

Robust calibration of numerical models based on Relative-regret

Robust Estimation of bottom friction

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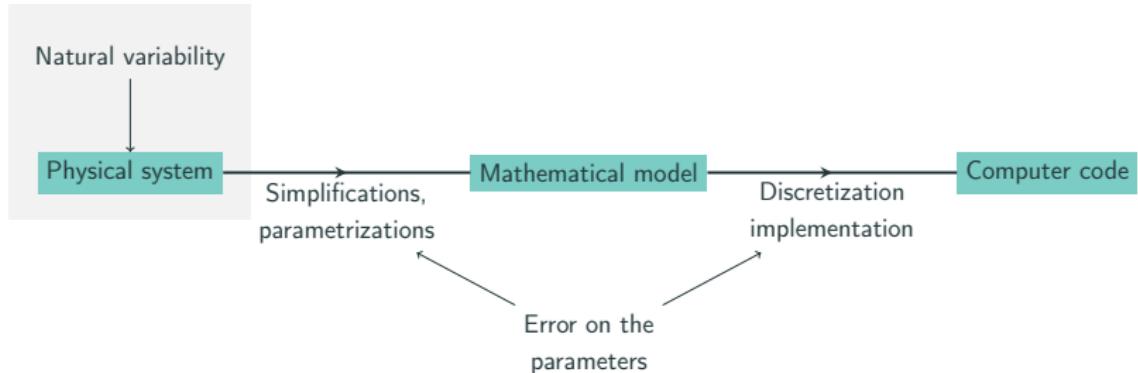
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Laboratoire Jean Kuntzmann

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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

Introduction

Calibration problem

Robust minimization

Surrogates

Conclusion

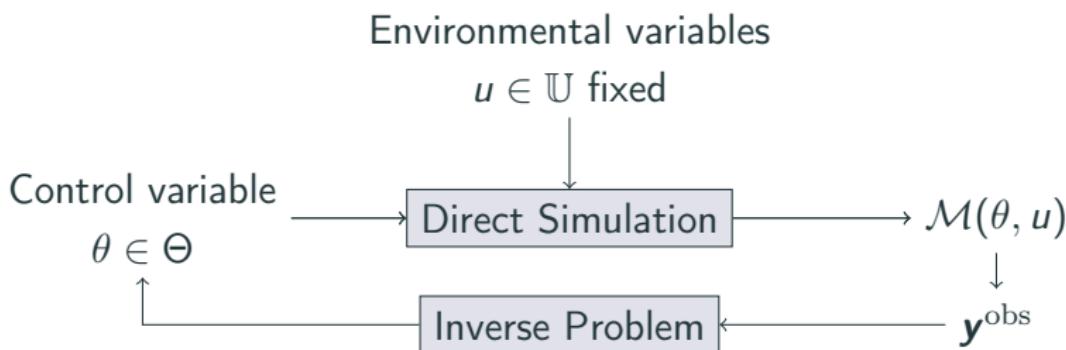
Calibration problem

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 $u \in \mathbb{U}$.

$$\hat{\theta} = \arg \min_{\theta \in \Theta} J(\theta) = \arg \min_{\theta \in \Theta} \frac{1}{2} \|\mathcal{M}(\theta, u) - \mathbf{y}^{\text{obs}}\|^2$$

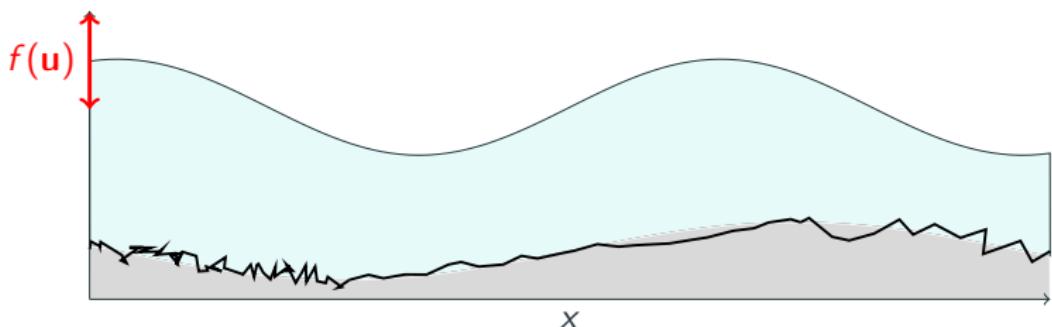
- Deterministic optimization problem
- Possibly add regularization
- Classical methods: Adjoint gradient and Gradient-descent

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]

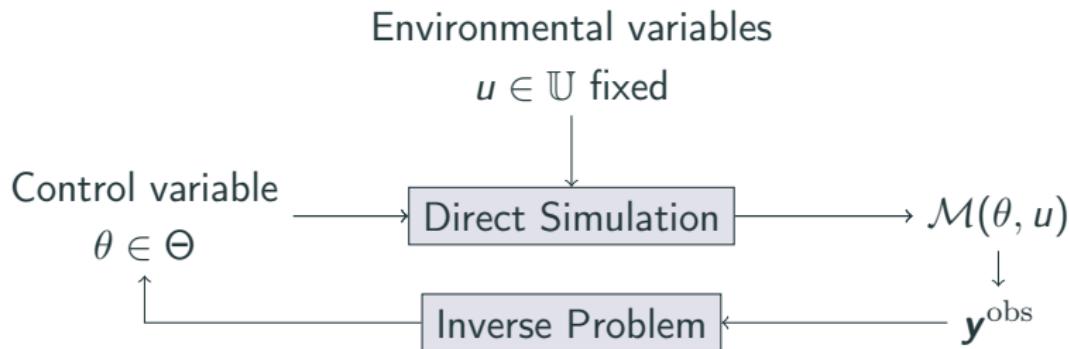
- Epistemic uncertainties: From a lack of knowledge, that can be reduced with more research/exploration
- Aleatoric uncertainties: From the inherent variability of the system studied, operating conditions

→ But where to draw the line?

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

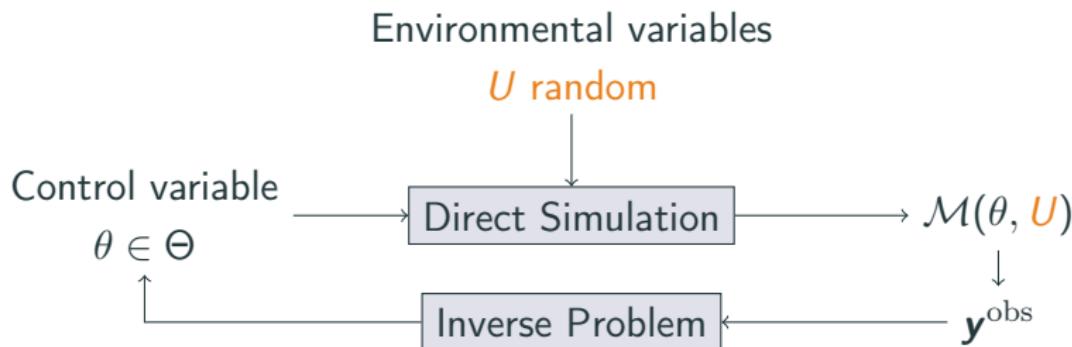
Aleatoric uncertainties

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:

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

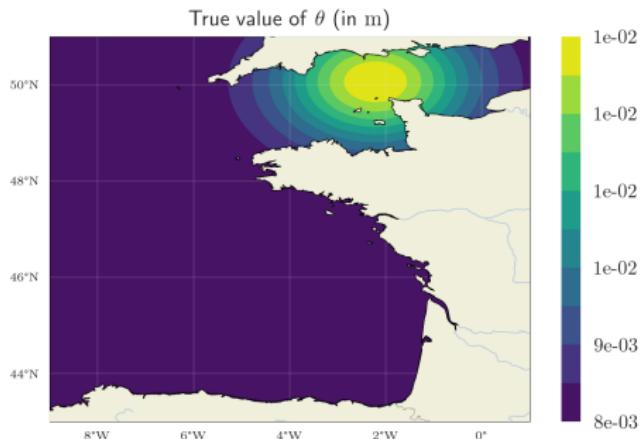
- The deterministic quadratic error is now

$$J(\theta, \textcolor{orange}{u}) = \frac{1}{2} \|\mathcal{M}(\theta, \textcolor{orange}{u}) - \mathbf{y}^{\text{obs}}\|^2$$

" $\hat{\theta} = \arg \min_{\theta \in \Theta} J(\theta, \textcolor{orange}{u})$ " but what can we do about u ?

Misspecification of u : twin experiment setup

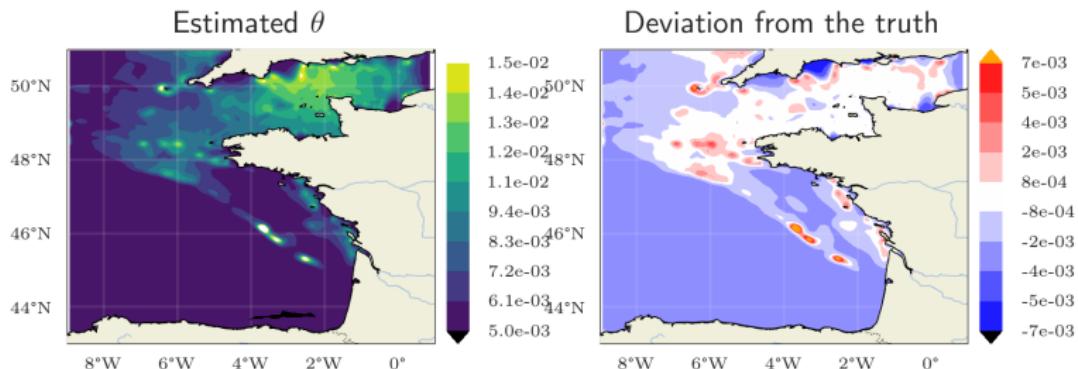
Minimization performed on $\theta \mapsto J(\theta, u)$, for different u :



Misspecification of u : twin experiment setup

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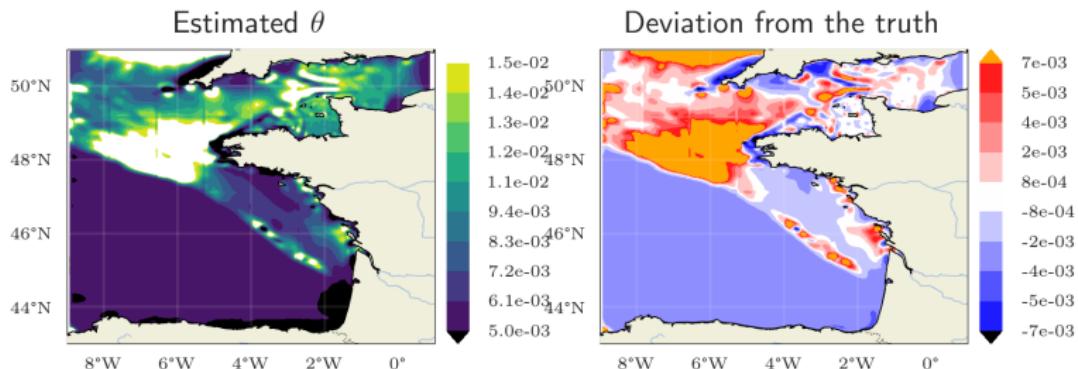
Well-specified model



Misspecification of u : twin experiment setup

Minimization performed on $\theta \mapsto J(\theta, u)$, for different u :

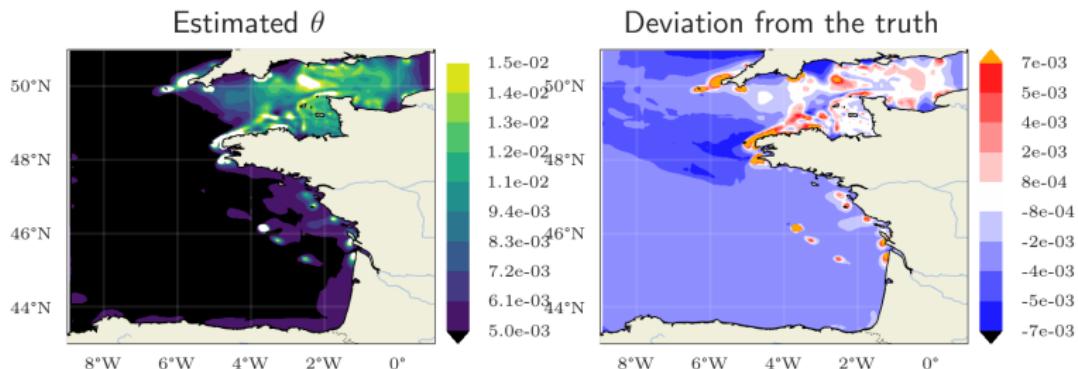
1% error on the amplitude of the M2 tide



Misspecification of u : twin experiment setup

Minimization performed on $\theta \mapsto J(\theta, u)$, for different u :

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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]:

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

- V-robustness [LSN04]:

$$\min_{\theta \in \Theta} \text{Var}_U [J(\theta, U)]$$

- Multiobjective [Bau12]:

Pareto frontier

- Best performance achievable given $u \sim U$

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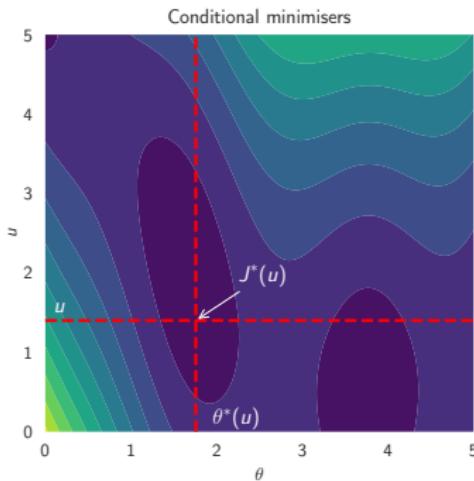
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How to take into account values not optimal, but not too far either
→ relaxation of the equality with $\alpha > 1$:

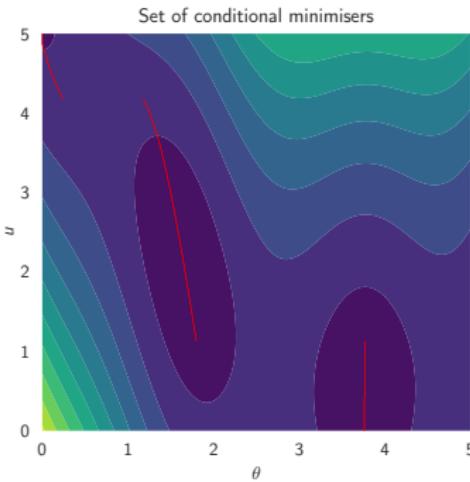
$$\Gamma_\alpha(\theta) = \mathbb{P}_U [J(\theta, U) \leq \alpha J^*(U)]$$

Illustration



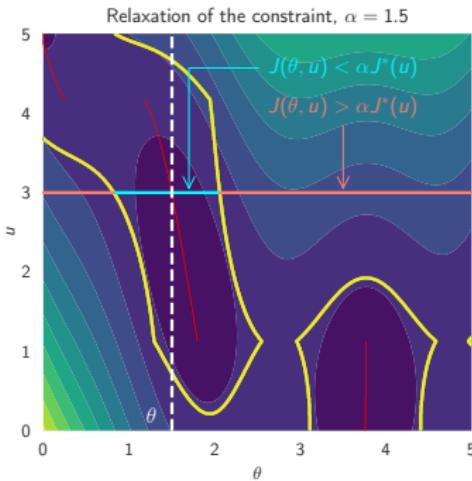
- Sample $u \sim U$, and solve
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Illustration



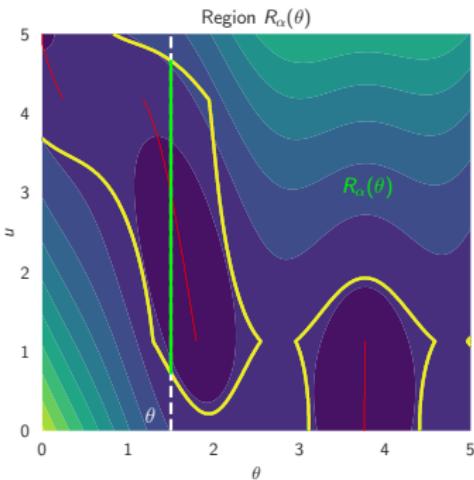
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- Set of conditional minimisers:
$$\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$$

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Illustration



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

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:

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

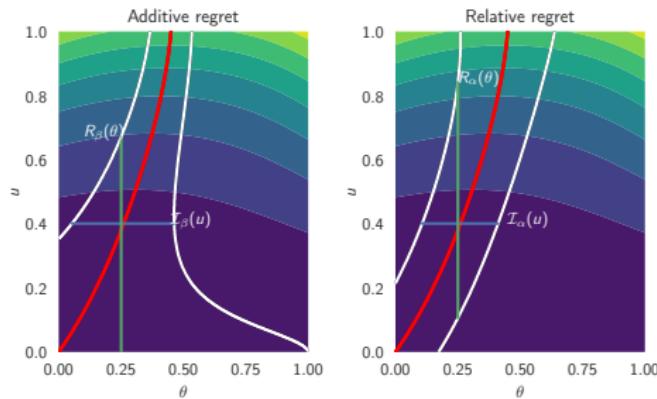
- Set a target probability $1 - \eta$, and find the smallest α .

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

Relative-regret family of estimators

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

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

Surrogates

How to compute $\hat{\theta}$ in a reasonable time?

Surrogates, and cost function

- Replace expensive model by a computationally cheap metamodel (~ plug-in approach)
 - Adapted sequential procedures e.g. EGO
- Kriging (Gaussian Process Regression) [Mat62, Kri51]

Surrogates, and cost function

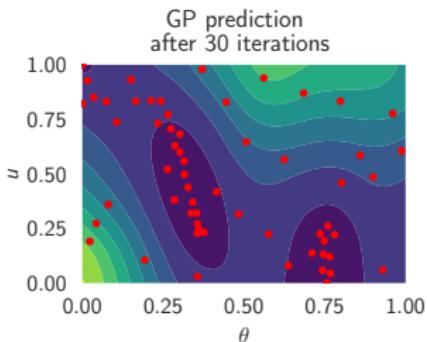
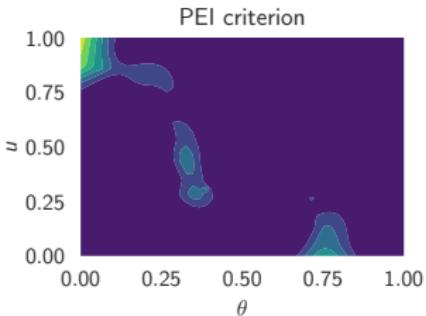
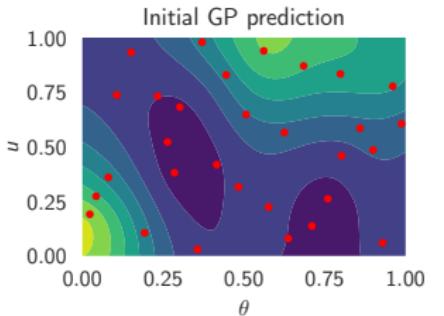
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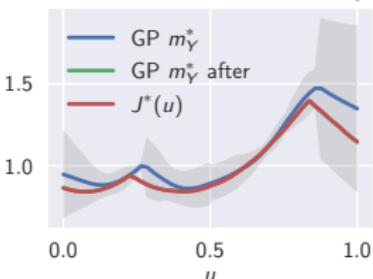
$Y \sim GP(m_Y(\cdot), C_Y(\cdot, \cdot))$ GP regression of J on $\Theta \times \mathbb{U}$, using an initial design $\mathcal{X} = \{((\theta_i, u_i), J(\theta_i, u_i))\}$

Estimation of θ^* , $J^*(u)$

Estimation of $J^*(u)$ and $\theta^*(u)$: Enrich the design according to PEI criterion [GBC⁺14].



Estimation of the conditional minimum function $J^*(u)$



GP of the “penalized” cost function

What about $J(\theta, u) - \alpha J^*(u)$?

$$Y \sim \text{GP}(m_Y(\cdot); C_Y(\cdot, \cdot)) \text{ on } \Theta \times \mathbb{U} \quad (4)$$

$$\Delta_\alpha = Y - \alpha Y^* \quad (5)$$

Still a GP

$$\Delta_\alpha(\theta, u) \sim \text{GP}(m_\alpha(\cdot); C_\alpha(\cdot, \cdot)) \quad (6)$$

$$m_\alpha(\theta, u) = m_Y(\theta, u) - \alpha m_Y^*(u) \quad (7)$$

$$\sigma_\alpha^2(\theta, u) = \sigma_Y^2(\theta, u) + \alpha^2 \sigma_{Y^*}^2(u) - 2\alpha C_Y((\theta, u), (\theta_Y^*(u), u)) \quad (8)$$

Estimate the “probability of failure” [BGL⁺12, EGL11]

$$\mathbb{P}_U [J(\theta, U) - \alpha J^*(U) \leq 0] \approx \mathbb{P}_U [\mathbb{P}_Y [\Delta_\alpha \leq 0]]$$

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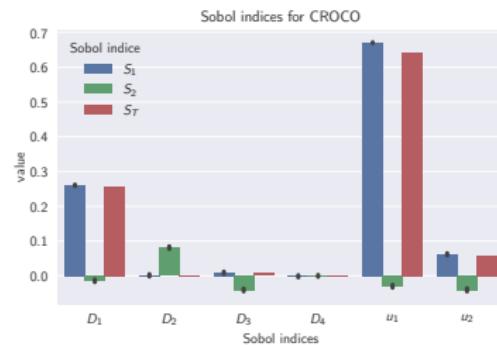
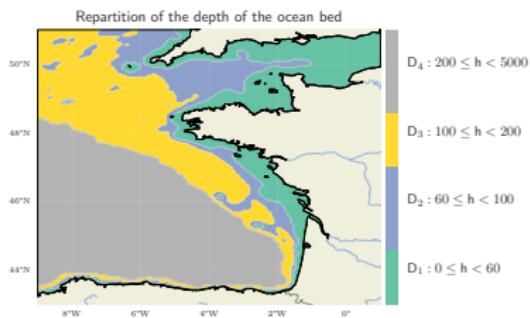
$$\mathbb{P}_U [J(\theta, U) - \alpha J^*(U) \leq 0] \approx \mathbb{P}_U [\mathbb{P}_Y [\Delta_\alpha \leq 0]]$$

Joint space or objective-oriented exploration

Because of $J^*(u)$, it is often not enough to select the point where the uncertainty is high. Generally, two main approaches can be considered

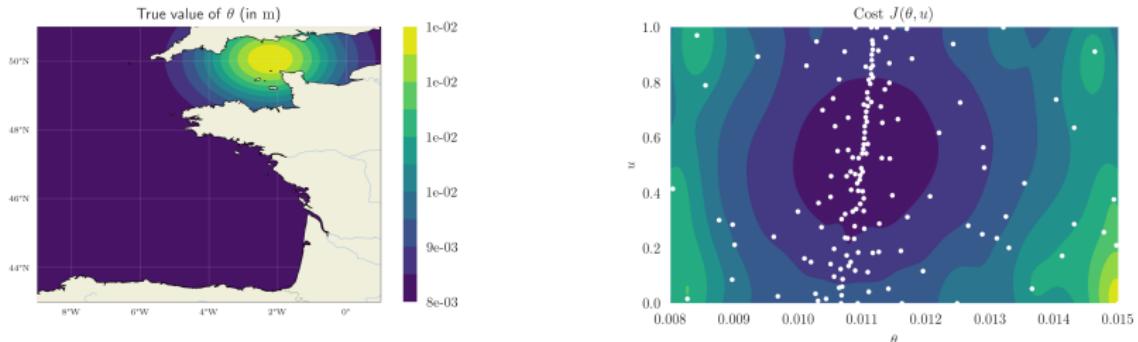
- Estimate the region $\{(\theta, u) \mid J(\theta, u) \leq \alpha J^*(u)\}$, then use the surrogate as a plug-in estimate to compute and maximize Γ_α
→ reduce uncertainty on the whole space
- Select a candidate $\tilde{\theta}$, such that uncertainty on the estimation of $\Gamma_\alpha(\tilde{\theta})$ is reduced
→ reduce uncertainty on $\{\tilde{\theta}\} \times \mathbb{U}$, with $\tilde{\theta}$ well-chosen.

Application to CROCO: Dimension reduction



Ad-hoc segmentation according to the depth, and sensitivity analysis: only the shallow coastal regions seem to have an influence.

Robust optimization



- $U \sim U[-1, 1]$ uniform r.v. that models the percentage of error on the amplitude of the M2 component of the tide
- The “truth” ranges from 8mm to 13mm.
- 11.0mm leads to a cost which deviates less than 1% from the optimal value with probability 0.77

Conclusion

Conclusion

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 → limited number of runs?
- In low dimension, CROCO very well-behaved.
- Dimensionality of the input space → reduction of the input space?

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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 :

$$r(\theta, u) = J(\theta, u) - J^*(u) = -\log \left(\frac{e^{-J(\theta, u)}}{\max_{\theta} \{ e^{-J(\theta, u)} \}} \right) \quad (9)$$

$$= -\log \left(\frac{\mathcal{L}(\theta, u)}{\max_{\theta \in \Theta} \mathcal{L}(\theta, u)} \right) \quad (10)$$

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

PEI criterion

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

$$\text{PEI}(\theta, u) = \mathbb{E}_Y [[f_{\min}(u) - Y(\theta, u)]_+] \quad (11)$$

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