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Title: *Parameter control in the presence of uncertainties*

with É. Arnaud, L. Debreu, A. Vidard



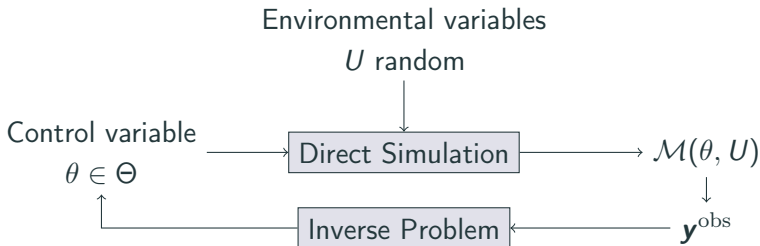
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1. Optimisation under Uncertainties
 - Notions of robustness in a calibration context
 - Regret-based family of estimators
2. Adaptive Strategies using GP for the estimation
 - GP formulation of the regret
 - SUR (Stepwise Uncertainty Reduction) strategies of design enrichment
 - AK-MCS (Adaptive Kriging Monte Carlo Sampling) for batch selection of points
3. Application: robust calibration of CROCO

Computer code and inverse problem

- Input
- θ : Control parameter
 - u : Environmental variables, realisations of r.v. U
- Output
- $\mathcal{M}(\theta, u)$: Quantity to be compared to observations



Regret-based formulations

- $(\theta, u) \mapsto J(\theta, u)$ objective function, *strictly positive*
 - Best performance given u : $J^* : u \mapsto \min_{\theta \in \Theta} J(\theta, u)$
- Find $\hat{\theta}$ such that $J(\hat{\theta}, U)$ “close to” $J^*(U) = J(\theta^*(U), U)$ with high enough probability

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- Regret: $r(\theta, u) = J(\theta, u) - J^*(u)$ or $r(\theta, u) = \frac{J(\theta, u)}{J^*(u)}$
 - $\Gamma_\alpha(\theta) = \mathbb{P}_U[r(\theta, U) \leq \alpha]$: Probability that the regret is below a level α

Regret-based family of estimators (Trappler et al., 2020)

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

Adaptive strategies for the estimation of Γ_α

Let $Z \sim \text{GP}(m_Z, C_Z^2)$ be a GP constructed on $\Theta \times \mathbb{U}$ based on J .
We use Z to estimate Γ_α

- Reduction of the *augmented* IMSE of $\Delta = Z - \alpha Z^*$
- Improve estimation of the set $\{\Delta \leq 0\}$, using probability of coverage
- Sampling in the margin of uncertainty of $\{\Delta \leq 0\}$, and transformations to get a batch of points (AK-MCS (Dubourg et al., 2011))

Adaptive strategies for the quantile of the regret

Under certain conditions, the ratio Z/Z^* is approximately log-normally distributed. Let us define $\Xi = \log Z/Z^*$

- Reduction of the augmented IMSE of Ξ
- Sampling in regions of interest, and subsequent transformations (QeAK-MCS (Razaaly, 2019))

Summary

Research topics

- Formulation of a notion of robustness using the regret
- Adaptive methods using GP for the estimation of Γ_α
- Application to the numerical model CROCO: robust estimation of the bottom friction

In progress

- Adaptive strategies for the *optimisation* (2-stage methods)
- Python package for adaptive methods (with scikit-learn)
- Improve scalability for CROCO

- Dubourg, V., Sudret, B., and Bourinet, J.-M. (2011). Reliability-based design optimization using kriging surrogates and subset simulation. *Structural and Multidisciplinary Optimization*, 44(5):673–690.
- Razaaly, N. (2019). *Rare Event Estimation and Robust Optimization Methods with Application to ORC Turbine Cascade*. These de doctorat, Université Paris-Saclay (ComUE).
- Trappler, V., Arnaud, É., Vidard, A., and Debreu, L. (2020). Robust calibration of numerical models based on relative regret. *Journal of Computational Physics*, page 109952.

“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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The minimizer can be seen as a random variable:

$$\theta^*(U) = \arg \min_{\theta \in \Theta} J(\theta, U)$$

→ estimate its density (how often is the value θ a minimizer)

$$p_{\theta^*}(\theta) = \mathbb{P}_U [J(\theta, U) = J^*(U)]$$

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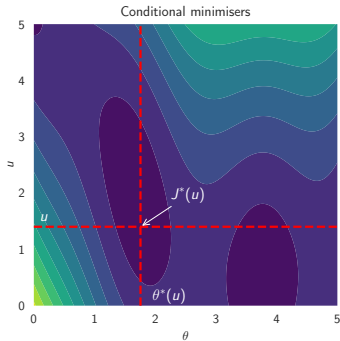
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How to take into account values not optimal, but not too far either

→ relaxation of the equality with $\alpha > 1$:

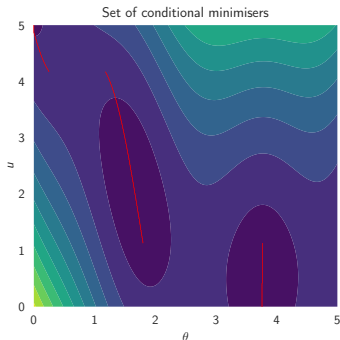
$$\Gamma_\alpha(\theta) = \mathbb{P}_U [J(\theta, U) \leq \alpha J^*(U)]$$

Relative-regret: illustration



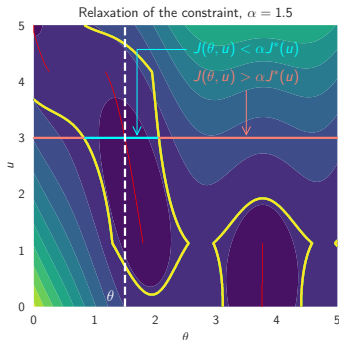
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Relative-regret: illustration



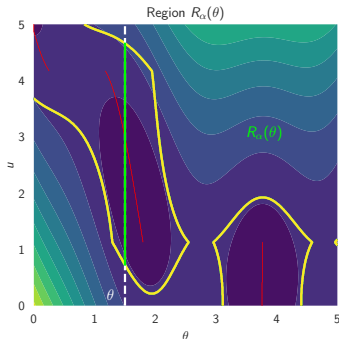
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- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$

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- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$
- Set $\alpha \geq 1$
- $R_\alpha(\theta) = \{u \mid J(\theta, u) \leq \alpha J^*(u)\}$
- $\Gamma_\alpha(\theta) = \mathbb{P}_U [U \in R_\alpha(\theta)]$

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:

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

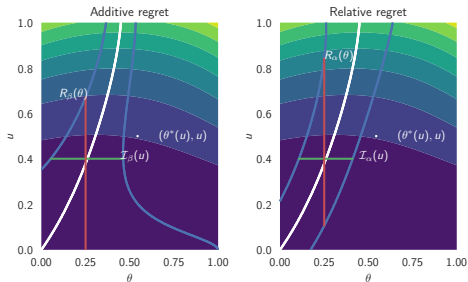
- Set a target probability $1 - \eta$, and find the smallest α .

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

Relative-regret family of estimators (Trappler et al., 2020)

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

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 :

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

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

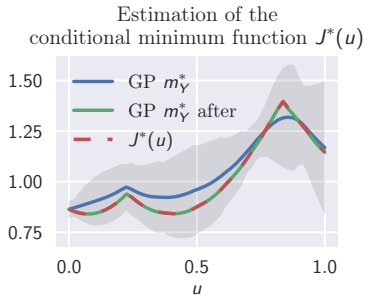
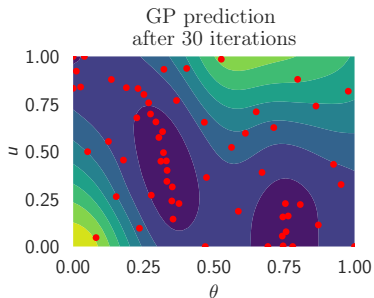
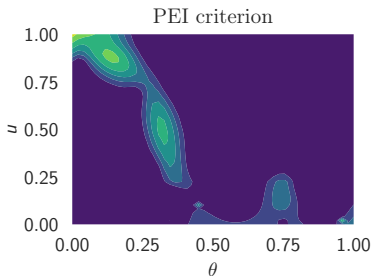
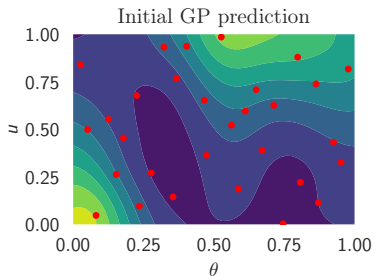
→ linked to misspecified LRT: maximize the probability of keeping \mathcal{H}_0 : θ valid instead of $\arg \max \mathcal{L}$.

$Z \sim \text{GP}(m_Z, C_Z)$ on $\Theta \times \mathbb{U}$

$$\text{PEI}(\theta, u) = \mathbb{E}_{Z(\theta, u)} \left[[f_{\min}(u) - Z(\theta, u)]_+ \right] \quad (6)$$

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

Illustration of the PEI



Principle of AK-MCS

