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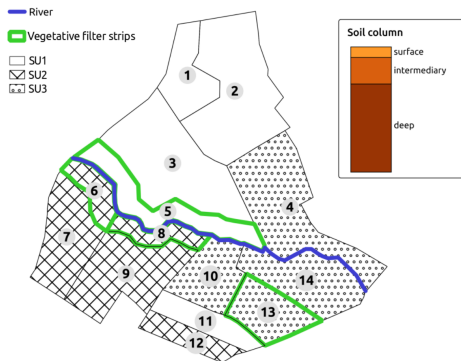
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Sensitivity analysis of a spatio-temporal hydrological model for water and pesticide transfers

Katarina Radišić
Emilie Rouzies, Claire Lauvernet, Arthur Vidard

10th International Conference on Sensitivity Analysis of Model Output
(SAMO) March 14-16, 2022

The PESHMELBA model Rouzies et al.^{1,2}



Landscape units and soil horizons, illustration from Rouzies et al.²

- simulates water and pesticide transfers at a catchment scale
- heterogeneous soil types
- 14 landscape units
- heterogeneous layers : soil horizons
- infiltration, surface runoff and lateral subsurface exchanges
- heterogeneous vegetation types
- large number of input parameters ($K = 145$)
- input parameters are independent
- expensive, process based, hydrologic model

1. ROUZIES, LAUVERNET, BARACHET et al., "From agricultural catchment to management scenarios", 2019.

2. ROUZIES, LAUVERNET, SUDRET et al., [How to perform global sensitivity analysis of a catchment-scale, distributed pesticide transfer model?](#), 2021.

1 Case study

2 Methodology

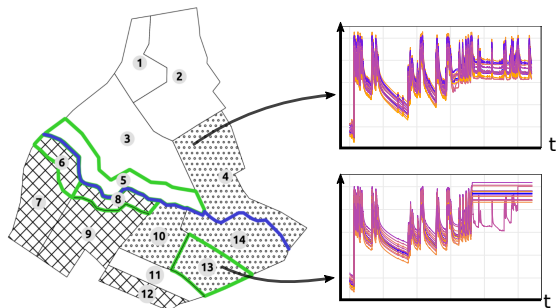
- Sobol' indices and PCE metamodels
- Functional principal components

3 Results

- Interpretation of principal components
- Validation of metamodels
- Sobol' indices

1. Case study

Sensitivity analysis on : **surface moisture outputs.**



$$\begin{bmatrix} Y^{(1)}(t) \\ Y^{(2)}(t) \\ \vdots \\ Y^{(14)}(t) \end{bmatrix} = \mathcal{M}(\mathbf{X}, t)$$

- time dependent outputs
- spatialized outputs
- large number of input parameters ($K = 52$ after screening)

Two types of behaviour :

$$\underbrace{\text{[oscillatory]}}_{\mathcal{G}_{plateau}}$$

$$\underbrace{\text{[oscillatory then steady]}}_{\mathcal{G}_{no_plateau}}$$

1 Case study

2 Methodology

- Sobol' indices and PCE metamodels
- Functional principal components

3 Results

- Interpretation of principal components
- Validation of metamodels
- Sobol' indices

2. Methodology

2.1. Sobol' indices and PCE metamodels

Polynomial Chaos Expansion (PCE), metamodel for analytical Sobol' indices calculation³, calculations were done in the UQLab⁴ Matlab environment.

$$\begin{aligned} Y &= \mathcal{M}(\mathbf{X}) \\ &= \sum_{\alpha \in \mathbb{N}^K} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) \end{aligned}$$

$$D = \text{Var}(Y)$$

$$S_i = \sum_{\substack{\alpha \in \mathbb{N}^K: \\ \alpha_i > 0, \alpha_{j \neq i} = 0}} y_{\alpha}^2 / D$$

$$\begin{aligned} Y &\approx \mathcal{M}_{PCE}(\mathbf{X}) \\ &= \sum_{\alpha \in \mathcal{A}_q^{K,p}} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) \end{aligned}$$

$$\hat{D} = \text{Var}(\mathcal{M}_{PCE}(\mathbf{X}))$$

$$\hat{S}_i = \sum_{\substack{\alpha \in \mathcal{A}_q^{K,p}: \\ \alpha_i > 0, \alpha_{j \neq i} = 0}} y_{\alpha}^2 / \hat{D}$$

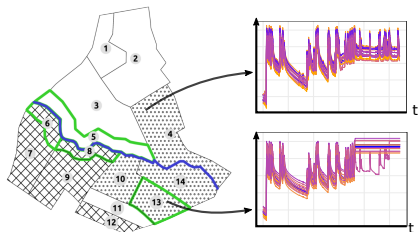
- Useful for models with large input spaces, needs little model simulations
- Scalar outputs → application to principal components (PC)

3. SUDRET, "Global sensitivity analysis using polynomial chaos expansions", 2008.

4. MARELLI et SUDRET, "UQLab", 2014.

2. Methodology

2.2. Functional principal components



$$\begin{bmatrix} Y^{(1)}(t) \\ Y^{(2)}(t) \\ \vdots \\ Y^{(14)}(t) \end{bmatrix} = \mathcal{M}(\mathbf{X}, t), \quad t \in \mathcal{T}$$

$$Y^{(m)}(t) = \mu^{(m)}(t) + \sum_{j=1}^{\infty} H_j^{(m)} \mathbf{v}_j^{(m)}(t)$$

$$Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} \mathbf{v}_1^{(m)}(t) + H_2^{(m)} \mathbf{v}_2^{(m)}(t)$$

$$H_1^{(m)} = \mathcal{M}_{PC1}^{(m)}(\mathbf{X})$$

$$\approx \mathcal{M}_{PC1, PCE}^{(m)}(\mathbf{X})$$

$$H_2^{(m)} = \mathcal{M}_{PC2}^{(m)}(\mathbf{X})$$

$$\approx \mathcal{M}_{PC2, PCE}^{(m)}(\mathbf{X})$$

1 Case study

2 Methodology

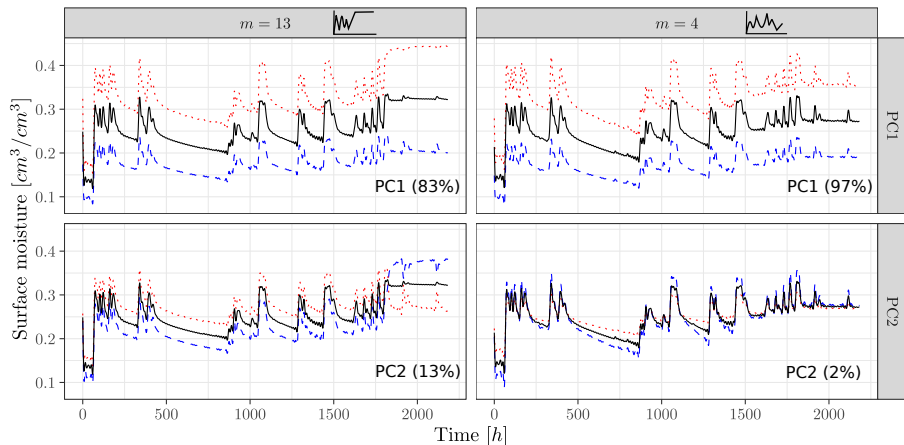
- Sobol' indices and PCE metamodels
- Functional principal components

3 Results

- Interpretation of principal components
- Validation of metamodels
- Sobol' indices

3. Results

3.1. Interpretation of principal components



$$\text{— } \mu^{(m)} \quad \text{... } \mu^{(m)} + 3\sqrt{\lambda_1^{(m)}}\mathbf{v}_1^{(m)} \quad \text{- - } \mu^{(m)} - 3\sqrt{\lambda_2^{(m)}}\mathbf{v}_2^{(m)}$$

3. Results

3.2 Validation of metamodels

| m | $\mathcal{M}_{PC1,PCE}^m$ | $\mathcal{M}_{PC2,PCE}^m$ |
|-----|---------------------------|---------------------------|
| 1 | 1.00 | NA |
| 2 | 0.99 | 0.80 |
| 3 | 0.99 | 0.77 |
| 4 | 0.99 | 0.99 |
| 5 | 0.99 | NA |
| 6 | 0.99 | 0.97 |
| 7 | 0.99 | 0.82 |
| 8 | 1.00 | NA |
| 9 | 0.99 | 0.80 |
| 10 | 0.99 | 0.98 |
| 11 | 1.00 | NA |
| 12 | 0.99 | 0.95 |
| 13 | 0.98 | 0.78 |
| 14 | 0.99 | 0.99 |

$$Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} \mathbf{v}_1^{(m)}(t) + H_2^{(m)} \mathbf{v}_2^{(m)}(t)$$

$$H_1^{(m)} \approx \mathcal{M}_{PC1,PCE}^{(m)}(\mathbf{X})$$

$$H_2^{(m)} \approx \mathcal{M}_{PC2,PCE}^{(m)}(\mathbf{X})$$

R^2 of the metamodels built on PC1 and PC2.

3. Results

3.2 Validation of metamodels

| m | $\mathcal{M}_{PC1,PCE}^m$ | $\mathcal{M}_{PC2,PCE}^m$ | \mathcal{G} |
|-----|---------------------------|---------------------------|-----------------------------|
| 1 | 1.00 | NA | $\mathcal{G}_{no_plateau}$ |
| 2 | 0.99 | 0.80 | $\mathcal{G}_{plateau}$ |
| 3 | 0.99 | 0.77 | $\mathcal{G}_{plateau}$ |
| 4 | 0.99 | 0.99 | $\mathcal{G}_{no_plateau}$ |
| 5 | 0.99 | NA | $\mathcal{G}_{no_plateau}$ |
| 6 | 0.99 | 0.97 | $\mathcal{G}_{no_plateau}$ |
| 7 | 0.99 | 0.82 | $\mathcal{G}_{plateau}$ |
| 8 | 1.00 | NA | $\mathcal{G}_{no_plateau}$ |
| 9 | 0.99 | 0.80 | $\mathcal{G}_{plateau}$ |
| 10 | 0.99 | 0.98 | $\mathcal{G}_{no_plateau}$ |
| 11 | 1.00 | NA | $\mathcal{G}_{no_plateau}$ |
| 12 | 0.99 | 0.95 | $\mathcal{G}_{no_plateau}$ |
| 13 | 0.98 | 0.78 | $\mathcal{G}_{plateau}$ |
| 14 | 0.99 | 0.99 | $\mathcal{G}_{no_plateau}$ |

$$Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} \mathbf{v}_1^{(m)}(t) + H_2^{(m)} \mathbf{v}_2^{(m)}(t)$$

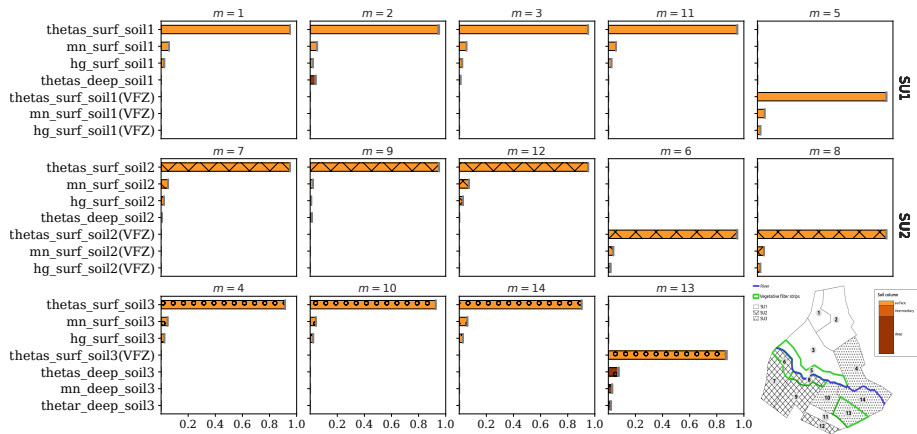
$$H_1^{(m)} \approx \mathcal{M}_{PC1,PCE}^{(m)}(\mathbf{X})$$

$$H_2^{(m)} \approx \mathcal{M}_{PC2,PCE}^{(m)}(\mathbf{X})$$

R^2 of the metamodels built on PC1 and PC2.

3. Results

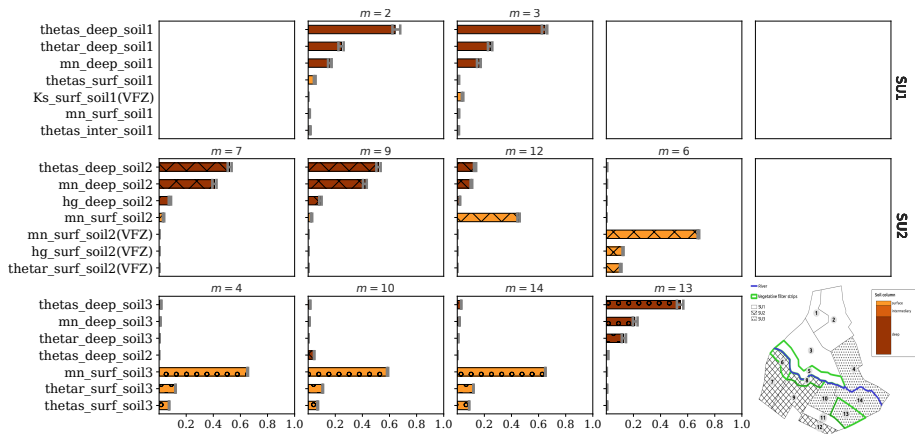
3.3 Sobol' indices



Total Sobol' indices on **PC1** per landscape unit with bootstrap confidence limits.

3. Results

3.3 Sobol' indices



Total Sobol' indices on **PC2** per landscape unit with bootstrap confidence limits.

- Successful application to surface moisture outputs.
 - Sobol' indices obtained with high precision.
 - Meaningful physical interpretations, increased comprehension of model behaviour.
 - information on the surface runoff type (infiltration excess runoff, saturation excess overland flow)
- Further adaptations
 - Cluster based SA for landscape units $\in \mathcal{G}_{plateau}$
 - Replace polynomial chaos expansion metamodel with more flexible metamodels (random forests or deep GP Gaussian processes)