Rethinking Aleatoric and Epistemic Uncertainty

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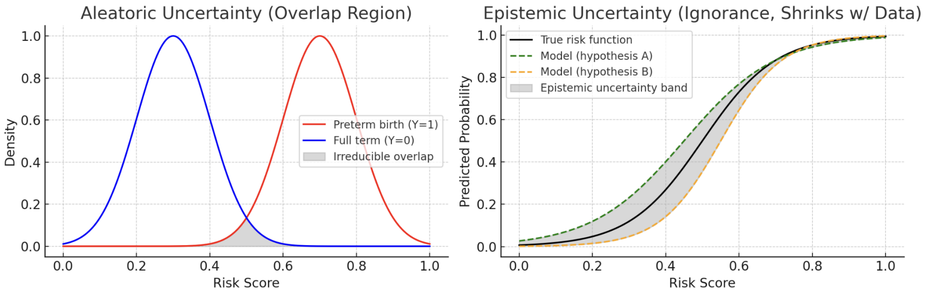
Presented by Mian Wei

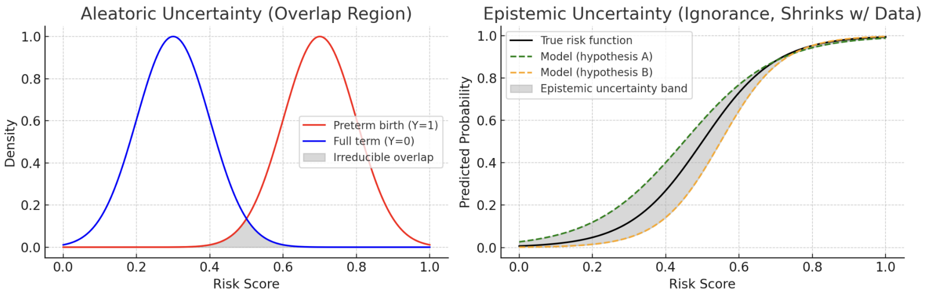
Aleatoric vs. Epistemic Uncertainty

We have a model to predict preterm birth, but there is predictive uncertainty. Should we use it cautiously, or should we collect more data and/or change the model?



- Aleatoric: Even with perfect features, some patients with identical profiles will deliver early, while others won't.
- Epistemic: Your dataset might be missing key variables or need better modeling.

Aleatoric vs. Epistemic Uncertainty



- Aleatoric: unavoidable risk → best to hedge.
- Epistemic: knowledge gap → best to reduce it.

Uncertainty Decomposition

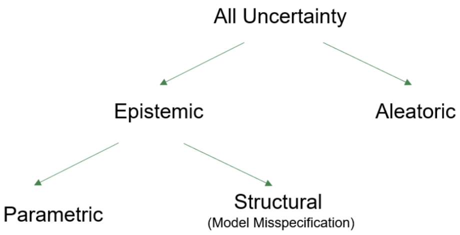


Figure: Adapted from [Che22]

- **Parametric**: uncertainty related to model parameter estimations under current model specification.
- **Structural**: the discrepancy between the assumed model specification and the true, unknown data-generating process

An area of ongoing debate

- Model-based prediction vs. the true data-generating process
- Uncertainty on unseen data
- Uncertainty vs. prediction accuracy
- Different approaches to epistemic uncertainty: density-based, information-based, variance-based, ...

Contribution of this paper:

- A critique of the popular uncertainty decomposition view
- A new decision-based framework for uncertainty

Notations

- an action, $a \in \mathcal{A}$
- a ground-truth variable, $z \in \mathcal{Z}$
- a loss function, $\ell : \mathcal{A} \times \mathcal{Z} \to \mathbb{R}$
- a policy $\pi \in \Pi$ that controls data generation
- some training data $y_{1:n} \sim p_{train}(y_{1:n}|\pi)$
- predictive model $p_n(z) = p(z; y_{1:n})$ or the predictive distribution $p_n(z) = \mathbb{E}_{p_n(\theta)}\left[p_n(z|\theta)\right]$, where $\theta \sim p_n(\theta) = p(\theta; y_{1:n})$ is a set of stochastic model parameters
- data generating process, $p_{train}(y_i|\pi(y_{<i}, y_{<i})$
- a ground-truth realization of z or a reference distribution, $p_{eval}(z)$

A Popular Decomposition View

Usual formula

$$\underbrace{\mathrm{EIG}_\theta}_{\text{“epistemic”}} = \underbrace{\mathrm{H}\left[p_n(z)\right]}_{\text{“total”}} - \underbrace{\mathbb{E}_{p_n(\theta)}\left[\mathrm{H}(p_n\left[z \mid \theta)\right]\right]}_{\text{“aleatoric”}}$$

- H: Shannon entropy
- EIG_θ: the expected information gain about θ from observing z

For finite n, epistemic and aleatoric uncertainty are only estimators of the true quantities and can be highly inaccurate.

Aleatoric uncertainty

"captures noise inherent in the observations" $\mathrm{H}[p_{\text{train}}(y_{1:n}\|\pi)]$ or $\mathrm{H}[p_{\text{eval}}(z)]$	$\neq$	"cannot be reduced even if more data were to be collected" $\mathrm{H}[p_\infty(z)]$	$\neq$	Expected parameter-conditional predictive entropy $\mathbb{E}_{p_n(\theta)}[\mathrm{H}[p_n(z\|\theta)]]$

Epistemic uncertainty

"uncertainty in the model parameters" $\mathrm{H}[p_n(\theta)]$	$\neq$	"can be explained away given enough data" $\mathrm{H}[p_n(z)] - \mathrm{H}[p_\infty(z)]$	$\neq$	Expected information gain in the model parameters $\mathrm{H}[p_n(z)] - \mathbb{E}_{p_n(\theta)}[\mathrm{H}[p_n(z\|\theta)]]$

Model world $\neq$ Real world

Decision-Based Fr

- Bayes-optimal action:

$$a_n^* = \arg\min_a \mathbb{E}_{p_n(z)}[\ell(a, z)]$$

- Loss-grounded uncertainty measure:

$$h[p_n(z)] = \mathbb{E}_{p_n(z)}[\ell(a_n^*, z)]$$

Takeaway: The choice of loss (and thus the uncertainty measure) depends on the decision problem at hand.

Expected Uncertainty Reduction (EUR)

Definition:

$$UR_z(y^+_{1:m}) = h[p_n(z)] - h[p_{n+m}(z)].$$

$$EUR^{\text{true}}_z(\pi, m) = \mathbb{E}_{p_{\text{train}}(y^+_{1:m}|\pi)}[\, UR_z(y^+_{1:m})\,].$$

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As $m \to \infty$, the decomposition:

$$h[p_n(z)] = \underbrace{EUR^{\text{true}}_z(\pi, \infty)}_{\text{Reducible}} + \underbrace{\mathbb{E}_{p_{\text{train}}(y^+_{1:m}|\pi)}[h[p_\infty(z)]]}_{\text{Irreducible}}.$$

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Compared with popular split:

$$H[p_n(z)] = \underbrace{\mathbb{E}_{p_n(\theta)}[H(p_n(z \mid \theta))]}_{\text{aleatoric}} + \underbrace{H[p_n(z)] - \mathbb{E}_{p_n(\theta)}[H(p_n(z \mid \theta))]}_{\text{BALD/epistemic}}$$

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- Paper's: decision/loss grounded, any learner, depends on data process.
- BALD: an *estimator*, not a universal decomposition.

EUR in Practice

Problem: We cannot access the true data-generating process or infinite data.

So we approximate with:

- Use model-based simulator $p_n(y^+_{1:m} \mid \pi')$ instead of true p_{train}.
- Use approximate update $q_{n+m}(z)$ instead of true $p_{n+m}(z)$.

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Estimator:

$$EUR^{\text{est}}_z(\pi', m) = h[p_n(z)] - \mathbb{E}_{p_n(y^+_{1:m} \mid \pi')}\big[h[q_{n+m}(z)]\big].$$

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Sources of error:

1. Simulator mismatch (p_n vs p_{train}).
2. Update approximation (q_{n+m} vs p_{n+m}).

Some Concepts

Predictive Uncertainty

- $h[p_n(z)] = \mathbb{E}_{p_n(z)}[\ell(a_n^*, z)]$
- How uncertain *my model* thinks the future is
- Subjective, depends on $p_n(z)$

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Predictive Performance

- $\mathrm{Perf}(p_n) = \mathbb{E}_{p_{\mathrm{eval}}}[\ell(a_n^*, z)]$
- How good the predictions are compared with reality
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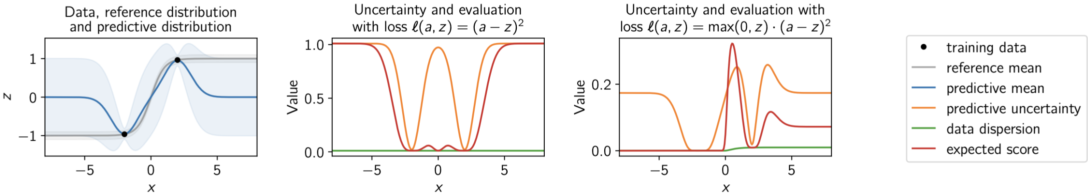
Data Dispersion

- Dispersion = entropy/variance of $p_{\mathrm{eval}}(z)$
- How random the world really is, regardless of the model
- World-based, not model-based

Some Concepts



Prop 1: Bayes estimator under quadratic loss = the posterior mean.
Prop 2: $h[p_n(z)]$ is the Bayes estimator of expected performance under p_{eval}.
Prop 3: $\mathbb{E}_{p_n(\theta)}[h[p_n(z \mid \theta))]$ is the Bayes estimator of data dispersion $h[p_{\text{eval}}(z)]$.

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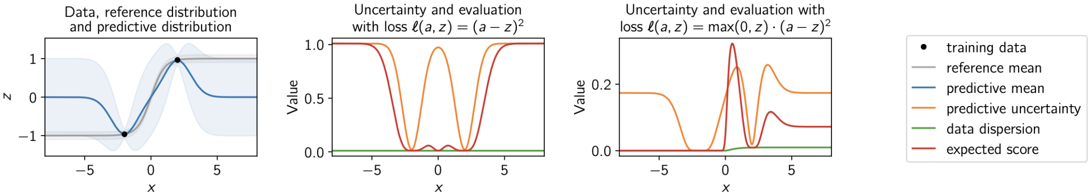

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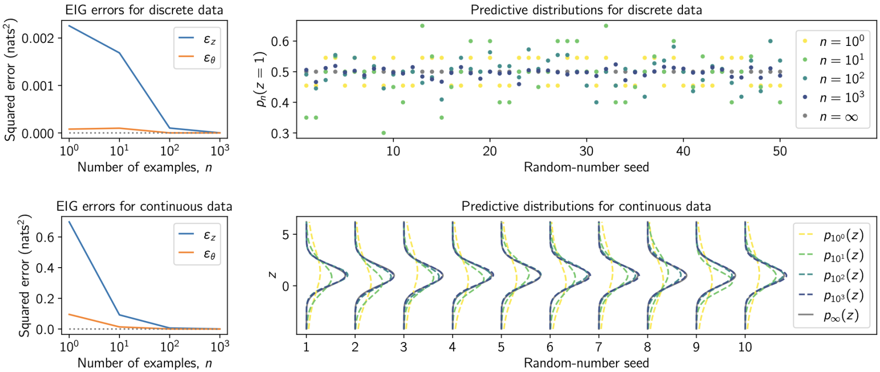
Takeaway: Model-based uncertainty $\neq$ truth; only *estimators* of performance/dispersion.

Re-reading BALD



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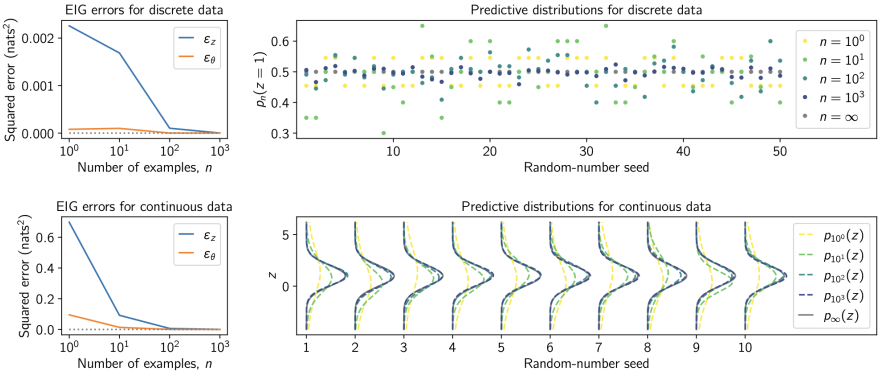

Takeaway:

- BALD is not the "epistemic uncertainty" truth. It's an estimator, and often poor for long-run reducibility.
- But good proxy for *short-run parameter IG* $\rightarrow$ explains success in active learning.

Decision-Theoretic Framework

Learning $\rightarrow$ Reasoning $\rightarrow$

Decision problem
$\ell : \mathcal{A} \times \mathcal{Z} \to \mathbb{R}$

Training data
$y_{1:n} \sim p_{\text{train}}(y_{1:n}|\pi)$

Predictive model
$p_n(z) = p(z; y_{1:n})$

Bayes-optimal action
$a_n^* = \arg\min_{a \in \mathcal{A}} \mathbb{E}_{p_n(z)}[\ell(a, z)]$

Uncertainty quantification

Predictive uncertainty
$h[p_n(z)] = \mathbb{E}_{p_n(z)}[\ell(a_n^*, z)]$

Expected uncertainty reduction

$$\begin{aligned} \text{EUR}_z^{\text{true}}(\pi, m) &= h[p_n(z)] - \mathbb{E}_{p_{\text{train}}(y_{1:m}^+|\pi)}[h[p_{n+m}(z)]] \\ &\approx h[p_n(z)] - \mathbb{E}_{p_n(y_{1:m}^+|\pi')}[h[q_{n+m}(z)]] \end{aligned}$$

Model evaluation

Proper scoring rule
$s(p_n, z) = \ell(a_n^*, z)$

Discrepancy function
$d(p_n, p_{\text{eval}}) = \mathbb{E}_{p_{\text{eval}}(z)}[s(p_n, z)] - h[p_{\text{eval}}(z)]$

Accommodation

Is it worth reading? Maybe.

1. Uncertainty is decision-specific, not one-size-fits-all.
2. Decomposition: reducible vs. irreducible (depends on DGS, not just model).
3. Model-based quantities are *estimators*, not ground truths.
4. BALD works in practice by estimating short-run parameter IG.

Cons:

1. The authors claim their decomposition is better, but the argument is unconvincing, as there are no experiments, no rigorous proof, and no empirical validation.
2. More like a conceptual critique + framework clarification paper.

Thank you! Any questions?

Shuo Chen.
Introduction and exemplars of uncertainty decomposition.
arXiv preprint arXiv:2211.15475, 2022.