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

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Introduction

PESHMELBA model

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

- 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

Landscape units and soil horizons, illustration from Rouzies et al.\textsuperscript{2}

\begin{enumerate}
\item Rouzies, Lauvernet, Barachet et al., “From agricultural catchment to management scenarios”, 2019.
\item Rouzies, Lauvernet, Sudret et al., \url{How to perform global sensitivity analysis of a catchment-scale, distributed pesticide transfer model?}, 2021.
\end{enumerate}
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   - Sobol’ indices and PCE metamodels
   - Functional principal components

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   - Interpretation of principal components
   - Validation of metamodels
   - Sobol’ indices
1. Case study

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

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

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

**Two types of behaviour:**
- $G_{\text{plateau}}$
- $G_{\text{no-plateau}}$
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2. Methodology
2.1. Sobol’ indices and PCE metamodels

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

\[
Y = \mathcal{M}(X) \\
= \sum_{\alpha \in \mathbb{N}^K} y_{\alpha} \psi_{\alpha}(X)
\]

\[
D = \text{Var}(Y) \\
S_i = \sum_{\alpha \in \mathbb{N}^K: \alpha_i > 0, \alpha_j \neq i = 0} y_{\alpha}^2 / D
\]

\[
Y \approx \mathcal{M}_{PCE}(X) \\
= \sum_{\alpha \in \mathcal{A}_q^{K,p}} y_{\alpha} \psi_{\alpha}(X)
\]

\[
\hat{D} = \text{Var}(\mathcal{M}_{PCE}(X)) \\
\hat{S}_i = \sum_{\alpha \in \mathcal{A}_q^{K,p}: \alpha_i > 0, \alpha_j \neq i = 0} y_{\alpha}^2 / \hat{D}
\]

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

---

2. Methodology
2.2. Functional principal components

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

\[
Y^{(m)}(t) = \mu^{(m)}(t) + \sum_{j=1}^{\infty} H_j^{(m)} v_j^{(m)}(t)
\]

\[
Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} v_1^{(m)}(t) + H_2^{(m)} v_2^{(m)}(t)
\]

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

\[
H_2^{(m)} = \mathcal{M}_{PC2}^{(m)}(\mathbf{X}) \approx \mathcal{M}_{PC2,PCE}^{(m)}(\mathbf{X})
\]
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3. Results

3.1. Interpretation of principal components

$m = 13$

$m = 4$

PC1 (83%)

PC1 (97%)

PC2 (13%)

PC2 (2%)

Surface moisture $[\text{cm}^3/\text{cm}^3]$

Time $[\text{h}]$

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

#### 3.2 Validation of metamodels

<table>
<thead>
<tr>
<th>m</th>
<th>$M_{PC1,PCE}^{m}$</th>
<th>$M_{PC2,PCE}^{m}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.00</td>
<td>NA</td>
</tr>
<tr>
<td>2</td>
<td>0.99</td>
<td>0.80</td>
</tr>
<tr>
<td>3</td>
<td>0.99</td>
<td>0.77</td>
</tr>
<tr>
<td>4</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>5</td>
<td>0.99</td>
<td>NA</td>
</tr>
<tr>
<td>6</td>
<td>0.99</td>
<td>0.97</td>
</tr>
<tr>
<td>7</td>
<td>0.99</td>
<td>0.82</td>
</tr>
<tr>
<td>8</td>
<td>1.00</td>
<td>NA</td>
</tr>
<tr>
<td>9</td>
<td>0.99</td>
<td>0.80</td>
</tr>
<tr>
<td>10</td>
<td>0.99</td>
<td>0.98</td>
</tr>
<tr>
<td>11</td>
<td>1.00</td>
<td>NA</td>
</tr>
<tr>
<td>12</td>
<td>0.99</td>
<td>0.95</td>
</tr>
<tr>
<td>13</td>
<td>0.98</td>
<td>0.78</td>
</tr>
<tr>
<td>14</td>
<td>0.99</td>
<td>0.99</td>
</tr>
</tbody>
</table>

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

\[
Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)} v_1^{(m)}(t) + H_2^{(m)} v_2^{(m)}(t)
\]

\[
H_1^{(m)} \approx M_{PC1,PCE}^{(m)}(X)
\]

\[
H_2^{(m)} \approx M_{PC2,PCE}^{(m)}(X)
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3.2 Validation of metamodels

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<tr>
<th>$m$</th>
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<th>$\mathcal{M}_{PC2,PCE}^m$</th>
<th>$G$</th>
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</thead>
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<tr>
<td>1</td>
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<td>$G_{\text{no plateau}}$</td>
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<td>$G_{\text{plateau}}$</td>
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$R^2$ of the metamodels built on PC1 and PC2.

\[ Y^{(m)}(t) \approx \mu^{(m)}(t) + H_1^{(m)}v_1^{(m)}(t) + H_2^{(m)}v_2^{(m)}(t) \]

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

\[ H_2^{(m)} \approx \mathcal{M}_{PC2,PCE}^{(m)}(X) \]
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.
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 $\in G_{plateau}$
  - Replace polynomial chaos expansion metamodel with more flexible metamodels (random forests or deep GP Gaussian processes)