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Method Article

Matlab/R workflows to assess critical choices in Global Sensitivity Analysis using the SAFE toolbox

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ABSTRACT

Global Sensitivity Analysis (GSA) is a set of statistical techniques to investigate the effects of the uncertainty in the input factors of a mathematical model on the model's outputs. The value of GSA for the construction, evaluation, and improvement of earth system models is reviewed in a companion paper by Wagener and Pianosi (2019). The present paper focuses on the implementation of GSA and provides a set of workflow scripts to assess the critical choices that GSA users need to make before and while executing GSA. The workflows proposed here can be adopted by GSA users and easily adjusted to a range of GSA methods. We demonstrate how to interpret the outcomes resulting from these different choices and how to revise the choices to improve GSA quality, using a simple rainfall-runoff model as an example. We implement the workflows in the SAFE toolbox, a widely used open source software for GSA available in MATLAB and R.

- The workflows aim to contribute to the dissemination of good practice in GSA applications.
- The workflows are well-documented and reusable, as a way to ensure robust and reproducible computational science.

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Specification Table

Subject Area:	*Earth and Planetary Sciences*
More specific subject area:	*Uncertainty and Sensitivity Analysis in Earth System Modelling*
Method name:	*Global Sensitivity Analysis*
Name and reference of original method:	*Wagener and Pianosi et al. (2019)* [1]
Resource availability:	*SAFE toolbox available at:* www.safetoolbox.info

Method details

Global Sensitivity Analysis (GSA) is a set of statistical techniques that allow to assess the effects of the uncertainty and variability in the input factors of a mathematical model on the model's output(s) [2]. GSA has been shown to improve the construction and evaluation of earth system models and to maximise the information content that is extracted from model predictions [1]. The application of GSA involves running Monte Carlo simulations and some post-processing of input-output samples. The latter typically consists of the calculation of a set of sensitivity indices for the different input factors of the model. GSA users need to make a number of choices to set-up their GSA application. All these choices can significantly affect the GSA results, i.e. the estimated sensitivity indices, the consequent ordering of the most influential input factors ('ranking' in the GSA jargon), and the identification of non-influential input factors ('screening'). Therefore, a thorough monitoring of the choices made is crucial to ensure the transparency and reproducibility of GSA results.

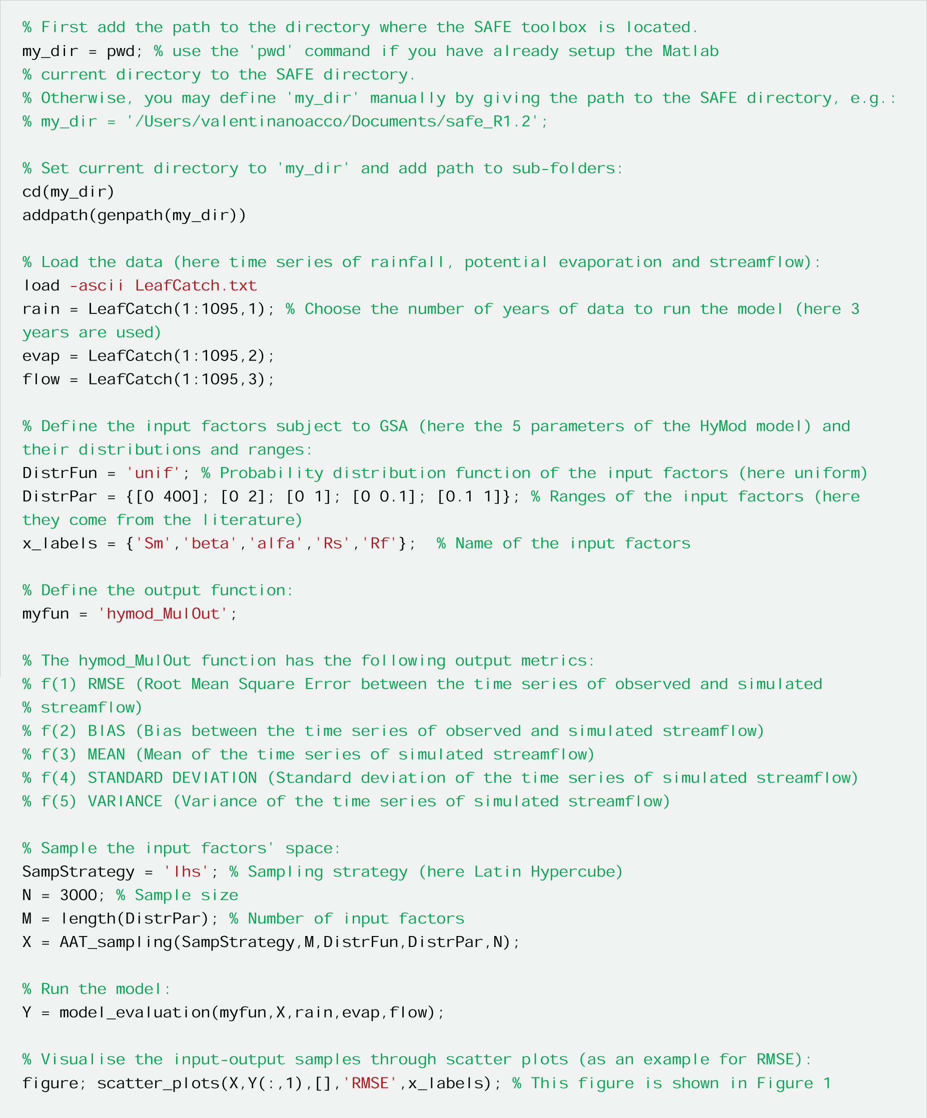
In the last decade the topic of reproducibility of scientific results has gained a growing interest, and concerns have been raised that a substantial number of scientific papers were falling short of this standard [3,4]. In particular, several papers (e.g. [5–7]) have stressed the importance of transparency and reproducibility in computational science to gain trust in the robustness of scientific results. Nonetheless, especially for large-scale, computationally expensive and time-consuming studies, the reproducibility quest might be difficult to achieve. One way to overcome this problem is to share the code that was developed to produce scientific results, along with well-documented and reusable workflows. The latter should combine the code and the data to produce the published scientific results [6].

In this paper, we will implement several GSA techniques by means of the SAFE (Sensitivity Analysis For Everybody) toolbox, which is available as Matlab code (SAFE version R1.1) and as an R package (SAFER version R1.0) [8]. A Python version of the SAFE toolbox is also currently under development. SAFE is an open source software which has been adopted so far by over 1700 academic users worldwide (by November 2018). The SAFE toolbox includes workflow scripts to guide users in applying GSA. The added value of the present paper is to provide workflows which make explicit the range of choices one should consider before and while running GSA, and to show the implications of different choices through practical examples. The rationale for the choices ('remarks') discussed in this paper is described in Section 2 of [1]. The workflows shown here aim to provide a basis for good practice and will help GSA users in their reproducibility quest. In fact, these workflows are generic and easy to customise. In turn, this will help in producing more transparent and robust GSA results, as the choices of the GSA users will be made explicit and the implications of these choices explored.

For illustration purposes, this paper uses the rainfall-runoff model HyMod, introduced by [9] and described in [10]. The model takes time series of precipitation and potential evapotranspiration as input and produces a time series of streamflow predictions as output. It includes five parameters: two parameters which control the soil moisture component and therefore the water balance ('beta' and 'Sm'), and three parameters which control the routing component and therefore the streamflow dynamics ('alfa' which partitions the flow between slow and fast reservoirs, and 'Rs' and 'Rf' which define the residence time of the slow and fast flow reservoirs, respectively). The application study site is the Leaf River catchment, a 1950 km^2 catchment located north of Collins, Mississippi, USA and described in [11].

Following this introduction, we provide an introductory code that sets-up the case study. Secondly, we discuss six critical choices in GSA applications. We provide below the code in Matlab/Octave and in the Supplementary material in R. The introductory code reports the basic steps that are necessary to generate the input-output samples that will be used in the subsequent remarks. Each remark can be run independently, but the order of the remarks follows what the authors believe is the natural sequence of choices GSA users would make in their analysis. For each remark, we report the code used to perform the analysis and the main figure showing the results, with a brief explanation of the results and their implications.

Introductory code to run before any subsequent analysis



```
% First add the path to the directory where the SAFE toolbox is located.
my_dir = pwd; % use the 'pwd' command if you have already setup the Matlab
% current directory to the SAFE directory.
% Otherwise, you may define 'my_dir' manually by giving the path to the SAFE directory, e.g.:
% my_dir = '/Users/valentinanoacco/Documents/safe_R1.2';

% Set current directory to 'my_dir' and add path to sub-folders:
cd(my_dir)
addpath(genpath(my_dir))

% Load the data (here time series of rainfall, potential evaporation and streamflow):
load -ascii LeafCatch.txt
rain = LeafCatch(1:1095,1); % Choose the number of years of data to run the model (here 3
years are used)
evap = LeafCatch(1:1095,2);
flow = LeafCatch(1:1095,3);

% Define the input factors subject to GSA (here the 5 parameters of the HyMod model) and
their distributions and ranges:
DistrFun = 'unif'; % Probability distribution function of the input factors (here uniform)
DistrPar = {[0 400]; [0 2]; [0 1]; [0 0.1]; [0.1 1]}; % Ranges of the input factors (here
they come from the literature)
x_labels = {'Sm','beta','alfa','Rs','Rf'};  % Name of the input factors

% Define the output function:
myfun = 'hymod_MulOut';

% The hymod_MulOut function has the following output metrics:
% f(1) RMSE (Root Mean Square Error between the time series of observed and simulated
% streamflow)
% f(2) BIAS (Bias between the time series of observed and simulated streamflow)
% f(3) MEAN (Mean of the time series of simulated streamflow)
% f(4) STANDARD DEVIATION (Standard deviation of the time series of simulated streamflow)
% f(5) VARIANCE (Variance of the time series of simulated streamflow)

% Sample the input factors' space:
SampStrategy = 'lhs'; % Sampling strategy (here Latin Hypercube)
N = 3000; % Sample size
M = length(DistrPar); % Number of input factors
X = AAT_sampling(SampStrategy,M,DistrFun,DistrPar,N);

% Run the model:
Y = model_evaluation(myfun,X,rain,evap,flow);

% Visualise the input-output samples through scatter plots (as an example for RMSE):
figure; scatter_plots(X,Y(:,1),[],'RMSE',x_labels); % This figure is shown in Figure 1
```

See Fig. 1

Remark 1: Multiple definitions of the model output are possible

The problem

GSA assumes that the output metric is a scalar output. Nonetheless most earth system models yield time- and/or space- distributed outputs, which then need to be summarised in a scalar output metric for the purpose of the GSA, such as a performance metric or a statistic of the simulated variables. A choice of which scalar output metric to use is then required. Therefore, it is important to analyse the impact that different choices have on the GSA results. This remark is discussed in section 2.1 of [1].

Implementation details

To illustrate this point, we use the Regional Sensitivity Analysis (RSA) method, also called Monte Carlo filtering [2], and first proposed by [12] and [13]. We use the implementation of RSA based on grouping, introduced in [10], where the output values are ranked and divided into a prescribed number of groups (here ten), each with equal number of output samples. For each group, the corresponding Cumulative Distribution Function (CDF) is derived for each input. Then, for each input, a sensitivity index that measures the difference between the CDFs for the various groups is derived. In the analysis below we compute the maximum vertical distance between the CDFs (i.e. the Kolmogorov-Smirnov statistic [14,15]). In this example, four definitions of the model output are considered: two performance metrics (the root mean squared error, denoted as ‘RMSE’, and the absolute mean error, denoted as ‘bias’) and two statistics (the mean and the standard deviation of the simulated streamflow).

The code

```
% Here the following output metrics are used from hymod_MulOut.m function:
% f(1) RMSE
% f(2) BIAS
% f(3) MEAN
% f(4) STANDARD DEVIATION

Y = Y(:,1:4); % Define the output metrics considered among those available in hymod_MulOut
n_out = size(Y,2); % Number of output metrics considered

flag = 2;  % Select the statistic to compute the sensitivity indices (here the maximum
vertical distance or Kolmogorov-Smirnov statistic between CDFs)
ngroup = 10; % Number of groups into which the output values are divided

for ii=1:n_out
    [Srsa(ii,:),idx(:,ii),Yk(:,ii)] = RSA_indices_groups(X,Y(:,ii),ngroup,flag); % Calculate
the sensitivity indices for each output metric
end

% Plot the sensitivity indices:
for ii = 1:n_out
    figure % This figure is shown in Figure 2
    boxplot1(Srsa(ii,:),x_labels,'Sensitivity index (RSA)')
end
```

The results

From Fig. 2 we can see that different definitions of the output metric result in different ordering of importance of the input factors. For instance, RMSE and the standard deviation of the simulated flow are mainly influenced by alfa, Rs and Rf (Fig. 2.a and. d), while bias and the mean of the simulated flow are mainly influenced by Sm and beta (Fig. 2.b and. c). This is expected, because different model outputs capture different model behaviours: in this example, RMSE and the standard deviation of the simulated flow highlight the model dynamics (which are controlled by alfa, Rs and Rf), while bias and the mean of the simulated flow highlight the water balance (which are controlled by Sm and beta).

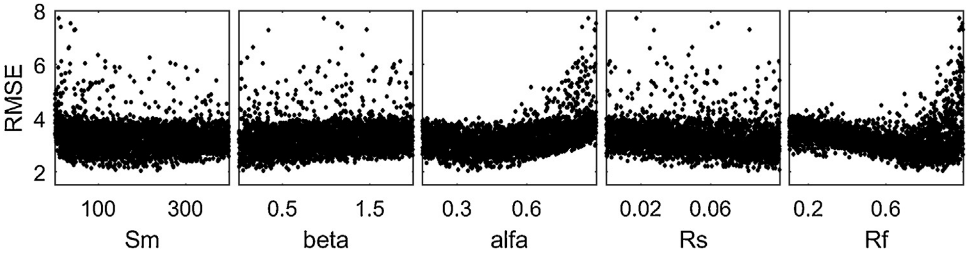


Fig. 1. Scatter plots of the output samples (RMSE of streamflow predictions) against the five input factors (the 5 model parameters: maximum soil moisture (Sm [mm]), exponent in the soil moisture routine (beta [−]), partition coefficient between fast and slow flow routing (alfa [-]), coefficient of slow reservoir residence time (Rs [1/dd]) and coefficient of fast reservoir residence time (Rf [1/dd])). Roughly uniformly scattered points (e.g. Sm) indicate low sensitivity, while clear patterns when moving along the horizontal axis (e.g. alfa) denote higher sensitivity.

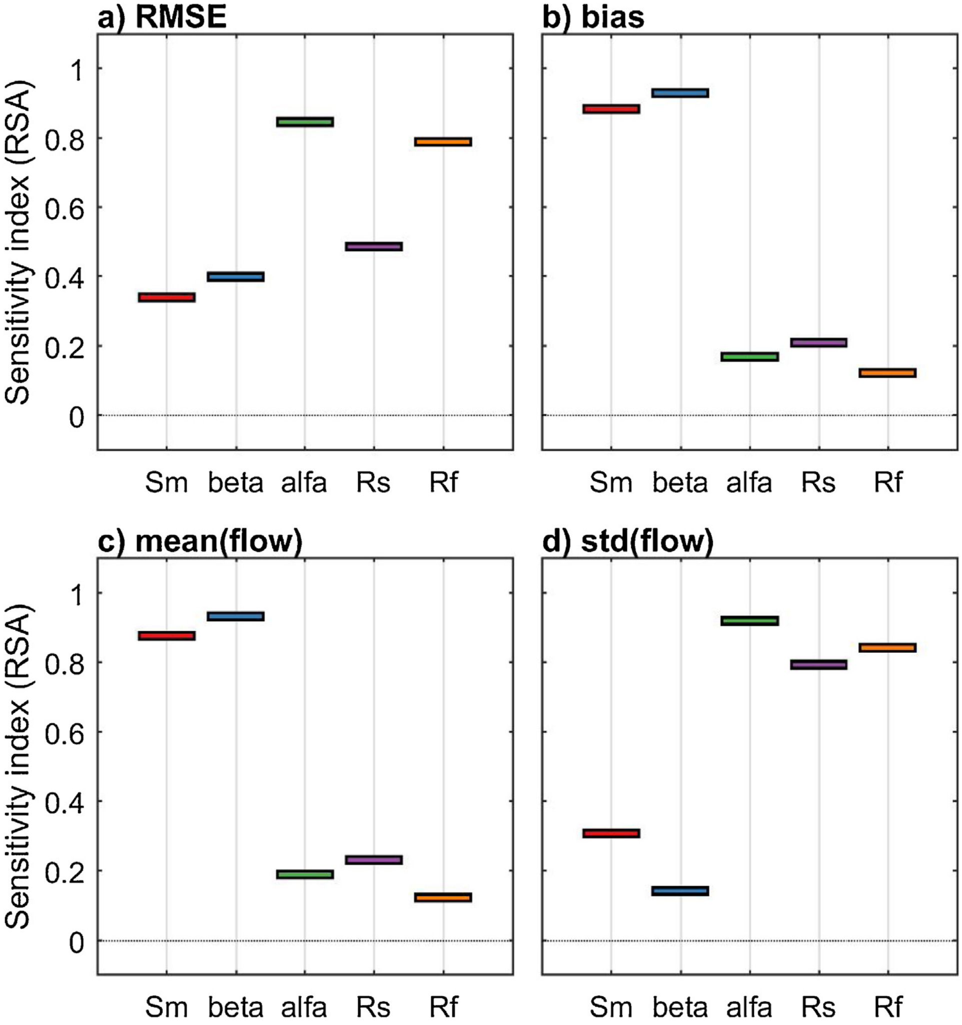


Fig. 2. Sensitivity indices of four different output metrics: a) RMSE, b) bias, c) the mean of the simulated flow, d) the standard deviation (std) of the simulated flow.

Interpretation of the results

Now we look for an explanation of the results obtained by plotting the input factors' CDFs. The additional code used is reported below and Fig. 3 provides detailed explanations.

```
% Plot input factors' CDFs:
for ii = 1:n_out
    figure; RSA_plot_groups(X,idx(:,ii),Yk(:,ii),[],x_labels); % Figure 3
end
```

Implications

The choice of the definition of the model output should be based on the intended use of the model. Multiple definitions of the model output are advised, as they allow further insight to be gained into the model behaviour, as well as to check whether the model behaves as expected.

Remark 2: Sample size also affects GSA results, so robustness of GSA results should be checked

The problem

The analytical computation of the sensitivity indices is generally not possible and sensitivity indices are typically approximated using an input-output sample obtained through Monte Carlo

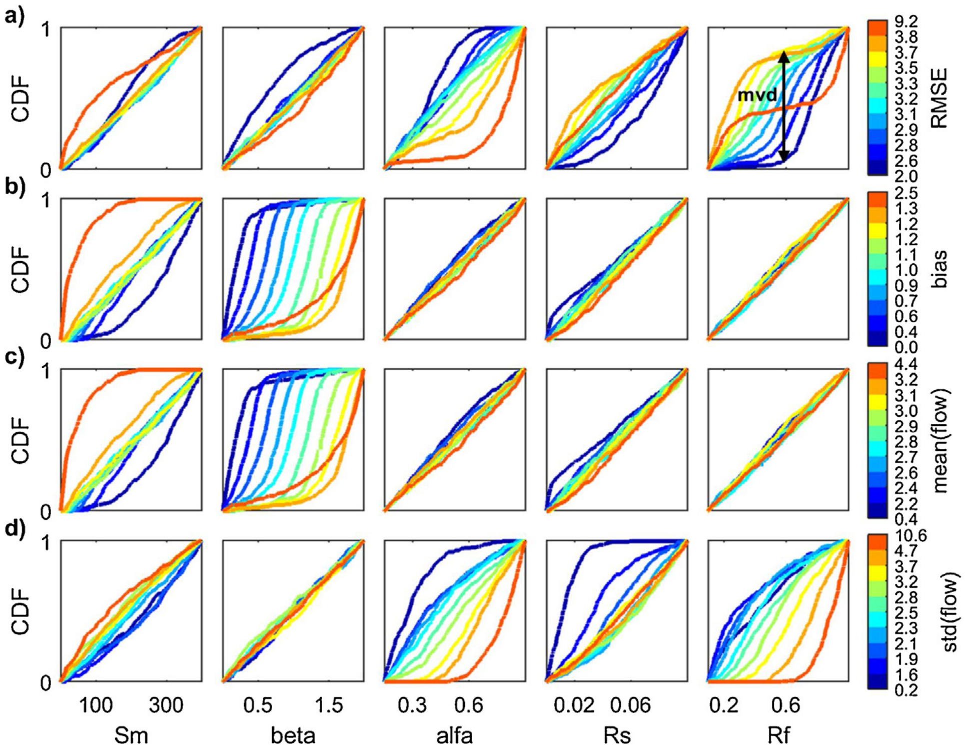


Fig. 3. Cumulative Distribution Functions (CDFs) of the input factors for the four definitions of the output metric: a) RMSE, b) bias, c) mean(flow), d) std(flow). The sensitivity index for each input in Fig. 2 was derived as the maximum vertical distance (mvd) between the above CDFs of each input factor (see the arrow in the right plot of Fig. 3.a). From this Figure we can see that the highest sensitivity of RMSE (a) and std(flow) (d) to parameters alfa, Rs and Rf is due to the larger spread between the CDFs of these input factors. A similar observation holds for bias (b) and mean(flow) (c), but in this case the largest spread among CDFs is that of input factors beta and alfa.

simulations. The choice of the sample size is therefore critical and should be evaluated so to find a good balance between the need for robust (i.e. sample independent) results and the need of limiting the computational cost of the analysis. In this section we demonstrate how to check that the sample size is large enough to obtain robust sensitivity analysis results, following the guidelines proposed in [16]. This remark is also discussed in section 2.5 of [1].

Implementation details

To illustrate this remark, we use the Elementary Effect Test (EET) [2], also called method of Morris [17]. The EET consists of calculating a number (r) of finite differences (also called Elementary Effects, EEs) for the different input factors at different points of the input factors' space. The sensitivity index is then computed as the mean of the EEs across the input factors' space. Contrary to RSA, the EET requires a tailored sampling strategy to calculate the sensitivity indices. Therefore, we cannot build on the samples drawn from the introductory code, and we need to derive a tailored input-output sample. In this application, the output metric is the performance metric RMSE.

The code

```
% Derive the tailored input factors' sample to perform Elementary Effect Test (EET):
r = 20; % Number of Elementary Effects (EEs)
design_type = 'radial'; % Design strategy to compute the EEs (here radial)
Xeet = OAT_sampling(r,M,DistrFun,DistrPar,SampStrategy,design_type); % EET requires One-At-a-Time sampling. The size of the input sample is (r*(M+1),M)

% Define the output function:
myfun = 'hymod_MulOut'; % We use the same output function as in the introductory code
iY = 1; % Define the index of the output metric(s) to consider, f(1) = RMSE

% Run the model:
Yeet = model_evaluation(myfun,Xeet,rain,evap,flow); % The size of the output sample is (r*(M+1),n_out), where n_out is the number of outputs produced by the output function (here 5)

% Calculate the sensitivity indices:
xmin = [0 0 0 0 0.1]; % Lower bound of input factors
xmax = [400 2 1 0.1 1]; % Upper bound of input factors
Seet = EET_indices(r,xmin,xmax,Xeet,Yeet(:,iY),design_type); % Calculate the mean of the absolute value of the EEs.

% Plot the sensitivity indices (Figure 4.a):
figure; boxplot1(Seet,x_labels,'Sensitivity index (EET)')
```

Now we repeat the estimation of the EET sensitivity indices using bootstrapping to derive confidence bounds around the sensitivity indices.

```
% Calculate the sensitivity indices using bootstrapping:
Nboot = 1000; % Number of bootstrap resamples
[Seet_m,~,~,~,~,Seet_lb,~,Seet_ub,~] = ...
EET_indices(r,xmin,xmax,Xeet,Yeet(:,iY),design_type,Nboot); % Calculate the mean of the absolute value of the EEs (Seet_m is the bootstrap mean, Seet_lb is bootstrap lower bound and Seet_ub is the bootstrap upper bound)

% Plot the sensitivity indices with confidence intervals (Figure 4.b):
figure; boxplot1(Seet_m,x_labels,'Sensitivity index (EET)',Seet_lb,Seet_ub)
```

And finally, we repeat the calculations with a larger number of input-output samples.

```
% Extend the tailored input factors' sample to perform the EET:
r_ext = 100; % Extended number of EEs
[Xeet_ext,Xeet_new] = ...
    OAT_sampling_extend(Xeet,r_ext,DistrFun,DistrPar,design_type); % Xeet_ext is the extended
sample of size (r_ext*(M+1),M) and Xeet_new is the new sample of size((r_ext-r)*(M+1),M)

% Run the model:
Yeet_new = model_evaluation(myfun,Xeet_new,rain,evap,flow) ; % New output sample of size
((r_ext-r)*(M+1),5)
Yeet_ext = [Yeet ; Yeet_new]; % Extended output sample of size (r_ext*(M+1),5)

% Assess the robustness of the results to the choice of sample size by using bootstrapping:
[Seet_ext_m,~,~,~,~,Seet_ext_lb,~,Seet_ext_ub] = ...
EET_indices(r_ext,xmin,xmax,Xeet_ext,Yeet_ext(:,iY),design_type,Nboot); % Calculate the mean
of the absolute value of the EEs.

% Plot the sensitivity indices with confidence intervals (Figure 4.c):
figure; boxplot1(Seet_ext_m,x_labels,'Sensitivity index (EET)',Seet_ext_lb,Seet_ext_ub)
```

The results

Interpretation of the results

By comparing Fig. 4.a and. b, which were both obtained using the same sample size (i.e. r = 20), we see the added value of deriving confidence bounds for the sensitivity indices. While Fig. 4.a indicates that alfa and Rf are highly influential and Sm, beta and Rs are little influential, Fig. 4.b shows that no robust conclusion can actually be drawn from the analysis because the confidence intervals of the input factors are overlapping. When we increase the sample size (Fig. 4.c), we observe a reduction in the width of the confidence intervals, as expected, which means that the results become more robust to the choice of the sample size. We now see a clear separation between highly influential (i.e. alfa and Rf) and little influential (i.e. Sm, beta and Rs) input factors. We also note that in this specific example the ordering of the input factors does not change when increasing the sample size, however in general this may not be the case.

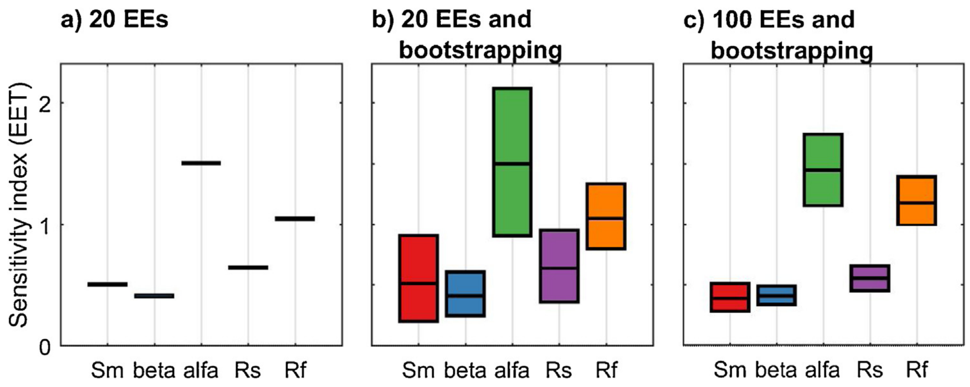


Fig. 4. EET sensitivity indices (mean of EEs) computed using: a) r = 20 EEs, b) r = 20 EEs and bootstrapping, and c) r = 100 EEs and bootstrapping. In Fig. 4.b–c the boxes represent the 95% bootstrap confidence intervals and the black lines indicate the bootstrap mean.

Implications

Assessing the robustness of the results via bootstrapping and visualising it through confidence intervals around the sensitivity indices is essential to check the robustness of the GSA results. The advantage of this method is that it does not require additional model executions. Wide and overlapping confidence intervals means that either the sample size should be increased if computationally affordable (as done in the above example), or the GSA user should opt for a less computationally demanding GSA method otherwise. The order of magnitude of the computational complexity of GSA methods is provided for instance in [18].

Remark 3: Method choice matters as it can result in different sensitivity estimates (so using multiple methods is advisable)

The problem

Sensitivity indices can be computed using different GSA methods relying on different rationales and assumptions. This section shows that different GSA methods can result in different sensitivity estimates. This remark is discussed in section 2.3 of [1].

Implementation details

We apply two GSA methods, namely Variance-Based Sensitivity Analysis (VBSA) described in [19] and a moment-independent method, called PAWN and described in [20,21]. VBSA relies on the variance decomposition proposed by [22] and consists of assessing the contributions to the variance of the model output from variations in the input factors. In this example, we use as sensitivity index the first-order (main effect) index, which measures the variance contribution from variations in an individual input factor alone (i.e. excluding interactions with other factors). Similar to the EET, VBSA requires a tailored sampling strategy and therefore we need to derive a tailored input-output sample.

In contrast to the VBSA method, the PAWN method estimates the effect of the input factors on the entire output distribution, instead of on its variance only. The method compares the output unconditional CDF, which is obtained by varying all input factors simultaneously, to the conditional CDFs that are obtained by varying all input factors but one, which is restrained to a prescribed conditioning interval [21]. For each input factor, we use *n* (here ten) conditional CDFs and calculate the average Kolmogorov-Smirnov (KS) statistic [14,15] (i.e. average maximum vertical distance) between the *n* conditional CDFs

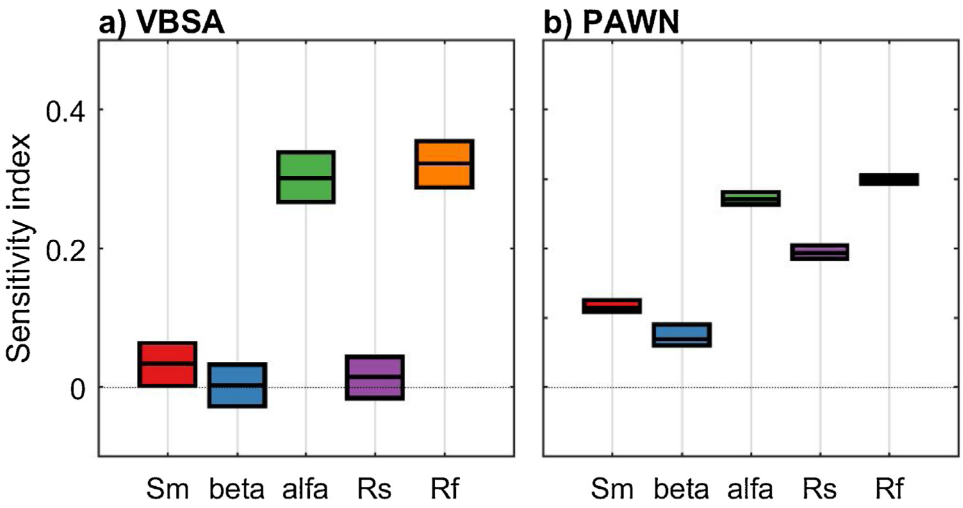


Fig. 5. Sensitivity indices calculated using a) the VBSA methods (main effects) and b) the PAWN method (mean value of the KS statistic across the conditioning intervals). The boxes represent the 95% bootstrap confidence intervals and the black lines indicate the bootstrap mean.

and the unconditional one, using the code available at https://www.safetoolbox.info/pawn-method/. In this example, the output scalar metric is the variance of the simulated flow.

The code

We perform Variance-Based Sensitivity Analysis (VBSA).

```
% Derive the tailored input factors' sample to perform VBSA:
N = 15000 ; % Base sample size. We note that the sample size is larger than the one used in
the introductory code. This is due to the fact that, in our example, VBSA requires is larger
sample size to produce robust results.
Xvbsa = AAT_sampling(SampStrategy,M,DistrFun,DistrPar,2*N); % Xvbsa has size (2*N,M)
[XA,XB,XC] = vbsa_resampling(Xvbsa) ; % Prepare the input samples needed to compute the
estimates of the VBSA sensitivity indices

% Define the output function:
myfun = 'hymod_MulOut'; % We use the same output function as in the introductory code
iY = 5; % Define the index of the output metric(s) to consider, f(5) = Variance of simulated
flow

% Run the model (warning: these lines may take some time to run):
YA = model_evaluation(myfun,XA,rain,evap,flow); % size (N,n_out) where n_out is the number of
outputs produced by the output function (here 5).
YB = model_evaluation(myfun,XB,rain,evap,flow); % size (N,n_out)
YC = model_evaluation(myfun,XC,rain,evap,flow); % size (N*M,n_out)

% Calculate the VBSA sensitivity indices using bootstrapping:
Nboot = 1000; % Number of bootstrap resamples
[Svbsa_M_m,~,~,~,Svbsa_M_lb,~,Svbsa_M_ub] = vbsa_indices(YA(:,iY),YB(:,iY),YC(:,iY),Nboot); %
Calculate the main effects

% Plot the VBSA sensitivity indices with confidence intervals:
figure; boxplot1(Svbsa_M_m,x_labels,'Sensitivity index (VBSA)',Svbsa_M_lb,Svbsa_M_ub) %
Figure 5.a
```

We perform PAWN.

```
% Calculate the sensitivity indices using the input/output sample given the introductory code
and using bootstrapping (Warning: the following line may take some time to run):
n = 10; % Number of conditioning intervals
Nboot = 1000; % Number of bootstrap resamples
[~,KS_mean] = pawn_indices_givendata(X,Y(:,iY),n,Nboot); % Calculate the PAWN sensitivity
indices: KS_mean (size (Nboot,M)) is the mean KS statistic across the n conditioning
intervals for the different bootstrap resamples.

% Calculate statistics across bootstrap resamples (mean, lower and upper bounds of
sensitivity indices):
alfa = 0.05; % Significance level for the confidence intervals estimated by bootstrapping
Spawn_m = mean(KS_mean); % Mean PAWN sensitivity index across bootstrap resamples
KS_sort = sort(KS_mean);
Spawn_lb = KS_sort(max(1,round(Nboot*alfa/2)),:); % Lower bound
Spawn_ub = KS_sort(round(Nboot*(1-alfa/2)),:); % Upper bound

% Plot the PAWN sensitivity indices with confidence intervals:
figure; boxplot1(Spawn_m,x_labels,'Sensitivity index (PAWN)',Spawn_lb,Spawn_ub) % Figure 5.b
```

The results

From Fig. 5.a, we see that Sm, beta and Rs have a similarly low value of the variance-based sensitivity index, with largely overlapping confidence intervals, while alfa and Rf have a much higher sensitivity index. By using PAWN (Fig. 5.b), we still infer that alfa and Rf are the two most influential input factors, however Rs appears to be the third most influential input factor, with a distinctively higher sensitivity index than Sm and beta. The relative importance of Rs is thus judged quite differently depending on the GSA method used. Therefore, in the interpretation of the results we will focus on the parameter Rs, as an example.

Interpretation of the results

Now we look for an explanation of the results obtained by examining the conditional and unconditional output distributions. The additional code used is reported below and Fig. 6 provides detailed explanations.

```
% For each input factor, compute the unconditional output and CDF (respectively YU and Fu),
the conditional outputs and CDFs for the n conditioning intervals (respectively YY and Fu) ,
the center of the n conditioning intervals (xc) and the KS statistics between conditional and
unconditional CDFs (KS):
[KS,~,YF,Fu,Fc,YY,xc,~,~,YU] = pawn_ks_givendata(X,Y(:,iY),n);

% Plot the unconditional (Fu) and conditional (Fc) CDFs for parameter Rs (Figure 6.a):
i = 4; % index of parameter Rs
figure; pawn_plot_cdf(YF,Fu,Fc(i,:),[],'Variance of flow')

% Compute the mean of the conditional outputs for Rs (this will allow to interpret the
provided by the VBSA method):
mC = nan(n,1); % mean of conditional outputs
for k=1:n % loop over conditioning intervals
    mC(k) = mean(YY{i,k});
end
disp(var(mC)) % Calculate and display the variance of the mean of the conditional output
(equal to 3)
disp(var(YU)) % Calculate and display the variance of the unconditional output (equal to 96)

% Plot the mean of the unconditional outputs to interpret the VBSA results of Figure 5.a:
col = gray(n); % Colours for the different conditioning intervals (grey scale)
figure % This figure is shown in Figure 6.b
for k=1:n
    hold on; plot(xc{i}(k),mC(k,i),'^k','MarkerFaceColor',col(k,:))
    % Plot means as grey triangles
end

% Plot the KS statistics between conditional and unconditional CDFs (KS) to interpret the
PAWN results of Figure 5.b:
figure % This figure is shown in Figure 6.c
for k=1:n
    hold on; plot(xc{i}(k),KS(k,i),'ok','MarkerFaceColor',col(k,:))
    % Plot KS-statistics as grey circles
end
```

From Fig. 6.a, we observe differences between the unconditional CDF and the conditional CDFs, and in particular over the lower range of values of the output (i.e. variance of flow below 10). As a result, the KS statistics shown in Fig. 6.c take high values, which explains the large value of the PAWN sensitivity index (Fig. 5.b). On the contrary, from Fig. 6.b, we observe little variation in the mean of the conditional CDFs across the conditioning intervals (values are between 6.9 and 12). We further estimate that the variance of the mean of conditional CDFs across the conditioning intervals is equal to 3, which is very small compared to the variance of the unconditional CDF which is equal to 93. This means that the contribution of Rs to the total output variance is very small. This explains the low value of the VBSA sensitivity index (Fig. 5.a).

Implications

The choice of the GSA method is critical as different methods focus on different aspects of the model input-output response and may therefore lead to different sensitivity estimates. In the example

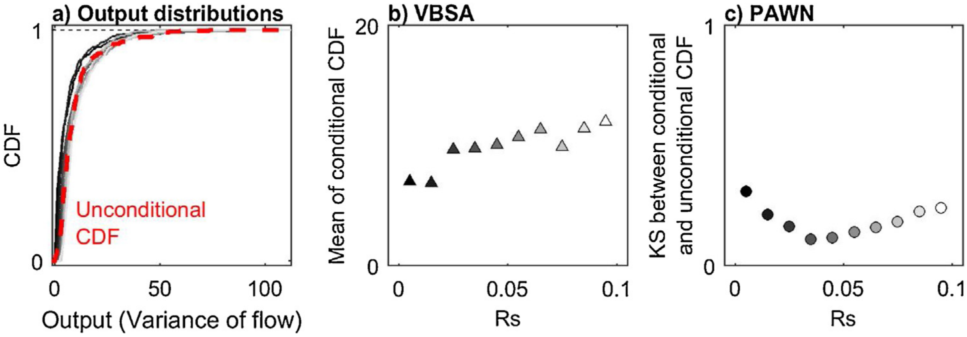


Fig. 6. Distribution and statistics of conditional and unconditional outputs (variance of simulated flow) for parameter Rs. a) Cumulative Distribution Functions (CDFs) of unconditional output (red dashed line) and of conditional outputs obtained by fixing the value of Rs within one of the ten conditioning intervals (grey lines). b) Mean of conditional outputs for the ten conditioning intervals (grey triangles). c) KS statistic between unconditional and conditional CDFs for the ten conditioning intervals (grey circles).

examined in this remark, the two methods used (VBSA and PAWN) analyse different aspects of the output distribution. This leads to slightly different conclusions, where the same parameter is considered uninfluential when only looking at the output variance (VBSA), and relatively influential when considering the entire output CDF (PAWN). It is also known that the different GSA methods have different ability to capture interactions among input factors as explained for instance in [2]. Interactions are further analysed in remark 4. Consequently, we advise that the choice of GSA method should depend on the objective of the analysis and, when possible, that the GSA user should aplply different methods to the same case study for a more exhaustive analysis of the model sensitivity. The task is facilitated by the increasing availability of sensitivity approximation techniques that can be applied to the same generic input-output sample (e.g. [23]).

Remark 4: GSA methods can measure direct and joint effects of input factors across their variability space

The problem

In complex dynamic models such as earth system models, input factors often have a high level of interactions, which means that the effect of a given input factor on the output(s) can be amplified or reduced depending on the value taken by the other input factors. Some GSA methods, such as

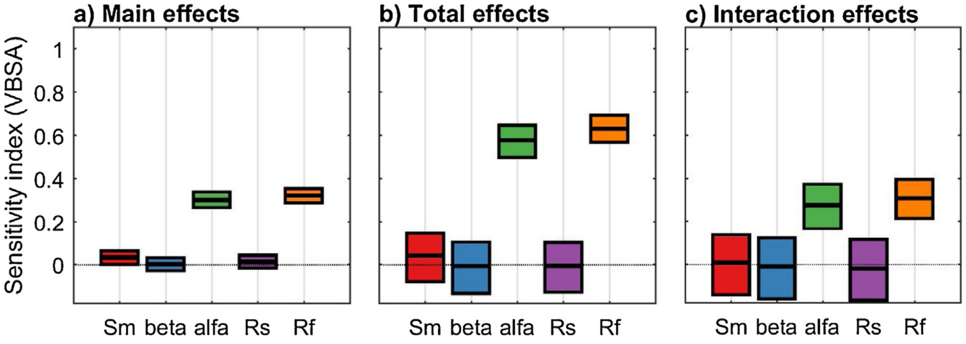


Fig. 7. Sensitivity indices calculated using the VBSA methods a) main effects indices, b) total effect indices and c) total interaction effect indices. The boxes represent the 95% bootstrap confidence intervals and the central black lines indicate the bootstrap mean.

Variance-Based Sensitivity Analysis introduced in remark 3, allow to capture input factors' interactions. This remark is discussed in section 2.2 of [1].

Implementation details

We calculate three sensitivity indices using the VSBA methods, i.e. (1) the main effect index (used in remark 3), which measures the direct effect of each input factor, (2) the total effect index, which measures the direct effect and the interaction effects with all other input factors and (3) the interaction effect index, which is the difference between total and main effect index. We use the same output metric and input-output samples generated in remark 3.

The code

We compute the main and total effect sensitivity index using VBSA.

```
% We use the output samples (YA, YB and YC) derived in remark 3

% Calculate the VBSA sensitivity indices using bootstrapping:
Nboot = 1000; % Number of bootstrap resamples
[Svbsa_M_m,Svbsa_T_m,~,~,Svbsa_M_lb,Svbsa_T_lb,...
    Svbsa_M_ub,Svbsa_T_ub,Svbsa_M_all,Svbsa_T_all] = ...
    vbsa_indices(YA(:,iY),YB(:,iY),YC(:,iY),Nboot); % Calculate the main effects (Svbsa_M_m,
Svbsa_M_lb, Svbsa_M_ub) and total effects (Svbsa_T_m, Svbsa_T_lb, Svbsa_T_ub). Svbsa_M_all
and Svbsa_T_all are the main and total effects respectively for the different bootstrap
resamples (matrix (Nboot,M)).

% Calculate interaction effects with bootstrapping as the difference between total and main
effects across bootstrap resamples:
Svbsa_I_all = Svbsa_T_all-Svbsa_M_all; % Total interactions, matrix (Nboot,M)

% Calculate statistics of interaction effects across bootstrap resamples (mean, lower and
upper bounds of sensitivity indices):
alfa = 0.05; % Significance level for the confidence intervals estimated by bootstrapping
Svbsa_I_m = mean(Svbsa_I_all); % Mean interactions across bootstrap resamples
Svbsa_I_sort = sort(Svbsa_I_all);
Svbsa_I_lb = Svbsa_I_sort(max(1,round(Nboot*alfa/2)),:); % Lower bound
Svbsa_I_ub = Svbsa_I_sort(round(Nboot*(1-alfa/2)),:); % Upper bound

% Plot the VBSA sensitivity indices with confidence intervals:
% Figure 7.a (main effects):
figure; boxplot1(Svbsa_M_m,x_labels,'Sensitivity index(VBSA)',Svbsa_M_lb,Svbsa_M_ub)
 % Figure 7.b (total effects):
figure; boxplot1(Svbsa_T_m,x_labels,'Sensitivity index (VBSA)',Svbsa_T_lb,Svbsa_T_ub)
% Figure 7.c (interaction effects):
figure; boxplot1(Svbsa_I_m,x_labels,'Sensitivity index (VBSA)',Svbsa_I_lb,Svbsa_I_ub)
```

The results

We observe that the total effect sensitivity index of parameters alfa and Rf (Fig. 7.b) is significantly higher than the main effect sensitivity index (Fig. 7.a). This means that these two parameters have an effect on the output not only through their individual variations but also through interactions, as we can see from Fig. 7.c which shows the total interaction effect index. Instead, the other three parameters (Sm, beta and Rs) have low main, total and interaction effect indices, and therefore these three parameters have a small effect, both direct and through interactions.

Interpretation of the results

Now we look for an explanation of the results by examining the two-dimensional scatter plots that allow to identify pairwise interactions (second order effects) between input factors. The additional code used is reported below and Fig. 8 provides detailed explanations.

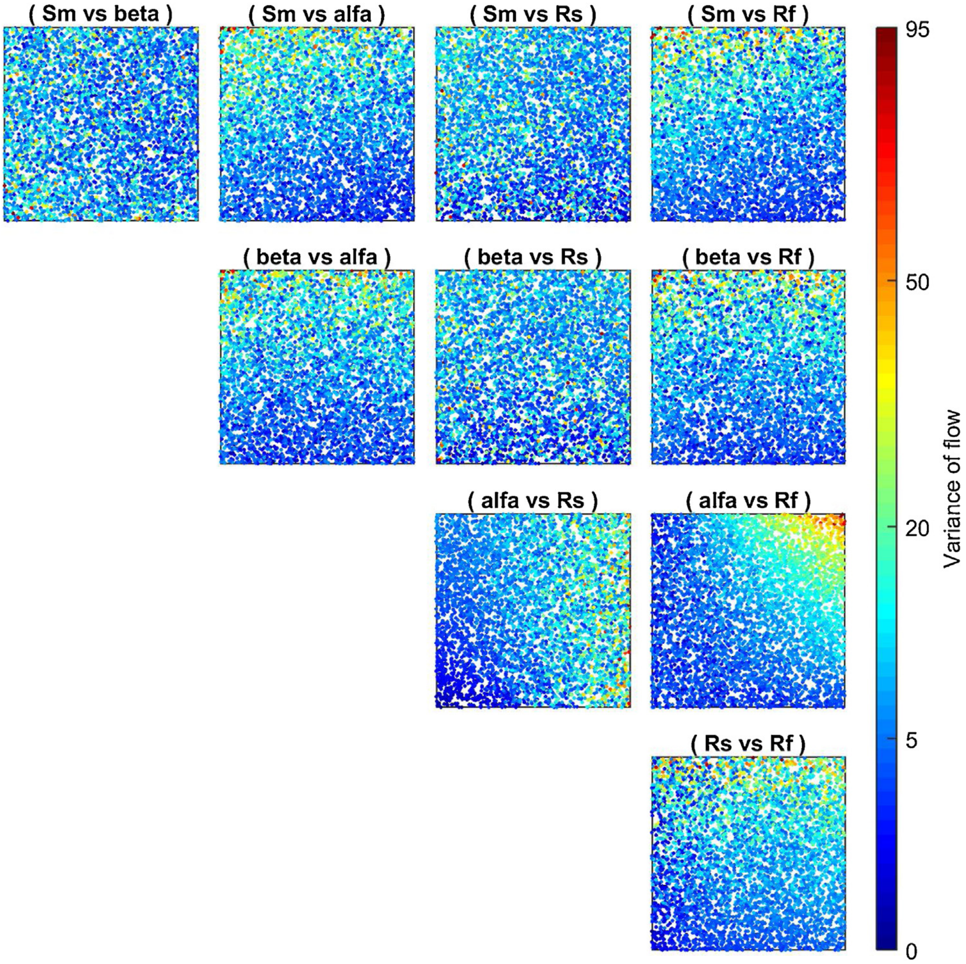


Fig. 8. Two-dimensional scatter plots. The colour indicates the value of the output (Variance of flow). The plot (alfa vs Rf) shows that high values of the variance (red colour) are obtained only when both alfa and Rf have values close to the upper bound of their range of variability. This means that these two input factors are interacting. On the contrary the other scatter plots do not show marked patterns and therefore the second order effects for the other pairs of input factors appear to be small.

```
% Rescale the output values for visualization purposes (Box-Cox transformation):
lambda = 0.5; % Parameter of the Box-Cox transformation
YA_boxcox = (YA.^lambda-1)/lambda; % Box-Cox transformation of YA

% Plot 2-dimensional scatter plots to visualize pairwise interactions:
scatter_plots_interaction(XA,YA_boxcox(:,iY),[],x_labels) % This figure is shown in Figure 8
```

Implications

It is important to use a GSA method that can detect parameter interactions, such as VBSA, if this information is relevant. In addition, as discussed in [24], scatter plot are easy-to-implement tools that can complement the results of a rigorous and quantitative GSA method and that provide insight into pairwise interactions between input factors. Nonetheless, complex interactions might not be visible from a scatterplot, that is why using VBSA, coupled with other methods, might be useful to highlight interactions between input factors.

Remark 5: The definition of the space of variability of the input factors has potentially a great impact on GSA

The problem

Sampling the input factors' space requires the definition of the distribution and range of the input factors. This section shows how the choice of the range of the input factors can impact the sensitivity indices. This remark is discussed in section 2.4 of [1].

Implementation details

We use RSA as in remark 1, but here we adopt the variant of RSA with threshold, where the input samples are divided into two groups ('behavioural' and 'non-behavioural'), whether their corresponding output falls above or below a prescribed threshold [12,13]. The output metric selected is the RMSE.

The code

```
% Set output threshold:
threshold = 2.5; %  Threshold for model output (here RMSE)
flag = 1; % Select the statistic to compute the sensitivity indices (here the maximum
vertical distance between the CDFs)

iY = 1; % Define the index of the output metric(s) to consider from those estimated in remark
1, f(1) = RMSE

% Perform RSA (find behavioural parameterisations):
[~,idxb] = RSA_indices_thres(X,Y(:,iY),threshold,flag) ;

% Calculate the sensitivity indices using bootstrapping:
Nboot = 1000; % Number of bootstrap resamples
[Srsa_m,~,Srsa_lb,Srsa_ub] = RSA_indices_thres(X,Y(:,iY),threshold,flag,Nboot); % Mean and
lower and upper bounds of the sensitivity indices (i.e. maximum vertical distance)

% Plot the sensitivity indices with confidence intervals with input factors' default ranges:
figure; boxplot1(Srsa_m,x_labels,'Sensitivity index (RSA)',Srsa_lb,Srsa_ub) % This figure is
shown in Figure 9.a
```

Now we repeat the estimation of the RSA sensitivity indices using modified input factors' ranges.

```
% Define new input factors' ranges:
DistrPar_2  = {[0 800]; [0 4]; [0 0.8]; [0 0.4]; [0.4 1]};

% Sample input factors' space:
X_2 = AAT_sampling(SampStrategy,M,DistrFun,DistrPar_2,N);

% Run the model:
Y_2 = model_evaluation(myfun,X_2,rain,evap,flow);

% Perform RSA (find behavioural parameterisations):
[~,idxb_2] = RSA_indices_thres(X_2,Y_2(:,iY),threshold,flag);

% Calculate the sensitivity indices using bootstrapping:
[Srsa_2_m,~,Srsa_2_lb,Srsa_2_ub] = RSA_indices_thres(X_2,Y_2(:,iY),threshold,flag,Nboot); %
Mean and lower and upper bounds of the sensitivity indices (i.e. maximum vertical distance)

% Plot the sensitivity indices with confidence intervals with input factors' modified ranges:
figure; boxplot1(Srsa_2_m,x_labels,'Sensitivity index (RSA)',Srsa_2_lb,Srsa_2_ub) % Figure
9.b
```

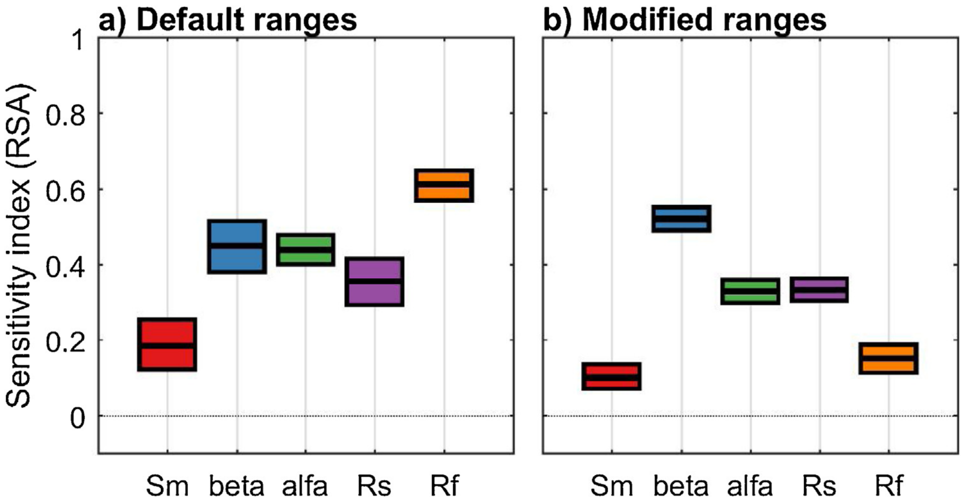


Fig. 9. Sensitivity indices calculated using a) the default ranges of the input factors taken from the literature and b) modified ranges. The boxes represent the 95% bootstrap confidence intervals and the central black lines indicate the bootstrap mean.

The results

The results reported in Fig. 9 show that changing the ranges of the input factors can change the sensitivity indices, as expected. In the specific, decreasing the range of Rf decreases its sensitivity index considerably, while decreasing the range of alfa slightly decreases its sensitivity index, and increasing considerably the range of Sm only slightly decreases its sensitivity index.

Interpretation of the results

Now we look for an explanation for the direction of change for the modified ranges by examining the ranges of the behavioural parameterisations using parallel coordinate plot. The additional code used is reported below and Fig. 10 provides detailed explanations.

```
% Parallel coordinate plot with default ranges:
figure; parcoor(X,x_labels,[],idxb) % This figure is shown in Figure 10.a

% Parallel coordinate plot with modified ranges:
figure; parcoor(X_2,x_labels,[],idxb_2) % This figure is shown in Figure 10.b
```

Implications

Changing the range of variability of an input factor can greatly change its sensitivity index. Therefore, careful consideration should be given to choose a range wide enough so that it includes all feasible (physical) values according to expert knowledge or literature values, but not too wide so that it excludes infeasible values. In this remark we varied the ranges of the input factors only (we used a uniform distribution). The effect of different distributions on the input factors' sensitivity estimates could also be tested, especially if a priory information is available on their distributions. Another implication is that sensitivity analysis and performance analysis go hand in hand, as discussed in greater detail in the next remark.

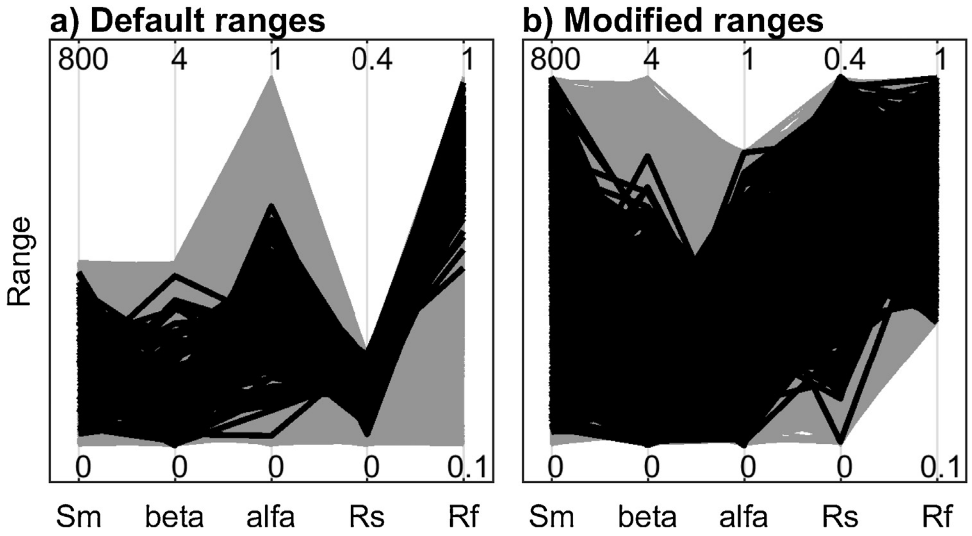


Fig. 10. Parallel coordinate plots representing the behavioural parameterisations (black lines) and the non-behavioural ones (grey lines) for the analysis with a) default input factors' ranges and b) modified ranges. In the case with modified ranges, we decreased the range of Rf. We see that the lower part of the default range of Rf provides non-behavioural parameterisations only (Fig. 10.a), while both behavioural and non-behavioural parameterisations can be found throughout the reduced range of Rf (Fig. 10.b). This explains the higher sensitivity index of Rf with the default ranges (Fig. 9.a) compared to the modified ranges (Fig. 9.b). Similarly, reducing the range for alfa (in this case decreasing its upper bound) has the effect of decreasing the sensitivity index of alfa (as shown in Fig. 9). In fact, alfa has most of its behavioural samples in the lower range and therefore the difference between behavioural and non-behavioural is reduced (as shown in Fig. 10). Fig. 10 allows analysis of the parameter ranges over the behavioural and non-behavioural parameter, thus explaining the direction of change in the sensitivity index of alfa and Rf shown in Fig. 9. For an explanation of the magnitude of change in the sensitivity indices, one could further analyse the Cumulative Distribution Functions of the parameters over the behavioural and non-behavioural parameter sets.

Remark 6: It may be necessary to remove poorly performing simulations to avoid that they dominate the estimation of sensitivity indices

The problem

Adopting input factors ranges that are too wide might result in the inclusion of poorly performing input factors values, which in turn might affect the sensitivity analysis results, as shown in remark 5. In this section, we analyse the effect of filtering out poorly performing input factors' sets based on their corresponding output values. We show the importance of running sensitivity analysis with and without the inclusion of poorly performing (sometimes called non-behavioural) simulations to assess their impact on the results. This remark forms part of the discussion in section 2.4 of [1].

Implementation details

We use RSA as in remark 1, i.e. with the implementation of RSA based on grouping. The output values are again divided into ten groups and the non-behavioural simulations are set to be those related to the highest (or lowest) performance metric (here set to be those with RMSE > 3.8, i.e. the group with the least performing simulations according to the performance metric chosen).

The code

We run RSA based on grouping as in remark 1, but here the confidence intervals of the sensitivity indices are also estimated with bootstrapping.

```
flag = 2;  % We select the maximum vertical distance or Kolmogorov-Smirnov statistic between
CDFs as statistics as in remark 1

iY = 1; % Define the index of the output metric(s) to consider, f(1) = RMSE
ngroup = 10; % Number of groups into which the output values are divided

% Calculate the respective groups of the samples (idx) and the range of Y in each group (Yk):
[~,idx,Yk] = RSA_indices_groups(X,Y(:,iY),ngroup,flag);

% Calculate the sensitivity indices using bootstrapping:
Nboot = 1000; % Number of bootstrap resamples
[Srsa_m,~,~,~,Srsa_lb,Srsa_ub] = RSA_indices_groups(X,Y(:,iY),ngroup,flag,Nboot); % Calculate
the mean and confidence intervals of the sensitivity indices (here the maximum vertical
distance). The output metric considered is RMSE.

% Plot the sensitivity indices with confidence intervals:
figure; boxplot1(Srsa_m,x_labels,'Sensitivity index (mvd)',Srsa_lb,Srsa_ub) % This is shown
in Figure 11.a
```

Now we remove the poorly performing simulations and rerun the analysis. First, we decide the value of the performance metric above (or below) which simulations are considered poorly performing

```
% Identify the poorly performing simulations to be removed:
Y_pp = Yk(10,iY); % Define the value above which we have poorly performing outputs (here
reference to the output groups' limit corresponding to a RMSE = 3.8 is made)
idx_pp = find(Yk(:,iY) >= Y_pp & Yk(:,iY) ~= Yk(end,iY)); % Index of the sets with poorly
performing output
Y_wp = Y(idx(:,iY) ~= idx_pp,iY); % Subsample of output where poorly performing values have
been excluded
X_wp = X(idx(:,iY) ~= idx_pp,:); % Subsample of input factors where poorly performing values
have been excluded

ngroup = 10; % Number of groups into which the output values are divided

% Calculate the respective group of the samples (idx_wp) and the range of Y in each group
(Yk_wp):
[~,idx_wp,Yk_wp] = RSA_indices_groups(X_wp,Y_wp,ngroup,flag);

% Calculate the sensitivity indices using bootstrapping:
[Srsa_wp_m,~,~,~,Srsa_wp_lb,Srsa_wp_ub] = RSA_indices_groups(X_wp,Y_wp,ngroup,flag,Nboot); %
Calculate the mean and confidence intervals of the sensitivity indices (here the maximum
vertical distance).

% Plot the sensitivity indices with confidence intervals calculated without poorly performing
simulations:
figure; boxplot1(Srsa_wp_m,x_labels,'Sensitivity index (RSA)',Srsa_wp_lb,Srsa_wp_ub)  % This
is shown in Figure 11.b
```

The results

The results reported in Fig. 11 show that removing the poorly performing simulations can change the sensitivity indices, as expected. In this specific case, it leads to a decrease in the sensitivity index of alfa.

Interpretation of the results

Now we look for an explanation of the results obtained by plotting the input factors' CDFs. The additional code used is reported below and Fig. 12 provides detailed explanations.

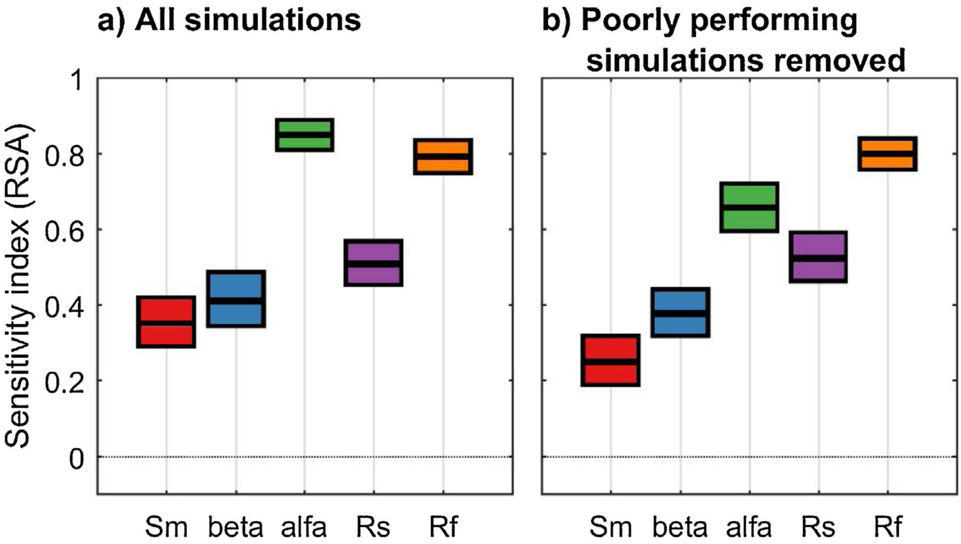


Fig. 11. Sensitivity indices calculated a) with all the simulations and b) with poorly performing simulations removed. The boxes represent the 95% bootstrap confidence intervals and the central black lines indicate the bootstrap mean.

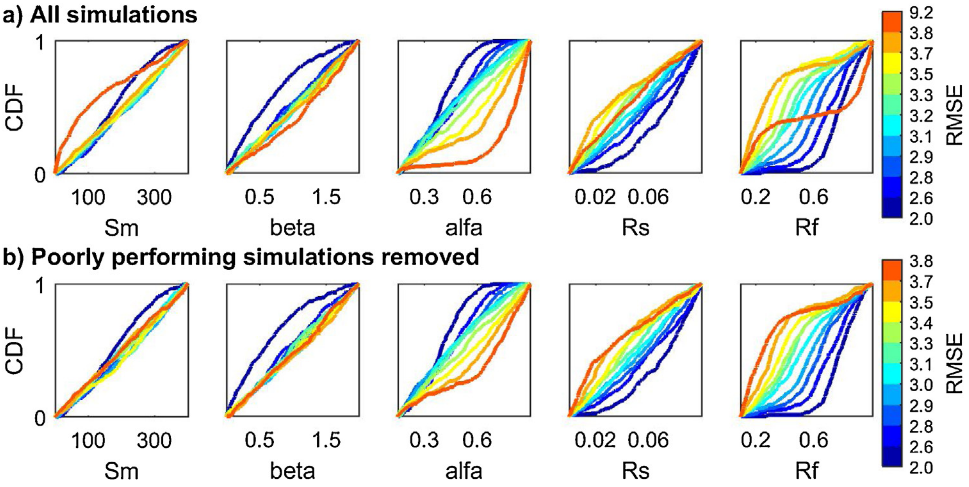


Fig. 12. Cumulative Distribution Functions (CDFs) of the input factors: a) when using all the simulations, b) when removing the poorly performing simulations. The sensitivity index for each input in Fig. 11 was derived as the maximum vertical distance (mvd) between the above CDFs (as explained in Fig. 3). We can see that the poorly performing simulations in Fig. 12.a (i.e. with RMSE > 3.8, red CDF) have been removed in Fig. 12.b. This has the effect of decreasing the mvd for alfa as it eliminates the red CDF of Fig. 12.a which stands out from the other CDFs for these two input factors. In fact, for alfa, the red CDF of Fig. 10.a shows that most of the worst performing samples of alfa are in its upper range. Instead, for example for Rf, the removal of poorly performing simulations (red CDF in Fig. 12.a) does not affect the mvd.

```
% Plot input factors' CDFs with all simulations:
figure; RSA_plot_groups(X,idx,Yk,[],x_labels,'RMSE'); % Figure 12.a

% Plot input factors' CDFs with poorly performing simulations removed:
figure; RSA_plot_groups(X_wp,idx_wp,Yk_wp,[],x_labels,'RMSE'); % Figure 12.b
```

Implications

Including poorly performing simulations can impact the results of the sensitivity analysis and might change how influential the input factors actually are. Therefore, an analysis of the subranges of values of the input factors which give poorly performing simulations should be carried out. The modeller should explicitly consider whether these subranges should be included in the sensitivity analysis or not.

Remark 7: Influential and non-influential input factors can be identified using a 'dummy' input factor

The problem

GSA is commonly applied to identify the non-influential input factors that can be set to any value within their space of variability with negligible effect on the output [2]. To set a threshold value on the sensitivity indices to separate influential and non-influential input factors (i.e. a screening threshold) [25], proposed to artificially introduce an additional 'dummy' input factor. Such a 'dummy' input factor is defined to have no impact on the output because it does not appear in the model equations. In this remark, we demonstrate the use of the 'dummy' input factor to screen influential and non-influential input factors. This remark forms part of the discussion in section 2.5 of [1].

The implementation

We use the PAWN method described in remark 3, because the method can be used for screening purposes [20]. As in remark 3, we apply PAWN to a generic input/output sample using the code available at https://www.safetoolbox.info/pawn-method/. This code also implements the computation of the PAWN sensitivity indices for the dummy input factor. We adopt as sensitivity index the maximum value of the KS statistic across the conditional CDFs. This sensitivity index is an appropriate

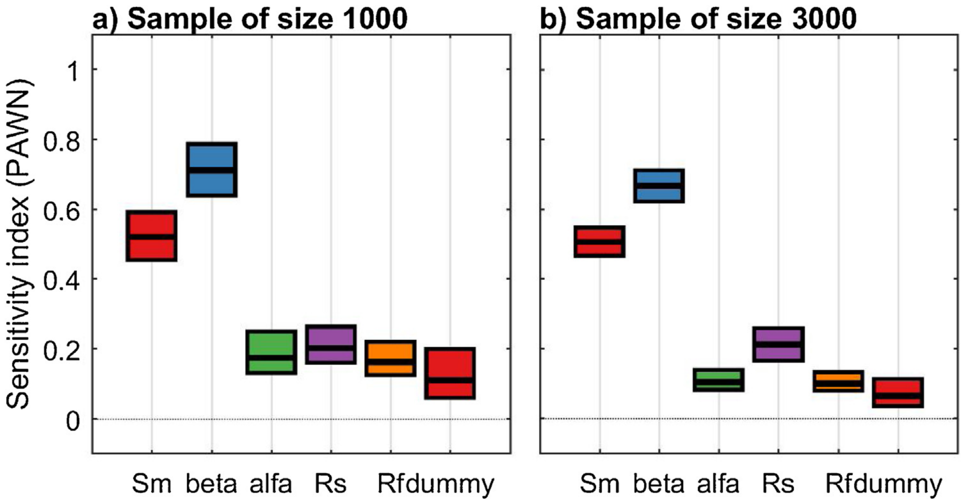


Fig. 13. PAWN sensitivity indices for the five model input factors and the additional 'dummy' input factor, calculated using an input/output sample a) of size 1000 and b) of size 3000. The boxes represent the 95% bootstrap confidence intervals and the central black lines indicate the bootstrap mean.

metric to identify non-influential input factors (and therefore for screening purposes) as it allows to detect whether an input factor has an effect on the output for at least one conditioning interval. The sensitivity index for the dummy input factor estimates the error in approximating the 'true' CDFs using the current input/output sample. The output metric selected to perform PAWN is the bias.

The code

We perform PAWN using a subsample of the input/output sample derived in the introductory code, to determine whether we could use a smaller sample to screen the input factors.

```
x_labels = {'Sm','beta','alfa','Rs','Rf','dummy'}; % Name of input factors (we add an
artificial 'dummy' input factor)

iY = 2; % Define the index of the output metric(s) to consider from those estimated in remark
1, f(2) = RMSE

% Calculate the sensitivity indices using bootstrapping for a subsample of the input/output
sample derived in the introductory code (warning: it may take some time to run these lines):
Nsub = 1000; % Size of the subsample
X_sub = X(1:Nsub,:); % Subsample of input factors
Y_sub = Y(1:Nsub,:); % Subsample of output
n = 10; %  Number of equally spaced intervals
Nboot = 1000; % Number of bootstrap resamples
[~,~,KS_max_sub,KS_dummy_sub] = pawn_indices_givendata(X_sub,Y_sub(:,iY),n,Nboot);
% Calculate PAWN sensitivity index:
% - KS_max_sub (size (Nboot,M)) is the maximum KS across the n conditioning intervals for the
Nboot bootstrap resamples and for the M model parameters analysed (we note that we use a
different index compared to remark 3 where we used the mean KS across the conditioning
intervals, because the objective here is to screen uninfluential input factors);
% - KS_dummy_sub (size (Nboot,1)) is the KS statistic for the dummy parameter.

% Calculate statistics across bootstrap resamples (mean, lower and upper bounds of
sensitivity indices):
alfa = 0.05; % Significance level for the confidence intervals estimated by bootstrapping
Spawn_sub_m = mean([KS_max_sub,KS_dummy_sub]); % Mean PAWN sensitivity index across bootstrap
resamples
KS_sort = sort([KS_max_sub,KS_dummy_sub]);
Spawn_sub_lb = KS_sort(max(1,round(Nboot*alfa/2)),:); % Lower bound
Spawn_sub_ub = KS_sort(round(Nboot*(1-alfa/2)),:); % Upper bound

% Plot the sensitivity indices with confidence intervals (Figure 13.a):
figure
boxplot1(Spawn_sub_m,x_labels,'Sensitivity index (PAWN)',Spawn_sub_lb,Spawn_sub_ub)
```

Now we repeat the calculation of the PAWN sensitivity indices using the entire input/output sample derived in the introductory code.

```
% Calculate the sensitiviy indices (warning: it may take some time to run the following
line):
[~,~,KS_max,KS_dummy] = pawn_indices_givendata(X,Y(:,iY),n,Nboot);

% Calculate statistics across bootstrap resamples (mean, lower and upper bounds of
sensitivity indices):
Spawn_m = mean([KS_max,KS_dummy]); % Mean PAWN sensitivity index across bootstrap resamples
KS_sort = sort([KS_max,KS_dummy]);
Spawn_lb = KS_sort(max(1,round(Nboot*alfa/2)),:); % Lower bound
Spawn_ub = KS_sort(round(Nboot*(1-alfa/2)),:); % Upper bound

% Plot the sensitivity indices with confidence intervals (Figure 13.b):
figure
boxplot1(Spawn_m,x_labels,'Sensitivity index (PAWN)',Spawn_lb,Spawn_ub)
```

The results

Interpretation of the results

From Fig. 13.a, we observe that the confidence intervals of the sensitivity index for three model input factors (alfa, Rs and Rf) are overlapping with the confidence intervals of the dummy input factor. On the other hand, the sensitivity index of Sm and beta are significantly higher than the sensitivity index of the dummy input factor. This means that, when using a sample of size 1000, we can conclude that Sm and beta are influential parameters, while alfa, Rs and Rf appear to be non-influential, because their sensitivity index is of the same order of magnitude as the approximation error of the CDFs. However, we observe that the confidence intervals on the sensitivity indices are rather wide, including for the low-sensitivity input factors. When using a larger sample size (Fig. 13.b), we observe a significant reduction in the width of the confidence intervals, which results in a clear separation between Rs and the dummy input factor. This means that we can robustly infer that Rs is an influential input factor using a sample of size 3000 (Fig. 13.b), while the sample of size 1000 was too small to robustly identify the non-influential input factors (Fig. 13.a).

Implications

The method discussed in this remark identifies the influential input factors as those factors that have a sensitivity index (and corresponding confidence intervals) higher than, (and not overlapping with), the sensitivity index of the dummy input factor. Input factors that have a sensitivity index lower than (or overlapping with) the dummy input factor can be considered non-influential, because their sensitivity index has the same magnitude as the approximation error of the sensitivity indices. However, the choice of the sample size is critical to obtain robust screening results (see further discussion on the choice of the sample size in remark 3). Specifically, it can be expected that the number of non-influential input factors identified using the 'dummy' approach will decrease with increasing sample size, as the approximation error of the sensitivity indices reduces.

Author contributions

V.N., F.S., F.P. and T.W. designed the study; V.N. and F.S. have contributed in equal measure to the preparation of the workflows and to the writing of the manuscript, with contributions from F.P. and T. W.; all authors have approved the final version of the manuscript.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.mex.2019.09.033.

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