Uncertainty Quantification in Machine Learning

From Aleatoric to Epistemic

Eyke Hüllermeier

Institute of Informatics, LMU Munich, Germany

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Introduction and motivation

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- Other sources of uncertainty exist: incorrect **model assumptions** (model misspecification), noisy or imprecise **data**, etc.
- **Trustworthy representation** of uncertainty is desirable and should be considered as a key feature of any machine learning method, all the more in safety-critical application domains.

Self-awareness of ML systems

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- Many applications require safe and reliable predictions, and hence a certain level of **self-awareness** of ML systems:
  - equip predictions with an appropriate **quantification of uncertainty**,
  - **reject** a decision in cases of high uncertainty (abstention) ,
  - deliver a credible **set-valued prediction** (partial abstention),
  - ...

Driver assistance systems: a safety-critical application

Adversarial examples

There is really but one thing to say about **this** sorry movie It should never have been made The first one one of my favourites An American Werewolf in London is a great movie with a good plot good actors and good FX But this one It stinks to heaven with a cry of helplessness

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- The **adversarial example** (right) is misclassified by a machine learning model trained on textual data, which changes its prediction due to a change of a single (actually unimportant) word (Sato *et al.*, 2018).

Lack of uncertainty-awareness

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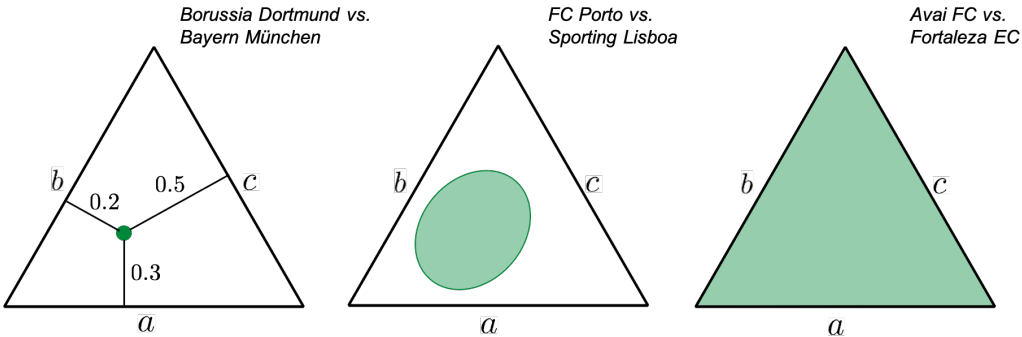
- Predictions by EfficientNet on test images from ImageNet: For the left image, the neural network predicts “typewriter keyboard” with certainty 83.14 %, for the right image “stone wall” with certainty 87.63 %.

Levels of self-awareness and uncertainty representation



Probability distributions $p = (p(a), p(b), p(c))$ on $\Omega = \{a, b, c\}$, for example $\Omega = \{\text{home wins}, \text{draw}, \text{away wins}\}$, as points in a Barycentric coordinate system.

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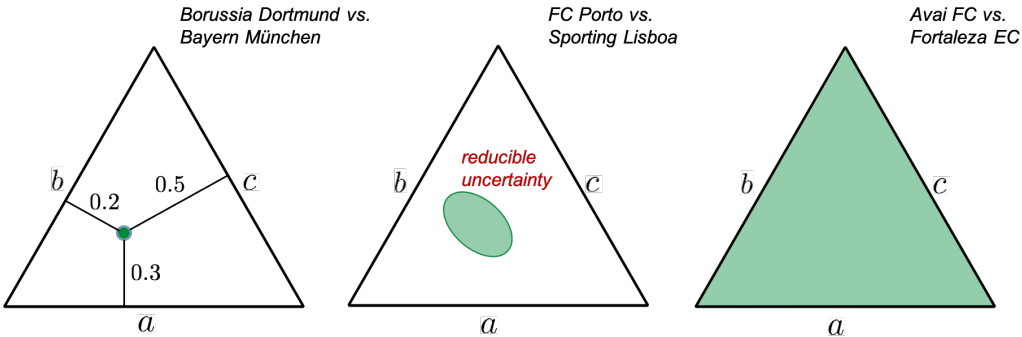

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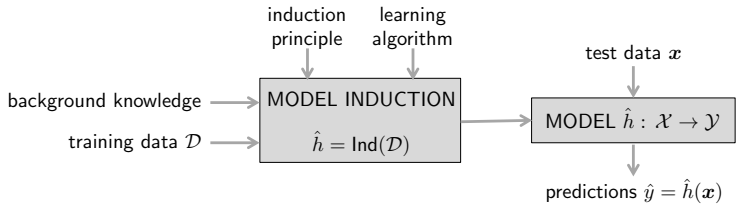

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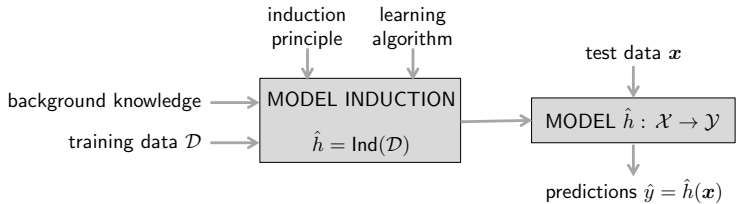
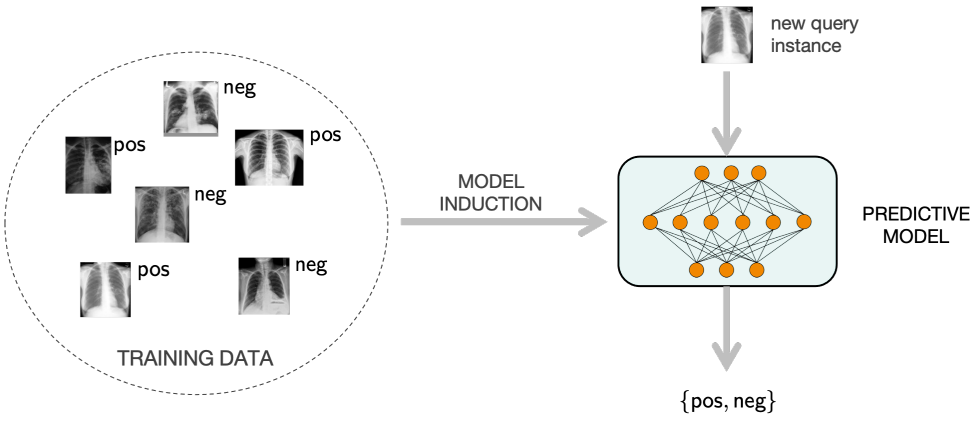


- Assuming a probabilistic data generating process $p(\boldsymbol{x}, y) = p(\boldsymbol{x})p(y \mid \boldsymbol{x})$, **probabilistic predictors** (estimating $p(y \mid \boldsymbol{x})$) are natural primitives.

Supervised learning



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- A learner is given access to a set of (i.i.d.) **training data**

$$\mathcal{D} := \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)\} \subset \mathcal{X} \times \mathcal{Y} \ ,$$

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- Given a **hypothesis space** $\mathcal{H} \subset \mathcal{Y}^{\mathcal{X}}$ and a loss function

$$\ell : \mathcal{Y} \times \mathcal{Y} \longrightarrow \mathbb{R} \, ,$$

  the goal of the learner is to induce a hypothesis $h^* \in \mathcal{H}$ with low **risk**

$$R(h) := \int_{\mathcal{X} \times \mathcal{Y}} \ell(h(\boldsymbol{x}), y) \, d \, P(\boldsymbol{x}, y) \ .$$

Classification and regression

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Then, however, a convex, (smooth) upper approximation is typically used as a surrogate for training.
- If predictions are **probabilities**
$$h(\boldsymbol{x}) = \hat{\boldsymbol{p}} = (\hat{p}_1, \dots, \hat{p}_K) \in \Delta_K \,,$$
the loss is defined on $\Delta_K \times \mathcal{Y}$; a common example is the logistic loss (log-loss)
$$\ell(\hat{\boldsymbol{p}}, y) = -\log(p_y) \,.$$

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- Correspondingly, there remains **uncertainty** regarding h^*, the approximation quality of $\hat{h}$ (in the sense of its proximity to h^*) and its true risk $R(\hat{h})$, as well as **predictive uncertainty** about $\hat{y}_q$ for an individual **query instance** $\boldsymbol{x}_q \in \mathcal{X}$.

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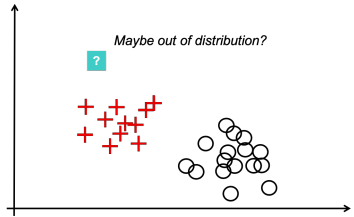
- A precise specification of the **problem setting** and **underlying assumptions** is an important prerequisite, not only for providing learning guarantees, but also for **uncertainty quantification**.



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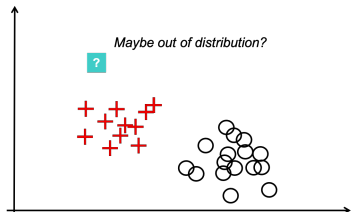

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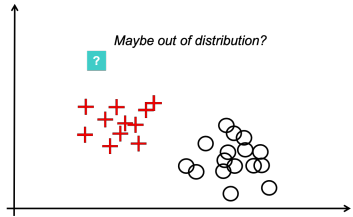

- Here, one might be quite sure about the class of the query under standard assumptions of binary classification, but much less so in a setting of **novelty detection**, where new classes may emerge.
- Likewise, assumptions such as **i.i.d. data generation** are really crucial (the past should be representative of the future).

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- The best point predictions (minimizing expected loss) are prescribed by the **pointwise Bayes predictor** f^*:

$$f^*(\boldsymbol{x}) := \operatorname*{arg\,min}_{\hat{y} \in \mathcal{Y}} \int_{\mathcal{Y}} \ell(y, \hat{y}) \, dP(y \mid \boldsymbol{x}) \,.$$

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- Due to model uncertainty, one cannot guarantee

$$h^*(\boldsymbol{x}) = f^*(\boldsymbol{x}),$$

or, in the case of probabilistic predictions $p^*(y \mid \boldsymbol{x}) := p(y \mid \boldsymbol{x}, h^*)$, that

$$p^*(\cdot \mid \boldsymbol{x}) = p(\cdot \mid \boldsymbol{x}).$$

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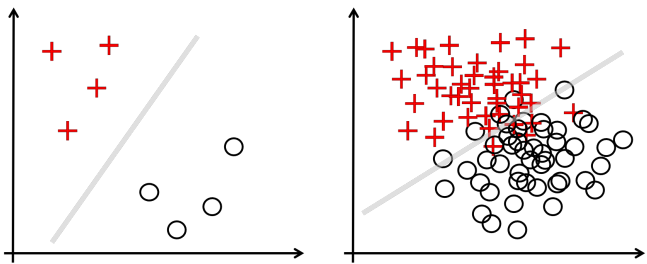

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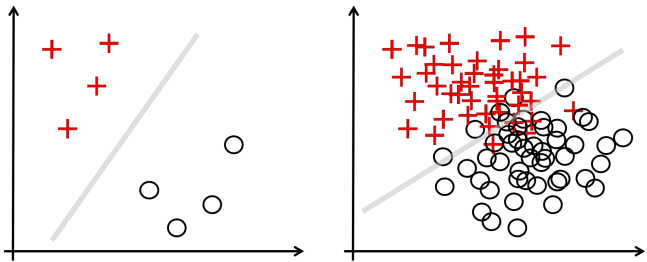

- We refer to the uncertainty about the discrepancy between $\hat{h}$ and h^* as **approximation uncertainty**.

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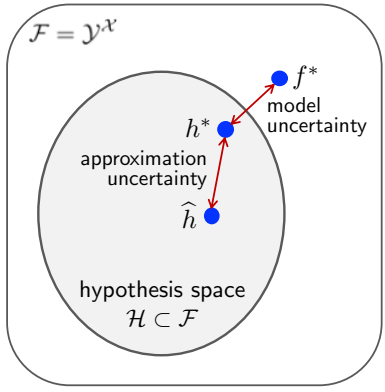

	point prediction	probability
ground truth	$f^*(\boldsymbol{x})$	$p(\cdot \mid \boldsymbol{x})$
best possible	$h^*(\boldsymbol{x})$	$p^*(\cdot \mid \boldsymbol{x}) = p(\cdot \mid \boldsymbol{x}, h^*)$
induced predictor	$\hat{h}(\boldsymbol{x})$	$\hat{p}(\cdot \mid \boldsymbol{x}) = p(\cdot \mid \boldsymbol{x}, \hat{h})$

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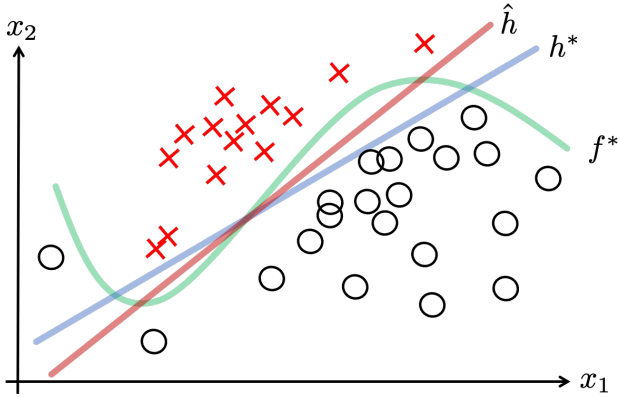

Agenda

1. Introduction
2. **Training probabilistic predictors**
3. Calibration
4. Set-valued (conformal) prediction
5. Epistemic uncertainty

Probabilistic models

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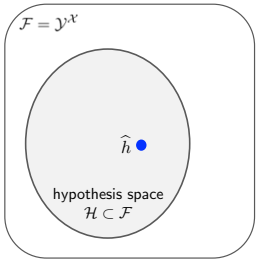
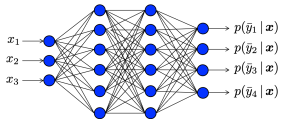
- Probabilistic learners produce a single probabilistic predictor $\hat{h}$:





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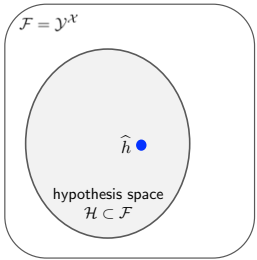

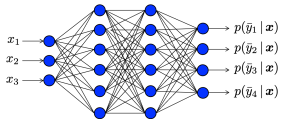

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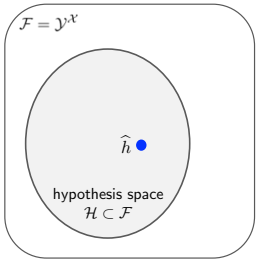

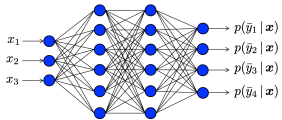

- Captures stochastic nature of dependence $p(y \mid \boldsymbol{x})$ between instances and outcomes, and hence **aleatoric uncertainty**.
- Yet, pretends full certainty about this dependence, thereby ignoring approximation and model uncertainty (epistemic uncertainty).

Maximum likelihood

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- Suppose that hypotheses h are (uniquely) identified by parameters $\boldsymbol{\theta} \in \Theta$, i.e.,

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- Under the i.i.d. assumption, ML estimation comes down to solving

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}\in\Theta} \prod_{i=1}^{N} P\big((\boldsymbol{x}_i, y_i) \,|\, \boldsymbol{\theta}\big) = \arg\max_{\boldsymbol{\theta}\in\Theta} \sum_{i=1}^{N} \log\, P\big((\boldsymbol{x}_i, y_i) \,|\, \boldsymbol{\theta}\big)$$

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- We can think of the above model as follows: First, an instance $\boldsymbol{x}$ is assigned a (latent) score (expressing the propensity for the positive class)

$$s = s(\boldsymbol{x}) = \big\langle \boldsymbol{\theta}, \boldsymbol{x} \big\rangle \,,$$

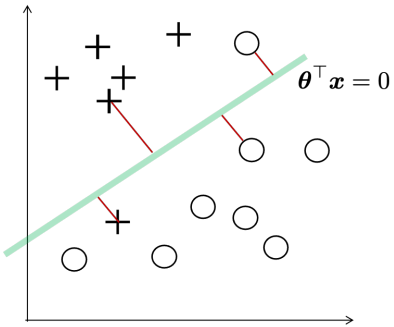
  which is then transformed into a probability via the (logistic) **link function**

$$\phi(s) = \frac{1}{1 + \exp(-s)} \,.$$

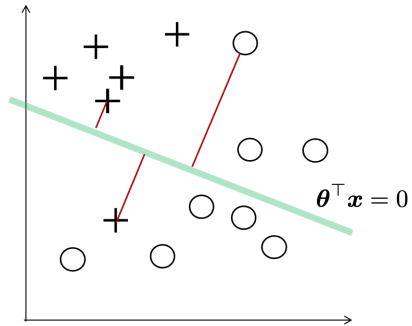
Logistic regression

Logistic regression

- The probability of a label y_i depends on the distance of $\boldsymbol{x}_i$ from the hyperplane defined by $\boldsymbol{\theta}^\top \boldsymbol{x} = 0$.



higher likelihood



lower likelihood

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- In order to learn $\boldsymbol{\theta}$, we can invoke the ML principle:

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- Probability is only maximised over the y_n, while the $\boldsymbol{x}_n$ are assumed to be fixed.
- Logistic regression is an example of **discriminative** learning, i.e., it learns a map

$$h : \boldsymbol{x} \mapsto p(Y \,|\, \boldsymbol{x}).$$

This is to be distinguished from **generative** learning, which essentially means learning the entire data-generating process in the form of the joint distribution $p(\boldsymbol{X}, Y)$.

Bayesian learning

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- In the Bayesian approach, learning corresponds to turning a **prior distribution** on $\mathcal{H}$ into a **posterior**:

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- Bayesian inference is very costly but can be done approximately, for example, using **ensemble methods**.
- An alternative is to commit to the hypothesis with maximum a-posteriori probability (**MAP** inference):

$$h_{MAP} = \arg\max_{h \in \mathcal{H}} p(h \mid \mathcal{D})\,.$$

Agenda

1. Introduction
2. Training probabilistic predictors
3. **Calibration**
4. Set-valued (conformal) prediction
5. Epistemic uncertainty

Proper scoring rules

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- Expressed in terms of predicted probability, the log-loss can then also be written as

$$\ell(\hat{\boldsymbol{p}}, y) = -\log \hat{p}_y \,.$$

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- A loss ℓ is a proper scoring rule if the expected loss minimiser coincides with the true probability $\boldsymbol{p}$:

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- Thus, given a query $\boldsymbol{x}$, a learner penalised by a (strictly) proper scoring rule has an incentive to predict the true (conditional) probability $\boldsymbol{p} = p(Y \mid \boldsymbol{x})$.
- For example, the **Brier score** $\sum_k (\hat{p}_k - y_k)^2$ is strictly proper, because

$$\sum_{k=1}^{K} p_k \cdot \left[(1 - \hat{p}_k)^2 + \sum_{j \neq k} (\hat{p}_j)^2 \right] = \sum_k (\hat{p}_k)^2 + \sum_k p_k (1 - 2\hat{p}_k)$$

  is minimised by $\hat{p}_k = p_k$ for all $k \in [K]$.

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- Define the **scoring function** on probability vectors $\hat{\boldsymbol{p}}, \boldsymbol{p}$ as

$$S(\hat{\boldsymbol{p}}, \boldsymbol{p}) := \mathbb{E}_{Y \sim \boldsymbol{p}} S(\hat{\boldsymbol{p}}, Y) = \sum_k S(\hat{\boldsymbol{p}}, y)\, p_k \,,$$

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- A scoring rule is proper if the **divergence**

$$d(\hat{\boldsymbol{p}}, \boldsymbol{p}) := S(\hat{\boldsymbol{p}}, \boldsymbol{p}) - S(\boldsymbol{p}, \boldsymbol{p})$$

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- $e(\boldsymbol{p}) := S(\boldsymbol{p}, \boldsymbol{p})$ is also called **entropy**.

Proper scoring rules

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- For the **log-loss**, we obtain a decomposition into KL-divergence and information (Shannon) entropy:

$$d(\hat{\boldsymbol{p}}, \boldsymbol{p}) = D_{KL}(\boldsymbol{p} \| \hat{\boldsymbol{p}}) = \sum_k p_k \cdot \log\left(\frac{p_K}{\hat{p}_k}\right)$$

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- The **0/1 loss** is a proper but not a strictly proper scoring rule.

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- The expectation of a strictly proper score can be decomposed as follows:

$$\mathbb{E}_{Y\sim\boldsymbol{p}}\, S(\hat{\boldsymbol{p}}, Y) = S(\hat{\boldsymbol{p}}, \boldsymbol{p}) = d(\hat{\boldsymbol{p}}, \boldsymbol{p}) + S(\boldsymbol{p}, \boldsymbol{p})\,,$$

  where the **entropy** $S(\boldsymbol{p}, \boldsymbol{p})$ is the unavoidable part of the loss (due to the need to predict the realisation of a random variable) and $d(\hat{\boldsymbol{p}}, \boldsymbol{p})$ the extra loss.

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$$\mathbb{E}\, S(\hat{\boldsymbol{p}}, Y) = \mathbb{E}\, d(\hat{\boldsymbol{p}}, \boldsymbol{c}) + \mathbb{E}\, e(\boldsymbol{c})\,,$$

  where the expectation is taken over $\mathcal{X} \times \mathcal{Y}$, and $c_k := p(y = k \mid \hat{\boldsymbol{p}})$, i.e., $\boldsymbol{c}$ is the true class distribution on those instances that receive the same prediction $\hat{\boldsymbol{p}}$.

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- $\mathbb{E}\, d(\hat{\boldsymbol{p}}, \boldsymbol{c})$ is called **calibration loss** and $\mathbb{E}\, e(\boldsymbol{c})$ **refinement loss**.

Calibration

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- Many ML methods naturally yield predictions in the form of **scores**

$$s_1, \ldots, s_K \in \mathbb{S} \subseteq \mathbb{R},$$

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$$\boldsymbol{s} = h(\boldsymbol{x}) = (s_1, \ldots, s_K) \in [0, 1]^K,$$

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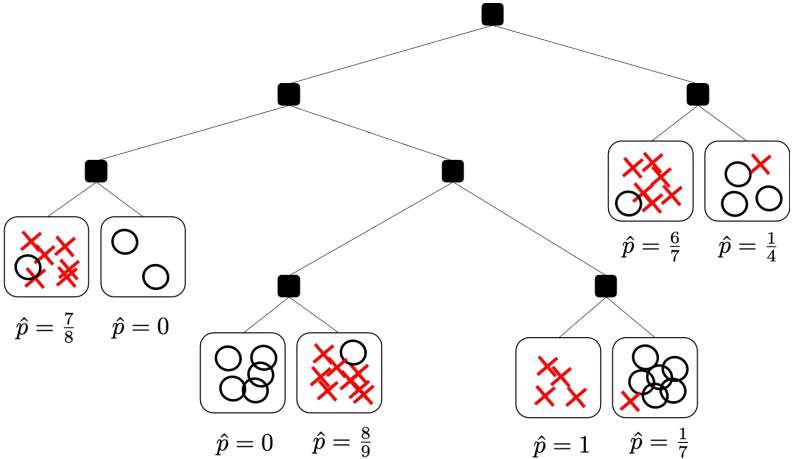
- Yet, calibration is a prerequisite for uncertainty-awareness and important for prediction, decision-making, cost-sensitive classification, etc.

Probability estimation with decision trees



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$$\hat{\boldsymbol{p}} = (\hat{p}_-, \hat{p}_+) = (1 - \hat{p}_+, \hat{p}_+) \in \Delta_2 \,,$$

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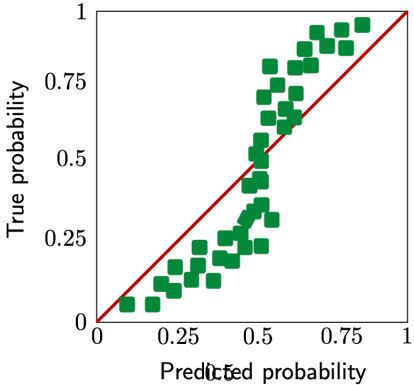
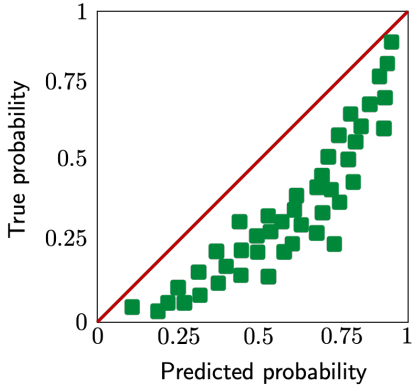
- In other words, a predicted probability vector is supposed to match empirical frequencies, at least in the long run.

Calibration





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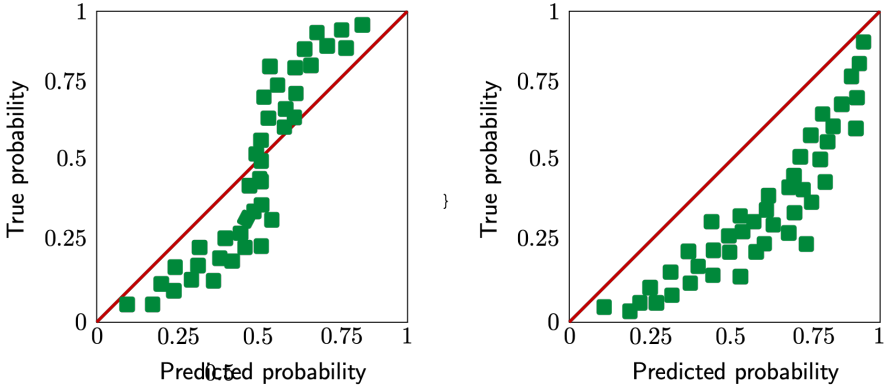
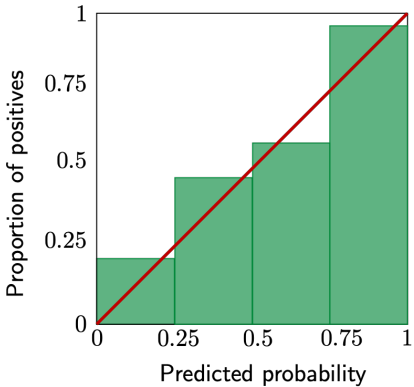
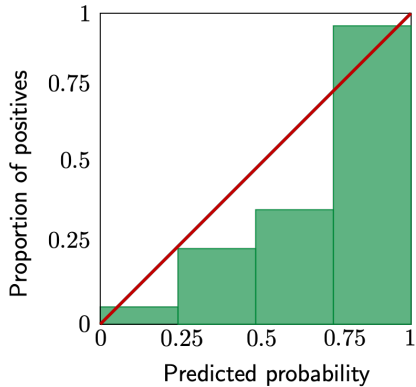


- Examples of miscalibration: bias toward 1/2 (left), systematic underestimation (right).

Reliability diagram





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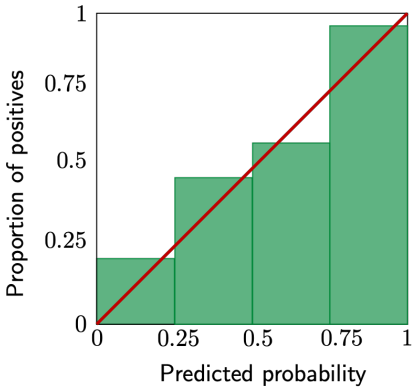

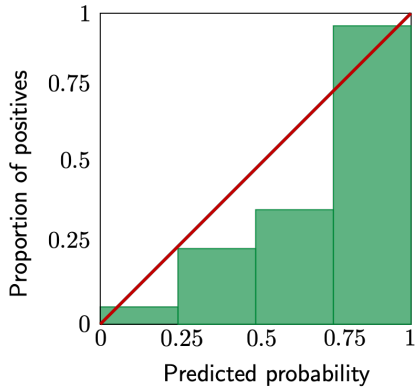

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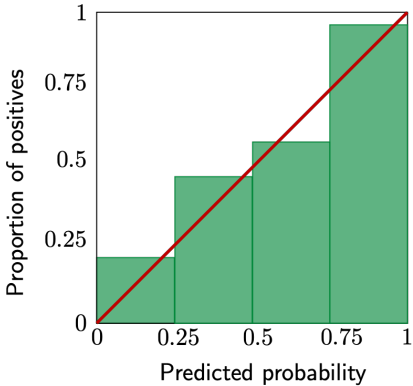

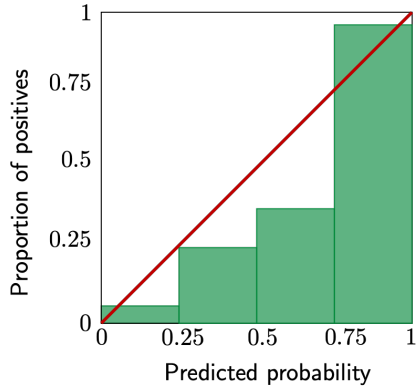

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- There is a trade-off in the choice of the width of the bins (more data per bin vs. more fine-granular assessment).

Calibration and scaling functions

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- Different **post-processing** (post-hoc) methods have been proposed for the purpose of calibration, i.e., to construct a **calibration function**

$$C : \mathbb{S} \longrightarrow [0, 1] \,,$$

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- NB: To make the distinction between (post-hoc) calibration and scaling, C is often called **scaling function** in the case where $\mathbb{S} \neq [0, 1]$.

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- This data should be different from the training data (used to learn the scoring classifier h). Otherwise, there is a risk of introducing a bias.

Empirical binning

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- **Binning** offers a first obvious approach: Partition $\mathbb{S}$ into bins (intervals) $B_1, \ldots, B_M$, and define $C(s) = \hat{p}_{J(s)}$, where $J(s)$ denotes the index of the bin of s (i.e., $s \in B_{J(s)}$).

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- $\hat{p}_1, \ldots, \hat{p}_M$ are chosen so as to minimise the **estimated calibration error** (ECE)

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- Binning is nonparametric and hence flexible, easy to train, and can directly minimise calibration error, albeit at the cost of (increased) groping loss.

Platt scaling

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- Another method is **Platt scaling**, which essentially applies logistic regression to predicted scores $s \in \mathbb{R}$, i.e., it fits a calibration function C such that

$$C_{\alpha,\beta}(s) = \frac{1}{1 + \exp(-\alpha \cdot s - \beta)},$$

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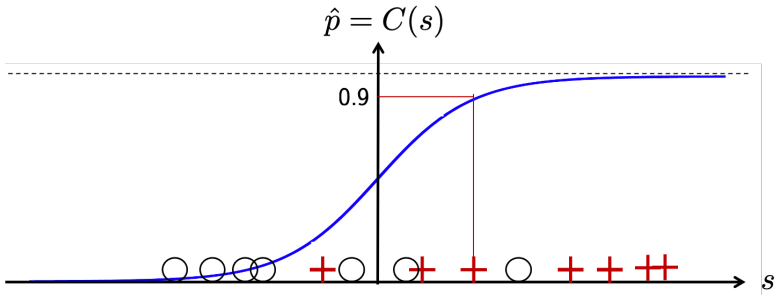
- Platt scaling is fast and easy to implement, but restricted to **sigmoidal calibration functions** (pushing scores from the center toward the extremes, hence coming with a risk of over-confidence).

Platt scaling



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- Although still restricted in a parametric way, Beta calibration is more flexible than Platt scaling and includes inverse sigmoids and the identity map (which helps prevent over-calibration and unnecessary adjustments).

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- Isotonic regression is more expensive in terms of training time and memory consumption.

Pair-adjacent violators algorithm (PAVA)

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- Let the scores observed for calibration be sorted (and without ties), such that

$$s_1 < s_2 < \ldots < s_N \,.$$

We then seek values $c_1 \leq c_2 \leq \ldots \leq c_N$ which minimize

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- **Initialise** one block B_n for each observation (s_n, y_n); the value of the block is $c(B_n) = y_n$ and the width is $w(B_n) = 1$.
- A **merge operation** combines two blocks B' and B'' into a new block B with width $w(B) = w(B') + w(B'')$ and value

$$c = \frac{w(B')c(B') + w(B'')c(B'')}{w(B') + w(B'')} \,.$$

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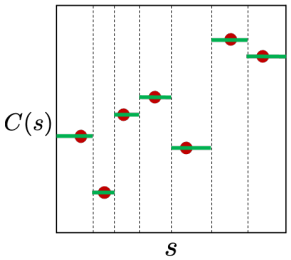
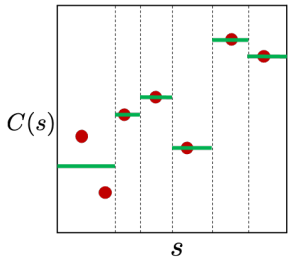
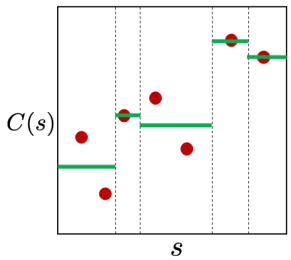
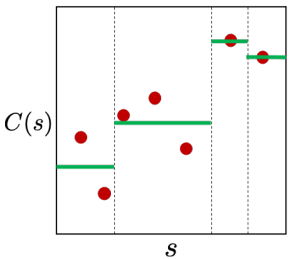
- PAVA iterates the following steps (the description is somewhat simplified to avoid notational overload):
  1. Find the first violating pair, namely, adjacent blocks B_i and B_{i+1} such that $c_i > c_{i+1}$; if there is no such pair, then stop.
  2. Merge B_i and B_{i+1} into a new block B.
  3. If $c(B) < c(B_{i-1})$ for the left neighbor block B_{i-1}, merge also these blocks and continue doing so until no more violations are encountered.
  4. Continue with (1).

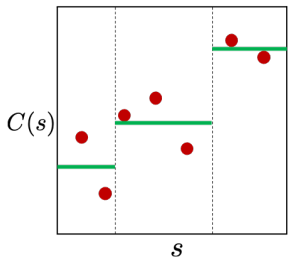
Pair-adjacent violators algorithm (PAVA)











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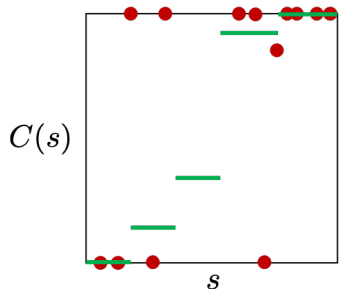
- Note that, in the case of binary classification, the target values are all in $\{0, 1\}$:



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- Then, however, the problem becomes conceptually more difficult (and is still a topic of ongoing research).
- Some concepts do not immediately generalise, for example isotonic regression (which assumes a ranking on scores, and rankings are inherently bipartite).
- While essentially coinciding for binary classification, the following definitions of calibration (leading to increasingly difficult problems) can be distinguished for more than two classes:
  - **Confidence calibration:** Calibration of the highest predicted probability
  - **Class-wise calibration:** Calibration of the marginal probabilities
  - **Multi-class calibration:** Calibration of the entire vector of predicted probabilities

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$\longrightarrow \qquad P\big(\, y \in \{2, 3, 9\} \,\big) \geq 0.9$

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- Given a sequence of training observations

$$(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_N, y_N), (\boldsymbol{x}_{N+1}, \bullet)$$

and a new query $\boldsymbol{x}_{N+1}$ with unknown outcome y_{N+1}, $\bullet$ is hypothetically replaced by each candidate, i.e., the hypothesis $y_{N+1} = y$ is tested for all $y \in \mathcal{Y}$:

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- Only those outcomes y for which this **hypothesis can be rejected** at a predefined level of confidence are excluded, while those for which the hypothesis cannot be rejected are collected to form the prediction set or **prediction region** $Y \subseteq \mathcal{Y}$.

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- The higher the score, the more "strange" the pattern $(\boldsymbol{x}, y)$, i.e., the less the data point $(\boldsymbol{x}, y)$ conforms to what one would expect to observe.

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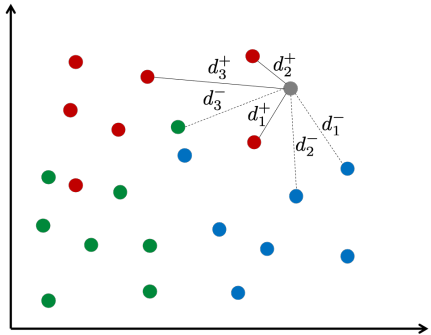
- Example of a nonconformity score based on nearest neighbors:

$$f(\boldsymbol{x}, y) = \frac{\sum_{i=1}^{k} d_i^+}{\sum_{i=1}^{k} d_i^-},$$

where d_i^+ is the distance from the i^{th} nearest neighbor labeled y, and d_i^- the distance from the i^{th} nearest neighbor labeled differently.



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- Under the assumption that the hypothetical choice of y_{N+1} is in agreement with the true data-generating process, and that this process has the property of **exchangeability**, every permutation σ has the same probability of occurrence.

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- However, the choice of this function has an important influence on the **efficiency** of conformal prediction, that is, the **size of prediction regions**: The more suitably the nonconformity function f is chosen, the smaller these sets will be.

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- There are various other extensions of CP, also for **conditional coverage**. Besides, instead of controlling coverage, there are variants for controlling more general notions of **risk** (Angelopoulos *et al.*, 2021).
- Uncertainty quantification with conformal prediction is
  - agnostic to the underlying model,
  - agnostic to the underlying data distribution (i.e., distribution-free),
  - valid for the finite sample case (not only asymptotically).

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- As opposed to aleatoric uncertainty, epistemic uncertainty can in principle be reduced on the basis of additional information.

Aleatoric versus epistemic uncertainty

H

$1/2$

T

$1/2$

H

$1/2$

T

$1/2$

“Not knowing the chance of mutually exclusive events and knowing the chance to be equal are two quite different states of knowledge"

Ronald Fisher (1890-1962)

Aleatoric versus epistemic uncertainty in ML

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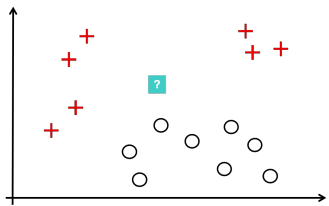

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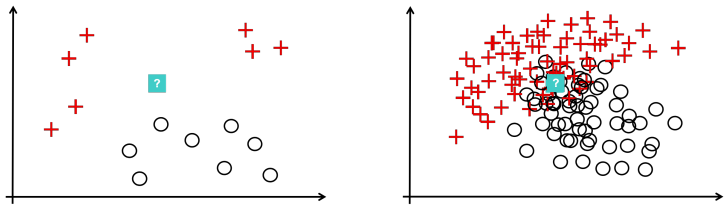

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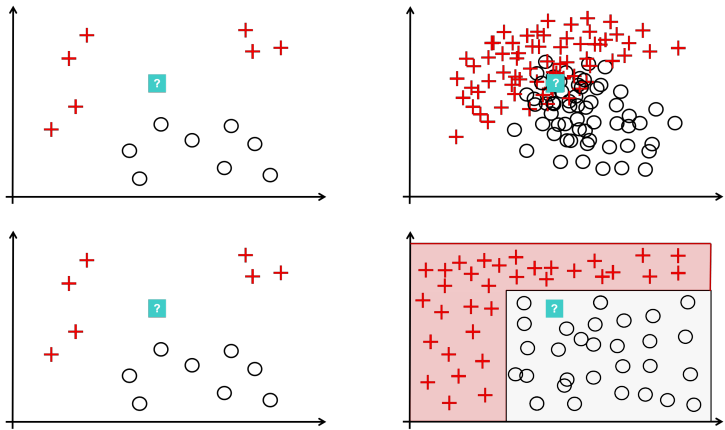

Aleatoric versus epistemic uncertainty in ML

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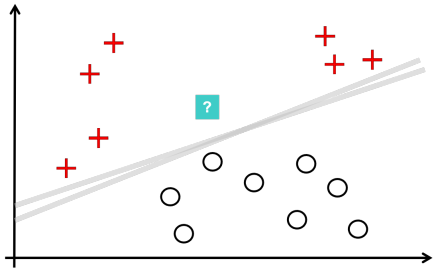
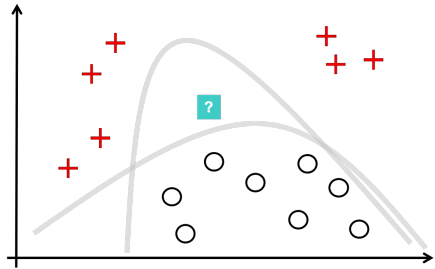
- ... but also on the underlying model assumptions:



strong prior



weaker prior

Uncertainty-aware learning

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- **Uncertainty quantification:** How to quantify the learner's uncertainty in terms of numbers? How to measure and disentangle the different types of uncertainty (aleatoric, epistemic, total)?

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- **Predict the next number**: 116, 304, 194, 341, 224, 654, 609, 625, 533, 91, 205, 35, 527, 611, 128, 235, 348, 912, 582, 52, 672, 20, 856, 904, 628, 273, 615, 105, 610, 862, 384, 705, 73, 794, 775, 156, **??**

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$$x \leftarrow x \times 237 \bmod 971$$

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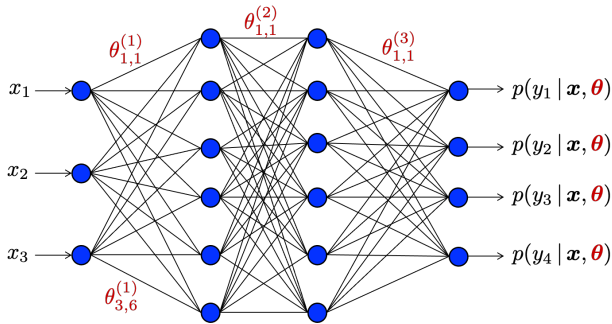
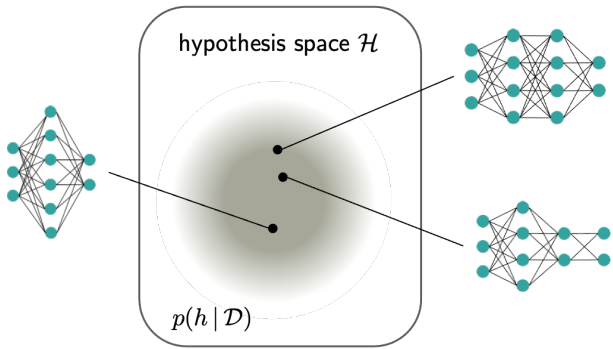
- Fixed weights $\boldsymbol{\theta}$ lead to a fixed probability $p(\cdot \mid \boldsymbol{x}, \boldsymbol{\theta})$.



The Bayesian approach

- A Bayesian learner maintains a probability distribution over the hypothesis space (probabilistic predictors).
- The less concentrated that distribution, the higher the learner's epistemic uncertainty.



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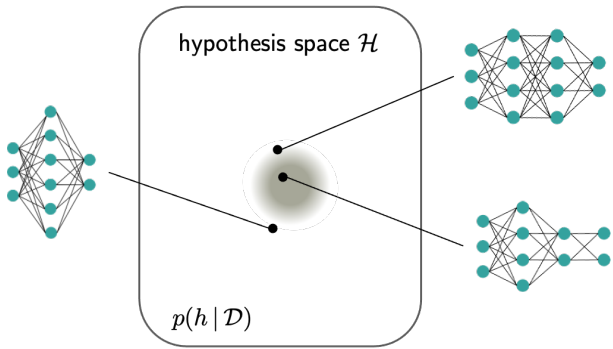
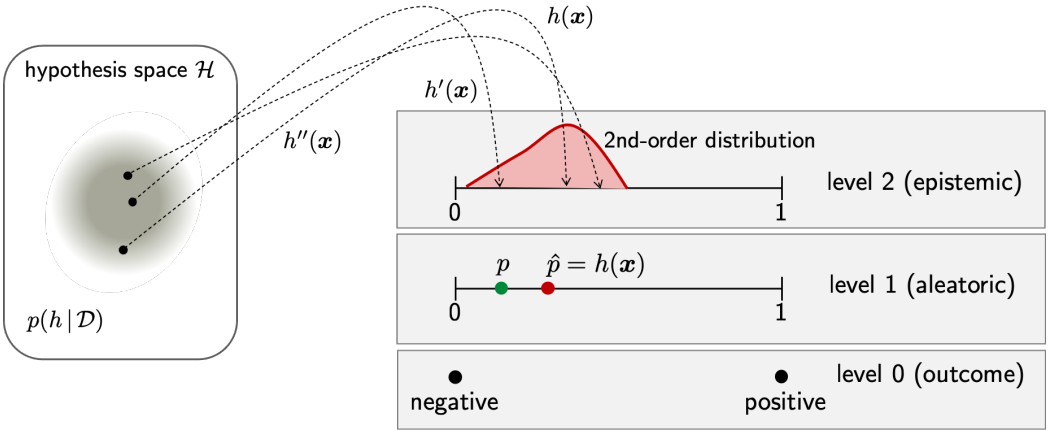


Posterior predictive distribution



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- What we seek is a **decomposition**

$$\underbrace{\mathrm{TU}(\boldsymbol{x})}_{\text{total uncertainty}} = \underbrace{\mathrm{AU}(\boldsymbol{x})}_{\text{aleatoric uncertainty}} + \underbrace{\mathrm{EU}(\boldsymbol{x})}_{\text{epistemic uncertainty}}$$

Uncertainty quantification

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- One idea is to model **epistemic uncertainty** as **mutual information** between outcomes and hypotheses (Depeweg *et al.*, 2018):

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- **Total uncertainty** = entropy of the predictive posterior distribution, in the case of discrete $\mathcal{Y}$ given by

$$\mathrm{TU}(\boldsymbol{x}) = H\big[\, p(y \mid \boldsymbol{x}) \,\big] = -\sum_{y \in \mathcal{Y}} p(y \mid \boldsymbol{x}) \log_2 p(y \mid \boldsymbol{x}) \,.$$

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- This uncertainty also includes the (epistemic) uncertainty about the network weights $\boldsymbol{\theta}$, but fixing a set of weights, i.e., considering a distribution $p(y \mid \boldsymbol{x}, \boldsymbol{\theta})$, removes the epistemic uncertainty.

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- Therefore, the expectation over the entropies of these distributions,

$$\mathbb{E}_{p(\boldsymbol{\theta} \mid \mathcal{D})} H\big[p(y \mid \boldsymbol{x}, \boldsymbol{\theta})\big] = \\ = -\int p(\boldsymbol{\theta} \mid \mathcal{D}) \left(\sum_{y \in \mathcal{Y}} p(y \mid \boldsymbol{x}, \boldsymbol{\theta}) \log_2 p(y \mid \boldsymbol{x}, \boldsymbol{\theta}) \right) d\,\boldsymbol{\theta} \ ,$$

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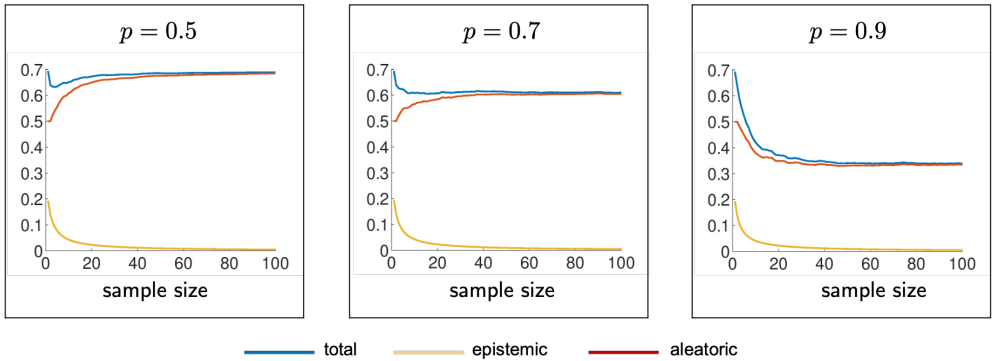
  is a measure of the **aleatoric uncertainty** (conditional entropy).
- Finally, the **epistemic uncertainty** is obtained as the difference

$$\mathrm{EU}(\boldsymbol{x}) := H\big[p(y \mid \boldsymbol{x})\big] - \mathbb{E}_{p(\boldsymbol{\theta} \mid \mathcal{D})} H\big[p(y \mid \boldsymbol{x}, \boldsymbol{\theta})\big] \ ,$$

  which equals the **mutual information** between y and $\boldsymbol{\theta}$.

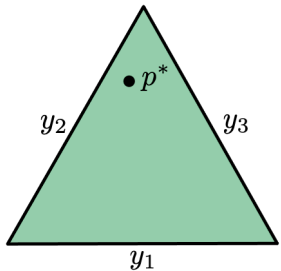
Example: coin flipping

- Tossing a coin with bias p, task is to predict the next outcome, hypothesis space equipped with Dirichlet distribution



Remarks

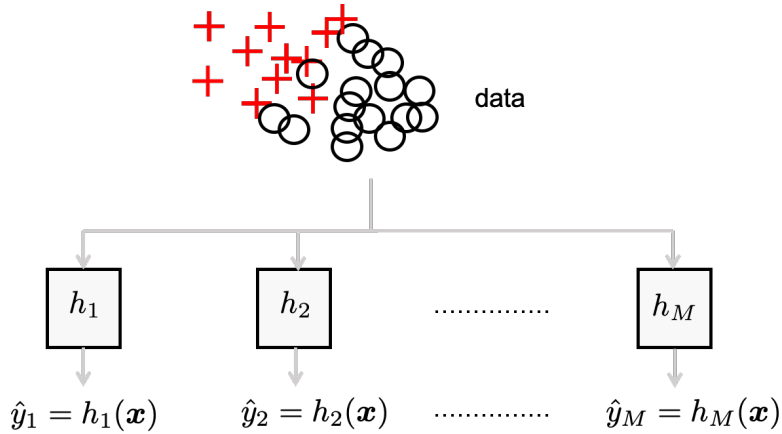
- Is a uniform distribution on $\Delta = \mathbb{P}(\mathcal{Y})$ (set of all distributions p on $\mathcal{Y}$) an adequate representation of **complete ignorance** (full epistemic uncertainty)?
- **Averaging** the (conditional) entropies over all p is meaningful only if all p are indeed **known** to be equally likely (aleatoric uncertainty is always $1/2$).
- But this is certainly not the case, as only one p^* can be the ground truth.



Remarks

- One may also question the **additive decomposition** $\mathrm{TU} = \mathrm{AU} + \mathrm{EU}$ itself.
- In the beginning, total uncertainty should be full ($\mathrm{TU} = 1$), and so should epistemic uncertainty ($\mathrm{EU} = 1$) — but this implies $\mathrm{AU} = 0$.
- This suggests a role of AU as a **lower bound** on (the true) aleatoric uncertainty.
- Indeed, epistemic uncertainty partially comprises aleatoric uncertainty (high EU implies high uncertainty about AU, showing interaction between both).

Ensemble methods for uncertainty quantification



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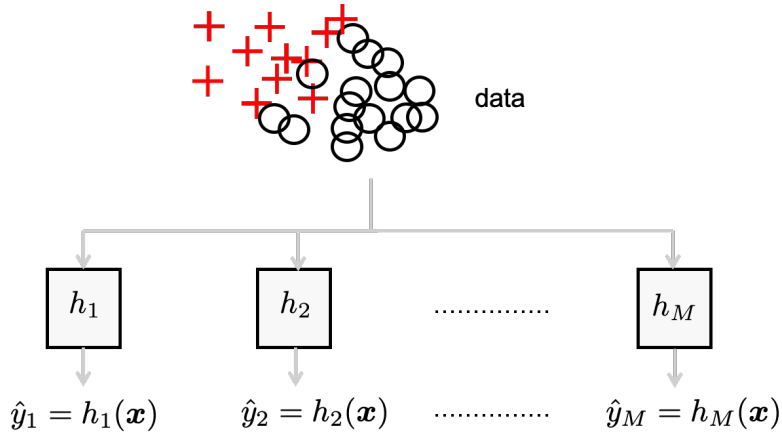

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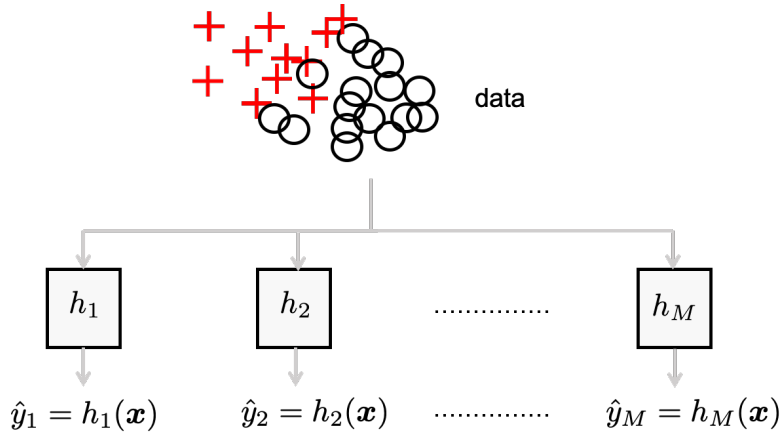

- Ensemble can be seen as an approximation of a distribution.
- Intuitively, diversity is an indicator of epistemic uncertainty.

Bayesian agents: Ensemble-based approximation

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- Based on an ensemble of hypotheses $h_1, \ldots, h_M$, producing respective predictions $p_1, \ldots, p_M$, an approximation of conditional entropy can be obtained by

$$\mathrm{AU}(\boldsymbol{x}) \coloneqq -\frac{1}{M} \sum_{i=1}^{M} \sum_{y \in \mathcal{Y}} p_i(y \mid \boldsymbol{x}) \log_2 p_i(y \mid \boldsymbol{x}) \,,$$

  an approximation of total uncertainty (Shannon entropy) by

$$\mathrm{TU}(\boldsymbol{x}) \coloneqq -\sum_{y \in \mathcal{Y}} \underbrace{\left(\frac{1}{M} \sum_{i=1}^{M} p_i(y \mid \boldsymbol{x}) \right)}_{\bar{p}(y \mid \boldsymbol{x})} \log_2 \underbrace{\left(\frac{1}{M} \sum_{i=1}^{M} p_i(y \mid \boldsymbol{x}) \right)}_{\bar{p}(y \mid \boldsymbol{x})} ,$$

  and an approximation of epistemic uncertainty (mutual information) by the difference.

Bayesian agents: Ensemble-based approximation

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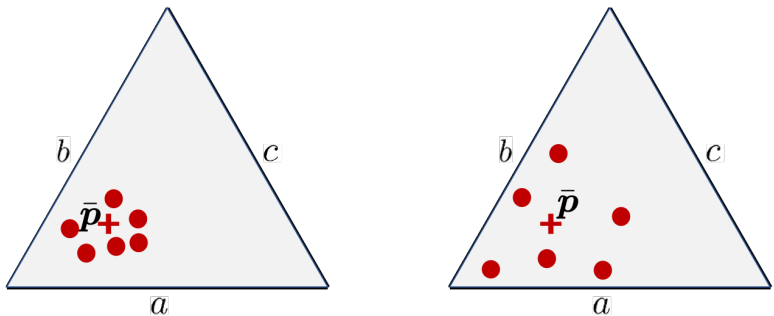
- Epistemic uncertainty thus defined is equivalent to **Jensen-Shannon divergence** of the distributions $p_i(y \mid \boldsymbol{x})$, $i = 1, \ldots, M$



low divergence

high divergence

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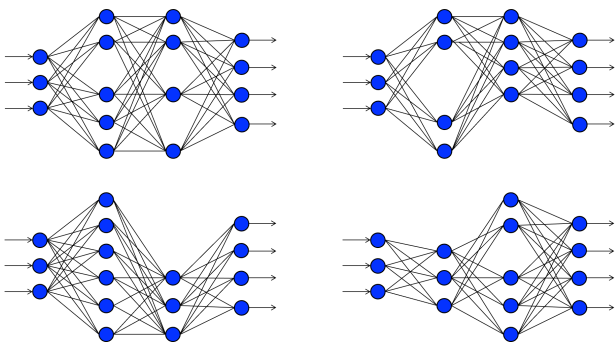
- Of course, any other ensemble technique could be used as well.



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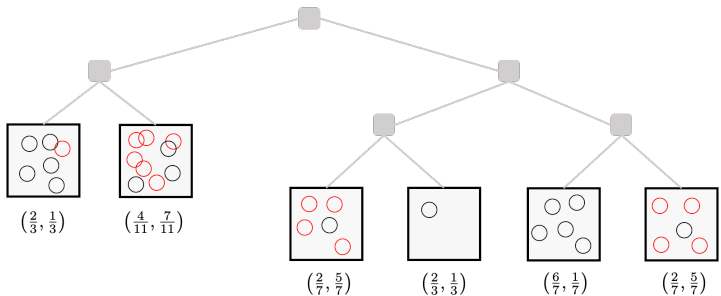
- We proposed an implementation based on **Random Forests**, using decision trees that predict probabilities in terms of (Laplace-corrected) relative frequencies (Shaker and Hüllermeier, 2020).



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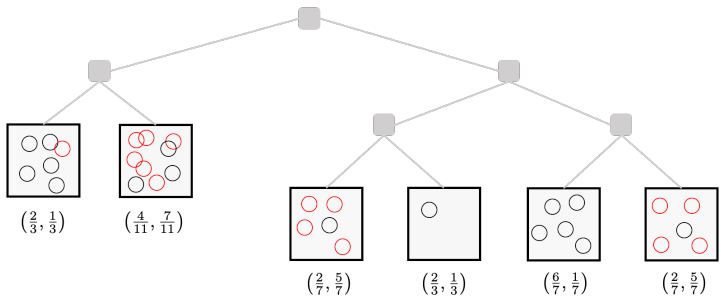

- Empirically, there are no significant performance differences between neural networks and random forests.

Direct (epistemic) uncertainty prediction

- Consider a (level-1) loss for **probabilistic predictions**:

$$\ell_1 : \mathbb{P}(\mathcal{Y}) \times \mathcal{Y} \longrightarrow \mathbb{R}$$

- Recall that ERM yields good (unbiased) predictors if ℓ_1 is a (strictly) **proper scoring rule**, which incentivises the learner to predict the true $p(y \mid \boldsymbol{x})$.
- **Question**: Can we do the same on the **epistemic level**, i.e., training a predictor

$$h : \mathcal{X} \longrightarrow \mathbb{P}(\mathbb{P}(\mathcal{Y}))$$

by minimising a **level-2 loss**

$$\ell_2 : \mathbb{P}(\mathbb{P}(\mathcal{Y})) \times \mathcal{Y} \longrightarrow \mathbb{R}\,,$$

such that the predictor represents its epistemic uncertainty in a faithful way?

The Dirichlet distribution

- A **Dirichlet distribution** $\mathrm{Dir}(\alpha)$ is specified by means of $K \geq 2$ positive real-valued parameters, i.e., a vector $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_K) \in \mathbb{R}_+^K$.

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- The probability density function is defined on the K simplex

$$\Delta_K = \left\{ \boldsymbol{\theta} = (\theta_1, \ldots, \theta_K)^\top \,|\, \theta_1, \ldots, \theta_K \geq 0, \sum_{k=1}^{K} \theta_k = 1 \right\}$$

and given as follows:

$$p(\boldsymbol{\theta} \,|\, \boldsymbol{\alpha}) = p(\theta_1, \ldots, \theta_K \,|\, \boldsymbol{\alpha}) = \frac{1}{\mathbb{B}(\boldsymbol{\alpha})} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1},$$

where the normalisation constant is the multivariate Beta function.

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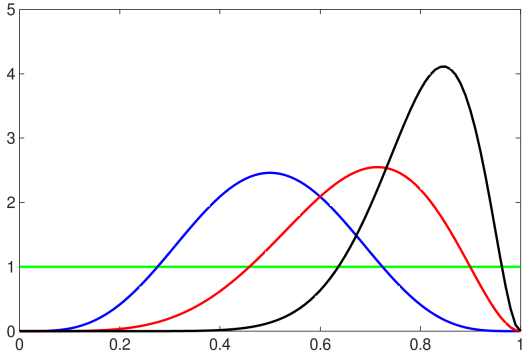
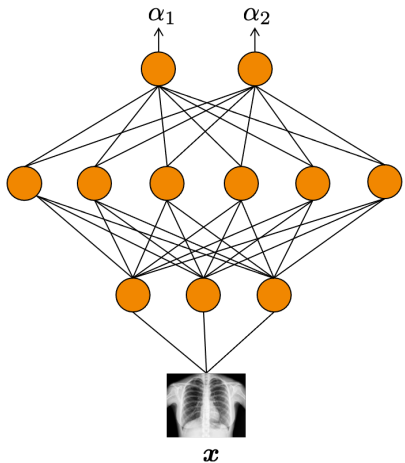
  where the normalisation constant is the multivariate Beta function.
- In Bayesian statistics, the Dirichlet distribution is commonly used as the conjugate prior of the **multinomial distribution**.

The Dirichlet distribution

- Dirichlet distribution with parameters $\boldsymbol{\alpha} = (\alpha_1, \alpha_2) = (1, 1)$, $(5, 5)$, $(3, 6)$, $(3, 12)$.



Predicting a Dirichlet distribution



Direct epistemic uncertainty prediction

- Several authors have proposed the minimisation of an empirical loss of the form

$$L = \frac{1}{N} \sum\nolimits_{n=1}^{N} \ell_2\big(Q^{(n)}, y^{(n)}\big) = \frac{1}{N} \sum\nolimits_{n=1}^{N} \mathbb{E}_{\boldsymbol{\theta} \sim Q}\, \ell_1 \left(\boldsymbol{\theta}, y^{(n)}\right) ,$$

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- Besides, a regularised version has been proposed:

$$L = \frac{1}{N}\sum_{n=1}^{N} \underbrace{\mathbb{E}_{\boldsymbol{\theta}\sim Q}\, \ell_1\left(\boldsymbol{\theta}, y\right) + \lambda\, d_{KL}\left(Q^{(n)}, Q_0\right)}_{\ell_2\left(Q^{(n)}, y^{(n)}\right)}$$

A negative result

- Informally, we define a level-2 loss function ℓ_2 as **appropriate** if the following holds for the empirical loss minimiser

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on any i.i.d. observational data sequence $y^{(1)}, y^{(2)}, \ldots$ with $y^{(i)} \sim \boldsymbol{\theta}^*$:

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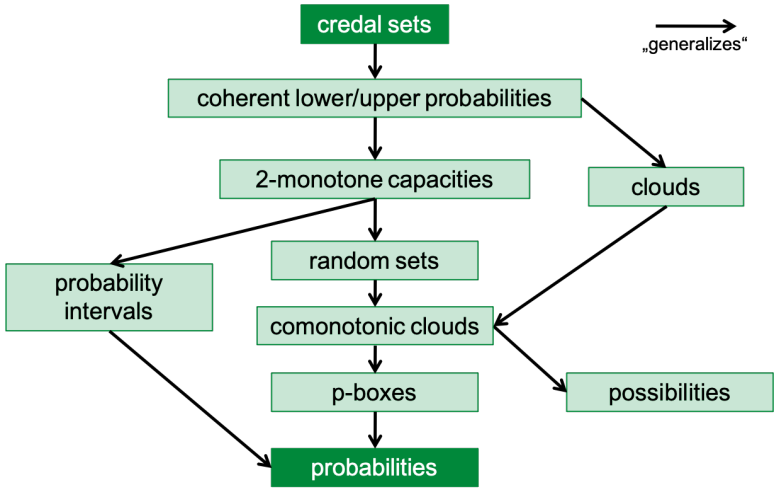
- Bengs *et al.* (2022) formally prove that a loss minimisation approach using a level-2 loss as specified above does not lead to an appropriate level-2 loss.

Generalised uncertainty calculi



Credal uncertainty representation

Probabilistic learner	Bayesian learner	Credal learner
$h : \mathcal{X} \longrightarrow \mathbb{P}(\mathcal{Y})$	$h : \mathcal{X} \longrightarrow \mathbb{P}(\mathbb{P}(\mathcal{Y}))$	$h : \mathcal{X} \longrightarrow 2^{\mathbb{P}(\mathcal{Y})}$

ENSEMBLE-BASED UNCERTAINTY QUANTIFICATION:
BAYESIAN VERSUS CREDAL INFERENCE

A PREPRINT

Mohammad Hossein Shaker
Department of Computer Science
Paderborn University
Paderborn, Germany
mhshaker@mail.upb.de

Eyke Hüllermeier
Institute of Informatics
University of Munich (LMU)
Munich, Germany
eyke@lmu.de

December 13, 2021

Possibilistic uncertainty representation

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- Senge *et al.* (2014) formalise the following principle in a mathematical way: Given a query $\boldsymbol{x}_q$, an outcome $y \in \mathcal{Y}$ is a **plausible** candidate if there exists a **plausible** hypothesis $h \in \mathcal{H}$ (compatible with the data) such that y is **strongly supported** by h (in the sense that $p(y \mid \boldsymbol{x}_q, h)$ is high).

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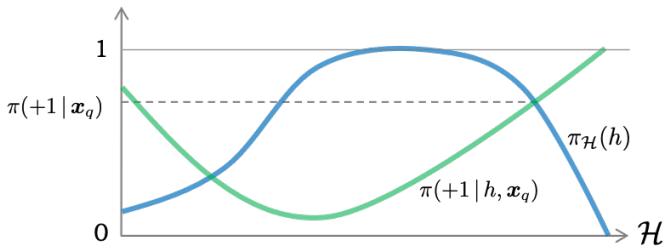
- Thus, they induce a graded (fuzzy) set of plausible candidate hypotheses instead of a single one, and consider the plausible outcomes under these candidates.



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- Usefulness of **generalized uncertainty calculi**?

More on this topic ...

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Aleatoric and epistemic uncertainty in machine learning: an introduction to concepts and methods

Eyke Hüllermeier ✉ & Willem Waegeman

Machine Learning **110**, 457–506 (2021) | Cite this article

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Abstract

The notion of uncertainty is of major importance in machine learning and constitutes a key element of machine learning methodology. In line with the statistical tradition, uncertainty has long been perceived as almost synonymous with standard probability and probabilistic predictions. Yet, due to the steadily increasing relevance of machine learning for practical applications and related issues such as safety requirements, new problems and challenges have recently been identified by machine learning scholars, and these problems may call for new methodological developments. In particular, this includes the importance of distinguishing between (at least) two different types of uncertainty, often referred to as *aleatoric* and *epistemic*. In this paper, we provide an introduction to the topic of uncertainty in machine learning as well as an overview of attempts so far at handling uncertainty in general and formalizing this distinction in particular.

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M.H. Shaker and E. Hüllermeier. Aleatoric and epistemic uncertainty with random forests. In *Proc. IDA, 18th Int. Symposium on Intelligent Data Analysis*, pages 444–456, Konstanz, Germany, 2020. Springer.

Epistemic uncertainty sampling

Open Access | Published: 18 June 2021

How to measure uncertainty in uncertainty sampling for active learning

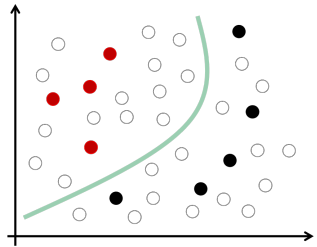
Vu-Linh Nguyen, Mohammad Hossein Shaker & Eyke Hüllermeier

Machine Learning (2021) | Cite this article

1033 Accesses | **1** Altmetric | Metrics

Abstract

Various strategies for active learning have been proposed in the machine learning literature. In uncertainty sampling, which is among the most popular approaches, the active learner sequentially queries the label of those instances for which its current prediction is maximally uncertain. The predictions as well as the measures used to quantify the degree of uncertainty, such as entropy, are traditionally of a probabilistic nature. Yet, alternative approaches to capturing uncertainty in machine learning, alongside with corresponding uncertainty measures, have been proposed in recent years. In particular, some of these measures seek to distinguish different sources and to separate different types of uncertainty, such as the reducible (epistemic) and the irreducible (aleatoric) part of the total uncertainty in a prediction. The goal of this paper is to elaborate on the usefulness of such measures for uncertainty sampling, and to compare their performance in active learning. To this end, we instantiate uncertainty sampling with different measures, analyze the properties of the sampling strategies thus obtained, and compare them in an experimental study.



Sampling in epistemically uncertain regions of the instance space is potentially more useful than sampling in aleatorically uncertain regions ...

Excursus: Hypothesis testing

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- If this nevertheless happens, i.e., $T \in R = \mathbb{R} \setminus A$, then H_0 is rejected and H_1 accepted.

Evaluation: accuracy-rejection curves

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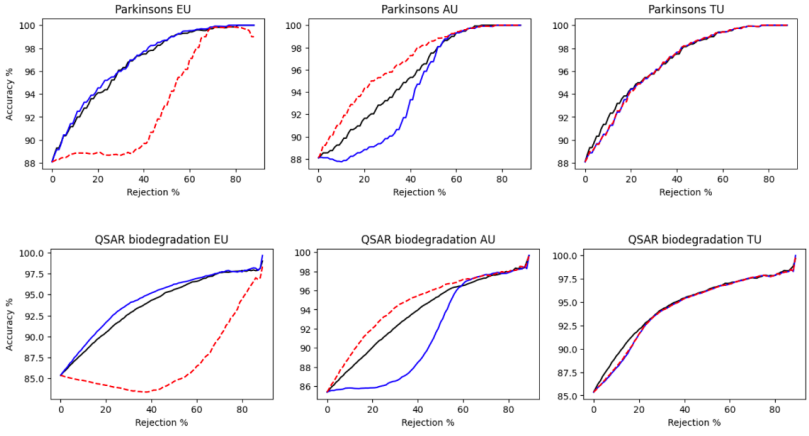
- Reject test instances for which (total, aleatoric, epistemic) uncertainty exceeds a certain threshold, measure accuracy on the remaining ones.



Facets of uncertainty

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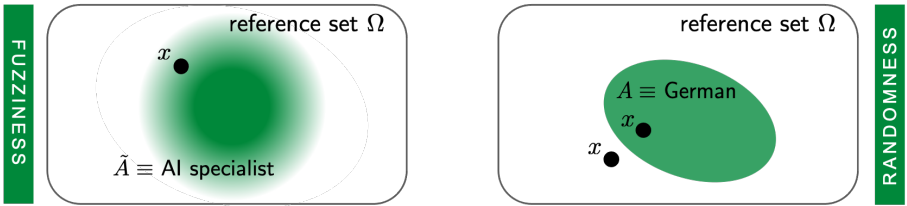
- Randomness, imprecision, inconsistency, ambiguity, vagueness, fuzziness, ...



"$x \in \tilde{A}$" uncertain due to non-sharp boundaries of $\tilde{A}$

$$\tilde{A}(x) = 0.7$$

"$x \in A$" for $A \subseteq \Omega$ uncertain due to lack of knowledge about x

$$P(A) = 0.7$$

"Fuzziness is orthogonal to probability theory – it focuses on the ambiguity of describing events, rather than the uncertainty about the occurrence or non-occurrence of events." | Judea Pearl (2000)

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$$P\left(T = k \,|\, \theta = \frac{1}{2}\right) = B(k, 1/2) = \binom{N}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{N-k} = \binom{N}{k} \left(\frac{1}{2}\right)^N$$

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- Probability is highest around $k = N/2$ and decreases toward both ends (very high or very low number of heads).
- Take $R = \{0, 1, \ldots, r\} \cup \{N - r, \ldots, N\}$, with r the largest number such that

$$P(T \in R) = \sum_{k=0}^{r} B(k, 1/2) + \sum_{k=N-r}^{N} B(k, 1/2) \leq \delta\,.$$

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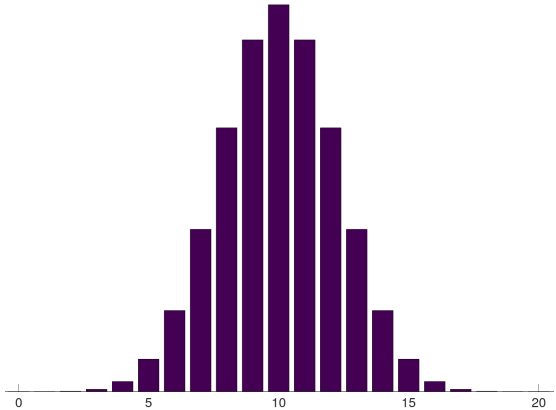

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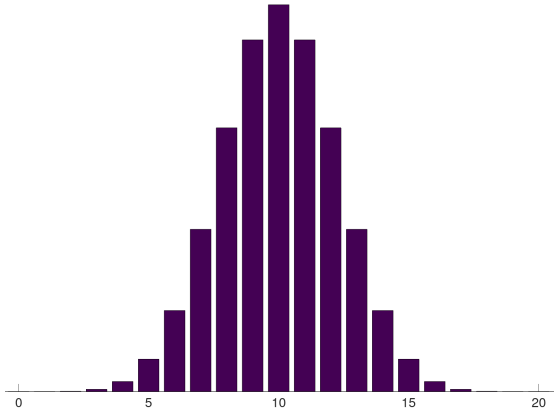

- For $R = \{0, 1, \ldots, 5\} \cup \{15, \ldots, 20\}$,

$$P(T \in R) = 0.041389 \leq 0.05$$

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- Also note that **nothing** can be concluded from the test in case H_0 is not rejected.
- In particular, not rejecting H_0 does not mean one can "accept" it:

$$P\left(\theta = \frac{1}{2} \mid T \in \{6, \ldots, 14\}\right) = ??$$

Exchangeability

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  is **symmetric** in its arguments.
- Exchangeability is weaker than the i.i.d. assumption (the latter implies the former but not the other way around).

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- This is computationally costly, as it possibly requires refitting a model to the data in each iteration.
- **Inductive conformal prediction** (ICP) is an alternative that is computationally less expensive.
- In the **split-conformal prediction** variant, ICP splits the training data $\mathcal{D}$ into
  - proper training data $\mathcal{D}_T$ of size $N - M$,
  - calibration data $\mathcal{D}_C = \left\{(\boldsymbol{x}_j, y_j)\right\}_{j=1}^{M}$ of size $M < N$.

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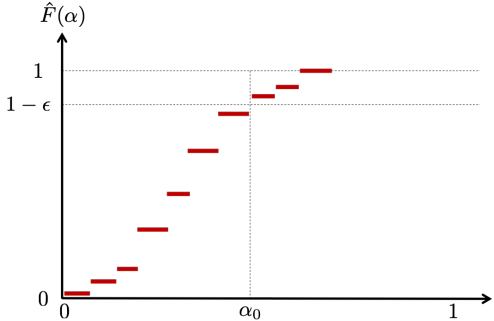

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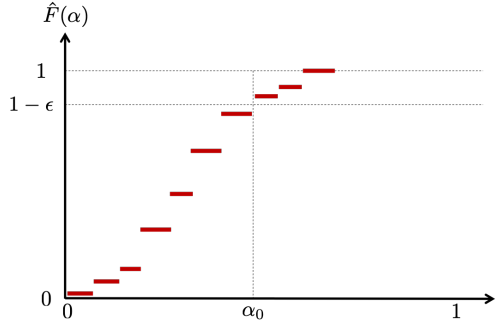

- With high probability, nonconformity of a "real" data point is $\leq \alpha_0$.

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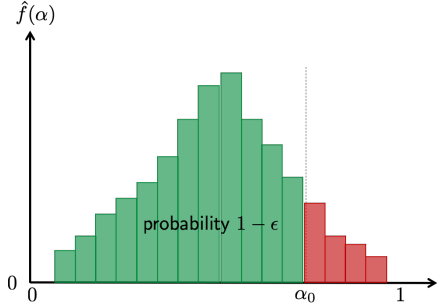

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- Imagine, for example, a probabilistic classifier h is trained on the proper training data, and nonconformity of $(\boldsymbol{x}, y)$ is defined as $\alpha = 1 - p(y)$, where $p = h(\boldsymbol{x})$.
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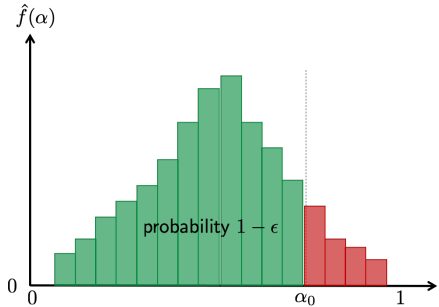

- With high probability, nonconformity of a "real" data point is $\leq \alpha_0$.

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- Assuming $\mathcal{D}$ to be an i.i.d. sample, and $(\boldsymbol{x}_q, y_q)$ sampled from the same distribution, the following estimate is provably correct:

$$1 - \epsilon \leq P\big(y_q \in Y(\boldsymbol{x}_q)\big) \leq 1 - \epsilon + \frac{1}{M+1}$$