Parameter control in the presence of uncertainties

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Why do we need models ?

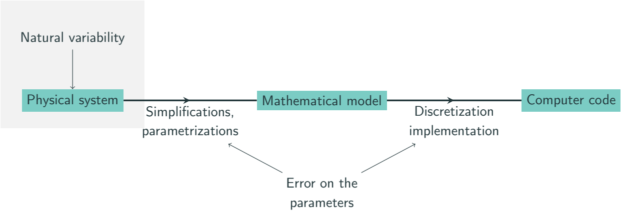
The ability to understand is essential in order to forecast, and to take decisions.

- Natural phenomenon 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
- The mathematical models can be used to construct numerical models, which are used for forecasts

Parametrization

A lot of choices are required to construct models, which depends on the scale we wish to represent

- Physical parameters, which represent some physical properties that influence the model.
- Additional parameters, introduced for numerical reasons



Uncertainties in the modelling

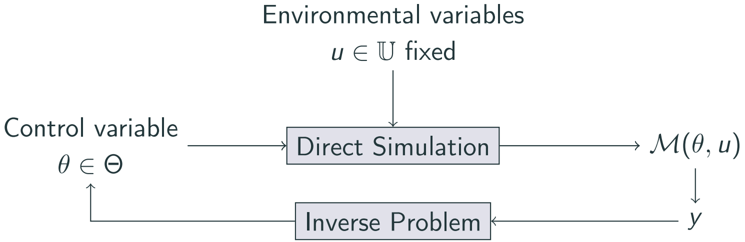
A fine tuning needed

$\rightarrow$ How well does the simulation using a set of parameters match the observations ?

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 $u \in \mathbb{U}$. By defining a notion of distance between $\mathcal{M}(\theta, u)$ and y:

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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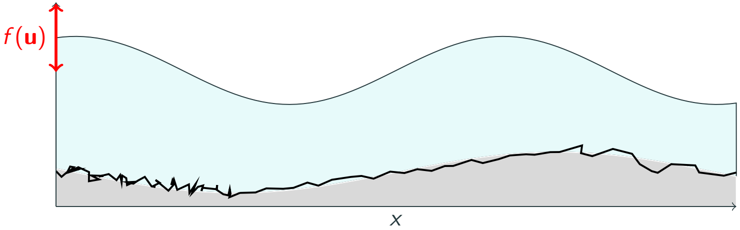
We can get an estimate by solving

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

- $\hat{\theta}$ depends inherently on u
- What if u does not reflect accurately the observations?
- Does $\hat{\theta}$ then 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



Outline

Introduction

Robustness in calibration

Adaptive strategies using Gaussian Processes

Calibration of a numerical model: Application to CROCO

Conclusion

Different types of uncertainties

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

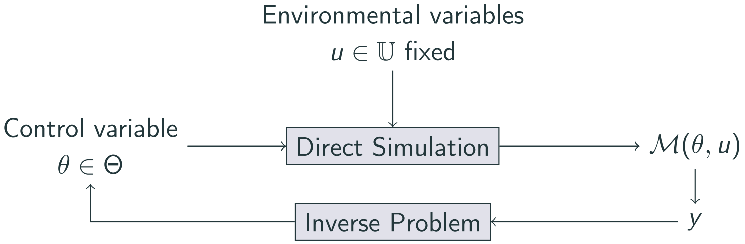
- Epistemic uncertainties: From a lack of knowledge, that can be reduced with more research/exploration
- Aleatoric uncertainties: From the inherent variability of the system studied, operating conditions

$\rightarrow$ 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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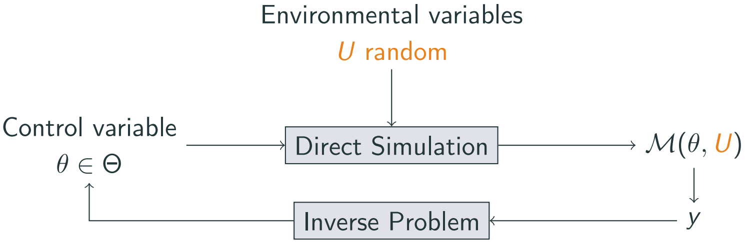

The cost function as a random variable

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

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

- The deterministic quadratic error is now

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

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

Misspecification of u: twin experiment setup

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

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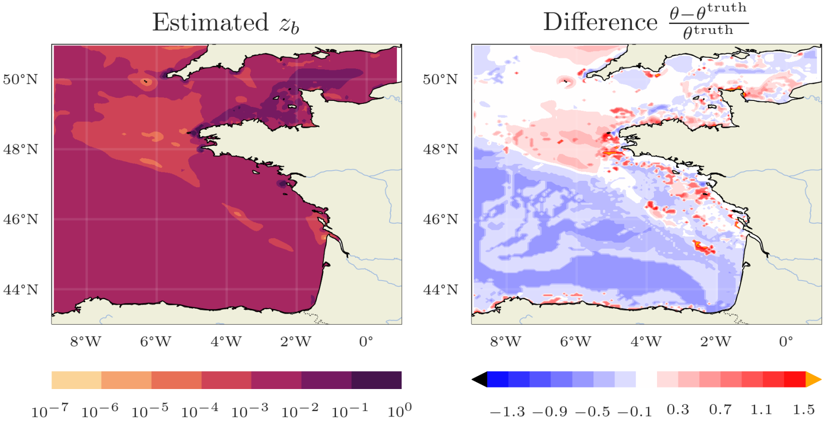

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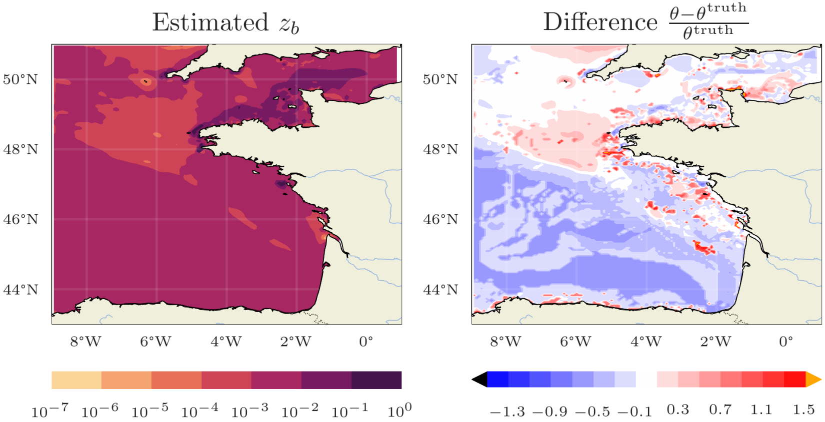

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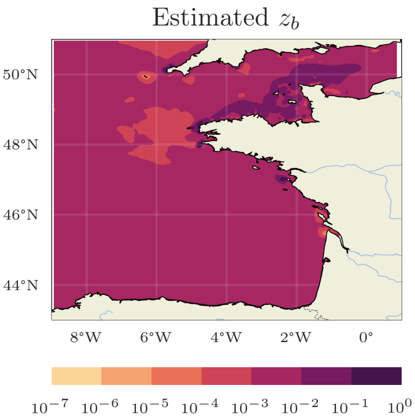

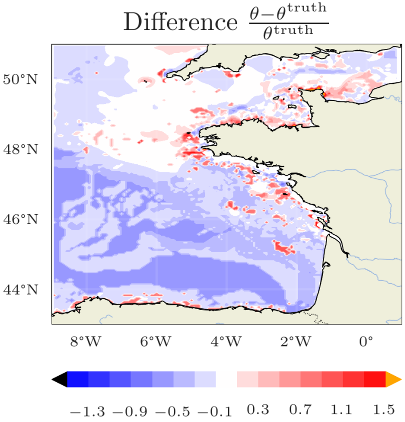

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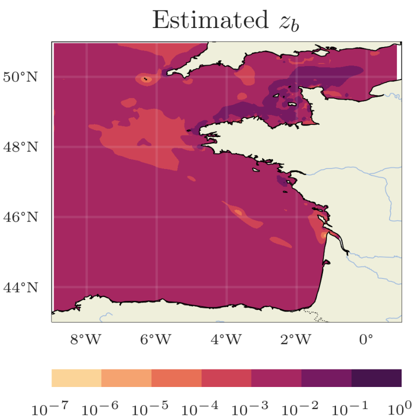

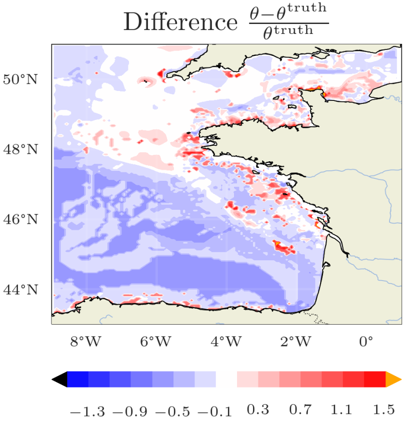

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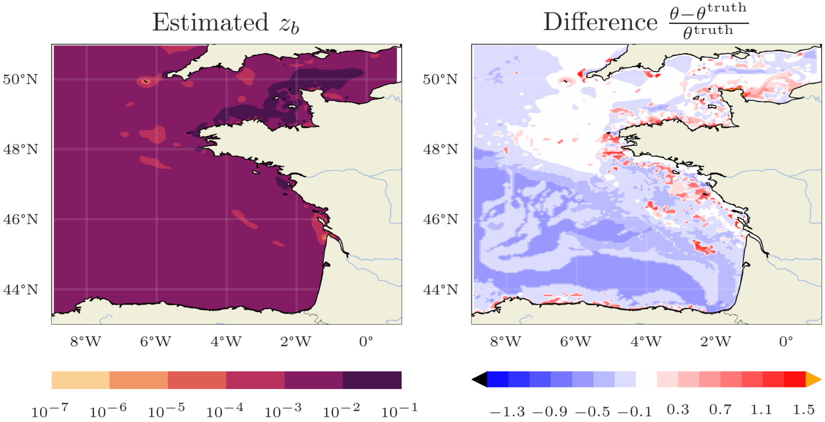

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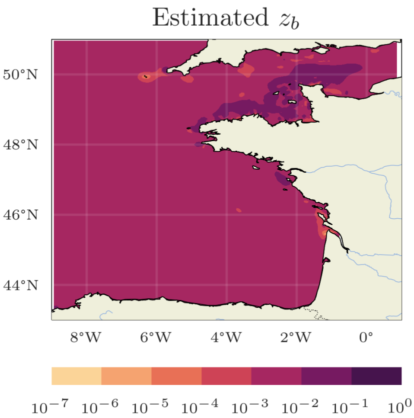

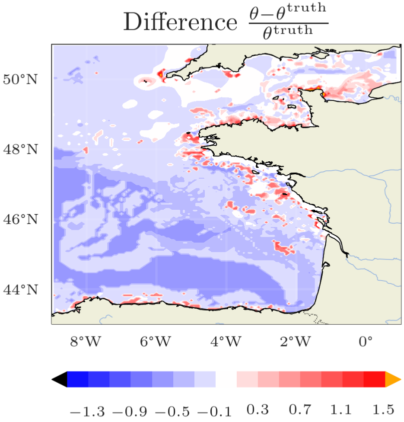

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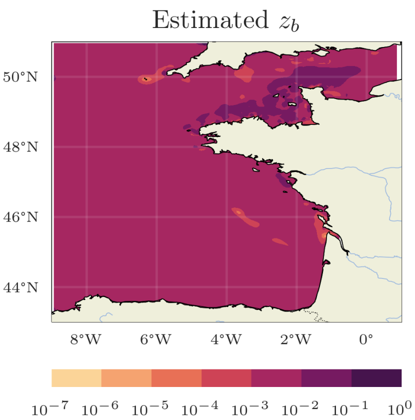

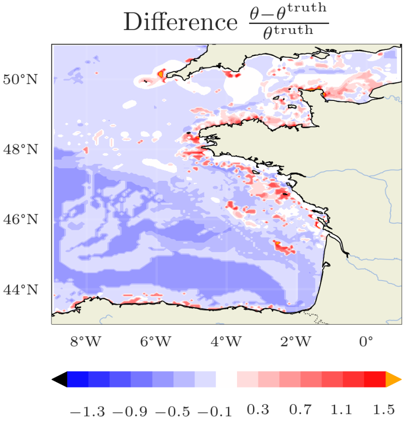

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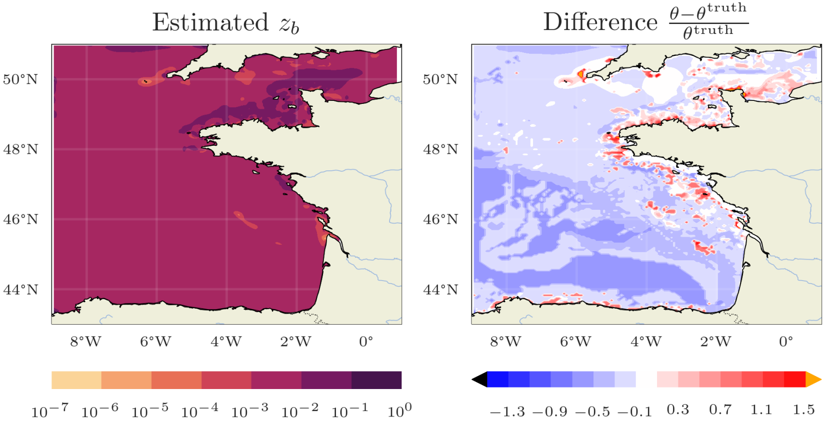

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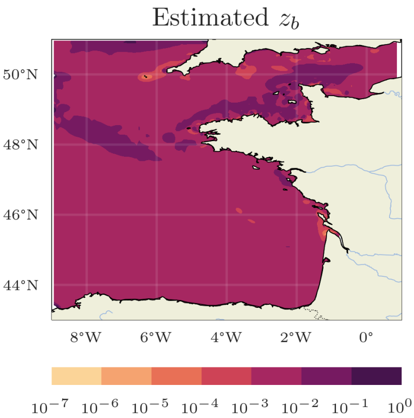

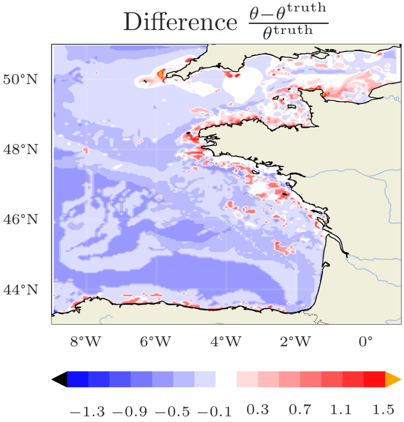

Robustness and estimation of parameters

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

Robustness in calibration

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Robust objectives of the objective function

- 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]:

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

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

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

- Multiobjective [Baudoui, 2012]:

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:

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

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

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

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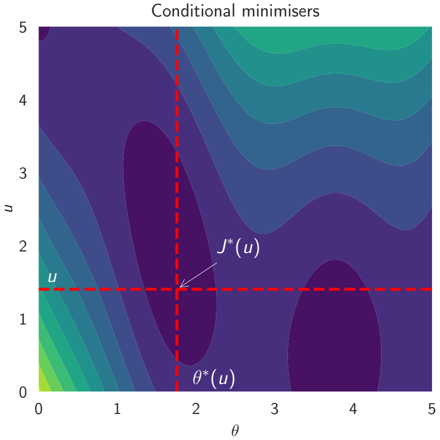
How to take into account values not optimal, but not too far either $\longrightarrow$ relaxation of the equality with $\alpha > 1$:

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

Trappler *et al.* [2020]

Construction of regions of acceptability



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

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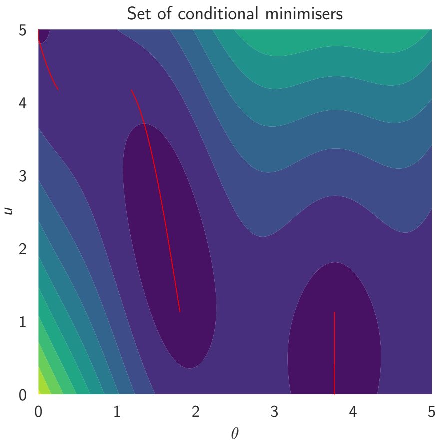

- Sample $u \sim U$, and solve $\theta^*(u) = \arg\min_{\theta \in \Theta} J(\theta, u)$
- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$

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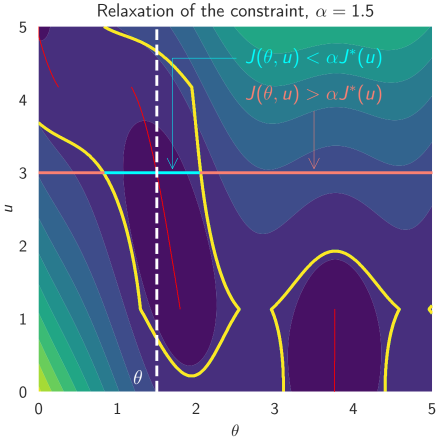

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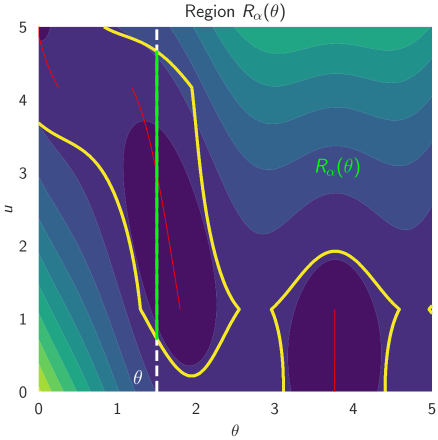

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- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$
- Set $\alpha \geq 1$
- $R_\alpha(\theta) = \{u \mid J(\theta, u) \leq \alpha J^*(u)\}$
- $\Gamma_\alpha(\theta) = \mathbb{P}_U\left[U \in R_\alpha(\theta)\right]$

Regret-based estimates

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

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

$$\max_{\theta\in\Theta} \Gamma_\alpha(\theta) = \max_{\theta\in\Theta} \mathbb{P}_U \left[J(\theta, U) \leq \alpha J^*(U)\right] \tag{3}$$

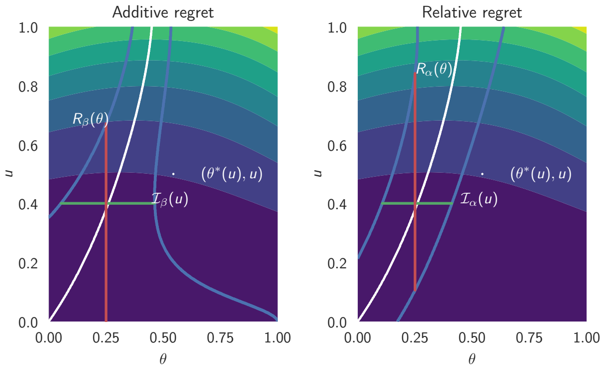
- Set a target probability $1-\eta$, and find the smallest α.

$$\inf\{\alpha \mid \max_{\theta\in\Theta} \Gamma_\alpha(\theta) \geq 1-\eta\} \tag{4}$$

Relative-regret family of estimators

$$\left\{\hat{\theta} \mid \hat{\theta} = \operatorname*{arg\,max}_{\theta\in\Theta} \Gamma_\alpha(\theta), \alpha > 1\right\} \tag{5}$$

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

Adaptive strategies using Gaussian Processes

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The computational bottleneck

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 of integrals)
- 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

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

Surrogates and cost function

- Replace expensive model by a computationally cheap metamodel ($\sim$ plug-in approach)
- Adapted sequential procedures e.g. EGO

$\rightarrow$ Kriging (Gaussian Process Regression)

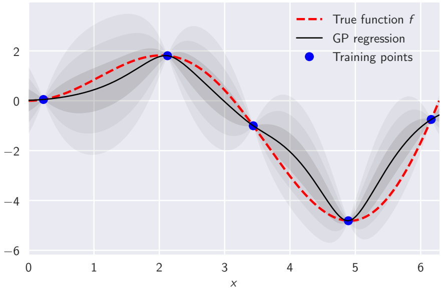
Gaussian Process Modelling

Let $x = (\theta, u) \in \Theta \times \mathbb{U} = \mathbb{X}$,
$f(x) = f((\theta, u)) = J(\theta, u)$
$\mathcal{X} = \{(x_i, f(x_i))\}_{1 \leq i \leq N}$ 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
- $Z(x) \sim \mathcal{N}\left(m_Z(x), \sigma_Z^2(x)\right)$



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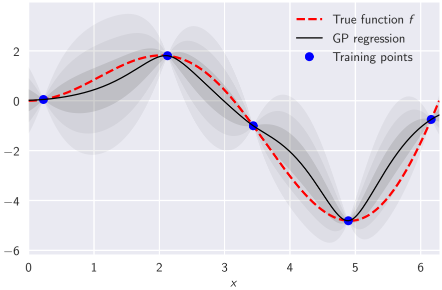


$\rightarrow$ Information on J using m_Z

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

Adaptive strategies

Adding and evaluating points to the design iteratively, with respect to some particular objective

- Explore the input space
- Optimize the unknown function f
- Level-sets or excursion sets: $\{x \in \mathbb{X} \mid f(x) \gtrless T\}$

From a design comprising n points $\mathcal{X}_n = \{(x_i, f(x_i))\}_{1 \leq i \leq n}$

- Construct GP of interest using $\mathcal{X}_n$
- Define a criterion $\kappa : \mathbb{X} \to \mathbb{R}$ which quantify the interest of evaluating a specific point
    - Optimize the criterion and add the optimizer to the design
    - Sample and cluster according to select a batch of points to evaluate

1-step criteria

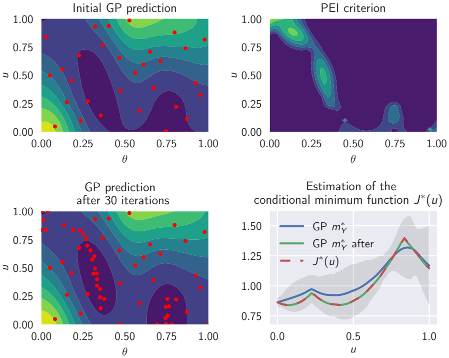
$$x_{n+1} = \arg\max_{x \in \mathbb{X}} \kappa(x) \tag{6}$$

$$\mathcal{X}_{n+1} = \mathcal{X}_n \cup \{(x_{n+1}, f(x_{n+1}))\} \tag{7}$$

- Optimization: PEI, EGO
- Exploration: prediction variance, aIMSE
- Contour/levelsets estimation: reliability index
- *PEI*

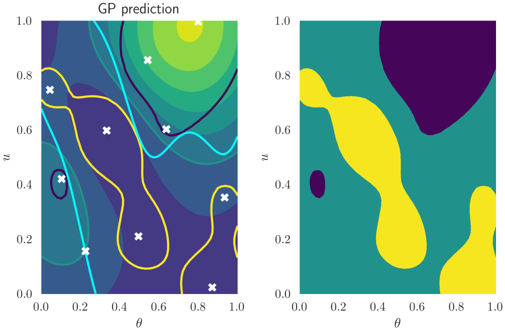
Estimation of θ^*, $J^*(u)$

Estimation of $J^*(u)$ and $\theta^*(u)$: Enrich the design according to PEI criterion Ginsbourger *et al.* [2014].



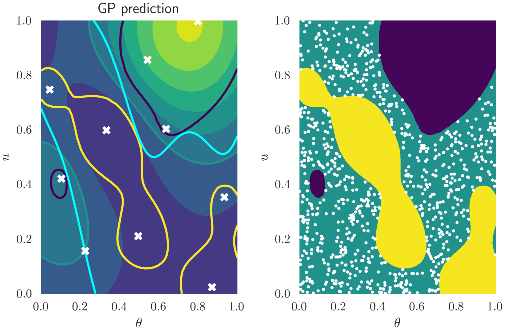
AK-MCS: Sampling-based methods

- Define sampling criterion (margin of uncertainty)



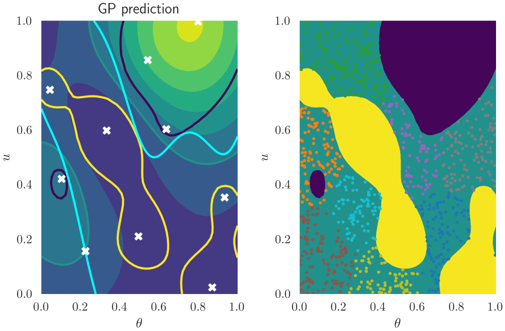
AK-MCS: Sampling-based methods

- Define sampling criterion (margin of uncertainty)
- Get Samples



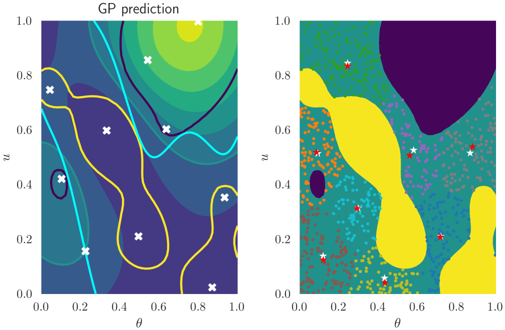
AK-MCS: Sampling-based methods

- Define sampling criterion (margin of uncertainty)
- Get Samples
- Cluster the samples



AK-MCS: Sampling-based methods

- Define sampling criterion (margin of uncertainty)
- Get Samples
- Cluster the samples
- Find closest sample to cluster centers, and add those



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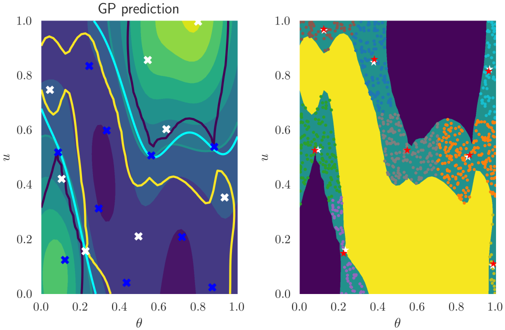

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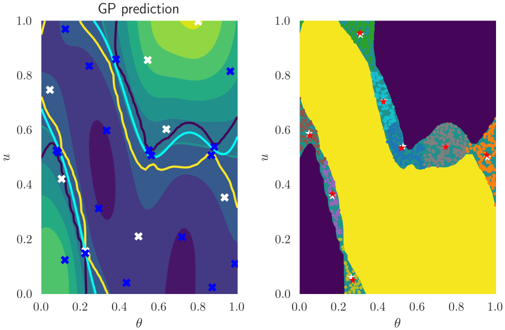

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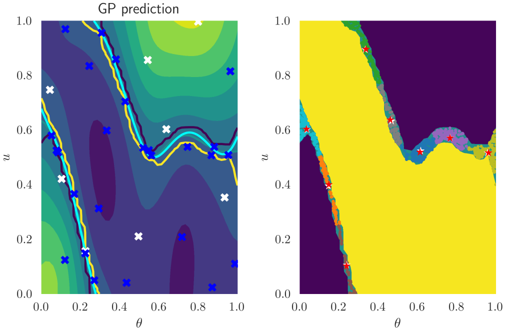

GP of the "penalized" cost function

With

$$Z \sim \mathrm{GP}\left(m_Z; C_Z\right) \text{ on } \Theta \times \mathbb{U} \tag{8}$$

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:

$$\Delta_\alpha(\theta, u) \sim \mathrm{GP}\left(m_{\Delta_\alpha}; C_{\Delta_\alpha}\right) \tag{9}$$

$$m_{\Delta_\alpha}(\theta, u) = m_Z(\theta, u) - \alpha m_Z^*(u) \tag{10}$$

$$\sigma^2_{\Delta_\alpha}(\theta, u) = \sigma^2_Z(\theta, u) + \alpha^2 \sigma^2_{Z^*}(u) - 2\alpha C_Z\left((\theta, u), (\theta_Z^*(u), u)\right) \tag{11}$$

GP of the "penalized" cost function

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

$$\Delta_\alpha(\theta, u) \sim \mathrm{GP}\left(m_{\Delta_\alpha}; C_{\Delta_\alpha}\right) \tag{9}$$

$$m_{\Delta_\alpha}(\theta, u) = m_Z(\theta, u) - \alpha m_Z^*(u) \tag{10}$$

$$\sigma^2_{\Delta_\alpha}(\theta, u) = \sigma^2_Z(\theta, u) + \alpha^2 \sigma^2_{Z^*}(u) - 2\alpha C_Z\left((\theta, u), (\theta_Z^*(u), u)\right) \tag{11}$$

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

$$\Xi(\theta, u) \sim \mathcal{N}\left(m_\Xi(\theta, u), \sigma^2_\Xi(\theta, u)\right) \tag{12}$$

$$m_\Xi(\theta, u) = \log \frac{m_Z(\theta, u)}{m^*_Z(u)} \tag{13}$$

$$\sigma^2_\Xi(\theta, u) = \frac{\sigma^2_Z(\theta, u)}{m_Z(\theta, u)^2} + \frac{\sigma^2_{Z^*}(u)}{m_{Z^*}(u)^2} - 2\frac{\mathrm{Cov}[Z(\theta, u), Z^*(u)]}{m_Z(\theta, u) m_{Z^*}(u)} \tag{14}$$

Computations using Δ_α or Ξ

Plug-in approximation

Instead of using directly Δ_α or Ξ, m_Δ and m_Ξ used instead

$$
\begin{aligned}
\Gamma_\alpha(\theta) &= \mathbb{P}_U\left[J(\theta, U) - \alpha J^*(U) \leq 0\right] && (15)\\
&\approx \mathbb{P}_U\left[m_{\Delta_\alpha}(\theta, U) \leq 0\right] && (16)\\
&\approx \mathbb{P}_U\left[m_\Xi(\theta, U) \leq \alpha\right] = F_{m_\Xi(\theta,U)}(\alpha) && (17)\\
& && (18)
\end{aligned}
$$

Estimate the "probability of failure" Bect *et al.* [2012]; Echard *et al.* [2011]
$\mathbb{P}_U\left[J(\theta, U) - \alpha J^*(U) \leq 0\right] \approx \mathbb{P}_U\left[\mathbb{P}_Z\left[\Delta_\alpha \leq 0\right]\right]$

Improving the plug-in estimation

Use sequential strategies to improve the estimation of Δ_α or Ξ

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
  $\rightarrow$ reduce uncertainty on the whole space
- Select a candidate $\tilde{\theta}$, such that uncertainty on the estimation of $\Gamma_\alpha(\tilde{\theta})$ is reduced
  $\rightarrow$ reduce uncertainty on $\{\tilde{\theta}\} \times \mathbb{U}$, with $\tilde{\theta}$ well-chosen.

Calibration of a numerical model: Application to CROCO

Introduction

Robustness in calibration

Adaptive strategies using Gaussian Processes

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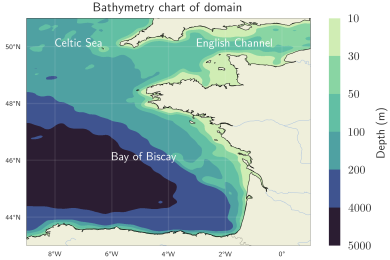
Conclusion

The numerical model CROCO

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

- Based on ROMS and AGRIF
- Solves the Shallow Water equations
- Grid resolution of $1/14^\circ$ (5.5 km)
- 15 684 cells located in the ocean



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

- Based on ROMS and AGRIF
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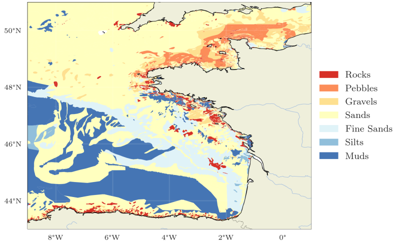
Repartition of the sediments



Modelling of the bottom friction

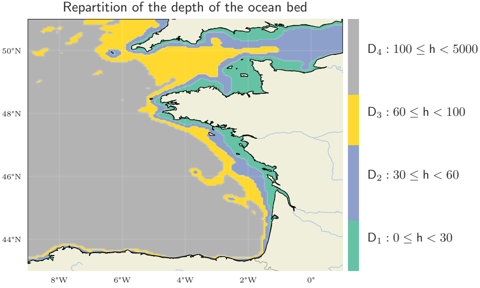
Quadratic friction coefficient

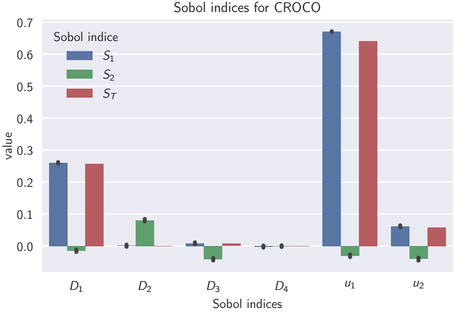
$$\tau_b = -C_d \|v_b\| v_b, \quad \text{with} \quad C_d = \left(\frac{\kappa}{\log\left(\frac{H}{z_b}\right) - 1}\right)^2 \tag{19}$$

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

SA on sediments

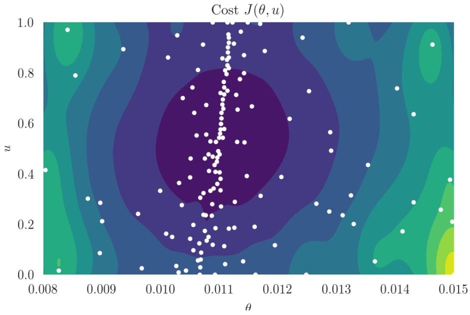
Application to CROCO: Dimension reduction





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

Robust optimization



- $U \sim \mathrm{U}[-1, 1]$ 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

Introduction

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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?

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