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Sensitivity analysis with external stochastic forcings: application to a water and pesticide transfer model

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Context: PESHMELBA

Landscape features speed up or slow down pesticide transfer from the plots to the river.

⇒ The configuration of the catchment can influence the water quality.
Context: PESHMELBA

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Figure: PESHMELBA\textsuperscript{a}, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

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**Figure:** PESHMELBA\(^a\), a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.


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Figure: PESHMELBA, a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.

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- → calibrate these model parameters with terrain observations
Context: PESHMELBA

Figure: PESHMELBA\(^a\), a process-based, physical, spatially distributed water and pesticide transfer model, representing pesticide fate in agricultural catchments, highly non-linear.


- Not all model parameters can be measured directly
- \(\rightarrow\) calibrate these model parameters with terrain observations
- Impact of external uncertainties on the calibration results
Context: model calibration
Context:

model calibration

\[ \theta_0 \rightarrow u_1 \]
Context: model calibration
Context: model calibration

$\theta_0 \rightarrow M(\theta_0, u_1)$
Context: model calibration
Context: model calibration

\[ |M(\theta_0, u_1) - y_{obs}|^2 = J(\theta_0, u_1) \]
Context: model calibration

\[
\left| M(\theta_0, u_1) - y_{obs} \right|^2 = J(\theta_0, u_1)
\]

\[
J(\theta_0)
\]
Context: model calibration

\[ |\mathcal{M}(\theta_0, u_2) - y_{obs}|^2 = J(\theta_0, u_2) \]

\[ J(\theta_0) \]

\[ J(\theta_0, u_1) \]
Context: model calibration

\[ |\mathcal{M}(\theta_0, u_2) - y_{\text{obs}}|^2 = J(\theta_0, u_2) \]
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\[ J(\theta_0, u_2) = |M(\theta_0, u_2) - y_{obs}|^2 \]
Context: model calibration

\[
|\mathcal{M}(\theta_0, U(\omega)) - y_{\text{obs}}|^2 = J(\theta_0, U(\omega))
\]
Before passing to calibration: a **sensitivity analysis on the cost function** can provide the information on the **identifiability** of the parameters, (Mai 2023).
1. Introduction: Sensitivity analysis

The variability in $J$ comes from two types of inputs:

1. Parameters ($\theta$): hydrodynamic soil properties.
2. Stochastic ($U(\omega)$): external forcing (rain).

Only the parameters can be controlled by the modeler. What is the sensitivity of the output to the parameters, given the uncertainty about the stochastic inputs? (Dell'Oca 2023)
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*What is the sensitivity of the output to the parameters, given the uncertainty about the stochastic inputs?* (Dell’Oca 2023)
2. Methodology: Sobol’ indices as random variables

$J : \mathcal{D} \times \Omega \rightarrow \mathbb{R},$

$(\theta, \omega) \mapsto J(\theta, U(\omega)),$
2. Methodology: Sobol’ indices as random variables

**Estimation of Sobol’ indices with polynomial chaos expansion,**\(^a\):

\[ J(\theta) = \sum_{\alpha \in N^K} c_\alpha \psi_\alpha(\theta) \approx \sum_{\alpha \in A} c_\alpha \psi_\alpha(\theta) \]

\[ \hat{S}_i = \sum_{\alpha \in A: \alpha_i > 0, \alpha_j \neq i = 0} c_\alpha^2 / D, \]

\[ D = \text{Var} \left[ \sum_{\alpha \in A} c_\alpha \psi_\alpha(\theta) \right] = \sum_{\alpha \in A} c_\alpha^2 \]

2. Methodology: metamodel validation

The $Q^2$ of the PCE metamodels are calculated on an independent test set for each rain:

We deem the metamodels a correct approximation of the original and proceed to Sobol' indices calculation.
3. Case study: moisture profiles

Rain

\[ M(\theta_0, U(\omega)) \]

\[ U(\omega) \]

\[ \omega \]

\[ \theta_0 \]

\[ M(\theta_0, U(\omega)) \]

Cumulated rain [mm]

Time [h]
3. Case study: moisture profiles
### 3. Case study: Sobol’ indices under one rain realization

**Soil column**

- surface
- intermediary
- deep

**Parameter**

- $\theta_s$.surf: water content at saturation (surface)
- $\theta_s$.inter: water content at saturation (intermediary)
- $\theta_s$.deep: water content at saturation (deep)
- $\theta_r$.deep: residual water content (deep)
- $mn$.deep: Van Genuchten retention curve parameter (deep)
- $hg$.deep: Van Genuchten retention curve parameter (deep)

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Unit</th>
<th>Distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_s$.surf</td>
<td>water content at saturation (surface)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N} (0.3375, 0.0338^2)$</td>
</tr>
<tr>
<td>$\theta_s$.inter</td>
<td>water content at saturation (intermediary)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N} (0.3322, 0.0332^2)$</td>
</tr>
<tr>
<td>$\theta_s$.deep</td>
<td>water content at saturation (deep)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N} (0.316, 0.0316^2)$</td>
</tr>
<tr>
<td>$\theta_r$.deep</td>
<td>residual water content (deep)</td>
<td>$[L^3 L^{-3}]$</td>
<td>$\mathcal{N} (0.0612, 0.0153^2)$</td>
</tr>
<tr>
<td>$mn$.deep</td>
<td>Van Genuchten retention curve parameter (deep)</td>
<td>$[-]$</td>
<td>$\mathcal{N} (0.1791, 0.0179^2)$</td>
</tr>
<tr>
<td>$hg$.deep</td>
<td>Van Genuchten retention curve parameter (deep)</td>
<td>$[-]$</td>
<td>$\mathcal{N} (-9.69, 0.969^2)$</td>
</tr>
</tbody>
</table>
4. Results: Sobol’ indices depending on rain

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\theta_{s,\text{surf}}$</th>
<th>$\theta_{s,\text{inter}}$</th>
<th>$\theta_{s,\text{deep}}$</th>
<th>$m_{\text{deep}}$</th>
<th>$\theta_{r,\text{deep}}$</th>
<th>$h_{g,\text{deep}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\hat{\mu}(S_t^T)$</td>
<td>0.11</td>
<td>0.17</td>
<td>0.58</td>
<td>0.09</td>
<td>0.10</td>
<td>&lt; 0.01</td>
</tr>
<tr>
<td>$\hat{\sigma}(S_t^T)$</td>
<td>0.04</td>
<td>0.07</td>
<td>0.19</td>
<td>0.11</td>
<td>0.11</td>
<td>&lt; 0.01</td>
</tr>
</tbody>
</table>
4. Results: Sobol’ indices depending on rain

- **θ_{s.surf}**
- **θ_{s.inter}**
- **θ_{s.deep}**
- **θ_{r.deep}**
- **mn_{deep}**

\[ \begin{array}{cccccc}
0.00 & 0.25 & 0.50 & 0.75 & 1.00 \\
0 & 10 & 20 & 30 & 0 \\
0 & 10 & 20 & 30 & 0 \\
0 & 20 & 40 & 60 & 0 \\
0 & 20 & 40 & 60 & 0 \\
0 & 20 & 40 & 60 & 0 \\
\end{array} \]

- **Time [h]**
- **Cumulated rain [mm]**

<table>
<thead>
<tr>
<th>Variable</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
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</thead>
<tbody>
<tr>
<td>θ_{s.surf}</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>θ_{s.inter}</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>θ_{s.deep}</td>
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</tr>
<tr>
<td>θ_{r.deep}</td>
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</tr>
<tr>
<td>mn_{deep}</td>
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<td></td>
</tr>
<tr>
<td>hg_{deep}</td>
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</tr>
</tbody>
</table>

- θ_{s.deep} is not 1st
- θ_{s.deep} is 1st
5. Conclusion:

1. Sobol’ indices were obtained for 6 input parameters in 200 different rain realizations.
2. the sensitivity analysis disentangles the variability in the parameters $\theta$ from the one in the stochastic forcing $\omega$.
3. the parameter $hg$ was found non-identifiable in all rain realizations.
4. the ranking of the input parameters varies depending on $\omega$

What’s next? :

1. other ways of synthesizing information of $S(\omega)$ ?
2. based on the sensitivity analysis results, implement a robust calibration method
3. study different model outputs, such as transferred pesticide mass.
4. study different stochastic inputs, such as pesticide application dates.
Bibliography I


Bibliography II


