Robust calibration of numerical models based on Relative-regret

Robust Estimation of bottom friction

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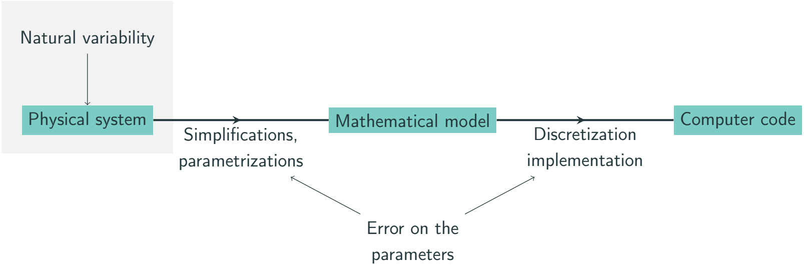
Uncertainties in the modelling



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

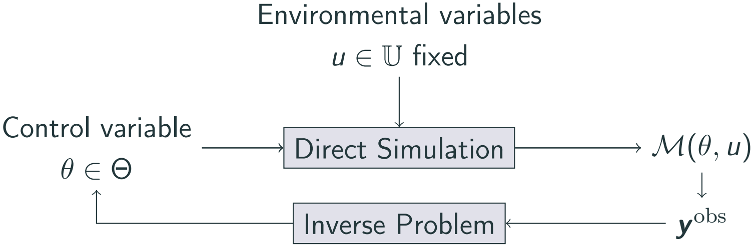
Outline

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 $u \in \mathbb{U}$.

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

$\rightarrow$ Deterministic optimization problem

$\rightarrow$ Possibly add regularization

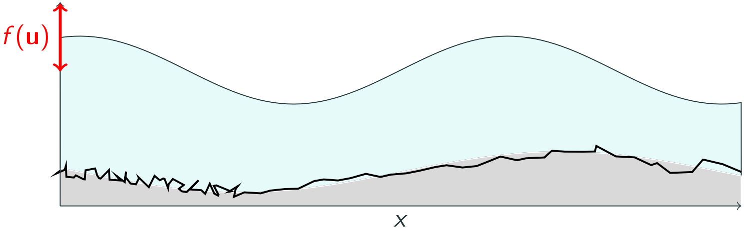
$\rightarrow$ Classical methods: Adjoint gradient and Gradient-descent

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]

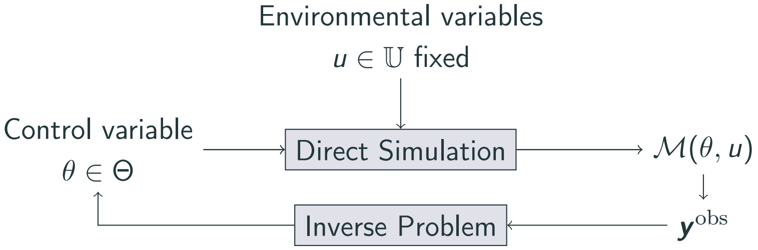
- Epistemic uncertainties: From a lack of knowledge, that can be reduced with more research/exploration
- Aleatoric uncertainties: From the inherent variability of the system studied, operating conditions

$\rightarrow$ 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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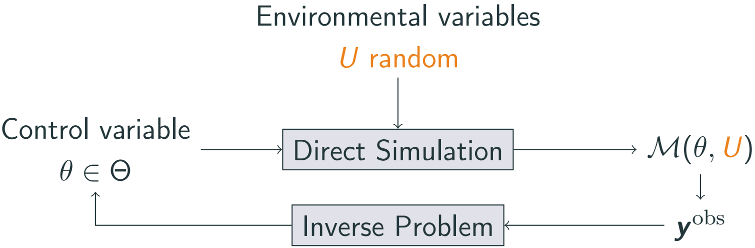


The cost function as a random variable

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

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

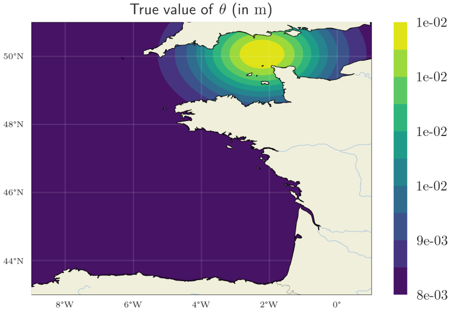
- The deterministic quadratic error is now

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

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

Misspecification of u: twin experiment setup

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



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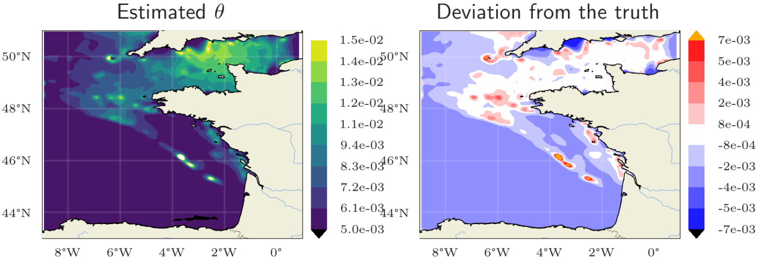
Well-specified model



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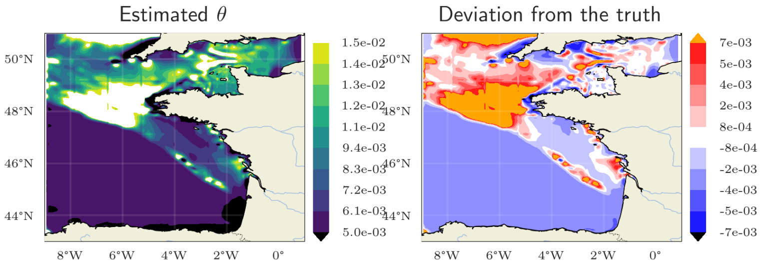
1% error on the amplitude of the M2 tide



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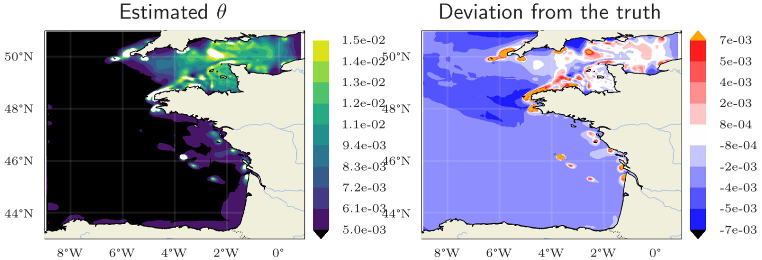

Robustness and estimation of parameters

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]:

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

- V-robustness [LSN04]:

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

- Multiobjective [Bau12]:

Pareto frontier

- Best performance acheivable 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:

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

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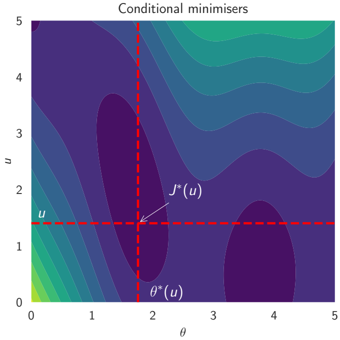
How to take into account values not optimal, but not too far either $\longrightarrow$ relaxation of the equality with $\alpha > 1$:

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

Illustration



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

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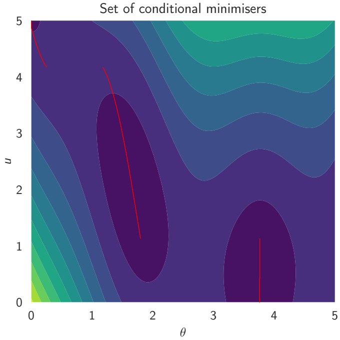

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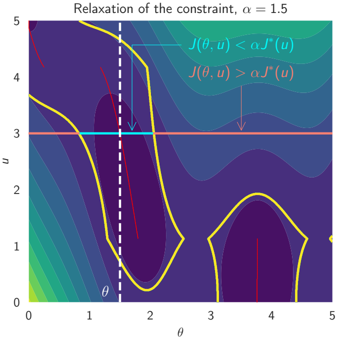

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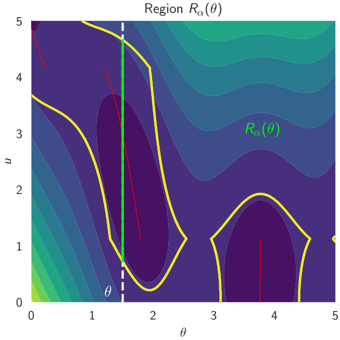


- Sample $u \sim U$, and solve $\theta^*(u) = \arg\min_{\theta \in \Theta} J(\theta, u)$
- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$
- Set $\alpha \geq 1$
- $R_\alpha(\theta) = \{u \mid J(\theta, u) \leq \alpha J^*(u)\}$
- $\Gamma_\alpha(\theta) = \mathbb{P}_U [U \in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

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:

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

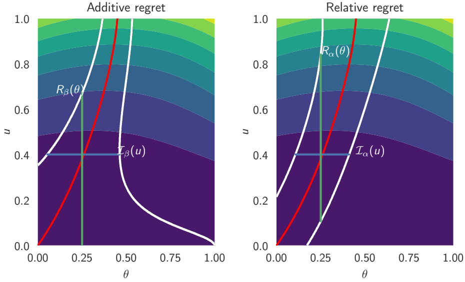
- Set a target probability $1 - \eta$, and find the smallest α.

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

More generally, let us define the RR family

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

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 ($\sim$ plug-in approach)
- Adapted sequential procedures e.g. EGO

$\rightarrow$ Kriging (Gaussian Process Regression) [Mat62, Kri51]

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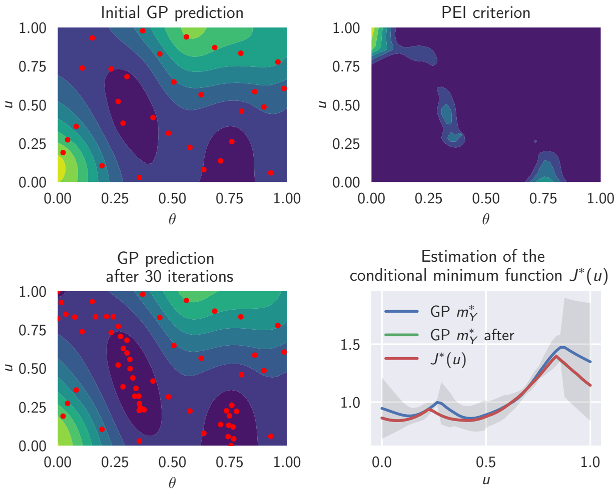
$\rightarrow$ Kriging (Gaussian Process Regression) [Mat62, Kri51]
$Y \sim \mathrm{GP}\left(m_Y(\cdot), C_Y(\cdot,\cdot)\right)$ GP regression of J on $\Theta \times \mathbb{U}$, using an initial design $\mathcal{X} = \{((\theta_i, u_i), J(\theta_i, u_i))\}$

Estimation of θ^*, $J^*(u)$

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



GP of the "penalized" cost function

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

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

$$\Delta_\alpha = Y - \alpha Y^* \tag{5}$$

Still a GP

$$\Delta_\alpha(\theta, u) \sim \mathrm{GP}\left(m_\alpha(\cdot); C_\alpha(\cdot,\cdot)\right) \tag{6}$$

$$m_\alpha(\theta, u) = m_Y(\theta, u) - \alpha m_Y^*(u) \tag{7}$$

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

Estimate the "probability of failure" [BGL+12, EGL11]
$\mathbb{P}_U\left[J(\theta, U) - \alpha J^*(U) \leq 0\right] \approx \mathbb{P}_U\left[\mathbb{P}_Y\left[\Delta_\alpha \leq 0\right]\right]$

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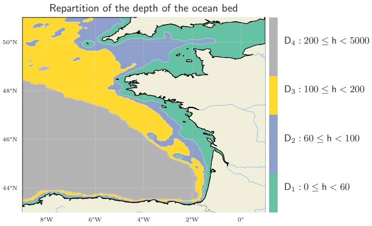
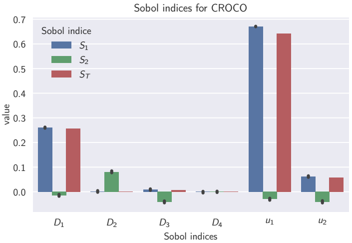
Joint space or objective-oriented exploration

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.

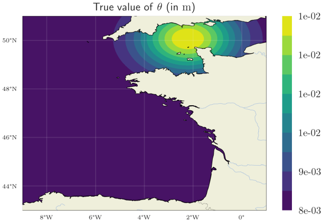
Application to CROCO: Dimension reduction

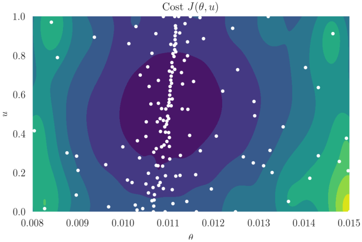




Ad-hoc segmentation according to the depth, and sensitivity analysis: only the shallow coastal regions seem to have an influence.

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

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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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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:

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

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

$\rightarrow$ 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 $\Theta \times \mathbb{U}$

$$\mathrm{PEI}(\theta, u) = \mathbb{E}_Y\left[\left[f_{\min}(u) - Y(\theta, u)\right]_+\right] \tag{11}$$

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