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Uncertainty quantification oriented active learning for surrogates of simulators with functional outputs

L. Brunel^{1,2}, M. Balesdent¹, L. Brevault¹, R. Le Riche² & B. Sudret³

ECCOMAS, Lisbon, Portugal

- 5 June 2024 -

¹ONERA, Paris Saclay University, ²LIMOS (CNRS, Mines Saint-Etienne and Université Clermont Auvergne), ³ETH Zürich

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Introduction

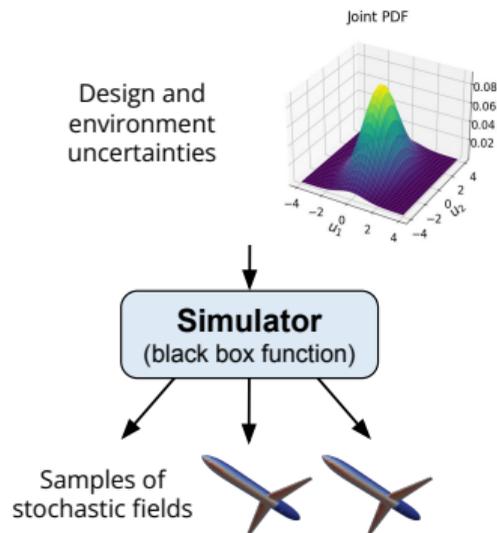
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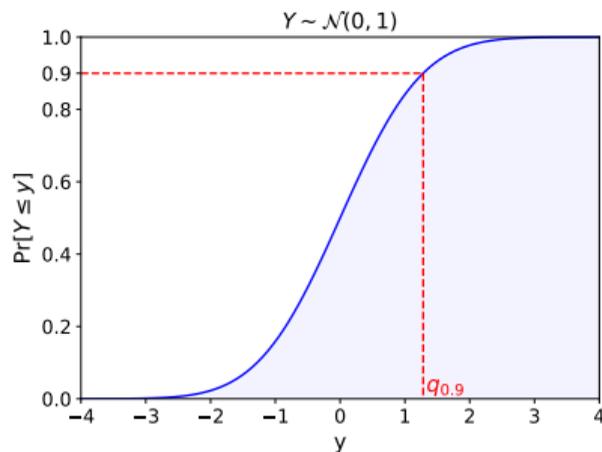


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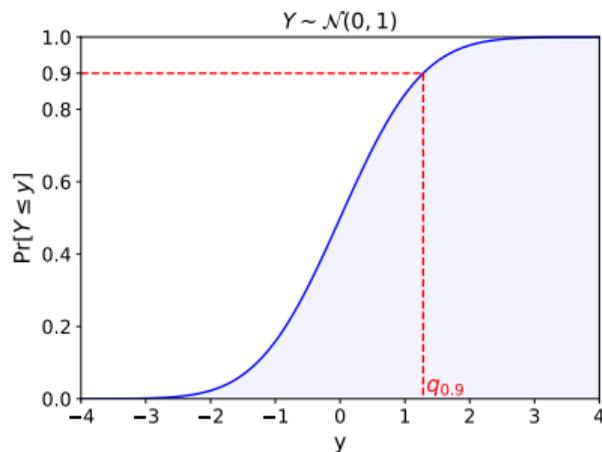


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- The estimation requires many runs of the costly simulator \Rightarrow need for **surrogate modeling**

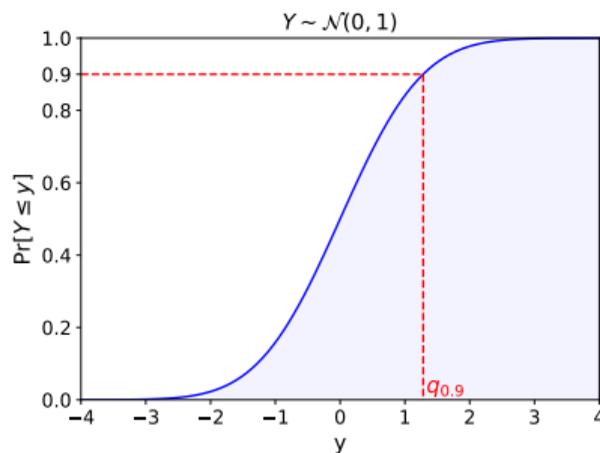


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Dimensionality reduction (DR)¹

- Exploits the spatial/temporal/*etc.* correlation of the field to describe it with a reduced set of **latent variables** z

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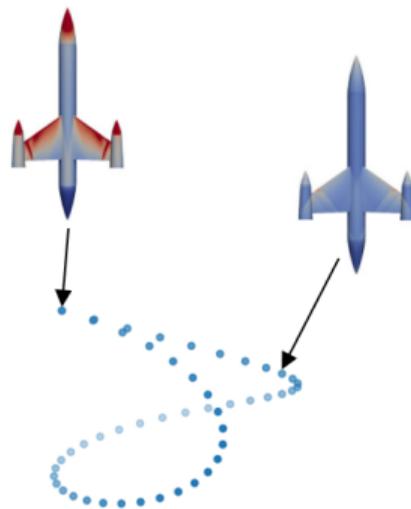
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- To each **snapshot** of the output field corresponds a point in the **low-dimensional latent space**

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- Example (on the right): snapshots are mapped to a 1-dimensional manifold



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Dimensionality reduction (DR)

Principal component analysis (PCA)²

- The mapping between the snapshots \mathbf{y} and the latent space is **linear**

$$\mathbf{y}(\mathbf{u}, x) = \sum_{i=1}^N \phi_i(x) z_i(\mathbf{u})$$

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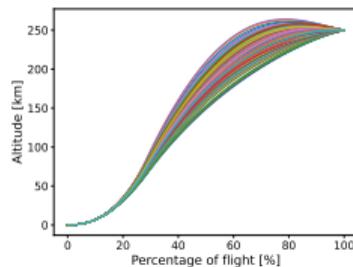
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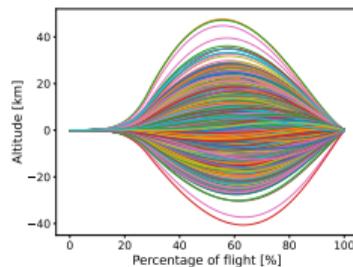
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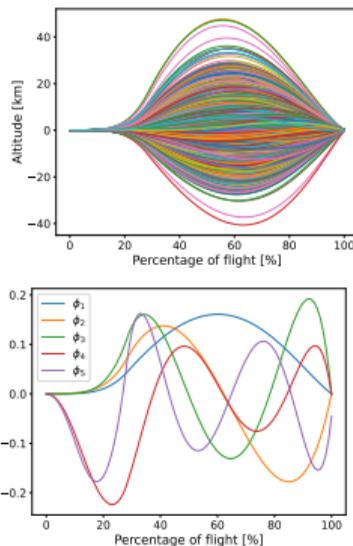
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Gaussian process regression³ in the latent space

- Probabilistic machine learning model

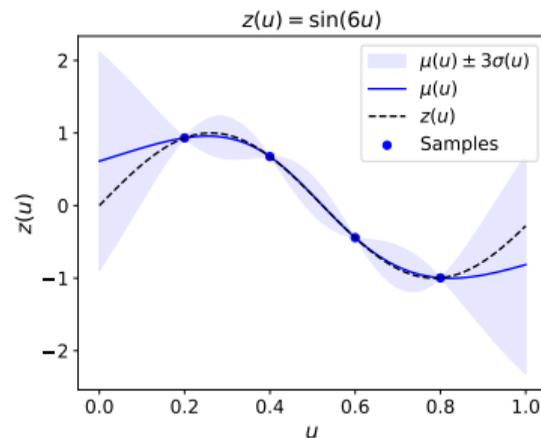


Figure: Gaussian process regression

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Gaussian process regression³ in the latent space

- Probabilistic machine learning model
- The latent variables are modeled by a **Gaussian process (GP)**:

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with $\mu_i(\cdot)$ the mean and $k_i(\cdot, \cdot)$ the covariance function

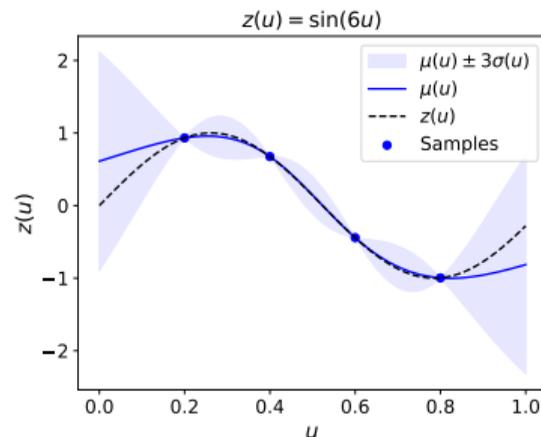


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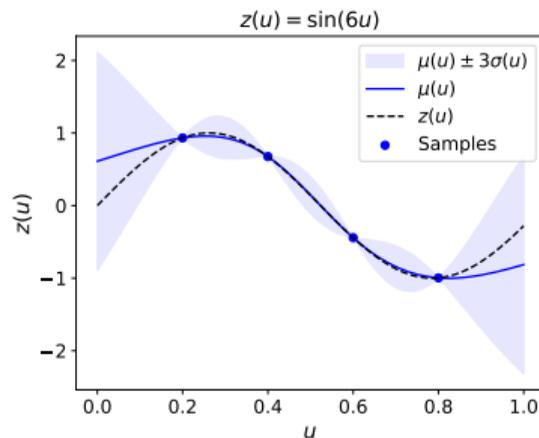


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- Used as the **latent surrogate model (LSM)**

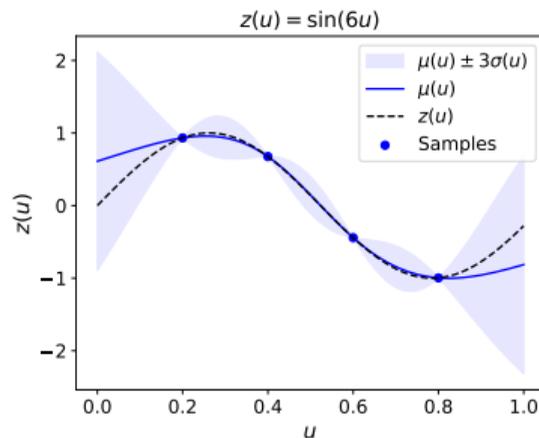
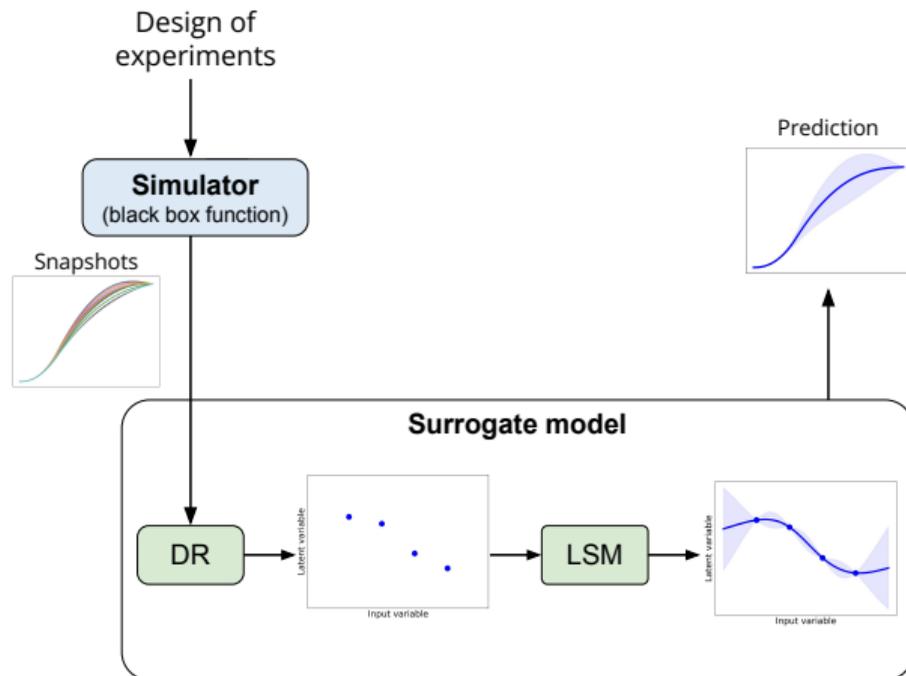


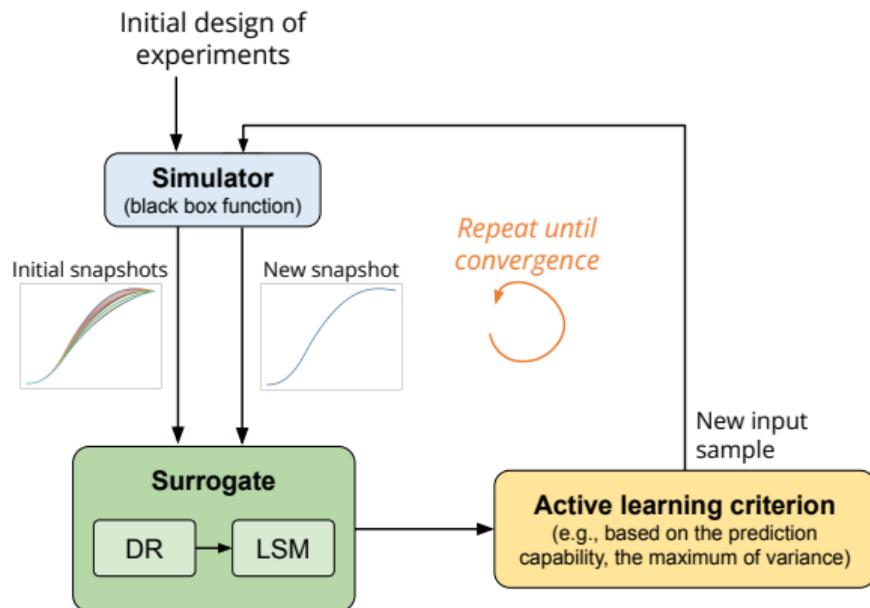
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Surrogate model with functional outputs



Active learning



UQ oriented active learning with scalar outputs

- The learning function $g(\cdot)$ is a compromise between points that are **close to the estimated quantile** \hat{q}_α (numerator) and points where the **prediction variance is high** (denominator)⁴

$$g(\mathbf{u}) = \frac{|\mu(\mathbf{u}) - \hat{q}_\alpha|}{\sigma(\mathbf{u})} \quad (2)$$

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- The sample that will be added is \mathbf{u}^* such that

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Extension to functional outputs

- Extension to functional outputs by taking the **integral of the field over the mesh** \mathcal{X}^5

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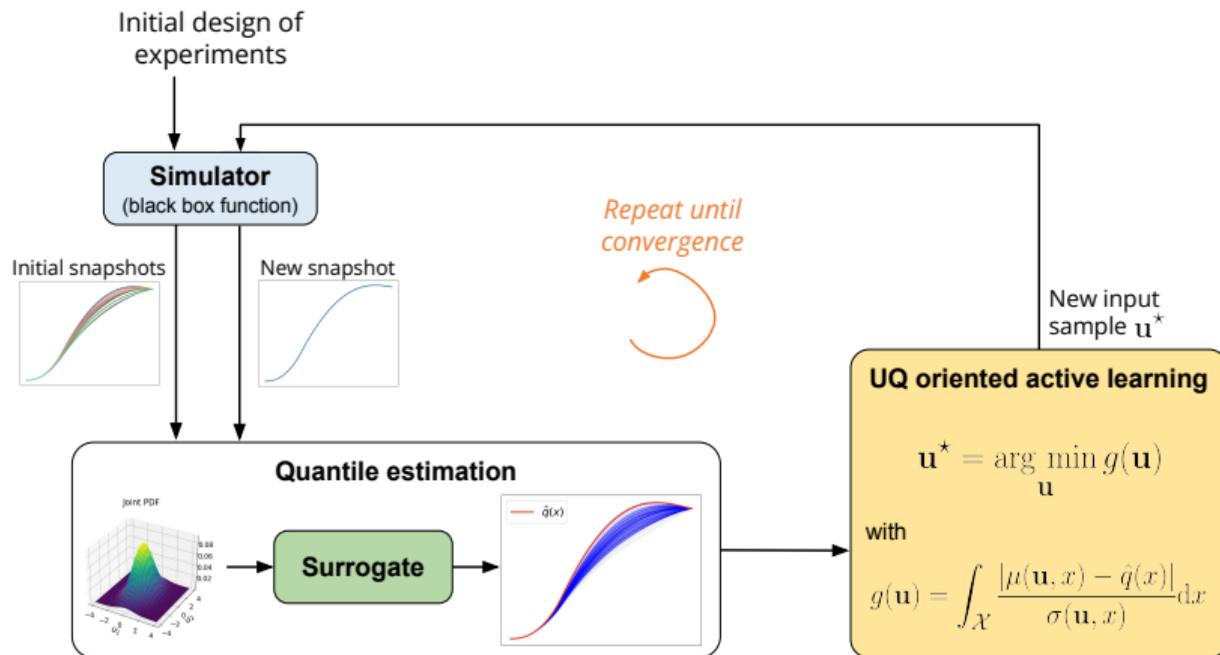
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UQ oriented active learning with functional outputs

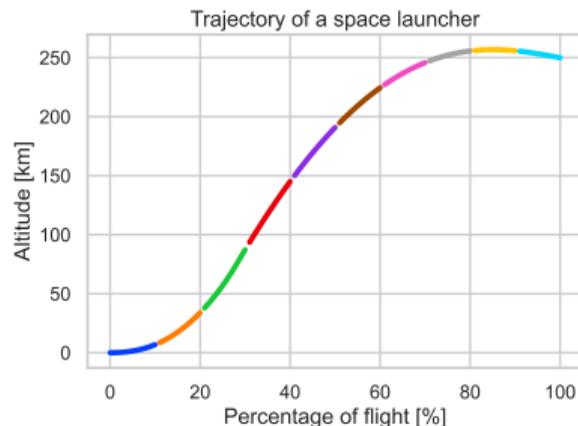


The problem with functional quantiles

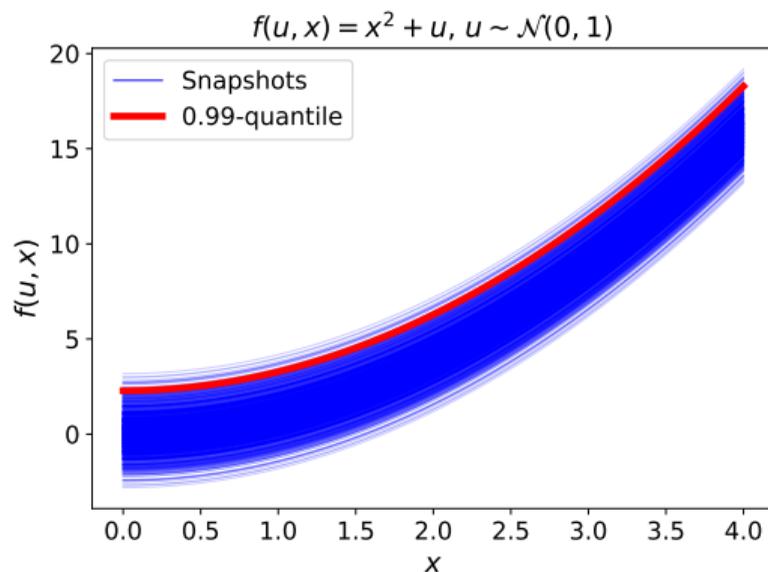
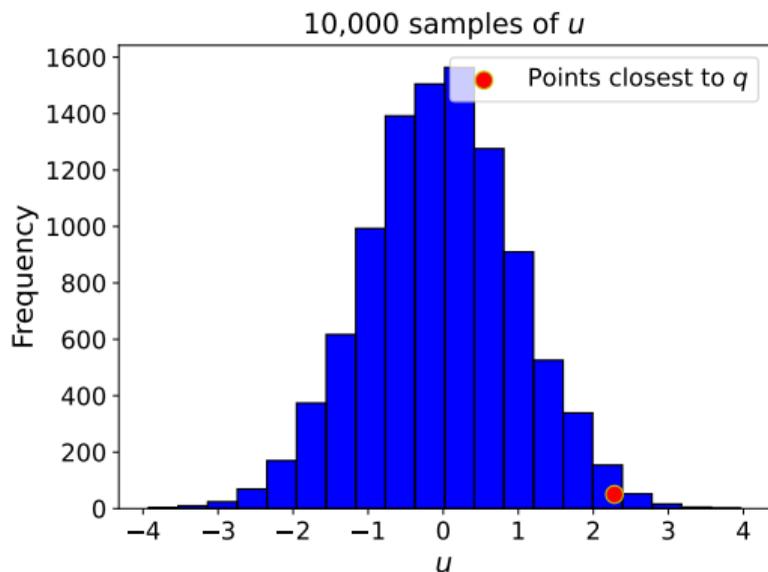
- With functional outputs, the quantile might not correspond to any snapshot but rather a **composition of snapshots**

The problem with functional quantiles

- With functional outputs, the quantile might not correspond to any snapshot but rather a **composition of snapshots**
- To illustrate, we divide the mesh into multiple sections and measure which snapshot is the closest to the quantile for each section

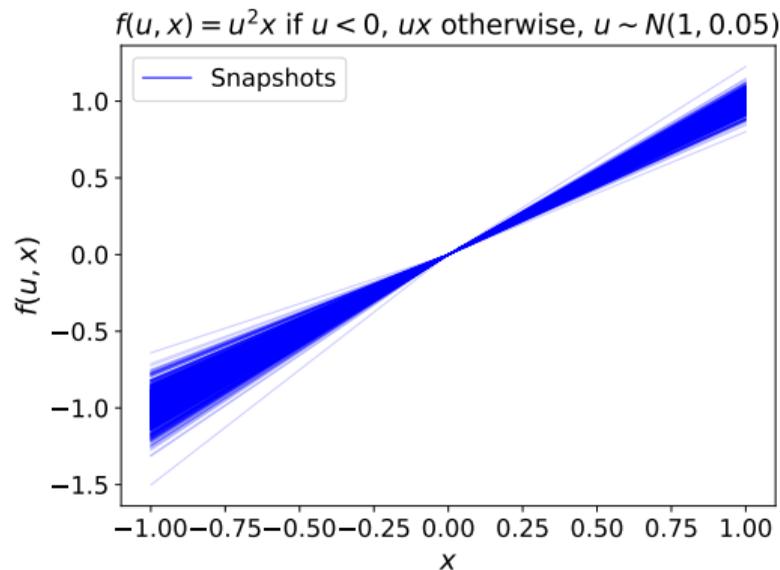
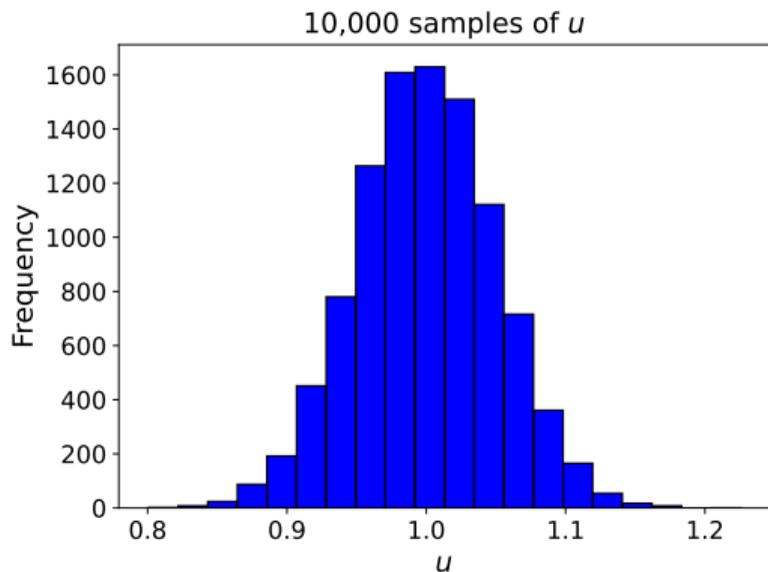


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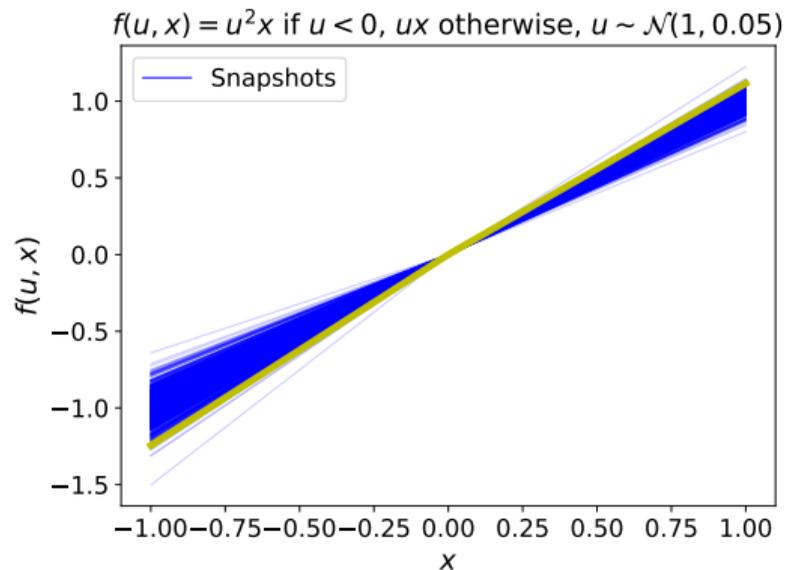
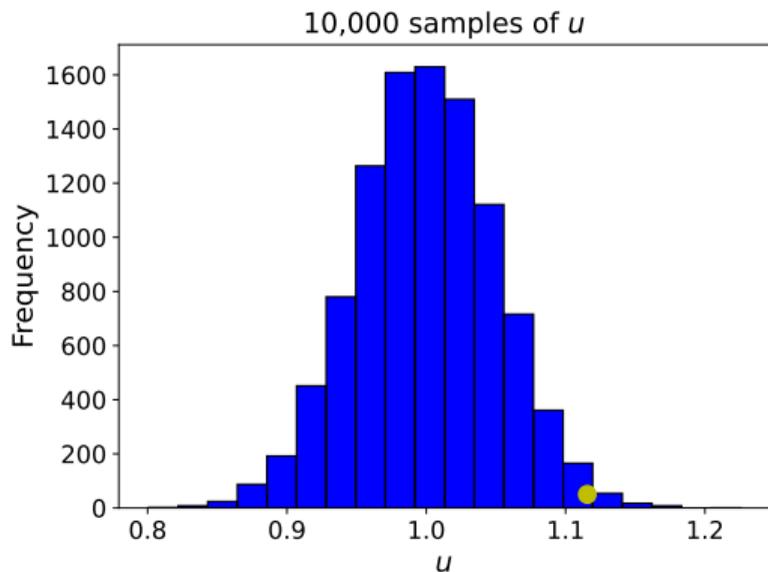


⇒ the quantile corresponds to a single snapshot, *i.e.*, one point in the input space

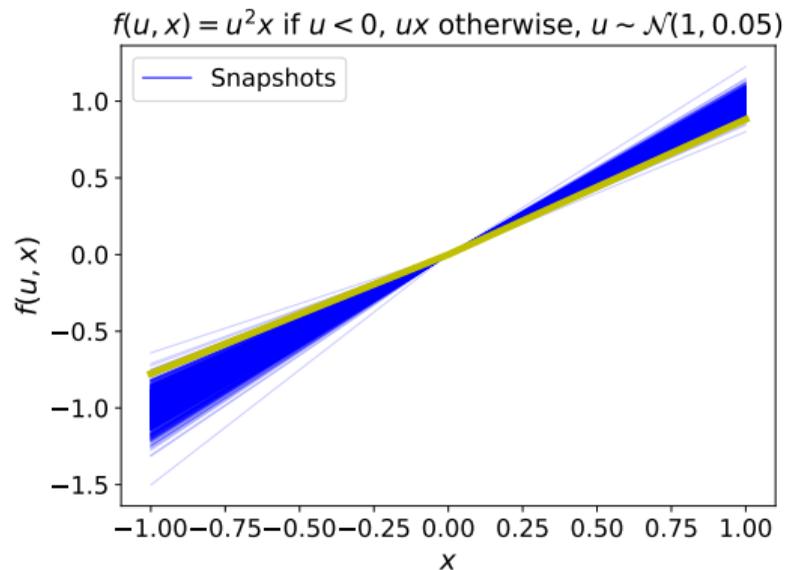
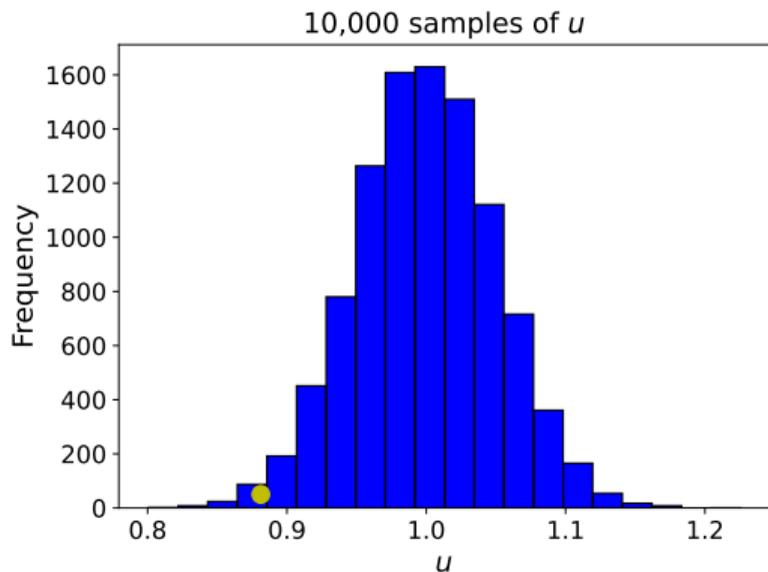
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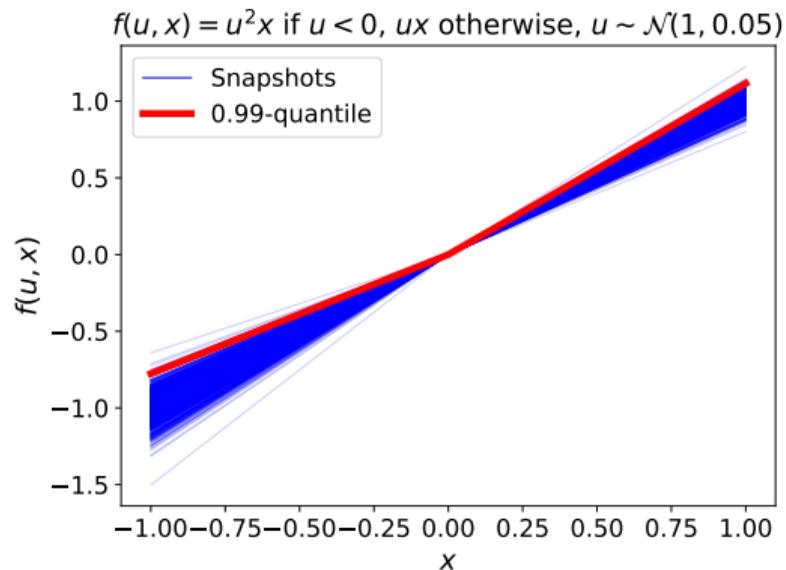
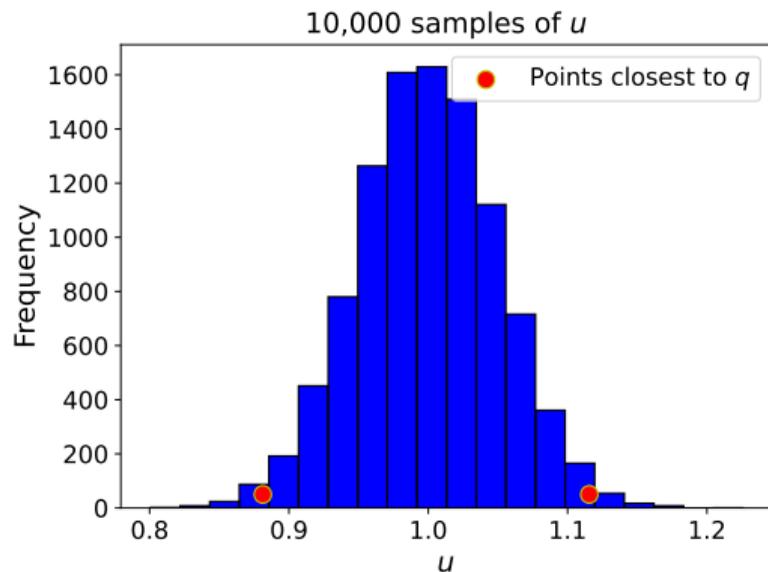
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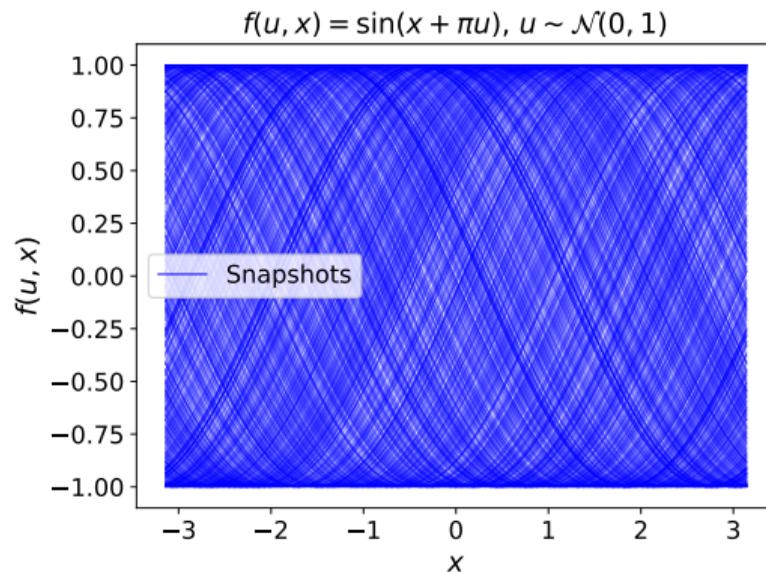
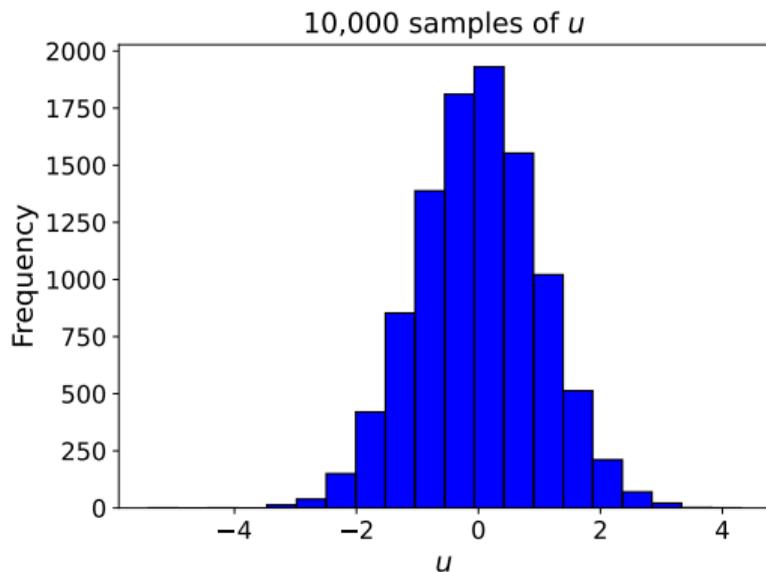


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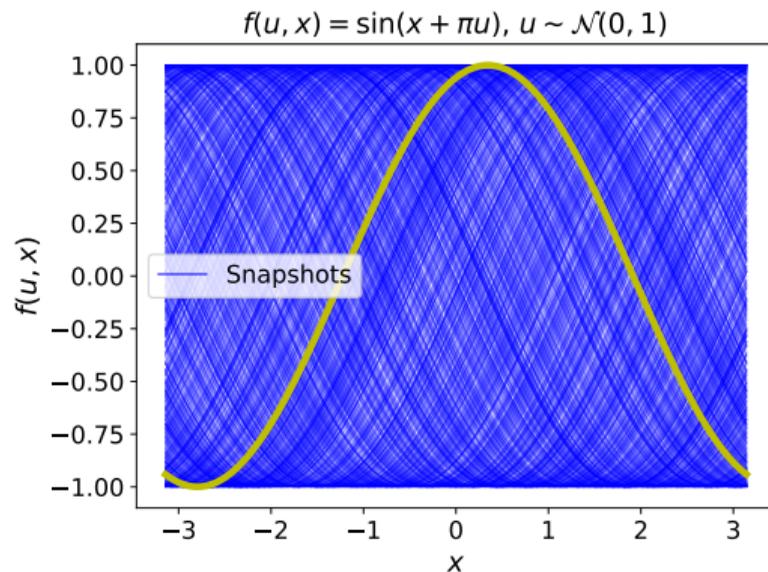
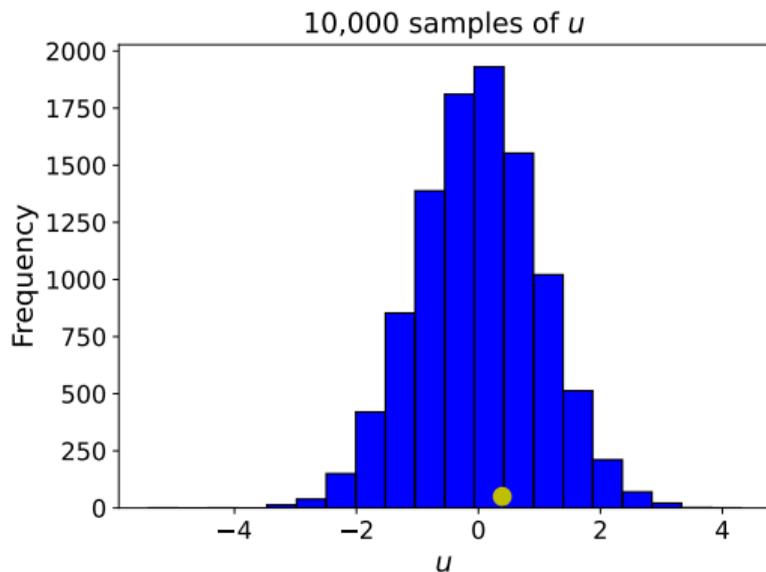


⇒ the quantile corresponds to two snapshots, *i.e.*, two points in the input space

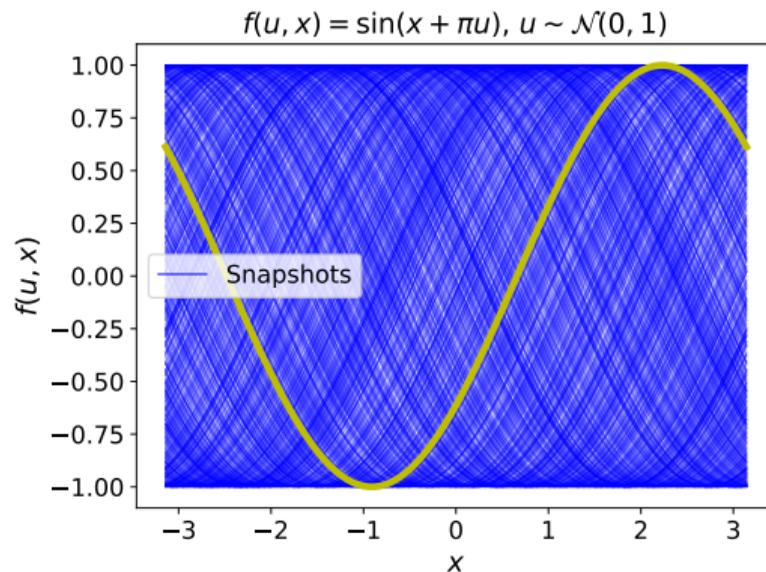
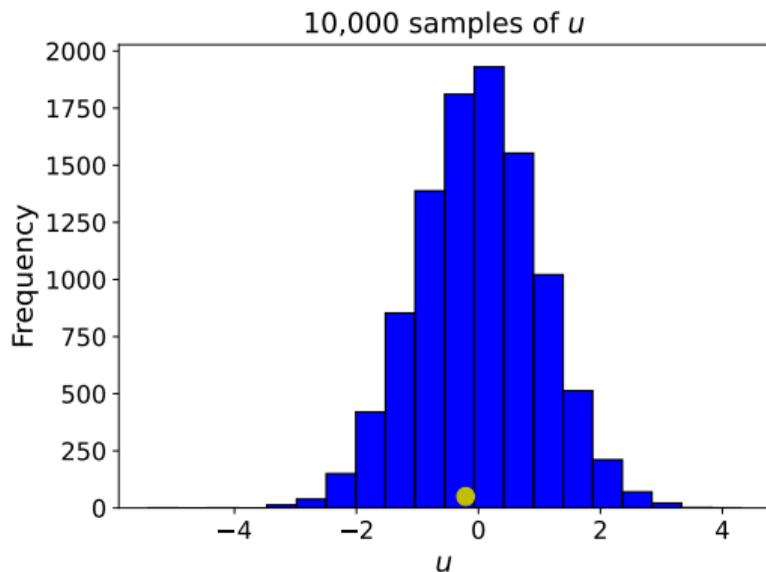
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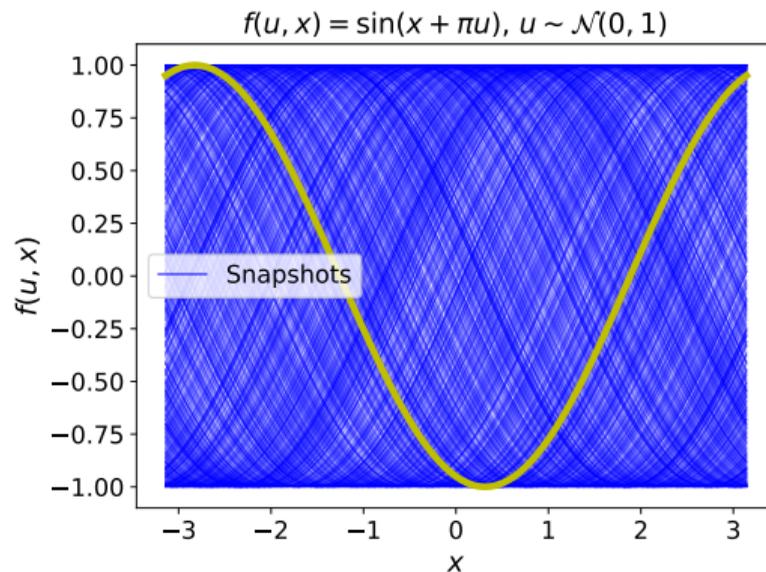
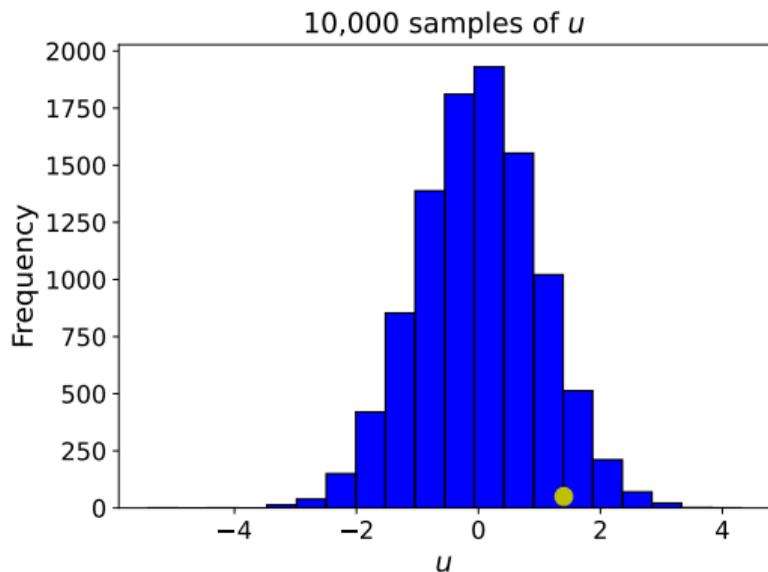
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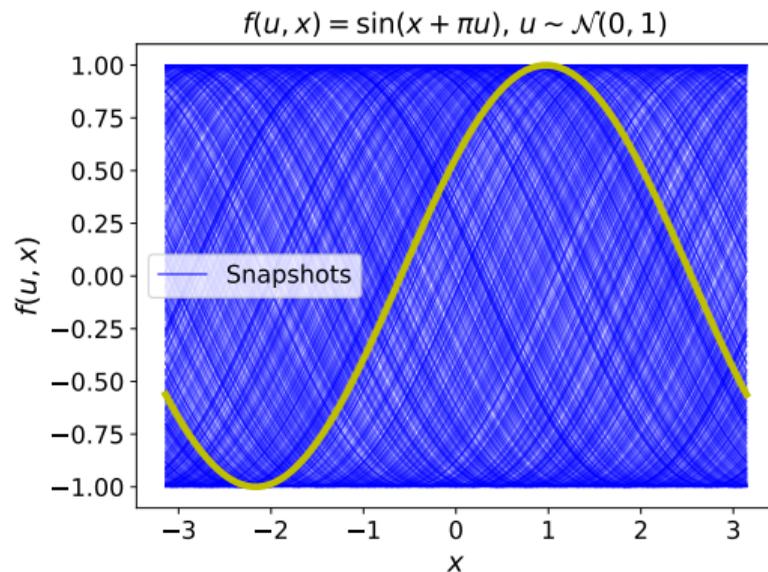
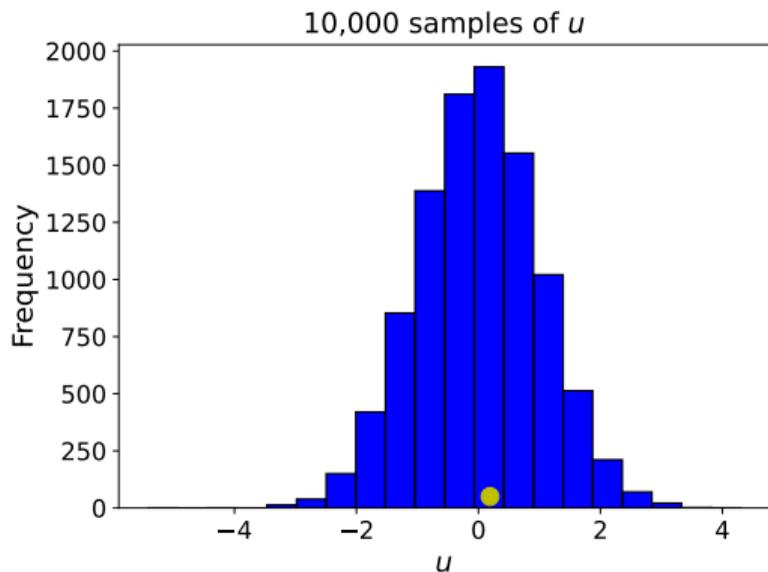
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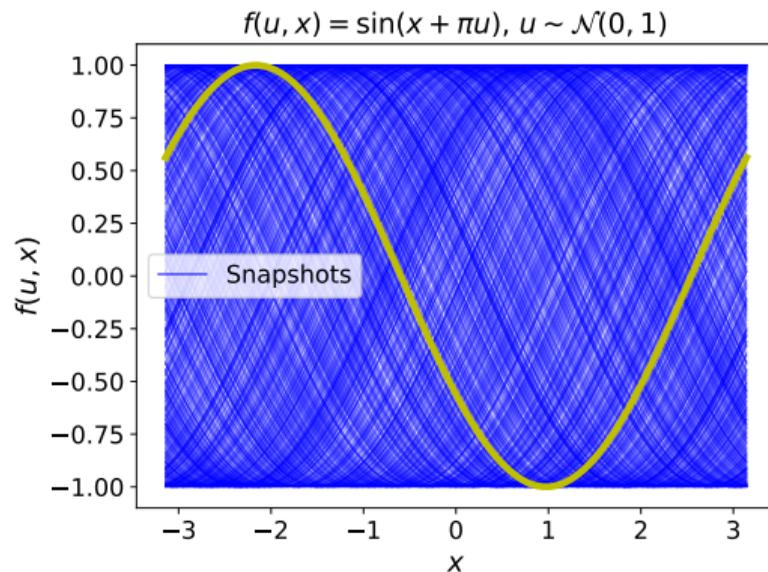
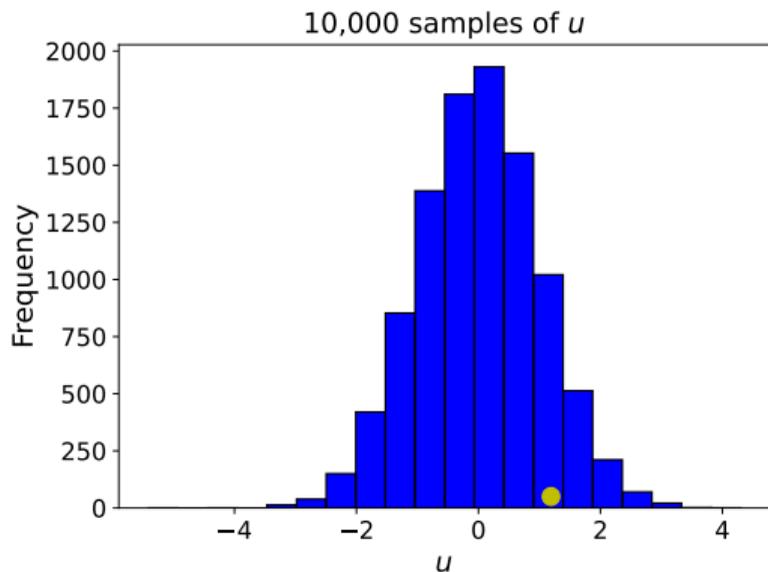
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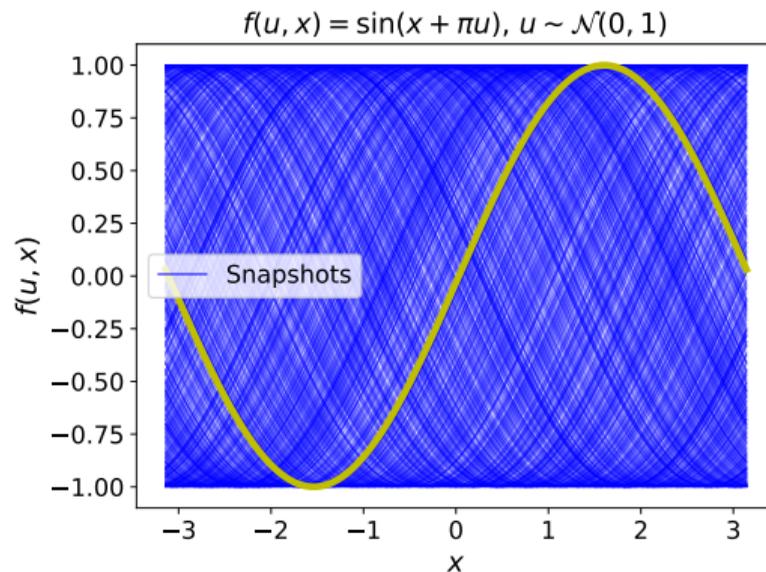
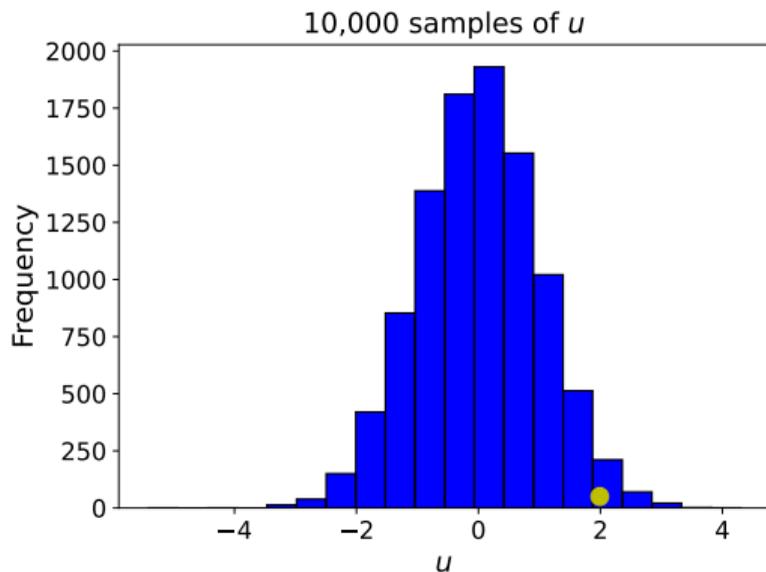
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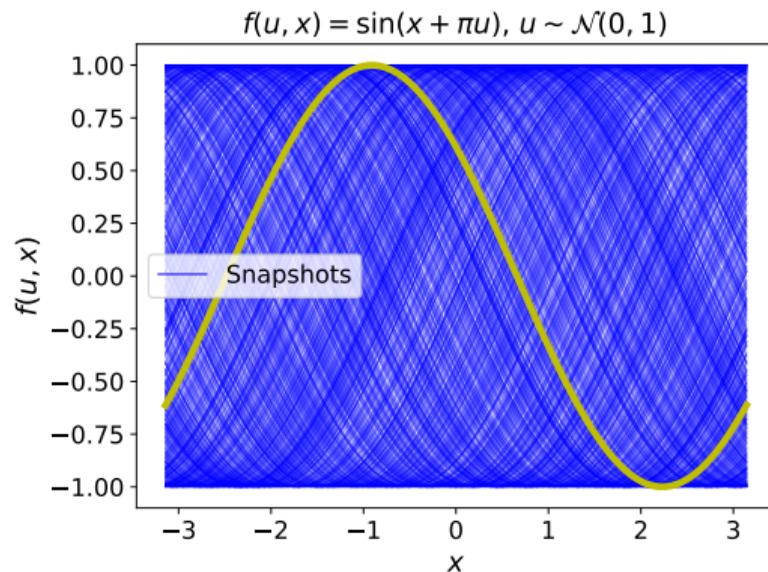
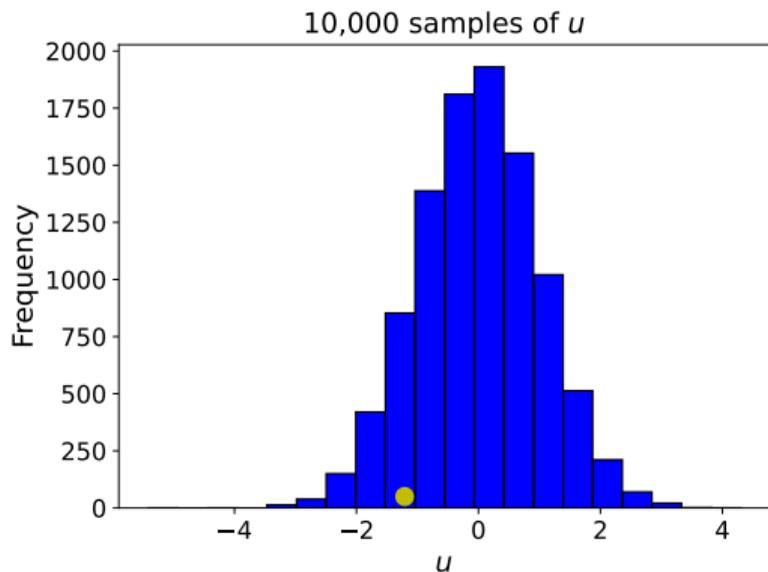
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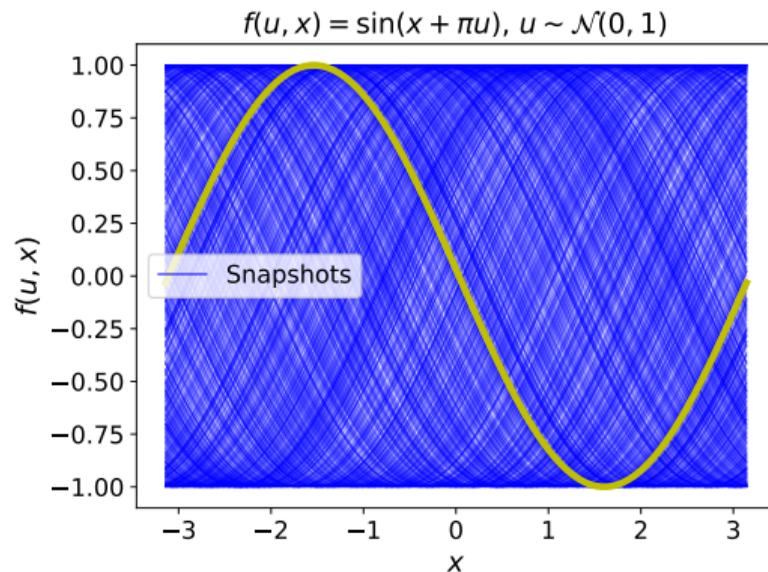
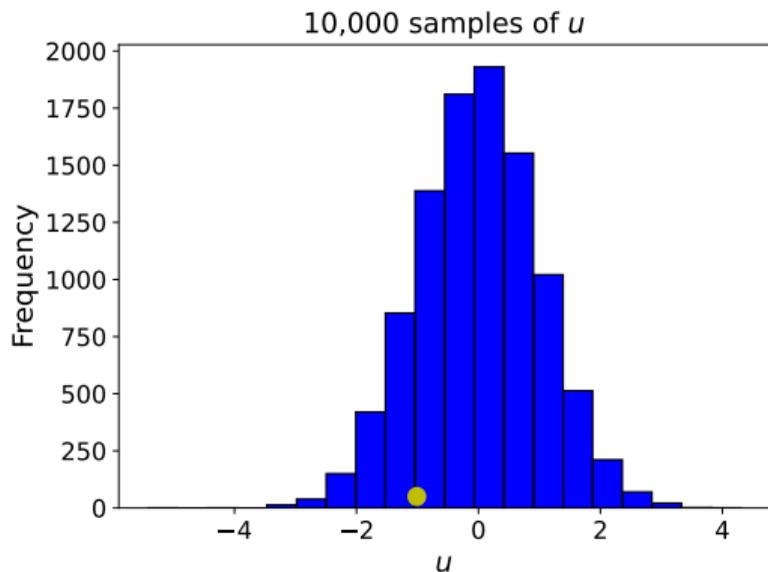
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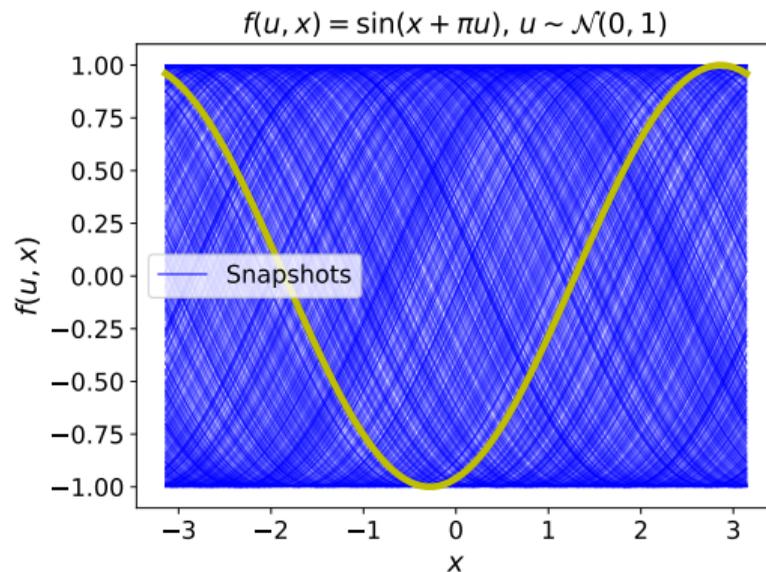
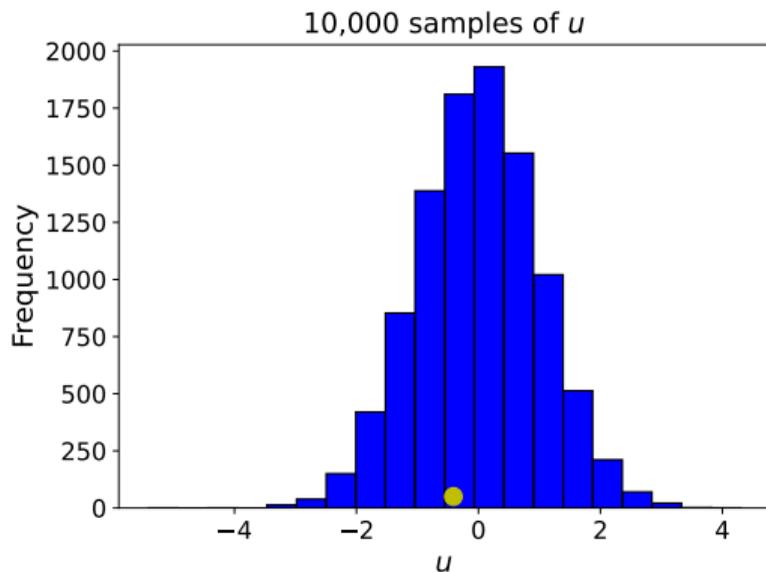
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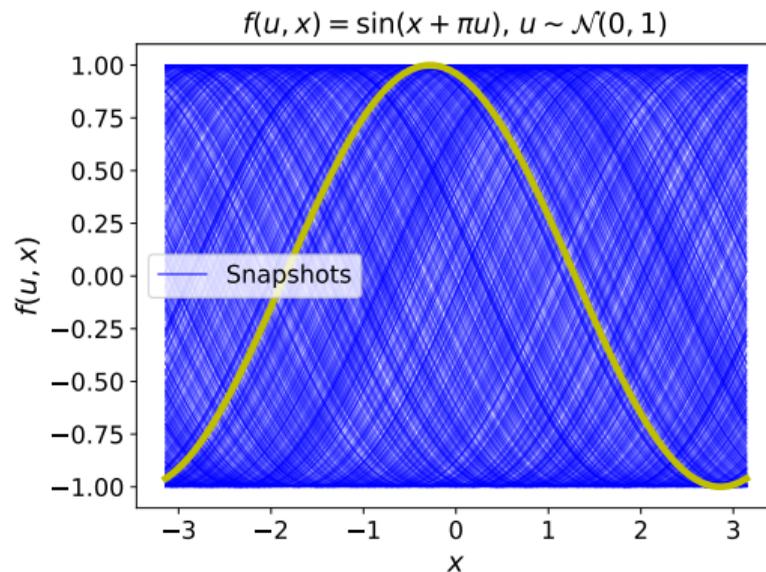
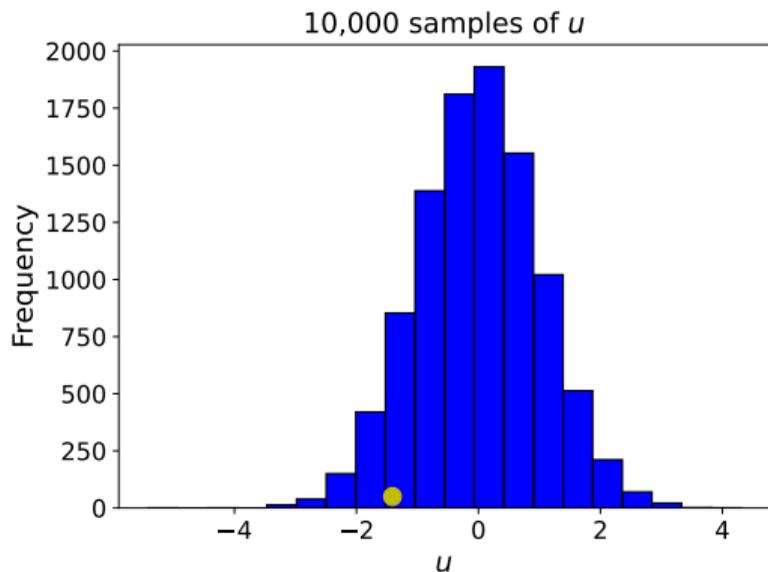
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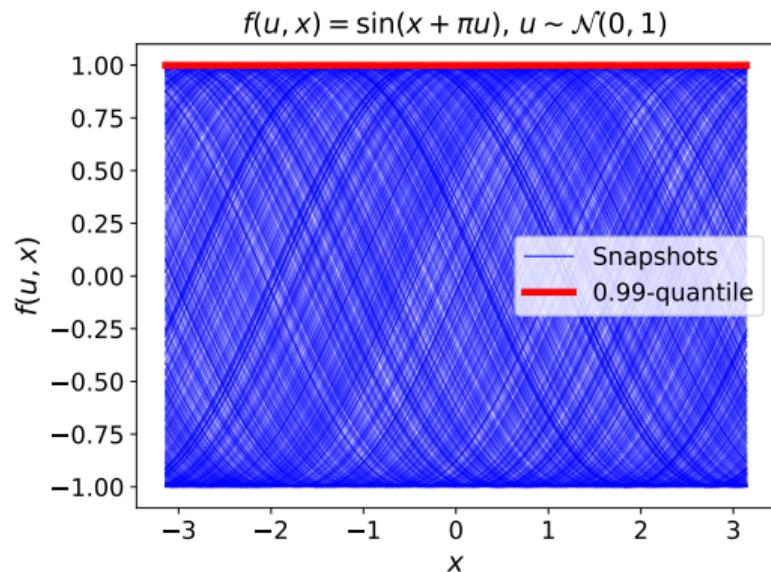
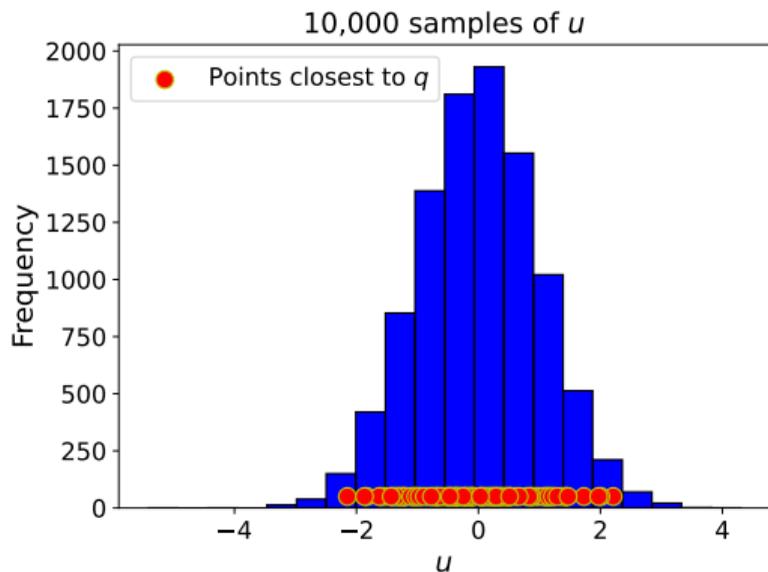
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The problem with functional quantiles



The problem with functional quantiles



⇒ the entire input space contributes to the quantile

Application to test cases

- Proposed approach compared to a **naive latin hypercube sampling** (LHS) scheme of the maximum budget and an active learning criterion based on the **maximization of the surrogate model variance**

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- **20 repetitions** for each test case and each criterion
- The performance is measured through the **mean relative error** (MRE) of the estimated quantile
- We do not solve the minimization problem (find \mathbf{u}^*), we rely on a discretization of the input space

Parametric test case to illustrate

Goal: compute the 99%-quantile of

$$f(\mathbf{u}, x) = \tilde{a} \exp\left(-\frac{1}{2} \times \frac{0.5 + 0.01\tilde{a} - x}{\ln(1 + u_1)}\right) \quad (6)$$

with $\tilde{a} = 1 + \sin(2nu_2)$, $n = 3$.

The distribution of the uncertain variables \mathbf{u} are $u_1 \sim \mathcal{U}(0.2, 0.4)$ and $u_2 \sim \mathcal{U}(0, \pi)$.

The mesh coordinate is $x \in [0, 1]$ with 101 nodes.

Parametric test case to illustrate

With 3 regions that activate the quantile

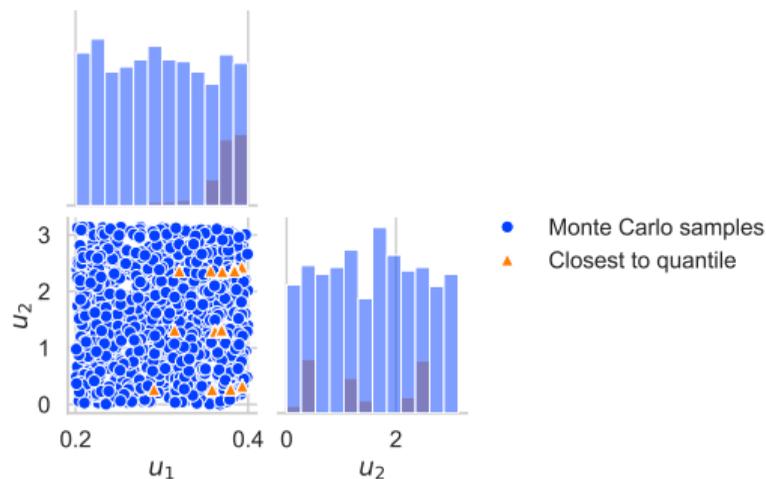


Figure: Distribution in the input space

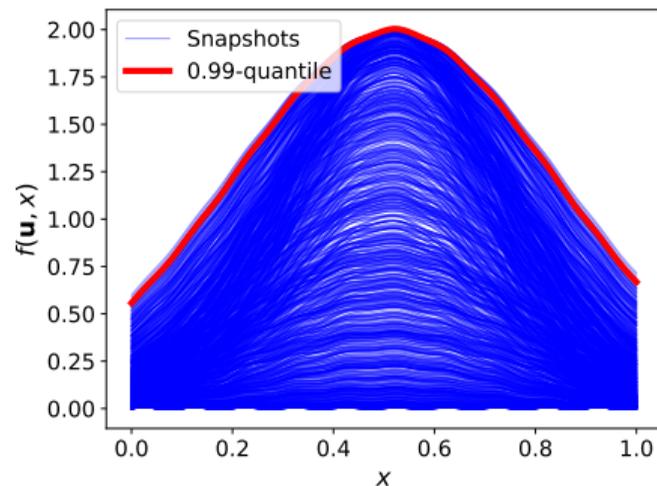
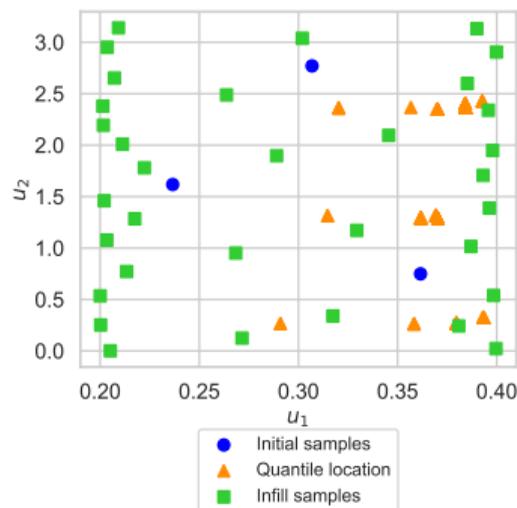
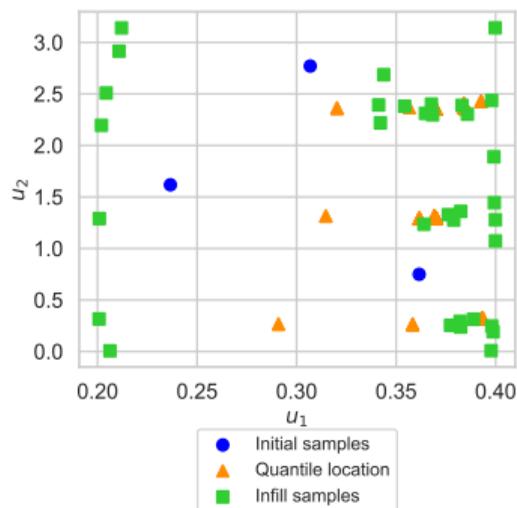


Figure: Snapshots and quantile

Parametric test case to illustrate

With 3 regions that activate the quantile



Input space for quantile oriented infill

Input space for variance based infill

Parametric test case to illustrate

With 3 regions that activate the quantile

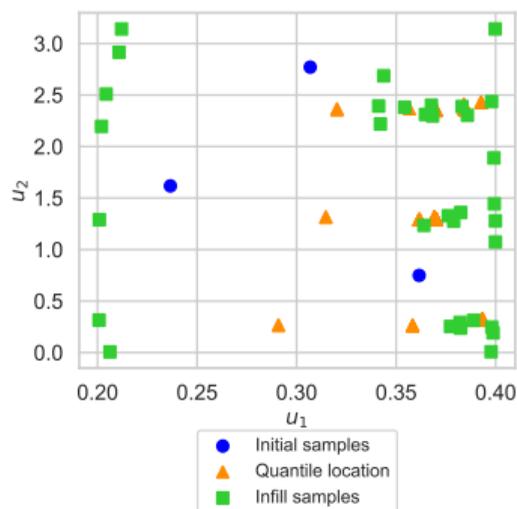


Figure: Input space for quantile oriented infill

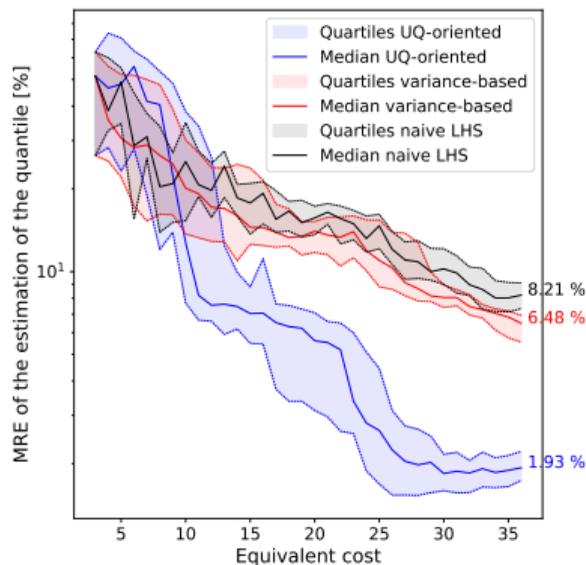


Figure: Convergence of the MRE

Trajectory of a space launcher test case

- Two-Stage-To-Orbit rocket (circular at 250 km)



Trajectory of a space launcher test case

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- The solver is the optimization of the trajectory



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- 99%-quantile: flight envelope for safety purposes



Trajectory of a space launcher test case

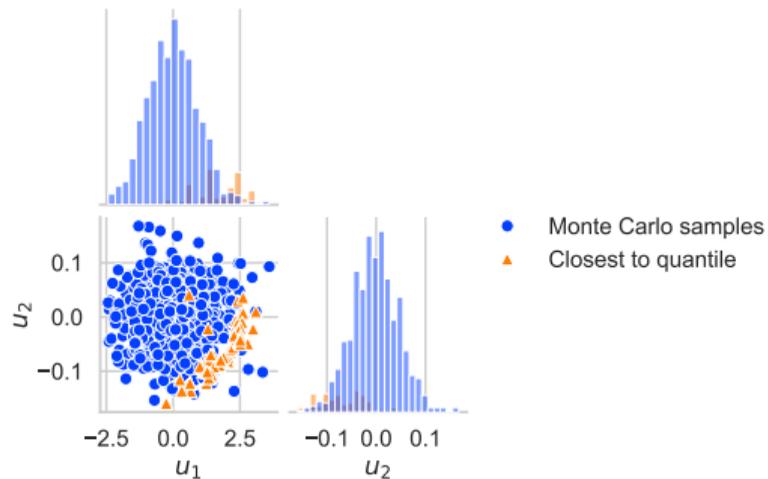


Figure: Distribution in the input space

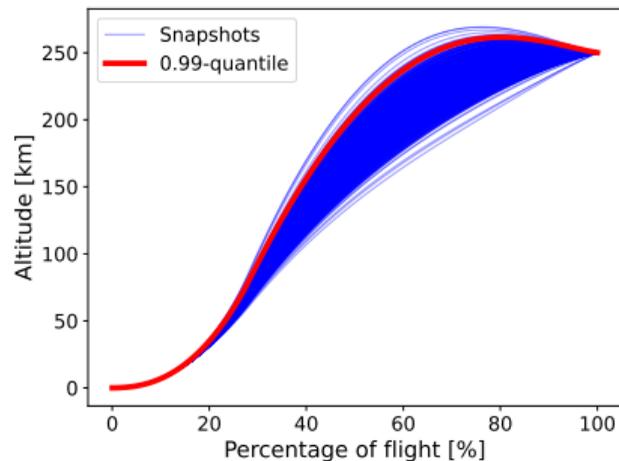
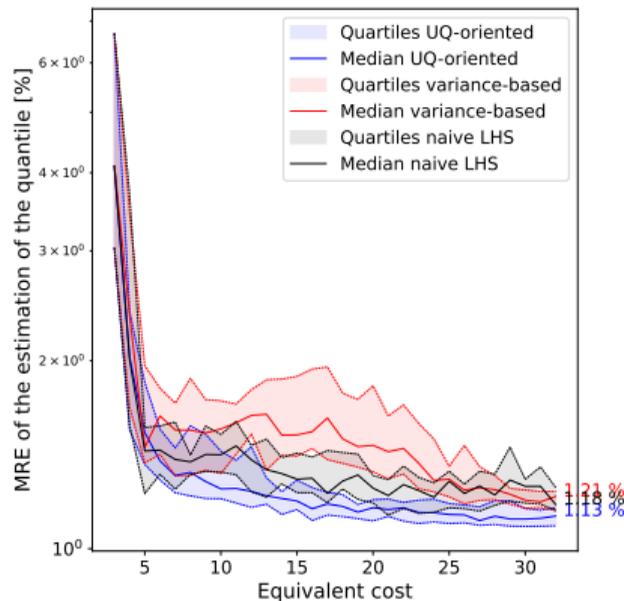
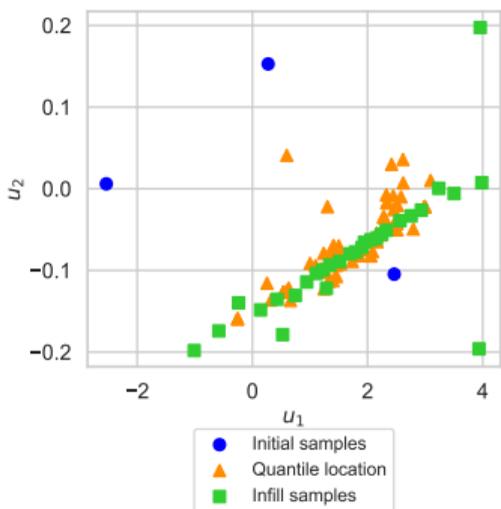


Figure: Snapshots and quantile

Trajectory of a space launcher test case



⇒ -11% median MRE at cost 10 and -7% at cost 20 over a naive LHS

Takeaways

- The proposed strategy behavior is as expected **adding samples in areas of the inputs space that contribute the most to the quantile** or that bear a large variance, and it appears to be beneficial

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- We cannot simply transpose scalar active learning strategies to simulators with functional outputs
- The effectiveness of our method is **highly dependent on which parts of the input space compose the quantile**, considering that the exact quantile is not known *a priori*

Future works

- Apply the method on **other test cases** (of increased dimensionality and complexity), in particular cases with varying quantile structure to better understand the effectiveness of the proposed method

Future works

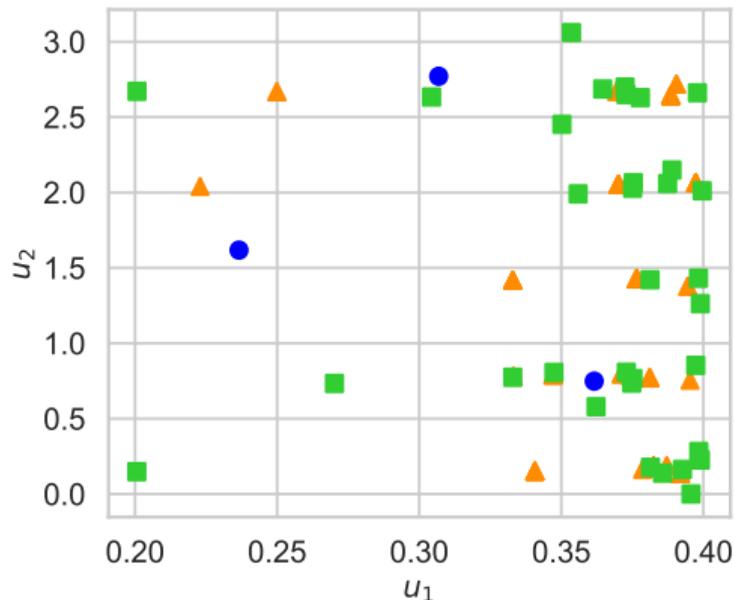
- Apply the method on **other test cases** (of increased dimensionality and complexity), in particular cases with varying quantile structure to better understand the effectiveness of the proposed method
- Extend it to **multi-fidelity** simulators to take advantage of the lower computational cost of lower-fidelity simulators

Thank you for listening!
Any questions?

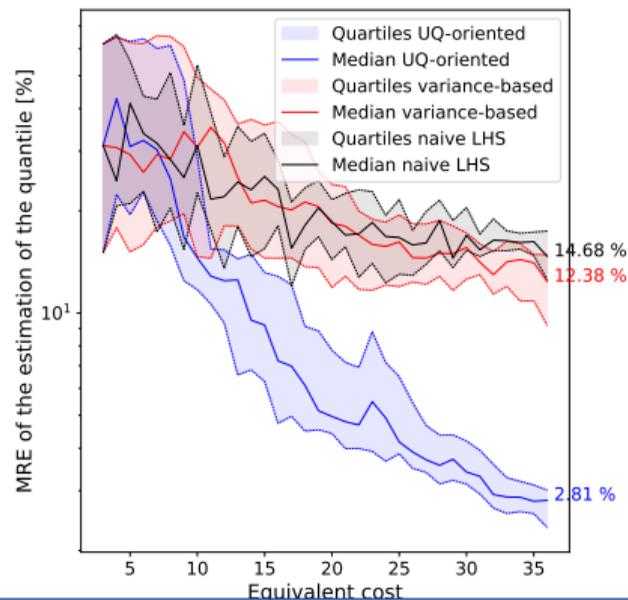
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Parametric test case to illustrate

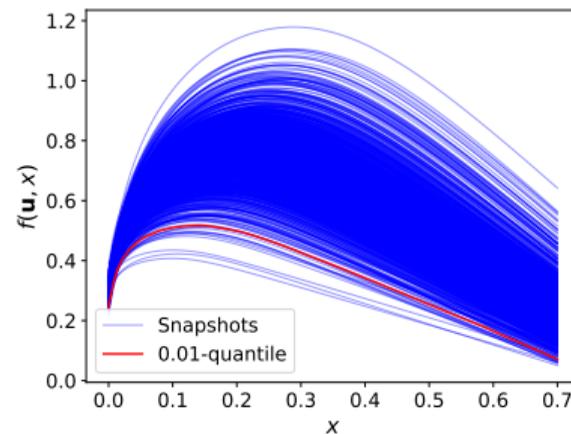
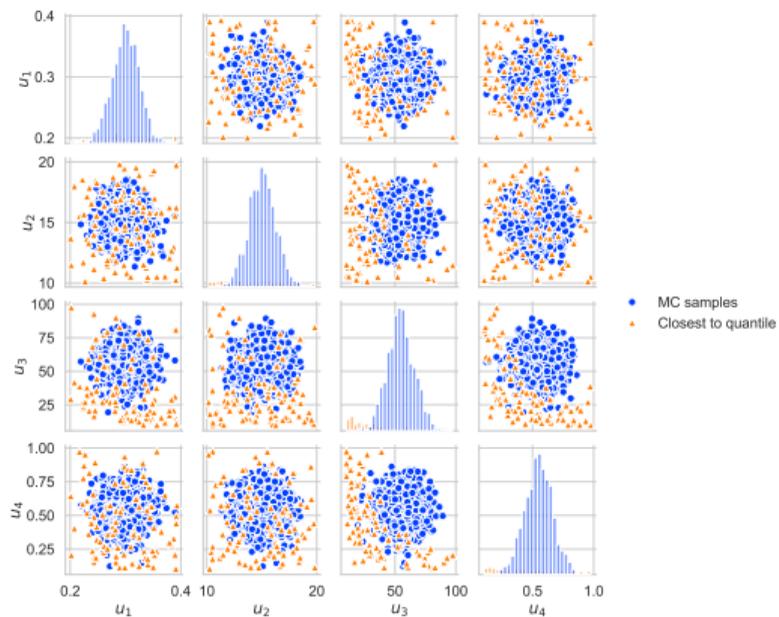
With 5 regions that activate the quantile



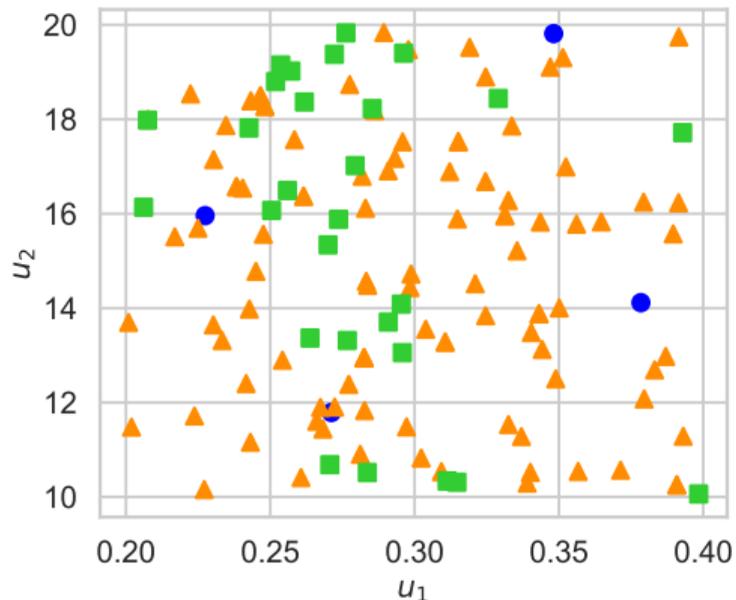
● Initial samples
▲ Quantile location



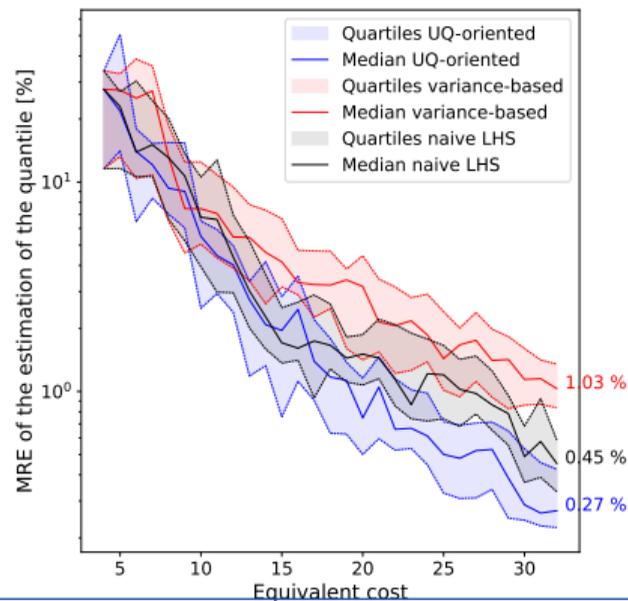
Viscous free fall



Viscous free fall



● Initial samples
▲ Quantile location



Viscous free fall

- Adds samples where we want them again
- Ecart moins important que sur le cas analytique
- Quand ce sera animé analyser l'ordre dans lequel les points sont ajoutés
- Le critère variance est moins intéressant qu'un LHS naif