Parameter control in the presence of uncertainties

Robust Estimation of Bottom friction

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Introduction

Processus of modelling of physical systems

Uncertainties and errors are introduced at each stage of the modelling, by simplifications, parametrizations...

In the end, we have a set of parameters we want to calibrate, but how can we be sure that this calibration is acting upon the errors of the modelling, and does not compensate the effect of the natural variability of the physical system?

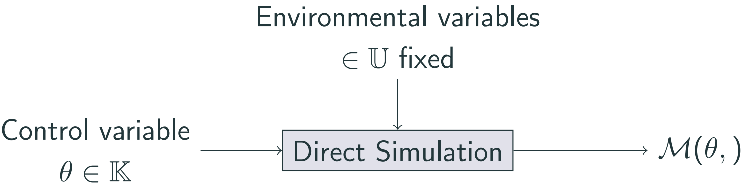
Outline

Deterministic problem

Computer code and inverse problem

Input
- $\boldsymbol{k}$: Control parameter
- $\boldsymbol{u}$: Environmental variables (fixed and known)

Output
- $\mathcal{M}(\boldsymbol{k}, \boldsymbol{u})$: Quantity to be compared to observations



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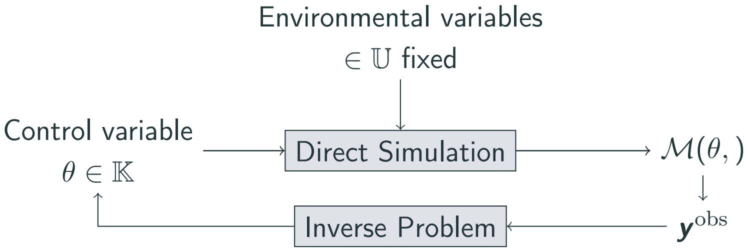


Data assimilation framework

We have $\boldsymbol{y}^{\mathrm{obs}} = \mathcal{M}(\boldsymbol{k}_{\mathrm{obs}}, \boldsymbol{u}_{\mathrm{obs}})$ with $\boldsymbol{u}_{\mathrm{obs}} = \boldsymbol{u}$

$$\hat{\boldsymbol{k}} = \underset{\boldsymbol{k}\in\mathbb{K}}{\arg\min}\, J(\boldsymbol{k}) = \underset{\boldsymbol{k}\in\mathbb{K}}{\arg\min}\, \frac{1}{2}\|\mathcal{M}(\boldsymbol{k}, \boldsymbol{u}) - \boldsymbol{y}^{\mathrm{obs}}\|^2$$

$\rightarrow$ Deterministic optimization problem

$\rightarrow$ Possibly add regularization

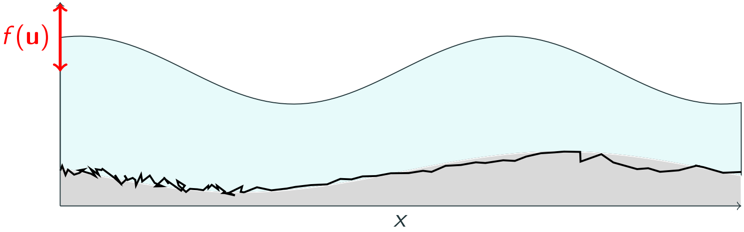
$\rightarrow$ Classical methods: Adjoint gradient and Gradient-descent

BUT

- What if $\boldsymbol{u} \neq \boldsymbol{u}_{\mathrm{obs}}$?
- Does $\hat{\boldsymbol{k}}$ compensate the errors brought by this misspecification?

Context

- The friction $\boldsymbol{k}$ of the ocean bed has an influence on the water circulation
- Depends on the type and/or characteristic length of the asperities
- Subgrid phenomenon
- $\boldsymbol{u}$ parametrizes the BC



Dealing with uncertainties

Different types of uncertainties

Epistemic or aleatoric uncertainties? [WHR+03]

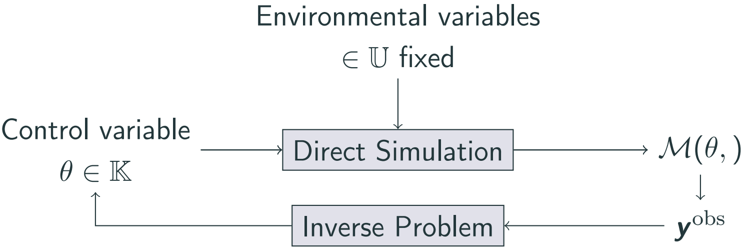
- Epistemic uncertainties: From a lack of knowledge, that can be reduced with more research/exploration
- Aleatoric uncertainties: From the inherent variability of the system studied, operating conditions

$\rightarrow$ 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 $\boldsymbol{u}$ fixed, we consider that $\boldsymbol{U}$ is a random variable (pdf $\pi(\boldsymbol{u})$), and the output of the model depends on its realization.



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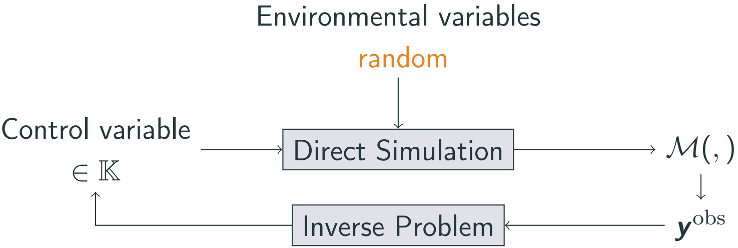


The cost function as a random variable

- Output of the computer code ($\boldsymbol{u}$ is an input):

$$\mathcal{M}(\boldsymbol{k}, \boldsymbol{u})$$

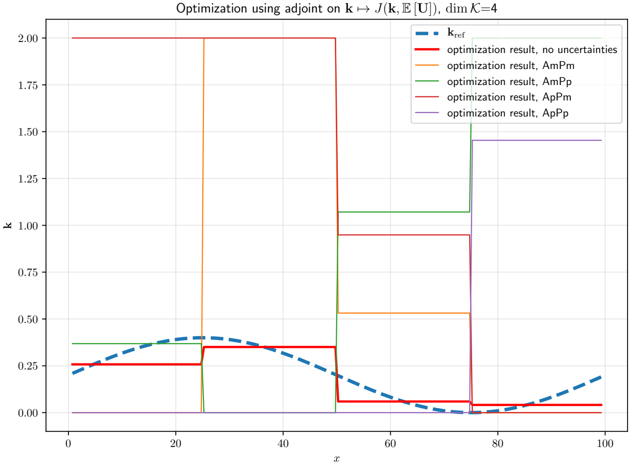
- The (deterministic) quadratic error is now

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

$$''\hat{\boldsymbol{k}} = \operatorname*{arg\,min}_{\boldsymbol{k}\in\mathbb{K}} J(\boldsymbol{k}, \boldsymbol{u})'' \text{ but what can we do about } \boldsymbol{u}?$$

Toy Problem: Influence of misspecification of $\boldsymbol{u}_{\mathrm{obs}}$

Minimization performed on $\boldsymbol{k} \mapsto J(\boldsymbol{k}, \mathbb{E}[\boldsymbol{U}])$, for different $\boldsymbol{u}_{\mathrm{obs}}$:
Naïve approach



Robust Estimation of parameters

- Main objectives:
  - Define criteria of robustness, based on $J(\boldsymbol{k}, \boldsymbol{u})$, that will depend on the final application
  - For each criterion, be able to compute an estimate $\hat{\boldsymbol{k}}$ in a reasonable time
- Questions to be answered along the way:
  - Good exploration of $\mathbb{U}$, based on the density of $\boldsymbol{U}$ (Design of Experiment: LHS, Monte-Carlo, OA,. . . ?)
  - Deal with dimension of $\mathbb{K}$?

Robust minimization

Criteria of robustness

Non-exhaustive list of “Robust” Objectives

- Worst case [MWP13]:

$$\min_{\boldsymbol{k} \in \mathbb{K}} \left\{ \max_{\boldsymbol{u} \in \mathbb{U}} J(\boldsymbol{k}, \boldsymbol{u}) \right\}$$

- M-robustness [LSN04]:

$$\min_{\boldsymbol{k} \in \mathbb{K}} \mathbb{E}_{\boldsymbol{U}} \left[J(\boldsymbol{k}, \boldsymbol{U}) \right]$$

- V-robustness [LSN04]:

$$\min_{\boldsymbol{k} \in \mathbb{K}} \mathbb{V}\mathrm{ar}_{\boldsymbol{U}} \left[J(\boldsymbol{k}, \boldsymbol{U}) \right]$$

- Multiobjective [Bau12]:

Pareto frontier

- Best performance attainable for each configuration $\boldsymbol{u} \sim \boldsymbol{U}$

“Most Probable Estimate”, and relaxation

Main idea: For each $\boldsymbol{u} \sim \boldsymbol{U}$, compare the value of the cost function to its optimal value $J^*(\boldsymbol{u})$ and define $\boldsymbol{k}^*(\boldsymbol{u}) = \arg\min_{\boldsymbol{k}\in\mathbb{K}} J(\boldsymbol{k}, \boldsymbol{u})$

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The minimizer as a random variable:

$$\boldsymbol{K}^* = \underset{\boldsymbol{k}\in\mathbb{K}}{\arg\min}\, J(\boldsymbol{k}, \boldsymbol{U})$$

$\longrightarrow$ estimate its density (how often is the value $\boldsymbol{k}$ a minimizer)

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

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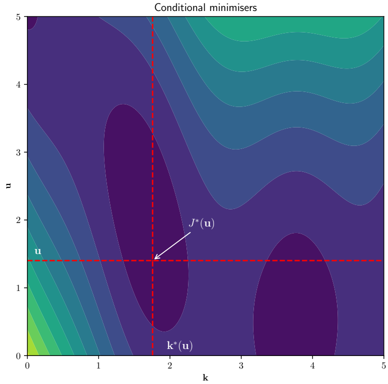
How to take into account values not optimal, but not too far either
$\longrightarrow$ relaxation of the equality with $\alpha > 1$:

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

Illustration



- Sample $\boldsymbol{u} \sim \boldsymbol{U}$, and solve $\boldsymbol{k}^*(\boldsymbol{u}) = \arg\min_{\boldsymbol{k}\in\mathbb{K}} J(\boldsymbol{k}, \boldsymbol{u})$

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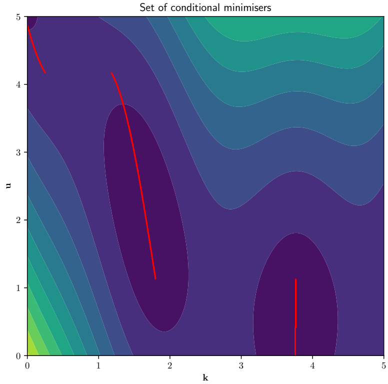

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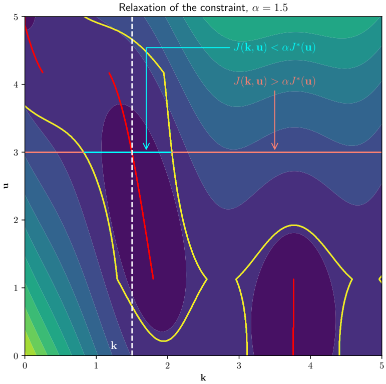

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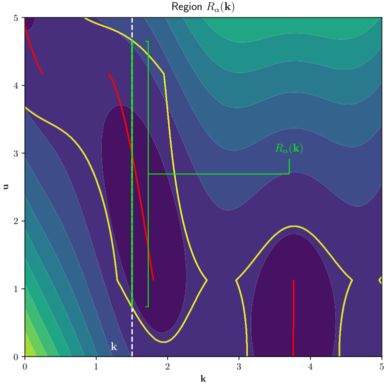

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- $R_\alpha(\boldsymbol{k}) = \{\boldsymbol{u} \mid J(\boldsymbol{k}, \boldsymbol{u}) < \alpha J^*(\boldsymbol{u})\}$
- $\Gamma_\alpha(\boldsymbol{k}) = \mathbb{P}_{\boldsymbol{U}}\left[\boldsymbol{U} \in R_\alpha(\boldsymbol{k})\right]$

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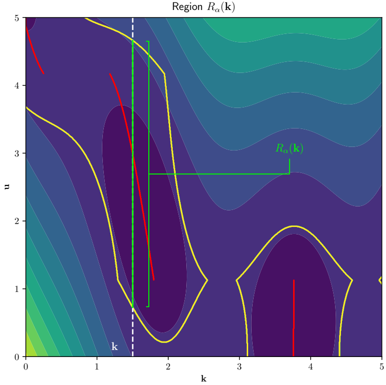

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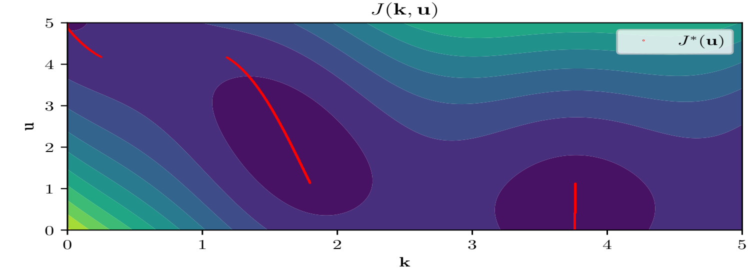
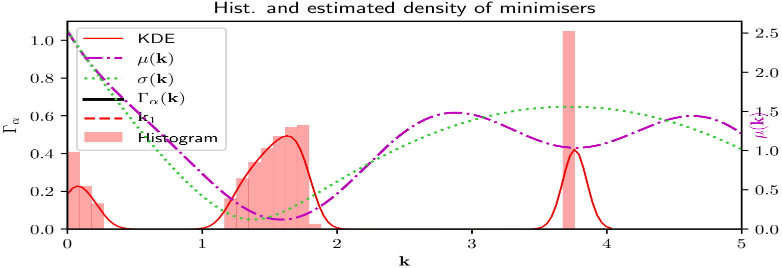
- $\Gamma_\alpha(\boldsymbol{k}) = \mathbb{P}_{\boldsymbol{U}}\left[\boldsymbol{U} \in R_\alpha(\boldsymbol{k})\right]$
- How to choose α? When $\max_{\boldsymbol{k}} \Gamma_\alpha(\boldsymbol{k})$ reaches fixed levels

Choosing a α





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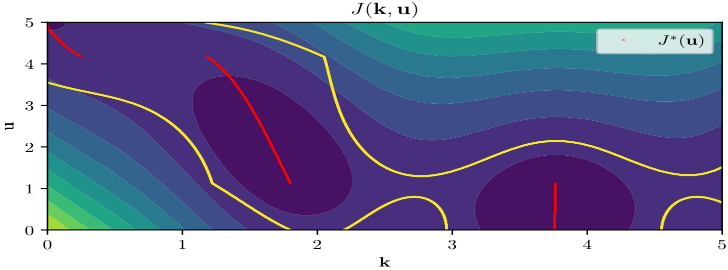

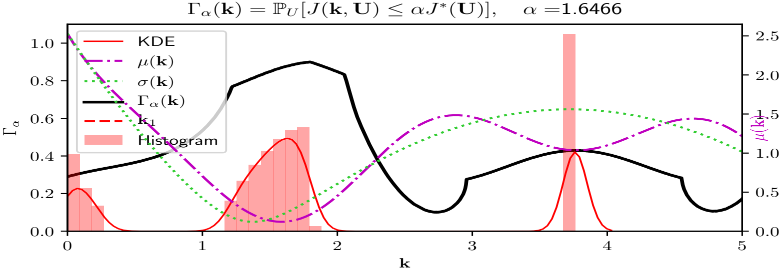

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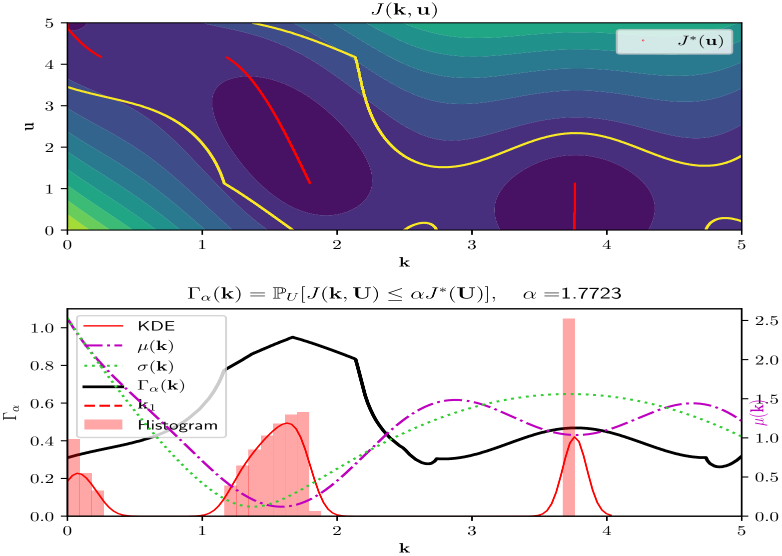

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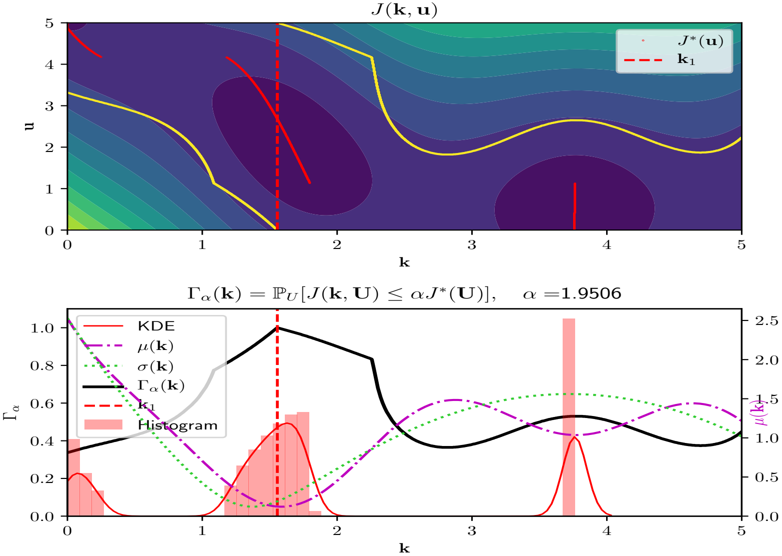

Bottlenecks and problems arising

- Computational Bottlenecks
  - Computer model: expensive to run $\rightarrow$ exhaustive computations unfeasible
  - $\dim \mathbb{K}$, $\dim \mathbb{U}$?: curse of dimensionality
- Calibration context
  - How to assess quality of predictions

Surrogates

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

Why surrogates?

- Replace expensive model by a computationally cheap metamodel ($\sim$ plug-in approach)
- Adapted sequential procedures e.g. EGO
- Uncertainties upon $\boldsymbol{u}$ may be incorporated directly in the surrogate

Environmental variables

$\boldsymbol{U}$ random

Control variable

$\boldsymbol{k} \in \mathcal{K}$

$$\boldsymbol{k} \longrightarrow \boxed{\text{Direct Simulation}} \longrightarrow \mathcal{M}(\boldsymbol{k}, \boldsymbol{u}) \longrightarrow J(\boldsymbol{k}, \boldsymbol{u})$$

Two main forms considered in UQ:

- Kriging (Gaussian Process Regression) [Mat62]
- Polynomial Chaos Expansion [XK02, Sud15]

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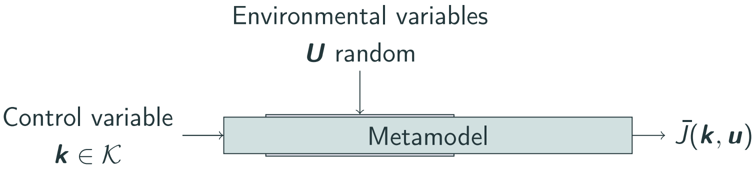

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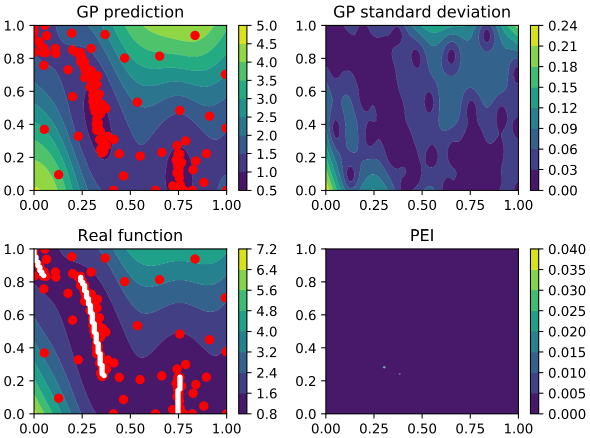
Estimation of K^*, $J^*(U)$

Iterative procedures to estimate set of conditional minimum/minimisers [GBC+14]



Conclusion

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Wrapping up

- Problem of a *good* definition of robustness
- Strategies rely heavily on surrogate models, to embed aleatoric uncertainties directly in the modelling

Perspective and future work

- Cost of computer evaluations $\rightarrow$ limited number of runs?
- Dimensionality of the input space $\rightarrow$ reduction of the input space?
- How to deal with uncontrollable errors $\rightarrow$ realism of the model?

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