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# Is the Volume of a Credal Set a Good Measure for Epistemic Uncertainty?

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# Lack of Uncertainty-Awareness of ML Systems

(a) “typewriter keyboard” with certainty **83.14 %**

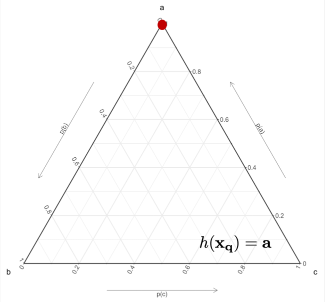
(b) “stone wall” with certainty **87.63 %**

Figure 1: Predictions by EfficientNet [Tan and Le, 2019] on test images from ImageNet.

# Aleatoric and Epistemic Uncertainty

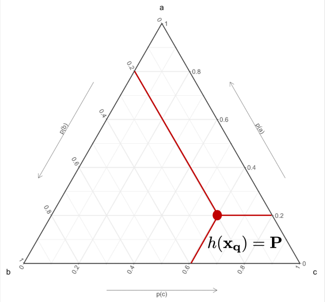
- **Aleatoric** uncertainty (AU)
  - refers to the notion of randomness, that is, the variability in the outcome which is due to inherently random effects,
  - is a property of the data-generating process, and as such irreducible.
- **Epistemic** uncertainty (EU)
  - refers to uncertainty caused by a lack of knowledge, i.e.,
  - to the epistemic state of the agent (e.g., learning algorithm),
  - can in principle be reduced on the basis of additional information (e.g., training data).

# Uncertainty Representation



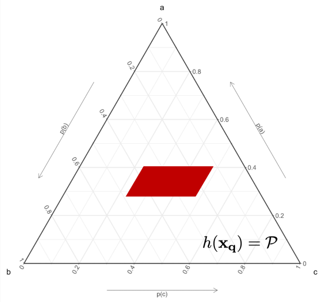

(a) **Hard Label Prediction**

$h_l : \mathcal{X} \to \mathcal{Y}$




(b) **Probabilistic Prediction**

$h_p : \mathcal{X} \to \mathbb{P}(\mathcal{Y})$




(c) **Credal Prediction**

$h_c : \mathcal{X} \to \mathrm{Cr}(\mathcal{Y})$

| | (a) | (b) | (c) |
|---|---|---|---|
| **AU aware?** | ✗ | ✓ | ✓ |
| **EU aware?** | ✗ | ✗ | ✓ |

## Formal Setting

### Definition (Credal set)

*Let $(\mathcal{Y}, \sigma(\mathcal{Y}))$ be a generic measurable space and denote by $\mathbb{P}(\mathcal{Y})$ the set of all probability measures on $(\mathcal{Y}, \sigma(\mathcal{Y}))$. A convex subset $\mathcal{P} \subseteq \mathbb{P}(\mathcal{Y})$ is called a credal set.*

In the following $\mathcal{Y}$ denotes a finite label space, i.e., $\mathcal{Y} = \{y_1, \dots, y_d\}$, where $d \in \mathbb{N}_{\geq 2}$. Further, we call

$$\overline{P}(A) := \sup_{P \in \mathcal{P}} P(A), \quad \text{for all} \quad A \in \sigma(\mathcal{Y})$$

upper probability (associated with a credal set $\mathcal{P}$), and

$$\underline{P}(A) := \inf_{P \in \mathcal{P}} P(A), \quad \text{for all} \quad A \in \sigma(\mathcal{Y})$$

lower probability, respectively.

## Vol($\mathcal{P}$): a good measure for EU, if $d = 2$

In the binary case Vol($\mathcal{P}$) satisfies a set of desirable axioms (see Abellán and Klir [2005], Jiroušek and Shenoy [2018], Hüllermeier et al. [2022]):

**A1** *Non-negativity* and *boundedness:*

(i) $\text{Vol}(\mathcal{P}) \geq 0$, for all $\mathcal{P} \in \text{Cr}(\mathcal{Y})$;

(ii) there exists $u \in \mathbb{R}$ such that $\text{Vol}(\mathcal{P}) \leq u$, for all $\mathcal{P} \in \text{Cr}(\mathcal{Y})$.

**A2** *Continuity*: $\text{Vol}(\cdot)$ is a continuous functional.

**A3** *Monotonicity*: for all $\mathcal{Q}, \mathcal{P} \in \text{Cr}(\mathcal{Y})$ such that $\mathcal{Q} \subset \mathcal{P}$, we have $\text{Vol}(\mathcal{Q}) \leq \text{Vol}(\mathcal{P})$.

## Vol($\mathcal{P}$): a good measure for EU, if $d = 2$

**A4** *Probability consistency*: Vol($\mathcal{P}$) reduces to 0 as the distance between $\overline{P}(A)$ and $\underline{P}(A)$ goes to 0, for all $A \in \sigma(\mathcal{Y})$.

**A5** *Sub-additivity*: Suppose $\mathcal{Y} = \mathcal{Y}_1 \times \mathcal{Y}_2$, and let $\mathcal{P}$ be a joint credal set on $\mathcal{Y}$ such that $\mathcal{P}'$ is the marginal credal set on $\mathcal{Y}_1$ and $\mathcal{P}''$ is the marginal credal set on $\mathcal{Y}_2$, respectively. Then, we have Vol($\mathcal{P}$) $\leq$ Vol($\mathcal{P}'$) + Vol($\mathcal{P}''$).

**A6** *Additivity*: If $\mathcal{P}'$ and $\mathcal{P}''$ are independent[1], **A5** holds with equality.

**A7** *Invariance*: Vol($\cdot$) is invariant to rotation and translation.

[1] Suitable notion of independence for credal sets, see Couso et al. [1999].

## Lack of Robustness in Higher Dimensions

For a generic compact set $K \in \mathbb{R}^d$ and a positive real $r$, the *$r$-packing* of $K$, denoted by $\text{Pack}_r(K)$, is the collection of sets $K'$ that satisfy the following properties

(i) $K' \subset K$,

(ii) $\cup_{x \in K'} B_r^d(x) \subset K$, where $B_r^d(x)$ denotes the ball of radius $r$ in space $\mathbb{R}^d$ centered at $x$,

(iii) the elements of $\{B_r^d(x)\}_{x \in K'}$ are pairwise disjoint,

(iv) there does not exist $x' \in K$ such that (i)-(iii) are satisfied by $K' \cup \{x'\}$.

The *packing number* of $K$, denoted by $N_r^{\text{pack}}(K)$, is given by $\max_{K' \in \text{Pack}_r(K)} |K'|$.

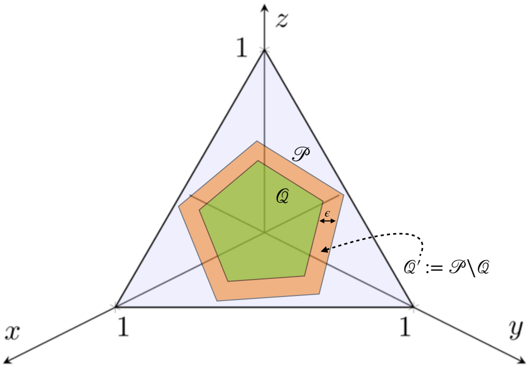
## Lack of Robustness in Higher Dimensions

Let $\mathcal{P} \subset \mathbb{P}(\mathcal{Y})$ be a compact credal set, and $\mathcal{Q} \subset \mathbb{P}(\mathcal{Y})$ such that:

(a) $\mathcal{Q} \subsetneq \mathcal{P}$, so that $\mathcal{Q}' := \mathcal{P} \setminus \mathcal{Q} \neq \emptyset$,

(b) $d_H(\mathcal{P}, \mathcal{Q}) = \varepsilon$, for some $\varepsilon > 0$,

(c) $\varepsilon$ is such that we can find $r > 0$ for which $N_r^{\text{pack}}(\mathcal{P}) \geq N_{r-\varepsilon}^{\text{pack}}(\mathcal{Q}')$.



## Lack of Robustness in Higher Dimensions

**Theorem**

*Let $\mathcal{Y}$ be a finite Polish space so that $|\mathcal{Y}| = d$, and let $\sigma(\mathcal{Y}) = 2^{\mathcal{Y}}$. Pick any compact set $\mathcal{P} \subset \mathbb{P}(\mathcal{Y})$, and any set $\mathcal{Q}$ that satisfies (a) - (c). The following holds*

$$\frac{Vol(\mathcal{P}) - Vol(\mathcal{Q}')}{Vol(\mathcal{P})} \geq 1 - \left(1 - \frac{\varepsilon}{r}\right)^d .$$

# Conclusion

We conclude with the following key takeaways:

- Representing uncertainty in terms of credal sets is appealing from a ML perspective,
- Volume of a credal set is a good measure of epistemic uncertainty in binary classification.
- Its effectiveness diminishes in the context of multi-class classification, despite being intuitively appealing.
- Feasibility and efficacy of geometric approaches to uncertainty quantification in ML?

# References

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