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Calibrating a hydrological model robustly to rain perturbations with stochastic surrogates

Katarina Radišić¹²

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¹INRAE, RiverLy, Lyon-Villeurbanne

²Univ. Grenoble-Alpes, Inria, CNRS, Grenoble-INP, LJK

Context

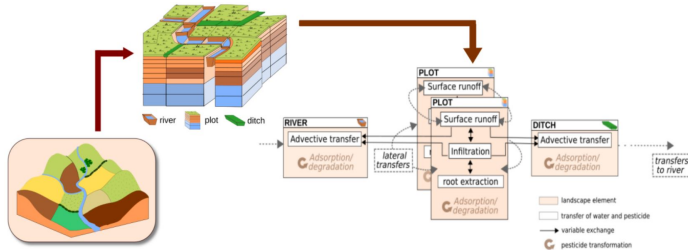
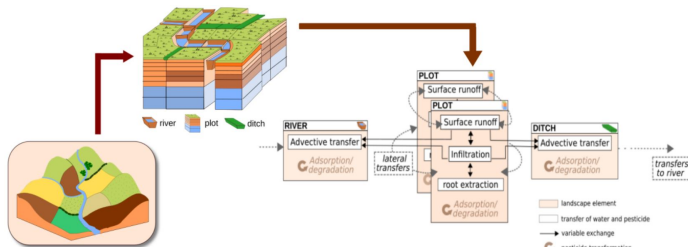


Figure: PESHMELBA^a, a process-based, spatially distributed water and pesticide transfer model, representing dynamical behavior of pesticides in agricultural catchments. Semi-conceptual, semi-physically based model, highly non-linear.

^aEmilie Rouzies et al. (June 2019). "From agricultural catchment to management scenarios: A modular tool to assess effects of landscape features on water and pesticide behavior". en. In: *Science of The Total Environment* 671, pp. 1144–1160.

Context



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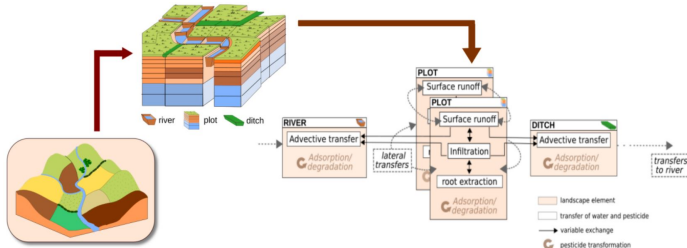


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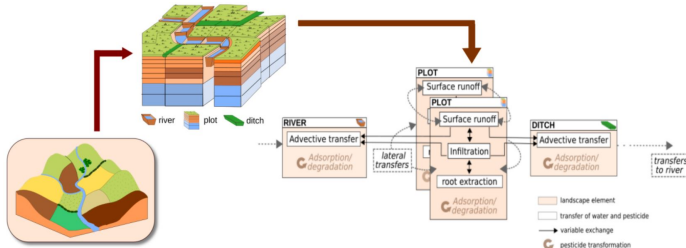
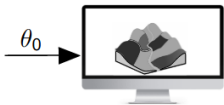


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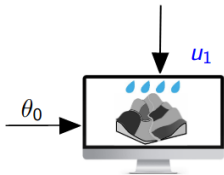
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- Not all model parameters can be measured directly
 - → calibrate these model parameters with terrain observations
- Impact of external uncertainties on the calibration results

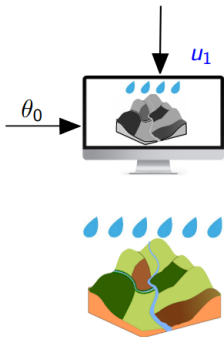
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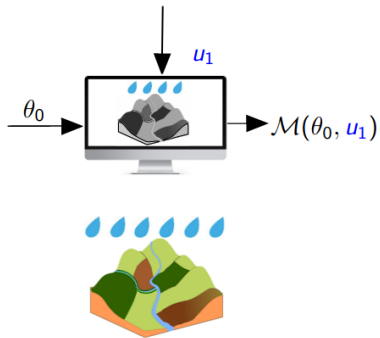
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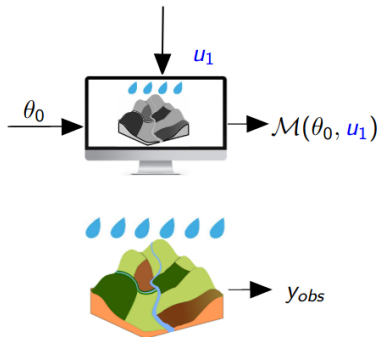
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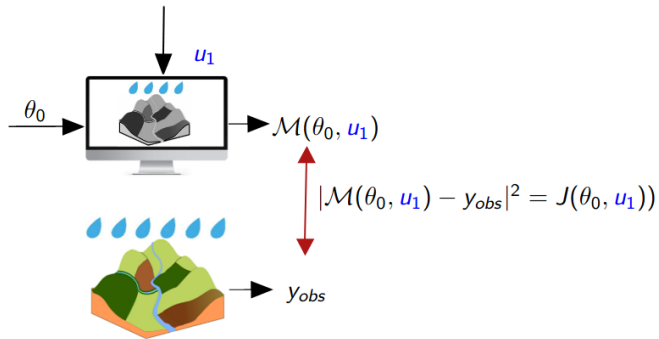
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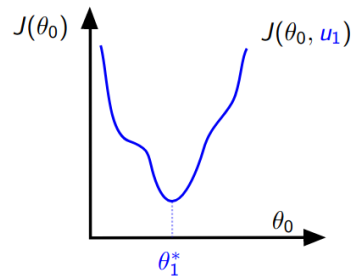
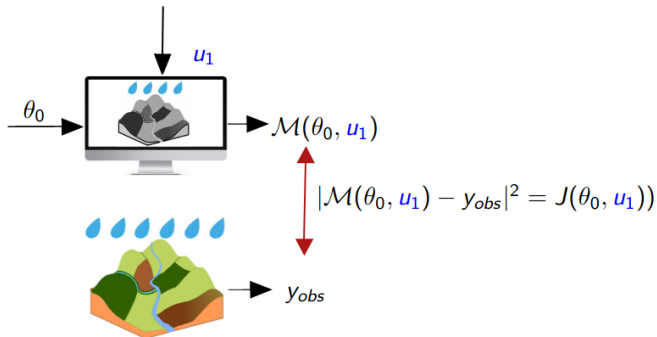
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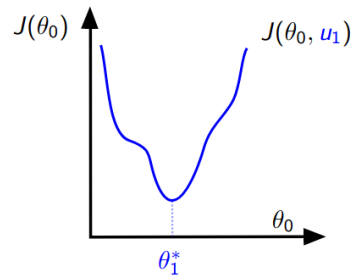
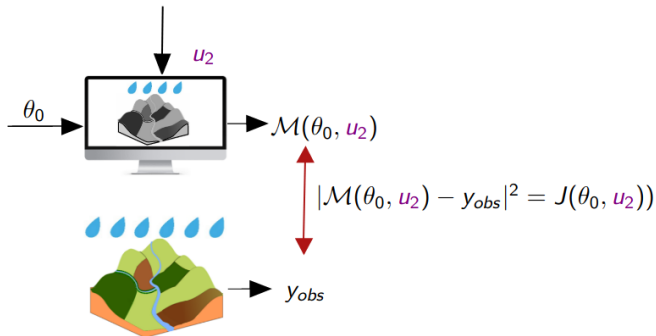
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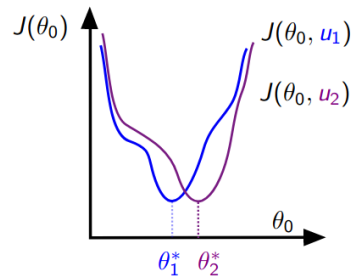
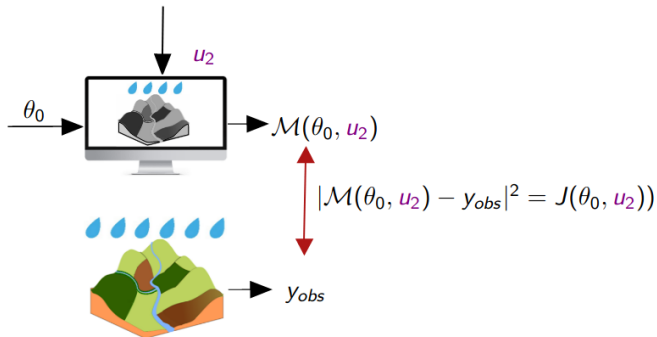
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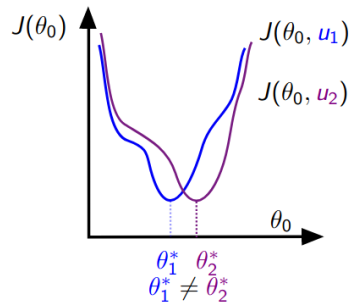
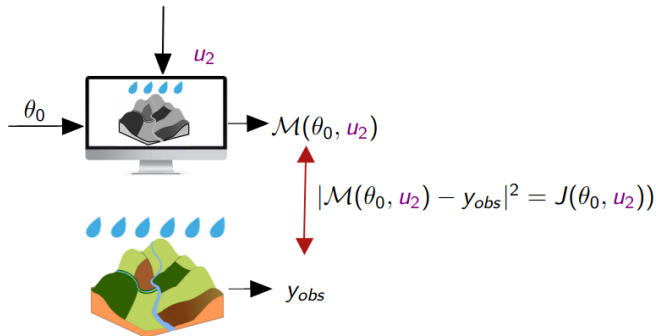
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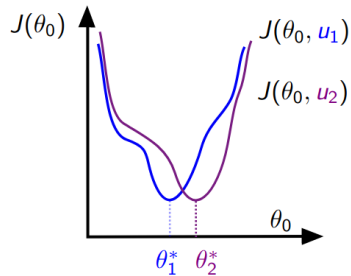
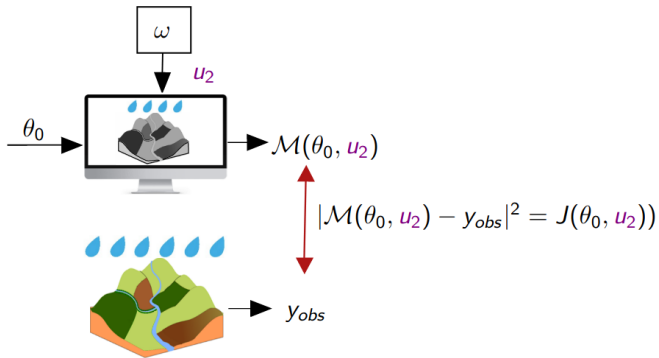
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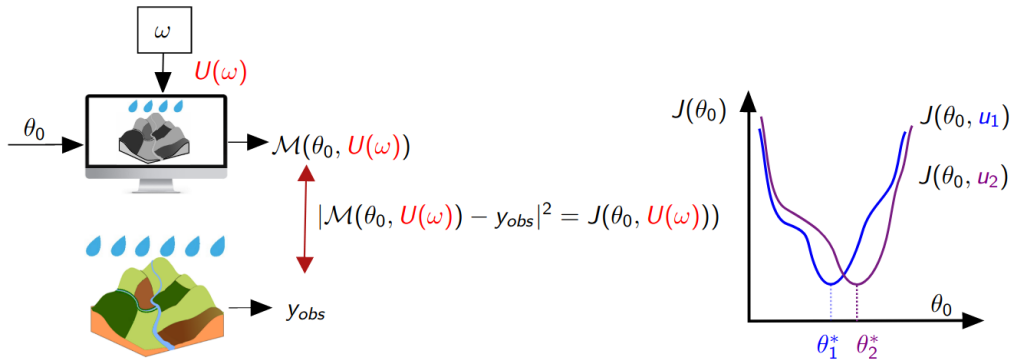
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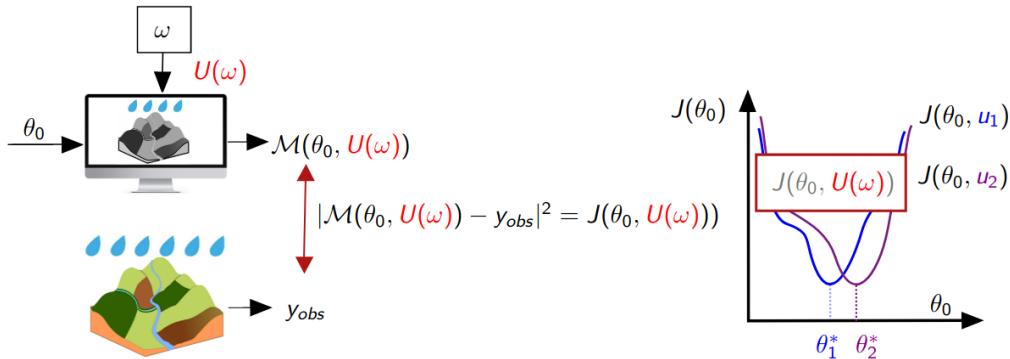
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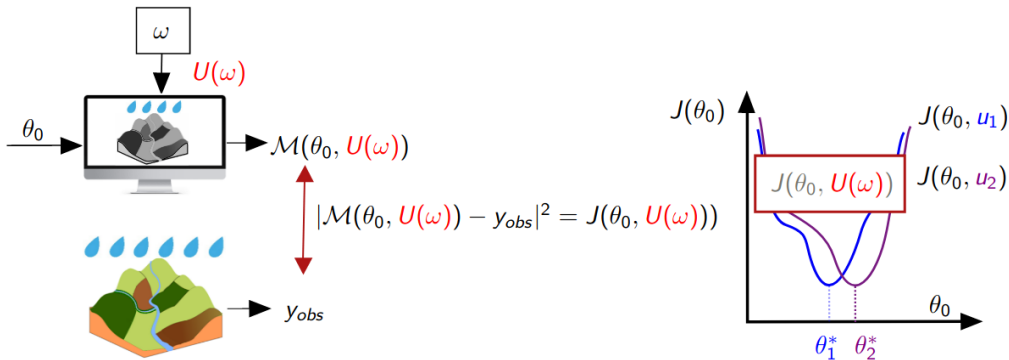
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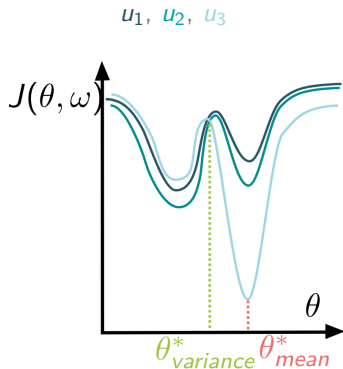


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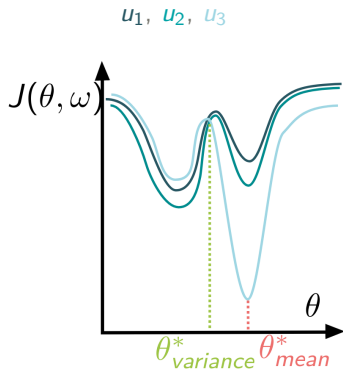
What does it mean to find a *robust* minimizer ?

Methods: Robust estimators



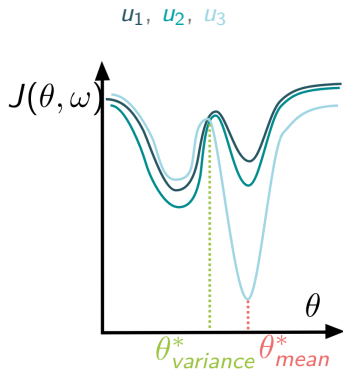
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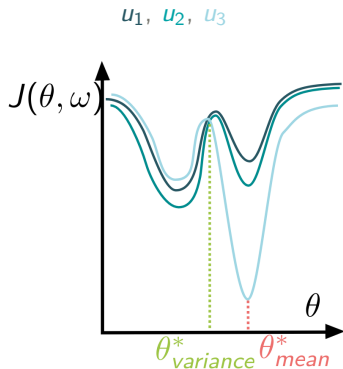
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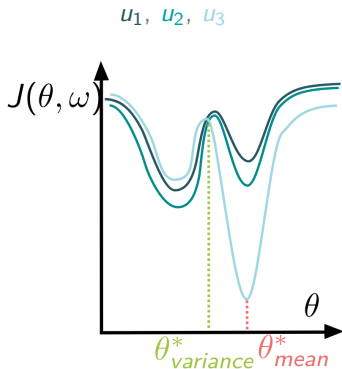
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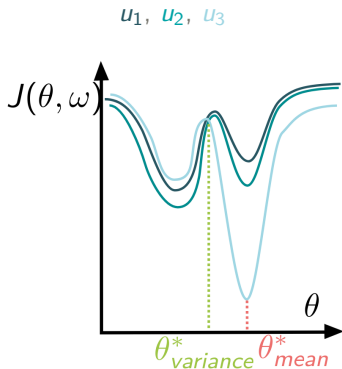
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- How to estimate the robust parameters from a limited number of model simulations?

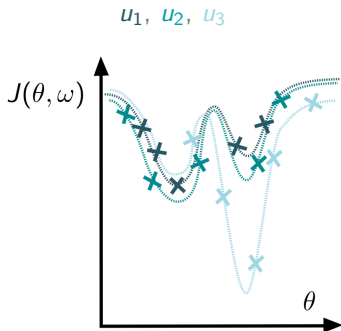
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→ Stochastic metamodel^a

^aNora Lüthen, Stefano Marelli, and Bruno Sudret (Mar. 2023). “A spectral surrogate model for stochastic simulators computed from trajectory samples”. en. In: *Computer Methods in Applied Mechanics and Engineering* 406, p. 115875.

Methods: Stochastic metamodel

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- representation of the impact of the variability of the rain on the cost function through a random variable in the latent space

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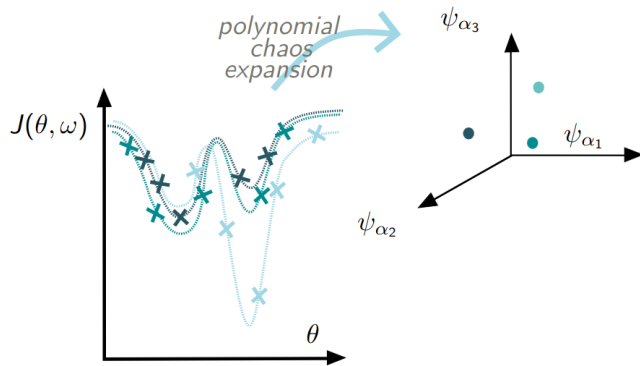
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$$\hat{J}(\boldsymbol{\theta}, \omega) = \textcolor{red}{\hat{\mu}}(\boldsymbol{\theta}) + \sum_{k=1}^K \sqrt{\lambda_k} \textcolor{blue}{Z}_k(\omega) \left(\sum_{\alpha \in \mathcal{A}} \textcolor{blue}{b}_{\alpha}^{(k)} \psi_{\alpha}(\boldsymbol{\theta}) \right)$$

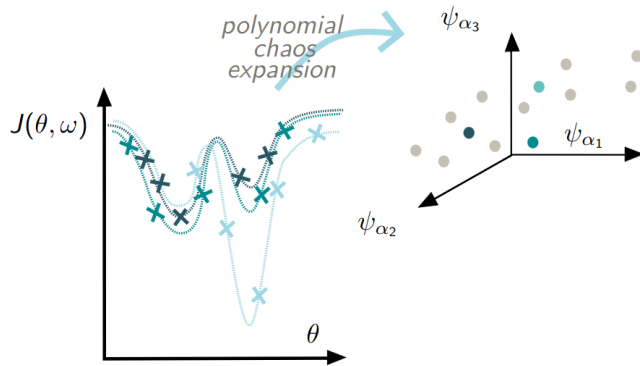
- PCE on each rain realization, then Principal component analysis on the PCE coefficients
- representation of the impact of the variability of the rain on the cost function through a random variable in the latent space
- the mean and variance are analytically available and independent of the distribution of Z

Methods: Stochastic metamodel



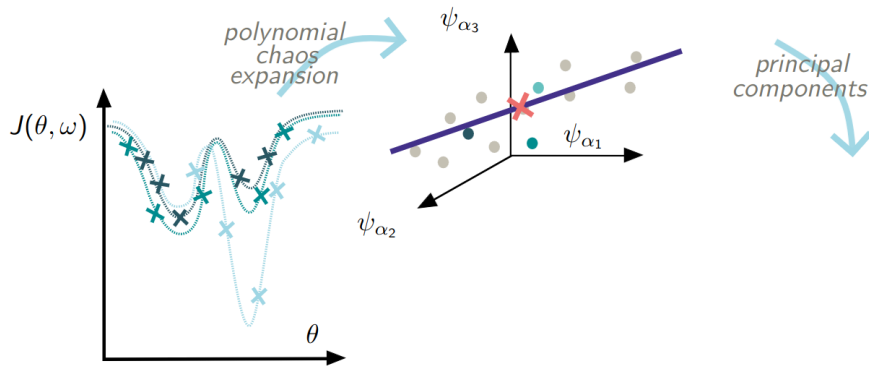
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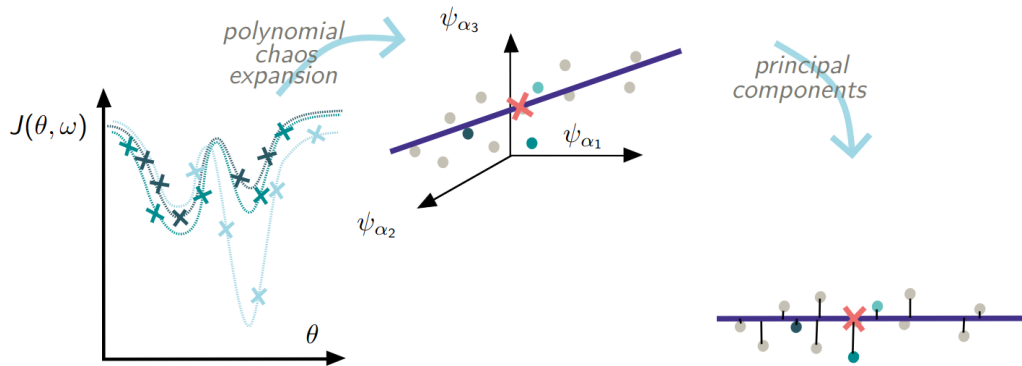
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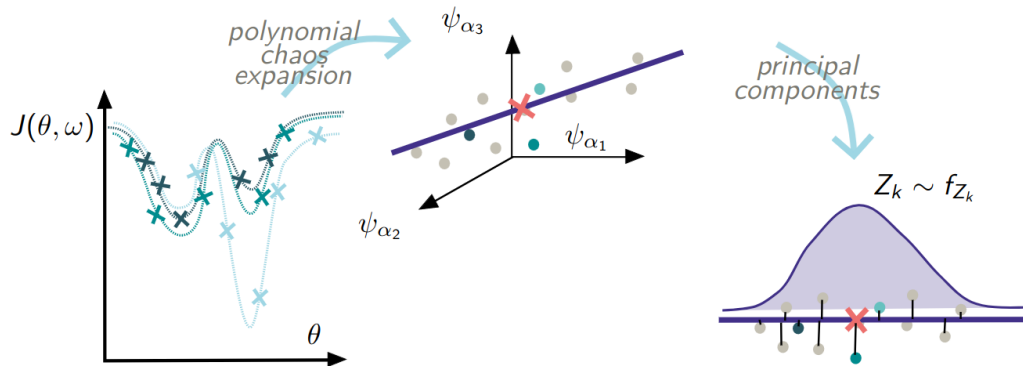
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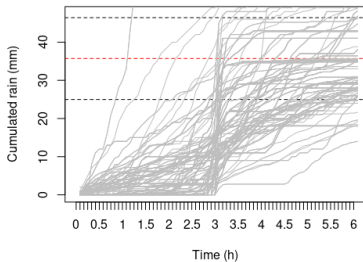
Case study: Moisture profile observations, twin experience

$$J(\theta, u) = (\mathcal{M}(\theta, u) - y_{true})^2$$

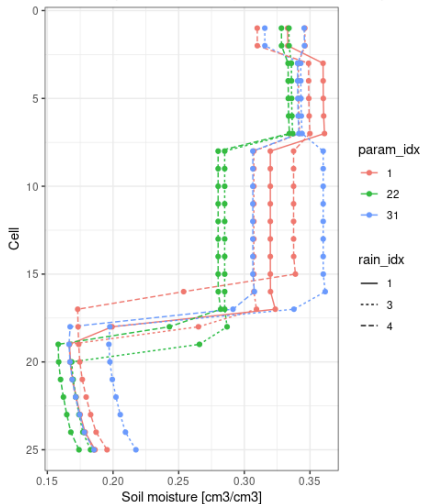
$$\theta \in \mathbb{R}^6$$

$$y_{true} \in \mathbb{R}^{25}$$

Season = S - Duration = 6h - Intensity = 35.7mm



Rain and parameter changes on the moisture profile



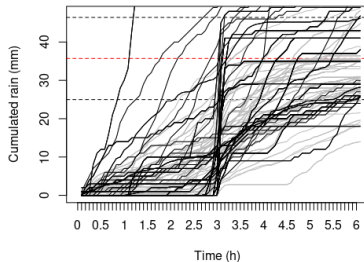
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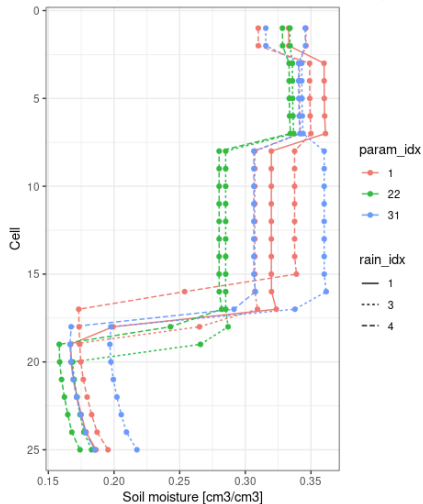
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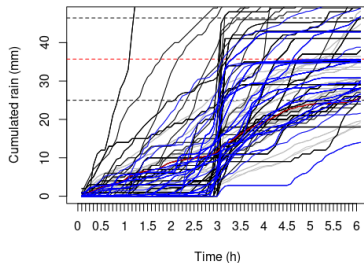
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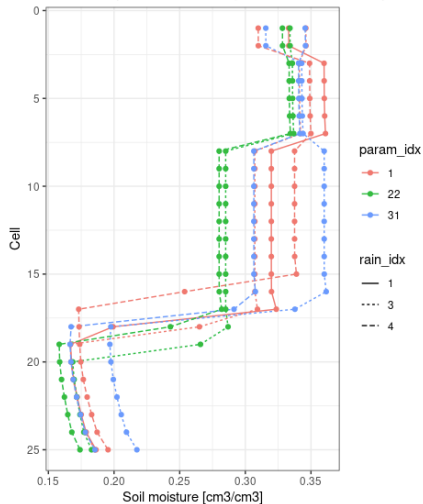
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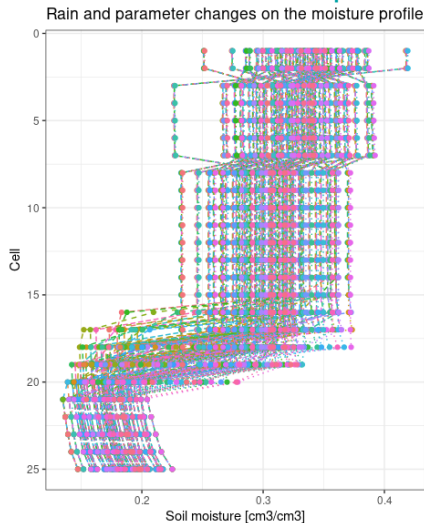
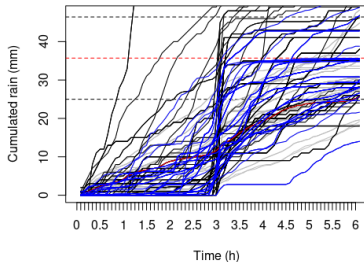
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Results: Conditional minimization

- PCE constructed conditionally to each train rain realization.
- Determination coefficients $R^2 > 0.95$
- Minimization BFGS conditionally to each rain realization.

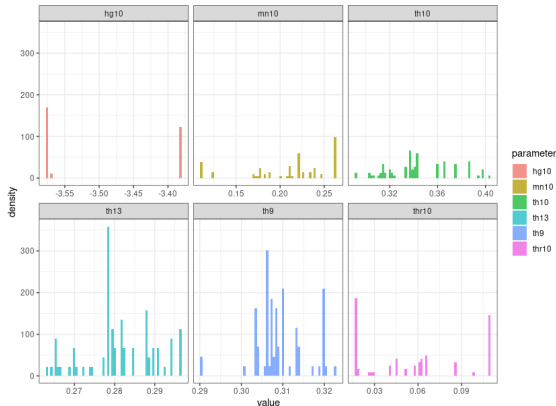


Figure: Histogram of conditional minimizers to each train rain realization.

Results: Validation of the emulator

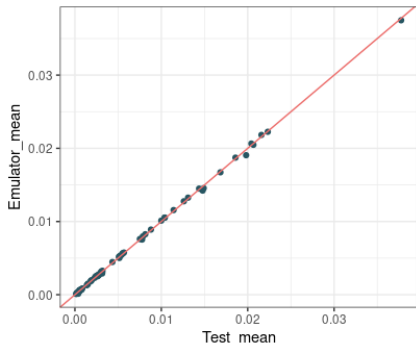


Figure: Comparison of the **train** and the **test** means $\mathbb{E}_U[J(\theta, U)]$.

$$\hat{J}(\theta, U(\omega)) = \hat{\mu}(\theta) + \sum_{k=1}^K \sqrt{\lambda_k} Z_k(\omega) \left(\sum_{\alpha \in \mathcal{A}} b_{\alpha}^{(k)} \psi_{\alpha}(\theta) \right)$$

- The emulator mean is a good estimator of the true mean.

Results: Validation of the emulator

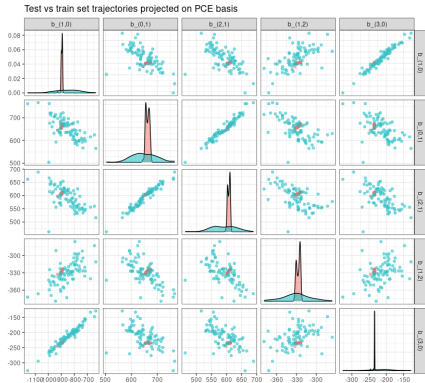


Figure: Comparison of the **train** and the **test** trajectories of PESHMELBA simulations, projected on the PCE basis.

$$\hat{J}(\theta, U(\omega)) = \hat{\mu}(\theta) + \sum_{k=1}^K \sqrt{\lambda_k} Z_k(\omega) \left(\sum_{\alpha \in \mathcal{A}} b_{\alpha}^{(k)} \psi_{\alpha}(\theta) \right)$$

- The emulator mean is a good estimator of the true mean.
- The **train** set and the **test** set do not present the same variabilities, thus the emulator does not reproduce correctly the impact of rain perturbations on the cost function.

Results: Validation of the emulator

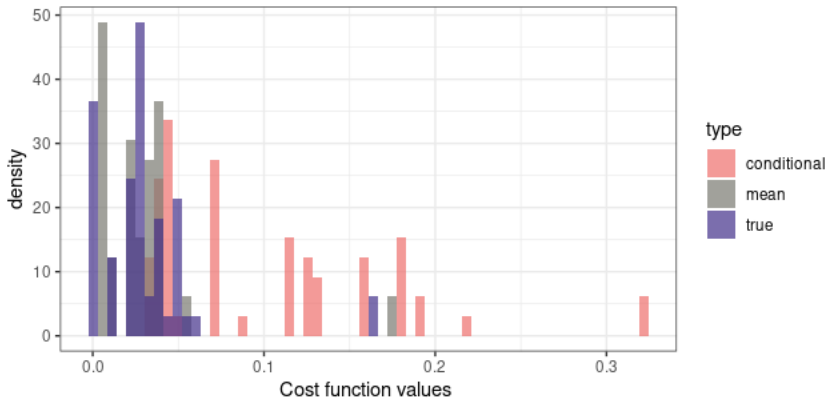


Figure: Cost function evaluated at the test rains, the simulations performed with the minimizer of the mean have a lower mean and variance than the one obtained with the minimizer conditioned on one rain realization.

Conclusion

- The PCE approximations on each conditioned rains have a determination coefficient $R^2 > 0.95$ and the approximation of the metamodel mean is good.
- The minimizer of the mean has lower cost function on unseen rains than a randomly chosen conditional minimizer.
- The variance of the metamodel is not a good estimate

What next ?

- work on the estimation of the variance
- study the Pareto-optimal minimizers
- augment rain perturbations
- minimize mean and variance with Gaussian Process based Efficient Global Optimization, compare the precision and number of model evaluations needed.
- observe another output, for example pesticide quantities in the river, interaction will be added.
- up the domain to the catchment scale

Thank you for your attention !

