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Spatial Pattern Oriented Multi-Criteria Sensitivity Analysis of a Distributed Hydrologic Model

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Abstract: Hydrologic models are conventionally constrained and evaluated using point measurements of streamflow, which represents an aggregated catchment measure. As a consequence of this single objective focus, model parametrization and model parameter sensitivity are typically not reflecting other aspects of catchment behavior. Specifically for distributed models, the spatial pattern aspect is often overlooked. Our paper examines the utility of multiple performance measures in a spatial sensitivity analysis framework to determine the key parameters governing the spatial variability of predicted actual evapotranspiration (AET). Latin hypercube one-at-a-time (LHS-OAT) sampling strategy with multiple initial parameter sets was applied using the mesoscale hydrologic model (mHM) and a total of 17 model parameters were identified as sensitive. The results indicate different parameter sensitivities for different performance measures focusing on temporal hydrograph dynamics and spatial variability of actual evapotranspiration. While spatial patterns were found to be sensitive to vegetation parameters, streamflow dynamics were sensitive to pedo-transfer function (PTF) parameters. Above all, our results show that behavioral model definition based only on streamflow metrics in the generalized likelihood uncertainty estimation (GLUE) type methods require reformulation by incorporating spatial patterns into the definition of threshold values to reveal robust hydrologic behavior in the analysis.

Keywords: mHM, remote sensing, spatial pattern, sensitivity analysis, GLUE, actual evapotranspiration

1 Introduction

Computer models are indispensable to perform costly experiments in an office environment e.g. distributed modeling of water fluxes across the hydrosphere. Physically based distributed hydrologic models have become increasingly complex due to the large number of incorporated parameters to represent a variety of spatially distributed processes. These models are typically calibrated against stream gauge observations i.e. a lumped variable of all hydrological processes at catchment scale. This can cause equifinality problems [1] and poor performance of the simulated spatial pattern of the model since optimizing the water balance and streamflow dynamics are the only concern. To solve this issue the community needs models with a flexible spatial parametrization and calibration frameworks that incorporate spatially distributed observations (e.g. remotely sensed evapotranspiration (ET)).

The basic idea behind any sensitivity analysis (SA) method is to relate the response of the model output to variations in the parameter values [2]. The SA methods can; therefore, enhance our control on spatiotemporal model behavior [3]. There are local (LSA) and global sensitivity analysis (GSA) methods that evaluate distinct and joint effects between different model parameters, respectively [4–6].
While LSA methods evaluate point sensitivity in parameter space [7] the GSA covers the entire parameter space and parameter interactions too [8,9]. This is from the fact that, GSA perturbs all parameters simultaneously to assess the inter relations [10]. The most well-known GSA methods are: Sobol’ method [11] and Fourier amplitude sensitivity test (FAST) [12]. The main effects (e.g. first-order sensitivity) and elementary effects, originally described by Morris [13], can be evaluated using both methods. The Morris method has been widely applied in hydrologic modeling. Herman et al. [14] were able to classify parameters of a spatially distributed watershed model as sensitive and not sensitive based on the Morris method with 300 times fewer model evaluations than the Sobol’ approach. The GSA methods are usually thought to be more appropriate to use in hydrologic applications than LSA methods since hydrological processes are non-linear and the interactions between the parameters have substantial effect on the results. However, the computational cost is crucial in applying the GSA methods in distributed hydrologic modelling [15,16]. The LSA methods gives fast results by assessing only one parameter at a time without interactions between parameters [17]. The local derivatives are however based on a certain initial set in the parameter space.

The foremost objective of our study is to assess the major driving parameters for the spatial patterns of actual evapotranspiration (AET) simulated by a catchment model. Furthermore, we address how the selected initial set of parameters can affect the LSA results and how many initial sets are required for a robust sensitivity analysis. We evaluate parameter sensitivities using a LSA method with random and behavioral initial parameter sets (each containing 100 initial parameter sets). We focus on both spatial patterns of AET over the basin and temporal hydrograph dynamics using multiple performance metrics to evaluate different aspects of the simulated maps and the hydrograph. Streamflow performance of a model has typically been the main concern in conventional model calibrations, whereas improving the simulated spatial pattern during calibration has rarely been targeted [18–24]. A unique feature of our study is evaluating the model’s sensitivity based on a set of ten spatial metrics that, unlike traditional cell-to-cell metrics, provide true pattern information. We include an innovative metric which utilizes empirical orthogonal function analysis [21] as well as the fractional skill score [25], among others, to evaluate the simulated spatial patterns. The added value of each metric is assessed based on a redundancy test. This is done to identify the most robust metric(s) with unique information content to apply in a subsequent spatial calibration study.

Recently it has been reported that the VIC model showed difficulty in simulating spatial variability and hydrologic connectivity [20]. Höllering et al [26] used hydrologic fingerprint-based sensitivity analysis using temporally independent and temporal dynamics of only streamflow data. They could identify two major driving parameters for evapotranspiration and soil moisture dynamics in different mesoscale catchments in Germany and reveal their relation to different streamflow characteristics. In our study, we applied the mesoscale hydrologic model (mHM) [27] which can simulate distributed variables using pedo-transfer functions (PTF) and related parameters. Additionally, a recently introduced dynamic ET scaling function (DSF) is used to increase the physical control on simulated spatial patterns of AET [28]. Ultimately, the identified important parameters for simulating both, stream discharge and spatial patterns of AET are used in a very recent model calibration study [28]. The novelty of the current study lies in using sensitivity maps showing difference between initial run and perturbation of a parameter and various spatial metrics to complement conventional SA with spatial pattern evaluation.

2 Materials

The Skjern river has a basin area of ~2500 km2 covered by mostly sandy soils (Figure 1) and dominated by agriculture (71%) and forest (15%) [19]. The maximum altitude in the basin is 130 m and annually averaged precipitation is around 1000 mm [29]. The monthly mean temperatures vary between 2 and 17 degrees Celsius whereas the annual mean streamflow is around 475 mm [30].
We use different products from the Moderate Resolution Imaging Spectroradiometer (MODIS) (Table 1) to generate leaf area index (LAI) and AET maps. The data are retrieved from NASA Land Processes Distributed Active Archive Center (LP-DAAC).

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Period</th>
<th>Spatial resolution</th>
<th>Remark</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>LAI</td>
<td>Fully distributed 8-day time varying LAI dataset</td>
<td>1990-2014</td>
<td>1 km</td>
<td>8 day to daily</td>
<td>MODIS and Mendiguren et al. [31]</td>
</tr>
<tr>
<td>AET</td>
<td>Actual evapotranspiration</td>
<td>1990-2014</td>
<td>1 km</td>
<td>daily</td>
<td>MODIS, TSEB</td>
</tr>
</tbody>
</table>

**Leaf Area Index (LAI)**

The Nadir BRDF Adjusted Reflectance (NBAR) from the MCD43B4 product is used to calculate the normalized vegetation index (NDVI) [32]. Subsequently the dataset are smoothed using a temporal filter available in the TIMESAT code [33,34]. Due to the low data availability of the MODIS LAI product at the latitudes of the study site during some periods of the year we derive a new empirical LAI equation based on the NDVI, Eq. (1).

Since in-situ measurements of LAI are scarce and typically limited to specific crops the reference LAI data used for the empirical equation is obtained from the LAI input tables for the Danish National Water Resources model [35,36]. The most common land use type in Denmark is cropland, ~80% of the total area. Boegh et al. [37] derived LAI using remote sensing data with an exponential function. In our case we used a similar approach in the following equation:
Using different equations for different land cover types is possible. However, imposing a land cover map on the remote sensing inputs can predispose the maps to show a spatial pattern controlled by land cover. To minimize this effect, we decided to apply a single equation to derive the LAI i.e. established based on the most abundant land cover type (agricultural) in the study area. The derived 8-day LAI product is later linearly interpolated to obtain daily LAI values for each pixel, which we find suitable for the study area, because temporal variability is limited at this time scale.

Actual Evapotranspiration (TSEB)

The Two Source Energy Balance (TSEB) model developed by Norman et al. [38] based on Priestly-Taylor approximation [39] is incorporated in this study to estimate AET based on MODIS data. The model inputs are solar zenith angle (SZA) and land surface temperature (LST) as well as height of canopy and albedo levels all derived from MODIS based observations. Other climate variables of incoming radiation and air temperature are retrieved from ERA interim reanalysis data [40]. One-at-a-time sensitivity analysis [41] of the TSEB model revealed that LST is the most sensitive parameter for AET (results not shown here). The TSEB model output was evaluated against field observations of eddy fluxes over three different land cover types before deriving the final maps of AET. The main purpose of including the remote sensing based AET estimations is to evaluate the spatial pattern performance of the model data during the growing season. All data were averaged across all years for calibration and validation periods to six monthly averaged spatial maps from April to September. This is from the fact that uncertainty is inevitable in the individual daily estimates of AET whereas the monthly maps show the general monthly patterns which are more robust. We refer to this this AET data as reference data to evaluate mHM based simulations of AET. We chose reference instead of observation, as the data are not purely observed but an energy balance model output using satellite observations.

2.2 Hydrologic model

The multiscale Hydrologic Model (mHM) has been developed as a distributed model delivering different outputs and fluxes at different model scales [27]. The direct runoff, slow and fast interflow and base flow are calculated for every grid cell. Finally, the runoff is routed through the basin domain using Muskingum flood routing method. The model applies pedo-transfer functions to regionalize soil parameters and is easily set-up for different platforms, e.g. Mac, Linux and Windows. The model contains 53 parameters for calibration. The study by Samaniego et al. [27] is the key reference describing model formulation and parameter description.

Meteorological input at different spatial scales can be handled internally by the model. This underlines the flexibility of mHM which operates at three spatial scales: morphologic data scale (L0), model scale (L1) and coarse meteorological data (L2). The model scale, i.e. L1, can have any value between L0 and L2. In our case, the Skjern model runs at daily time scale at 1x1 km resolution whereas the soil inputs have 250x250 m resolution. The meteorological data sets, i.e. P, ETref and Tavg, were resampled from 10-20 km resolution to 1x1 km [28].

Table 2 Setup of newly introduced parameters for dynamic scaling function (DSF) for sensitivity analysis: parameter types, initial values and range.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Description</th>
<th>Initial value**</th>
<th>Lower bound</th>
<th>Upper Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>ET&lt;sub&gt;ref&lt;/sub&gt;-a</td>
<td>-</td>
<td>Intercept</td>
<td>0.95</td>
<td>0.5</td>
<td>1.2</td>
</tr>
<tr>
<td>ET&lt;sub&gt;ref&lt;/sub&gt;-b</td>
<td>-</td>
<td>Base Coefficient</td>
<td>0.2</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>ET&lt;sub&gt;ref&lt;/sub&gt;-c</td>
<td>-</td>
<td>Exponent Coefficient</td>
<td>-0.7</td>
<td>-2</td>
<td>0</td>
</tr>
</tbody>
</table>

**Recommended initial values for calibration only. Different initial values are tested in our sensitivity analysis framework.

3 Methods

In this study, we applied the Latin-hypercube sampling strategy combined with a local sensitivity analysis approach [17]. We test ten sophisticated performance measures (hereinafter called objective functions) to identify most important parameters. Three of these metrics, i.e. Nash-Sutcliffe Efficiency (NSE, Nash and Sutcliffe [42]), Kling-Gupta Efficiency (KGE, Gupta et al., [43]) and percent bias (PB), focus on simulated streamflow, whereas the remaining objective functions focus on the spatial distribution of AET (Table 3). Although PB is included in KGE equation, the PB that reflects errors in the water balance is evaluated separately to consider volume error in addition to the streamflow timing.

Table 3 Overview of the ten metrics which are used in the sensitivity analysis. First three metrics are regarding time series of streamflow while the latter seven are used to evaluate spatial patterns of AET.

<table>
<thead>
<tr>
<th>Description</th>
<th>Best value</th>
<th>Abbreviation</th>
<th>Group</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nash-Sutcliffe Efficiency</td>
<td>1.0</td>
<td>NSE</td>
<td>Streamflow</td>
<td>[42]</td>
</tr>
<tr>
<td>Kling-Gupta Efficiency</td>
<td>1.0</td>
<td>KGE</td>
<td>Streamflow</td>
<td>[43]</td>
</tr>
<tr>
<td>Percent Bias</td>
<td>0.0</td>
<td>PB</td>
<td>Streamflow</td>
<td></td>
</tr>
<tr>
<td>Goodman and Kruskal’s Lambda</td>
<td>1.0</td>
<td>λ</td>
<td>Spatial pattern</td>
<td>[44]</td>
</tr>
<tr>
<td>Theil’s Uncertainty coefficient</td>
<td>1.0</td>
<td>U</td>
<td>Spatial pattern</td>
<td>[45]</td>
</tr>
<tr>
<td>Cramér’s V</td>
<td>1.0</td>
<td>V</td>
<td>Spatial pattern</td>
<td>[46]</td>
</tr>
<tr>
<td>Map Curves</td>
<td>1.0</td>
<td>MC</td>
<td>Spatial pattern</td>
<td>[47]</td>
</tr>
<tr>
<td>Empirical Orthogonal Function</td>
<td>0.0</td>
<td>EOF</td>
<td>Spatial pattern</td>
<td>[21]</td>
</tr>
<tr>
<td>Fraction Skill Score</td>
<td>1.0</td>
<td>FSS</td>
<td>Spatial pattern</td>
<td>[25]</td>
</tr>
<tr>
<td>Pearson Correlation Coefficient</td>
<td>1.0</td>
<td>PCC</td>
<td>Spatial pattern</td>
<td>[48]</td>
</tr>
</tbody>
</table>

3.1 Objective functions focusing on spatial patterns

The objective functions focusing on streamflow, i.e. NSE, KGE and PB, are all well-known and therefore not presented in detail. In the following, we focus on introducing the spatial objective functions. Seven objective functions are used to evaluate the pattern similarity between the reference AET from TSEB and the simulated AET from mHM. Five of the seven spatial pattern oriented metrics are calculated based on the spatial overlap of categorical maps. [49]. In this study, we used three classes to transform the continuous patterns of AET into categorical maps: 1) below the 15th percentile, 2) above the 85th percentile and 3) the remaining grids between highest 15% and lowest 15% values. The empirical orthogonal functions analysis does not require categorical maps and therefore does not need to be transformed. The fractional skill score is based on categorical maps but uses more bins in the classification than the three mentioned above. The applied spatial metrics are all bias insensitive, which we consider favorable to conduct a meaningful pattern comparison. The overall water balance error is well represented by streamflow observations and therefore represented in the respective objective functions. Moreover AET is simulated in mm/day whereas the remote sensing reference is given in
W/m². The two units are closely related, but vary in range, therefore applying bias insensitive metrics is inevitable.

**Goodman and Kruskal’s lambda**

Goodman and Kruskal’s lambda ($\lambda$) is a similarity metric for contingency tables. It has an optimal value of one indicating perfect match and lowest value of zero indicating no overlap [50]. $\lambda$ is calculated as:

$$\lambda = \frac{\sum_{i=1}^{m} \max_j(c_{ij}) + \sum_{j=1}^{n} \max_i(c_{ij}) - \max_i(c_{ij}) - \max_j(c_{ij})}{2N - \max_i(c_{ij}) - \max_j(c_{ij})}$$

(2)

Where N is the total number of grids; $m$ and $n$ are the number of classes in the observed and simulated maps to be compared. $c_{ij}$ is the grid numbers for the class $i$ in first map (A) and to class $j$ in the second map (B); $c_{i+}$ is the grid numbers contained in category $i$ in map A; $c_{+j}$ is the grid numbers contained in category $j$ in map B; $\max_i(c_{ij})$ is the grid numbers in the modal class of map A, i.e. the class with largest number of grids; and $\max_j(c_{ij})$ is the number of class in map B with a given class of map A.

**Theil’s Uncertainty coefficient**

Theil’s Uncertainty ($U$) is a measure of percent reduction in error. It is also known as average mutual information [50]. It yields the same value when the reference map is A or B i.e. symmetric; therefore, a reference does not need to be defined. Unlike $\lambda$ which accounts for modal class, Theil’s $U$ considers the whole distribution of the data. It is based on entropy, joint entropy and average mutual information [45,49]. The information content (entropy) of map A is calculated as

$$H(A) = -\sum_{i=1}^{m} \frac{c_{i+}}{N} \log \left( \frac{c_{i+}}{N} \right).$$

(3)

The same notation as $\lambda$ is used for Theil’s $U$ equation below. Similarly for map B:

$$H(B) = -\sum_{j=1}^{n} \frac{c_{+j}}{N} \log \left( \frac{c_{+j}}{N} \right).$$

(4)

The joint entropy is then calculated as:
\begin{equation}
H(A, B) = - \sum_{i=1}^{m} \sum_{j=1}^{n} \frac{c_{ij}}{N} \log \left( \frac{c_{ij}}{N} \right).
\end{equation}

The shared information by map A and B is estimated by average mutual information \( I(A; B) \) based on the entropy of two maps minus the joint entropy:

\begin{equation}
I(A; B) = H(A) + H(B) - H(A, B).
\end{equation}

The uncertainty coefficient is then calculated as:

\begin{equation}
U = 2 \cdot \frac{I(A; B)}{H(A) + H(B)}.
\end{equation}

**Cramér’s V**

Cramér’s V is a metric based on Pearson’s \( X^2 \) statistic calculated from the contingency table of the map A and B \cite{46}. Recently, Speich et al. \cite{49} used this metric to assess the similarity of different bivariate maps for Switzerland. In their case the variable pairs snowmelt and runoff as well as precipitation and PET, have been selected to describe the water balance in Swiss catchments. The \( \chi^2 \) statistics can be calculated by

\begin{equation}
\chi^2 = \sum_{i=1}^{m} \sum_{j=1}^{n} \frac{(c_{ij} - c_{i+}c_{+j}/N)^2}{c_{i+}c_{+j}/N}
\end{equation}

with using the same notation of \( c_{ij} \), \( c_{i+} \) and \( c_{+j} \) as for the metrics above. In addition, \( m \) and \( n \) shows the number of grids in map A and B, respectively. \( \chi^2 \) yields always non-negative values. Zero values only appear in the case when \( c_{ij} = c_{i+}c_{+j}/N \). The zero value hence indicates no similarity between the map pairs. There has been different modifications of \( \chi^2 \) \cite{50} but the simplest and most widely used form has been proposed by Cramér \cite{46}. V is a transformation of \( X^2 \) as shown below:

\begin{equation}
V = \sqrt{\frac{\chi^2}{N \cdot (\min(m, n) - 1)}}
\end{equation}
In an earlier study, Rees [50] used Cramér’s V together with two other categorical association metrics (U and λ) to assess the similarity of two thematic maps from Landsat images. All three metrics, investigated in that study, appeared to work well as they produced significantly high values for the maps that are reasonably similar and low values for those maps that obviously differ. Rees [50] recommended to use Cramér’s V for three reasons: 1) this metric is relatively simple to calculate, 2) it is symmetric giving the same value when the reference map is A or B, 3) it performs slightly better than U and λ in discriminating between two different maps or approving two similar maps.

Mapcurves

Mapcurves (MC) is a measure of goodness-of-fit (GOF) indicating the degree of match between two categorical maps [49]. It has an optimal value of one whereas the lowest value is zero. For each pair of classes \(i, j\), between the two maps A and B, the algorithm calculates GOF using the following equation:

\[
GOF_{ij} = \frac{c_{ij}}{c_{i+} + c_{+j}}
\]  

In the following equations, the equations are presented for class A (i.e. index \(i\)), as the category A represents observed maps and B indicates simulated maps (i.e. index \(j\)). Thus the calculation for class B is analogous. The GOF values are added up for each group of the observed map (A):

\[
G_{A,i} = \sum_{j=1}^{n} G_{ij}
\]  

Where \(n\) is the grid numbers in the map (A). Note that the size of maps should match each other for this comparison. The GOF values are organized in ascending order to estimate the vector \(G'_{A}\). The values 0 and 1 are included in the series of \(G'_{A}\) to integrate the function later. The length of \(G'_{A}\) is hence \(m+2\). For each GOF value \(i \in G'_{A}\), the MC is calculated as a segment of classes that have a GOF more than or equal to \(i\):

\[
f_A(i) = \frac{\sum_{k=1}^{m}[G_{A,k} \geq i]}{m} ; i \in G'_{A}
\]  

The MC value is then calculated by integrating \(f(x)\) between zero and one. A trapezoid rule is applied as follows to calculate the area under the curve. It has a best value of one.

\[
MC_A = \sum_{i=1}^{n} \left( G'_{A,i+1} - G'_{A,i} \right) f_A(x + 1) + \frac{\left( G'_{A,i+1} - G'_{A,i} \right) \left( f_A(x + 1) - f_A(x) \right)}{2}
\]
Empirical Orthogonal Functions

The Empirical-Orthogonal-Functions (EOF) analysis is a frequently applied tool to study the spatio-temporal variability of environmental and meteorological variables [51,52]. The most important feature of the EOF analysis is that it decomposes the variability of a spatio-temporal dataset into two crucial components i.e. time invariant orthogonal spatial patterns (EOFs) and a set of loadings that are time variant [28]. Perry et al. [51] give a brief description of the mathematical background of the EOF analysis. The EOF based similarity score (SEOF) at time \( x \) is formulated as:

\[
S_{\text{SEOF}}^x = \sum_{i=1}^{n} w_i \left| \text{load}_{i}^{\text{sim}(x)} - \text{load}_{i}^{\text{obs}(x)} \right|
\]  

(14)

where \( n \) is the number of EOFs and \( w_i \) represents the covariation contribution of the \( i \)’th EOF. In our study, we focus on the overall AET pattern performance and thus we average \( S_{\text{SEOF}} \) from the individual months of the growing season into a single overall skill score.

Fractions Skill Score

Roberts and Lean [25] introduced the fractions skill score (FSS) to the atmospheric science community to establish a quantitative measure of how the skill of precipitation products varies for different spatial scales. Fractions relate to occurrences of values exceeding a certain threshold at a given window size (scale) and are compared between model and observation at individual grids. Most commonly, the thresholds represent percentiles which have the purpose to eliminate any impact of a potential bias. Hence, FSS assesses the spatial performance of a model as a function of threshold and scale and has been implemented by Gilleland et al. [53], Wolff et al. [54] and others to spatially validate precipitation forecasts. In summary, the following steps are performed during the FSS methodology: (1) truncate the observed \( A \) and simulated \( B \) spatial patterns into binary patterns for each threshold of interest, (2) compute fractions \( A(n) \) and \( B(n) \) within a given spatial scale \( n \) based on the number of grids that exceed the threshold and lie within the window of size \( n \) by \( n \) and (3) estimate the mean-squared-error (MSE) and standardize it with a worst-case MSE that returns zero spatial agreement between \( A \) and \( B \) (\( \text{MSE}_{\text{ref}} \)). The MSE is based on all grids \( (N_{nx}N_{ny}) \) that define the catchment area with dimension \( N_x \) and \( N_y \). For a certain threshold the FSS at scale \( n \) is given by:

\[
\text{FSS}_{(n)} = 1 - \frac{\text{MSE}_{(n)}}{\text{MSE}_{(n)\text{ref}}}
\]

(15)

where

\[
\text{MSE}_{(n)} = \frac{1}{N_{nx}N_{ny}} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} [A_{(n)ij} - B_{(n)ij}]^2
\]

(16)

and

\[
\text{MSE}_{(n)\text{ref}} = \frac{1}{N_{nx}N_{ny}} \left[ \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} A_{(n)ij}^2 + \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} B_{(n)ij}^2 \right]
\]

(17)

FSS ranges from zero to one, where one indicates a perfect agreement between observed and simulated patterns and zero reflects the worst possible performance. To our knowledge, Koch et al. [55] have been the first transferring FSS from the atmosphere- to the hydrological-community and applied it on spatial patterns of land-surface variables simulated by a hydrological catchment model. The flexibility of FSS, in terms of scale and threshold, is very desirable in hydrological modelling applications where uncertainties in model forcing and parameters as well as scale differences between model and observation hinder a meaningful validation at native scales. In this study, FSS is implemented in an automated manner. In order to reduce the computational time an overall FSS score is computed based on an average of six selected percentiles with individual thresholds. We decided to tolerate placement errors of extreme percentiles (1% and 99% that focus on the bottom and top 1% of AET, respectively) more than moderate percentiles (20% and 80%) by assessing the first at a larger scale (25 km) than the
latter (5 km). In addition, the 5th and 95th percentiles, that represent the top and bottom 5% of AET grids, are assessed at 15 km scale. The average of these six percentiles is used as the overall FSS score.

3.2 Latin-hypercube sampling one-factor-at-a-time sensitivity analysis

We used Latin-hypercube (LH) sampling in combination with a local sensitivity analysis method. This is an integration of a global sampling method with a local SA method changing one factor at a time (OAT). In other words, one perturbation at a time depends on the local derivatives based on a certain initial point in the parameter space [17]. A similar design based on random perturbation at a time following trajectories was firstly proposed by Morris [13]. SA based on Monte Carlo simulation is robust but requires a larger number of simulations. Alternatively, the LHS is based on a stratified sampling method that divides the parameter values into N strata with probability of occurrence having a value of 1/N. This feature leads to a more robust sensitivity analysis with a given number of initial values [17]. Here, we test whether behavioral initial parameter sets result in different parameter identification compared to random initial parameter sets. In addition, we use 100 different initial sets to assess if/when the accumulated relative sensitivities become stable. We can then evaluate how many initial samples were required to get a robust results using LHS-OAT.

4 Results

4.1 Exploration of spatial metrics characteristics

The spatial performance metrics are examined to gain more insight in their reliability and to understand whether any of them provides redundant information. This is an important step before including them into the sensitivity analysis and model calibration, because the ability to discriminate between a good and a poor spatial pattern performance is an essential characteristic of a metric. We compared 12 synthetic land surface temperature (LST) maps of a subbasin of Skjern (~1000 km²), i.e. all perturbed differently, with a reference LST map using the spatial metrics applied in this study. The details about the applied perturbation strategies can be found in Table 1 of Koch et al. [21]. In that study, Koch et al. [21] conducted an online based survey with the aim to use the well trained human perception to rank the 12 synthetic LST maps in terms of their similarity to the reference map. The obtained results were subsequently used to benchmark a set of spatial performance metrics. The same procedure is incorporated in this study to get a better understanding of the metrics selected for this study. We included the survey results in our study and assessed the coefficient of determination $R^2$ between the human perception and the spatial metrics. This helps to differentiate between metrics that contain redundant and those with unique information content. Figure 2 shows two distinct examples, i.e. one noisy perturbation and one slightly similar map to the reference map, to better explain the results presented in Table 4, that summarizes the spatial scores for the 12 maps sorted based on the survey similarity index (last column).

Figure 2. Two synthetic LST maps for Ahlergaarde subbasin of Skjern to compare the spatial metrics. Map 9 (left) is generated using a noisy perturbation while map 6 (right) is more similar to the reference map (middle)
Map 9 is ranked as the second least similar map as compared to the reference map. Map 10 that is perturbed with an overall bias of +2 is ranked as a perfect agreement by all metrics. This confirms that all of our spatial metrics are bias insensitive. In addition, map 1 is identified as the most similar map to the reference map by the human perception and all other metrics.

Table 4 Comparison of 12 perturbed maps [21] based on spatial metrics. The first seven columns presents the metrics used in this study while the last column gives the survey similarity reported in Koch et al. [21]. Map 1 has the highest similarity which means that it is the most similar map to the reference while map 7 is the least similar.

<table>
<thead>
<tr>
<th>MAP_ID</th>
<th>(\lambda)</th>
<th>U</th>
<th>V</th>
<th>MC</th>
<th>EOF*</th>
<th>FSS</th>
<th>PCC</th>
<th>Survey Similarity</th>
</tr>
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<tr>
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<td>0.81</td>
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<tr>
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<td>0.87</td>
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<td>0.50</td>
<td>0.08</td>
<td>0.89</td>
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<td>0.77</td>
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<td>0.36</td>
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<tr>
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<td>0.70</td>
<td>0.29</td>
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<td>0.28</td>
<td>0.73</td>
<td>-0.01</td>
<td>0.10</td>
</tr>
</tbody>
</table>

*Highest EOF value is zero for similar maps.

Following the \(R^2\) values in Table 5, 72.2% of the variance in the human perception is explained by the EOF analysis. The PCC, V and FSS metrics also perform well in discriminating spatial maps with respect to the human perception as benchmark. However, the U metric explains the lowest variance (40.9%) which indicates that it should not be included in the model calibration, because we trust the well trained human perception as a reference. Moreover, the spatial metrics, i.e. \(\lambda\), U, V and MC, are highly correlated (italic fonts in Table 5). All are based on transforming the data into a three category system, which results in redundancy between the four given metrics. This shows that not all of them are required for model calibration. However, we will still evaluate the sensitivity results based on all given spatial metrics in the following sections.

Table 5 Coefficient of determination (\(R^2\)) between spatial metrics and survey similarity. Bold values mark metrics with highest ability to reproduce survey similarity.Italic values highlight spatial metrics which are highly correlated.

<table>
<thead>
<tr>
<th>(R^2) score</th>
<th>(\lambda)</th>
<th>U</th>
<th>V</th>
<th>MC</th>
<th>EOF</th>
<th>FSS</th>
<th>PCC</th>
<th>Survey Similarity</th>
</tr>
</thead>
<tbody>
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<td>(\lambda)</td>
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<td>0.88</td>
<td>0.97</td>
<td>0.71</td>
<td>0.51</td>
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<tr>
<td>U</td>
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<td>0.99</td>
<td>0.99</td>
<td>0.72</td>
<td>0.59</td>
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</tr>
<tr>
<td>V</td>
<td>1</td>
<td>0.93</td>
<td>0.90</td>
<td>0.90</td>
<td>0.72</td>
<td>0.59</td>
<td>0.63</td>
<td>0.41</td>
</tr>
<tr>
<td>MC</td>
<td>1</td>
<td>0.77</td>
<td>0.61</td>
<td>0.61</td>
<td>0.72</td>
<td>0.59</td>
<td>0.63</td>
<td>0.41</td>
</tr>
<tr>
<td>EOF</td>
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<td>0.79</td>
<td>0.96</td>
<td>0.96</td>
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<td>0.96</td>
<td>0.96</td>
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</tr>
<tr>
<td>FSS</td>
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<tr>
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<td>0.69</td>
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<td>0.69</td>
<td>0.69</td>
</tr>
<tr>
<td>Survey Similarity</td>
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<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>
4.2 Latin-hypercube sampling one-factor-at-a-time sensitivity analysis

In this study, we apply LHS-OAT sensitivity analysis with 47 parameters using both random and behavioral sets of initial parameter values. Initially we selected 100 random initial parameter sets using the lower and upper limits of the parameters. Subsequently, we generate 10,000 random initial samples to select 100 behavioral sets among these. For that we start running each of the 10,000 random set, one at a time, and evaluate the simulated discharge. We continue the model runs until we reach 100 behavioral sets that all result in NSE above 0.5. This is from the fact that we are interested in investigating only the plausible region of the parameter space as we know the calibration will never end up outside this region in either way. We also ensure that the selected 100 behavioral sets are uniformly distributed to the different probability bins since we tested only the first ~2400 random initial parameter sets to have 100 behavioral sets.

In total, we execute mHM about ~11800 times in forward mode using the parameter estimation tool PEST [41]. This is from the fact that we run the model ~4700 times (47 parameters x 100 LHS-OAT) for random and ~4700 times for behavioral initial sets, and additional ~2400 runs for the selection of behavioral set as described above. Figure 3 shows the average accumulated relative parameter sensitivities over the 100 behavioral (NSE > 0.5) initial parameter sets and one at a time parameter perturbations. Relative sensitivities are normalized values by the highest sensitive parameter. Therefore, the most sensitive parameter results in one. It should be noted that we only show the results of behavioral initial sets as they are similar to those from the random initial sets. Here, the colored lines show the most important parameters. Other parameters are presented in gray color only. One of the soil moisture related parameter (rotfrcroffore) is always the most sensitive parameter for all objective functions except for KGE where one parameter of the PTF, i.e. related to sandy soils, is the most sensitive one as compared to the other 47 parameters of mHM. The rankings of important parameters are converged and similar for all spatial objective functions while different parameters are highlighted using stream flow related objective functions. The five most sensitive parameters based on spatial objective functions are soil moisture related, PTF and ET related parameters. Further, ETref-a parameter seems to be the second most important parameter affecting streamflow dynamics of the Skjern River model (see PB at Figure 3 and Figure 4), whereas another PTF parameter is ranked as the second most important parameter affecting KGE.
Figure 3. Average accumulated relative parameter sensitivities over 100 behavioral (NSE > 0.5) initial parameter sets and one at a time parameter perturbations. The different colors indicate different model processes. The red coded parameters refer to soil moisture, yellow to evapotranspiration, ice blue to interflow, light blue to percolation and dark blue to geology.
Figure 4 shows the average of 100 maps where each reflects the impact of a perturbation per parameter based on the 100 behavioral (NSE > 0.5) parameter sets as initial points. Each of these 100 perturbation maps (sensitivity maps) are calculated as absolute difference between the initial run and the perturbation that is further normalized by the initial run i.e. NMAD (%) = abs(perturbation-initial) / initial. We then use the average of 100 runs as a final sensitivity map. The maps in Figure 4 are informative in several ways. First, they show that some of the parameters have a uniform (light green map) or no effect (dark blue map) on the spatial pattern distribution, whereas other parameters have a high control on spatial variability (e.g. rotfrcofperv, ptfkssand and ETref-a). Second, we can recognize different patterns on the maps such as land cover patterns (see Figure 1) from root fraction maps (especially the one for pervious areas), LAI patterns from ETref-c map and soil patterns from pedo-transfer function maps (e.g. ptfkconst). The geoparam 2, 3 and 4 parameters are also identified as sensitive influencing streamflow dynamics (see KGE at Figure 3). However, their maps are not shown at Figure 4 as they are similar to the map for geoparam 1 (uniform effect). Further, the map for the ptflowdb parameter is completely dark blue showing that it has no effect on the simulated spatial pattern of AET.
4.3 Random parameter sets based on the 17 sensitive parameters evaluated against NSE and FSS

Figure 5 illustrates the simulated spatial AET performance as a function of streamflow model performance based on 1700 randomly generated parameter sets only constrained by the parameter bounds and evaluated against observed streamflow and spatial patterns of AET. Only the results of 329 parameter sets from 1700 total random sample resulting a minimum NSE of 0.0 are shown in these two plots i.e. the left plot shows NSE vs FSS and right plot shows NSE vs EOF. In the GLUE based uncertainty analysis framework, numerous random parameter sets are sampled and, from those, only the parameter sets that deliver a performance level that is above a predefined minimum threshold are retained and classified as behavioral models [56]. As a rule of thumb 10% of the random parameter sets should be behavioral. Demirel et al. [57] generated 120,000 parameter sets for a conceptual hydrologic model and around 10,000 (~9%) parameter sets were selected using a threshold i.e. NSE above 0.4. This performance measure has been widely used in rainfall-runoff model optimizations and subsequent GLUE studies. Additional performance measures can constrain the solution space and decrease the number of behavioral models. Wambura et al. [24] showed that while 100 out of 1000 random parameter sets satisfied the hydrograph performance evaluation based on NSE above 0.65 threshold, only 80 behavioral models could be identified with two performance measures i.e. NSE and index of volumetric fit. Similarly, in this study the behavioral models from a discharge criteria (NSE above 0.5) exhibit very different spatial AET performances varying from ~0.1 to ~0.8 for both FSS and EOF (Figure 5). Using a simple 10% (~35 parameter sets) cut-off provide a subjective threshold value of above 0.5 for FSS and below 0.15 for EOF. Together with NSE above 0.5 these two thresholds enable an identification of a more robust selection of behavioral model regions shown with a green box shown in Figure 5. It should be noted that the number of runs that satisfy both spatial metrics and NSE is 20 that is considerably less than using only one spatial metric. Both spatial metrics clearly indicate that the set of behavioral models is narrowed considerably by adding spatial pattern to the definition of combined behavioral threshold. Therefore, inclusion of MODIS AET to the sensitivity analysis only improves the quality and robustness of the behavioral model selection. Moreover, the results from Figure 5 illustrate the potential of spatial pattern evaluation to discriminate between behavioral parameter sets from more than a pure NSE perspective and how it can minimize equifinality issues.
Figure 5. Scatter plot of 329 (NSE>0.0) model runs from a total of 1700 random parameter sets as a function of spatial fit a) FSS b) EOF between remote sensing actual evapotranspiration and simulated actual evapotranspiration from mHM. Green-box in both figures show the new behavioral regions when spatial and temporal thresholds are applied together.

5 Discussion

In this study, we identified important parameters for streamflow dynamics and spatial patterns of AET by incorporating different spatial and temporal performance metrics in a LHS-OAT sensitivity analysis combined with spatial sensitivity maps. We first analyzed the suitability of spatial performance metrics for sensitivity analysis. The results suggest that a good combination of performance metrics that are complimentary should be included in a sensitivity analysis. Most importantly, the metrics should be able to separate similar and dissimilar spatial patterns. We concluded this by benchmarking a set of performance metrics against the human perception, which is a reliable and well trained reference for comparing spatial patterns. Furthermore, redundant metrics need to be identified and excluded from the analysis.

Another important point is that the modeler has to select or design a model parametrization scheme that allows the simulated spatial patterns to change while minimizing the number of model parameters. Otherwise the efforts towards a spatial model calibration will be inadequate. Here, the mHM model is selected due to its flexibility through the pedo-transfer functions.

Once the appropriate spatial performance metrics and model are selected, model evaluation against relevant spatial observations can be conducted. Such modelling schemes can be easily incorporated with any parameter sensitivity analysis. In our study, the identified parameters that are sensitive to either streamflow or spatial patterns will be used in a subsequent calibration framework. With this study, we ensure that we select the best combination of objective functions for model calibration and simultaneously reduce the computational costs of model calibration by reducing the number of model parameters.

5.1 Utility of the multi-criteria spatial sensitivity analysis

In this study, we showed that the LHS-OAT method can reduce the computational burden of the GSA methods like Sobol’. To compensate the weakness of one-at-a time perturbation we
incorporated different random and behavioral initial sets in our study. This makes the combined approach simple and robust when used with appropriate multiple metrics. It should be noted that LHS-OAT has been validated in different study areas [3,17]. Although the parameter interactions are not evaluated explicitly, the identified parameters seem to be the most important and relevant parameters for calibration. This might stem from the fact that parameters in mHM are not highly interacting with each other as already shown in Cuntz et al. [16]. The resultant maps at Figure 4 are instrumental to decide which parameter has spatial effect on the results. The average accumulated relative parameter sensitivities become stable, i.e. unchanging parameter ranking, after ~20 initial parameter sets used in LHS-OAT. This corresponds to 940 model simulations (20 x 47) including 47 mHM parameters evaluated in LHS-OAT. These are much less number of runs as compared to first and second order sensitivity analysis based on Sobol’ requiring minimum 104 - 105 model simulations [58,59]. The gain in computational costs is mostly done to the fact that we are not mainly interested in quantitative sensitivity indexes rather than the importance ranking of the model parameters.

6 Conclusions

The effect of hydrologic model parameters on the spatial distribution of AET has been evaluated with LHS-OAT method and maps. This is done to identify the most sensitive parameters to both streamflow dynamics and monthly spatial patterns of AET. To increase the model’s ability on changing simulated spatial patterns during calibration, we introduced a new dynamic scaling function using actual vegetation information to update reference evapotranspiration at the model scale. Moreover the uncertainties arising from random and behavioral Latin-hypercube sampling are addressed. The following conclusions can be drawn from our results:

- Based on the detailed analysis of spatial metrics, the EOF, FSS and Cramér’s V are found to be relevant (non-redundant) pair for spatial comparison of categorical maps. Further, the PCC metric can provide an easy understanding of map association although it can be very sensitive to extreme values.
- Based on the results from sensitivity analysis, the vegetation and soil parametrization mainly control the spatial pattern of the actual evapotranspiration. Besides, the interception, recharge and geological parameters are also important for changing streamflow dynamics. Their effect on spatial actual evapotranspiration pattern is substantial but uniform over the basin. For interception the lacking effect on the spatial pattern of AET is due to the exclusion of rainy day in the spatial pattern evaluation.
- More than half of the 47 parameters included in this study have either little or no effect on simulated spatial patterns, i.e. non-informative parameters, in the Skjern basin with chosen setup. In total, only 17 of 47 mHM parameters are selected for a subsequent spatial calibration study.
- The sensitivity maps are consistent with parameter types as they reflect land cover, LAI and soil maps of the Skjern basin.
- Combining NSE with a spatial metric strengthens the physical meaningfulness and robustness of selecting behavioral models.

Our results are in line with the study by Cornelissen et al. [22] showing that the spatial parameterization directly affects the monthly AET patterns simulated by the hydrologic model. Further, Berezowski et al. [3] used a similar sort of Latin-Hypercube One-factor-At-a-Time algorithm for sensitivity analysis of model parameters affecting simulated snow distribution patterns over Biebrza River catchment, Poland. However, to our knowledge this is the first study incorporating sensitivity maps with wide range of spatial performance metrics. The LHS-OAT method is easy to apply and informative when used with bias-insensitive spatial metrics. The framework is transferrable to other catchments in the world. Even other metrics can be added to the spatial metric group if not redundant with the current ones.

In this study we could exemplify the impact of selecting thresholds of 0.5 for FSS and 0.15 for EOF on the selection of behavioral models although the hydrologic community lack experience with
the use of these metrics. The general consensus threshold for streamflow NSE is 0.5, however, this threshold is also arbitrary and slightly differs from one study to another. It is anticipated that once the spatial metrics are more often used in the hydrologic practices, the expertise will grow in identifying suitable performance metrics and threshold value for a satisfying spatial performance. Particularly for the GLUE type uncertainty analysis methods and other model calibration frameworks, a new spatiotemporal perspective for behavioral model definition is indispensable.

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Author Contributions: Mehmet C. Demirel and Simon Stisen designed the sensitivity analysis framework, conducted model runs and prepared some of the figures. Julian Koch conducted experiments on human perception, provided some of the metric codes (EOF and FSS), and prepared some of the figures. Gorka Mendiguren prepared remote sensing data, mean monthly reference raster images and post processing python codes.

Conflicts of Interest: The authors declare no conflict of interest.

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