



HAL
open science

Regret-based calibration using GPs

Victor Trappier, Élise Arnaud, Laurent Debreu, Arthur Vidard

► **To cite this version:**

Victor Trappier, Élise Arnaud, Laurent Debreu, Arthur Vidard. Regret-based calibration using GPs. Journées CIROQUO 2022, May 2022, Grenoble, France. hal-03681091

HAL Id: hal-03681091

<https://hal.science/hal-03681091v1>

Submitted on 30 May 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Regret-based calibration using GPs

Victor Trappier^{‡, §}, Élise Arnaud[‡], Laurent Debreu[‡], Arthur Vidard[‡]

victor.trappier@inria.fr

[‡] AIRSEA Research team (INRIA) – Laboratoire Jean Kuntzmann

[§] AI4Sim R&D team (ATOS)



JOURNÉES CIROQUO, GRENOBLE 2022

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...)

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

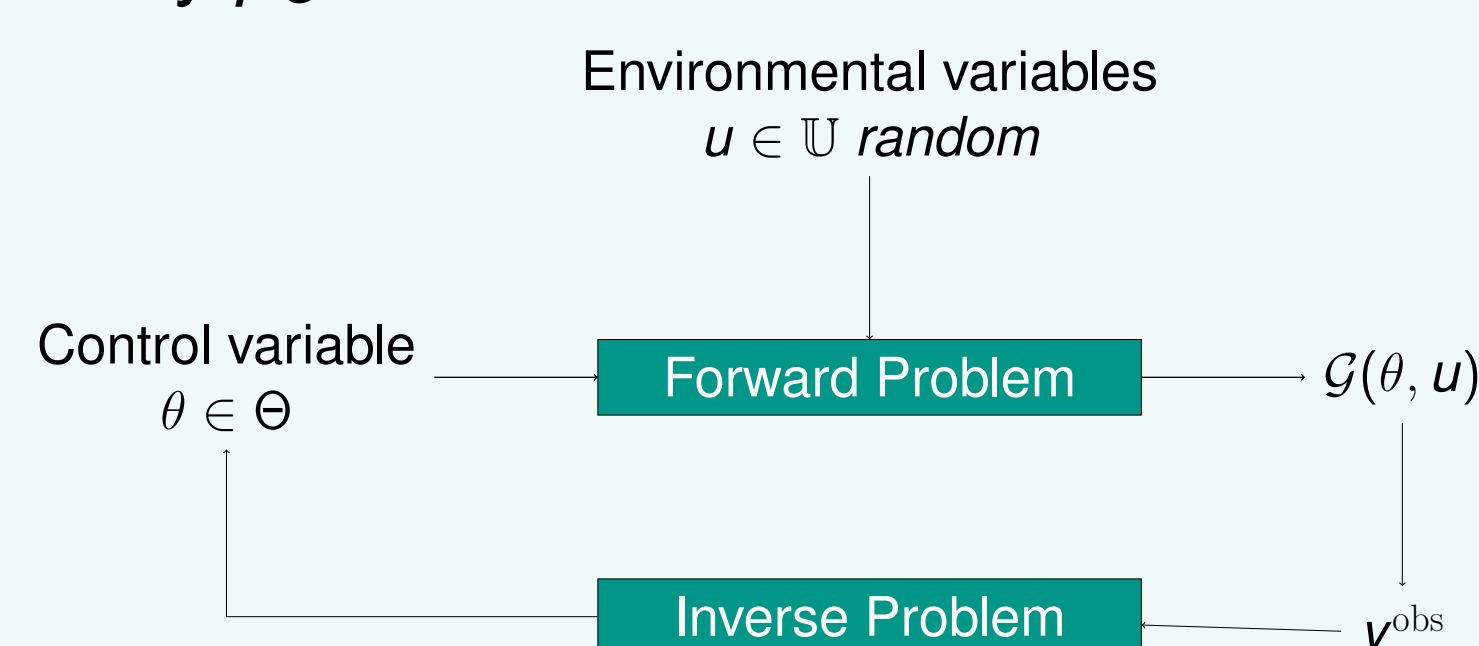
Given some observations y^{obs} , the MSE is

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

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

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

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

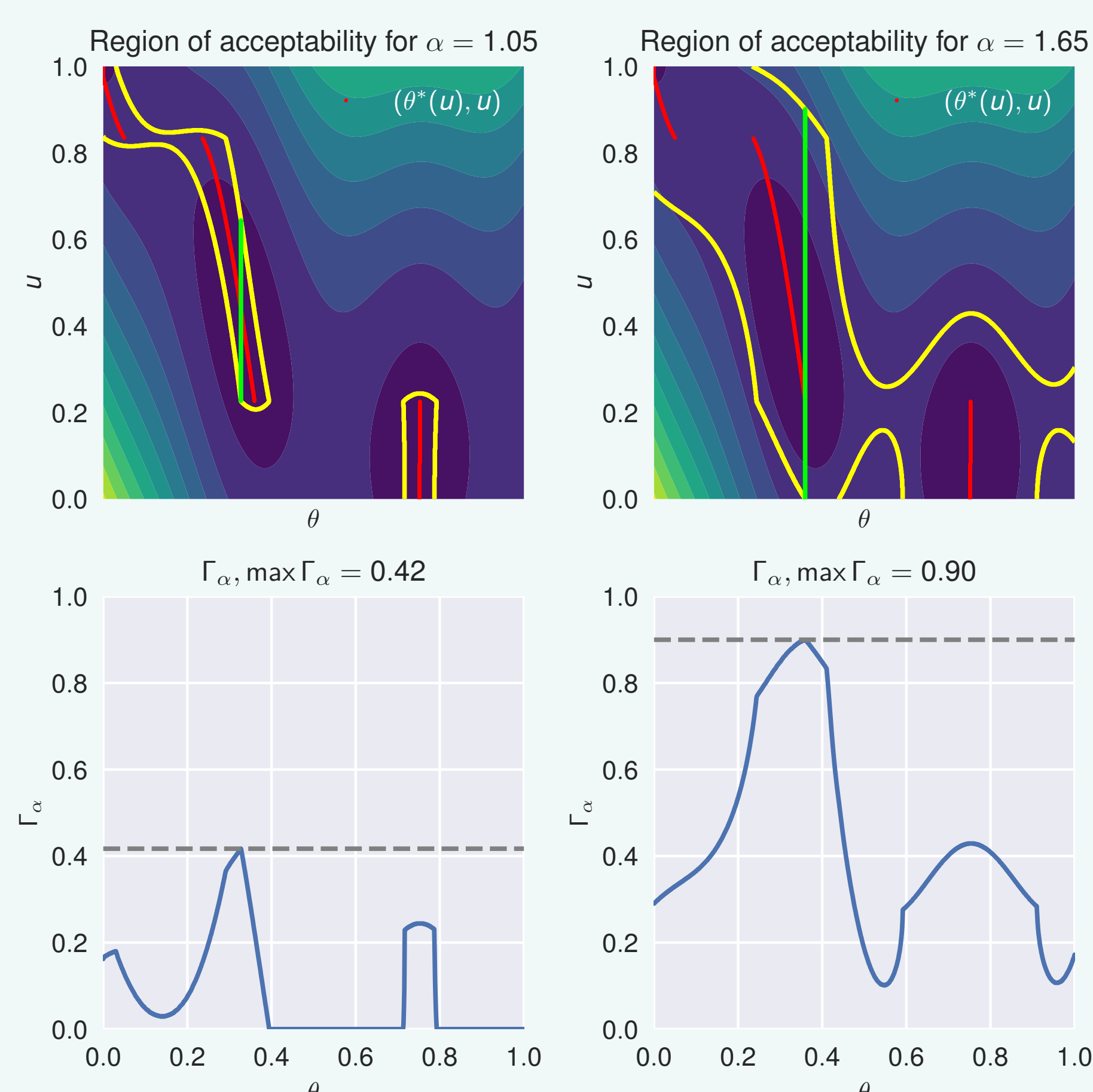
α -acceptability [TAVD20]

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

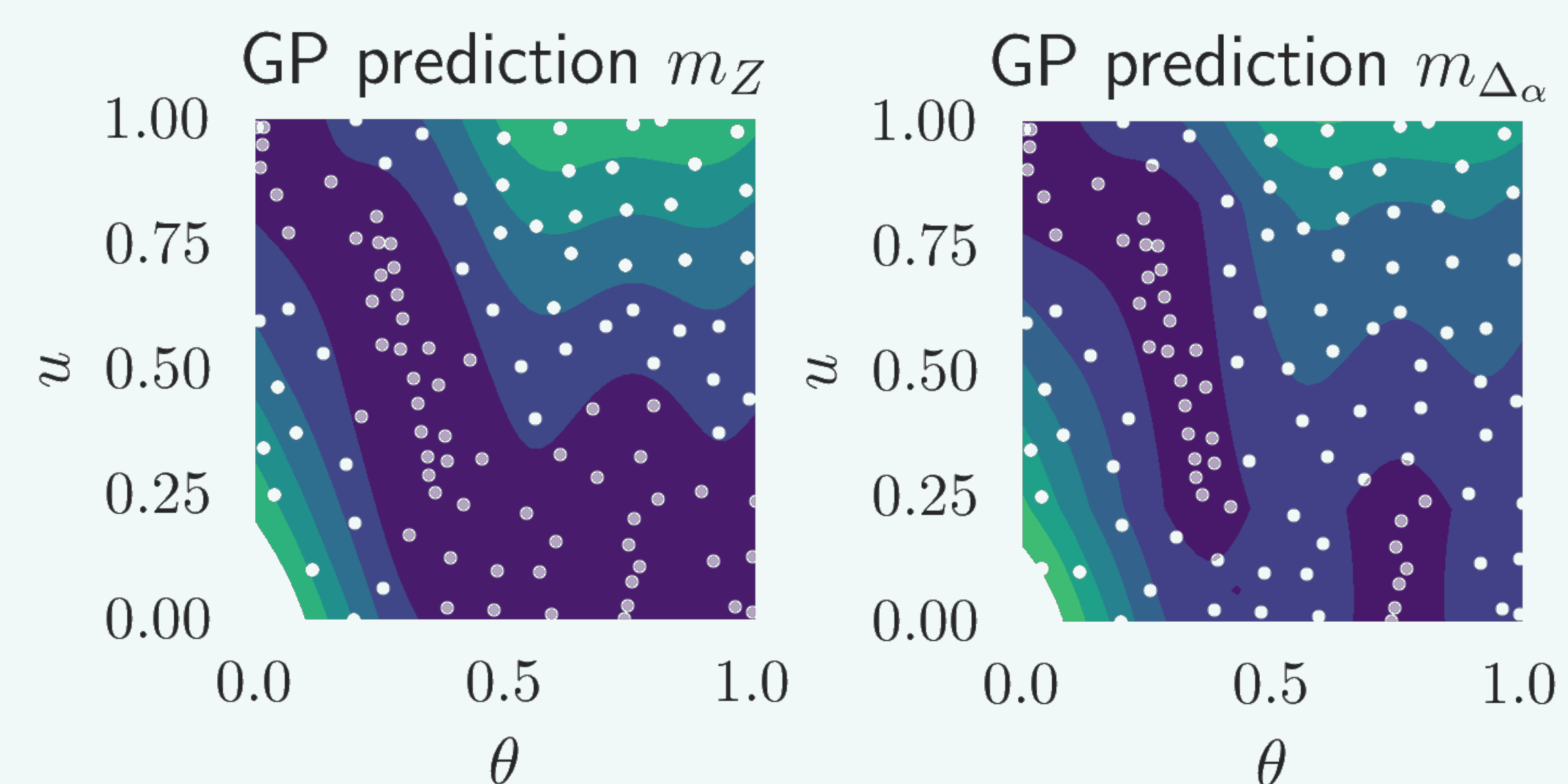
Approximation error (θ, u) comes from:

- ▶ 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:

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



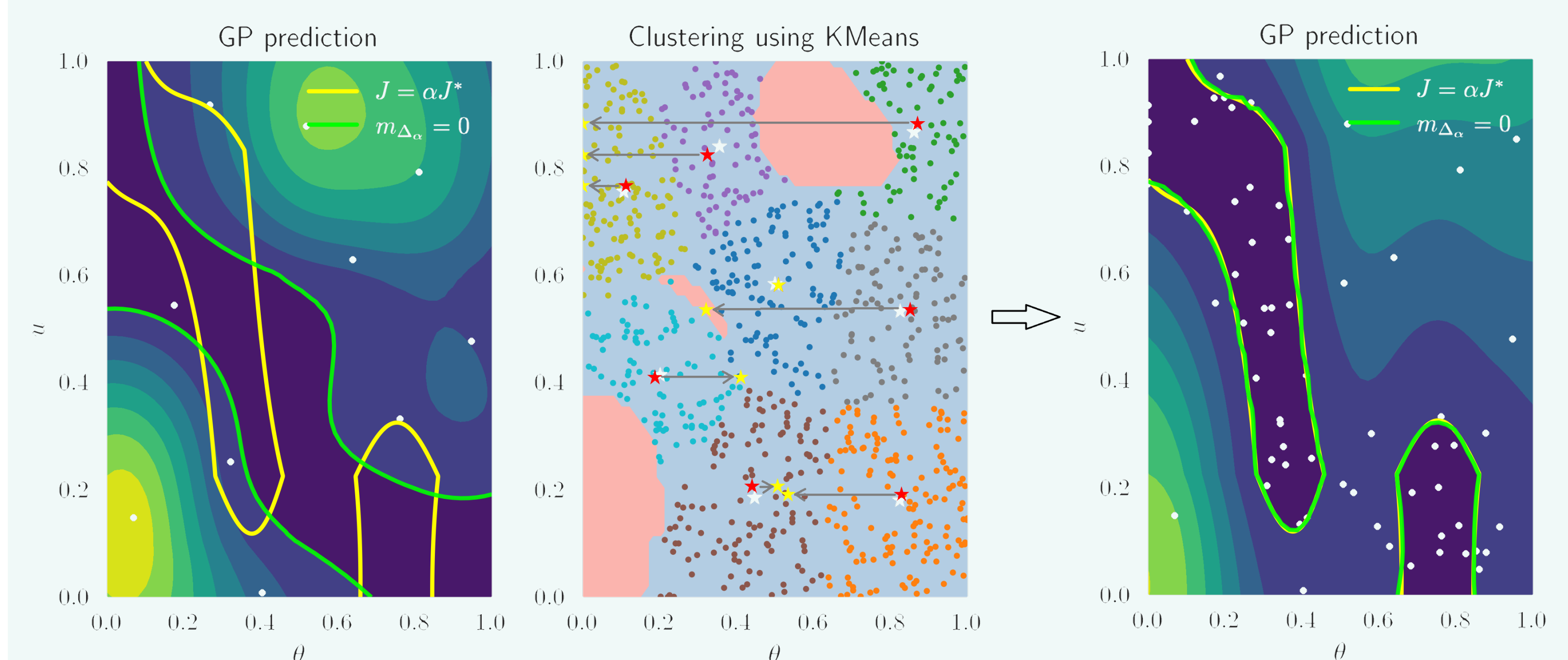
k-batch approach ([DSB11])

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^*

References

Maria J. Bayarri, James O. Berger, Rui Paulo, Jerry Sacks, John A. Cafeo, 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.