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

Katarina Radišić, Emilie Rouzies, Claire Lauvernet, Arthur Vidard

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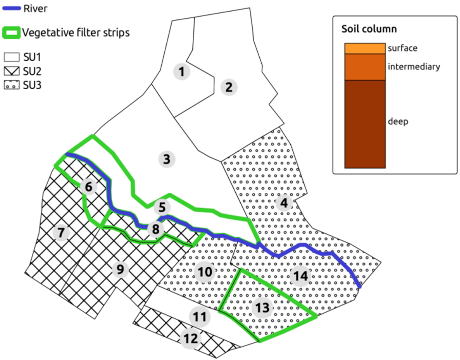
The PESHMELBA model Rouzies et al.[1,2]



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.

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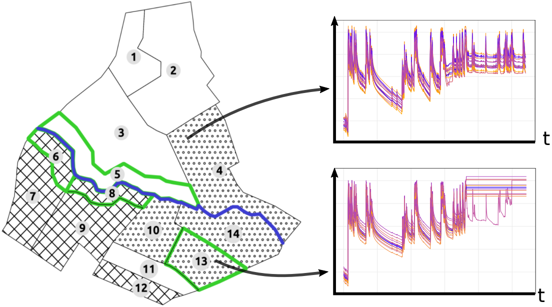
1. Case study

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



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

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

Two types of behaviour :

$\mathcal{G}_{plateau}$

$\mathcal{G}_{no\_plateau}$

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Polynomial Chaos Expansion (PCE), metamodel for analytical Sobol' indices calculation [3], calculations were done in the UQLab [4] Matlab environment.

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

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

$$D = Var(Y)$$

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

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

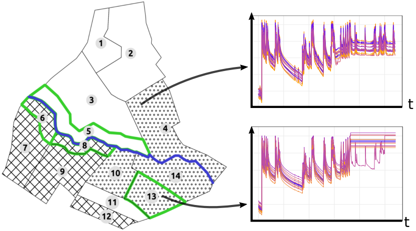
$$\hat{S}_i = \sum_{\substack{\alpha \in \mathcal{A}_q^{K,p}: \\ \alpha_i > 0, \alpha_{j \neq i} = 0}} y_\alpha^2 / \hat{D}$$

- 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



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

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

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

$$H_1^{(m)} = \mathcal{M}_{PC1}^{(m)}(\boldsymbol{X}) \qquad H_2^{(m)} = \mathcal{M}_{PC2}^{(m)}(\boldsymbol{X})$$

$$\boxed{\approx \mathcal{M}_{PC1,PCE}^{(m)}(\boldsymbol{X})} \qquad \boxed{\approx \mathcal{M}_{PC2,PCE}^{(m)}(\boldsymbol{X})}$$

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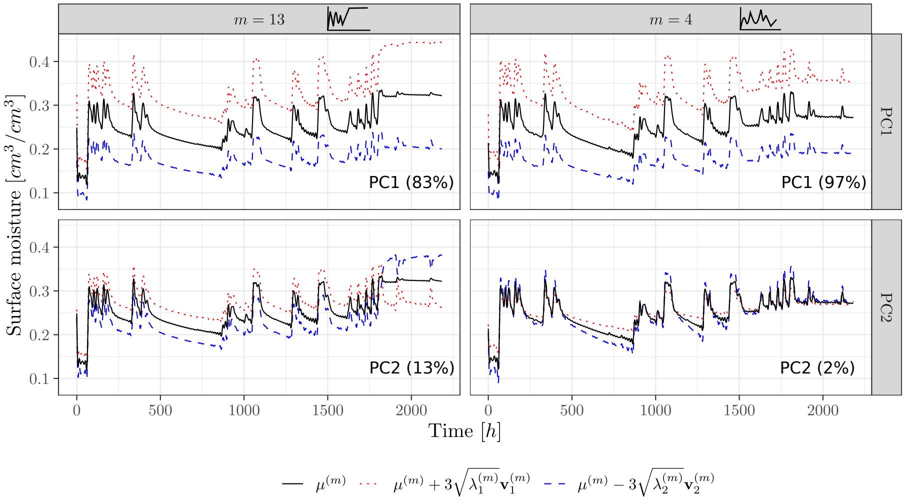


$m = 13$
$m = 4$
0.4
0.3
0.2
0.1
Surface moisture $[cm^3/cm^3]$
PC1 (83%)
PC1 (97%)
PC2 (13%)
PC2 (2%)
PC1
PC2
0
500
1000
1500
2000
Time $[h]$
$\mu^{(m)}$
$\mu^{(m)} + 3\sqrt{\lambda_1^{(m)}}\mathbf{v}_1^{(m)}$
$\mu^{(m)} - 3\sqrt{\lambda_2^{(m)}}\mathbf{v}_2^{(m)}$

m	$\mathcal{M}^{m}_{PC1,PCE}$	$\mathcal{M}^{m}_{PC2,PCE}$
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

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

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

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

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

m	$\mathcal{M}^m_{PC1,PCE}$	$\mathcal{M}^m_{PC2,PCE}$	$\mathcal{G}$
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**	$\mathcal{G}_{no\_plateau}$

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

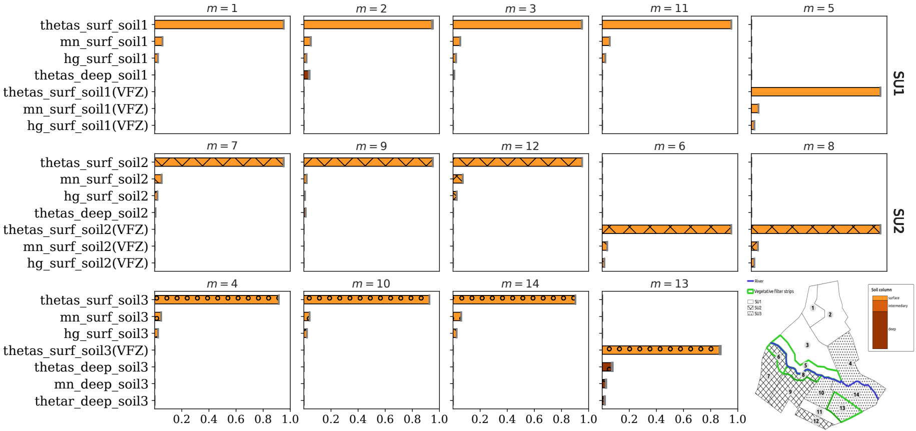
$$Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)}\mathbf{v}_1^{(m)}(t) + H_2^{(m)}\mathbf{v}_2^{(m)}(t)$$

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

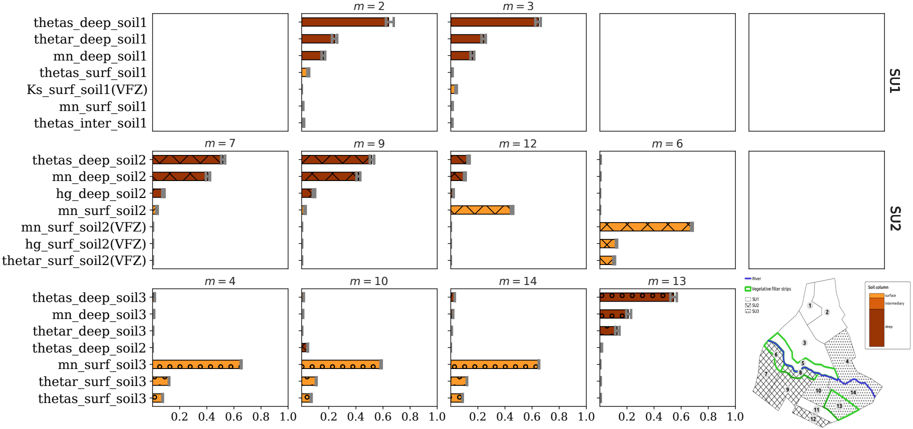
$$H_2^{(m)} \approx \mathcal{M}^{(m)}_{PC2,PCE}(\boldsymbol{X})$$

3. Results

3.3 Sobol’ indices



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



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

Conclusion

- 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)