Parameter control in the presence of uncertainties

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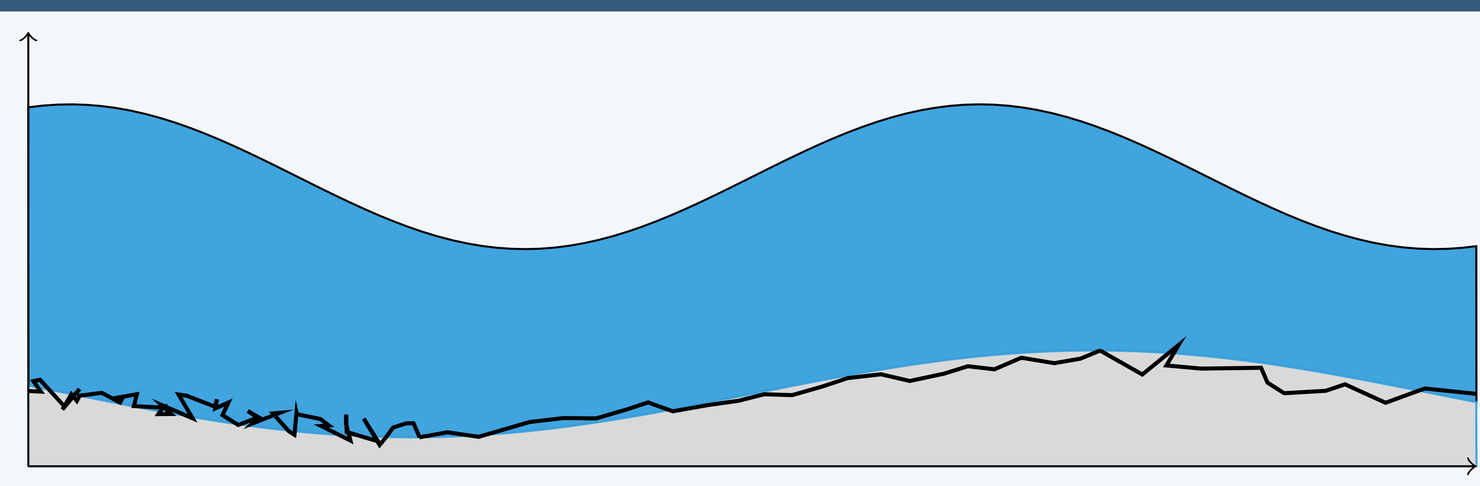
How can one calibrate a numerical model so that it performs reasonably well for different random operating conditions ?

Objectives

- Define suitable definitions of robustness in the field of computer code calibration
- Develop efficient techniques and algorithms in order to estimate those parameters
- Deal with the high-dimension of the parameter spaces: Dimension reduction

Background: estimation of the bottom friction in a shallow water model



The calibration problem is to be able to find a value of $\boldsymbol{k} \in \mathcal{K}$ denoted $\hat{\boldsymbol{k}}$ that matches the best the observations $\boldsymbol{y}_{\text{obs}}$. We define a loss function, that is the misfit between the observations to the model.

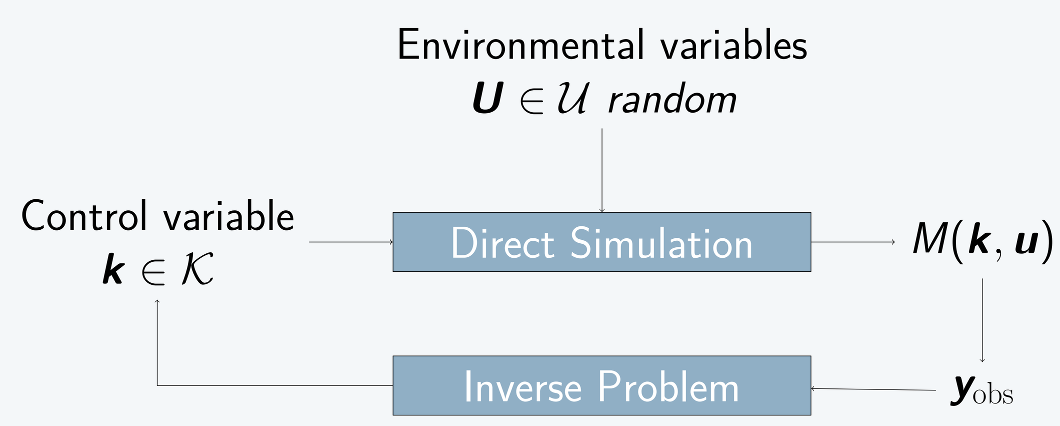
$$J(\boldsymbol{k}) = \frac{1}{2}\|M(\boldsymbol{k}) - \boldsymbol{y}_{\text{obs}}\|^2_{\Sigma^{-1}}$$

and we have to perform the following minimisation problem, usually with the help of the adjoint method

$$\hat{\boldsymbol{k}} = \operatorname*{arg\,min}_{\boldsymbol{k} \in \mathcal{K}} J(\boldsymbol{k})$$

Stochastic Inverse Problem

Now, $\boldsymbol{u} \in \mathcal{U} \sim \boldsymbol{U}$ of density p_U and $\boldsymbol{y}_{\text{obs}} = M(\boldsymbol{k}_{\text{ref}}, \boldsymbol{u}_{\text{ref}})$



The loss function is now

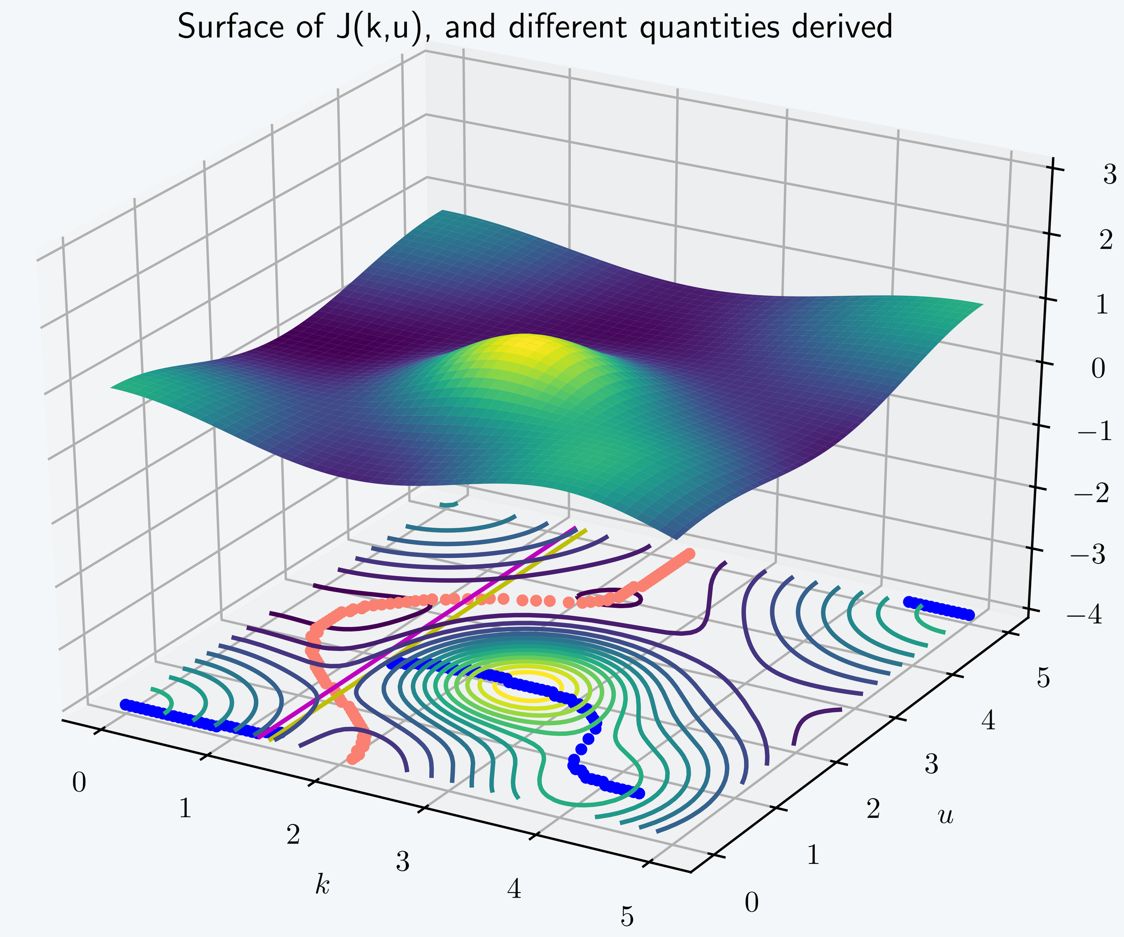
$$\underbrace{J(\boldsymbol{k}, \boldsymbol{U}) = \frac{1}{2}\|M(\boldsymbol{k}, \boldsymbol{U}) - \boldsymbol{y}_{\text{obs}}\|^2_{\Sigma^{-1}}}_{\text{Random variable}}$$

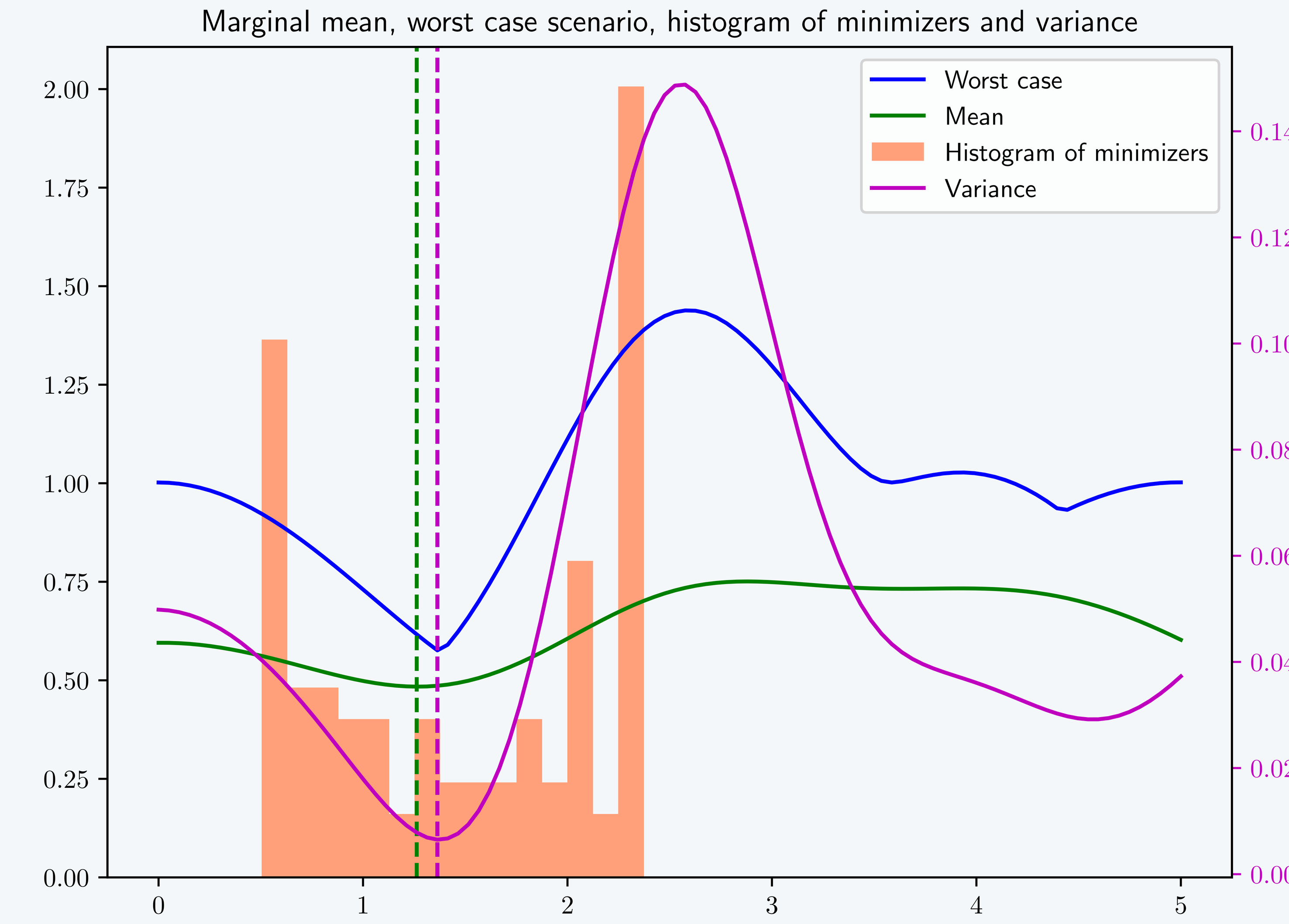
- What criteria to use to "optimize" in a sense J ?
- Evaluating J is time consuming. How to deal with a limited budget of evaluations ?

Which criterion to choose ?

- Global minimum
$$(\boldsymbol{k}^*, \boldsymbol{u}^*) = \operatorname*{arg\,min}_{(\boldsymbol{k},\boldsymbol{u})} J(\boldsymbol{k}, \boldsymbol{u}) \quad \text{and} \quad \hat{\boldsymbol{k}}_{\text{global}} = \boldsymbol{k}^*$$
- Assuming that the environmental variables have little influence:
$$J_{\mathbb{E}}(\boldsymbol{k}) = J(\boldsymbol{k}, \mathbb{E}[\boldsymbol{U}]) \quad \text{and} \quad \hat{\boldsymbol{k}}_{\mathbb{E}} = \operatorname*{arg\,min}_{\boldsymbol{k}} J_{\mathbb{E}}(\boldsymbol{k}) \qquad \text{(Classical methods)}$$
$\longrightarrow$ Those approaches are not robust: inherent variability of $\boldsymbol{U}$ not taken into account
- Consider the worst-case scenario
$$J_{\text{w}}(\boldsymbol{k}) = \max_{\boldsymbol{u} \in \mathcal{U}} J(\boldsymbol{k}, \boldsymbol{u}) \quad \text{and} \quad \hat{\boldsymbol{k}}_{\text{wc}} = \operatorname*{arg\,min}_{\boldsymbol{k}} J_{\text{w}}(\boldsymbol{k}) \qquad \text{(Explorative EGO)}$$
- The solution gives good results on average:
$$\mu(\boldsymbol{k}) = \mathbb{E}_U[J(\boldsymbol{k}, \boldsymbol{U})] \quad \text{and} \quad \hat{\boldsymbol{k}}_{\mu} = \operatorname*{arg\,min}_{\boldsymbol{k}} \mu(\boldsymbol{k}) \qquad \text{(Iterative EGO)}$$
- The estimate gives steady results:
$$\sigma^2(\boldsymbol{k}) = \mathbb{V}\text{ar}_U[J(\boldsymbol{k}, \boldsymbol{U})] \quad \text{and} \quad \hat{\boldsymbol{k}}_{\sigma^2} = \operatorname*{arg\,min}_{\boldsymbol{k}} \sigma^2(\boldsymbol{k}) \qquad \text{(PCE gradient)}$$
- Compromise between Mean and Variance $\rightarrow$ multiobjective optimization problem:
$$\text{Pareto front of } (\mu(\boldsymbol{k}), \sigma^2(\boldsymbol{k})) \qquad \text{(Layered kriging)}$$
- Probability of being below threshold $T \in \mathbb{R}$: Reliability analysis
$$R_T(\boldsymbol{k}) = \mathbb{P}\left[J(\boldsymbol{k}, \boldsymbol{U}) \leq T\right], \quad \hat{\boldsymbol{k}}_{R_T} = \operatorname*{arg\,max} R_T(\boldsymbol{k}) \qquad \text{(GP simulations)}$$
- We define $T_\alpha(\boldsymbol{U}) = \alpha \min_{\boldsymbol{k}} J(\boldsymbol{k}, \boldsymbol{U})$, for $\alpha \geq 1$, and $R_\alpha = R_{T_\alpha}$
Distribution of minimizers: $T_{\min} = T_1(\boldsymbol{U}) = \min_{\boldsymbol{k}} J(\boldsymbol{k}, \boldsymbol{U})$
$$R_{\min}(\boldsymbol{k}) = \mathbb{P}\left[J(\boldsymbol{k}, \boldsymbol{U}) \leq T_{\min}\right] = \mathbb{P}\left[\boldsymbol{k} = \operatorname*{arg\,min}_{\tilde{\boldsymbol{k}}} J(\tilde{\boldsymbol{k}}, \boldsymbol{U})\right]$$
(Estimation and maximization of density)

2D Illustration





General methods

- Design of Experiment
  - Efficient exploration of the input space: LHS, space filling designs
- Statistical/Probabilistic aspects
  - Bayesian/Frequentist approach: Markov-chain based methods, study of the posterior distribution
  - Choice of prior on $\boldsymbol{K}$ to take into account specific information on spatial variation of the friction
  - Marginalization with respect to $\boldsymbol{U}$
- Surrogate modelling
  - Kriging (Gaussian Process Regression)
  - Polynomial Chaos Expansion
- Optimization
  - Adjoint method provides the gradient of the cost function $\rightarrow$ Adapt principles of gradient descent on specific objectives
  - Adaptative sampling: based on surrogate, choose the next point to be evaluated based on a specific criterion: EGO, IAGO and more general *Stepwise Uncertainty Reduction* strategies

Conclusion and perspectives

- Several objectives can be defined, often concurrent
- Choice of criterion of robustness is application-dependent
- Scalability of methods in high dimension ? Need to perform Dimension reduction on $\mathcal{K}$ and $\mathcal{U}$

References