Parameter control in the presence of uncertainties

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Why do we need models ?

The ability to understand is essential in order to forecast, and to take decisions.

- Natural phenomena are often very complex to understand in their entirety
- Mathematical models are simplified versions, which allow to study the relationships between some observed (or not) quantities
- Mathematical models can be used to construct numerical models, which are used for forecasts

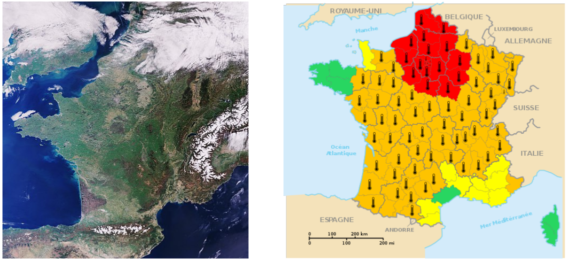
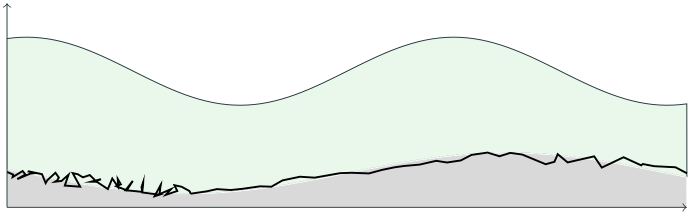


Figure 1: From the reality to predictions

Modelling of the bottom friction

Example: the bottom friction

- Ocean domain discretized
- Bottom of the ocean is not completely smooth
- Energy is dissipated through turbulences because of the asperities
- The water current at the surface is affected
- The friction is taken into account at a cell level



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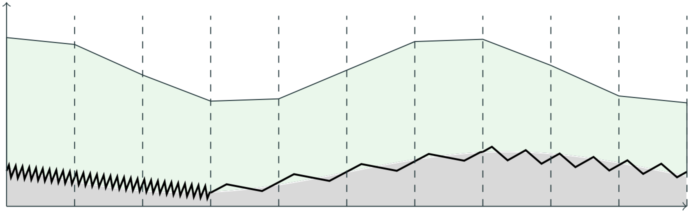
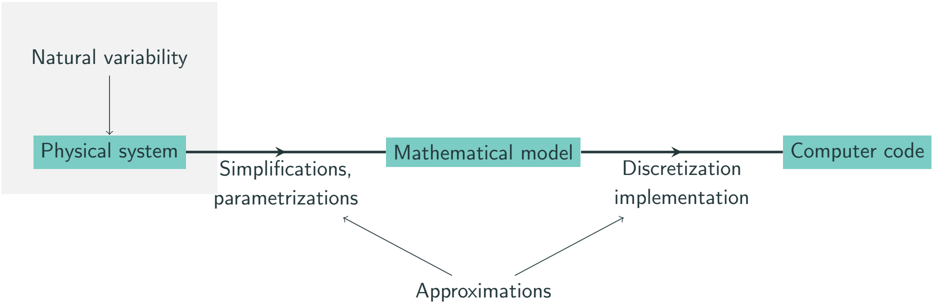


The modelling process

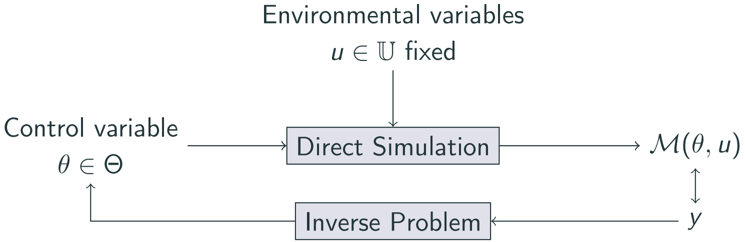


→ How well can we calibrate the model, so that it depicts *accurately* the reality ?

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 y



Data assimilation framework

Let $u \in \mathbb{U}$, assumed fixed and known

Objective function

We define J as the squared difference between the output of the model and the observations

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

$\rightarrow$ the smaller J is, the better the fit is

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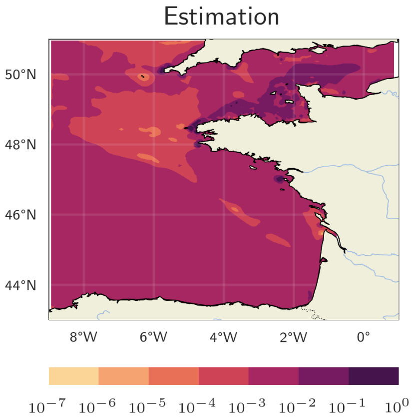
We can get an estimate by solving an optimisation problem:

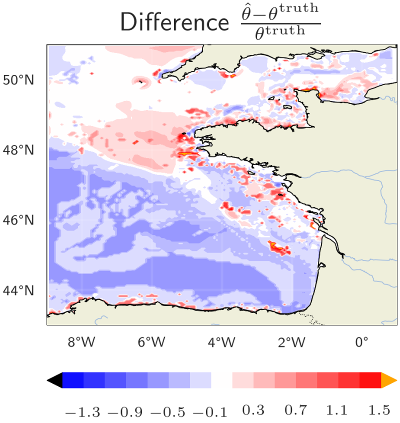
$$\min_{\theta \in \Theta} J(\theta, u) = J(\hat{\theta}, u) \tag{2}$$

- $\hat{\theta}$ depends inherently on u
- What if u is uncertain by nature ?
- Does $\hat{\theta}$ compensate the errors brought by variability? ($\sim$ overfitting)

An example: Misspecification of u

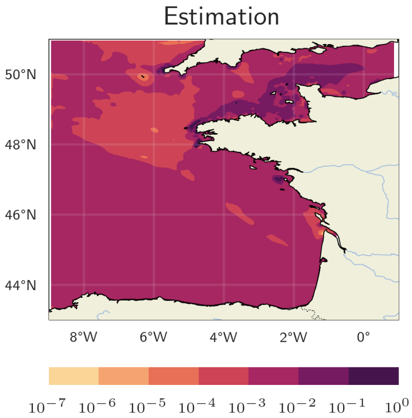
Minimization of $\theta \mapsto J(\theta, u)$, for different u, which parametrizes some boundary conditions:
$u = (0.0, 0.0)$

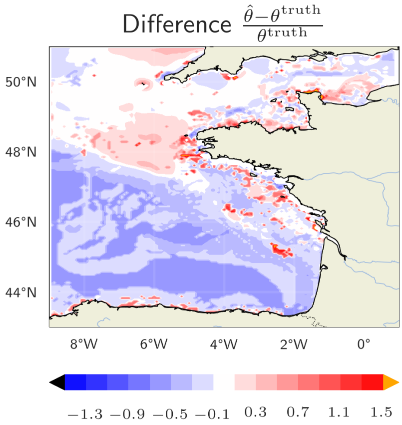




An example: Misspecification of u

Minimization of $\theta \mapsto J(\theta, u)$, for different u, which parametrizes some boundary conditions: $u = (0.0, 0.5)$





An example: Misspecification of u

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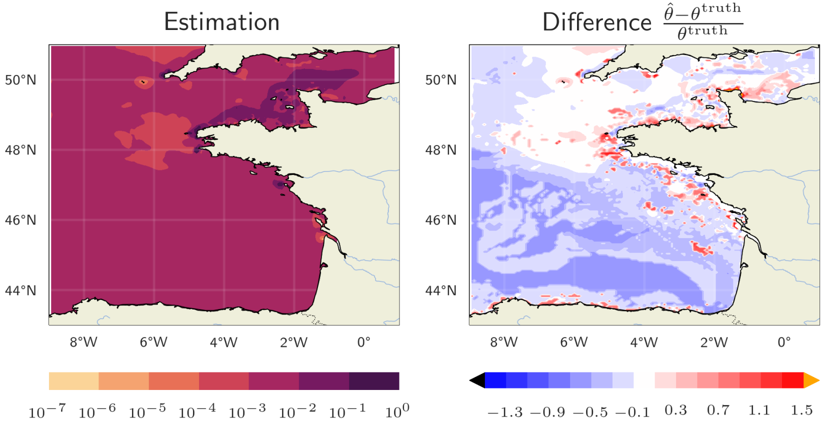
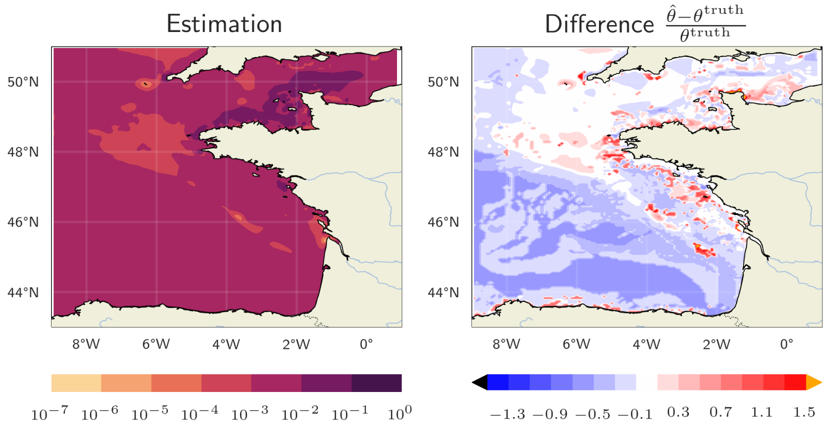
$u = (0.0, 1.0)$



An example: Misspecification of u

Minimization of $\theta \mapsto J(\theta, u)$, for different u, which parametrizes some boundary conditions:
$u = (0.5, 0.0)$



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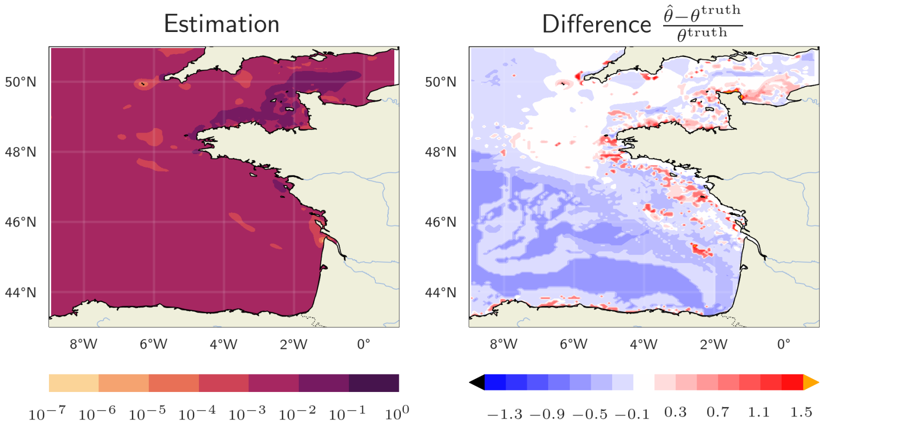

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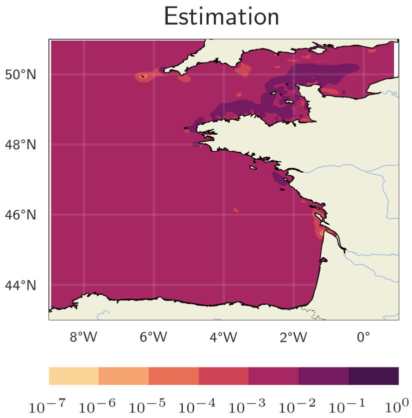

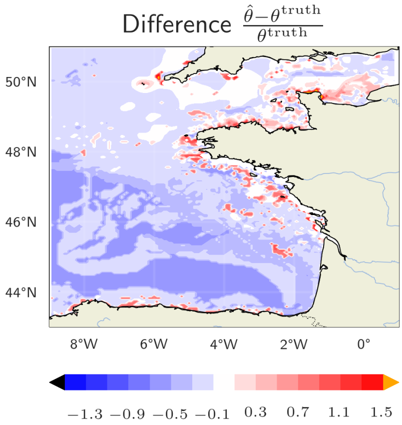

An example: Misspecification of u

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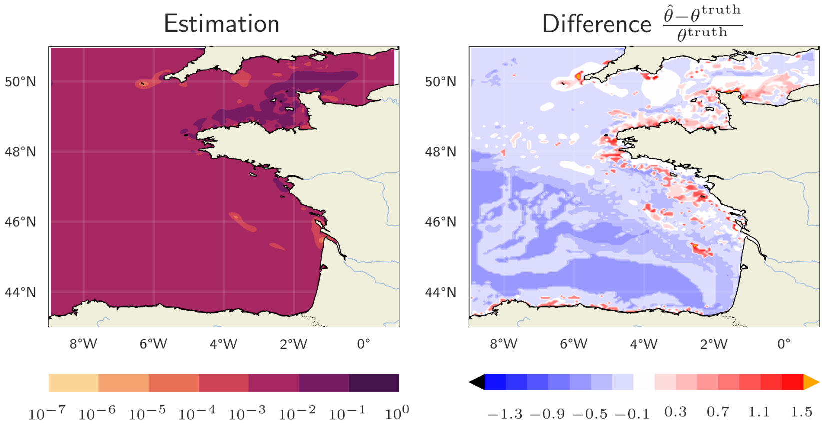

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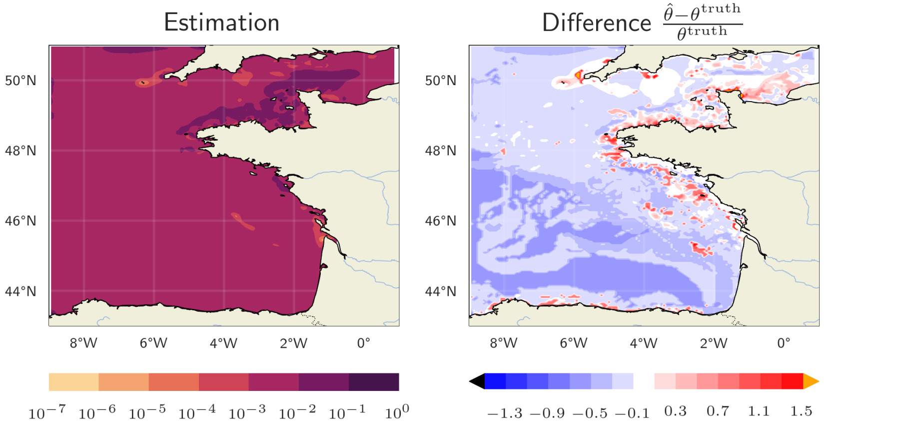

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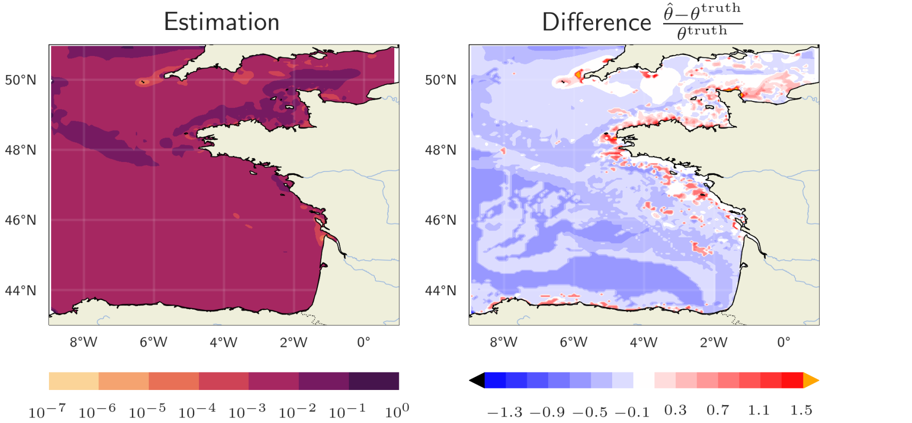


A definition of robustness ?

Robustness

$\hat{\theta}$ can be considered "robust" if $J(\hat{\theta}, u)$ gives "good enough" performances when u varies

Main objectives:

- Define quantitative criteria of robustness
- Develop methods in order to compute robust estimates efficiently
- Apply those methods to the robust calibration of CROCO

Outline

Robustness in calibration

Different types of uncertainties

Epistemic or aleatoric uncertainties? [Walker *et al.* , 2003]

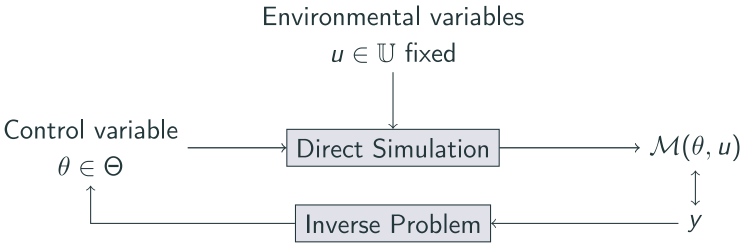
- Epistemic uncertainties: From a lack of knowledge, that can be reduced with more research/exploration
- Aleatoric uncertainties: Inherent variability of the system studied, operating conditions that we cannot afford to research further

- θ: Control parameter, needs to be tuned
- u: Environmental variable: subject to natural variability

Our goal is to take into account the aleatoric uncertainties (=the assumed variability of the environmental conditions) in the estimation of the control parameter (=reduction of the epistemic uncertainties).

Aleatoric uncertainties as a random variable

- U: random variable of known distribution, with support $\mathbb{U}$
- u is a sample of U



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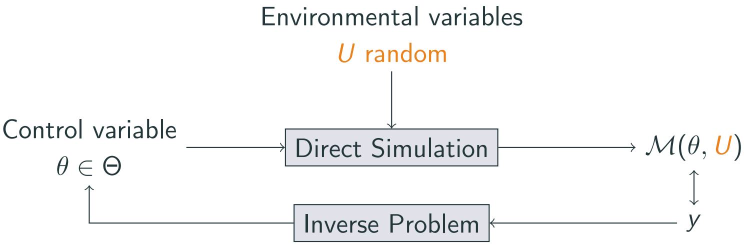

The objective function as a random variable

- The computer code is *still* deterministic, and takes θ and u as inputs (from the user):

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

- Due to the previous assumptions, the quadratic error J is now considered as a random variable, indexed by θ

$$J(\theta, U) = \frac{1}{2}\|\mathcal{M}(\theta, U) - y\|^2$$

Robust objectives of the objective function

We are looking for $\hat{\theta}$, such that $J(\hat{\theta}, U)$ gives "good performances"

- Worst case [Marzat *et al.* , 2013]:

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

- M-robustness [Lehman *et al.* , 2004]:

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

- Multiobjective [Baudoui, 2012]:

$$\text{Pareto frontier of } \left(\mathbb{E}_U \left[J(\theta, U) \right], \mathbb{V}\mathrm{ar}_U \left[J(\theta, U) \right] \right)$$

- Reliability

$$\min_{\theta \in \Theta} Q_U(J(\theta, U); p)$$

- Regret-based estimates

The notion of relative-regret

Given $u \in \mathbb{U}$, how well can we calibrate the model ?

- The best performance is $\min_{\theta \in \Theta} J(\theta, u) = J^*(u)$
- How does $J^*(u)$ compare to $J(\theta, u)$?
- What is the cost of choosing θ instead of $\theta^*(u) = \arg\min_\theta J(\theta, u)$?

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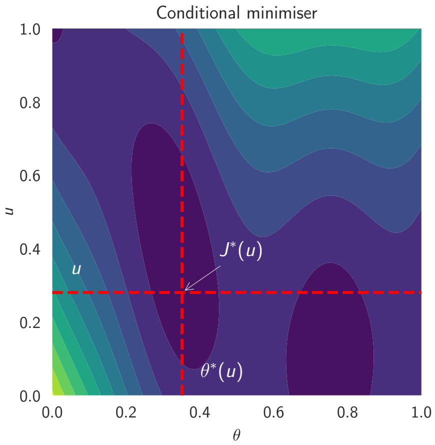
The relative-regret, α-acceptability

- We define the relative-regret as the ratio $\frac{J(\theta,u)}{J^*(u)}$
- (θ, u) said α-acceptable if $\frac{J(\theta,u)}{J^*(u)} \leq \alpha \Rightarrow J(\theta, u) \leq \alpha J^*(u)$

Construction of regions of acceptability

$$J(\theta,u)=\frac{1}{51.95}\left[\left(x_2-\frac{5.1}{4\pi^2}x_1^2+\frac{5}{\pi}x_1-6\right)^2+\left(10-\frac{10}{8\pi}\right)\cos(x_1)-44.81\right]+2,\quad x_1=15\theta-5,\quad x_2=15u$$



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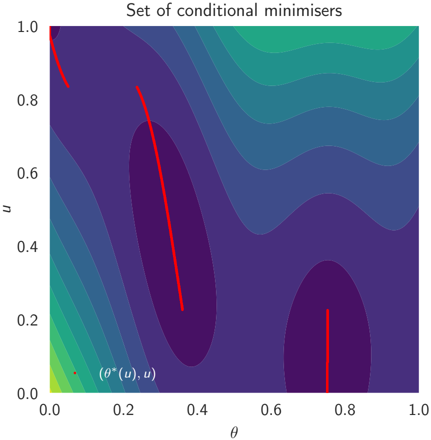

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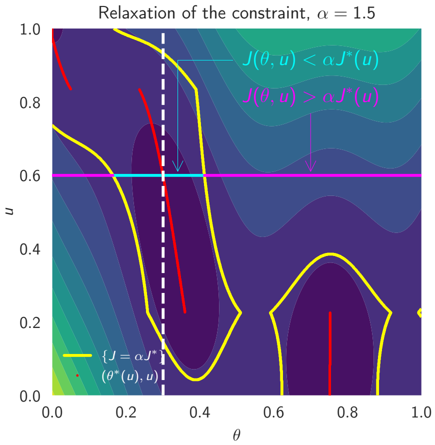

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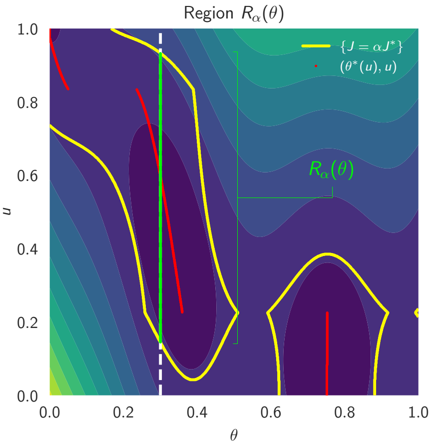

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- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$
- Set $\alpha > 1$
- $R_\alpha(\theta) = \{u \mid J(\theta, u) \leq \alpha J^*(u)\}$
- $\Gamma_\alpha(\theta) = \mathbb{P}_U\left[U \in R_\alpha(\theta)\right]$

Γ_α as a measure of robustness

- probability that θ is close enough to the optimal value
- probability that the relative-regret is less than α

Regret-based estimates

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

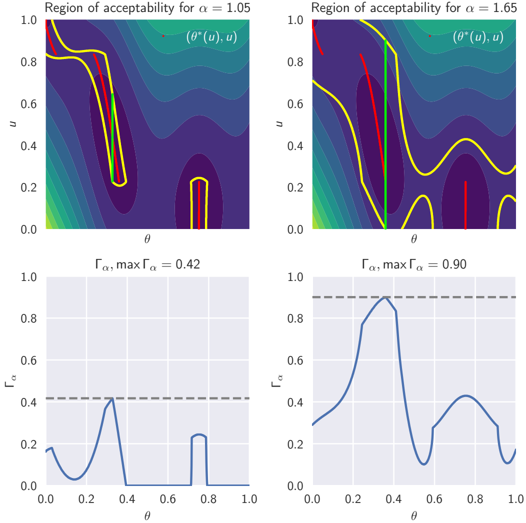
Relative-regret family of estimators [Trappler *et al.* , 2020]

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

- $\hat{\theta}$: calibrated value of the control parameter
- α: range of variation from the optimal value
- $p = \Gamma_\alpha(\hat{\theta})$: probability of being within this range

$\rightarrow$ the relative-regret is bounded by α with probability p

Conservative or optimistic estimate



By acting either on α or on p, we can choose a level of robustness

- α small: Optimistic, good performances but maybe not often
- α large: Conservative, performances controlled with high probability
- Choose p, in order to ensure a certain level of confidence

Relation between α, p as optimisation problems

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

$$\max_{\theta\in\Theta} \Gamma_\alpha(\theta) = \max_{\theta\in\Theta} \mathbb{P}_U\left[J(\theta, U) \leq \alpha J^*(U)\right] \tag{4}$$

$\rightarrow$ Probability maximization

- Set a target probability p, find the smallest α such the probability p is reached

$$\inf\{\alpha \mid \max_{\theta\in\Theta} \Gamma_\alpha(\theta) \geq p\} \tag{5}$$

$\rightarrow$ Quantile minimization

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Adaptive strategies using Gaussian Processes

The computational bottleneck

$$\max_{\theta\in\Theta} \Gamma_\alpha(\theta) = \underbrace{\max_{\theta\in\Theta}}_{\text{expensive}} \overbrace{\mathbb{P}_U}^{\text{expensive}} \left[\underbrace{J(\theta, U)}_{\text{expensive}} \leq \alpha \overbrace{J^*(U)}^{\text{expensive}}\right] \tag{6}$$

In general, getting estimates can be very expensive:

- Estimate statistical quantities ($\mathbb{E}_U$, $\mathbb{P}_U$)
  - $\rightarrow$ Sufficient exploration of $\mathbb{U}$ with respect to $\mathbb{P}_U$ (Monte-Carlo methods, numerical integration)
- Optimize those quantities with respect to $\theta \in \Theta$
  - $\rightarrow$ Focus on regions of interest of Θ
  - $\rightarrow$ Take into account the uncertainty on the estimation

$\Rightarrow$ requires a lot of computational effort (*i.e.* extensive number of calls to J)

How to make the best use of a specific budget of evaluations ?

Surrogates and cost function

Given a set comprising points and their evaluations $\mathcal{X} = \{(x_i, J(x_i))\}_{1 \leq i \leq n}$ (*training set*), we can construct an approximation of the expensive function J

$\rightarrow$ Polynomial interpolation, Gaussian Process Regression (Kriging), Polynomial Chaos Expansion

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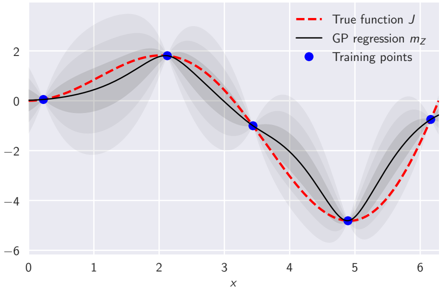
- It replaces the expensive original function J by a computationally cheap surrogate ($\sim$ plug-in approach)
- It can be adapted for sequential strategies

Let $x = (\theta, u) \in \Theta \times \mathbb{U} = \mathbb{X}$, $J(x) = J(\theta, u)$
$\mathcal{X} = \{(x_i, J(x_i))\}_{1 \leq i \leq N}$ initial design of experiments ($\sim$ training points)

GP regression [Matheron, 1962; Krige, 1951]

$Z \sim \mathrm{GP}(m_Z, C_Z)$ is the GP constructed on $\mathcal{X}$ with $m_Z : \mathbb{X} \to \mathbb{R}$ and $C_Z : \mathbb{X}^2 \to \mathbb{R}$

- m_Z: GP (or kriging) regression
- C_Z: covariance function
- $\sigma_Z^2 : x \mapsto C_Z(x, x)$ variance function
- $Z(x) \sim \mathcal{N}\left(m_Z(x), \sigma_Z^2(x)\right)$



Gaussian Process Regression

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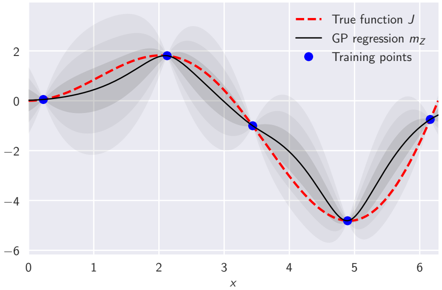

$\to$ m_Z is an approximation of J

$\to$ Information on prediction error with σ_Z^2

Adaptive strategies

$Z \sim \mathrm{GP}(m_Z, C_Z)$ constructed using $\mathcal{X}_n = \{(x_i, J(x_i))\}_{1 \leq i \leq n}$

As a surrogate, m_Z is a cheap alternative to J in order to compute Γ_α,

- still an approximation based on $\mathcal{X}_n$
- is it accurate enough for this purpose ?

Adaptive methods: enrichment of the design

- Choosing iteratively the most relevant point(s) to add to the design
- ... until the budget of evaluations runs out

$\Rightarrow$ Definition of a criterion κ, that measures the relevancy

$\Rightarrow$ How to exploit such criterion ?

Objectives of adaptive strategies

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

- m_Z should be a good approximation of J
- m_Z should be strictly positive
- Good approximation of J^* ?

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- Enrich the design for the estimation of J^* and ensure positivity as well
  $\rightarrow$ PEI criterion
- Improve the estimation of $J - \alpha J^*$ globally
  $\rightarrow$ Reduction of the IMSE using a 1-step criterion
- Improve the estimation of the set $\{J - \alpha J^* \leq 0\}$
  $\rightarrow$ AK-MCS: enrichment using batches of points

1-step criteria

Let κ be such a criterion measuring the relevancy of points:

- κ is constructed using the properties of the GP
- $\kappa(x)$ measures how *interesting* would be the evaluation of x

Selection of the next point and update of the design

Given a GP Z, constructed using $\mathcal{X}_n = \{(x_i, J(x_i))\}_{1 \leq i \leq n}$

$$x_{n+1} = \arg\max_{x \in \mathbb{X}} \kappa(x) = \arg\max_{x \in \mathbb{X}} \kappa(x; Z; \mathcal{X}_n) \tag{7}$$

$$\mathcal{X}_{n+1} = \mathcal{X}_n \cup \{(x_{n+1}, J(x_{n+1}))\} \tag{8}$$

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Different criteria caters to different objectives

- Optimization: PI, EGO [Jones *et al.* , 1998; Hernández-Lobato *et al.* , 2014]
- Exploration: prediction variance, aIMSE
- Contour/levelsets estimation: reliability index [Bect *et al.* , 2012; Picheny *et al.* , 2010]

Estimation of $\theta^*(u)$, $J^*(u)$ with the PEI

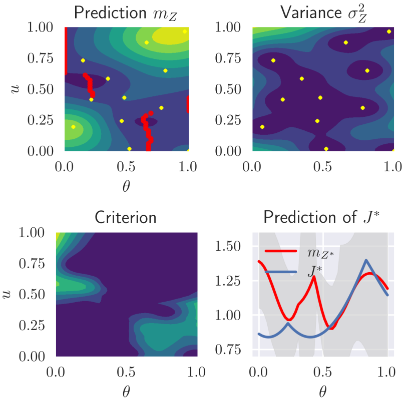
$$\Gamma_\alpha(\theta) = \mathbb{P}_U\left[J(\theta, U) \leq \alpha J^*(U)\right]$$

$\rightarrow$ Need to have a good approximation of the conditional minimum and minimisers:
$m_{Z^*}(u) = \min_\theta m_Z(\theta, u)$, and $\theta^*_Z(u) = \arg\min_\theta m_Z(\theta, u)$

PEI [Ginsbourger *et al.* , 2014]

Profile Expected Improvement:
$\kappa(\theta, u) = \mathbb{E}_{Z(\theta,u)}\left[(f_{\min}(u) - Z(\theta, u))_+\right]$ and close form available due to the GP properties of Z

Design enriched iteratively using the PEI criterion, one point at a time:
m_{Z^*} becomes a more accurate approximation of J^*



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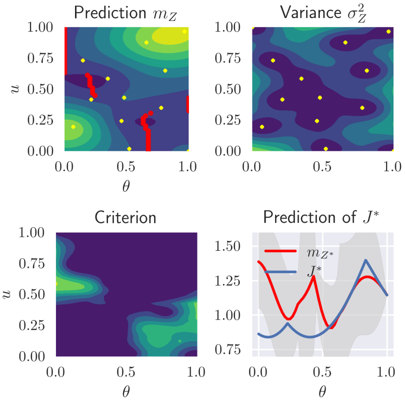

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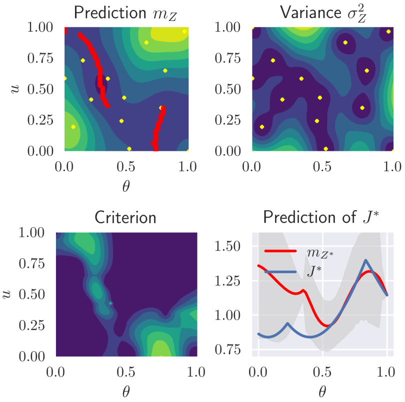

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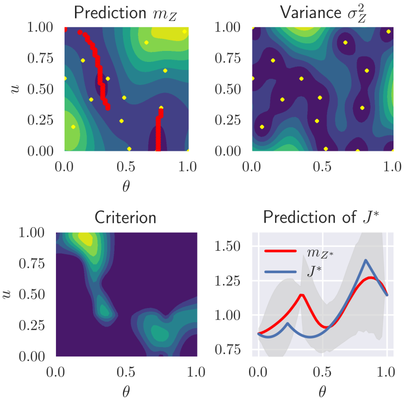

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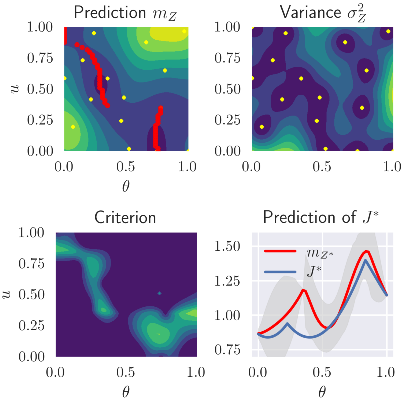

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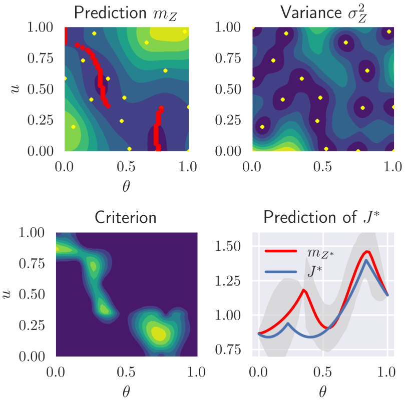

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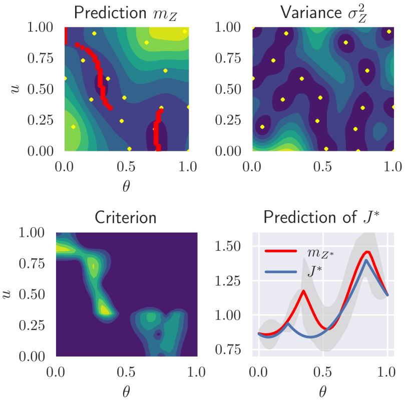

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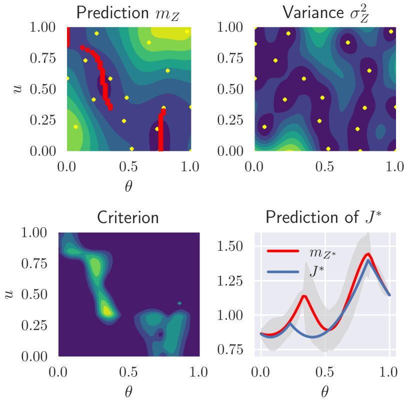

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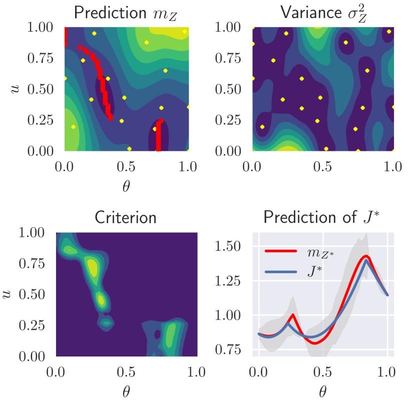

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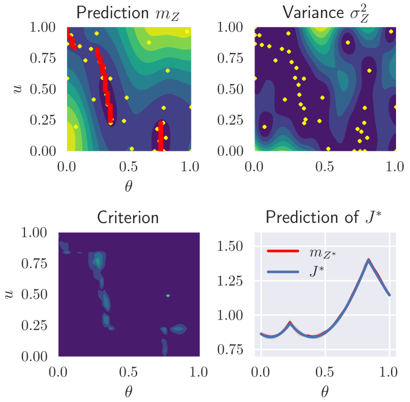

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GP formulation

- $\Delta_\alpha = Z - \alpha Z^*$ is a GP

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Improving the plug-in estimation of Δ_α

$\rightarrow$ We want to define a criterion κ in order to reduce the global uncertainty

Integrated Mean Square Error

Uncertainty associated with the GP Δ_α using the design $\mathcal{X}_n$

$$\mathrm{IMSE}(\mathcal{X}_n) = \int_{\mathbb{X}} \sigma^2_{\Delta_\alpha}(x)\,\mathrm{d}x \tag{11}$$

After having chosen *and evaluated* the next point x_+, we want the IMSE to be as small as possible

$$\min_{x_+} \overbrace{\mathrm{IMSE}\left(\mathcal{X}_n \cup \{(x_+, \underbrace{J(x_+)}_{\text{unknown}})\}\right)}^{\kappa} \tag{12}$$

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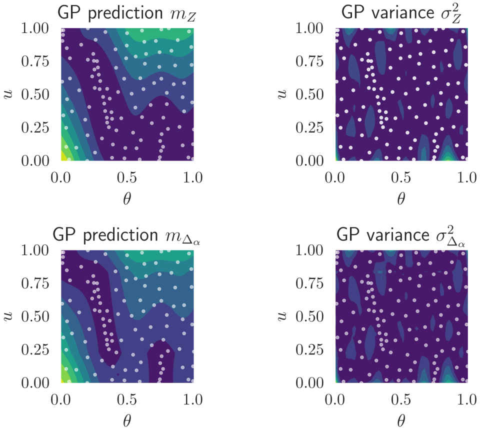
x_{n+1} presents the smallest IMSE on average once evaluated

Numerical illustration for Δ_α



$\rightarrow$ Explore the whole input space $\mathbb{X} = \Theta \times \mathbb{U}$, but intensification also near the conditional minimisers

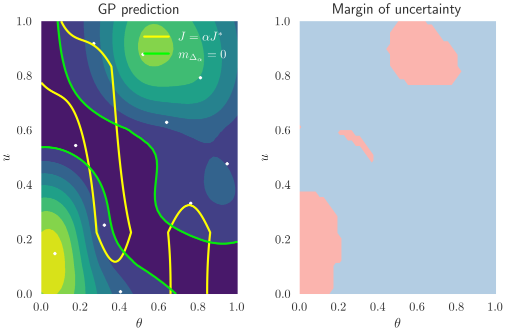
Sampling-based methods: AK-MCS

Given $\mathbb{M} \subset \mathbb{X}$, margin of uncertainty

Selection of a batch of K points and update of the design

Example: estimation of the set $\{\Delta_\alpha < 0\}$:

$$g(x) = \begin{cases} 1 \text{ if } x \in \mathbb{M} \\ 0 \text{ elsewhere} \end{cases}$$



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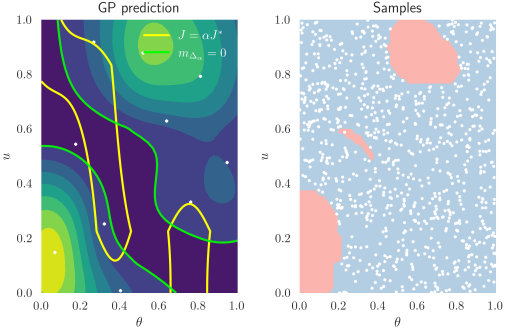

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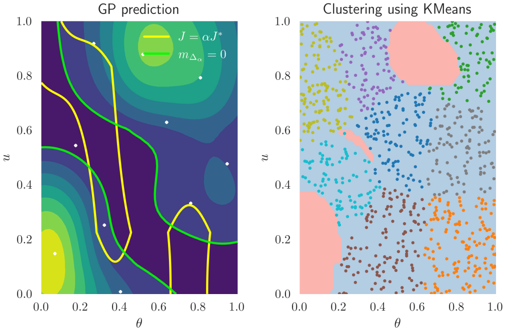

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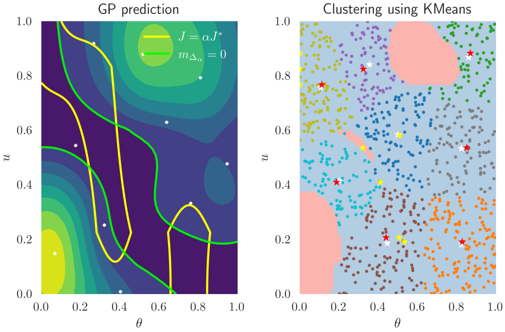

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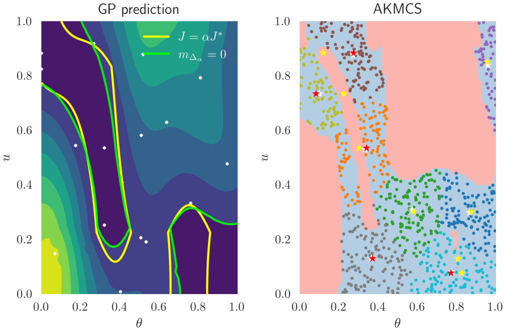

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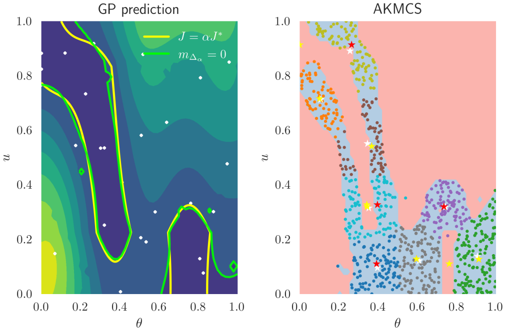

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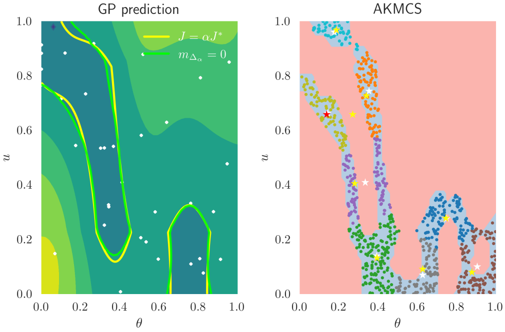

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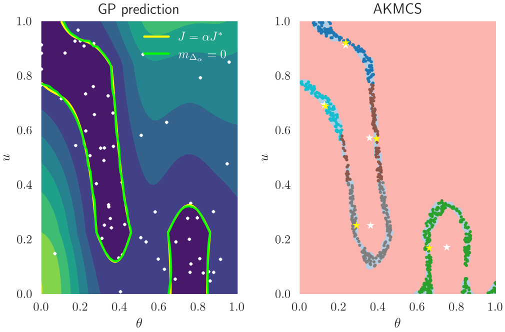


Computations using Δ_α or Ξ

Recalling that $\Gamma_\alpha(\theta) = \mathbb{P}_U\left[J(\theta, U) - \alpha J^*(U) \leq 0\right] = \mathbb{P}_U\left[\frac{J(\theta,U)}{J^*(U)} \leq \alpha\right]$

Plug-in and sample average approximation

- J is replaced by m_Z
- $J - \alpha J^*$ is replaced by $m_{\Delta_\alpha} \to \alpha$ fixed, estimation of probability
- $\frac{J}{J^*}$ is replaced by $m_\Xi \to p$ fixed, estimation of quantile

$$\begin{aligned} \Gamma_\alpha(\theta) &\approx \mathbb{P}_U\left[m_{\Delta_\alpha}(\theta, U) \leq 0\right] && (13) \\ &\approx \mathbb{P}_U\left[m_\Xi(\theta, U) \leq \log \alpha\right] && (14) \end{aligned}$$

Outer probability approximated using Monte-Carlo since m_{Δ_α} and m_Ξ are cheaper to evaluate than J

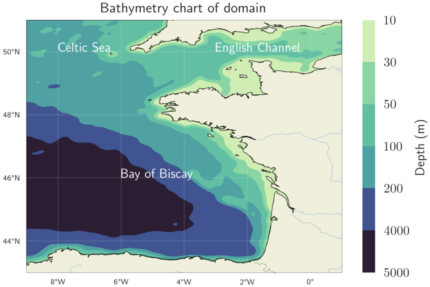
Robust calibration of CROCO

The numerical model CROCO

Coastal and **R**egional **O**cean **CO**mmunity model

- Solves the Shallow Water equations
- Grid resolution of $1/14^{\circ}$ (5.5 km)
- 15 684 cells located in the ocean

$\rightarrow$ Academic toy problem



The Shallow water equations

ζ sea-water height, $\mathbf{v}$ velocity vector

$$\mathcal{M}: \begin{cases} \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{x} \cdot \nabla)\mathbf{v} + 2\boldsymbol{\Omega} \wedge \mathbf{v} & = & -g\nabla H + \frac{\boldsymbol{\tau}_b}{\rho H} + F \\ \frac{\partial \zeta}{\partial t} + \nabla(H \cdot \mathbf{v}) & = & 0 \\ \zeta & = & \mathrm{BC}(u) \text{ at the boundary} \end{cases} \tag{15}$$

- $\boldsymbol{\tau}_b = \boldsymbol{\tau}_b(\theta)$: bottom shear stress $\rightarrow$ depends on the control parameter θ
- $\mathrm{BC}(u)$: tidal boundary conditions $\rightarrow$ depends on the environmental variable u

Model and objective function

- Output of the model: $\mathcal{M}(\theta, u) = (\zeta_{i,t}(\theta, u))_{\substack{1 \leq i \leq N_{\mathbf{Mesh}} \\ 1 \leq t \leq N_{\mathbf{time}}}}$
- Observations: $y = \mathcal{M}(\theta^{\mathrm{truth}}, u^{\mathrm{truth}})$, truth values defined later
- Objective function: $J(\theta, u) = \|\mathcal{M}(\theta, u) - y\|^2 = \sum_{i,t}(\zeta_{i,t}(\theta, u) - y_{i,t})^2$

Modelling of the bottom friction

Quadratic friction coefficient

Let $\boldsymbol{\tau}_b$ be the shear stress at the bottom, and v_b the velocity vector at the bottom

$$\boldsymbol{\tau}_b = -C_d \|v_b\| v_b, \quad \text{with} \quad C_d = \left(\frac{\kappa}{\log\left(\frac{H}{z_b}\right) - 1} \right)^2 \tag{16}$$

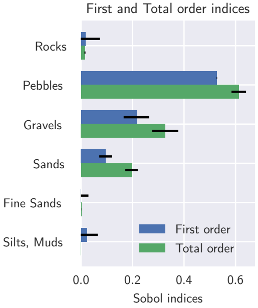
and we define the control parameter as $\theta = \log z_b$

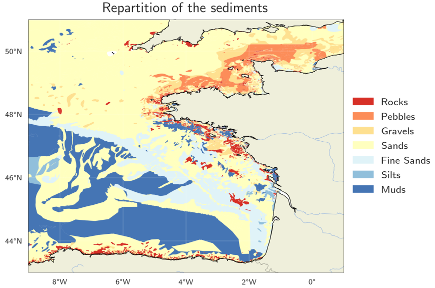
- We assume that the friction is uniform and constant for each of the sediment type
- The effect on the water circulation (through $\boldsymbol{\tau}_b$) depends also on the water height H
- θ^{truth}: one specific value for each sediment type

Due to the water height, influence of each sediment type is not the same $\Rightarrow$ Sensitivity analysis

Sensitivity analysis on the friction associated with the sediments

Global Sensitivity Analysis with Sobol' indices [Sobol, 2001, 1993]: quantify the influence of each input variable on J





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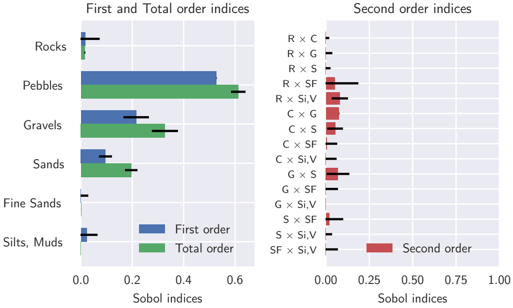
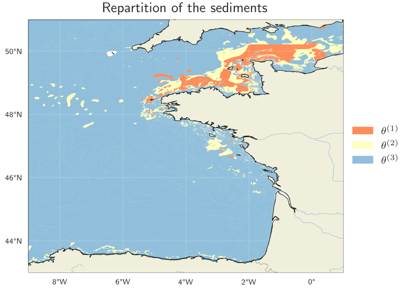




The control variable is then $\theta = (\theta^{(1)}, \theta^{(2)}, \theta^{(3)}) \in \Theta$

- $\theta^{(1)}$: Pebbles
- $\theta^{(2)}$: Gravels
- $\theta^{(3)}$: Other sediments (in deeper water)

Control parameter and environmental variable

- Aleatoric uncertainty on boundary conditions
- u parametrizes an error on the amplitude of the M_2 and S_2 tide components.
- We assume that $U \sim \mathcal{U}(\mathbb{U})$, with $\mathbb{U} = [0, 1]^2$

Recap of the problem

- $\theta = (\theta^{(1)}, \theta^{(2)}, \theta^{(3)}) \in \Theta \subset \mathbb{R}^3$
- $u \in \mathbb{U} = [0, 1]^2$
- $U \sim \mathcal{U}(\mathbb{U})$

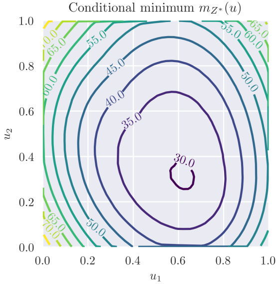
- $\theta^{\text{truth}} \in \mathbb{R}^6 \neq \Theta$
- $u^{\text{truth}} = (0.5, 0.5)$
- $y = \mathcal{M}(\theta^{\text{truth}}, u^{\text{truth}})$
- $J(\theta, u) = \|\mathcal{M}(\theta, u) - y\|^2$

Initial design, preliminary analysis

- Initial design evaluated $\mathcal{X}_{\mathrm{LHS}} = \{(x_i, J(x_i))\}_{1\leq i\leq n}$, LHS on $\Theta \times \mathbb{U}$
- $J^* > 0$ by definition, but m_{Z^*} ?

Initial design, preliminary analysis

- Initial design evaluated $\mathcal{X}_{\mathrm{LHS}} = \{(x_i, J(x_i))\}_{1\leq i \leq n}$, LHS on $\Theta \times \mathbb{U}$
- $J^* > 0$ by definition, but m_{Z^*} ?
    - Improve first m_{Z^*} using PEI criterion to ensure $m_{Z^*} > 0$



Global minimum not attained at the truth value of the environmental parameter

$\rightarrow$ Compensation of errors due to the dimension reduction

Robust calibration

With this preliminary analysis, we can choose α

- we set $\alpha = 1.3$: with which probability can we stay within 30% of the optimal value ?
- we enrich the design by looking to reduce globally the IMSE using κ

	$\theta^{(1)}$	$\theta^{(2)}$	$\theta^{(3)}$	
$\hat{\theta}_\alpha$, $\alpha = 1.3$	-3.43	-5.20	-6.48	$\Gamma_\alpha(\hat{\theta}_\alpha) = 0.93$
$\hat{\theta}_{\text{global}}$	-3.516	-5.078	-6.346	
θ^{truth}	-3.689	-4.962	n.a.	

In this case:

- $\hat{\theta}_\alpha^{(1)} > \hat{\theta}_{\text{global}}^{(1)} > \theta^{\text{truth},(1)}$
- $\hat{\theta}_\alpha^{(2)} < \hat{\theta}_{\text{global}}^{(2)} < \theta^{\text{truth},(2)}$
- $\hat{\theta}_\alpha^{(3)} < \hat{\theta}_{\text{global}}^{(3)}$

Computational overview

- Total of 500 runs of the numerical model
  - 100 for the initial LHS
  - 200 with the PEI criterion
  - 200 for the reduction of the IMSE
- Each iteration for the reduction of the IMSE requires
  - Evaluation of an integral of dimension $1 + \dim(\Theta \times \mathbb{U})$
  - Optimization of this integral in a space of dimension $\dim \Theta$

  $\rightarrow$ Dependent on the ability to compute m_{Z^*}, m_{Δ_α}, $\sigma^2_{\Delta_\alpha}$

  $\rightarrow$ As is, limits severely the possibility of increased dimension
- For sampling-based methods:
  - Size of margin of uncertainty decreases

  $\rightarrow$ Sampling becomes increasingly difficult

Conclusion

Conclusion: overview

Notion of robustness

- Notion of robustness is context dependent
- Relative-regret estimates control the deviation from the *optimal value*
- α can reflect risk-adverse or risk-seeking preferences

Adaptive methods for computations

- GP used as tools for plug-in estimation
- Allow to derive sequential strategies for enrichment of the design
- Can be adapted for batch evaluations

Conclusion: perspectives

Computational improvements

- Dimension of the input space $\Theta \times \mathbb{U}$ can be limiting
  - $\rightarrow$ Reduction of the input space required
- Adaptive methods still require expensive or difficult tasks (optimization, sampling, integration)
  - $\rightarrow$ 2-stages methods
  - $\rightarrow$ Focus computational effort for optimization

Perspectives

- Study of CROCO with a more complex configuration
- Study and compare robust estimates in predictions
- Discrepancy between $J^*(U)$ and $J(\hat{\theta}, U)$ in terms of r.v.
- Include gradient information in the procedures ?

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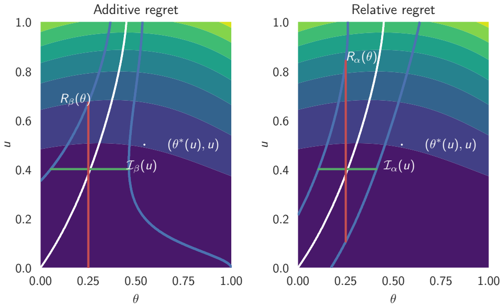
Relative or additive regret



- 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

Modelling of $J(\theta, u) - \alpha J^*(u)$ using Δ_α

Let $Z \sim \mathrm{GP}\left(m_Z; C_Z\right)$ on $\Theta \times \mathbb{U}$, constructed using $\{(\theta_i, u_i), J(\theta_i, u_i))\}$

We define $Z^*(u) = Z(\theta_Z^*(u), u)$, with $\theta_Z^*(u) = \min_\theta m_Z(\theta, u)$, and $\Delta_\alpha = Z - \alpha Z^*$:

The GP Δ_α

As a linear combination of GP, Δ_α is a GP as well:

$$\Delta_\alpha \sim \mathrm{GP}\left(m_{\Delta_\alpha}; C_{\Delta_\alpha}\right) \tag{17}$$

$$m_{\Delta_\alpha}(\theta, u) = m_Z(\theta, u) - \alpha m_Z^*(u) \tag{18}$$

$$\sigma^2_{\Delta_\alpha}(\theta, u) = \sigma^2_Z(\theta, u) + \alpha^2 \sigma^2_{Z^*}(u) - 2\alpha C_Z\left((\theta, u), (\theta_Z^*(u), u)\right) \tag{19}$$

Approximation of the ratio

Let us assume that $Z^* > 0$ with high enough probability: $\Xi(\theta, u) = \log \frac{Z(\theta,u)}{Z^*(u)}$ is approximately normal

Log-normal approximation of the ratio of GP

$$\Xi(\theta, u) \sim \mathcal{N}\left(m_\Xi(\theta, u), \sigma^2_\Xi(\theta, u)\right) \tag{20}$$

$$m_\Xi(\theta, u) = \log \frac{m_Z(\theta, u)}{m^*_Z(u)} \tag{21}$$

$$\sigma^2_\Xi(\theta, u) = \frac{\sigma^2_Z(\theta, u)}{m_Z(\theta, u)^2} + \frac{\sigma^2_{Z^*}(u)}{m_{Z^*}(u)^2} - 2\frac{\mathrm{Cov}[Z(\theta, u), Z^*(u)]}{m_Z(\theta, u)m_{Z^*}(u)} \tag{22}$$

Objective-oriented exploration: 2-stage methods

Instead of reducing *globally* the uncertainty, we can look directly to optimize Γ_α

- Select a candidate $\tilde{\theta}$ with "high potential" to optimize Γ_α
- Find the point x_{n+1} which reduces the most a measure of uncertainty on $\{\tilde{\theta}\} \times \mathbb{U}$

IMSE given a candidate $\tilde{\theta}$

$$\mathrm{IMSE}(\mathcal{X}_n; \tilde{\theta}) = \int_{\{\tilde{\theta}\} \times \mathbb{U}} \sigma_\Phi^2(x)\,\mathrm{d}x \tag{23}$$

$x_{n+1} = (\theta_{n+1}, u_{n+1})$ presents the smallest IMSE (given $\tilde{\theta}$) on average once evaluated.

$\tilde{\theta} \neq \theta_{n+1}$ in general