UQ of the 4th kind, Uncertainty Quantification of the 4th kind; optimal posterior accuracy-uncertainty tradeoff with the minimum enclosing ball,


Supported by AFOSR, JPL and BL with the following target applications

Greenland contribution to sea level by 2050: The role of meltwater in shaping the future ice sheet

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3 main approaches to uncertainty quantification

- **Worst case**: min and max (conservative)
  Not good at assimilating data.
- **Bayesian**: Brittle with respect to the choice of prior. MCMC to compute posteriors (slow)
- **Decision/Game Theory** (Minimax, identifies a prior). Suffers from the curse of dimensionality in approximating an optimal prior. The notion of risk is an averaged one (average with respect to data)

**We have discovered a 4th one**

- Hybrid between all 3 above and hypothesis testing
- Does not suffer from the curse of dimensionality
- Fast
- Notion of risk posterior to measurements
- Contains a Bayesian interpretation (direct computation of an optimal posterior)
- Optimal in the robustness vs accuracy tradeoff
Given $x \sim P(\cdot | \theta^\dagger)$ estimate $\varphi(\theta^\dagger)$ and quantify the uncertainty of the estimate.
Solution

$\theta \in \Theta_x(\alpha)$: Non-rarity assumption on the data

$\Theta_x(\alpha) := \{\theta \in \Theta : \bar{p}(x|\theta) \geq \alpha\}$: Likelihood region

$\bar{p}(x|\theta) := \frac{p(x|\theta)}{\sup_{\theta \in \Theta} p(x|\theta)}$: Relative likelihood

$p(\cdot|\theta)$: density of $P(\cdot|\theta)$

$0 \leq \alpha \leq 1$

$\beta_\alpha := \sup_{\theta \in \Theta} P\left(\{x' \in X : \theta \notin \Theta_{x'}(\alpha)\} | \theta\right)$: $p$-value

Significance level: (max in $\theta$) probability that the assumption is wrong

$1 - \beta_\alpha$: Confidence level that the assumption is true
\( \theta \in \Theta_x(\alpha) \): Non-rarity assumption on the data

\[ \Theta_x(\alpha) := \{ \theta \in \Theta : \bar{p}(x|\theta) \geq \alpha \} \]: Likelihood region

\[ \bar{p}(x|\theta) := \frac{p(x|\theta)}{\sup_{\theta \in \Theta} p(x|\theta)} \]: Relative likelihood

\[ \beta_\alpha := \sup_{\theta \in \Theta} P\left( \{ x' \in X : \theta \notin \Theta_{x'}(\alpha) \} \mid \theta \right) \]: p-value

When \( \alpha \approx 1 \), \( \Theta_x(\alpha) \) concentrates around the MLE but the max probability \( \beta_\alpha \) that \( \theta^\dagger \notin \Theta_x(\alpha) \) is high.
\[ \theta \in \Theta_x(\alpha) : \text{Non-rarity assumption on the data} \]

\[ \Theta_x(\alpha) := \{ \theta \in \Theta : \bar{p}(x|\theta) \geq \alpha \} : \text{Likelihood region} \]

\[ \bar{p}(x|\theta) := \frac{p(x|\theta)}{\sup_{\theta \in \Theta} p(x|\theta)} : \text{Relative likelihood} \]

\[ \beta_\alpha := \sup_{\theta \in \Theta} P \left( \{ x' \in X : \theta \notin \Theta_{x'}(\alpha) \} | \theta \right) : p\text{-value} \]

When \( \alpha \approx 0 \), \( \Theta_x(\alpha) \) covers most of the domain and the max probability \( \beta_\alpha \) that \( \theta^\dagger \notin \Theta_x(\alpha) \) is low.
Choose

\[ \alpha := \max \{ \alpha' \mid 1 - \beta_{\alpha'} \geq 0.95 \} \]

With probability at least 0.95, \( \theta_x(\alpha) \) contains the true (data generating) parameter \( \theta^\dagger \).

Play adversarial game in \( \Theta_x(\alpha) \)

**Player I**

Selects \( \pi \in \mathcal{P}(\Theta_x(\alpha)) \)

\[ \pi_x := \frac{\bar{p}(x \mid \cdot)\pi}{\int_{\Theta} \bar{p}(x \mid \theta) d\pi(\theta)} \]

**Player II**

Selects \( d \in V \)

\[ \max \quad \min \]

\[ \mathbb{E}_{\theta \sim \pi_x} \left[ \| \varphi(\theta) - d \|^2 \right] \]
Choose
\[ \alpha := \max \{ \alpha' \mid \beta_{\alpha'} \leq 0.05 \} \]

With probability at least 0.95, \( \theta_x(\alpha) \) contains the true (data generating) parameter \( \theta^\dagger \).

Identification of optimal posterior

Player I
Selects \( \pi \in \mathcal{P}(\Theta_x(\alpha)) \)

Player II
Selects \( d \in V \)

\[ \max \quad \min \]
\[ \mathbb{E}_{\theta \sim \pi} \left[ \| \varphi(\theta) - d \|^2 \right] \]
**Theorem**

\[ B: \text{Min enclosing ball of } \varphi(\Theta_x(\alpha)) \]

**Optimal decision** \( d \): Center of \( B \)

**Optimal posterior:** \[ \pi = \sum_{i=1}^{\dim(V)+1} \pi_i \delta_{\theta_i} \]

\[ \varphi(\theta_i) \in \partial B \]

**Risk** \( \mathbb{E}_{\theta \sim \pi} [\| \varphi(\theta) - d \|^2] \): Squared radius \( R^2 \) of \( B \)
Consider the Lotka-Volterra predator-prey model.

\[
\frac{dx}{dt} = \theta_1 x - \eta xy \\
\frac{dy}{dt} = \xi xy - \theta_2 y
\]

Given

\[
x^{(t)} = \begin{bmatrix} x_t \\ y_t \end{bmatrix} = m(t; \theta) + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0, \sigma^2 I), \quad t \in \{0, \frac{1}{10}, \ldots, 20\}
\]

Estimate \((\theta_1, \theta_2)\)
Min enclosing ball and optimal decision

- Feasible Region Boundary: $\partial \Theta_P(\alpha)$
- Minimum Enclosing Ball: $B$
- Optimized Center
- Truth: $\theta^*$
- Optimized Boundary Points: $S$
Solution map and support points of optimal posterior

$$\theta \mapsto m(t; \theta), \ t \in T.$$
Example

$\theta^\dagger \in [-\tau, \tau]$ unknown

Given $x \sim \mathcal{N}(\theta^\dagger, \sigma^2)$ estimate $\theta^\dagger$

Solution

$x = 1.5$, $\sigma = 1$, $\tau = 3$
Example

Estimate the probability that a biased coin lands on heads from the observation of $n$ independent tosses of that coin.

$\theta^\dagger \in [0, 1]$

Given $Y_1, \ldots, Y_n$ i.i.d. ($P(Y_i = 1) = \theta^\dagger$, $P(Y_i = 0) = 1 - \theta^\dagger$) estimate $\theta^\dagger$.

Solution

$n = 5$, 4 heads
Example

Consider two independent biased coins with unknown probabilities $\theta_1^\dagger$ and $\theta_2^\dagger$ of landing on head. Given $n_1$ tosses of coin 1 and $n_2$ tosses of coin 2 estimate $\theta_1^\dagger$ and $\theta_2^\dagger$.

$n_1 = 4$, 3 heads and 1 tail for coin 1

$n_2 = 6$, 5 heads and 1 tail for coin 2