



HAL
open science

Calibration robuste d'un modèle hydrologique de transfert de pesticides par métamodélisation

Katarina Radišić, Claire Lauvernet, Arthur Vidard

► To cite this version:

Katarina Radišić, Claire Lauvernet, Arthur Vidard. Calibration robuste d'un modèle hydrologique de transfert de pesticides par métamodélisation. JMSC 2024 - 5ème édition des Journées de Modélisation des Surfaces Continentales, Jun 2024, Strasbourg, France. pp.1-49. hal-04622409

HAL Id: hal-04622409

<https://hal.inrae.fr/hal-04622409>

Submitted on 24 Jun 2024

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.



Distributed under a Creative Commons Attribution 4.0 International License

Calibration robuste d'un modèle hydrologique de transfert de pesticides par métamodélisation

Katarina Radišić¹²³
Claire Lauvernet¹, Arthur Vidard²

¹INRAE, RiverLy, Lyon-Villeurbanne

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

³ED MSTII

Table of contents

Introduction

Model calibration = minimization of a cost function

Methods

Robust minimizers

Case study

PESHMELBA

Moisture profiles

Results

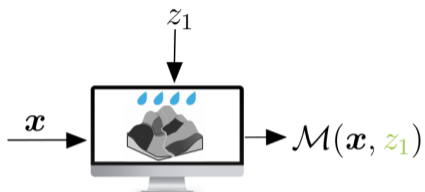
Problem formulation

Minimizers

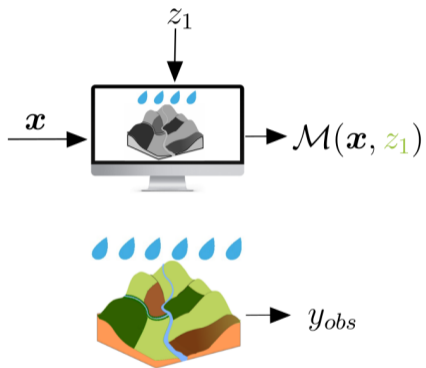
New simulations cost function

Conclusion

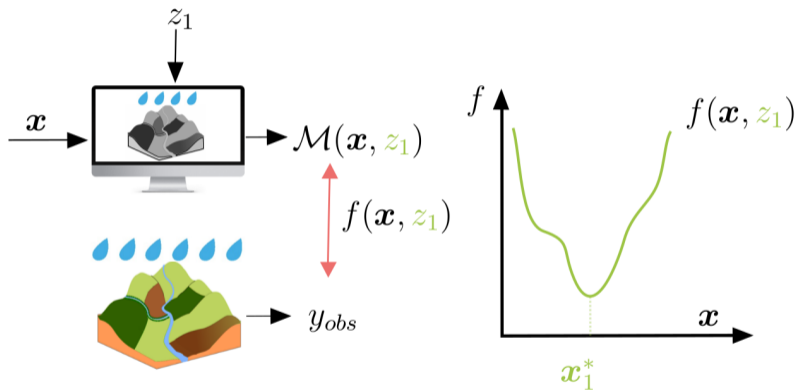
Introduction: Model calibration = minimization of a cost function



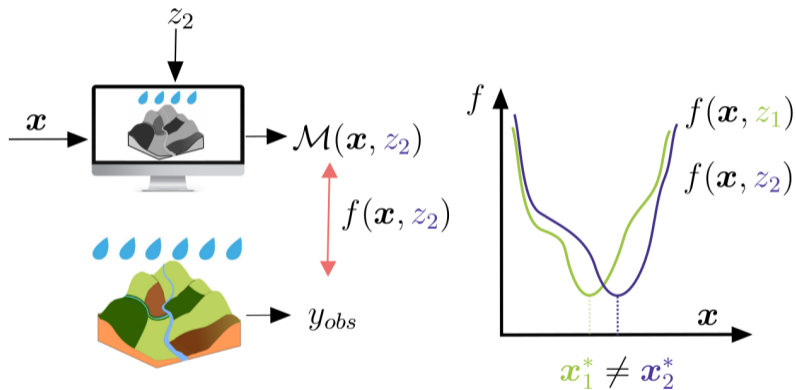
Introduction: Model calibration = minimization of a cost function



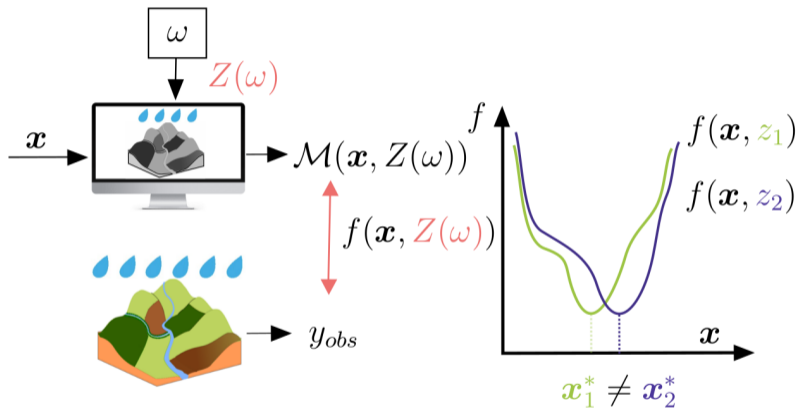
Introduction: Model calibration = minimization of a cost function



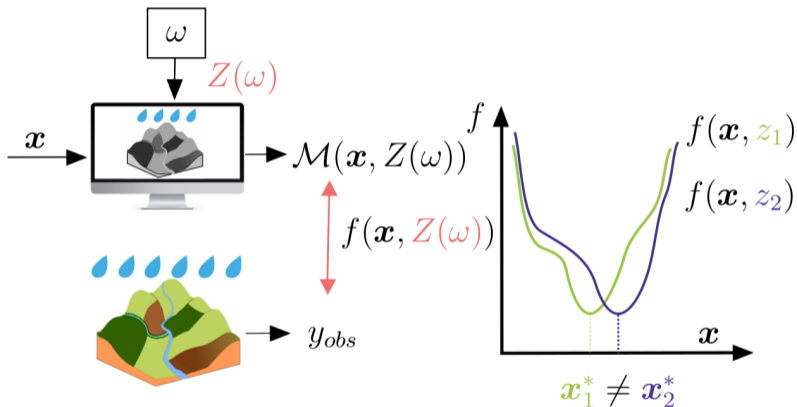
Introduction: Model calibration = minimization of a cost function



Introduction: Model calibration = minimization of a cost function



Introduction: Model calibration = minimization of a cost function



How to minimize a stochastic function? → **robust calibration**

Table of contents

Introduction

Model calibration = minimization of a cost function

Methods

Robust minimizers

Case study

PESHMELBA

Moisture profiles

Results

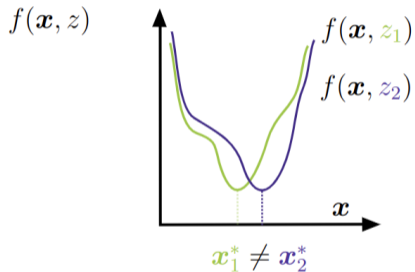
Problem formulation

Minimizers

New simulations cost function

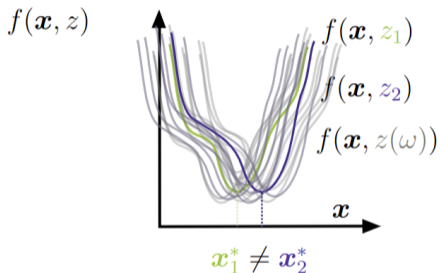
Conclusion

Methods: Robust minimizers



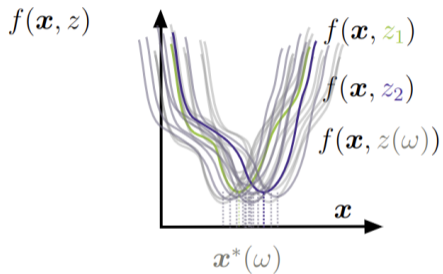
What criterion for the minimization of a stochastic cost function ?

Methods: Robust minimizers



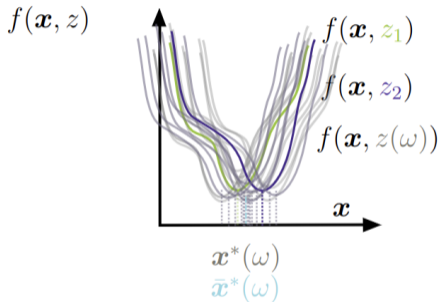
What criterion for the minimization of a stochastic cost function ?

Methods: Robust minimizers



What criterion for the minimization of a stochastic cost function ?

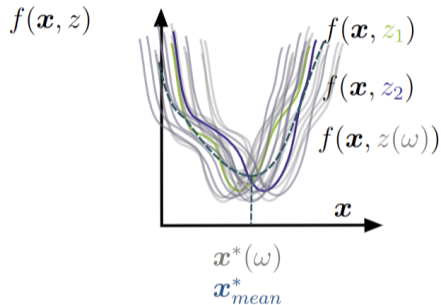
Methods: Robust minimizers



What criterion for the minimization of a stochastic cost function ?

$$\bar{\mathbf{x}}^* = \mathbb{E}_{\omega}[\operatorname{argmin}_{\mathbf{x}} f(\mathbf{x}, \omega)],$$

Methods: Robust minimizers

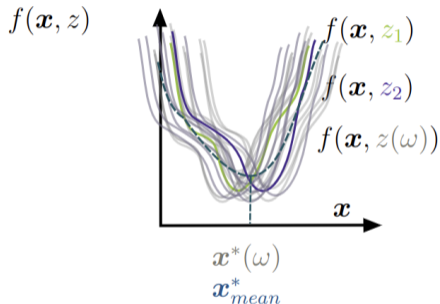


What criterion for the minimization of a stochastic cost function ?

$$\bar{x}^* = \mathbb{E}_{\omega}[\underset{x}{\operatorname{argmin}} f(x, \omega)],$$

$$x_{mean}^* = \underset{x}{\operatorname{argmin}} \mathbb{E}_{\omega}[f(x, \omega)],$$

Methods: Robust minimizers



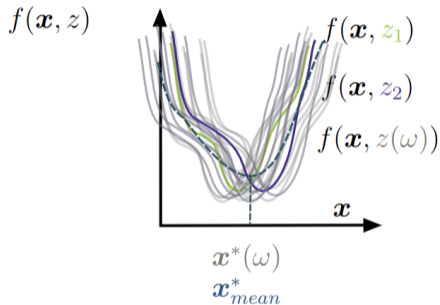
What criterion for the minimization of a stochastic cost function ?

$$\bar{\mathbf{x}}^* = \mathbb{E}_{\omega} [\operatorname{argmin}_{\mathbf{x}} f(\mathbf{x}, \omega)],$$

$$\mathbf{x}_{mean}^* = \operatorname{argmin}_{\mathbf{x}} \mathbb{E}_{\omega} [f(\mathbf{x}, \omega)],$$

$$\mathbf{x}_{\nabla ar}^* = \operatorname{argmin}_{\mathbf{x}} \nabla ar_{\omega} [f(\mathbf{x}, \omega)],$$

Methods: Robust minimizers



What criterion for the minimization of a stochastic cost function ?

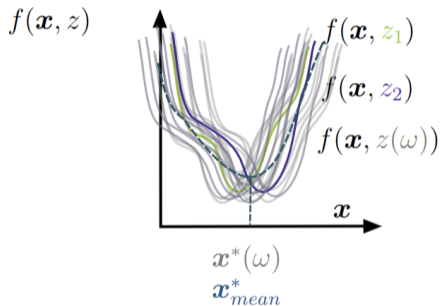
$$\bar{\mathbf{x}}^* = \mathbb{E}_{\omega} [\underset{\mathbf{x}}{\operatorname{argmin}} f(\mathbf{x}, \omega)],$$

$$\mathbf{x}_{mean}^* = \underset{\mathbf{x}}{\operatorname{argmin}} \mathbb{E}_{\omega} [f(\mathbf{x}, \omega)],$$

$$\mathbf{x}_{\nabla ar}^* = \underset{\mathbf{x}}{\operatorname{argmin}} \nabla ar_{\omega} [f(\mathbf{x}, \omega)],$$

...

Methods: Robust minimizers



What criterion for the minimization of a stochastic cost function ?

$$\bar{\mathbf{x}}^* = \mathbb{E}_{\omega}[\operatorname{argmin}_{\mathbf{x}} f(\mathbf{x}, \omega)],$$

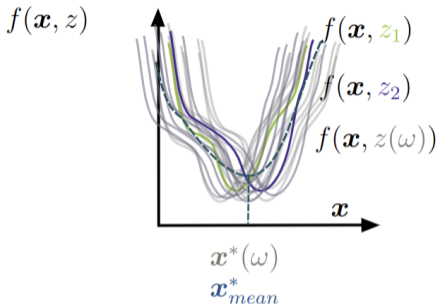
$$\mathbf{x}_{mean}^* = \operatorname{argmin}_{\mathbf{x}} \mathbb{E}_{\omega}[f(\mathbf{x}, \omega)],$$

$$\mathbf{x}_{\nabla ar}^* = \operatorname{argmin}_{\mathbf{x}} \nabla ar_{\omega}[f(\mathbf{x}, \omega)],$$

...

Very expensive simulations

Methods: Robust minimizers



What criterion for the minimization of a stochastic cost function ?

$$\bar{x}^* = \mathbb{E}_{\omega} [\operatorname{argmin}_x f(x, \omega)],$$

$$x^*_{mean} = \operatorname{argmin}_x \mathbb{E}_{\omega} [f(x, \omega)],$$

$$x^*_{\nabla ar} = \operatorname{argmin}_x \nabla ar_{\omega} [f(x, \omega)],$$

...

Very expensive simulations

How to limit number of model evaluations ?

→ Metamodels = approximation of the original model (*or of the cost function*):
linear regression, neural networks ...

- **Polynomial Chaos Expansion**, Marelli and Sudret 2014
 - can be used for a large number of input parameters (+)
 - uses one-shot experimental designs (can be parallelized) (+)
 - approximate the cost function globally (-)
 - have to be validated (-)

Table of contents

Introduction

Model calibration = minimization of a cost function

Methods

Robust minimizers

Case study

PESHMELBA

Moisture profiles

Results

Problem formulation

Minimizers

New simulations cost function

Conclusion

Case study: PESHMELBA

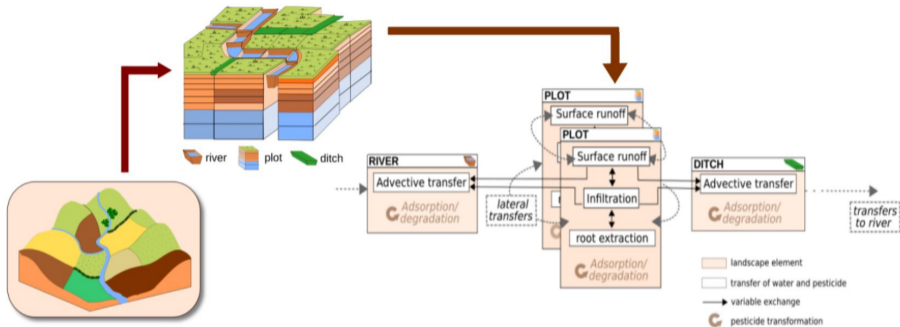


Figure: PESHMELBA model, Rouzies et al. 2019

Case study: PESHMELBA

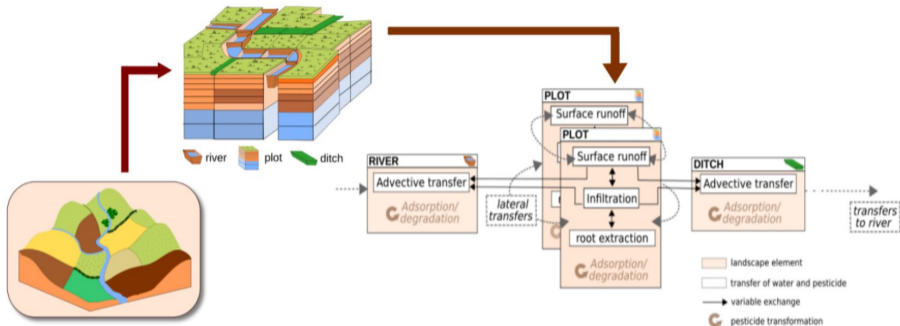


Figure: PESHMELBA model, Rouzies et al. 2019

- process-oriented, physically-based, coupling with landscape features

Case study: PESHMELBA

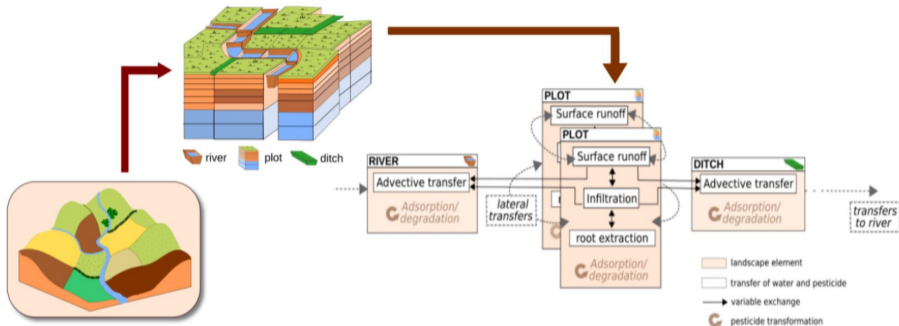


Figure: PESHMELBA model, Rouzies et al. 2019

- process-oriented, physically-based, coupling with landscape features
- simulates water and pesticide transfers on an agricultural catchment

Case study: PESHMELBA

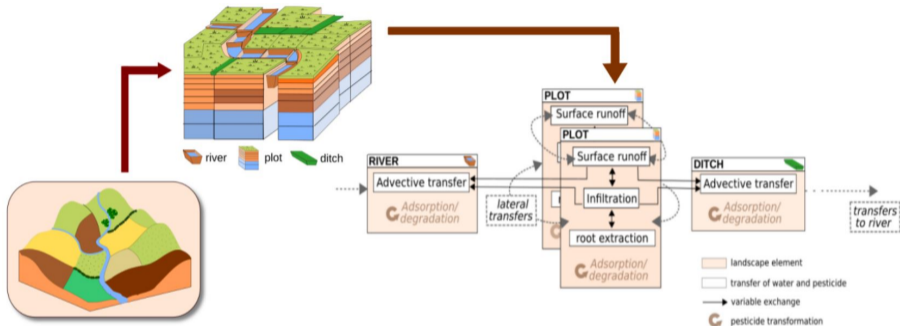


Figure: PESHMELBA model, Rouzies et al. 2019

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

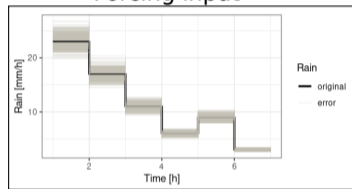
Case study: Moisture profiles

A simplified case study: moisture profile of one plot

Case study: Moisture profiles

A simplified case study: moisture profile of one plot

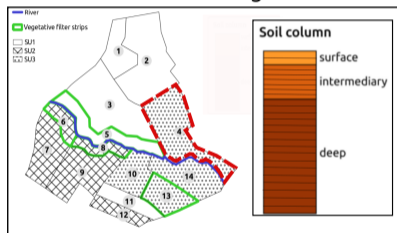
Forcing input



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)

PESHMELBA configuration



Observation = moisture profile of parcel 4

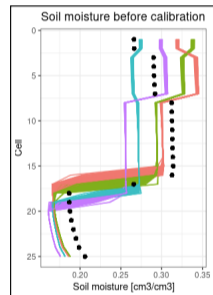


Table of contents

Introduction

Model calibration = minimization of a cost function

Methods

Robust minimizers

Case study

PESHMELBA

Moisture profiles

Results

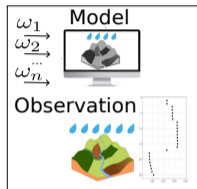
Problem formulation

Minimizers

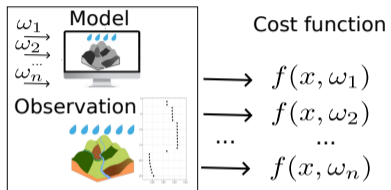
New simulations cost function

Conclusion

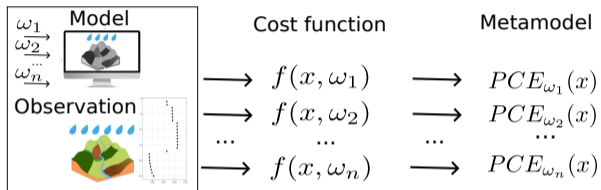
Results: Problem formulation



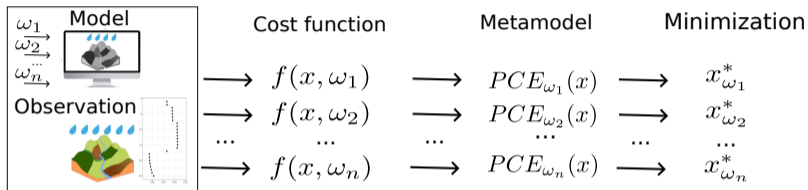
Results: Problem formulation



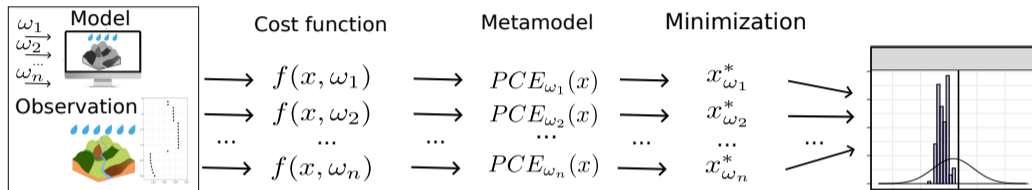
Results: Problem formulation



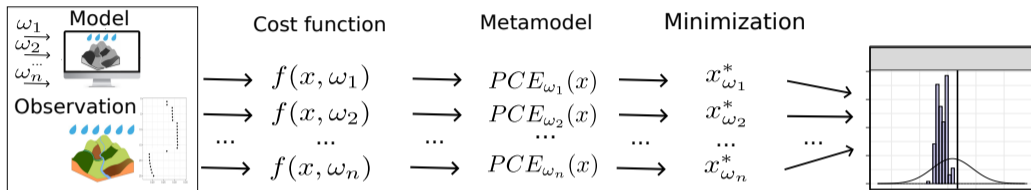
Results: Problem formulation



Results: Problem formulation

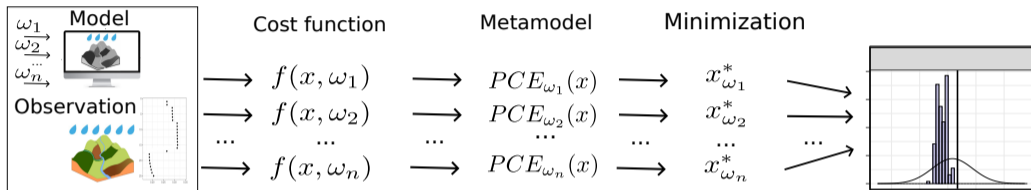


Results: Problem formulation



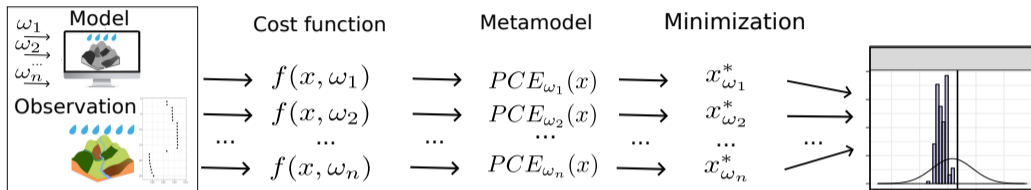
- the spread of minimizer histogram = the uncertainty propagation from forcings to calibrated values

Results: Problem formulation



- the spread of minimizer histogram = the uncertainty propagation from forcings to calibrated values
- all metamodels show very good R2 values > 0.95 (validation).

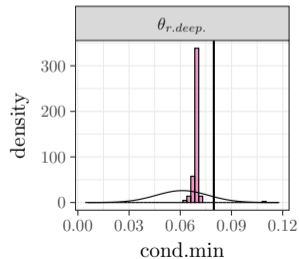
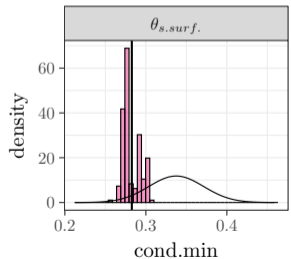
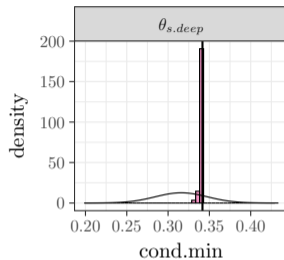
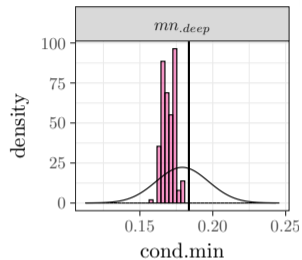
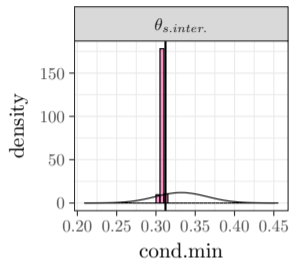
Results: Problem formulation



- the spread of minimizer histogram = the uncertainty propagation from forcings to calibrated values
- all metamodels showed very good R2 values > 0.95 .

Next: Compare classic minimizers with robust minimizers : x_{mean}^ and \bar{x}^* .*

Results: Minimizers



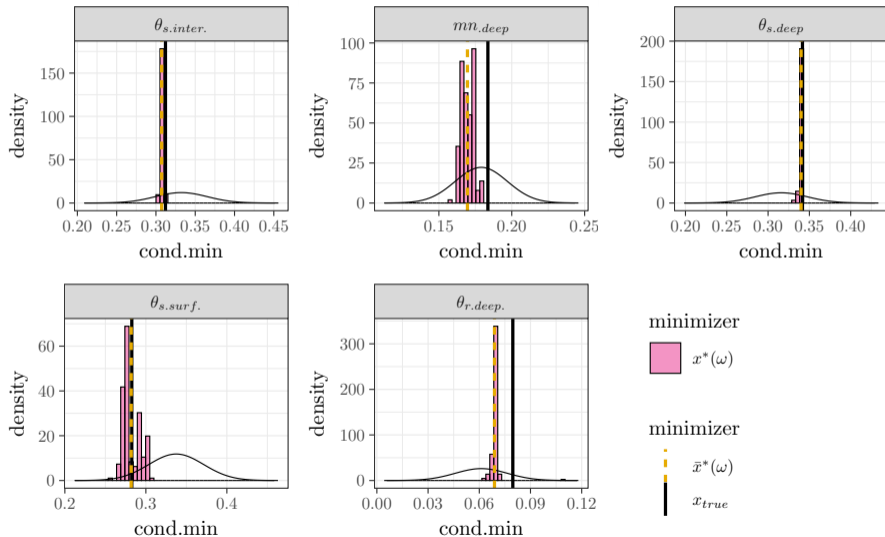
minimizer

 $x^*(\omega)$

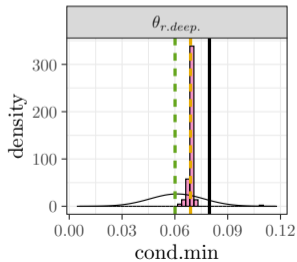
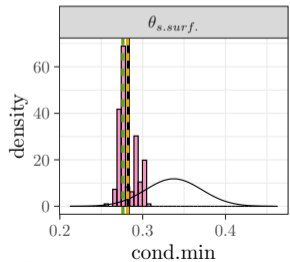
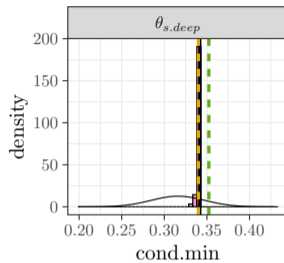
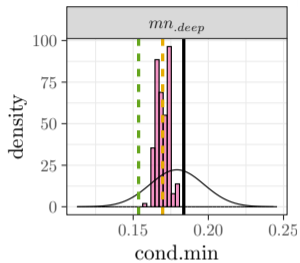
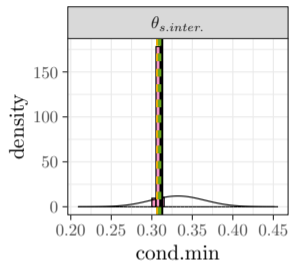
minimizer

 x_{true}

Results: Minimizers



Results: Minimizers



minimizer

$x^*(\omega)$

minimizer

x_{mean}^*

$\bar{x}^*(\omega)$

x_{true}

Results: New simulations cost function

Is the calibration better with robust minimizers ?

Results: New simulations cost function

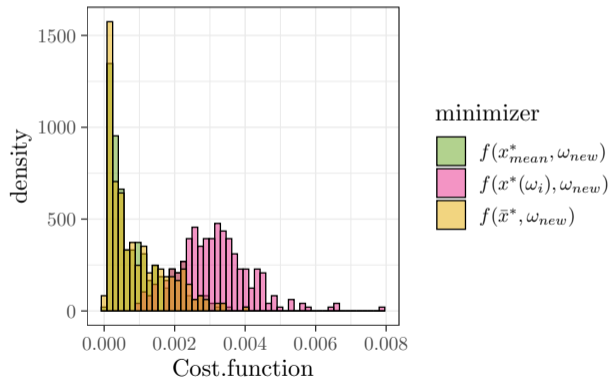
Is the calibration better with robust minimizers ?

→ compare cost function for new realisations of forcing uncertainty.

Results: New simulations cost function

Is the calibration better with robust minimizers ?

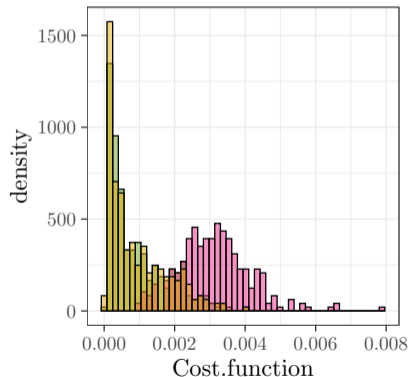
→ compare cost function for new realisations of forcing uncertainty.



Results: New simulations cost function

Is the calibration better with robust minimizers ?

→ compare cost function for new realisations of forcing uncertainty.



minimizer

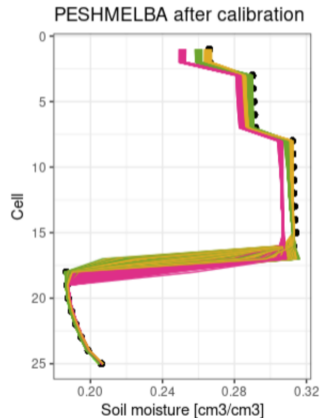
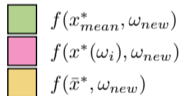


Table of contents

Introduction

Model calibration = minimization of a cost function

Methods

Robust minimizers

Case study

PESHMELBA

Moisture profiles

Results

Problem formulation

Minimizers

New simulations cost function

Conclusion

Conclusion:

1. a method is proposed to calibrate models by taking external factors into account (here, rainfall, but the method is valid for any forcing: discretization, evapotranspiration, given a representative sample).

Conclusion:

1. a method is proposed to calibrate models by taking external factors into account (here, rainfall, but the method is valid for any forcing: discretization, evapotranspiration, given a representative sample).
2. the interest of the method and the chosen robust minimizers is illustrated on a simple case study

Conclusion:

1. a method is proposed to calibrate models by taking external factors into account (here, rainfall, but the method is valid for any forcing: discretization, evapotranspiration, given a representative sample).
2. the interest of the method and the chosen robust minimizers is illustrated on a simple case study

What's next :

- complexify case study, passage to catchment scale, study propagation of uncertainty on pesticide application dates to the model calibration

Conclusion:

1. a method is proposed to calibrate models by taking external factors into account (here, rainfall, but the method is valid for any forcing: discretization, evapotranspiration, given a representative sample).
2. the interest of the method and the chosen robust minimizers is illustrated on a simple case study

What's next :

- complexify case study, passage to catchment scale, study propagation of uncertainty on pesticide application dates to the model calibration
- compare Polynomial Chaos Expansion metamodelization with other metamodelization methods

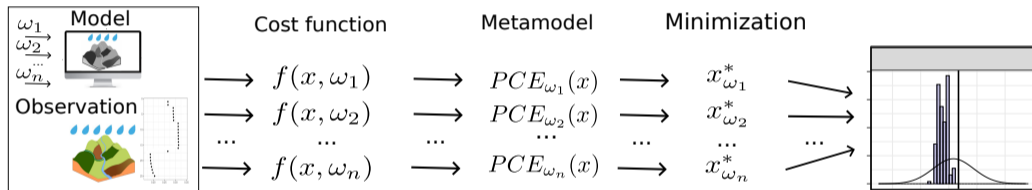
Conclusion:

1. a method is proposed to calibrate models by taking external factors into account (here, rainfall, but the method is valid for any forcing: discretization, evapotranspiration, given a representative sample).
2. the interest of the method and the chosen robust minimizers is illustrated on a simple case study




What's next :

- complexify case study, passage to catchment scale, study propagation of uncertainty on pesticide application dates to the model calibration
- compare Polynomial Chaos Expansion metamodelization with other metamodelization methods
- reduce the number of rain simulations used, interpolation in the rains → stochastic metamodel, Lüthen, Marelli, and Sudret 2023

Conclusion:



Bibliography I

-  Lüthen, Nora, 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. DOI: [10.1016/j.cma.2022.115875](https://doi.org/10.1016/j.cma.2022.115875).
-  Marelli, Stefano and Bruno Sudret (July 2014). “UQLab: A Framework for Uncertainty Quantification in Matlab”. en. In: *Vulnerability, Uncertainty, and Risk*. University of Liverpool, United Kingdom: American Society of Civil Engineers, pp. 2554–2563. DOI: [10.1061/9780784413609.257](https://doi.org/10.1061/9780784413609.257).
-  Rouzies, Emilie 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. DOI: [10.1016/j.scitotenv.2019.03.060](https://doi.org/10.1016/j.scitotenv.2019.03.060).