Robust calibration of a water and pesticide transfer model at the catchment scale

Katarina Radišić, Claire Lauvernet, Arthur Vidard

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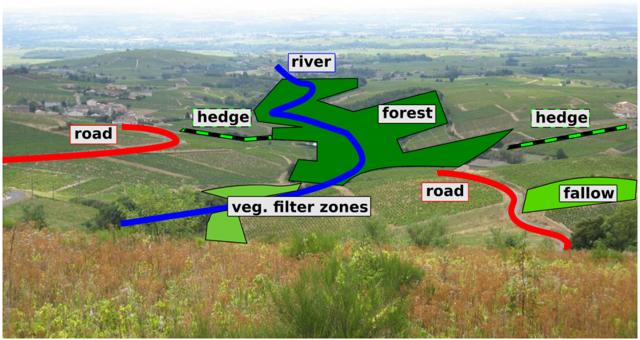
Context: Pesticide transfer dynamics

Landscape features speed up or slow down pesticide transfer from the plots to the river.

⇒ The configuration of the catchment influences the water quality.

Context: Pesticide transfer dynamics

Landscape features speed up or slow down pesticide transfer from the plots to the river.



⇒ The configuration of the catchment influences the water quality.

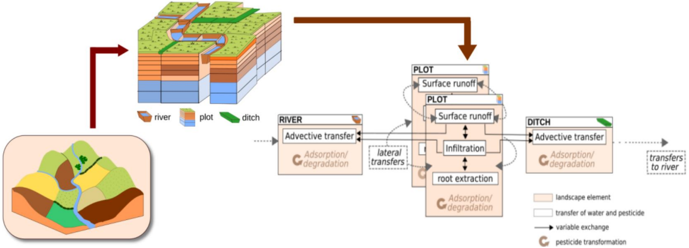


Figure: PESHMELBA model, [7].

- process-oriented, physically-based, coupling with landscape features
- simulates water and pesticide transfers on an agricultural catchment
- distributed model, numerous parameters to calibrate

- not all **parameters** can be measured
- → **calibration** of parameters through field observations

- calibration sensitive to **forcing uncertainties**

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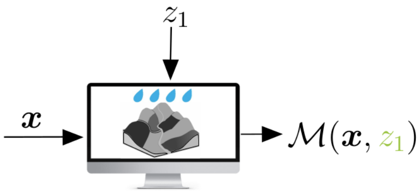
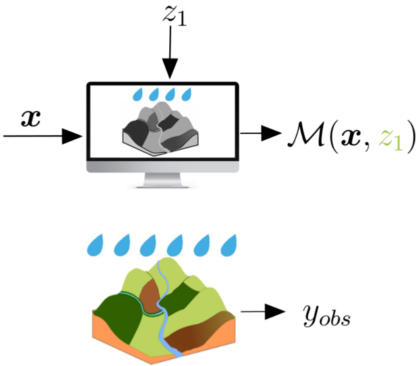

z_1
$\boldsymbol{x}$
$\mathcal{M}(\boldsymbol{x}, z_1)$


z_1
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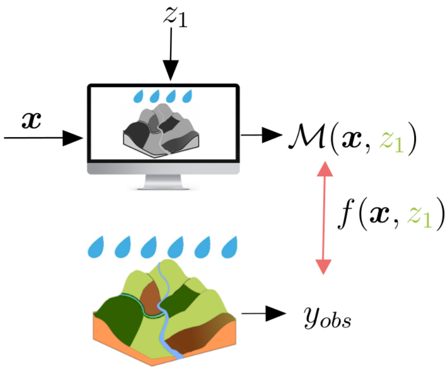
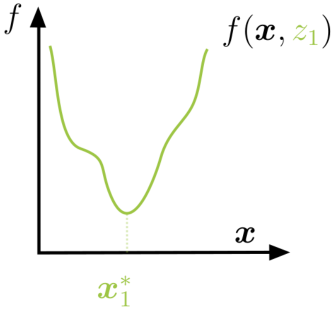
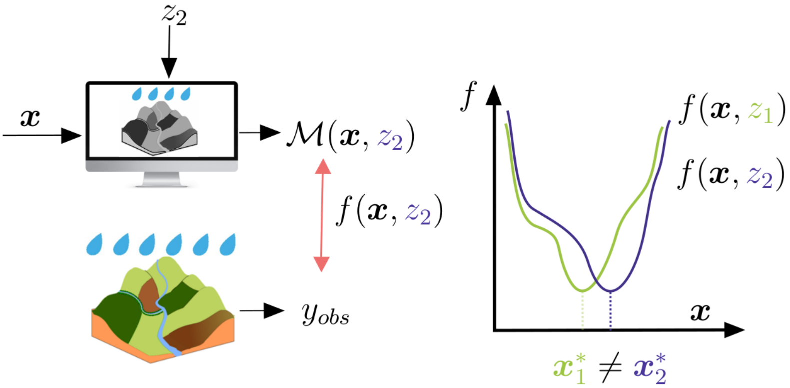
y_{obs}


z_1
$\boldsymbol{x}$
$\mathcal{M}(\boldsymbol{x}, z_1)$
$f(\boldsymbol{x}, z_1)$
y_{obs}


f
$f(\boldsymbol{x}, z_1)$
$\boldsymbol{x}$
$\boldsymbol{x}_1^*$

Introduction: Classic calibration



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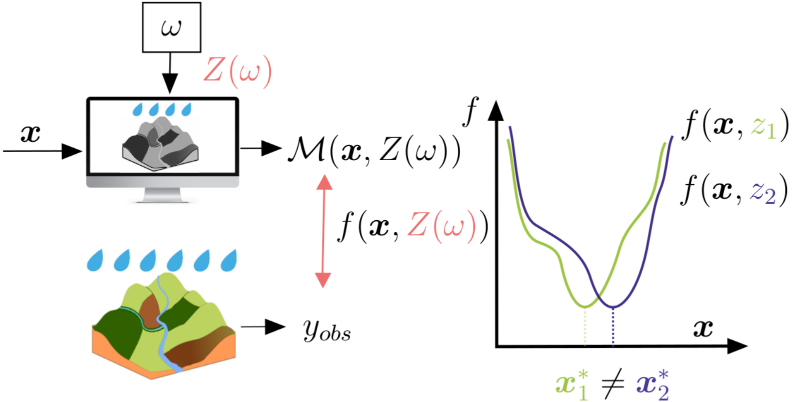
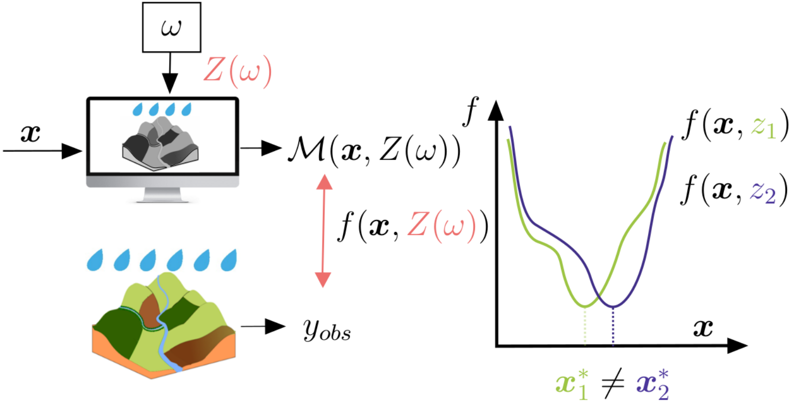
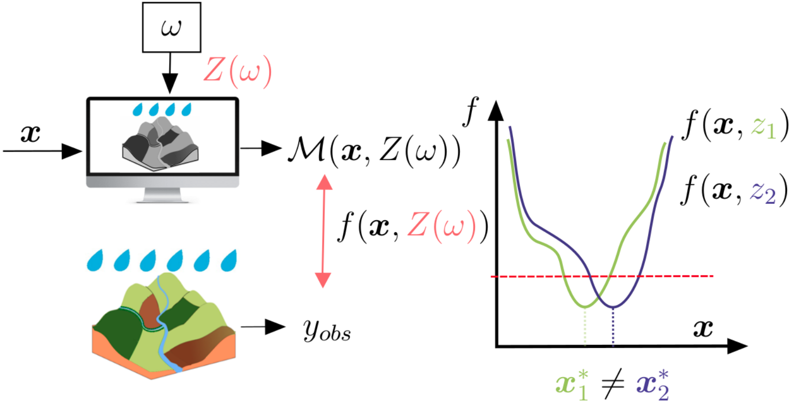


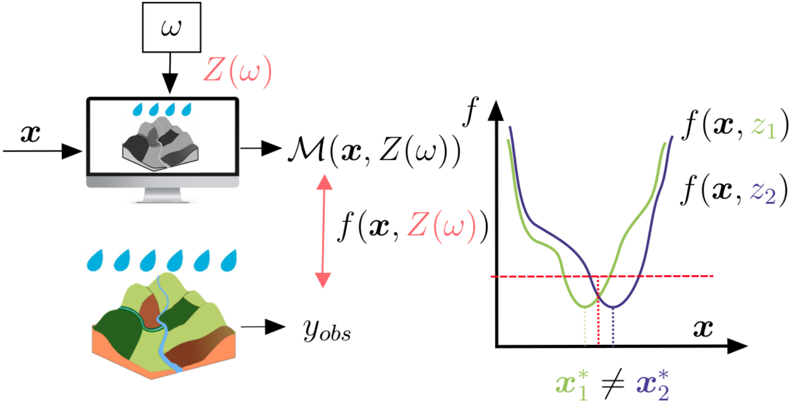


Calibration robuste *: satisfait des conditions d'optimalité sous un ensemble de forçages*

Introduction: Classic calibration



Calibration robuste *: satisfait des conditions d'optimalité sous un ensemble de forçages*



***Robust calibration**: satisfies optimality conditions under a set of forcings*

Introduction: Robust calibration

1. Find $\boldsymbol{x}^*_{robust}$ minimizing a QoI: the mean $\mathbb{E}$, the variance $\mathbb{V}ar$, or Pareto of the two [2, 6].
2. other definitions of robustness, excursion sets, relative regret [1, 8].

→ a thing in common : **computationally expensive**

- metamodel on the QoI of interest, or
- metamodel on the entire $\mathcal{D}_X \times \Omega$,

→ however the parametrization of Ω is highly model specific [5].

Our approach:

- take a non-intrusive approach in the space Ω [9, 4]
- estimate a stochastic emulator $\hat{f}_s(\boldsymbol{x}, \omega) \approx f_s(\boldsymbol{x}, \omega)$ over the whole space $\mathcal{D}_X \times \Omega$ [3]

→ use $\hat{f}_s(\boldsymbol{x}, \omega)$ to estimate different $\boldsymbol{x}^*_{robust}$

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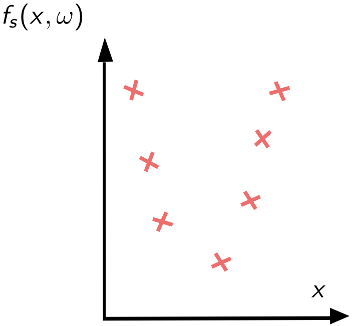
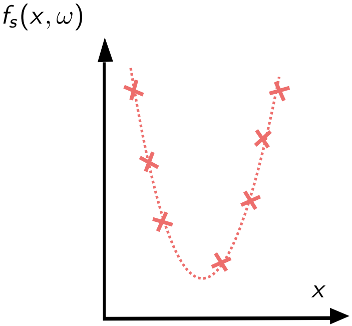
Methodology: Polynomial chaos expansion (PCE)



$f_s(\boldsymbol{x}, \omega_1) \approx$

Methodology: Polynomial chaos expansion (PCE)



$$f_s(\boldsymbol{x}, \omega_1) \approx f_{PCE}^{(1)}(\boldsymbol{x})$$

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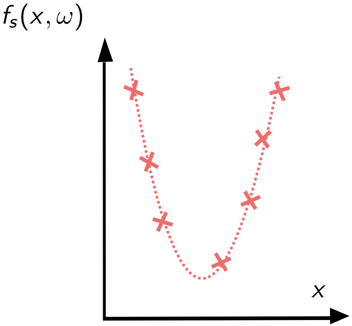

$$f_s(\boldsymbol{x}, \omega_1) \approx f_{PCE}^{(1)}(\boldsymbol{x}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} c_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

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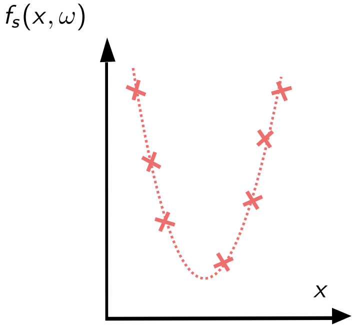

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$$= c_{\boldsymbol{\alpha}_1} \psi_{\boldsymbol{\alpha}_1}(\boldsymbol{x}) + c_{\boldsymbol{\alpha}_2} \psi_{\boldsymbol{\alpha}_2}(\boldsymbol{x}) + c_{\boldsymbol{\alpha}_3} \psi_{\boldsymbol{\alpha}_3}(\boldsymbol{x})$$

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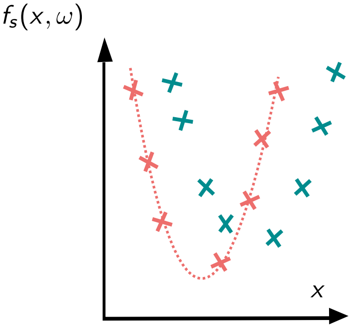

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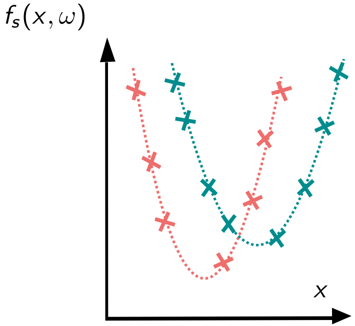

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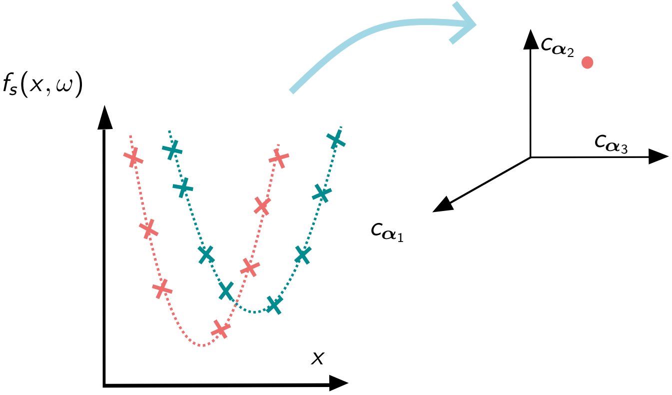

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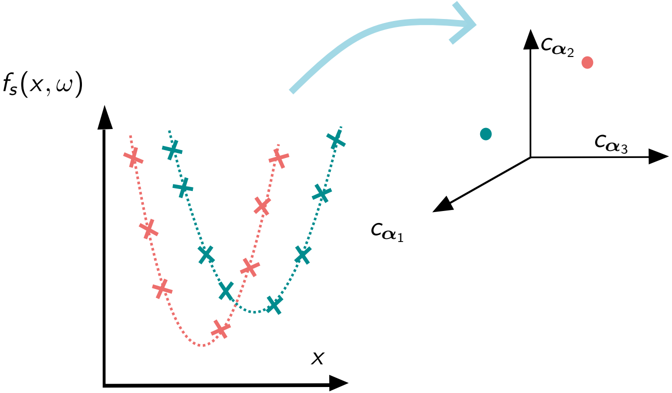
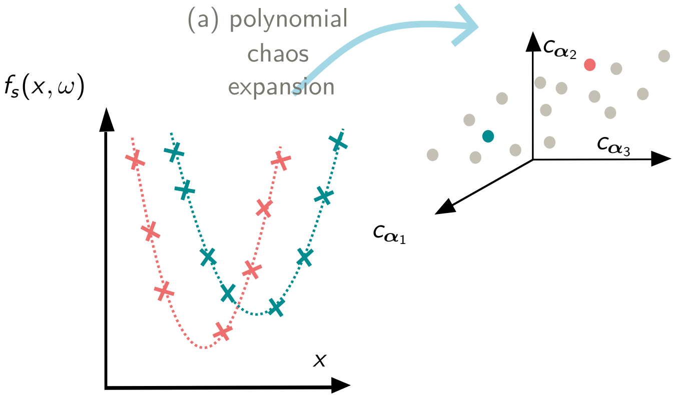


Methodology: Stochastic emulator $\hat{f}_s$: Fitting



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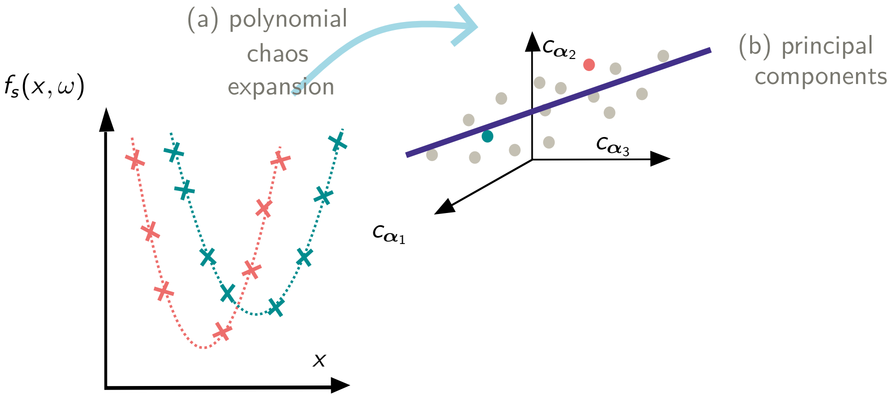

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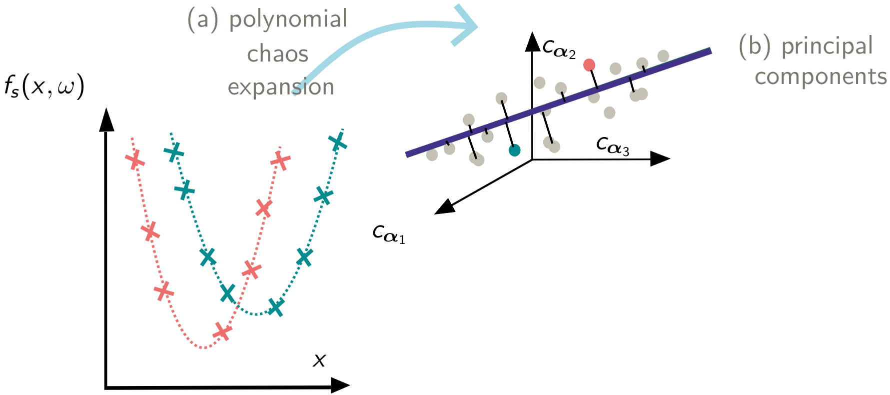

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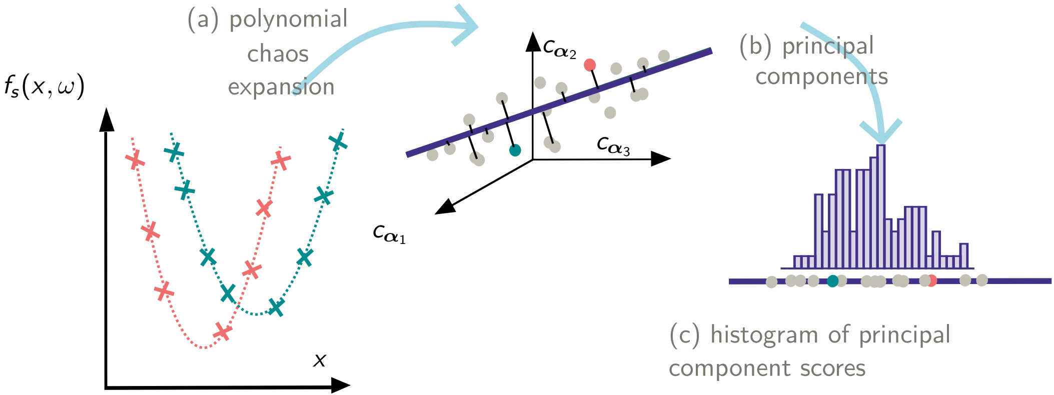

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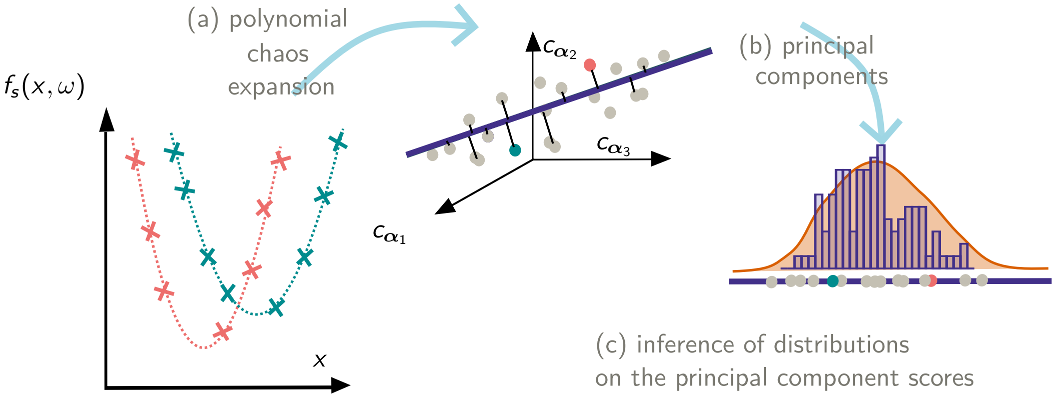
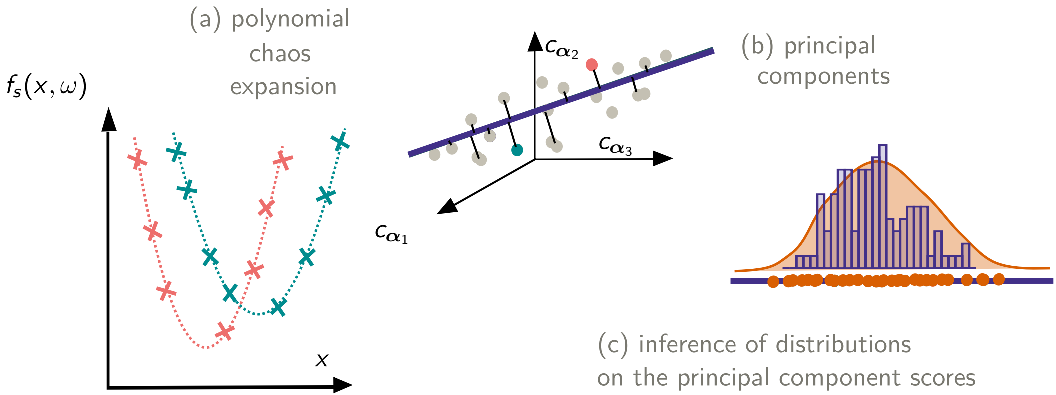


(c) inference of distributions on the principal component scores

Methodology: Stochastic emulator $\hat{f}_s$: Generate new trajectories



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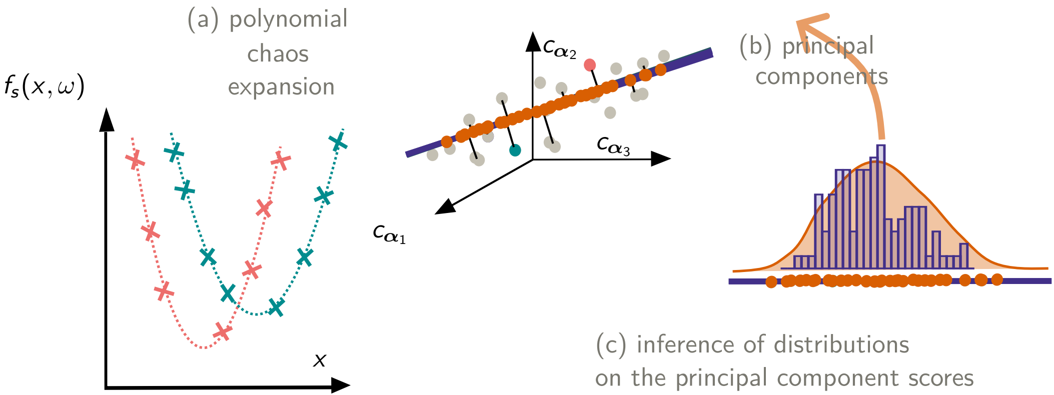

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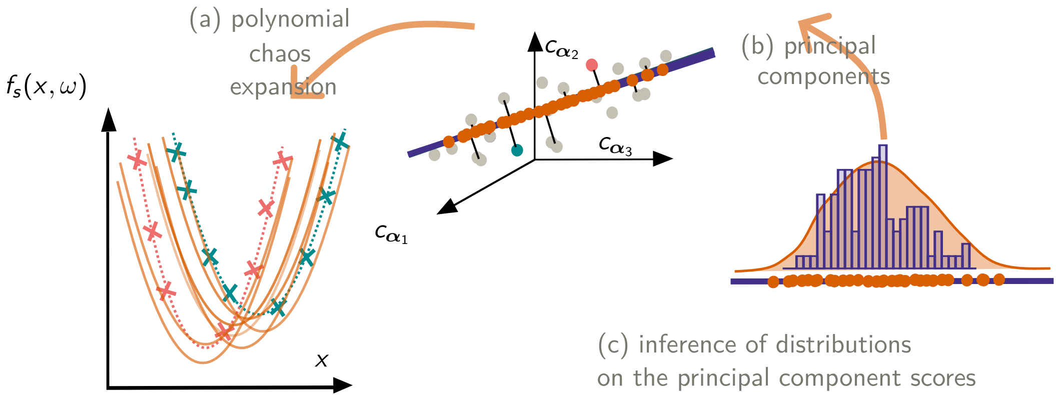
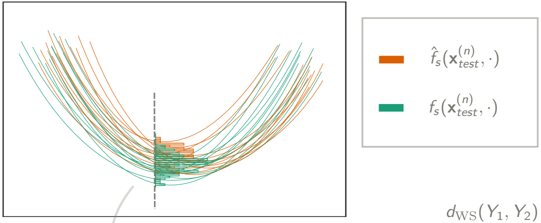


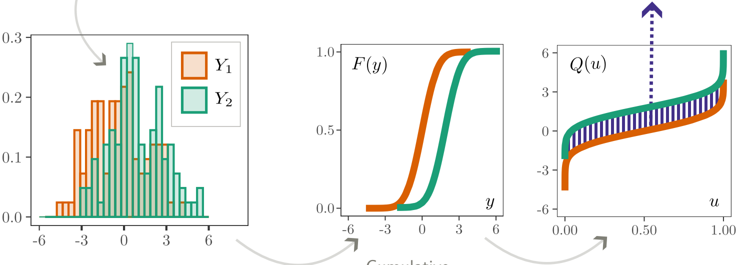
Methodology: Stochastic emulator $\hat{f}_s$: Validation vs f_s

Averaged normalized Wasserstein distance

Cost function: metamodel and test



$$d_{\mathrm{WS}}(Y_1, Y_2) = \sqrt{\int_0^1 \left(Q_1(u) - Q_2(u)\right)^2 \, \mathrm{d}u}$$

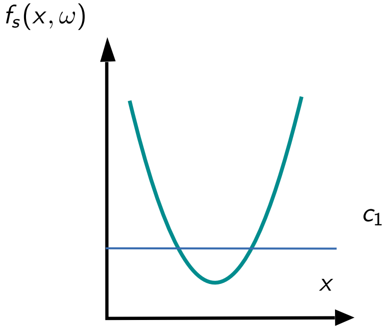


Histograms in one test point

Cumulative density function

Quantile function

Methodology: Robust calibration with $\hat{f}_s$



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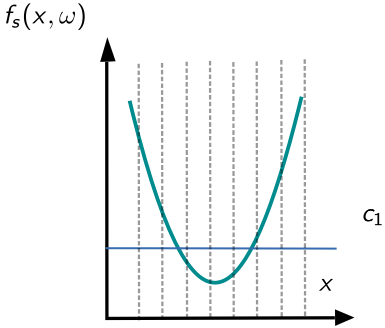

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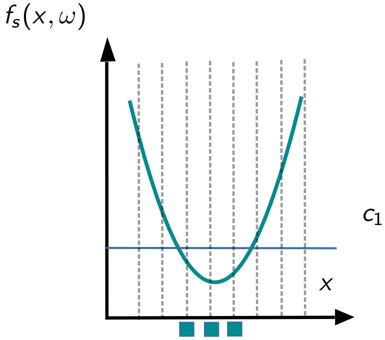

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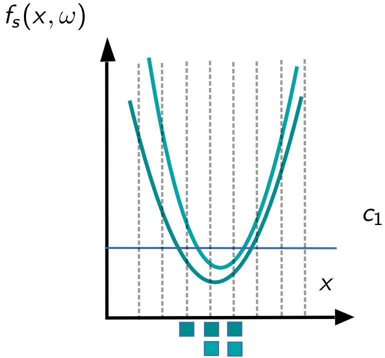

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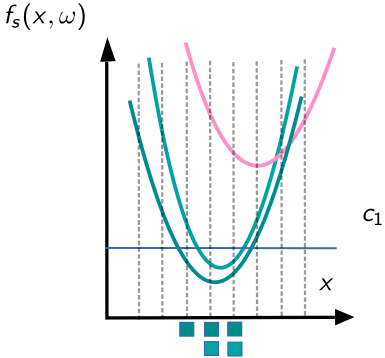

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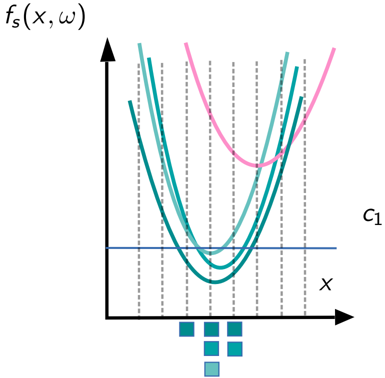

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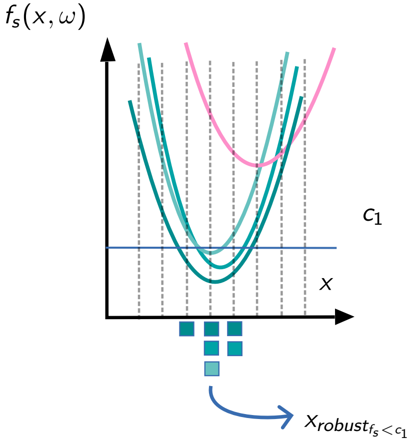

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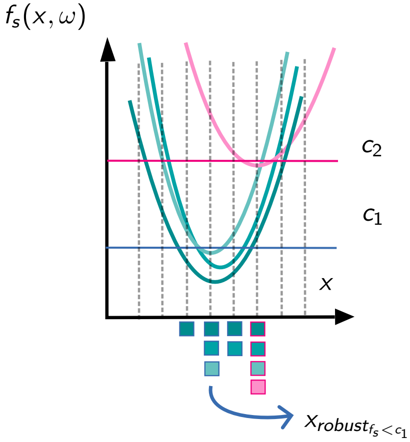

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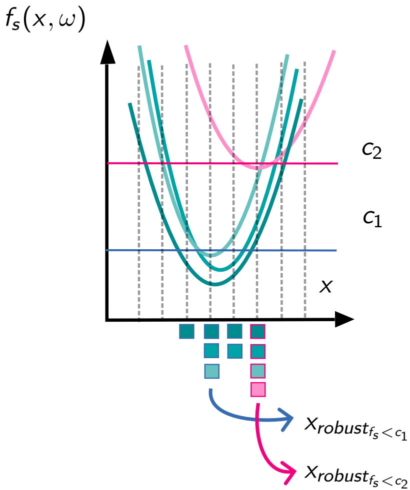

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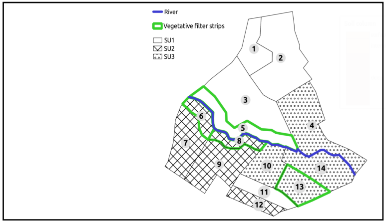
Case study: Moisture profiles

(c) PESHMELBA configuration



- parameters x (prior GSA), 5 params.
- forcing uncertainty Ω, rain error
- observation y_{obs}, moisture profile
- cost function f

Case study: Moisture profiles

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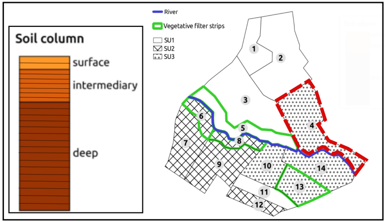

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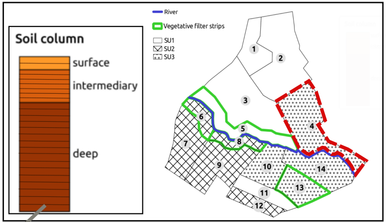

(b) Parameters to calibrate

Name	Definition
$\theta_{s.surf.}$	water content at saturation (surface)
$\theta_{s.inter.}$	water content at saturation (intermediary)
$\theta_{s.deep}$	water content at saturation (deep)
$\theta_{r.deep}$	residual water content (deep)
$mn_{.deep}$	Van Genuchten retention curve parameter (deep)

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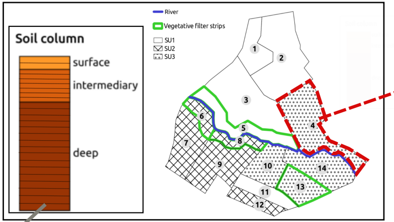

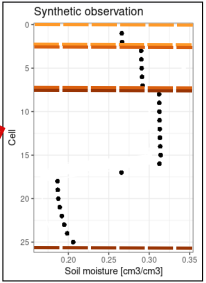

(d) Observation:
moisture profile of plot 4

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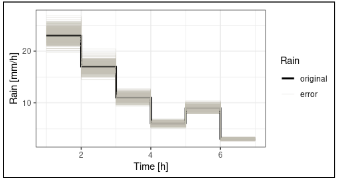
Case study: Moisture profiles

(a) Forcing input



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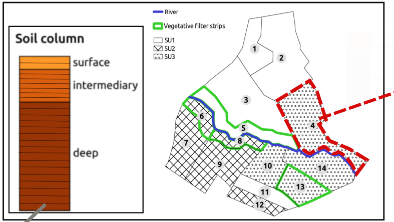

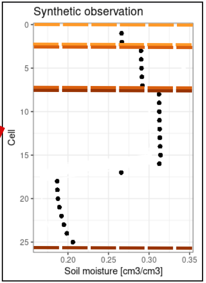

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INRAE

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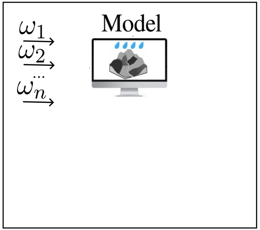
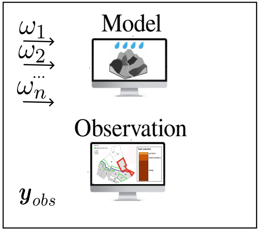
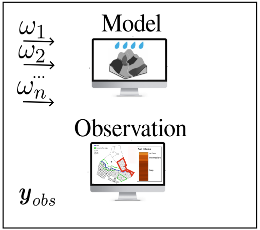

Model
ω_1
ω_2
...
ω_n

Results: Overview





Cost function

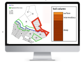
$$\longrightarrow f_s^{(1)}(x)$$
$$\longrightarrow f_s^{(2)}(x)$$
...
$$\longrightarrow f_s^{(n)}(x)$$

Results: Overview

$\omega_1 \longrightarrow$, $\omega_2 \longrightarrow$, …, $\omega_n \longrightarrow$

Model

Observation



$\boldsymbol{y}_{obs}$

Cost function		Metamodel
$\longrightarrow f_s^{(1)}(x)$	$\longrightarrow$	$f_{s\_PCE}^{(1)}(x)$
$\longrightarrow f_s^{(2)}(x)$	$\longrightarrow$	$f_{s\_PCE}^{(2)}(x)$
…		…
$\longrightarrow f_s^{(n)}(x)$	$\longrightarrow$	$f_{s\_PCE}^{(n)}(x)$

Results: Overview

$\omega_1 \longrightarrow$

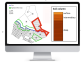
$\omega_2 \longrightarrow$

$\cdots$

$\omega_n \longrightarrow$

Model

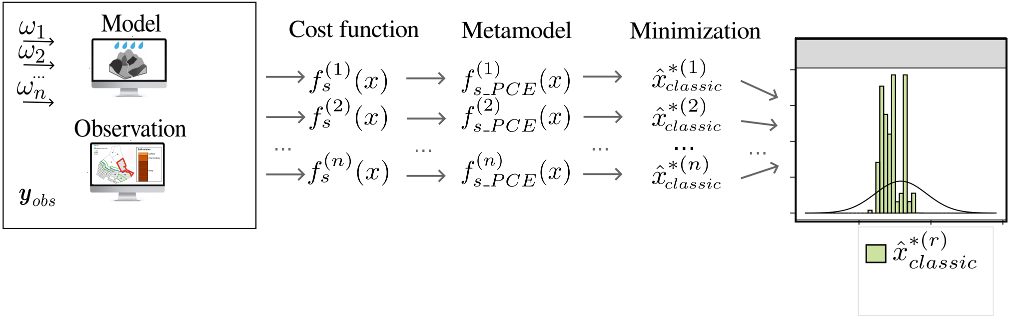
Observation



$\boldsymbol{y}_{obs}$

Cost function	Metamodel	Minimization
$\longrightarrow f_s^{(1)}(x)$	$\longrightarrow f_{s\_PCE}^{(1)}(x)$	$\longrightarrow \hat{x}_{classic}^{*(1)}$
$\longrightarrow f_s^{(2)}(x)$	$\longrightarrow f_{s\_PCE}^{(2)}(x)$	$\longrightarrow \hat{x}_{classic}^{*(2)}$
$\cdots$	$\cdots$	$\cdots$ $\cdots$
$\longrightarrow f_s^{(n)}(x)$	$\longrightarrow f_{s\_PCE}^{(n)}(x)$	$\longrightarrow \hat{x}_{classic}^{*(n)}$

Results: Overview



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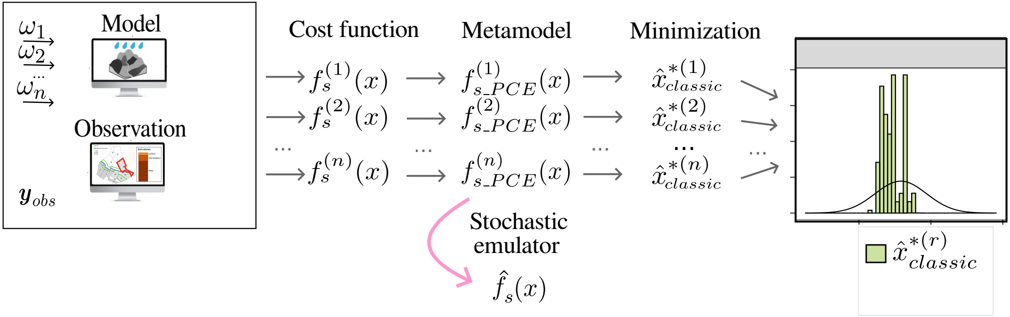

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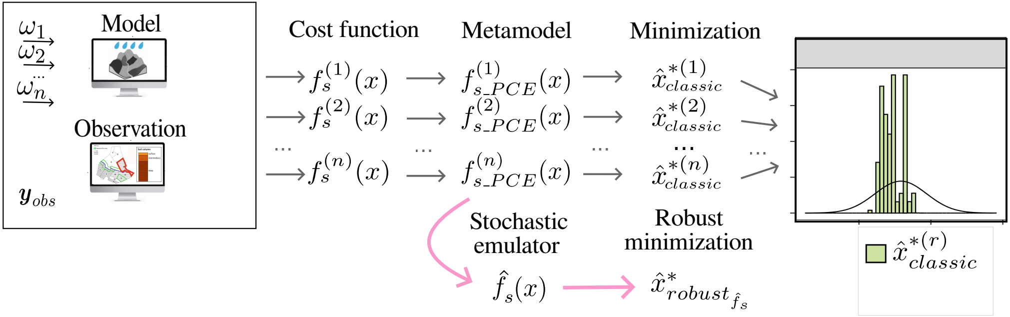

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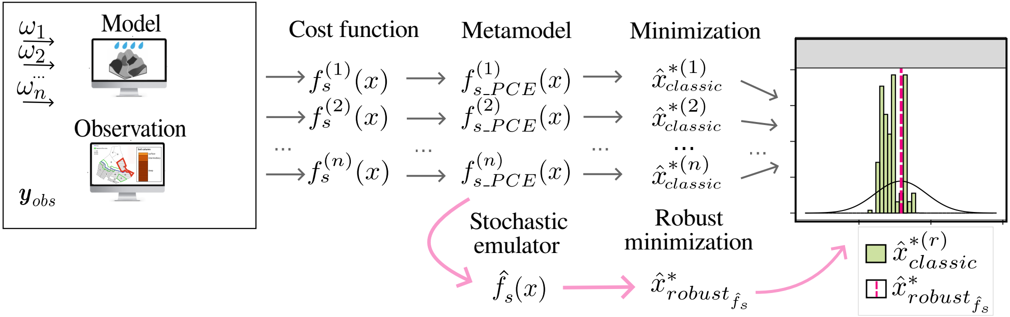
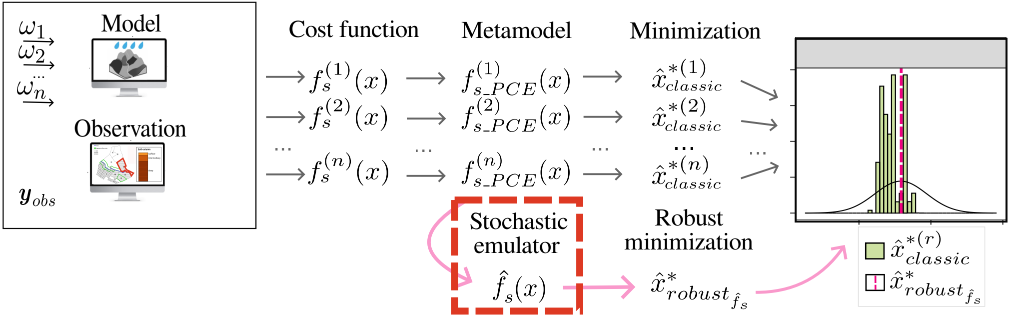


1. Fit and validate $\hat{f}_s$.
2. Get robust calibration for different thresholds c.
3. Compare robust calibration to classic approach.

Results: Overview



1. **Fit and validate $\hat{f}_s$.**
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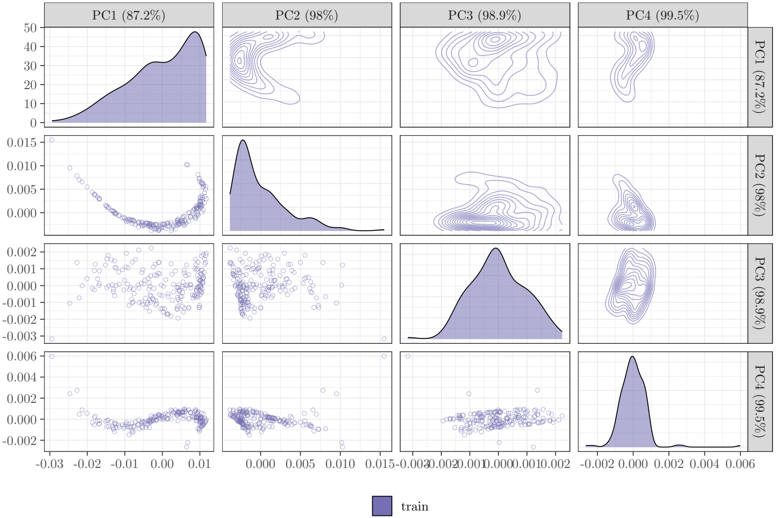
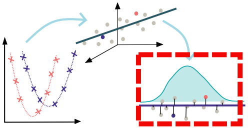
Results: Fit and validate $\hat{f}_s$





latent space *original (test set) vs metamodel*

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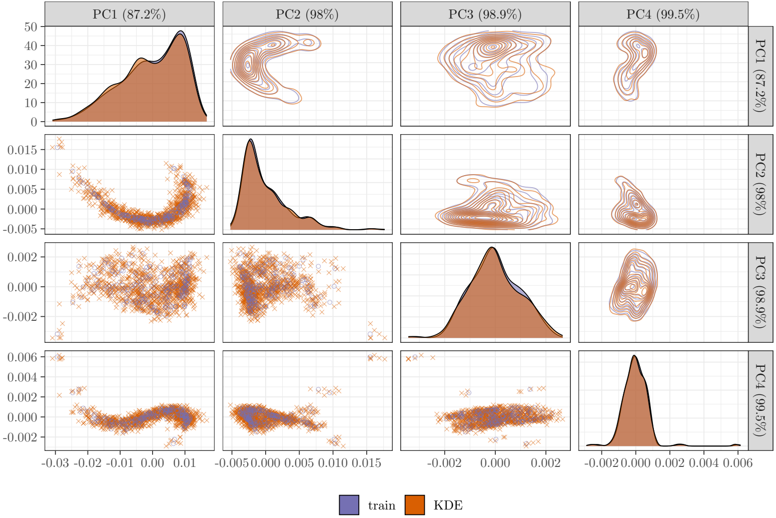

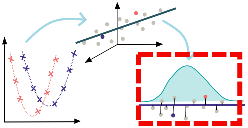

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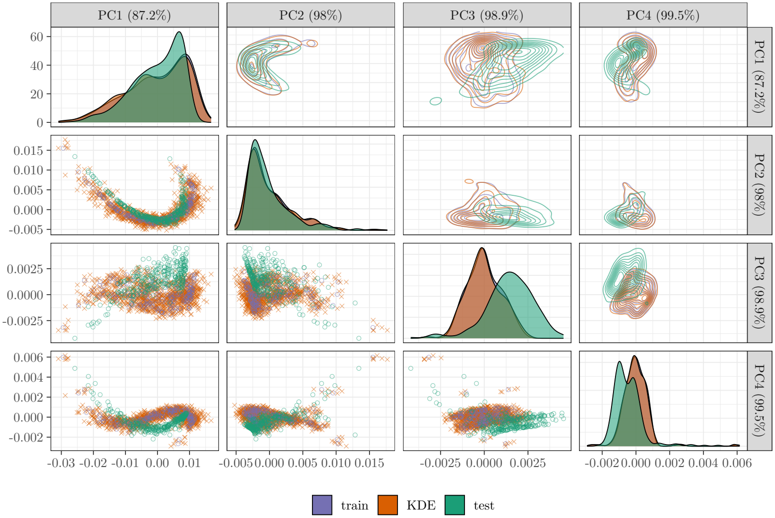

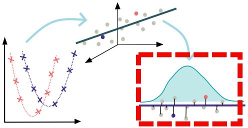

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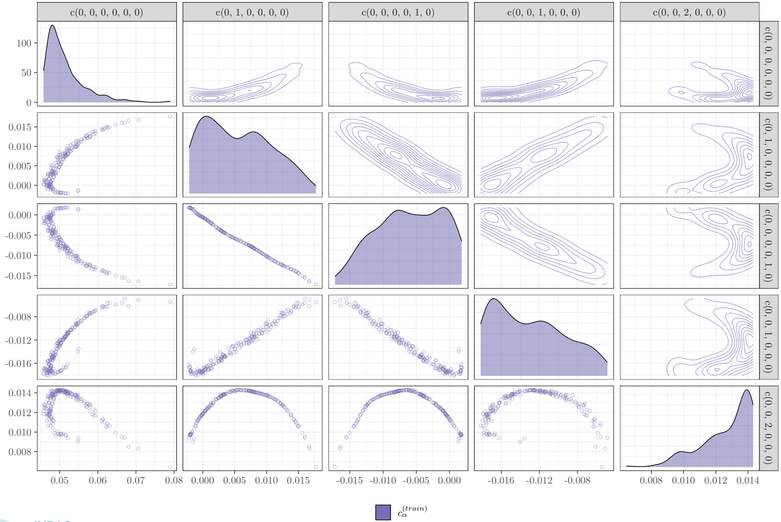

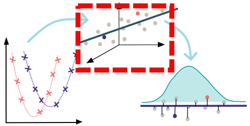

coefficients space
original (test set) vs metamodel

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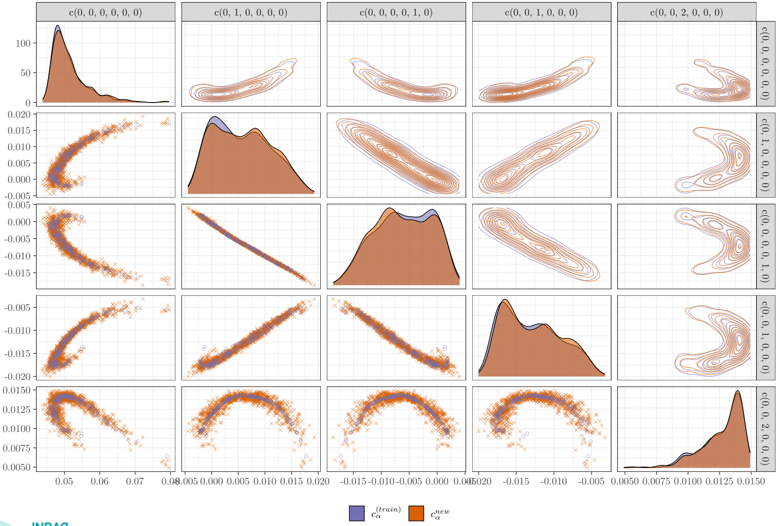

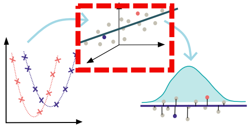

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INRAE

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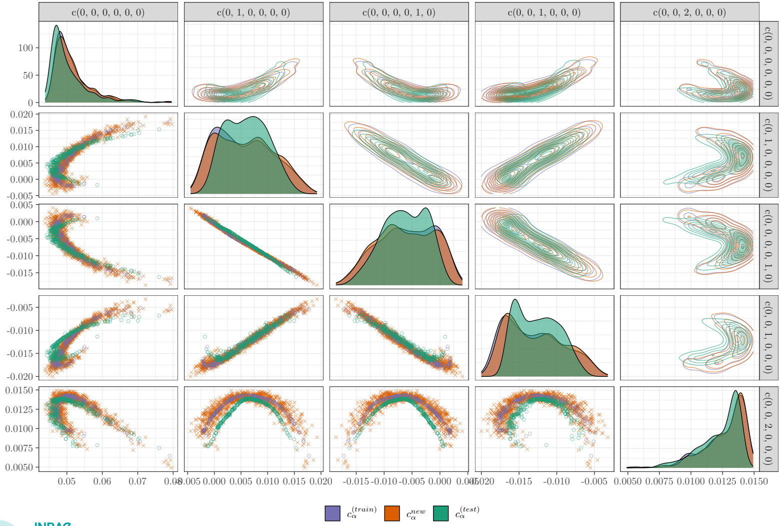

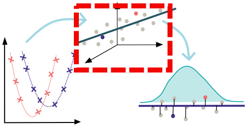

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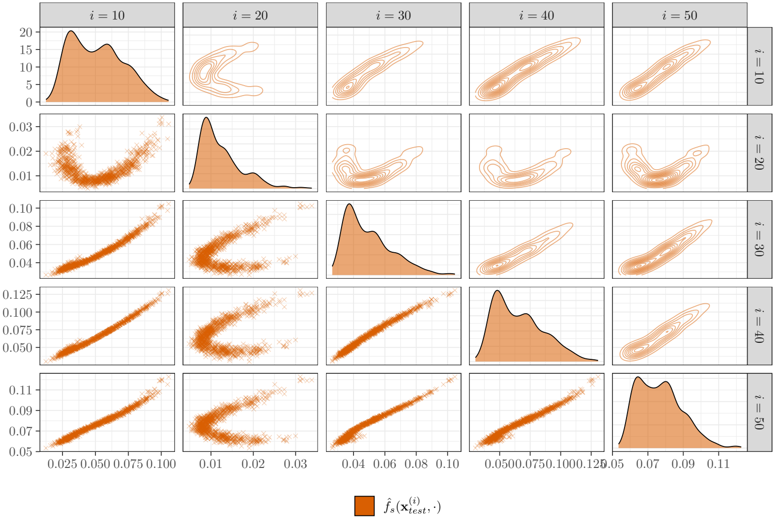

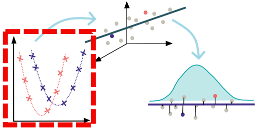

physical space (cost function values)
original (test set) vs metamodel

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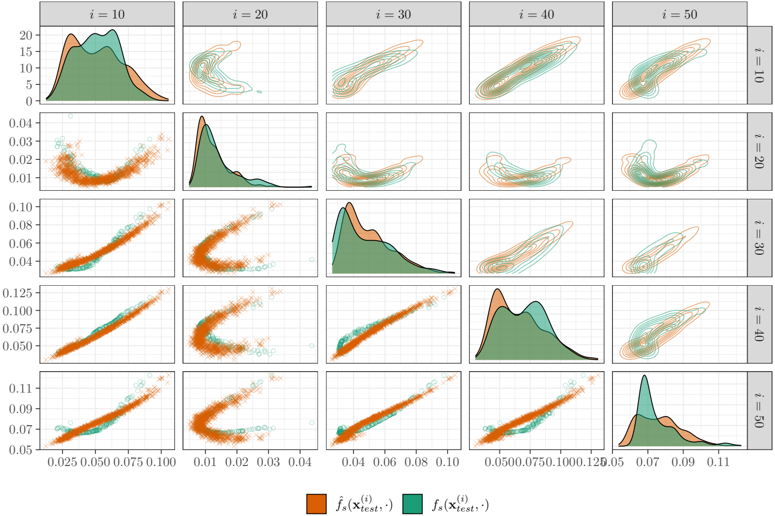

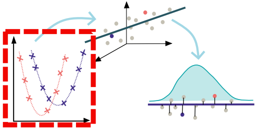

physical space (cost function values)

original (test set) vs metamodel

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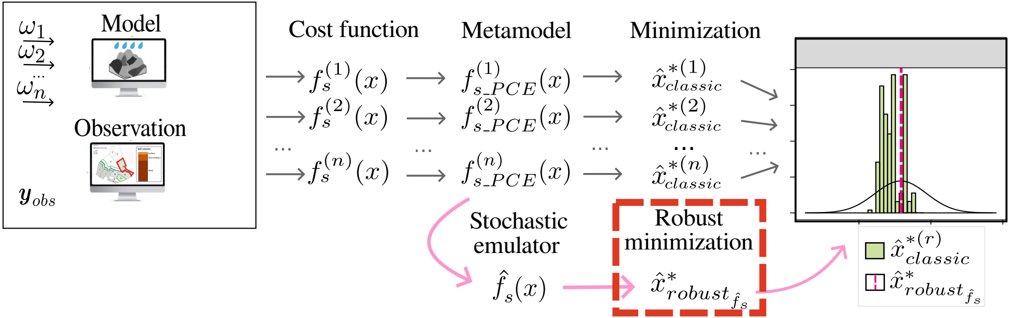
Results: Robust calibration with different thresholds c



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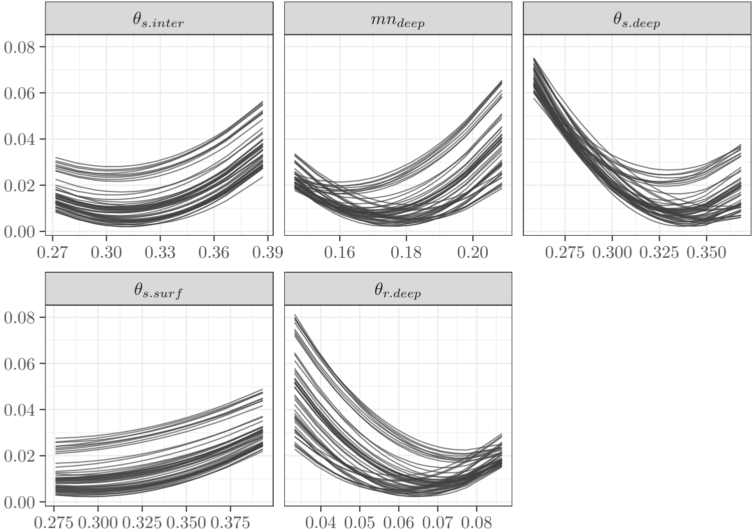

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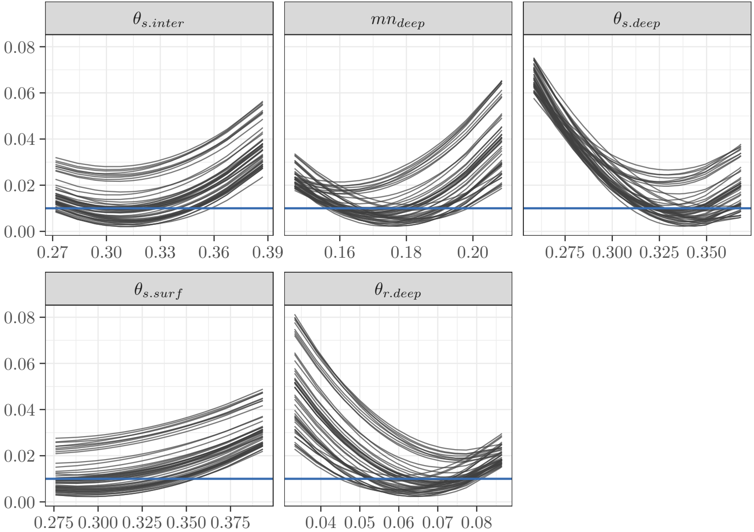

INRAE

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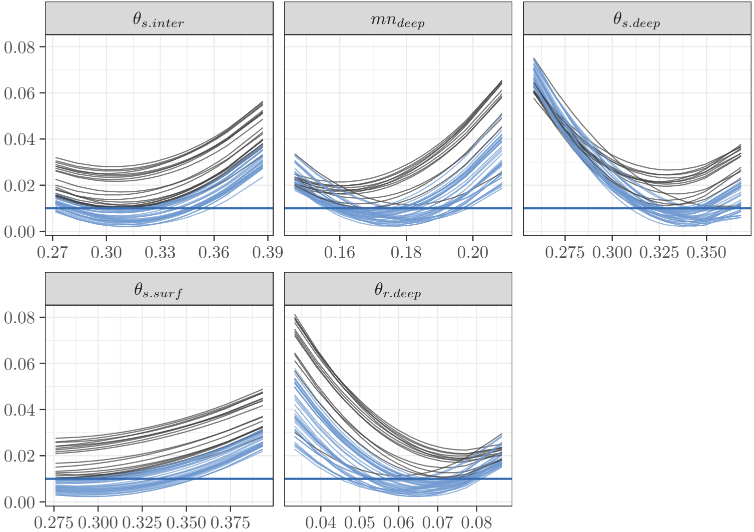

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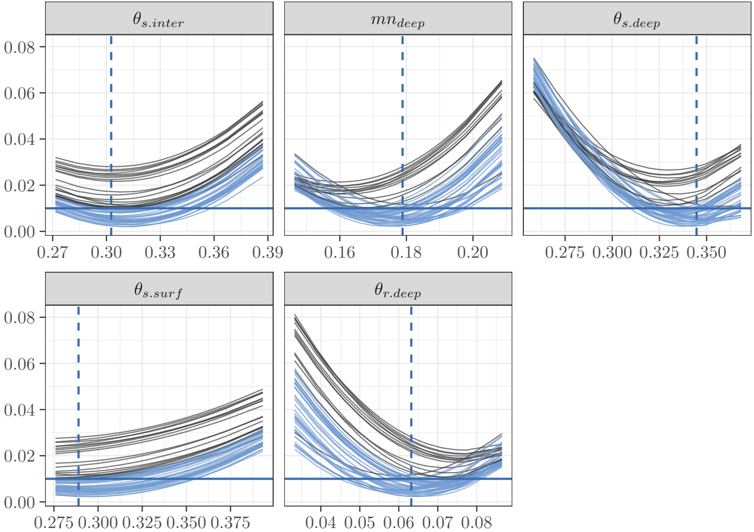

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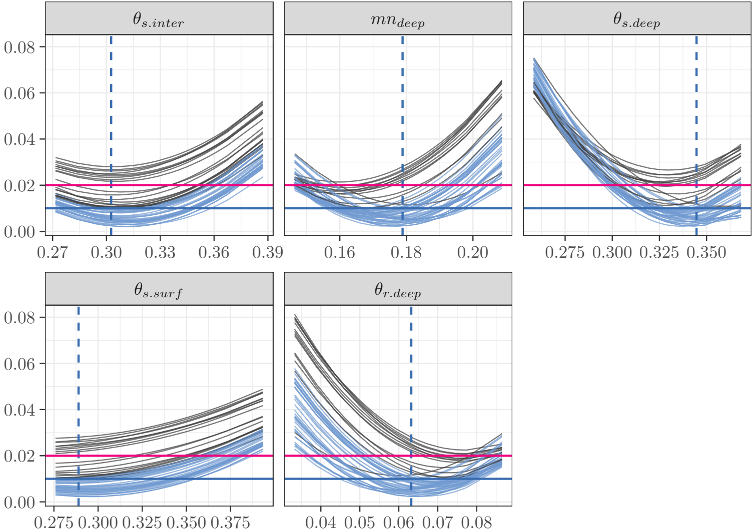

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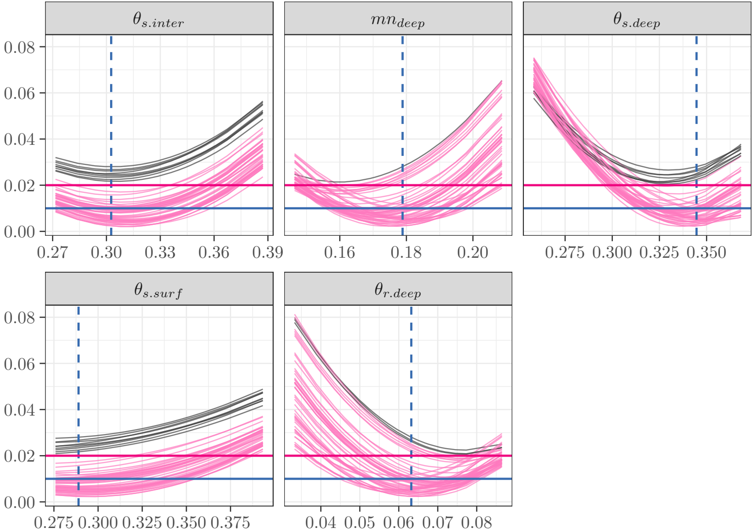

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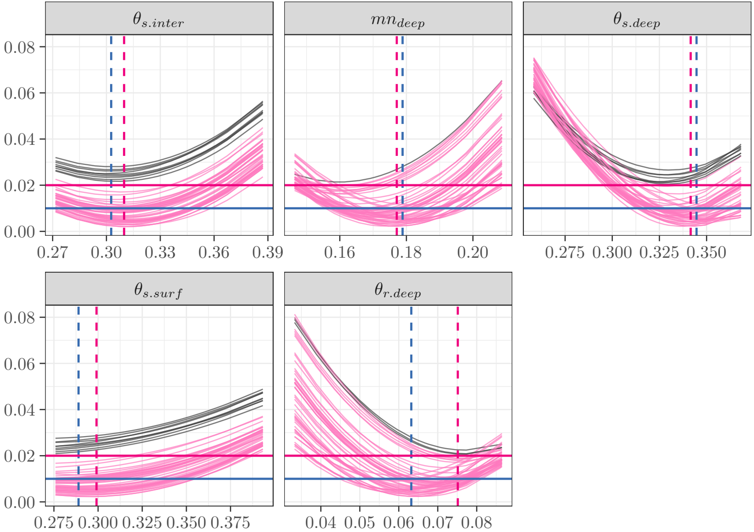

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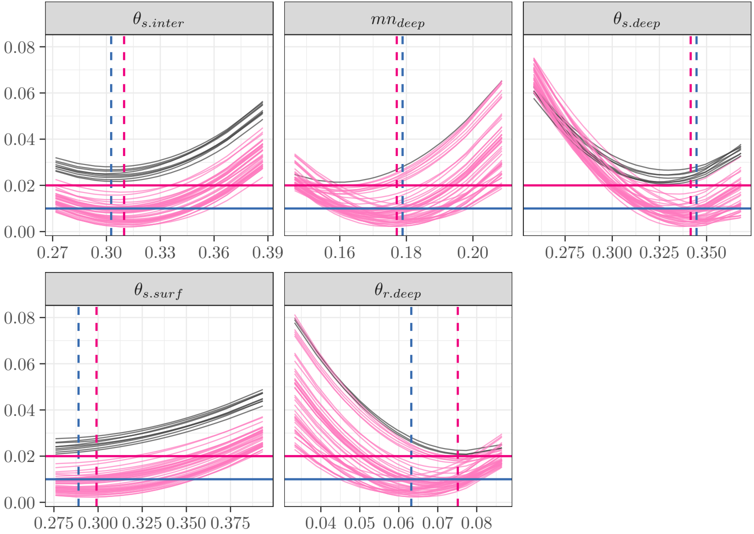

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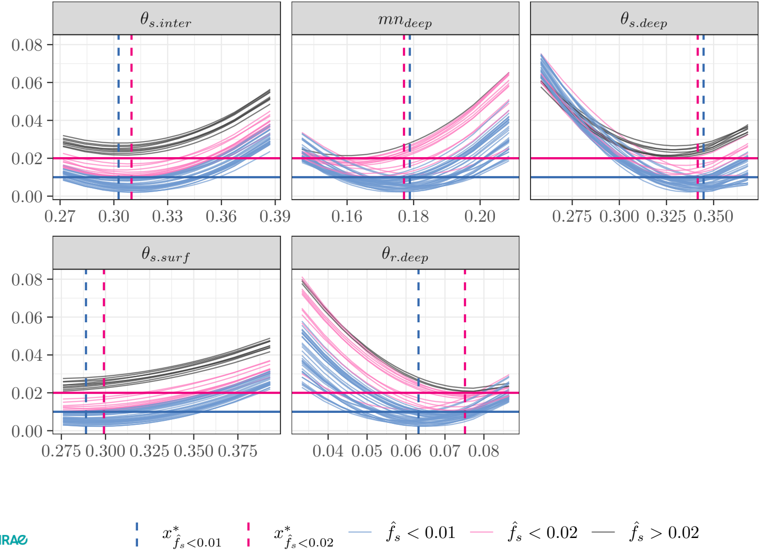

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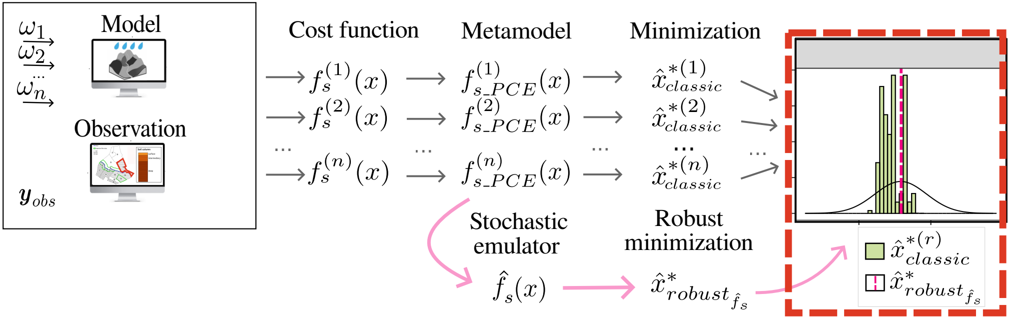
Results: Compare robust calibration with classic approach



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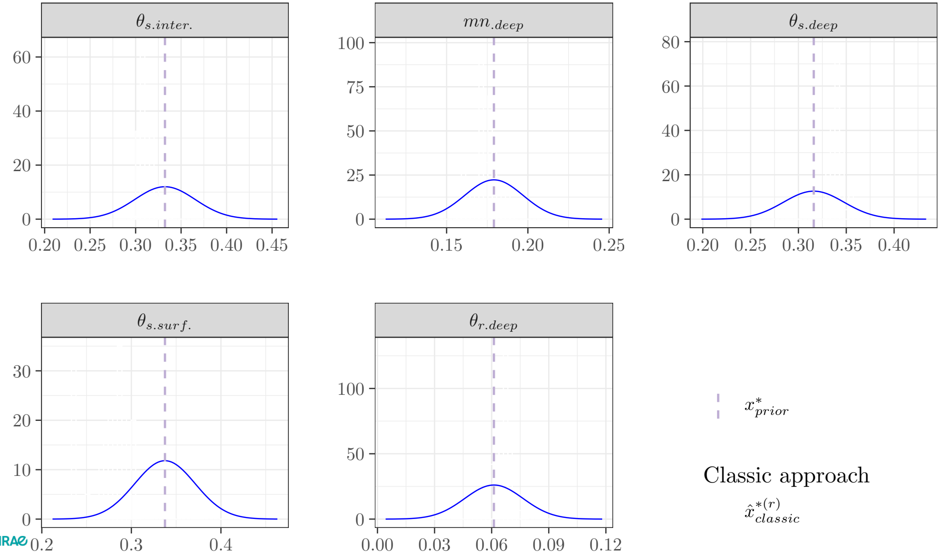

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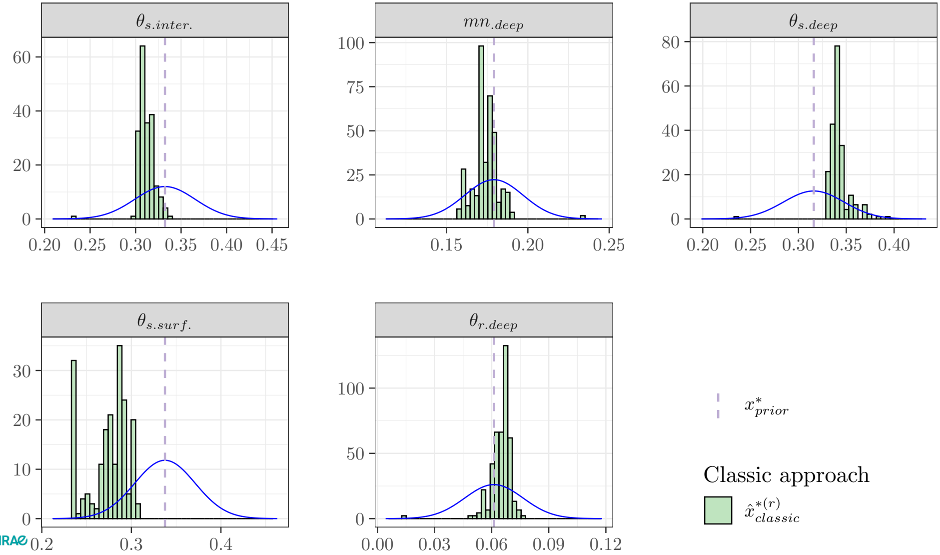

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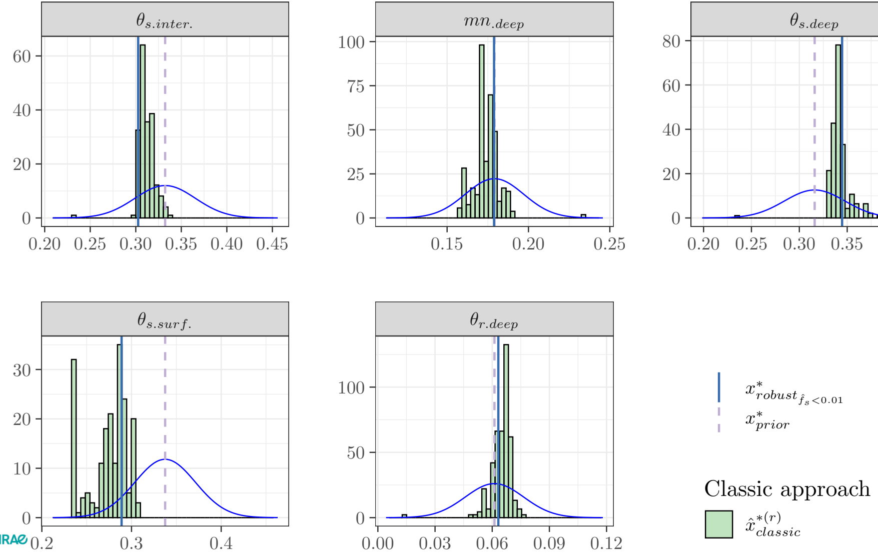

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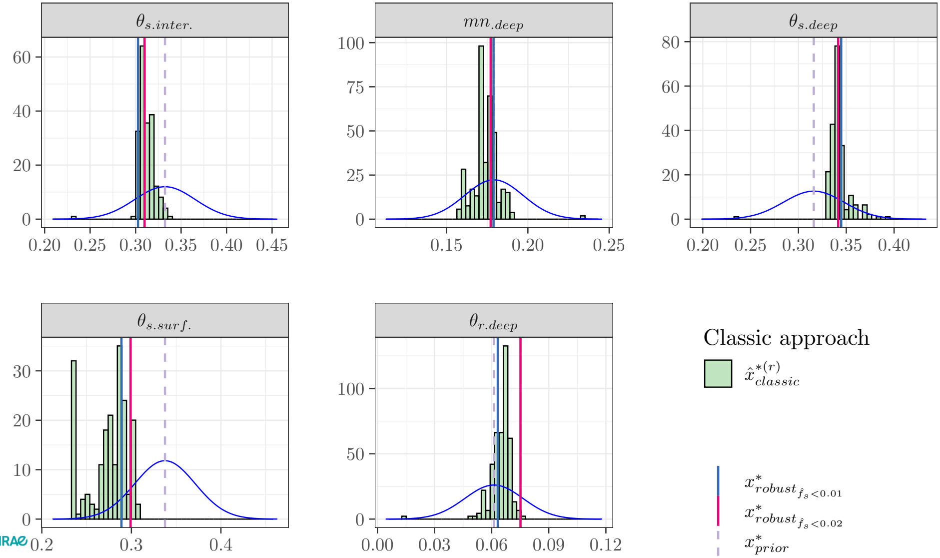

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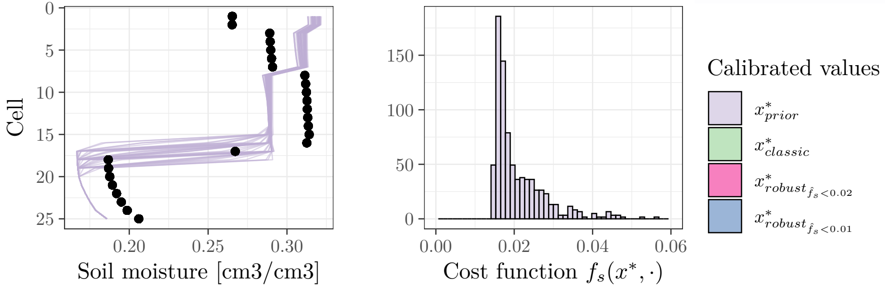

	$\overline{f_s(\boldsymbol{x}^*, \cdot)}$	$\overline{\mathbb{1}_{\{f_s(\boldsymbol{x}^*,\cdot)>0.01\}}}$	$\overline{\mathbb{1}_{\{f_s(\boldsymbol{x}^*,\cdot)>0.02\}}}$	$\max(f_s(\boldsymbol{x}^*, \cdot))$	$\mathrm{Var}(f_s(\boldsymbol{x}^*, \cdot))$
$\boldsymbol{x}^*_{prior}$	0.0209	0.99	0.39	0.057	4.57e-05

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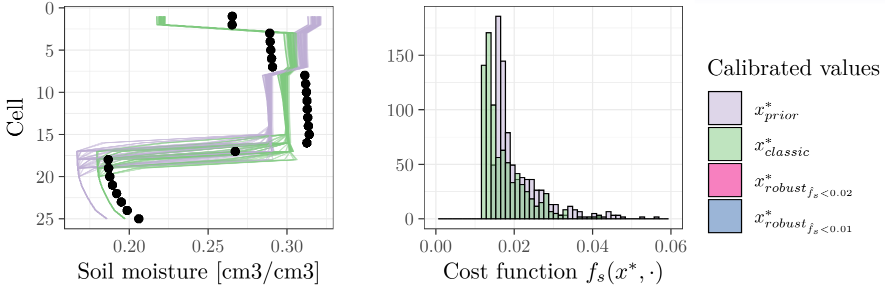

	$\overline{f_s(\boldsymbol{x}^*, \cdot)}$	$\overline{\mathbb{1}_{\{f_s(\boldsymbol{x}^*,\cdot)>0.01\}}}$	$\overline{\mathbb{1}_{\{f_s(\boldsymbol{x}^*,\cdot)>0.02\}}}$	$\max(f_s(\boldsymbol{x}^*, \cdot))$	$\mathrm{Var}(f_s(\boldsymbol{x}^*, \cdot))$
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$\hat{\boldsymbol{x}}^*_{classic}$	0.0173	0.99	0.25	0.042	**2.91e-05**

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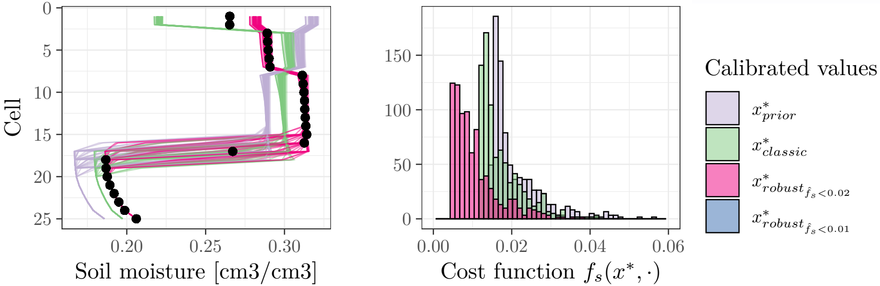

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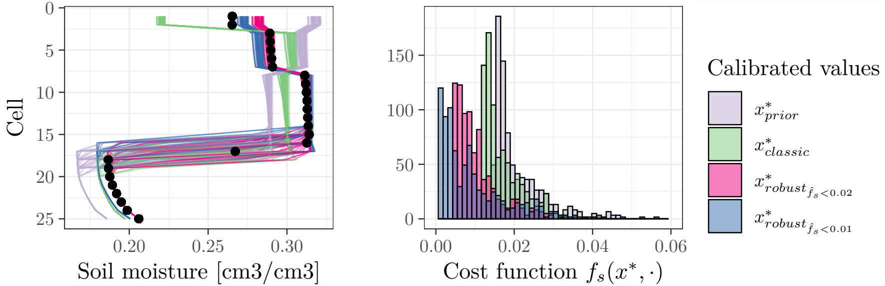

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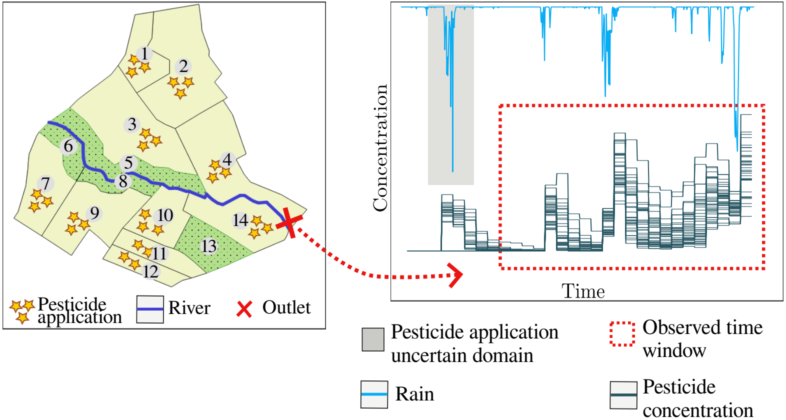
Results: Pesticide concentration at outlet



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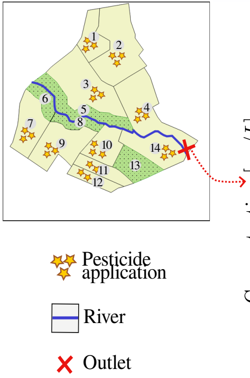

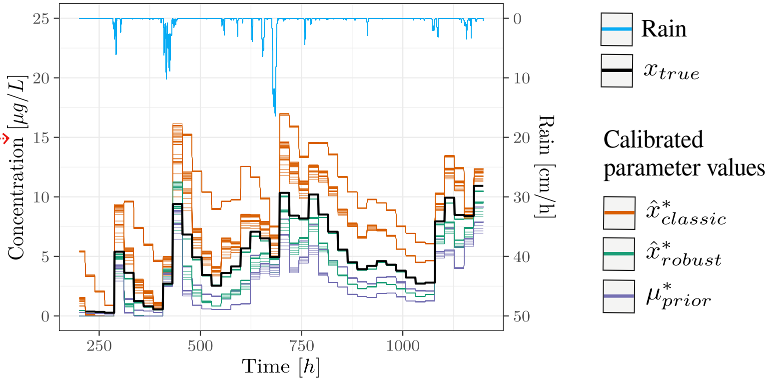

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- Development and comparison with adaptive methods [2].
- Study and definition of robustness criteria for pesticide concentrations.
- Another definition of Ω: natural variability, interannual variability, or uncertainty in future projections.

Bibliography I

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Average norm. wass. distance w.r.t. number of training trajectories and size of the latent space I