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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...)

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

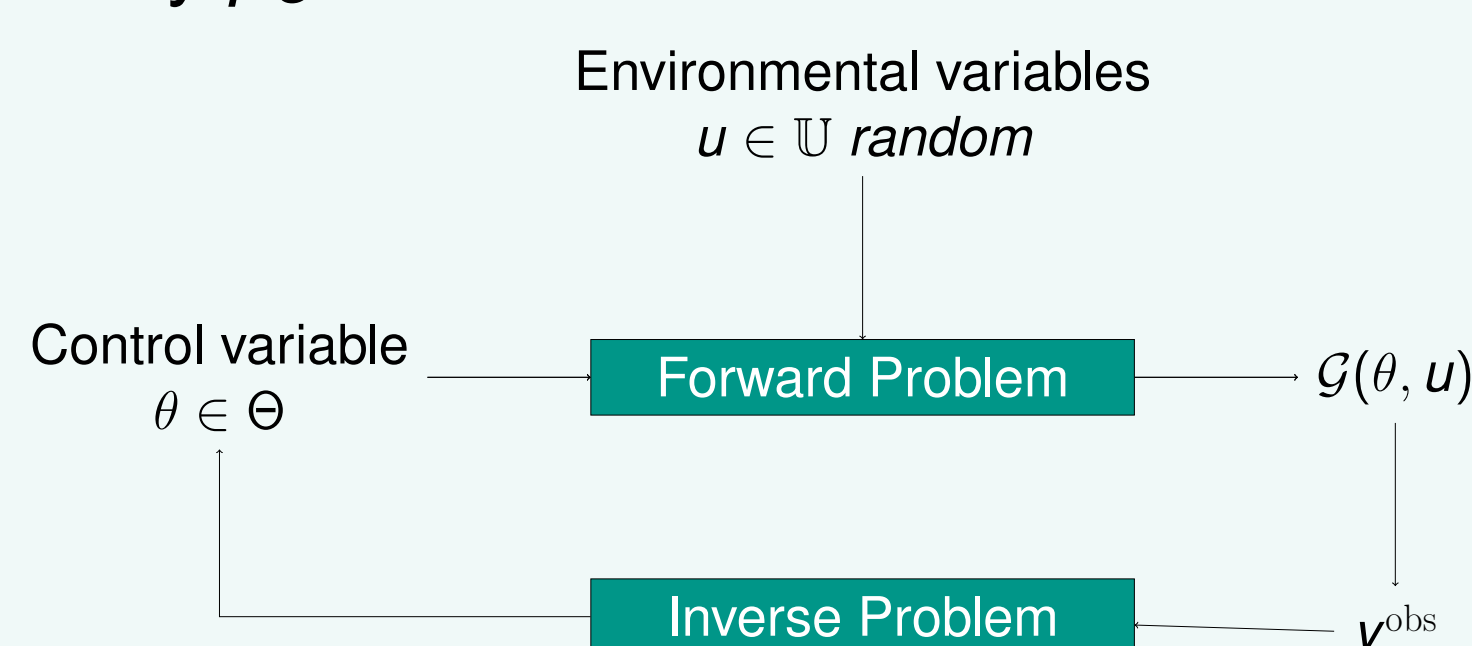
Given some observations y^{obs} , the MSE is

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

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 θ , 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 θ

- ▶ 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

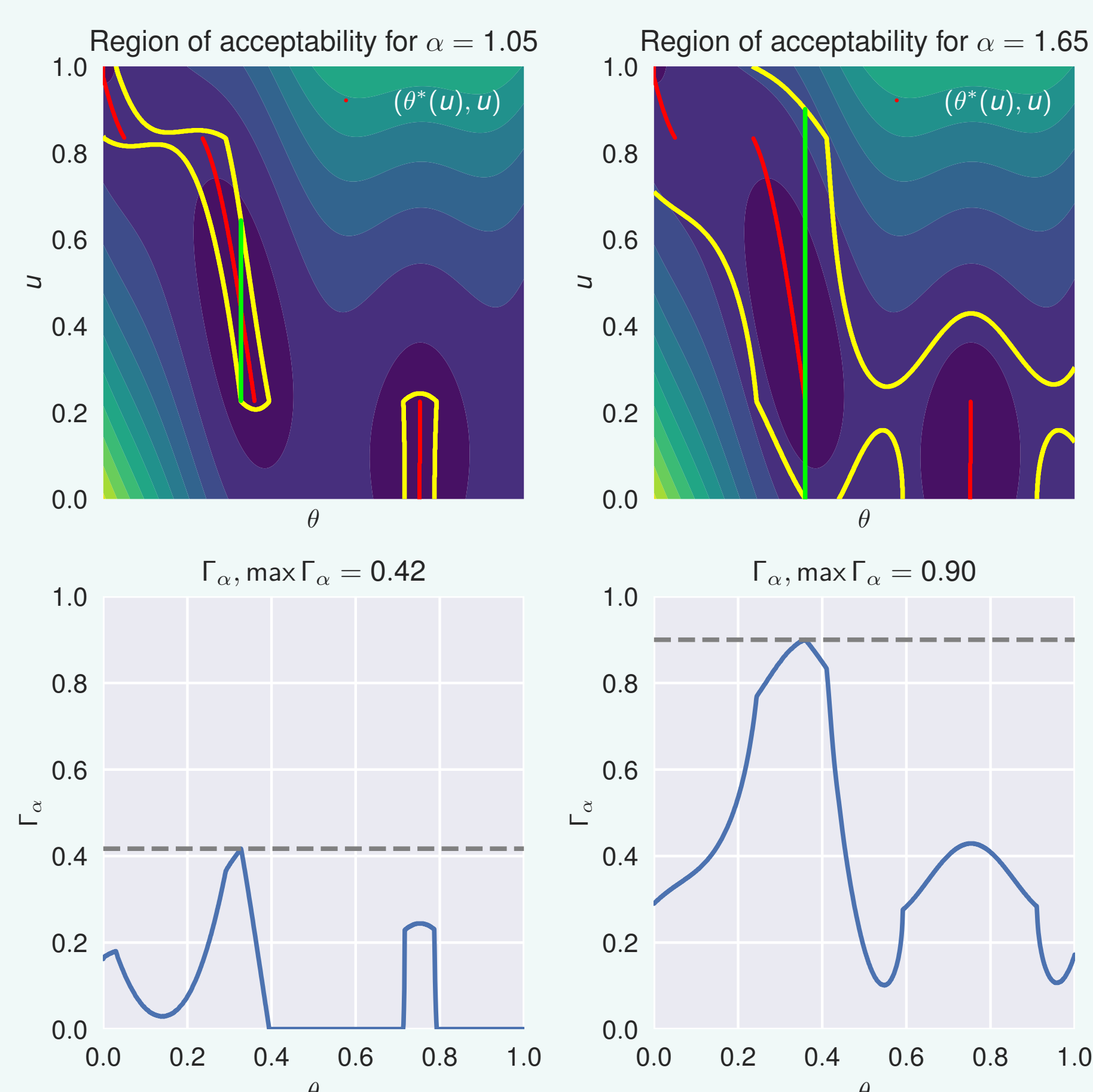
α -acceptability [TAVD20]

Given $u \in \mathbb{U}$

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

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

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



- ▶ Large α : Conservative, performances controlled with high probability
 - ▶ Small α : 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

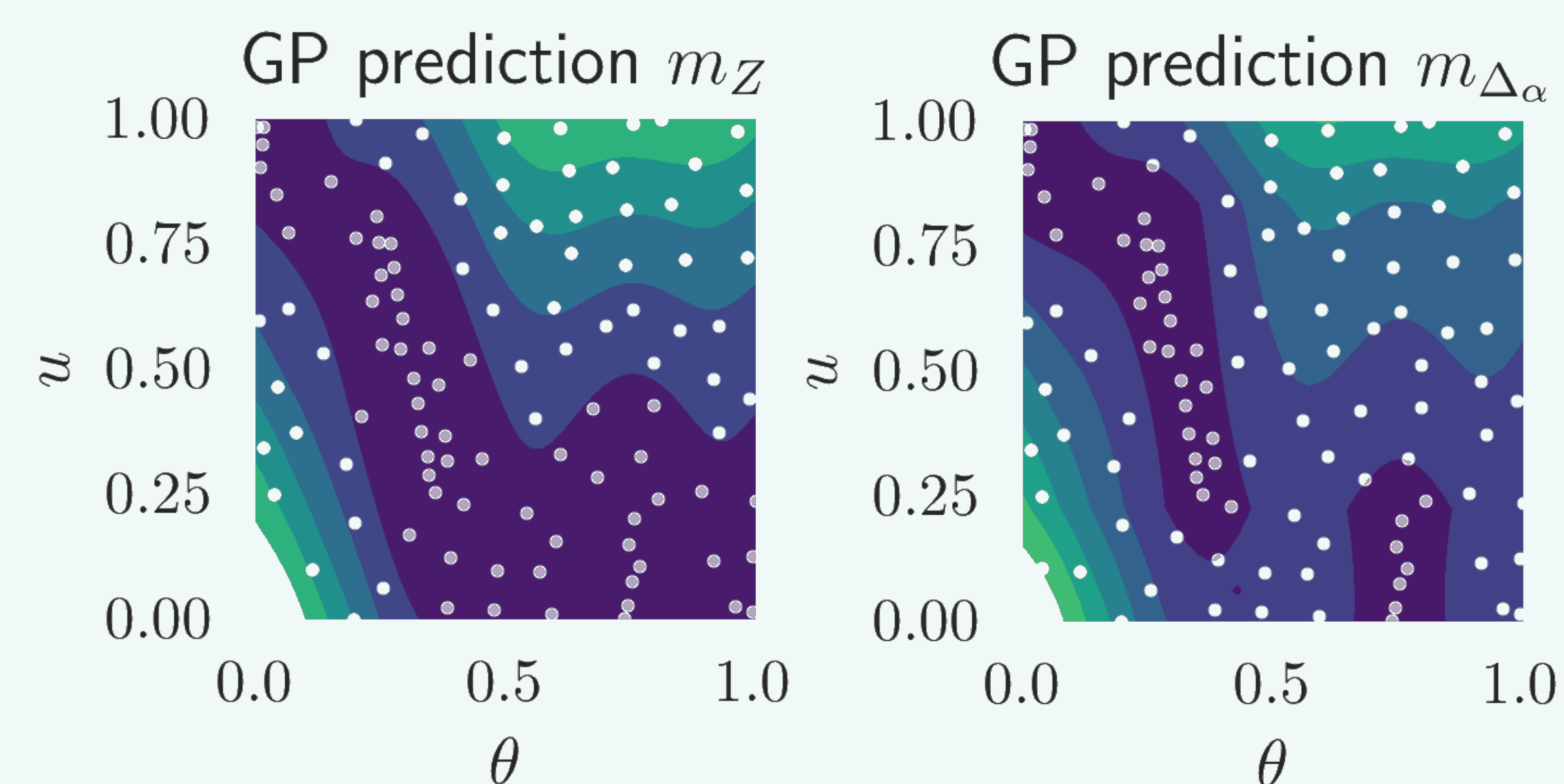
Approximation error (θ, u) comes from:

- ▶ 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:

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



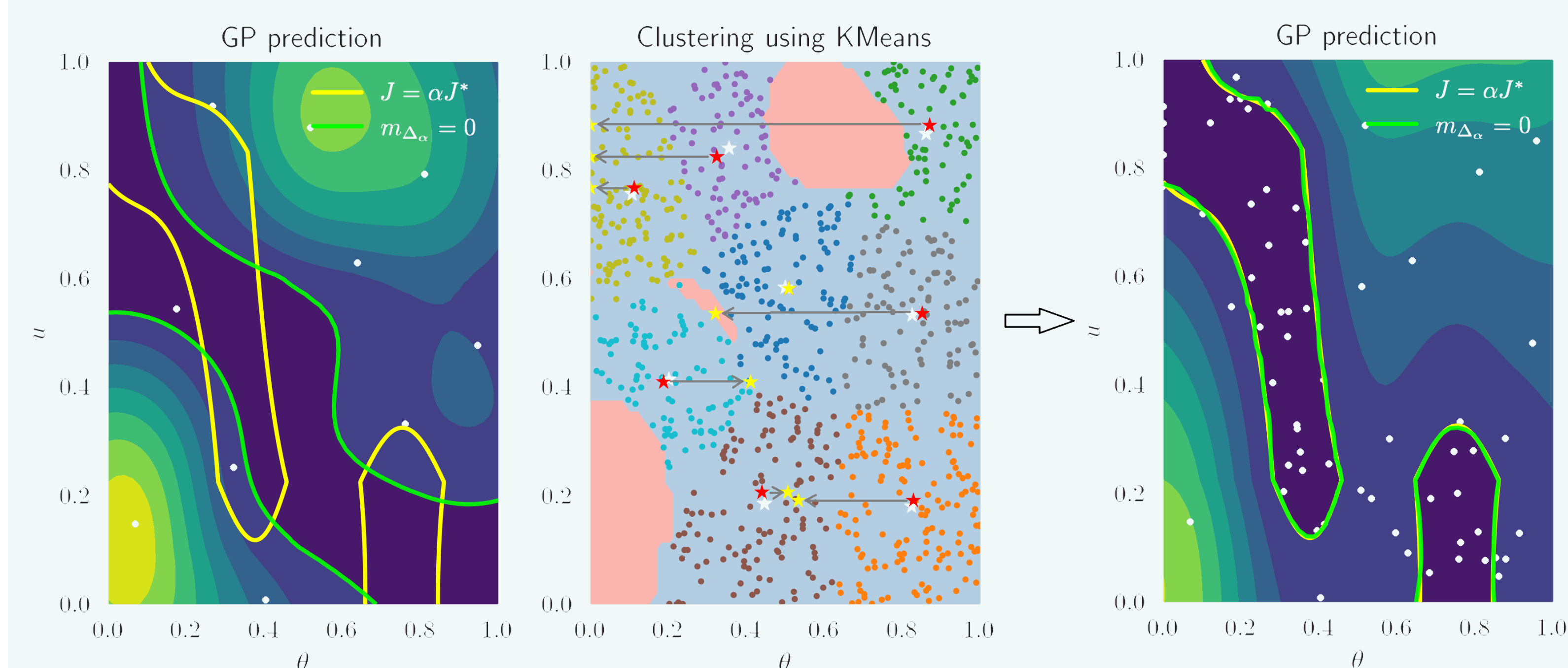
k-batch approach ([DSB11])

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

- ▶ 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^*

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