Parameter control in the presence of uncertainties

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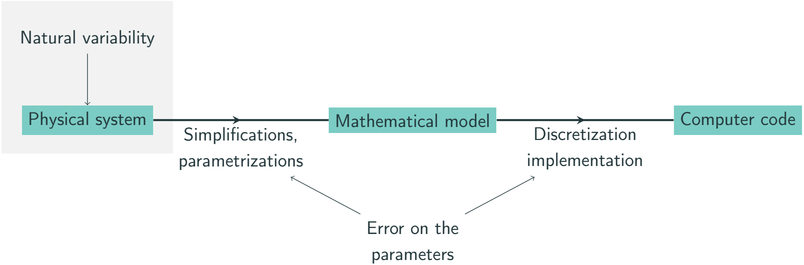
Uncertainties in the modelling



Does reducing the error on the parameters leads to the compensation of the unaccounted natural variability of the physical processes ?

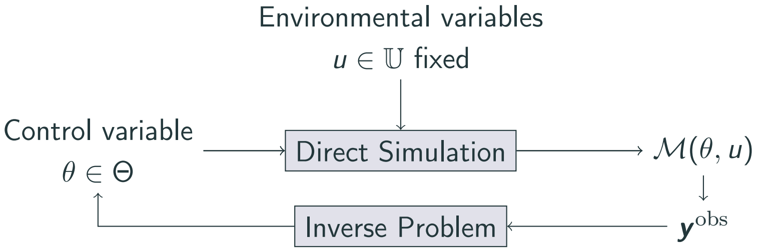
Outline

Calibration problem

Computer code and inverse problem

Input
- θ: Control parameter
- u: Environmental variables (fixed and known)

Output
- $\mathcal{M}(\theta, u)$: Quantity to be compared to observations



Data assimilation framework

Let $u \in \mathbb{U}$.

$$\hat{\theta} = \underset{\theta \in \Theta}{\arg\min}\, J(\theta) = \underset{\theta \in \Theta}{\arg\min}\, \frac{1}{2} \|\mathcal{M}(\theta, u) - \boldsymbol{y}^{\mathrm{obs}}\|^2$$

→ Deterministic optimization problem

→ Possibly add regularization

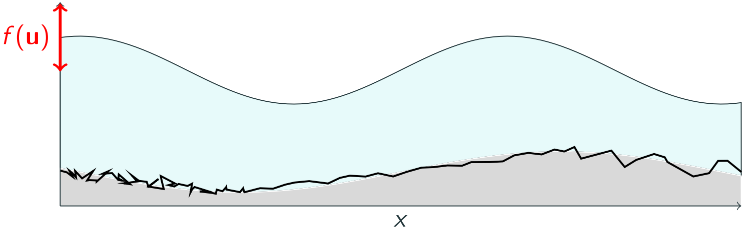
→ Classical methods: Adjoint gradient and Gradient-descent

BUT

- What if u does not reflect accurately the observations?
- Does $\hat{\theta}$ compensate the errors brought by this random misspecification? ($\sim$overfitting)

Context

- The friction θ of the ocean bed has an influence on the water circulation
- Depends on the type and/or characteristic length of the asperities
- Subgrid phenomenon
- u parametrizes the BC



Different types of uncertainties

Epistemic or aleatoric uncertainties? [WHR+03]

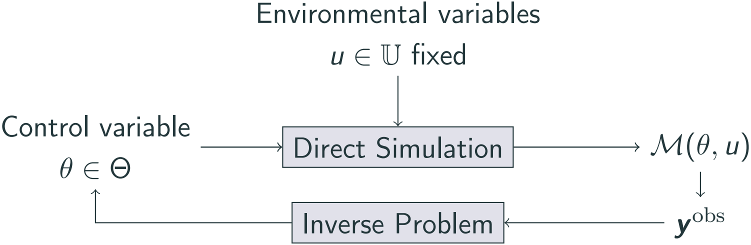
- Epistemic uncertainties: From a lack of knowledge, that can be reduced with more research/exploration
- Aleatoric uncertainties: From the inherent variability of the system studied, operating conditions

$\rightarrow$ But where to draw the line?

Our goal is to take into account the aleatoric uncertainties in the estimation of our parameter.

Aleatoric uncertainties

Instead of considering u fixed, we consider that $u \sim U$ r.v. (with known pdf $\pi(u)$), and the output of the model depends on its realization.



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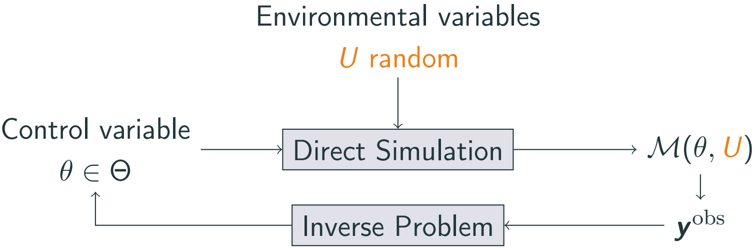


The cost function as a random variable

- The computer code is deterministic, and takes θ and u as input:

$$\mathcal{M}(\theta, u)$$

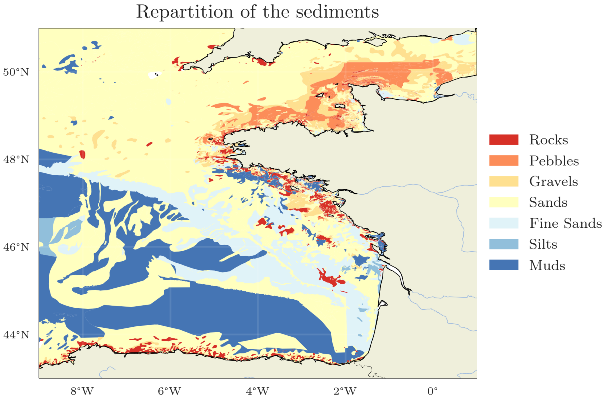
- The deterministic quadratic error is now

$$J(\theta, u) = \frac{1}{2}\|\mathcal{M}(\theta, u) - \boldsymbol{y}^{\mathrm{obs}}\|^2$$

$$''\hat{\theta} = \underset{\theta \in \Theta}{\arg\min}\, J(\theta, u)'' \text{ but what can we do about } u?$$

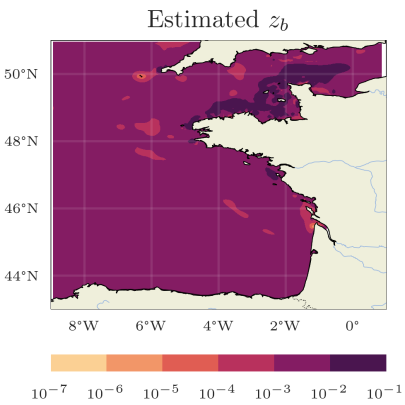
Misspecification of u: twin experiment setup

Minimization performed on $\theta \mapsto J\left(\theta, u^b\right)$, for different u^b:



Minimization performed on $\theta \mapsto J\left(\theta, u^b\right)$, for different u^b:

Well-specified model: $u^b = (0.5, 0.5)$



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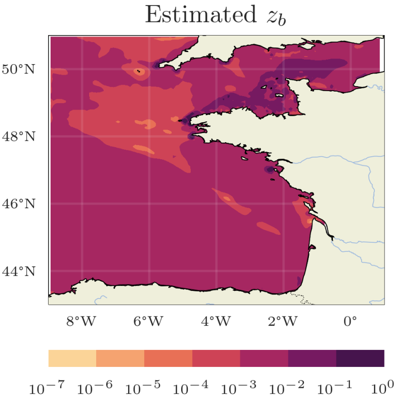

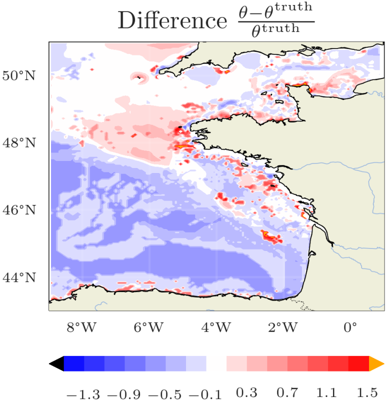

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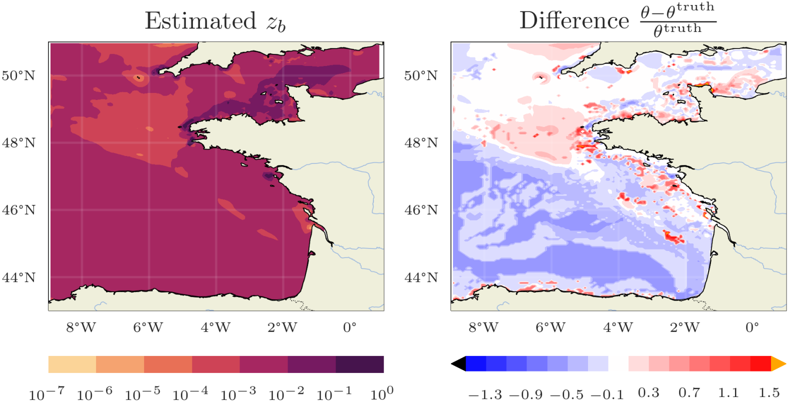

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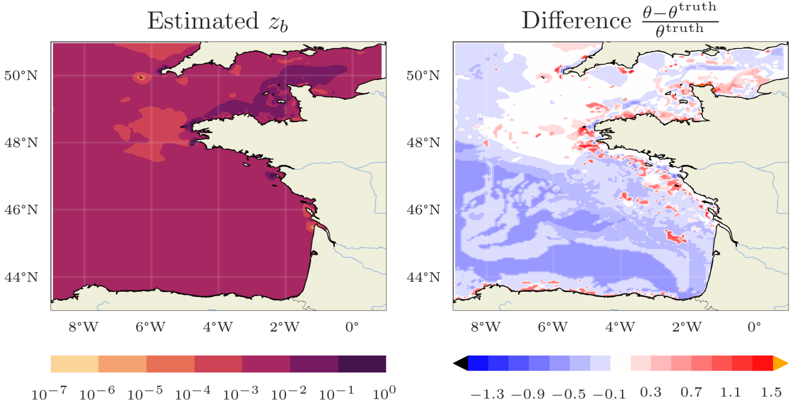

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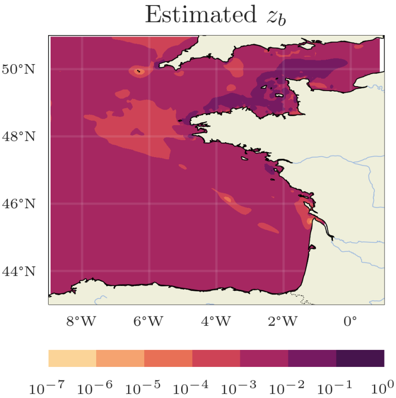

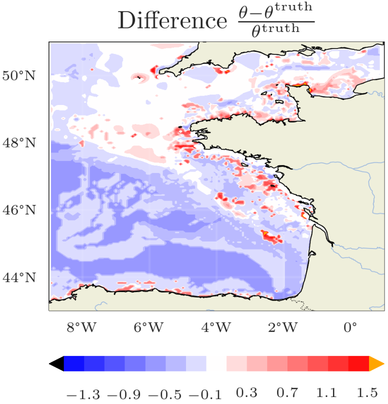

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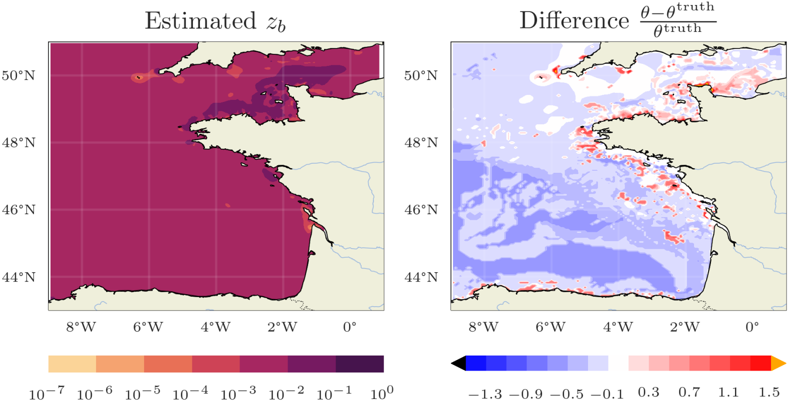

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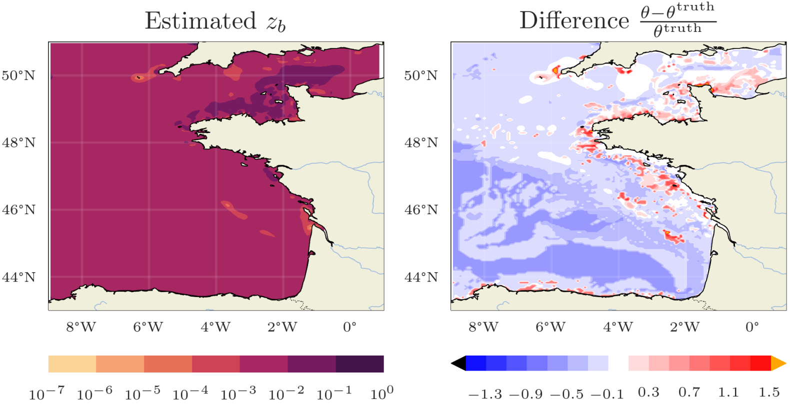

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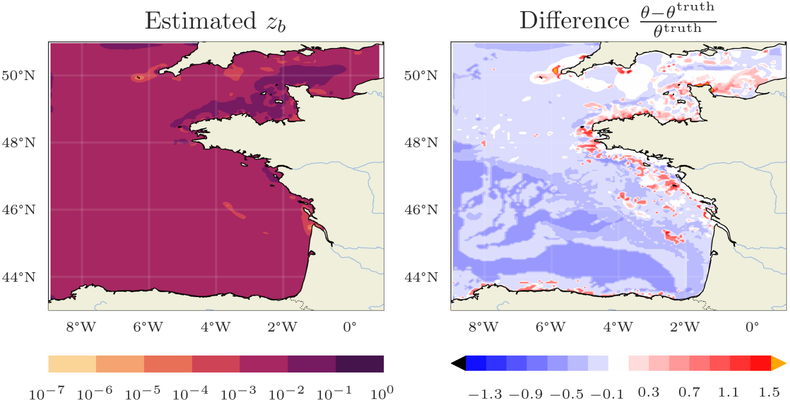

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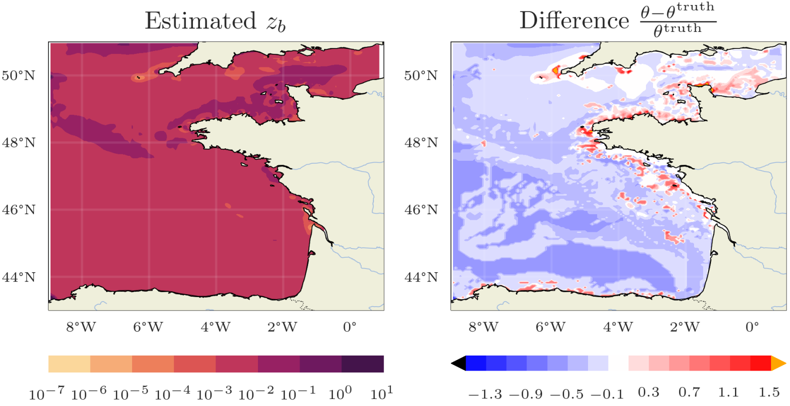

Robustness and estimation of parameters

Robustness: get good performances when the environmental parameter varies

- Define criteria of robustness, based on $J(\theta, u)$, that will depend on the final application
- Be able to compute them in a reasonable time

Robust minimization

Criteria of robustness

Non-exhaustive list of "Robust" Objectives

- Worst case [MWP13]:

$$\min_{\theta \in \Theta} \left\{ \max_{u \in \mathbb{U}} J(\theta, u) \right\}$$

- M-robustness [LSN04]:

$$\min_{\theta \in \Theta} \mathbb{E}_U \left[J(\theta, U) \right]$$

- Multiobjective [Bau12]:

Pareto frontier

- Best performance achievable given $u \sim U$, regret-based robustness

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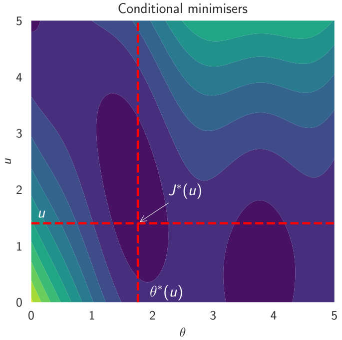
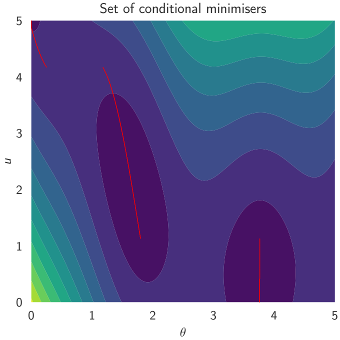
Relative-regret: illustration



- Sample $u \sim U$, and solve $\theta^*(u) = \arg\min_{\theta \in \Theta} J(\theta, u)$

Relative-regret: illustration



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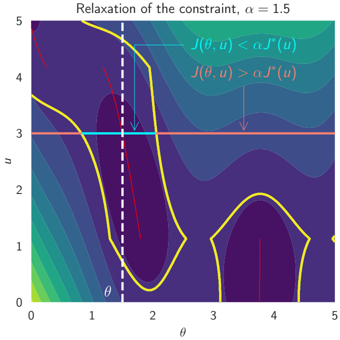

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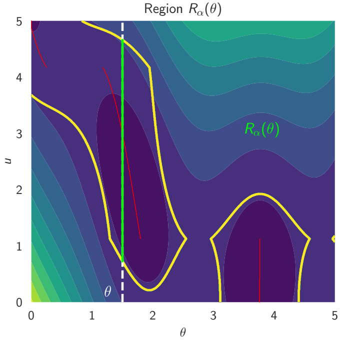

- Sample $u \sim U$, and solve $\theta^*(u) = \arg\min_{\theta\in\Theta} J(\theta, u)$
- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$
- Set $\alpha \geq 1$
- $R_\alpha(\theta) = \{u \mid J(\theta, u) \leq \alpha J^*(u)\}$
- $\Gamma_\alpha(\theta) = \mathbb{P}_U\left[U \in R_\alpha(\theta)\right]$

Getting an estimator

$\Gamma_\alpha(\theta)$: probability that the cost (thus θ) is α-acceptable

- If α known, maximize the probability that θ gives acceptable values:

$$\max_{\theta \in \Theta} \Gamma_\alpha(\theta) = \max_{\theta \in \Theta} \mathbb{P}_U \left[J(\theta, U) \leq \alpha J^*(U) \right] \tag{1}$$

- Set a target probability $1 - \eta$, and find the smallest α.

$$\inf\{\alpha \mid \max_{\theta \in \Theta} \Gamma_\alpha(\theta) \geq 1 - \eta\} \tag{2}$$

Relative-regret family of estimators [TAVD20]

$$\left\{ \hat{\theta} \mid \hat{\theta} = \arg\max_{\theta \in \Theta} \Gamma_\alpha(\theta), \alpha > 1 \right\} \tag{3}$$

Conclusion

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Wrapping up

- Problem of a *good* definition of robustness
- Tuning α or η reflects risk-seeking or risk-adverse strategies
- Strategies rely heavily on surrogate models, to embed aleatoric uncertainties directly in the modelling

Perspectives

- Cost of computer evaluations $\rightarrow$ limited number of runs?
- In low dimension, CROCO very well-behaved.
- Dimensionality of the input space $\rightarrow$ reduction of the input space?

Vincent Baudoui.
***Optimisation Robuste Multiobjectifs Par Modèles de Substitution*.**
PhD thesis, Toulouse, ISAE, 2012.

Julien Bect, David Ginsbourger, Ling Li, Victor Picheny, and Emmanuel Vazquez.
Sequential design of computer experiments for the estimation of a probability of failure.
Statistics and Computing, 22(3):773–793, May 2012.

B. Echard, N. Gayton, and M. Lemaire.
AK-MCS: An active learning reliability method combining Kriging and Monte Carlo Simulation.
Structural Safety, 33(2):145–154, March 2011.

David Ginsbourger, Jean Baccou, Clément Chevalier, Frédéric Perales, Nicolas Garland, and Yann Monerie.
Bayesian Adaptive Reconstruction of Profile Optima and Optimizers.
SIAM/ASA Journal on Uncertainty Quantification, 2(1):490–510, January 2014.

Daniel G. Krige.
A statistical approach to some basic mine valuation problems on the Witwatersrand.
Journal of the Southern African Institute of Mining and Metallurgy, 52(6):119–139, 1951.

Jeffrey S. Lehman, Thomas J. Santner, and William I. Notz.
Designing computer experiments to determine robust control variables.
Statistica Sinica, pages 571–590, 2004.

Georges Matheron.
***Traité de Géostatistique Appliquée. 1 (1962)*, volume 1.**
Editions Technip, 1962.

Julien Marzat, Eric Walter, and Hélène Piet-Lahanier.
Worst-case global optimization of black-box functions through Kriging and relaxation.
Journal of Global Optimization, 55(4):707–727, April 2013.

Victor Trappler, Élise Arnaud, Arthur Vidard, and Laurent Debreu.
Robust calibration of numerical models based on relative regret.
Journal of Computational Physics, page 109952, November 2020.

Warren E. Walker, Poul Harremoës, Jan Rotmans, Jeroen P. van der Sluijs, Marjolein BA van Asselt, Peter Janssen, and Martin P. Krayer von Krauss.
Defining uncertainty: A conceptual basis for uncertainty management in model-based decision support.
Integrated assessment, 4(1):5–17, 2003.

"Most Probable Estimate", and relaxation

Given $u \sim U$, the optimal value is $J^*(u)$, attained at $\theta^*(u) = \arg\min_{\theta \in \Theta} J(\theta, u)$.

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$\longrightarrow$ estimate its density (how often is the value θ a minimizer)

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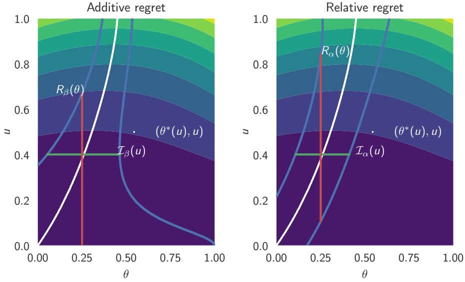
How to take into account values not optimal, but not too far either $\longrightarrow$ relaxation of the equality with $\alpha > 1$:

$$\Gamma_\alpha(\theta) = \mathbb{P}_U\left[J(\theta, U) \leq \alpha J^*(U)\right]$$

Why the relative regret ?



- Relative regret
    - α-acceptability regions large for flat and bad situations ($J^*(u)$ large)
    - Conversely, puts high confidence when $J^*(u)$ is small
    - No units $\rightarrow$ ratio of costs

Notions of regret

Let $J^*(u) = \min_{\theta \in \Theta} J(\theta, u)$ and $\theta^*(u) = \arg\min_{\theta \in \Theta} J(\theta, u)$. The regret r:

$$r(\theta, u) = J(\theta, u) - J^*(u) = -\log\left(\frac{e^{-J(\theta,u)}}{\max_\theta\{e^{-J(\theta,u)}\}}\right) \tag{4}$$

$$= -\log\left(\frac{\mathcal{L}(\theta, u)}{\max_{\theta\in\Theta} \mathcal{L}(\theta, u)}\right) \tag{5}$$

$\rightarrow$ linked to misspecified LRT: maximize the probability of keeping $\mathcal{H}_0$: θ valid instead of $\arg\max \mathcal{L}$.

PEI criterion

$Y \sim \mathrm{GP}(m_Y(\cdot), C_Y(\cdot,\cdot))$ on $\Theta \times \mathbb{U}$

$$\mathrm{PEI}(\theta, u) = \mathbb{E}_Y\left[\left[f_{\mathrm{min}}(u) - Y(\theta, u)\right]_+\right] \tag{6}$$

where $f_{\mathrm{min}}(u) = \max\left\{\min_i J(\theta_i, u_i), \min_{\theta\in\Theta} m_Y(\theta, u)\right\}$