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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.\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

\begin{itemize}
  \item River
  \item Vegetative filter strips
  \item SU1
  \item SU2
  \item SU3
\end{itemize}

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

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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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   - Functional principal components

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1. Case study

Sensitivity analysis on: surface moisture outputs.

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

Two types of behaviour:
- $G_{\text{plateau}}$
- $G_{\text{no-plateau}}$

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

1 Case study

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   • Validation of metamodels
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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.

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

\[ D = \text{Var}(Y) \]

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

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

\[ \hat{D} = \text{Var}(\mathcal{M}_{PCE}(X)) \]

\[ \hat{S}_i = \sum_{\alpha \in \mathcal{A}_{q,p}^K: \alpha_i > 0, \alpha_j \neq i = 0} y_\alpha^2 / \hat{D} \]

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

---

2. Methodology

2.2. Functional principal components

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

\[
Y^{(m)}(t) = \mu^{(m)}(t) + \sum_{j=1}^{\infty} H^{(m)}_j v^{(m)}_j(t)
\]

\[
Y^{(m)}(t) \approx \mu^{(m)}(t) + H^{(m)}_1 v^{(m)}_1(t) + H^{(m)}_2 v^{(m)}_2(t)
\]

\[
H^{(m)}_1 = \mathcal{M}^{(m)}_{PC1}(X) \approx \mathcal{M}^{(m)}_{PC1,PCE}(X)
\]

\[
H^{(m)}_2 = \mathcal{M}^{(m)}_{PC2}(X) \approx \mathcal{M}^{(m)}_{PC2,PCE}(X)
\]
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

$m = 13$

$\mu^{(m)}$ - solid line,
$\mu^{(m)} + 3\sqrt{\lambda_1^{(m)}}\nu_1^{(m)}$ - dashed line,
$\mu^{(m)} - 3\sqrt{\lambda_2^{(m)}}\nu_2^{(m)}$ - dotted line.

$m = 4$

PC1 (97%)

PC2 (2%)
## 3. Results

### 3.2 Validation of metamodels

<table>
<thead>
<tr>
<th>m</th>
<th>$\mathcal{M}_{PC1,PCE}^m$</th>
<th>$\mathcal{M}_{PC2,PCE}^m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.00</td>
<td>NA</td>
</tr>
<tr>
<td>2</td>
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<td>0.80</td>
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<tr>
<td>3</td>
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<td>0.77</td>
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<tr>
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<td>0.99</td>
</tr>
<tr>
<td>5</td>
<td>0.99</td>
<td>NA</td>
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<tr>
<td>6</td>
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<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.

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

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

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

#### 3.2 Validation of metamodels

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

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

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

<table>
<thead>
<tr>
<th>$m$</th>
<th>$\mathcal{M}_{PC1,PCE}^{m}$</th>
<th>$\mathcal{M}_{PC2,PCE}^{m}$</th>
<th>$G$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.00</td>
<td>NA</td>
<td>$G_{no_plateau}$</td>
</tr>
<tr>
<td>2</td>
<td>0.99</td>
<td>0.80</td>
<td>$G_{plateau}$</td>
</tr>
<tr>
<td>3</td>
<td>0.99</td>
<td>0.77</td>
<td>$G_{plateau}$</td>
</tr>
<tr>
<td>4</td>
<td>0.99</td>
<td>0.99</td>
<td>$G_{no_plateau}$</td>
</tr>
<tr>
<td>5</td>
<td>0.99</td>
<td>NA</td>
<td>$G_{no_plateau}$</td>
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<td>$G_{no_plateau}$</td>
</tr>
</tbody>
</table>

$R^2$ 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.
**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 $\in G_{\text{plateau}}$
  - Replace polynomial chaos expansion metamodel with more flexible metamodels (random forests or deep GP Gaussian processes)