Fan, Ulrich Paquet, Jakub M. Tomczak, and Cheng Zhang
 768 (eds.), *Advances in Neural Information Processing Systems 38: Annual Conference on Neural*
 769 *Information Processing Systems 2024, NeurIPS 2024, Vancouver, BC, Canada, December 10 -*
 770 *15, 2024*, 2024.

771 Tobias Weber, Balint Mucsanyi, Lenard Rommel, Thomas Christie, Lars Kasuschke, Marvin
 772 Pfortner, and Philipp Hennig. laplax - laplace approximations with JAX. *CoRR*, abs/2507.17013,
 773 2025.

774 Samuel S Wilks. The large-sample distribution of the likelihood ratio for testing composite hypoth-
 775 eses. *The annals of mathematical statistics*, 9(1):60–62, 1938.

776 Han Xiao, Kashif Rasul, and Roland Vollgraf. Fashion-mnist: a novel image dataset for benchmark-
 777 ing machine learning algorithms. *CoRR*, abs/1708.07747, 2017.

778 Adam X. Yang, Maxime Robeyns, Xi Wang, and Laurence Aitchison. Bayesian low-rank adaptation
 779 for large language models. In *The Twelfth International Conference on Learning Representations,*
 780 *ICLR 2024, Vienna, Austria, May 7-11, 2024*. OpenReview.net, 2024.

781 Xiaohua Zhai, Basil Mustafa, Alexander Kolesnikov, and Lucas Beyer. Sigmoid loss for language
 782 image pre-training. In *IEEE/CVF International Conference on Computer Vision, ICCV 2023,*
 783 *Paris, France, October 1-6, 2023*, pp. 11941–11952. IEEE, 2023.

784 Sheng Zhang, Yanbo Xu, Naoto Usuyama, Hanwen Xu, Jaspreet Bagga, Robert Tinn, Sam Pre-
 785 ston, Rajesh Rao, Mu Wei, Naveen Valluri, Cliff Wong, Andrea Tupini, Yu Wang, Matt Mazzola,
 786 Swadheen Shukla, Lars Liden, Jianfeng Gao, Angela Crabtree, Brian Piening, Carlo Bifulco,
 787 Matthew P. Lungren, Tristan Naumann, Sheng Wang, and Hoifung Poon. A multimodal biomedical
 788 foundation model trained from fifteen million image–text pairs. *NEJM AI*, 2(1), 2024.

789 Bolei Zhou, Agata Lapedriza, Aditya Khosla, Aude Oliva, and Antonio Torralba. Places: A 10
 790 million image database for scene recognition. *IEEE Trans. Pattern Anal. Mach. Intell.*, 40(6):
 791 1452–1464, 2018.

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810 **ORGANIZATION OF THE APPENDIX**
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812 We structure the appendix as follows: Appendix **A** provides a proof for Proposition **2.1** and Propo-
813 sition **3.1**, followed by a detailed description of our implementation in Appendix **B**. Appendix **C**
814 describes the newly introduced *credal spider plots* in detail, before we give details about the differ-
815 ent setups of our experiments in Appendix **D**. We finish with additional results in Appendix **E** and
816 two ablation studies in Appendix **F**.

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864 **A PROOFS**
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866 *Proof of Proposition 2.1.* Write $\gamma(h) = L(h) / \sup_{g \in \mathcal{H}} L(g) \in [0, 1]$, $\mathcal{C}_\alpha = \{h \in \mathcal{H} : \gamma(h) \geq \alpha\}$,
 867 and $\mathcal{Q}_{\mathbf{x}, \alpha} = \{p(\cdot | \mathbf{x}, h) : h \in \mathcal{C}_\alpha\}$. If $0 < \alpha_2 \leq \alpha_1 \leq 1$ and $h \in \mathcal{C}_{\alpha_1}$, then $\gamma(h) \geq \alpha_1 \geq \alpha_2$, hence
 868 $h \in \mathcal{C}_{\alpha_2}$. Thus $\mathcal{C}_{\alpha_1} \subseteq \mathcal{C}_{\alpha_2}$ and, by applying the prediction map, $\mathcal{Q}_{\mathbf{x}, \alpha_1} \subseteq \mathcal{Q}_{\mathbf{x}, \alpha_2}$. Consequently,
 869 for each class k , $\underline{p}_k(\mathbf{x}; \alpha_1) = \inf_{h \in \mathcal{C}_{\alpha_1}} p_k(\mathbf{x}, h) \geq \inf_{h \in \mathcal{C}_{\alpha_2}} p_k(\mathbf{x}, h) = \underline{p}_k(\mathbf{x}; \alpha_2)$, and similarly
 870 $\bar{p}_k(\mathbf{x}; \alpha_1) = \sup_{h \in \mathcal{C}_{\alpha_1}} p_k(\mathbf{x}, h) \leq \bar{p}_k(\mathbf{x}; \alpha_2)$.
 871

872 If an MLE h^{ML} exist, then $\gamma(h^{\text{ML}}) = 1$ and \mathcal{C}_1 is the set of MLEs. In particular, if the (predictive)
 873 MLE is unique at \mathbf{x} (e.g., the MLE is unique, or all MLEs agree at \mathbf{x}), then

874
$$\mathcal{Q}_{\mathbf{x}, 1} = \{p(\cdot | \mathbf{x}, h^{\text{ML}})\} \quad \text{and} \quad [\underline{p}_k(\mathbf{x}; 1), \bar{p}_k(\mathbf{x}; 1)] = \{p_k(\mathbf{x}, h^{\text{ML}})\}.$$

 875

876 As $\alpha \downarrow 0$, the sets \mathcal{C}_α increase to $\{h \in \mathcal{H} : L(h) > 0\}$, hence $\mathcal{Q}_{\mathbf{x}, \alpha} \uparrow \{p(\cdot | \mathbf{x}, h) : L(h) > 0\}$.
 877 For an increasing family of sets, coordinate-wise infima over $\mathcal{Q}_{\mathbf{x}, \alpha}$ decrease to the infimum over the
 878 union, and suprema increase to the supremum. Therefore,
 879

880
$$\underline{p}_k(\mathbf{x}; \alpha) \downarrow \inf_{\{h: L(h) > 0\}} p_k(\mathbf{x}, h), \quad \bar{p}_k(\mathbf{x}; \alpha) \uparrow \sup_{\{h: L(h) > 0\}} p_k(\mathbf{x}, h),$$

 881

882 as claimed. This completes the proof. \square
 883

884 *Proof of Proposition 3.1.* (a) For each n , define $\phi_n(c) := \log p_{y^{(n)}}^{(n)}(c)$. Then
 885

886
$$\phi_n(c) = \langle \mathbf{e}_{y^{(n)}}, c \rangle - \log \sum_{\ell=1}^K \exp(z_\ell^{(n)} + c_\ell) + \text{const}(z^{(n)}),$$

 887

888 hence ϕ_n is C^∞ . Direct differentiation yields
 889

890
$$\nabla \phi_n(c) = \mathbf{e}_{y^{(n)}} - p^{(n)}(c), \quad \nabla^2 \phi_n(c) = -\left(\text{Diag}(p^{(n)}(c)) - p^{(n)}(c) p^{(n)}(c)^\top\right) \preceq 0,$$

 891

892 so each ϕ_n is concave, and thus $\Delta\ell(c) = \sum_n \phi_n(c) - \sum_n \phi_n(0)$ is C^∞ and concave. The Hessian
 893 matrices in the sum are positive semi-definite with nullspace containing $\text{span}\{\mathbf{1}\}$, since $(\text{Diag}(p) -$
 894 $pp^\top)\mathbf{1} = 0$; therefore $\nabla^2 \Delta\ell(c) \prec 0$ on H provided at least two classes appear. Concavity implies
 895 that every level-set $\{c : \Delta\ell(c) \geq \tau\}$ is convex. Non-emptiness follows from $\Delta\ell(0) = 0 \geq \log \alpha$.
 896

897 To see compactness of $F_H(\alpha)$ when at least two classes appear, fix $d \in H \setminus \{0\}$ and consider $c = td$
 898 with $t \rightarrow \infty$. Then
 899

900
$$\Delta\ell(td) = \sum_{n=1}^N \left(\langle \mathbf{e}_{y^{(n)}}, td \rangle - \log \sum_{\ell=1}^K e^{z_\ell^{(n)} + td_\ell} \right) + \text{const} = t \sum_{j=1}^K N_j d_j - \sum_{n=1}^N \log \sum_{\ell=1}^K e^{z_\ell^{(n)} + td_\ell} + \text{const}.$$

 901

902 As $t \rightarrow \infty$, $\log \sum_{\ell} e^{z_\ell^{(n)} + td_\ell} = t \max_{\ell} d_\ell + O(1)$, hence
 903

904
$$\Delta\ell(td) = t \left(\sum_{j=1}^K N_j d_j - N \max_{\ell} d_\ell \right) + O(1).$$

 905

906 Because $d \in H$ and at least two d_ℓ differ, we have $\sum_j N_j d_j < N \max_{\ell} d_\ell$. Thus $\Delta\ell(td) \rightarrow -\infty$
 907 along every ray in H , proving coercivity on H , and hence compactness of $F_H(\alpha)$.
 908

909 (b) Follows by differentiating
 910

911
$$\log p_k(\mathbf{x}; c) = (z_k(\mathbf{x}) + c_k) - \log \sum_{\ell=1}^K e^{z_\ell(\mathbf{x}) + c_\ell}.$$

 912

913 The gradient and Hessian are as stated, and negative semi-definiteness of the Hessian shows
 914 concavity. The coordinate-wise monotonicity is immediate from $\partial \log p_k / \partial c_i = \delta_{ik} - p_i(\mathbf{x}; c)$ together
 915 with $p_i(\mathbf{x}; c) \in (0, 1)$.
 916

918 (c) Since $\log p_k(\mathbf{x}; \cdot)$ is concave and $F(\alpha)$ is convex, $\sup_{c \in F(\alpha)} \log p_k(\mathbf{x}; c)$ is a concave maximization, i.e., a convex optimization problem. Existence of an optimizer on $F_H(\alpha)$ follows from compactness; invariance along $\text{span}\{\mathbf{1}\}$ yields uniqueness only modulo translations by 1. The equality between $\sup p_k$ and $\exp(\sup \log p_k)$ follows from strict monotonicity of the exponential.

919 (d) Because $\log p_k(\mathbf{x}; \cdot)$ is concave, minimizing p_k is equivalent to minimizing a concave function, which is not a convex optimization problem in general. Nevertheless, on the compact convex
920 set $F_H(\alpha)$, a minimizer exists and is attained at an extreme point by standard results on concave
921 functions over convex compact sets.

922 This completes the proof. □

923 *Proof of Corollary 3.1.* Fix $k \in \{1, \dots, K\}$ and restrict the multivariate objects of Proposition 3.1
924 to the affine line $c = t \mathbf{e}_k$, $t \in \mathbb{R}$.

925 (a) Since $\Delta\ell(\cdot)$ is concave on \mathbb{R}^K by Proposition 3.1(a), its restriction $t \mapsto \Delta\ell_k(t)$ is concave on \mathbb{R} ;
926 non-emptiness follows from $\Delta\ell_k(0) = 0 \geq \log \alpha$. Moreover, if $0 < N_k < N$, then $\Delta\ell_k(t) \rightarrow -\infty$
927 as $t \rightarrow +\infty$ (terms with $y^{(n)} \neq k$ decay like $-t$) and as $t \rightarrow -\infty$ (terms with $y^{(n)} = k$ decay like
928 t), so $F_k(\alpha)$ is a compact interval $[t_k^-, t_k^+]$. If $N_k \in \{0, N\}$, the same tail check shows $F_k(\alpha)$ is a
929 closed (possibly half-infinite) interval.

930 (b) From Proposition 3.1(b), $\nabla \log p_k(\mathbf{x}; c) = \mathbf{e}_k - p(\mathbf{x}; c)$. Along the line $c = t \mathbf{e}_k$,

$$931 \frac{d}{dt} \log p_k(\mathbf{x}; t) = (\mathbf{e}_k - p(\mathbf{x}; t \mathbf{e}_k))^\top \mathbf{e}_k = 1 - p_k(\mathbf{x}; t),$$

932 hence $\frac{d}{dt} p_k(\mathbf{x}; t) = p_k(\mathbf{x}; t)(1 - p_k(\mathbf{x}; t)) > 0$. Thus $t \mapsto p_k(\mathbf{x}; t)$ is strictly increasing.

933 (c) Since $F_k(\alpha)$ is an interval and $t \mapsto p_k(\mathbf{x}; t)$ is strictly increasing, the infimum/supremum over
934 $F_k(\alpha)$ are attained at the endpoints:

$$935 p_k(\mathbf{x}) = p_k(\mathbf{x}; t_k^-), \quad \bar{p}_k(\mathbf{x}) = p_k(\mathbf{x}; t_k^+).$$

936 (d) The feasible set can be written as $\{t \in \mathbb{R} : -\Delta\ell_k(t) \leq -\log \alpha\}$, where $-\Delta\ell_k$ is convex.
937 Minimizing t (resp. $-t$) over this convex set is a convex program whose optimizer is exactly the left
938 (resp. right) endpoint t_k^- (resp. t_k^+). In the half-infinite cases $N_k \in \{0, N\}$ the same conclusions
939 hold with the appropriate limits $t_k^- = -\infty$, $t_k^+ = +\infty$ (so $p_k(\mathbf{x}; t_k^-) = 0$ or $p_k(\mathbf{x}; t_k^+) = 1$).

940 This completes the proof. □

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972 **B IMPLEMENTATION DETAILS**
973974 In this section, we provide a detailed description of how our method EffCre is practically imple-
975 mented, including the optimization procedure, the evaluation of probability intervals, and the steps
976 taken to ensure computational efficiency.
977978 As discussed in Section 3, given the logits of the MLE, our method essentially solves two con-
979 vex optimization problems per class to determine the boundaries—namely, the lower and upper
980 probabilities—of a plausible interval according to the relative likelihood constraint. Specifically, for
981 each class logit of the MLE, we add a value to the logit to perturb the resulting probability, thereby
982 deriving a bound for the plausible probability interval as a result of the optimization. In practice, we
983 use the `minimize` function from SciPy (Virtanen et al., 2020) to optimize this value, with the rela-
984 tive likelihood threshold as a constraint, an initial solution of 0, and bounds set to $(-10000, 10000)$.
985 Roughly speaking, each optimization produces a constant that is added to a single class logit, giving
986 the lower (or upper) bound of the plausible probability interval for that class. As a result, applying
987 our method to a dataset requires solving $2K$ convex optimization problems for each value of α .988 The constants obtained by our method, EffCre, can then be used to evaluate our method on test data
989 instances, thus, constructing probability intervals, and thereby credal sets. Each interval bound is
990 directly associated with a specific relative likelihood, which served as the constraint during the opti-
991 mization. For models we trained ourselves, we use the training dataset to evaluate the log-likelihood
992 and compare it with that of the maximum likelihood estimator (MLE) predictor to compute the rela-
993 tive likelihood, as described in Section 2. When the *original* training data is unavailable, we instead
994 use a subset of the target dataset to compute the relative likelihood budget. For example, in the case
995 of CLIP, we do not have access to the *original* training data, which spans many benchmark dataset
996 in addition to a large sample of images from the internet. Since we want to make credal predictions
997 for CIFAR-10, we use the respective train split of CIFAR-10 to compute the (relative) log-likelihoods
998 in order to solve the optimization problem described above. Credal predictions are then made using
999 the respective test split of the dataset.
10001001 In general, our setup allows for straightforward computation of alpha-cuts once results for
1002 multiple alpha values have been obtained, a task made feasible by the efficiency of our
1003 method. The implementation is simple and intuitive; for further clarity, we refer to the
1004 function `classwise_adding_optim_logit` in the code <https://anonymous.4open.science/r/efficient-credal-prediction/>.
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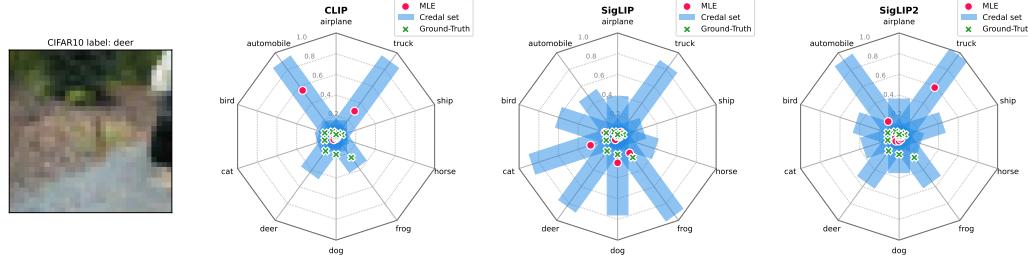
1026 C GUIDE ON INTERPRETING CREDAL SPIDER PLOTS

1028 So far, the quantitative evaluation of credal sets has mainly been restricted to the three class setting,
 1029 due to the inability to visualize credal sets in a $(K - 1)$ -simplex for $K > 3$. As many machine learning
 1030 problems involve more than three classes and as a visual representation of the output of models
 1031 can give useful insight, it is important to be able to have such a visual representation. To enable this,
 1032 we propose *credal spider plots*—these plots offer an intuitive way to evaluate the interval-based
 1033 credal sets. Given an instance that we want to evaluate, we plot the different classes as variables
 1034 in the spider diagram and generate bars, starting at the lower probability and ending at the upper
 1035 probability, for each class, which represent the (plausible) probability intervals. The ground-truth
 1036 distributions is then plotted as multiple dots (depending on the number of classes with non-zero
 1037 probability mass) on the radii corresponding to the given probability mass of a class. As our method
 1038 relies on the maximum likelihood estimate (MLE), we additionally plot the MLE in a similar way.
 1039

1040 In Section 4.4, we sort instances in descending order by the aleatoric and epistemic uncertainty
 1041 associated with the predicted credal set using measures by [Abellán et al. \(2006\)](#) that have been
 1042 proposed on the basis of a number of suitable axioms. Specifically,

$$\overline{S}(Q_x) = \underbrace{S(Q_x)}_{\text{TU}(Q_x))} + \underbrace{(\overline{S}(Q_x) - S(Q_x))}_{\text{AU}(Q_x))} + \underbrace{S(Q_x)}_{\text{EU}(Q_x))} \quad (7)$$

1043 Therefore, maximum aleatoric uncertainty (lower entropy) will manifest itself in the credal spider
 1044 plot for K classes as having intervals that include $1/K$ for all K classes. The maximum epistemic
 1045 uncertainty (difference upper and lower entropy) is obtained by having similar plausible intervals as
 1046 for aleatoric uncertainty, but additionally, the plausible interval for (at least) one class should admit
 1047 a probability of 1. Besides, this instance-wise coverage and efficiency can also easily be observed from
 1048 the credal spider plot by evaluating whether the ground-truth point fall into the plausible intervals
 1049 and by considering the average length of the aforementioned intervals, respectively.
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 1061 **Figure 7: Example credal spider plots for CLIP, SigLIP, and SigLIP-2.** used for illustration
 1062 purposes. The credal spider plots includes the maximum likelihood estimate, the plausible intervals,
 1063 and the ground-truth distribution.
 1064

1080 **D EXPERIMENTAL SETUP**
10811082 **D.1 MODELS**
10831084 **Multilayer Perceptron** We train multilayer perceptron on the ChaosNLI dataset. The model
1085 consists of four linear layers with dimensions $[768 - 256 - 64 - 16 - 3]$, employing ReLU activations
1086 for all hidden layers, while the output layer uses a Softmax function to produce probability distribu-
1087 tions from the logits. For training, we adopt hyperparameters similar to those identified as optimal
1088 in Javanmardi et al. (2024) (see Table 1).
10891090 **ResNet18** For experiments on CIFAR-10, we employ the ResNet-18 implementation and train-
1091 ing configuration from <https://github.com/kuangliu/pytorch-cifar>. This variant
1092 is tailored to CIFAR-10 and is trained entirely from scratch, without ImageNet pretraining.
10931094 **TabPFN** TabPFN (Tabular Prior-data Fitted Network) (Hollmann et al., 2022) is a transformer-
1095 based foundation model developed for supervised classification and regression tasks on small to
1096 medium-sized tabular datasets, typically up to 10,000 samples and 500 features. Pre-trained on
1097 approximately 130 million synthetic datasets generated via structural causal models, TabPFN learns
1098 to approximate Bayesian inference through a single forward pass, eliminating the need for task-
1099 specific tuning. It adeptly handles numerical and categorical features, missing values, and outliers.
1100 We use TabPFN for all experiments with tabular data as presented in Section 4.3. The model
1101 is publicly accessible under a *custom license based on Apache 2.0*, which includes an enhanced
1102 attribution requirement.
11031104 **CLIP** CLIP (Contrastive Language–Image Pretraining) (Radford et al., 2021) is a multimodal
1105 neural network that learns visual concepts from natural language supervision. Trained on 400 mil-
1106 lion image-text pairs sourced from the internet, CLIP can understand images in the context of nat-
1107 ural language prompts, enabling zero-shot classification across various tasks without task-specific
1108 tuning. It employs a vision transformer architecture to process images and a causal language model
1109 to process text, aligning both modalities in a shared embedding space. This design allows CLIP
1110 to generalize to a wide range of visual tasks by interpreting textual descriptions directly. We em-
1111 ploy CLIP to assess our method’s performance in zero-shot classification tasks, demonstrating its
1112 applicability to large-scale models without the need for task-specific training. The model is publicly
1113 available under the MIT License, permitting both academic and commercial use.
11141115 **SigLIP** SigLIP (Sigmoid Loss for Language-Image Pretraining) (Zhai et al., 2023) is a multi-
1116 modal vision-language model that enhances the CLIP framework by employing a pairwise sigmoid
1117 loss function instead of the traditional softmax loss. This modification allows for more efficient
1118 scaling to larger batch sizes while maintaining or improving performance at smaller batch sizes.
1119 SigLIP utilizes separate image and text encoders to generate representations for both modalities,
1120 aligning them in a shared embedding space. The model has demonstrated superior performance in
1121 zero-shot image classification tasks compared to CLIP, achieving an ImageNet zero-shot accuracy
1122 of 84.5% with a batch size of 32,000. Same as for CLIP, we demonstrate with SigLIP the ability
1123 to construct credal sets based on large-scale models. SigLIP is publicly available under the Apache
2.0 license, facilitating research and application in various domains.
11241125 **SigLIP-2** SigLIP-2 (Sigmoid Loss for Language-Image Pretraining 2) (Tschannen et al., 2025)
1126 is a multilingual vision-language encoder. Building upon the original SigLIP, SigLIP-2 in-
1127 tegrates advanced pretraining techniques—including captioning-based pretraining, self-supervised
1128 losses (self-distillation and masked prediction), and online data curation—to enhance semantic un-
1129 derstanding, localization, and dense feature extraction. The model demonstrates improved per-
1130 formance in zero-shot classification, image-text retrieval, and transfer tasks, particularly when extract-
1131 ing visual representations for Vision-Language Models. Notably, SigLIP-2 introduces a dynamic
1132 resolution variant, NaFlex, which supports multiple resolutions and preserves the native aspect ratio,
1133 making it suitable for applications sensitive to image dimensions. We use SigLIP-2 in a similar
fashion as SigLIP and CLIP for large-scale experiments. The model is publicly available under
the Apache 2.0 license, facilitating research and application across various domains.
1134

BiomedCLIP BiomedCLIP (Zhang et al., 2024) is a multimodal biomedical foundation model, pretrained on the PMC-15M dataset—a collection of 15 million figure-caption pairs extracted from over 4.4 million scientific articles in PubMed Central. Utilizing PubMedBERT as the text encoder and Vision Transformer as the image encoder, BiomedCLIP is tailored for biomedical vision-language processing through domain-specific adaptations. It has demonstrated state-of-the-art performance across various biomedical tasks, including cross-modal retrieval, image classification, and visual question answering, outperforming previous models such as BioViL in radiology-specific tasks like RSNA pneumonia detection. The model is publicly available under the Apache 2.0 license, facilitating research and application in the biomedical domain.

Hyperparameters For certain experiments in our empirical evaluation, we use pre-trained (foundation) models, which do not require training and thus do not need hyperparameter specifications. In contrast, for the coverage-efficiency experiments on CIFAR-10, ChaosNLI, and QualityMRI, we train models from scratch using a dataset-specific set of hyperparameters, summarized in Table 1. Multiple configurations were evaluated, and the best-performing setup was selected individually for each dataset. To ensure comparability, all methods—our approach as well as the baselines—share the same hyperparameter settings within a given dataset. The only exception is CreBNN, which, when trained with the Adam optimizer (Kingma & Ba, 2015), requires a KL-divergence penalty of $1e - 7$ and weight decay set to zero. When instead using SGD combined with a cosine annealing learning rate schedule (Loshchilov & Hutter, 2017), CreBNN additionally needs a momentum of 0.9 to achieve stable training.

Table 1: Hyperparameters used for each dataset.

Hyperparameter	ChaosNLI	CIFAR-10	QualityMRI
Model	FCNet	ResNet18	ResNet18
Epochs	300	200	200
Learning rate	0.01	0.1	0.01
Weight decay	0.0	0.0005	0.0005
Optimizer	Adam	SGD	SGD
Ensemble members	20	20	20
LR scheduler	-	CosineAnnealing	CosineAnnealing

D.2 DATASETS

ChaosNLI ChaosNLI, introduced by Nie et al. (2020), is a large-scale dataset created to investigate human disagreement in natural language inference (NLI). It includes 100 annotations per example for 3,113 instances from SNLI and MNLI, as well as 1,532 examples from the α NLI dataset, totaling around 464,500 annotations. In line with Javanmardi et al. (2024), we focus only on the SNLI and MNLI portions, which we refer to simply as ChaosNLI for convenience. Each entry provides rich metadata, including a unique identifier, the count of labels assigned by annotators, the majority label, the full label distribution, the distribution’s entropy, the original text, and the original label from the source dataset. ChaosNLI facilitates detailed study of variability in human judgments, highlighting examples where disagreement is high and illustrating the limitations of treating the majority label as definitive ground truth. The dataset is publicly accessible under the *CC BY-NC 4.0 License*. For our experiments, we use the precomputed 768-dimensional embeddings, available at <https://github.com/alireza-javanmardi/conformal-credal-sets>, with further details on their generation provided by Javanmardi et al. (2024).

QualityMRI Introduced by Obuchowicz et al. (2020), the QualityMRI dataset is part of the Data-Centric Image Classification (DCIC) Benchmark, which studies the role of dataset quality in shaping model performance. It consists of 310 magnetic resonance images that cover different quality levels, providing a resource for assessing MRI image quality. The dataset is distributed under the *Creative Commons BY-SA 4.0 License*.

CIFAR-10 CIFAR-10, introduced by Krizhevsky et al. (2009) and Geoffrey Hinton in 2009, is a widely adopted benchmark in machine learning and computer vision. It consists of 60,000 color

1188 images with a resolution of 32×32 pixels, evenly divided among 10 classes: airplane, automobile,
 1189 bird, cat, deer, dog, frog, horse, ship, and truck. The dataset is split into 50,000 training images
 1190 and 10,000 test images, organized into five training batches and a single test batch, each containing
 1191 10,000 images. CIFAR-10 is publicly available and has been extensively used for training and
 1192 evaluating machine learning models. While the original dataset does not explicitly define a license,
 1193 versions distributed through platforms such as TensorFlow datasets are provided under the *Creative
 1194 Commons Attribution 4.0 License*.

1195
 1196 **CIFAR-10H** CIFAR-10H provides human-generated soft labels for the 10,000 images in the
 1197 CIFAR-10 test set, reflecting the variability in human judgments for image classification. Introduced
 1198 by [Peterson et al. \(2019\)](#), the dataset contains 511,400 annotations from 2,571 workers on
 1199 Amazon Mechanical Turk, with each image receiving around 51 labels. Each annotation assigns an
 1200 image to one of the ten CIFAR-10 classes, allowing the creation of a probability distribution over
 1201 labels for every image. CIFAR-10H is publicly available under the *Creative Commons BY-NC-SA
 4.0 License*.

1202
 1203 **CIFAR-100** CIFAR-100, introduced by [Krizhevsky et al. \(2009\)](#), consists of 60,000 color images
 1204 at a resolution of 32×32 pixels, organized into 100 classes with 600 images per class. Each im-
 1205 age carries both a “fine” label, indicating its specific class, and a “coarse” label corresponding to
 1206 one of 20 broader superclasses. The dataset is divided into 50,000 training images and 10,000 test
 1207 images. CIFAR-100 is derived from the Tiny Images dataset and is widely used for benchmarking
 1208 image classification models. While the original dataset does not define a license, versions distributed
 1209 through platforms such as TensorFlow Datasets are available under the *Creative Commons Attribu-
 1210 tion 4.0 License*.

1211
 1212 **SVHN** The SVHN dataset, introduced by [Netzer et al. \(2011\)](#), contains over 600,000 32×32
 1213 RGB images of digits (0–9) extracted from real-world house numbers in Google Street View. It is
 1214 organized into three subsets: 73,257 images for training, 26,032 for testing, and an additional set
 1215 of 531,131 images for extended training. SVHN is intended for digit recognition tasks and requires
 1216 minimal preprocessing. Although the original dataset does not specify a license, versions distributed
 1217 through platforms like TensorFlow Datasets are available under the *Creative Commons Attribution
 4.0 License*.

1218
 1219 **Places365** Places365, introduced by [Zhou et al. \(2018\)](#), is a large-scale dataset for scene recog-
 1220 nition, comprising 1.8 million training images spanning 365 scene categories. The validation set
 1221 contains 50 images per category, while the test set includes 900 images per category. An expanded
 1222 variant, Places365-Challenge-2016, incorporates an additional 6.2 million images and 69 new scene
 1223 categories, bringing the total to 8 million images across 434 categories. Although the original dataset
 1224 does not specify a license, versions distributed through platforms such as TensorFlow Datasets are
 1225 available under the *Creative Commons Attribution 4.0 License*.

1226
 1227 **FMNIST** Fashion-MNIST (FMNIST), introduced by [Xiao et al. \(2017\)](#), contains 70,000
 1228 grayscale images of Zalando products, each sized 28×28 pixels and categorized into 10 classes,
 1229 including T-shirt/top, Trouser, and Sneaker. The dataset is divided into 60,000 training images and
 1230 10,000 test images, and it is commonly used as a modern replacement for the original MNIST
 1231 dataset in machine learning benchmarks. *FMNIST is publicly released under the MIT License*.

1232
 1233 **ImageNet** ImageNet, introduced by [Deng et al. \(2009\)](#), is a large-scale image dataset structured
 1234 according to the WordNet hierarchy, comprising over 14 million images spanning more than 20,000
 1235 categories. Its ILSVRC subset, commonly referred to as ImageNet-1K, contains 1,281,167 training
 1236 images, 50,000 validation images, and 100,000 test images across 1,000 classes. *The dataset is
 1237 freely accessible to researchers for non-commercial purposes*.

1238
 1239 **TabArena Benchmark Data** TabArena ([Erickson et al., 2025](#)) is a continuously maintained
 1240 benchmarking system designed for evaluating tabular machine learning models. It comprises 51
 1241 manually curated datasets representing real-world tabular tasks, including both classification and
 regression problems. Each dataset has been evaluated across 9 to 30 different splits, ensuring ro-
 bust performance assessments. The datasets encompass a diverse range of domains, such as finance,

1242 healthcare, and e-commerce, providing a comprehensive foundation for benchmarking various
 1243 machine learning models. This diversity ensures that evaluations reflect the complexities and nuances
 1244 found in real-world tabular data scenarios. We use 7 different datasets with IDs 46906, 46930,
 1245 46941, 46958, 46960, 46963, 46980 from the benchmark to validate our method in different ex-
 1246 periments. Each of the datasets contains a classification task with 2 or more classes and a number
 1247 of instances between 898 and 12,684. The datasets are publicly accessible and released under the
 1248 *Apache 2.0 license*, ensuring permissive use and redistribution for research purposes.

1250 D.3 BASELINES

1251 Below, we provide detailed descriptions of the baseline implementations used in this paper, relying
 1252 on the implementations provided by Löhrt et al. (2025).

1253 **Credal Prediction based on Relative Likelihood (CreRL)** The implementation of Credal Pre-
 1254 diction based on Relative Likelihood (Löhrt et al., 2025) is provided in <https://github.com/timoverse/credal-prediction-relative-likelihood>. We use the provided code
 1255 to perform all experiments involving CreRL. Similar to our method, the CreRL defines plausibility
 1256 in terms of the relative likelihood of a model. One significant difference is that, while CreRL tries
 1257 to find sufficiently diverse hypotheses that satisfy the relative likelihood criterion, therefore having
 1258 to train an ensemble of model, we directly obtain the plausible probability intervals by varying the
 1259 logits of the maximum likelihood estimate.

1260 **Credal Wrapper (CreWra)** The Credal Wrapper (Wang et al., 2025a) was initially implemented
 1261 in TensorFlow, but then reimplemented in PyTorch to ensure compatibility with other baselines. It
 1262 follows a standard ensemble learning approach, training multiple models independently. Like our
 1263 method, the Credal Wrapper constructs credal sets using class-wise upper and lower probability
 1264 bounds, making it well-aligned with our implementation.

1265 **Credal Ensembling (CreEns $_{\alpha}$)** Our implementation adheres closely to the specifications outlined
 1266 in Nguyen et al. (2025). The method extends standard ensemble training, adapting the inference
 1267 stage by ranking predictions according to a distance metric and including only the top $\alpha\%$ of closest
 1268 predictions when forming the credal sets. In our experiments, we employ the Euclidean distance
 1269 and test multiple α values.

1270 **Credal Deep Ensembles (CreNet)** Since the official Credal Deep Ensembles implementation was
 1271 provided only in TensorFlow, it was reimplemented by Löhrt et al. (2025) in PyTorch to integrate
 1272 seamlessly with other baselines. The version maintains the key design choices of the original, espe-
 1273 cially regarding the architecture and loss function. In particular, the models' final linear layers are
 1274 replaced with a head that outputs $2 \times$ classes values corresponding to upper and lower probability
 1275 bounds, followed by batch normalization and the custom IntSoftmax activation. The loss function
 1276 applies standard cross-entropy to the upper bounds, while for the lower bounds, gradients are prop-
 1277 agated only for the $\delta\%$ of samples exhibiting the largest errors, in line with Wang et al. (2025b). For
 1278 our experiments, we adopt $\delta = 0.5$ as recommended in the original work.

1279 **Credal Bayesian Deep Learning (CreBNN)** The method proposed by Caprio et al. (2024a) was
 1280 reimplemented by Löhrt et al. (2025) using only the high-level description from the original work.
 1281 The ensemble consists of Bayesian neural networks (BNNs), each trained via variational inference
 1282 with distinct priors: the prior means μ are drawn from $[-1, 1]$ and the standard deviations σ from
 1283 $[0.1, 2]$, ensuring a diverse prior set. At inference time, we sample once from each BNN to generate
 1284 a finite collection of probability distributions, and the credal set is defined as the convex hull of these
 1285 samples.

1286 **Evidential Deep Learning** Our implementation of Evidential Deep Learning follows (Sensoy
 1287 et al., 2018) as closely as possible. We use a single model and include a SoftPlus activation function
 1288 after the last layer to ensure the output is non-negative. We use the Type II Maximum Likelihood as
 1289 a loss function and the KL-divergence as a regularization term as described in (Sensoy et al., 2018).

1296 The regularization term is scaled by $\lambda_i = \min(1, i/10)$ at epoch i as also done in the original work.
 1297 At inference time, the model predicts the evidence for each class, which can then be used to compute
 1298 the parameters of the corresponding Dirichlet distribution.
 1299
 1300
 1301

1302 **Deep Deterministic Uncertainty** For the Deep Deterministic Uncertainty method (Mukhoti
 1303 et al., 2023), we used the original implementation provided in <https://github.com/omegafragger/DDU>. This approach uses a single model to reason about uncertainty. In the
 1304 original paper, the authors apply additional techniques—including spectral normalization and residual
 1305 connections—to encourage more regularized embeddings in feature-space. For our comparison,
 1306 we omit these techniques to ensure a fair comparison, as integrating such modifications into
 1307 a pre-trained model would require re-training the model. Thus, we rely on the identical, trained
 1308 ResNet18, which is also used for the other experiments. At inference time, epistemic uncertainty
 1309 can be quantified through density estimation in feature-space: a normal distribution is fit to the em-
 1310 beddings of training data for each class, and epistemic uncertainty is computed on the basis of the
 1311 likelihood of new embeddings under this distribution.
 1312
 1313

D.4 COMPUTE RESOURCES

1315 All experiments in this work were conducted using the computing resources listed in Table 2, with
 1316 an estimated total GPU usage of approximately 820 hours.
 1317

1318 **Table 2:** Specifications of Computing Resources
 1319

1320 Component	1321 Specification
1322 CPU	1323 AMD EPYC MILAN 7413 Processor, 24C/48T 2.65GHz 128MB L3 Cache
1323 GPU	1324 2 × NVIDIA A40 (48 GB GDDR each)
1324 RAM	1325 128 GB (4x 32GB) DDR4-3200MHz ECC DIMM
1325 Storage	2 × 480GB Samsung Datacenter SSD PM893

1326
 1327
 1328 **D.5 GENERATING SEMI-SYNTHETIC GROUND-TRUTH DISTRIBUTIONS**
 1329

1330 Due to a lack of ground-truth distributions, the evaluation of credal predictors remains non-trivial.
 1331 While a number of datasets have a (test) set that includes multiple human annotations—such as the
 1332 ones used in this work—most of the commonly-used benchmarking datasets do not provide these.
 1333 Therefore, we use a simple method to generate semi-synthetic datasets that include (conditional)
 1334 ground-truth distributions. The general idea is as follows: given a training set $\mathcal{D}_{\text{train}}$, we either train a
 1335 model or retrieve a strong model from a model hub. The trained or retrieved model is then considered
 1336 to be the ground-truth model h^* and ground-truth distributions may be generated by collecting the
 1337 predicted distributions $p(\cdot | \mathbf{x}, h^*)$ based on instances from the $\mathcal{D}_{\text{train}}$ or $\mathcal{D}_{\text{test}}$. The model that is to
 1338 be evaluated (in terms of coverage and efficiency) is then trained on the same instances $\mathbf{x} \in \mathcal{D}_{\text{train}}$,
 1339 but the labels are sampled from $p(\cdot | \mathbf{x}, h^*)$. Thereafter, the model can be evaluated using the test
 1340 set.
 1341

1342 For example, in Section 4.3, we train a RandomForest with the default parameters from scikit-
 1343 learn (Pedregosa et al., 2011) with the exception of maximum depth; this is set to 5 to prevent
 1344 the predicted distributions too “peaked”. The RandomForest is assumed to be the ground-truth
 1345 model h^* and its prediction for an instance \mathbf{x} is taken to be the *ground-truth* conditional distribution
 1346 $p(\cdot | \mathbf{x}, h^*)$. The TabPFN model is then trained on the same instances \mathbf{x} , but the labels y are
 1347 realizations sampled from the distribution $p(\cdot | \mathbf{x}, h^*)$. The model is then evaluated on the test set,
 1348 for which the ground-truth distributions are also generated by the RandomForest h^* .
 1349

1348 We refer to this as *semi-synthetic*, because, while the generated distribution is not (necessarily) the
 1349 ground-truth, under the assumption that the used model is sufficiently well-trained, they should be
 “close” to the ground-truth.

1350
1351 D.6 TURNING CLIP-BASED MODELS INTO ZERO-SHOT CLASSIFIERS

1352 To demonstrate the usefulness and flexibility of our method for producing credal sets for any black-
 1353 box model structure without the need for retraining, we apply it to multi-modal CLIP-based models.
 1354 Contrastive Language–Image Pretraining (CLIP) (Radford et al., 2021) introduced a mechanism to
 1355 pre-train models that share embeddings across two modalities. The training data consists of a large
 1356 corpus of images and their corresponding descriptions (e.g., captions or alternative text from web-
 1357 sites). The central idea is to align each image with its textual description: images and their captions
 1358 should be close in the embedding space, while mismatched pairs should be far apart. To achieve this,
 1359 two modality-specific encoders are trained to produce embeddings of equal dimension, from which a
 1360 similarity score (e.g., cosine similarity) is computed. Captions that accurately describe an image re-
 1361 ceive high similarity scores, whereas unrelated captions receive low scores. This training paradigm
 1362 and model architecture have since been refined by subsequent works, yielding better-performing or
 1363 more specialized models. For example, BiomedCLIP (Zhang et al., 2024), trained on biomedical
 1364 data from PubMed, achieves superior performance on medical tasks. Similarly, the SigLIP (Zhai
 1365 et al., 2023) and SigLIP-2 (Tschannen et al., 2025) families adapt the training procedure and ex-
 1366 tend the datasets to include multilingual text sources, resulting in improved performance on general
 1367 tasks (Zhai et al., 2023; Tschannen et al., 2025).

1368 **Zero-Shot Prediction.** Zero-shot image classification with CLIP-based models proceeds by refor-
 1369 mulating the label set into natural-language *templates*. For each candidate class, a short descriptive
 1370 text is created (e.g., the template “a photo of a [label]” yields “a photo of a dog” or “a photo of a
 1371 cat”). These textual descriptions are embedded by the text encoder, while the input image is embed-
 1372 ded by the image encoder. The similarity between the image embedding and each text embedding
 1373 is then computed, typically using cosine similarity. The resulting similarity values can be treated
 1374 as logits, where the highest-scoring label determines the predicted class. Importantly, this formu-
 1375 lation also makes it straightforward to restrict classification to any subset of labels without training
 1376 a new classifier, since one can simply retain and compare the logits corresponding to the labels
 1377 of interest. This procedure enables CLIP-based models to serve as flexible, task-agnostic classi-
 1378 fiers without requiring any additional training, and has proven effective across diverse downstream
 1379 domains (Radford et al., 2021; Zhang et al., 2024; Zhai et al., 2023; Tschannen et al., 2025).

1380 **Templates for Multi-Lingual Datasets.** Zero-shot classification can be extended to multi-lingual
 1381 datasets by translating labels into the target language and constructing corresponding templates. For
 1382 example, in our experiments we used the English template “This is a photo of a [label]” alongside a
 1383 Swahili template “Hii ni picha ya [label]”, allowing classification in either language. Models such
 1384 as SigLIP-2 (Tschannen et al., 2025), trained on multilingual data, further improve robustness in
 1385 this setting.

1386 **Model Performance.** To illustrate the effectiveness of different CLIP-based models in our setting,
 1387 we report their zero-shot classification accuracy on CIFAR-10, ImageNet, and DermMNIST (see
 1388 Table 3). The results show that while standard CLIP performs strongly on general-purpose datasets,
 1389 specialized variants such as BiomedCLIP yield improved performance on domain-specific tasks,
 1390 and recent multilingual models like SigLIP and SigLIP-2 further enhance accuracy on broad
 1391 benchmarks.

1392 **Table 3:** Zero-shot classification accuracy (%) of CLIP-based models on CIFAR-10 (EN = English,
 1393 SW = Swahili, FR = French, ZH = Chinese), ImageNet, and DermMNIST.

1395 1396 1397 Model	1398 1399 1400 1401 CIFAR-10				1402 ImageNet	1403 DermaMNIST
	1398 EN	1399 SW	1400 FR	1401 ZH		
CLIP	88.97%	9.11%	85.97%	33.73%	57.14%	24.74%
SigLIP	92.17%	15.33%	84.05%	91.28%	72.83%	8.28%
SigLIP2	93.91%	10.21%	92.21%	93.85%	69.87%	11.67%
BiomedCLIP	–	–	–	–	–	45.89%

1404 **E ADDITIONAL EXPERIMENTAL RESULTS**
 1405

1406 **E.1 COVERAGE VERSUS EFFICIENCY**
 1407

1408 In addition to the datasets provided in Section 4.1, we present an additional comparison to the base-
 1409 lines in the form of the QUALITYMRI dataset. Figure 8 shows that our approach Pareto dominates the
 1410

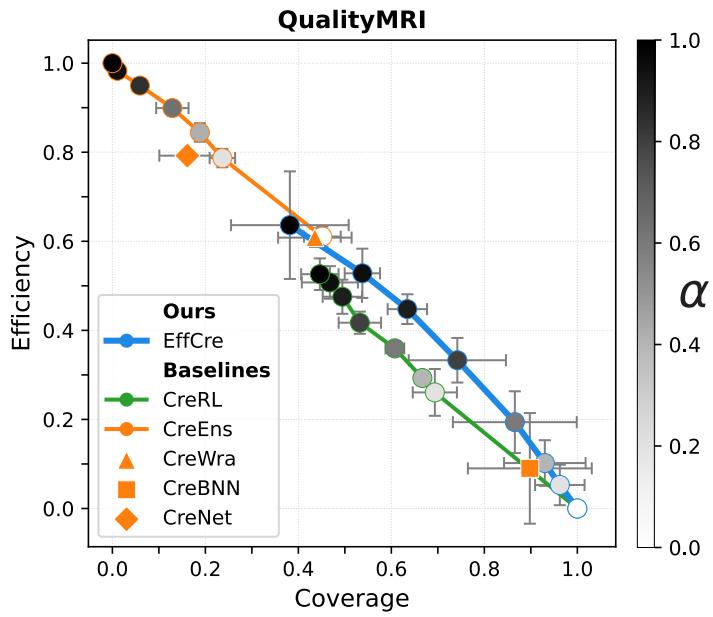


Figure 8: Coverage versus Efficiency. Our method, EffCre, is compared to baselines on QUALITYMRI.

CreRL method, while having a similar coverage and efficiency to CreBNN for $\alpha = 0.4$. However, our method allows a trade-off between coverage and efficiency beyond that, allowing the exploration of regions with a better efficiency or better coverage. Our method is Pareto incomparable to the CreEns, because CreEns does not reach the high coverage region (while having higher efficiency, whereas our method does (while having lower efficiency). It should be noted that reaching the high coverage area, as our method does, is especially important in medical settings, as is the case for the QualityMRI dataset.

E.2 OUT-OF-DISTRIBUTION DETECTION

For this experiment, we trained a ResNet18 on CIFAR-10, which serves as the in-distribution dataset. At evaluation time, we consider both the in-distribution data and five out-of-distribution datasets to compute epistemic uncertainty values with our method. These values are then used to separate ID from OOD samples, with performance measured via AUROC. In addition to the results in Section 4.2, Table 5 reports AUROC scores across different α values for our method, and Table 4 states the corresponding [training and inference times](#) for each method. Furthermore, Appendix F.1 presents an ablation study on the effect of the ensemble size for OOD detection performance.

Table 4: Training and inference time in seconds for models trained on CIFAR10. Mean with standard deviation over three runs. Computed based on ensembles with 10 members.

Method	Training time	Inference time
EffCre	2136.33 ± 1.70	1.50 ± 0.02
CreRL	12675.84 ± 412.68	11.46 ± 0.12
CreWra	21363.34 ± 33.99	11.44 ± 0.19
CreEns	21363.34 ± 33.99	11.44 ± 0.23
CreNet	24996.65 ± 180.12	11.41 ± 0.18
CreBNN	29796.67 ± 12.94	12.74 ± 1.1

Table 5: Out-of-Distribution Detection.

Method	SVHN	Places365	CIFAR-100	FMNIST	ImageNet
EffCre _{0.0}	0.478±0.006	0.478±0.005	0.480±0.005	0.486±0.002	0.481±0.002
EffCre _{0.2}	0.474±0.003	0.474±0.001	0.473±0.002	0.474±0.002	0.473±0.003
EffCre _{0.4}	0.303±0.100	0.389±0.072	0.335±0.040	0.325±0.057	0.338±0.035
EffCre _{0.6}	0.415±0.010	0.428±0.007	0.440±0.017	0.404±0.024	0.435±0.008
EffCre _{0.8}	0.744±0.009	0.721±0.009	0.720±0.007	0.733±0.012	0.700±0.008
EffCre _{0.9}	0.854±0.005	0.827±0.006	0.822±0.004	0.860±0.005	0.796±0.005
EffCre _{0.95}	0.885±0.003	0.862±0.005	0.854±0.003	0.907±0.002	0.826±0.004
EffCre _{1.0}	0.894±0.015	0.886±0.008	0.868±0.005	0.933±0.010	0.844±0.006
CreRL _{0.95}	0.917±0.013	0.910±0.001	0.901±0.000	0.945±0.004	0.878±0.002
CreWra	0.957±0.003	0.916±0.001	0.916±0.000	0.952±0.000	0.890±0.001
CreEns _{0.0}	0.955±0.001	0.913±0.000	0.914±0.001	0.949±0.001	0.888±0.000
CreBNN	0.907±0.006	0.885±0.002	0.880±0.002	0.935±0.002	0.859±0.002
CreNet	0.943±0.003	0.918±0.000	0.912±0.000	0.951±0.002	0.884±0.001

In the main paper, we focused exclusively on comparing credal predictors in order to ensure a consistent evaluation of methods within a single framework (that of credal predictors). This allows us to isolate the effect of the credal predictor from the influence of other factors such as the uncertainty measure or the base model. Here, we additionally compare our method to other methods that allow for uncertainty quantification with a single model. In particular, we compare EffCre to evidential deep learning (EDL) (Sensoy et al., 2018) and deep deterministic uncertainty (DDU) quantification (Mukhoti et al., 2023). For evidential deep learning, the epistemic uncertainty quantification is computed by

$$\text{EU} = \frac{K}{S},$$

where K is the number of classes and $S = \sum_{k=1}^K (z_k + 1)$ denotes the sum of the predicted parameters of the Dirichlet distribution for an input for \mathbf{x} . Deep deterministic uncertainty quantifies epistemic uncertainty on the basis of the likelihood of the embedding of an input

$$\text{EU} = \sum_{k=1}^K q(e | k)q(k),$$

where q represents the density function of a normal distribution. The implementation details are described in Appendix D.3. The results are presented in Table 6. When compared to EDL, our

Table 6: Out-of-Distribution Detection.

Method	SVHN	Places365	CIFAR-100	FMNIST	ImageNet
EDL	0.938±0.010	0.889±0.001	0.887±0.001	0.940±0.005	0.866±0.001
DDU	0.973±0.001	0.969±0.001	0.873±0.002	0.892±0.010	0.969±0.000

method (EffCre_{1.0}) performs on par with EDL on Places365, while being slightly outperformed on the remaining datasets. However, it is important to emphasize that EDL requires re-training the model with a specific activation and loss function, hence it cannot be applied directly in standard settings, specifically if the training data is not available. In contrast, our method can be applied without re-training, making it compatible with a broader range of settings such as the ones using TabPFN and CLIP presented in the manuscript. Our method outperforms DDU on FMNIST, while being weaker on other datasets. Moreover, while DDU is also a post-training method, it requires access to the embeddings generated by the model, whereas our method does not. EffCre, by operating on logits, can be applied on top of black-box models, which enables it to be directly applied in more general settings, such as large language models, which form an interesting direction for future work. Overall, there is no clear winner across the evaluated methods, and drawing definitive conclusions remains challenging. Besides the stark differences in the working of the

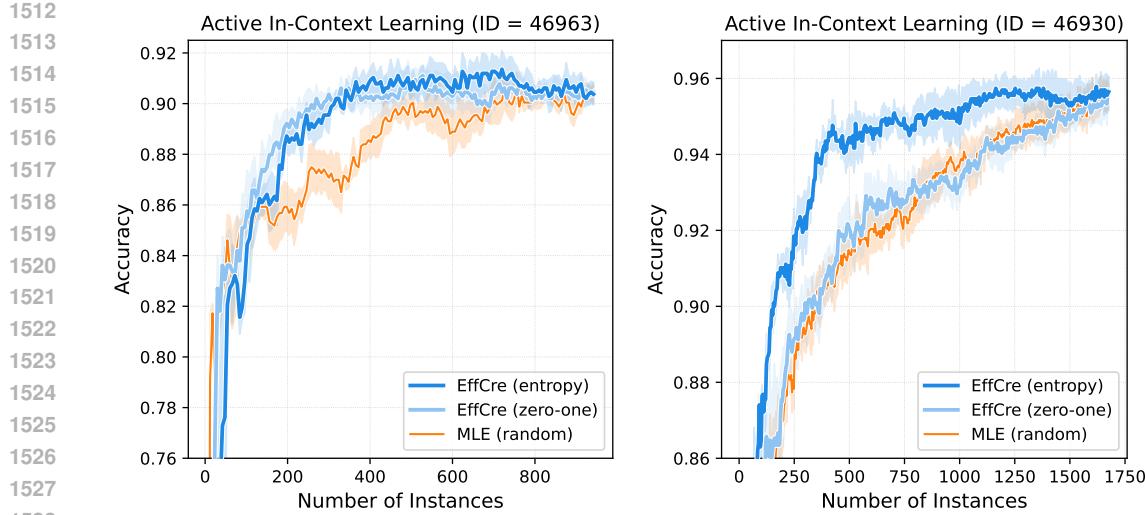


Figure 9: Active In-Context Learning with TabPFN. Performance on TabArena datasets 46963, and 46930 versus the random baseline.

methods, the OOD detection task itself comes with numerous caveats (Li et al., 2025), meaning that performance on this task can only be taken as a proxy of the quality of the epistemic uncertainty representation.

Additionally, although these methods also rely on a single (re-trained) model, they differ from the other (credal) approaches in that they do not produce credal sets. We consider this distinction to be particularly important, as the credal set predictors quantify a fundamentally different form of epistemic uncertainty than DDU. Indeed, the credal set represents an epistemic uncertainty with respect to the predicted probability distribution, which will directly affect the subsequent decision-making. DDU, however, quantifies a form of epistemic uncertainty about the “familiarity” of an input, derived from its density relative to the training data. It is not immediately clear how this should influence the decision-making process that follows.

E.3 IN-CONTEXT LEARNING WITH TABPFN

We compute coverage and efficiency for our method used with TabPFN with all multi-class TABARENA datasets. As discussed in Section 4.3, the datasets do not come with ground-truth distributions. Therefore, we construct *semi-synthetic* distributions that serve as the ground-truth. In Appendix D.5, we give a detailed explanation of our approach. Note that we consider the resulting distributions to only be a proxy of the “true” ground-truth distributions. In addition to computing the coverage and efficiency, we perform active in-context learning. In Section 4.3 and the results that will follow, this is done by first splitting the data, in a stratified manner, to have a 0.3 test split. The remaining 0.7 split is then split into an initial training set and the sampling pool, again stratified, such that the initial training set contains $2K$ instances, where K is the number of classes. At every iteration, the predictor is “allowed” to sample $2K$ instances from the pool, based on its epistemic uncertainty, which is a common setup in active learning (Nguyen et al., 2019; Margraf et al., 2024). This is done until the pool is exhausted—and, hence, until the performance converges to what would be obtained with a traditional train-test split. The goal is thus, to select at every iteration samples that are most informative, i.e. the samples that will give the greatest performance increase at that iteration. In addition to the results in Section 4.3, we present active in-context learning results for two additional TABARENA datasets: 46963 and 46930. Figure 9 shows the results for our method using epistemic uncertainty sampling based on (5) and (6) compared to the random baseline. Conform the results presented in Section 4.3, our method applied to TABPFN provides a valuable advantage over the random baseline in terms of accuracy.

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E.4 ZERO-SHOT CLASSIFICATION WITH CLIP-BASED MODELS

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Extending on the examples shown in Section 4.4, we create additional credal spider plots for CLIP-based models in Figures 10 to 12. Figure 11 highlights challenging natural images with high uncertainty in CLIP, Figure 12 examines medical images from DERMAMNIST, and Figure 10 analyzes cross-lingual predictions on CIFAR-10. Together, these visualizations complement the quantitative results reported in Table 3 by showcasing how credal spider plots reveal distinct uncertainty patterns that align with the models’ performance across domains.

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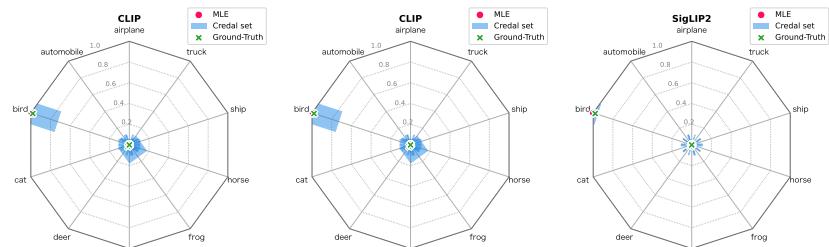
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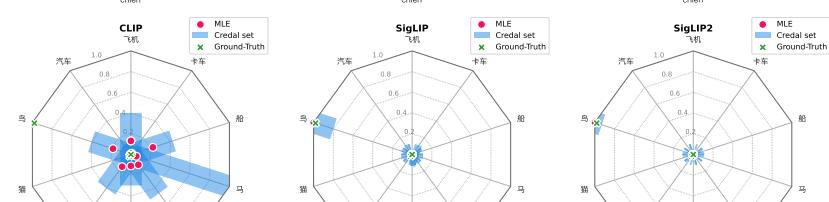
(English)



(French)



(Chinese)



(Swahili)

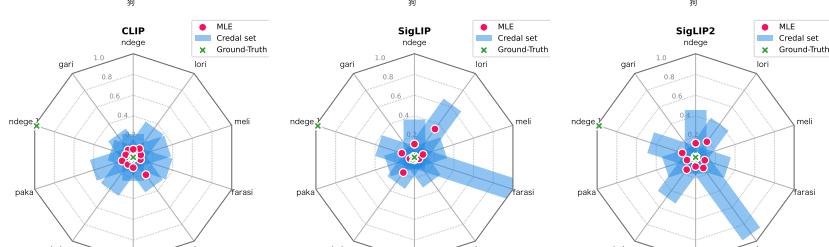


Figure 10: Credal spider plots for an image of a bird with CLIP, SigLIP, and SigLIP-2 across different languages. In English, all models confidently predict the image as *bird*. In French, SigLIP-2 maintains the correct maximum likelihood prediction but shows increased uncertainty toward *cat*. In Chinese, CLIP exhibits high uncertainty across all classes, indicating difficulties in this language, whereas SigLIP and SigLIP-2 remain as confident as in English. In Swahili, all models struggle and display high uncertainty across all classes; notably, *bird* and *airplane* share the same word in Swahili, complicating the prediction. These examples align well with models' performances across the different languages (see Table 3).

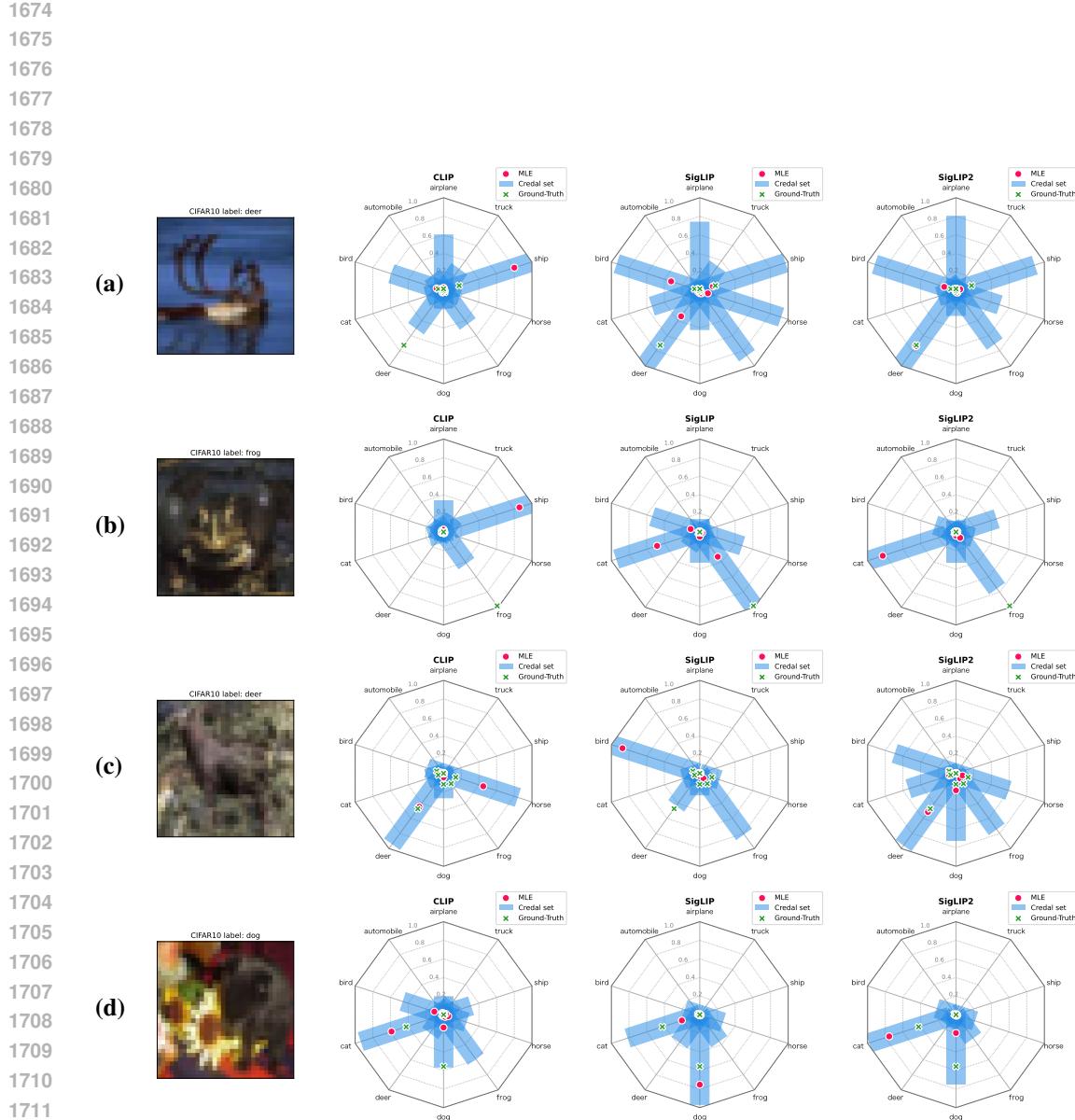


Figure 11: Comparison of credal sets for CLIP, SigLIP, and SigLIP-2 on observations with high uncertainty with CLIP. Observation **(a)** shows a swimming deer, where the MLE is ship. High uncertainty is spread across ship, two sky-related classes (airplane, bird), the amphibious frog, and the correct class deer. Both SigLIP models exhibit similar patterns with even greater uncertainty. Observation **(b)** depicts a dark image of a frog misclassified as ship, with high uncertainty again on that class; both SigLIP models additionally assign probability to cat. Observation **(c)** is a challenging deer image, where annotators themselves showed high disagreement. CLIP is confident it is either deer or horse, while SigLIP favors bird or frog, and SigLIP-2 remains certain it is an animal but not which. Observation **(d)** illustrates a case where human annotators are nearly evenly split between cat and dog, and the uncertainties of all three models capture this ambiguity.

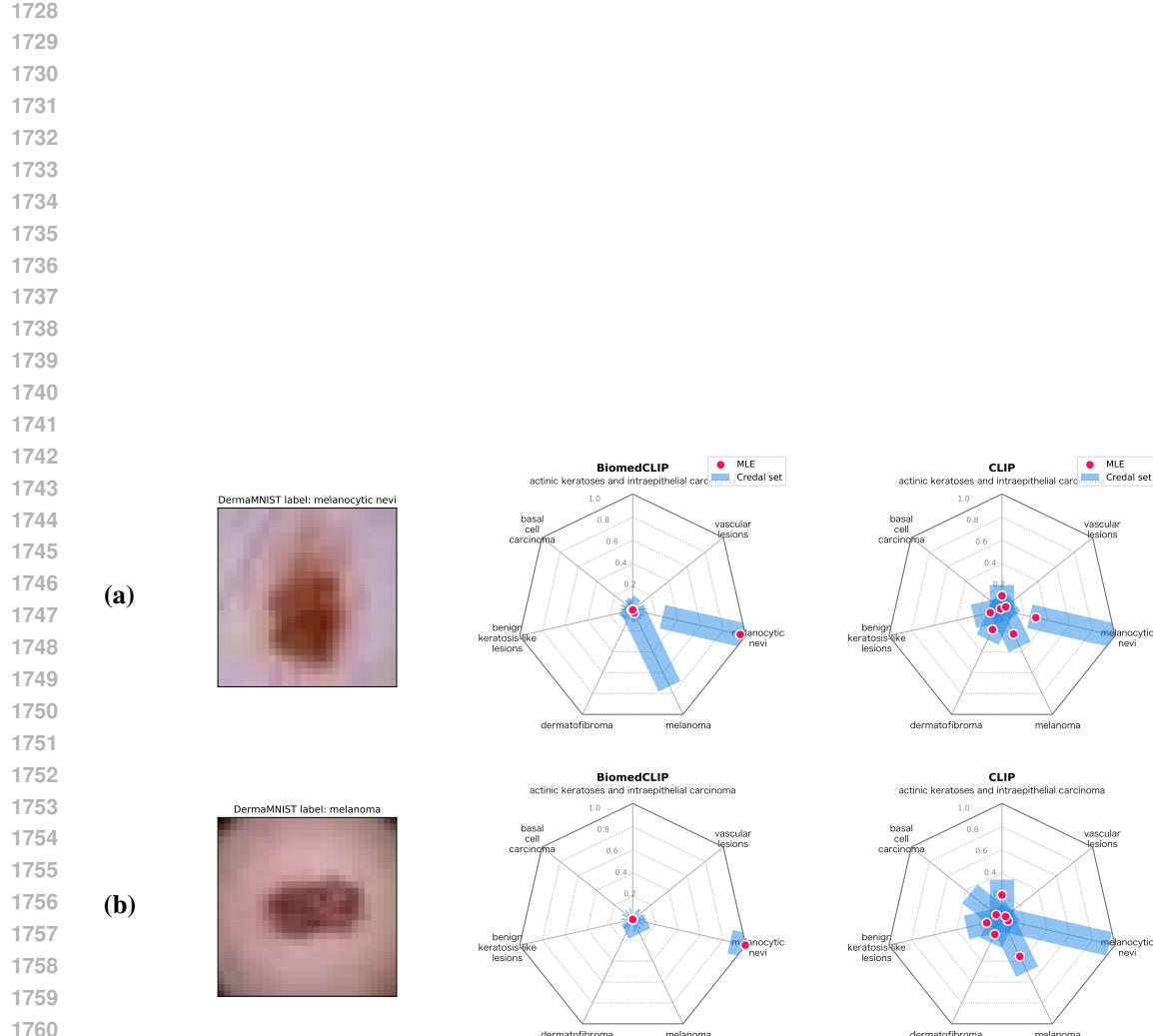


Figure 12: Comparison of credal sets for BiomedCLIP and CLIP on DERMAMNIST for a melanocytic nevi **(a)** and a melanoma **(b)**. While BiomedCLIP demonstrates higher overall performance than CLIP (see Table 3), it misclassifies the melanoma with high confidence and low uncertainty, which could be dangerous if applied in medical contexts. Interestingly, CLIP classifies the melanoma correctly, albeit with greater uncertainty. Both models predict the melanocytic nevi correctly, though BiomedCLIP shows increased uncertainty toward the related melanoma class, suggesting a more challenging case.

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1782 **F ABLATIONS**
17831784 This section contains additional ablation experiments.
17851786 **F.1 NUMBER OF ENSEMBLE MEMBERS IN OUT-OF-DISTRIBUTION DETECTION**
17871788 We provide an additional ablation study on the impact of the ensemble size on out-of-distribution
1789 performance. Table 7 and Figure 13 demonstrate once more the efficiency of our approach: it
1790 requires only a single trained model. In contrast, ensemble-based baselines typically rely on at least
1791 five members and benefit from larger ensembles to improve performance.
17921793 **Table 7:** Ablation of different numbers of trained ensemble members for Out-of-Distribution De-
1794 tection.

Method	Members	SVHN	Places365	CIFAR-100	FMNIST	ImageNet
EffCre _{0.95}	1	0.885 \pm 0.003	0.862 \pm 0.005	0.854 \pm 0.003	0.907 \pm 0.002	0.826 \pm 0.004
CreRL _{0.95}	5	0.917 \pm 0.012	0.894 \pm 0.002	0.885 \pm 0.002	0.928 \pm 0.004	0.863 \pm 0.002
CreWra	5	0.943 \pm 0.006	0.904 \pm 0.001	0.905 \pm 0.001	0.939 \pm 0.001	0.879 \pm 0.001
CreEns _{0.0}	5	0.938 \pm 0.007	0.898 \pm 0.001	0.900 \pm 0.001	0.929 \pm 0.001	0.874 \pm 0.001
CreBNN	5	0.843 \pm 0.006	0.829 \pm 0.006	0.831 \pm 0.007	0.851 \pm 0.007	0.809 \pm 0.007
CreNet	5	0.938 \pm 0.003	0.908 \pm 0.001	0.900 \pm 0.001	0.941 \pm 0.003	0.871 \pm 0.002
CreRL _{0.95}	10	0.921 \pm 0.010	0.905 \pm 0.002	0.896 \pm 0.001	0.940 \pm 0.002	0.872 \pm 0.002
CreWra	10	0.953 \pm 0.004	0.911 \pm 0.001	0.912 \pm 0.000	0.948 \pm 0.001	0.886 \pm 0.001
CreEns _{0.0}	10	0.949 \pm 0.001	0.907 \pm 0.001	0.909 \pm 0.002	0.941 \pm 0.002	0.883 \pm 0.001
CreBNN	10	0.880 \pm 0.009	0.856 \pm 0.002	0.859 \pm 0.002	0.886 \pm 0.001	0.838 \pm 0.001
CreNet	10	0.944 \pm 0.001	0.915 \pm 0.001	0.908 \pm 0.001	0.949 \pm 0.001	0.881 \pm 0.001
CreRL _{0.95}	20	0.917 \pm 0.013	0.910 \pm 0.001	0.901 \pm 0.000	0.945 \pm 0.004	0.878 \pm 0.002
CreWra	20	0.957 \pm 0.003	0.916 \pm 0.001	0.916 \pm 0.000	0.952 \pm 0.000	0.890 \pm 0.001
CreEns _{0.0}	20	0.955 \pm 0.001	0.913 \pm 0.000	0.914 \pm 0.001	0.949 \pm 0.001	0.888 \pm 0.000
CreBNN	20	0.907 \pm 0.006	0.885 \pm 0.002	0.880 \pm 0.002	0.935 \pm 0.002	0.859 \pm 0.002
CreNet	20	0.943 \pm 0.003	0.918 \pm 0.000	0.912 \pm 0.000	0.951 \pm 0.002	0.884 \pm 0.001

1815 **F.2 α -VALUES FOR ACTIVE IN-CONTEXT LEARNING**
18161817 We provide an additional ablation on the effect that the α -value has on the performance of our
1818 method in active in-context learning. We evaluate runs for values $\alpha \in \{0.2, 0.4, 0.6, 0.8, 0.9, 0.95\}$.
1819 In Figure 14, we provide the results for the TabArena datasets with OpenML (Bischl et al., 2025)
1820 id 46941, 46963, and 46930. For the sake of legibility, we only consider the zero-one-loss-based
1821 epistemic uncertainty measure (6).
18221823 We observe that higher α values consistently improve performance across all three datasets until
1824 the performance converges at $\alpha = 0.8$. In particular, lower α values result in larger predicted
1825 sets with high epistemic uncertainty, which reduces the meaningful separation between instances.
1826 Consequently, the optimal order for selecting instances during active learning is lost when α is small,
1827 explaining the drop in performance.
18281829 **F.3 ACCURACY AND EXPECTED CALIBRATION SCORE EVALUATION FOR SINGLE MODELS**
18301831 If we have to commit to a precise probabilistic prediction, a natural choice is to use the maximum
1832 likelihood estimate, which is a theoretically well-established approach. If, additionally, a class-
1833 wise prediction is sought, the argmax class can be predicted. To provide a sense of the quality of
1834 the underlying models trained for our experiments, we report standard supervised-learning metrics,
1835 namely accuracy and expected calibration error, for each individual model in Table 8 based on
1836 the original CIFAR-10 test set. This serves as a sanity check to ensure a fair comparison with the
1837 baselines. For our experiments with TabPFN and CLIP models we use the pre-trained models.
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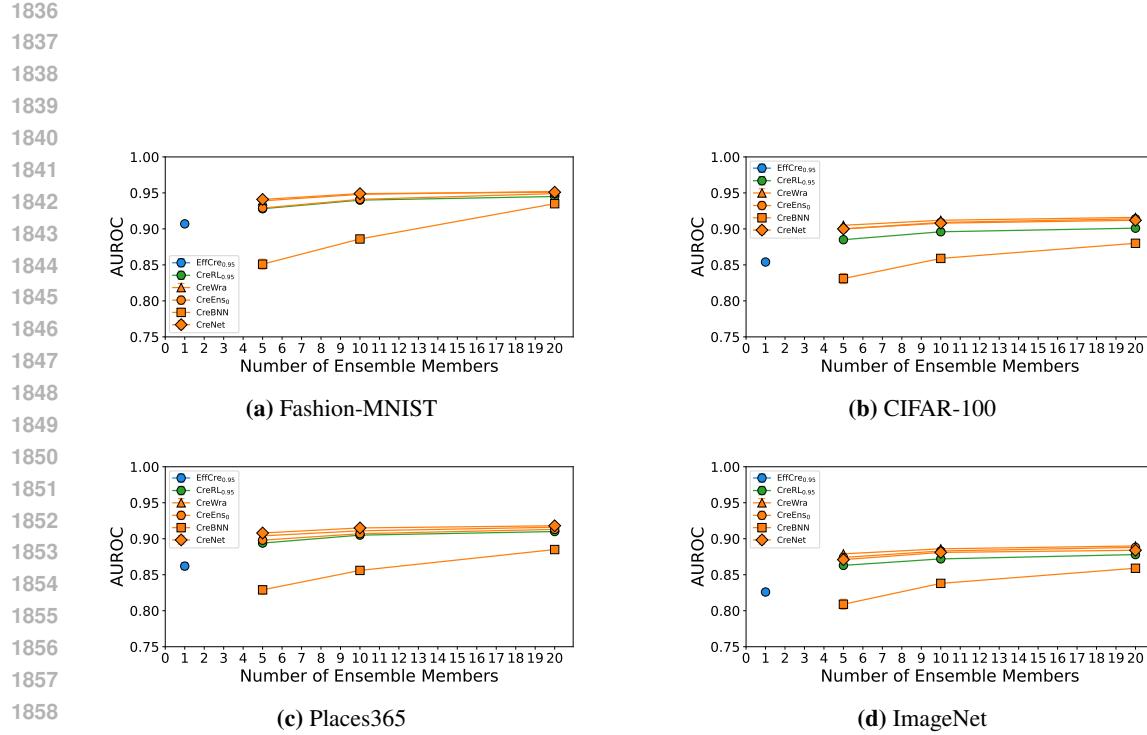


Figure 13: Out-of-distribution detection performance (based on AUROC score) as a function of ensemble size. CIFAR-10 is the in-distribution data while various datasets are used as OOD data.

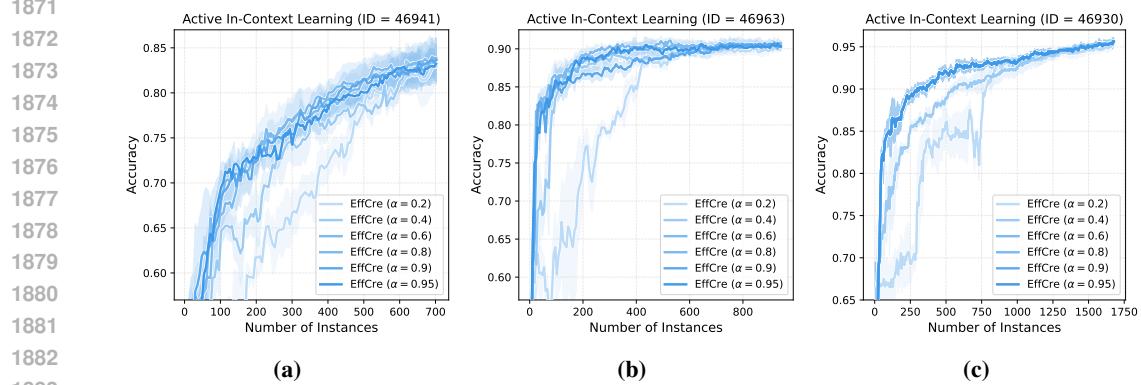


Figure 14: Active In-Context Learning with TabPFN. Performance on TabArena datasets 46941, 46963, 46930 for different values of α .

1890	1891	1892	1893	1894	Method	Model	CIFAR10		ChaosNLI		QualityMRI	
							ECE	Acc	ECE	Acc	ECE	Acc
1896	EffCre	1	0.04 ± 0.00	0.93 ± 0.00	0.04 ± 0.01	0.61 ± 0.01	0.30 ± 0.05	0.49 ± 0.05				
1897	CreRL _{0.8}	1	0.04 ± 0.00	0.94 ± 0.00	0.09 ± 0.03	0.60 ± 0.02	0.33 ± 0.09	0.48 ± 0.04				
1898		2	0.06 ± 0.01	0.87 ± 0.01	0.13 ± 0.01	0.57 ± 0.01	0.35 ± 0.08	0.50 ± 0.05				
1899		3	0.06 ± 0.00	0.87 ± 0.00	0.10 ± 0.01	0.56 ± 0.01	0.37 ± 0.10	0.51 ± 0.02				
1900		4	0.06 ± 0.00	0.88 ± 0.00	0.09 ± 0.01	0.58 ± 0.01	0.30 ± 0.09	0.49 ± 0.03				
1901		5	0.06 ± 0.00	0.89 ± 0.00	0.12 ± 0.01	0.60 ± 0.00	0.38 ± 0.09	0.48 ± 0.04				
1902		6	0.06 ± 0.00	0.89 ± 0.00	0.10 ± 0.01	0.57 ± 0.01	0.30 ± 0.08	0.49 ± 0.07				
1903		7	0.06 ± 0.01	0.88 ± 0.01	0.09 ± 0.01	0.59 ± 0.02	0.34 ± 0.04	0.51 ± 0.04				
1904		8	0.06 ± 0.01	0.90 ± 0.00	0.11 ± 0.01	0.60 ± 0.01	0.33 ± 0.09	0.49 ± 0.04				
1905		9	0.06 ± 0.00	0.90 ± 0.01	0.09 ± 0.01	0.59 ± 0.00	0.35 ± 0.10	0.47 ± 0.03				
1906		10	0.06 ± 0.00	0.91 ± 0.00	0.09 ± 0.01	0.39 ± 0.01	0.38 ± 0.09	0.49 ± 0.04				
1907	CreWra	1	0.03 ± 0.00	0.94 ± 0.00	0.12 ± 0.02	0.60 ± 0.01	0.39 ± 0.02	0.48 ± 0.03				
1908		2	0.03 ± 0.00	0.95 ± 0.00	0.11 ± 0.01	0.60 ± 0.01	0.39 ± 0.02	0.51 ± 0.04				
1909		3	0.03 ± 0.00	0.94 ± 0.00	0.12 ± 0.02	0.59 ± 0.01	0.38 ± 0.02	0.48 ± 0.03				
1910		4	0.03 ± 0.00	0.94 ± 0.00	0.15 ± 0.01	0.57 ± 0.02	0.34 ± 0.01	0.49 ± 0.02				
1911		5	0.03 ± 0.00	0.94 ± 0.00	0.13 ± 0.01	0.55 ± 0.01	0.37 ± 0.03	0.46 ± 0.01				
1912		6	0.03 ± 0.00	0.94 ± 0.00	0.10 ± 0.01	0.59 ± 0.02	0.38 ± 0.04	0.48 ± 0.04				
1913		7	0.03 ± 0.00	0.94 ± 0.00	0.12 ± 0.01	0.59 ± 0.01	0.39 ± 0.02	0.46 ± 0.05				
1914		8	0.03 ± 0.00	0.94 ± 0.00	0.13 ± 0.01	0.59 ± 0.01	0.34 ± 0.01	0.51 ± 0.06				
1915		9	0.03 ± 0.00	0.94 ± 0.00	0.12 ± 0.02	0.59 ± 0.01	0.33 ± 0.02	0.48 ± 0.04				
1916		10	0.03 ± 0.00	0.94 ± 0.00	0.10 ± 0.01	0.58 ± 0.02	0.34 ± 0.04	0.47 ± 0.04				
1917	CreEns	1	0.03 ± 0.00	0.94 ± 0.00	0.07 ± 0.03	0.59 ± 0.08	0.31 ± 0.02	0.46 ± 0.03				
1918		2	0.03 ± 0.00	0.94 ± 0.00	0.12 ± 0.03	0.58 ± 0.01	0.33 ± 0.02	0.48 ± 0.04				
1919		3	0.03 ± 0.00	0.94 ± 0.00	0.11 ± 0.02	0.60 ± 0.00	0.34 ± 0.04	0.47 ± 0.04				
1920		4	0.03 ± 0.00	0.94 ± 0.00	0.14 ± 0.01	0.57 ± 0.02	0.38 ± 0.04	0.48 ± 0.04				
1921		5	0.03 ± 0.00	0.94 ± 0.00	0.07 ± 0.03	0.59 ± 0.08	0.31 ± 0.02	0.46 ± 0.03				
1922		6	0.03 ± 0.00	0.94 ± 0.00	0.12 ± 0.03	0.58 ± 0.01	0.33 ± 0.02	0.48 ± 0.04				
1923		7	0.03 ± 0.00	0.94 ± 0.00	0.09 ± 0.03	0.60 ± 0.01	0.32 ± 0.01	0.48 ± 0.02				
1924		8	0.03 ± 0.00	0.94 ± 0.00	0.11 ± 0.02	0.59 ± 0.01	0.38 ± 0.03	0.48 ± 0.03				
1925		9	0.03 ± 0.00	0.94 ± 0.00	0.15 ± 0.01	0.57 ± 0.02	0.34 ± 0.01	0.49 ± 0.02				
1926		10	0.03 ± 0.00	0.94 ± 0.00	0.13 ± 0.01	0.55 ± 0.01	0.37 ± 0.03	0.46 ± 0.01				
1927	CreNet	1	0.03 ± 0.00	0.93 ± 0.00	0.10 ± 0.01	0.57 ± 0.02	0.38 ± 0.04	0.48 ± 0.05				
1928		2	0.03 ± 0.00	0.94 ± 0.00	0.12 ± 0.01	0.59 ± 0.01	0.39 ± 0.02	0.47 ± 0.03				
1929		3	0.02 ± 0.01	0.94 ± 0.00	0.13 ± 0.01	0.59 ± 0.00	0.34 ± 0.01	0.51 ± 0.06				
1930		4	0.03 ± 0.00	0.94 ± 0.00	0.10 ± 0.01	0.59 ± 0.01	0.37 ± 0.02	0.47 ± 0.03				
1931		5	0.03 ± 0.00	0.94 ± 0.00	0.11 ± 0.04	0.58 ± 0.01	0.33 ± 0.02	0.48 ± 0.04				
1932		6	0.03 ± 0.00	0.95 ± 0.00	0.11 ± 0.02	0.59 ± 0.01	0.39 ± 0.02	0.50 ± 0.04				
1933		7	0.03 ± 0.00	0.92 ± 0.01	0.12 ± 0.01	0.59 ± 0.01	0.39 ± 0.02	0.47 ± 0.03				
1934		8	0.02 ± 0.01	0.94 ± 0.00	0.13 ± 0.01	0.59 ± 0.00	0.34 ± 0.01	0.51 ± 0.06				
1935		9	0.03 ± 0.00	0.94 ± 0.02	0.12 ± 0.02	0.58 ± 0.01	0.33 ± 0.02	0.48 ± 0.04				
1936		10	0.03 ± 0.01	0.94 ± 0.00	0.10 ± 0.01	0.58 ± 0.02	0.34 ± 0.04	0.48 ± 0.03				
1937	CreBNN	1	0.64 ± 0.00	0.87 ± 0.00	0.10 ± 0.04	0.49 ± 0.07	0.15 ± 0.14	0.54 ± 0.11				
1938		2	0.64 ± 0.01	0.87 ± 0.02	0.09 ± 0.03	0.49 ± 0.07	0.15 ± 0.14	0.54 ± 0.11				
1939		3	0.65 ± 0.00	0.88 ± 0.01	0.10 ± 0.05	0.49 ± 0.08	0.15 ± 0.04	0.54 ± 0.11				
1940		4	0.65 ± 0.01	0.88 ± 0.01	0.07 ± 0.00	0.44 ± 0.00	0.17 ± 0.12	0.54 ± 0.11				
1941		5	0.65 ± 0.00	0.88 ± 0.00	0.07 ± 0.00	0.44 ± 0.00	0.24 ± 0.13	0.54 ± 0.12				
1942		6	0.65 ± 0.01	0.88 ± 0.01	0.13 ± 0.05	0.55 ± 0.08	0.28 ± 0.14	0.46 ± 0.11				
1943		7	0.64 ± 0.00	0.87 ± 0.00	0.11 ± 0.03	0.53 ± 0.06	0.14 ± 0.15	0.44 ± 0.09				
1944		8	0.63 ± 0.01	0.86 ± 0.02	0.13 ± 0.04	0.55 ± 0.07	0.19 ± 0.07	0.53 ± 0.13				
1945		9	0.63 ± 0.01	0.85 ± 0.04	0.12 ± 0.05	0.53 ± 0.07	0.19 ± 0.07	0.51 ± 0.11				
1946		10	0.63 ± 0.00	0.86 ± 0.01	0.12 ± 0.04	0.54 ± 0.07	0.17 ± 0.12	0.52 ± 0.12				

Table 8: Comparison of ECE and accuracy of single models per method across datasets.