Provable Uncertainty Decomposition via Higher-Order Calibration

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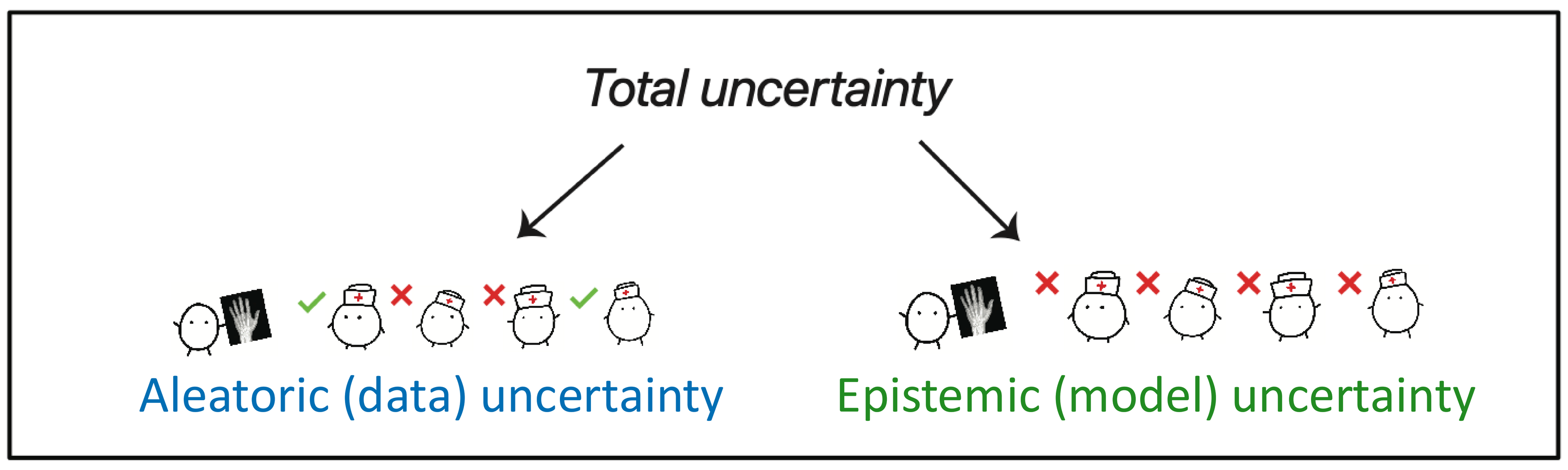
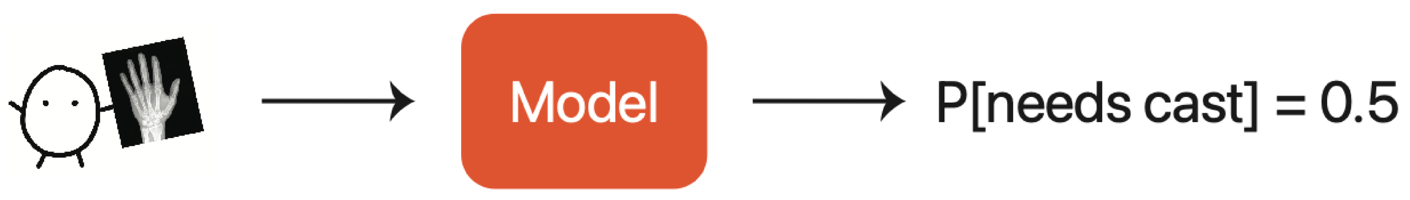
Overview

Decomposing model uncertainty reveals which factors drive prediction errors, and can help practitioners pinpoint where models need improvement.



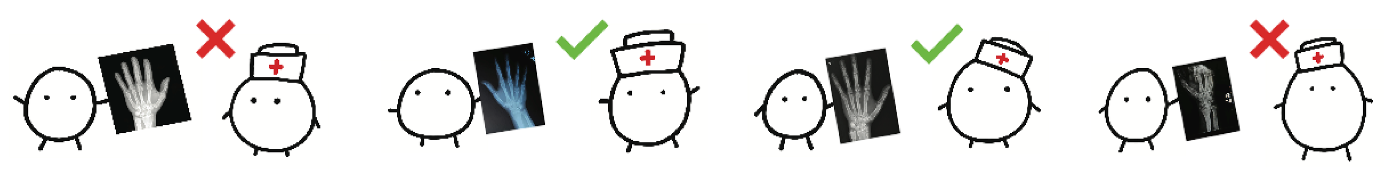
We give a principled method for decomposing the predictive uncertainty of a model into aleatoric and epistemic components with **explicit semantics relating them to the real-world data distribution.**

Motivation



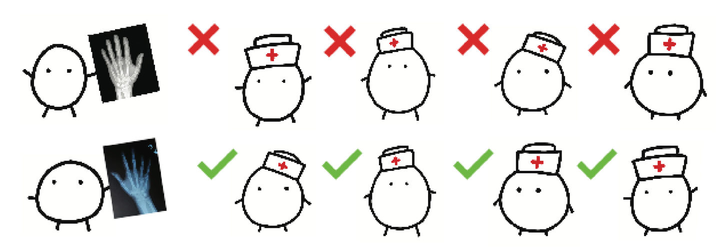
A classifier says a patient needs a cast with confidence 50%

What does this mean, really?

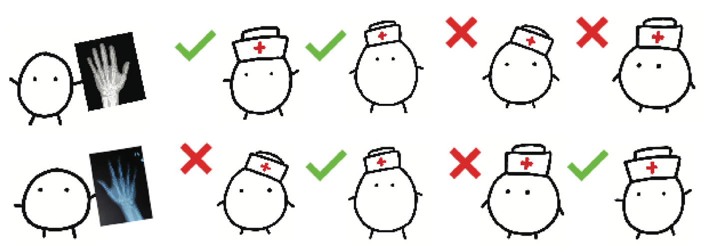


If the model is *calibrated*, then scans assigned that prediction have a 50% chance of needing a cast: it's now a probability

Calibration grounds our prediction in reality. But it's not the whole story! Let's ask multiple doctors per image:



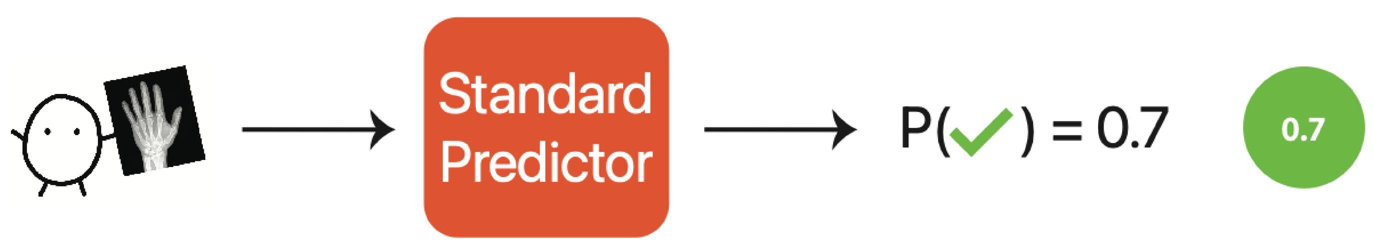
Scenario 1: Our model is *epistemically* uncertain because it can't tell two different sets of images apart!

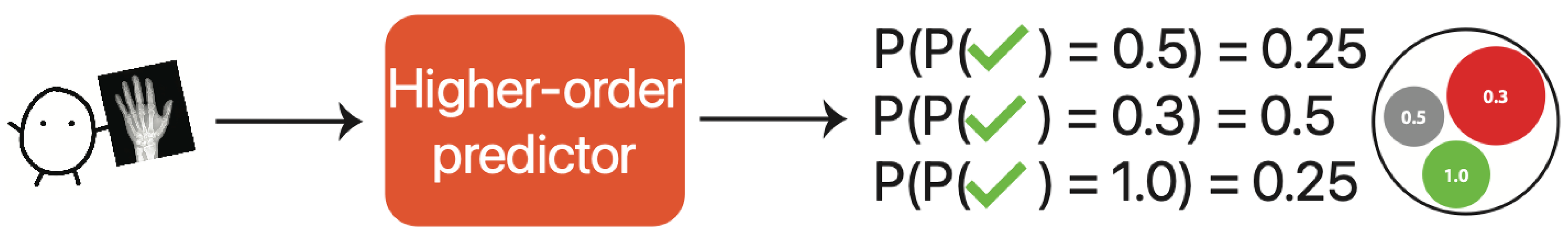


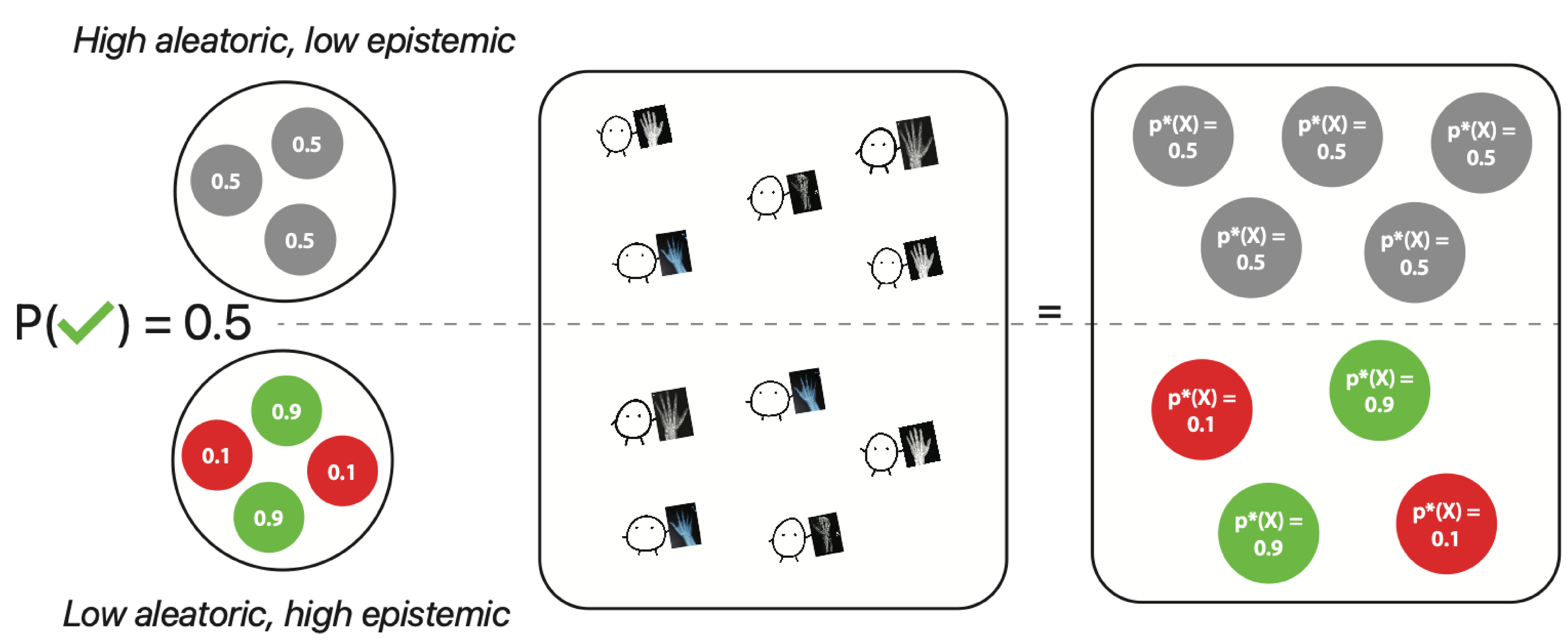
Scenario 2: Our model is good, but now the images are ambiguous. Uncertainty is aleatoric.

Definition

We work with "higher-order" predictors (e.g. ensembles, BNNs, etc.):







A higher-order predictor is higher-order calibrated (HOC) when its prediction matches the ground truth mixture. HOC <-> good uncertainty decompositions!

The Mutual Uncertainty Decomposition

Given a higher-order prediction p(x) ∈ ΔΔY, the mutual uncertainty decomposition defines a concrete way to decompose the predictive uncertainty into aleatoric and epistemic components:

$$\underbrace{H(\mathbb{E}_{v\sim p(x)}[v])}_{\substack{\text{total/predictive uncertainty}\\ TU(p(x))}} = \underbrace{\mathbb{E}_{v\sim p(x)}[H(v)]}_{\substack{\text{aleatoric uncertainty}\\ AU(p(x))}} + \underbrace{H(\mathbb{E}_{v\sim p(x)}[v]) - \mathbb{E}_{v\sim p(x)}[H(v)]}_{\substack{\text{epistemic uncertainty}\\ EU(p(x))}}$$

Ideally, uncertainty estimates would be grounded in reality.

True aleatoric uncertainty: $AU^*(x) = H(\mathbb{E}[y|x])$

Theorem: When p is HOC, the estimated aleatoric uncertainty of each level set is equal to the average true aleatoric uncertainty. I.e., for any π ∈ ΔY,

$$AU(\pi) = \mathbb{E}[AU^*(x)|p(x) = \pi]$$

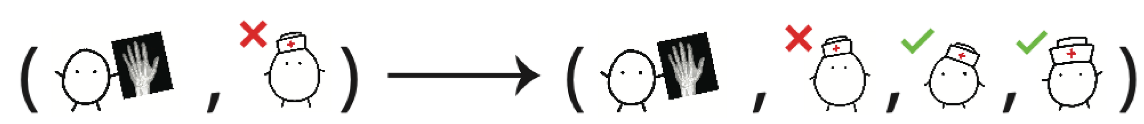
Proof:

$$AU(\pi) = \mathbb{E}_{v\sim\pi}[H(v)] = \mathbb{E}[H(\mathbb{E}[y|x])|p(x) = \pi] = \mathbb{E}[AU^*(x)|p(x) = \pi]$$

HOC guarantee

k-th Order Calibration

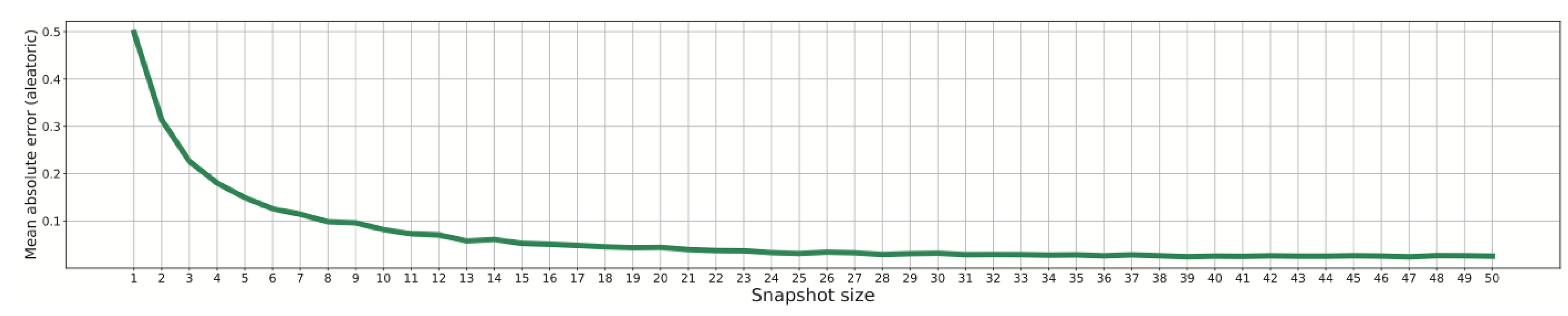
Perfect HOC is difficult to achieve in practice. We propose a tractable relaxation of HOC, k-th order calibration, that only needs k-snapshots.



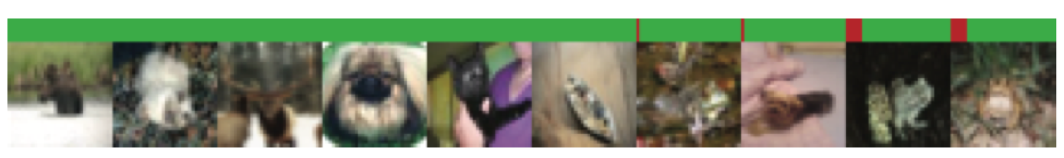
A k-th-order-calibrated model gives good estimates of the first k moments of the ground truth mixture!

Can be achieved two ways:
1. Post-process a regular, first-order predictor using a calibration set of k-snapshots by treating each k-snapshot as an empirical label distribution.
2. Predict k-snapshots directly in an extended label space.

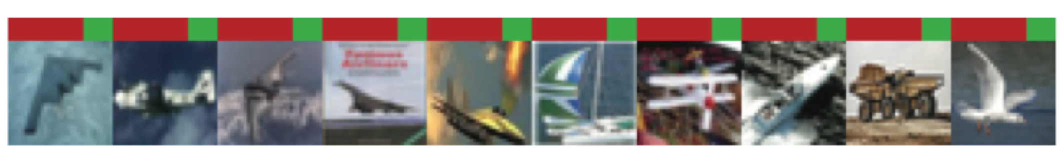
Results



HOC improves as k increases (O(1 / sqrt(k)))



Aleatoric images are very ambiguous



Epistemic images are just unusual

CIFAR decompositions