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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

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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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   - Sobol’ indices and PCE metamodels
   - Functional principal components

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   - Interpretation of principal components
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   - 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)
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 calculation\(^3\), calculations were done in the UQLab\(^4\) Matlab environment.

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

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

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

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

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

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

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

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2. Methodology

2.2. Functional principal components

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

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

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

\[ H_2^{(m)} = \mathcal{M}_{PC2}^{(m)}(X) \approx \mathcal{M}_{PC2,PCE}^{(m)}(X) \]
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3. Results
3.1. Interpretation of principal components

- PC1 (83%)
- PC2 (13%)
- PC1 (97%)
- PC2 (2%)

\[ m = 13 \]

\[ m = 4 \]

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

Time \[ [\text{h}] \]

\[ \mu^{(m)} \quad \mu^{(m)} + 3\sqrt{\lambda_1^{(m)} v_1^{(m)}} \quad \mu^{(m)} - 3\sqrt{\lambda_2^{(m)} v_2^{(m)}} \]
### 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>
<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>
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<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.

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

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

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

3.2 Validation of metamodels

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<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>
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<tr>
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<td>0.99</td>
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$H_1^{(m)} \approx \mathcal{M}_{PC1,PCE}^{(m)}(X)$

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

$R^2$ 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.
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)