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# Regret-based calibration using GPs

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

## Objectives

- ▶ Define the notion of **regret** in a calibration context
- ▶ Develop **efficient** methods and algorithms in order to estimate those parameters

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

Let  $u$  be some operating conditions (configuration, boundary conditions...)

$$\mathcal{G} : \underbrace{\theta}_{\text{bottom friction}}, \underbrace{u}_{\text{config}} \mapsto \underbrace{\mathcal{G}(\theta, u)}_{\text{SSH}}$$

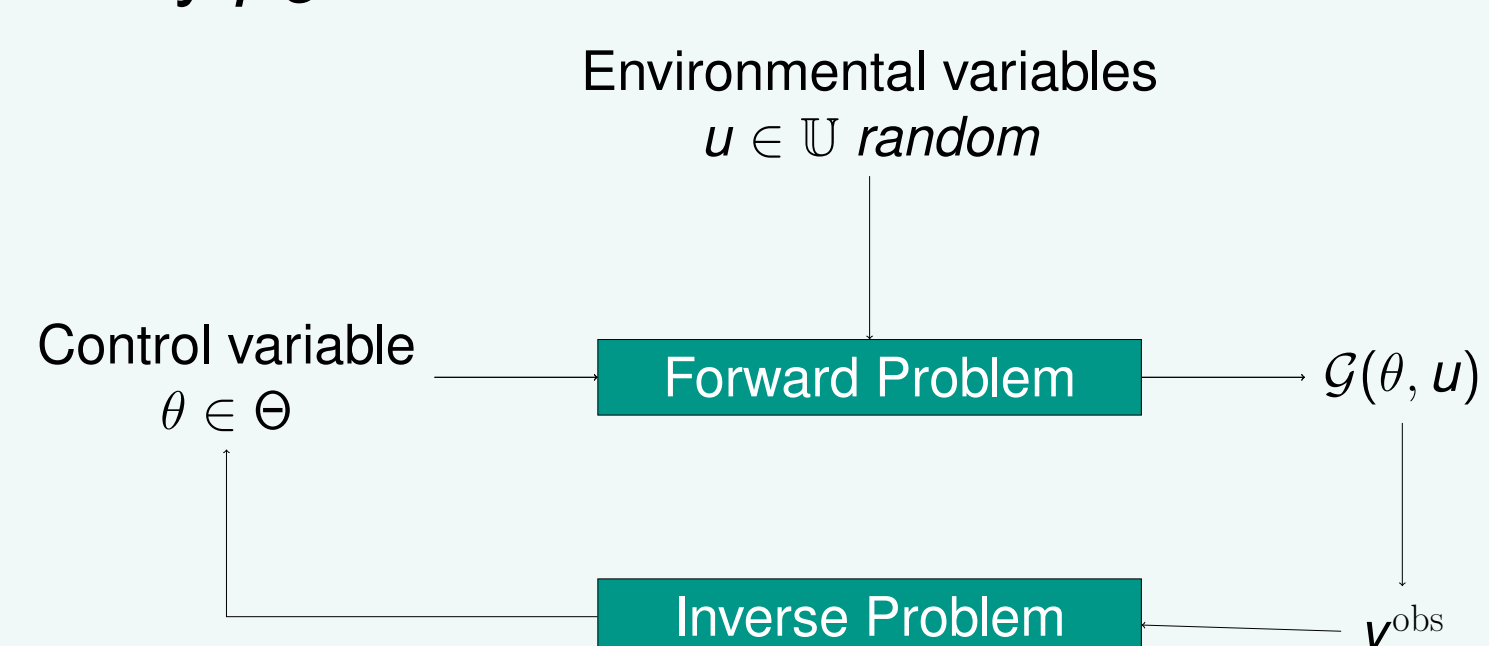
Given some observations  $y^{\text{obs}}$ , the MSE is

$$J(\theta) = \frac{1}{2} \|\mathcal{G}(\theta, u) - y^{\text{obs}}\|_{\Sigma^{-1}}^2$$

and the estimate  $\hat{\theta}$  is defined as

$$\hat{\theta} = \arg \min_{\theta \in \Theta} J(\theta)$$

Now,  $u \in \mathbb{U} \sim U$  of density  $p_U$



For all  $\theta$ , the loss function is now

$$J(\theta, U) = \frac{1}{2} \|\mathcal{G}(\theta, U) - y^{\text{obs}}\|_{\Sigma^{-1}}^2$$

Random variable

or equivalently,

$\{J(\theta, U) \mid \theta \in \Theta\}$  is a family of random variable indexed by  $\theta$

- ▶ How to choose a  $\hat{\theta} \in \Theta$ , such that " $\hat{\theta} = \arg \min J(\theta, U)$ " ?

## (Relative)-regret based calibration

- ▶ For a fixed  $u \in \mathbb{U}$ , the best attainable value is

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

We want to find  $\hat{\theta}$  so that

$J(\hat{\theta}, U)$  close to  $J^*(U)$  with high probability

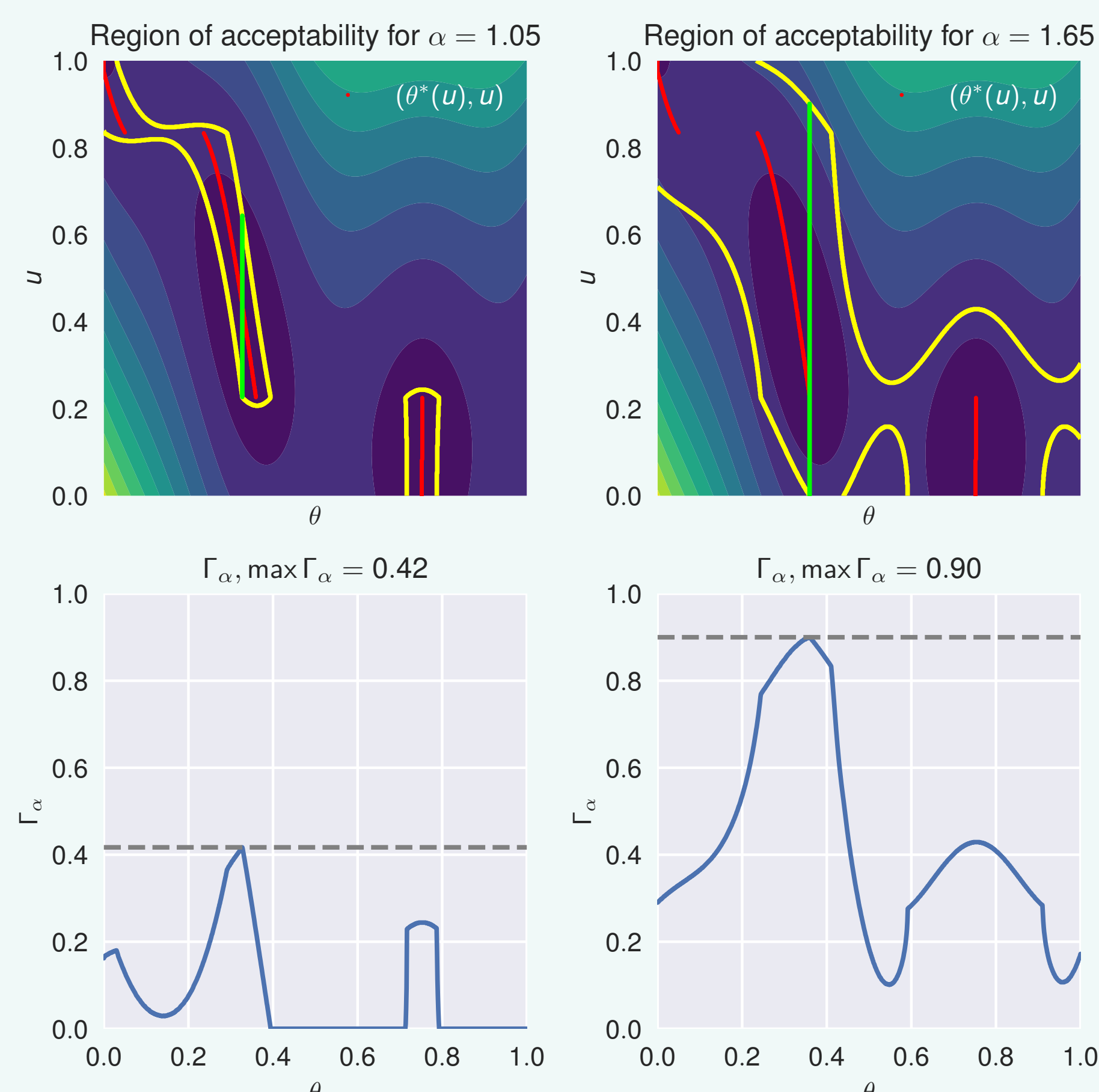
### $\alpha$ -acceptability [TAVD20]

Given  $u \in \mathbb{U}$

$\hat{\theta}$  is  $\alpha$ -acceptable if  $J(\hat{\theta}, u) \leq \alpha \cdot J^*(u)$

- ▶ Find  $\hat{\theta}$  which is  $\alpha$ -acceptable with the highest probability:

$$\hat{\theta}_\alpha = \arg \max_{\theta} \mathbb{P}_U [J(\theta, U) \leq \alpha \cdot J^*(U)]$$



- ▶ Large  $\alpha$ : Conservative, performances controlled with high probability
  - ▶ Small  $\alpha$ : Optimistic, good performances but less frequently
- Good knowledge of  $J$  globally and around the conditional minimisers is required.

## Computing regret-based estimates using GP regression

Two approaches:

- ▶ Reduce approximation error of  $J - \alpha J^*$
- ▶ Improve estimation of the set  $\mathcal{A}_\alpha = \{J - \alpha J^* \leq 0\}$

Let  $Z \sim \text{GP}(m_Z, \sigma_Z^2)$  modelling  $J$  over  $\Theta \times \mathbb{U}$

- ▶ Define  $\Delta_\alpha(\theta, u) = Z(\theta, u) - \alpha Z^*(u)$  with  $Z^*(u)$  approximation of  $J^*$  computed using  $m_Z$ :

$$Z^* \sim \text{GP} \left( m_{Z^*} = \min_{\theta} m_Z, \sigma_{Z^*}^2 \right)$$

## Reduction of the expected IMSE

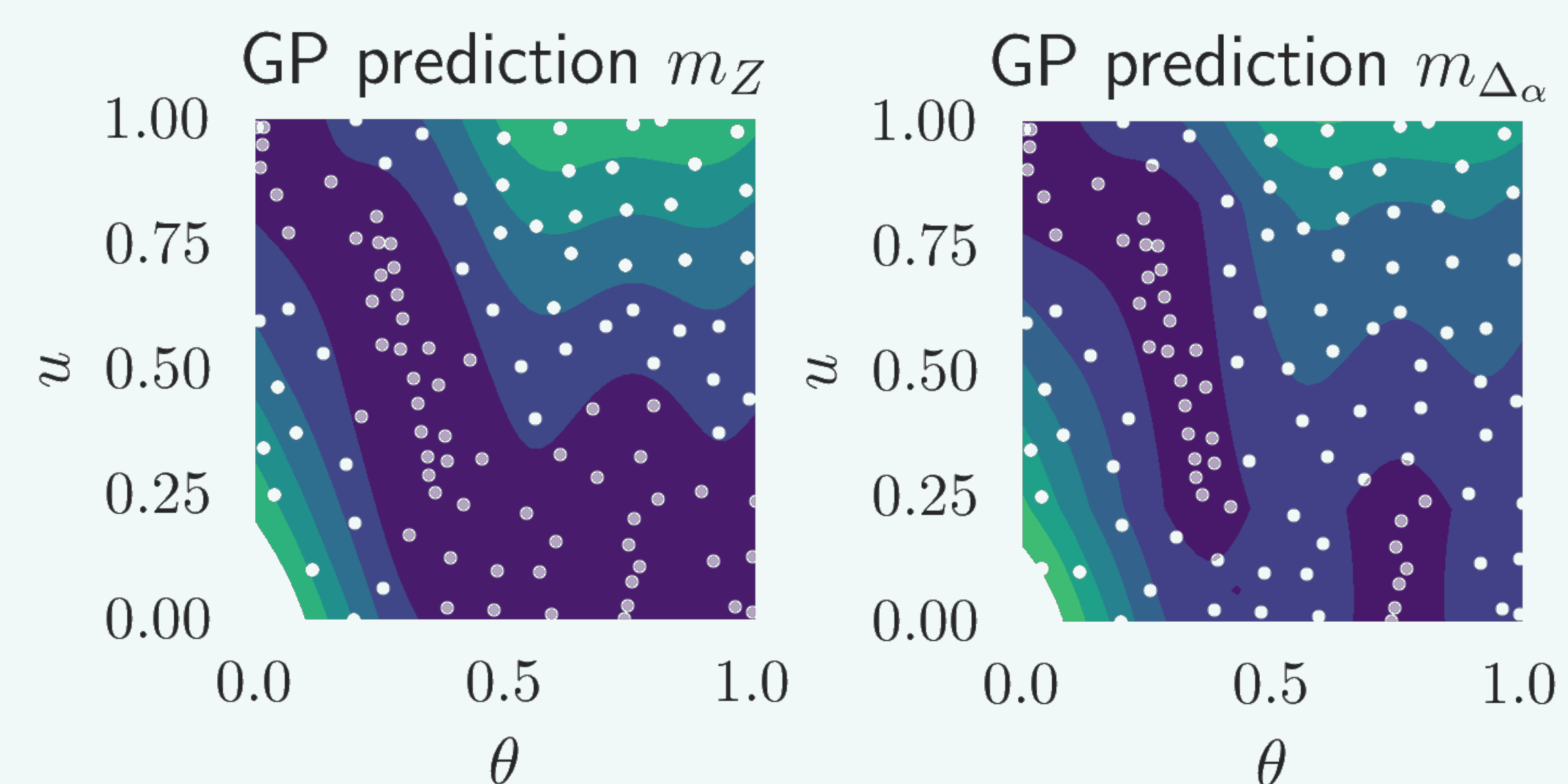
Approximation error  $(\theta, u)$  comes from:

- ▶ Uncertainty on the value of the function  $J$ :  $\rightarrow Z(\theta, u)$
- ▶ Uncertainty on the conditional minimiser  $J^*$ :  $\rightarrow Z^*(u)$

$$\text{IMSE}(\Delta_\alpha) = \int_{\Theta \times \mathbb{U}} \sigma_{\Delta_\alpha}^2(\theta, u) d\theta du$$

→ global measure of the approximation error. We want the smallest IMSE once a point is added to the design:

$$(\theta_{\text{new}}, u_{\text{new}}) = \arg \min_{\theta, u} \mathbb{E}_Z [\text{IMSE}(\Delta_\alpha \cup Z(\theta, u))]$$



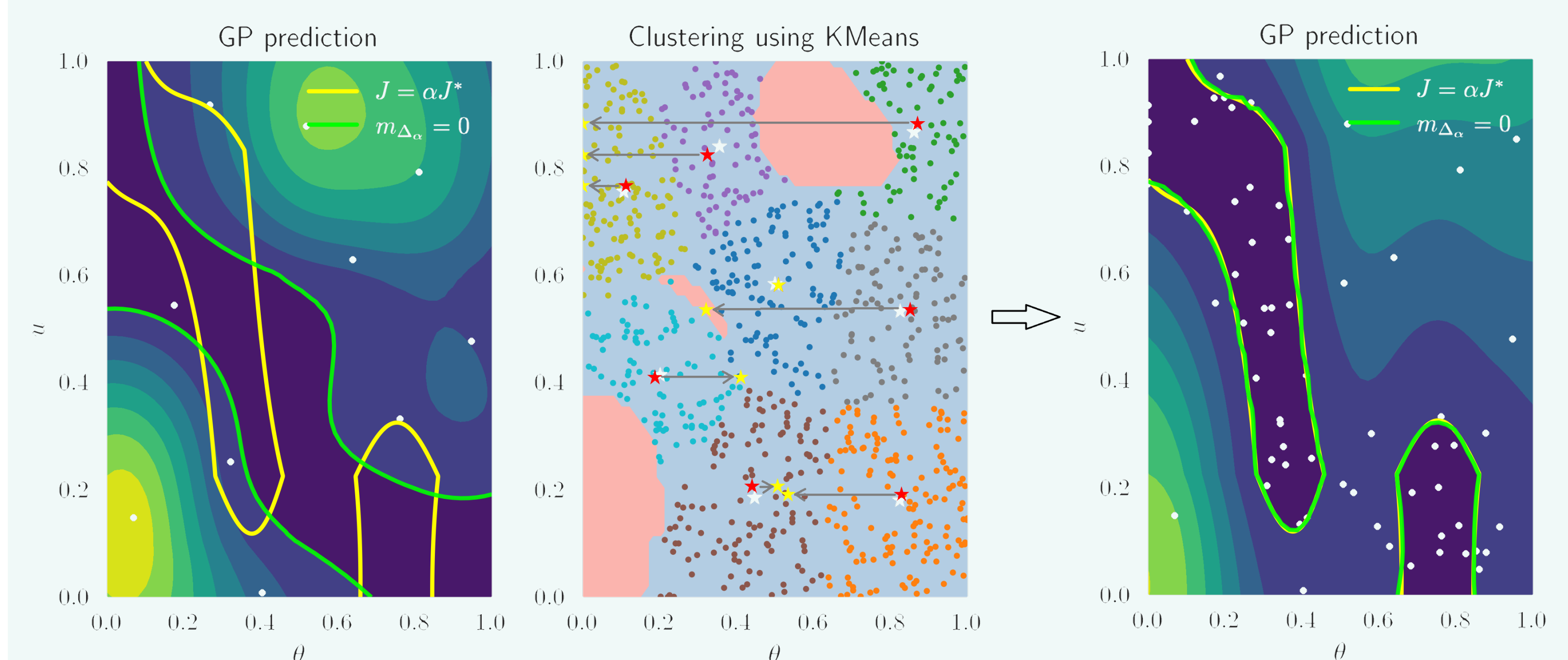
## k-batch approach ([DSB11])

Improve the "classifier"  $(\theta, u) \in \mathcal{A}_\alpha$  by sampling in margin of uncertainty based on  $\Delta_\alpha$

- ▶ Define the probability of coverage

$$\pi_\alpha(\theta, u) = \mathbb{P}_Z [Z(\theta, u) - \alpha Z^*(u) \leq 0]$$

- ▶ Define  $\mathbb{M} = \{\pi_\alpha \in [\eta; 1 - \eta]\}$  → points where the classifier is not too "confident"
- ▶ Sample points in  $\mathbb{M}$ , and find centers of clusters using  $k$ -means.
- ▶ Adjust centroids to reduce either uncertainties on  $Z$  or on  $Z^*$



## Conclusion and perspectives

- ▶ Many criteria of robustness can be defined
- ▶ We propose regret based estimate, which can translate **risk-adverse** or **risk-seeking** strategies
- ▶ We propose adaptive enrichment methods to compute those estimates
- ▶ Alternatively, we can consider the optimization of the quantile  $Q_U \left( \frac{J(\theta, U)}{J^*(U)}, p \right)$
- ▶ Similar iterative methods can be derived using a GP approximation of  $Z/Z^*$

## References

Maria J. Bayarri, James O. Berger, Rui Paulo, Jerry Sacks, John A. Cafoe, James Cavendish, Chin-Hsu Lin, and Jian Tu. A framework for validation of computer models. *Technometrics*, 49(2):138–154, 2007.  
 V. Dubourg, B. Sudret, and J.-M. Bourinet. Reliability-based design optimization using kriging surrogates and subset simulation. *Structural and Multidisciplinary Optimization*, 44(5):673–690, November 2011.  
 Albert Tarantola. *Inverse Problem Theory and Methods for Model Parameter Estimation*. SIAM, Society for Industrial and Applied Mathematics, Philadelphia, Pa, 2005.  
 Victor Trappier, Élise Arnaud, Arthur Vidard, and Laurent Debreu. Robust calibration of numerical models based on relative regret. *Journal of Computational Physics*, page 109952, November 2020.  
 Victor Trappier. *Contrôle de Paramètre En Présence d'incertitudes*. These de doctorat, Université Grenoble Alpes, June 2021.