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An Integrated, Fast and Easily Useable Software Toolbox Allowing Comparative and Complementary Application of Various Parameter Sensitivity Analysis Methods

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Abstract: The analysis of parameter sensitivity in environmental models is an excellent technique to assess a model's behavior, to determine its potential utility, to support its calibration, and to identify areas of improvement. Recent work on comparing sensitivity analysis methods shows that the methods available today are complementary, i.e. multiple methods should be used to assess a model. We present a software toolbox for global sensitivity analysis which supports the investigation of parameter sensitivity using different methods. The toolbox includes *Regional Sensitivity Analysis*, *Morris Method*, and a *Sobols method*. The majority of these methods require input data from a Monte-Carlo-Sampling which has to be carried out in advance, others demand for special properties of the sampling. Therefore, in most cases, huge computational effort has to be spent to generate several sampling data. To overcome this deficit the data from a single Monte-Carlo-Sampling is used to train an *Artificial Neural Network (ANN)* which imitates the original model. By using this approach, arbitrary samplings can be easily drawn from the ANN-based emulator. This approach also gives an objective measure of the quality of the sampling itself and provides criteria on how many samples are required to get representative results. The sensitivity toolbox is part of the OPTAS module in the Jena Adaptable Modelling System. We will present the developed sensitivity analysis toolbox and examples of its application to the hydrological model J2000 in a catchment located in Germany. Special attention is paid to the emulation of the model with the newly developed ANN approach which produced very promising results.

Keywords: Sensitivity Analysis, Morris Method, Regional Sensitivity Analysis, Artificial Neural Network

1 INTRODUCTION

This article illustrates the capabilities of a sensitivity analysis toolbox which uses a metamodel based on an *Artificial Neural Network (ANN)* to incorporate the power of several widely-used sensitivity analysis methods computationally efficiently.

Saltelli [2004] defines sensitivity analysis (SA) as *"The study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input."* Environmental modeling sensitivity analysis can be used in various ways, e.g. (i) A priority ranking of the input-factors and parameters of a model can be assessed. Factors with strong influence on the model output should be handled very carefully during model setup, while factors without influence could be neglected and can be considered as candidates for model simplification. The same ranking can also be used to guide to process of model improvement. (ii) Sensitivity Analysis helps to improve the knowledge about the model and can be used to work out characteristic properties. (iii) The robustness of the model parameters can be estimated. The presence of very sensitive input factors and parameters may indicate for flaws in the underlying assumptions of the model. (iv) The calibration of the model can be supported [Saltelli, 2004].

Recent studies have shown that the SA methods available today have distinct capabilities of model assessment [Yang, 2011]. Consequently, to get the most out of sensitivity analysis, multiple SA methods have to be applied. Usually, they require an extensive sampling of the model's input and/or parameter space to assess its behavior. Unfortunately, each method demands distinct sampling properties (e.g. information about partial derivatives), so that such a sampling often cannot be reused. Hence, huge computational effort has to be spent to do this work several times. To overcome this deficit, a single quasi-random sampling is used to generate a meta-model based on an Artificial Neural Network (ANN), which imitates the original model.

2 METHODS

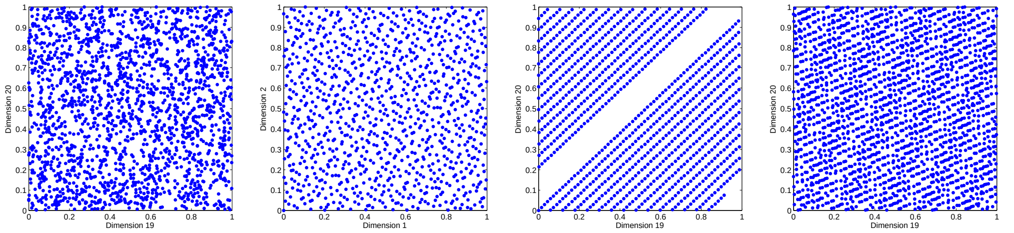
In the following, $f(\theta) \rightarrow O$ will denote an environmental model, which maps a model input $\theta \in \Omega$ onto a model response O. For the sake of simplicity, O is supposed here to be a scalar quantity and Ω an n-dimensional hypercube.

2.1 Sample Generation

Most SA methods require an (i) uncorrelated (ii) uniformly distributed, and (iii) representative sampling of the parameter space, which is easily generated by drawing as many samples from a uniform probability distribution as needed. Unfortunately, such samplings tend to cover the parameter space non-uniformly by forming clusters and gaps (Shirley [1991], see figure 1(a)). When they are used for statistical analysis, clusters are overemphasized and gaps excluded. Thus, large samplings are needed to compute reliable statistical measures [Saltelli et al., 2008].

The quasi-random sequence of Halton [1960] overcomes this deficit by exploring the parameter space more efficiently (Figure 1(b)). But high dimensional Halton Sequences show strong correlations between their elements, in case the sequence is terminated too early, which is clearly shown in Figure 1(c). However, excellent samplings can be generated (see Figure 1(d)) with the *Leaped Halton-Sequence*, which avoids this problem by using only every L-th element [Kocis and Whiten, 1997].

To setup the meta-model, a multi-step procedure is carried out: (i) First, the Leaped Halton Sequence is used to generate an initial sampling. (ii) The sampling is used to train an *Artificial Neuronal Network* in such a way that it imitates the model response. (iii) A K-fold cross-validation is used to estimate the agreement between the real model $f(\theta)$ and the meta-model $\tilde{f}(\theta)$. In case the test fails, i.e. the agreement is not acceptable, additional samples are generated and the procedure is repeated. Otherwise, the information content of the sampling is sufficient to reproduce most of the characteristics of the original model f. Hence, further exploration of the input space would not lead to much additional information, so that the procedure can be terminated successfully. The meta-model is now able to dynamically generate samplings with arbitrary properties.



(a) Sampling drawn from a uniform random distribution (b) Halton-Sequence in dimension 1 and 2 (c) Halton-Sequence in dimension 19 und 20 (d) Leaped Halton-Sequence in dimension 19 und 20

Figure 1: Comparison of four different samplings with 2,000 elements each.

The flow chart (Figure 2) summarizes this process. In the software application, an Artificial Neuronal Network consisting of an input layer, one hidden layer, and an output layer, is used. The input layer contains $n + 1$ neurons, which equals the number of input factors plus an additional node to model a constant bias. The hidden layer consists of $1/2 \cdot (n + 1)$ neurons and the output layer has one neuron. The activation function of the hidden layer is a sigmoid function and that of the output layer is a linear function. Prior to the training process a linear transformation normalizes the training set. The application uses the *Java and DotNet Neural Network Framework Encog*[1] [Heaton Research, 2012] and the *Resilient Propagation* learning rule [Riedmiller and Braun, 1992].

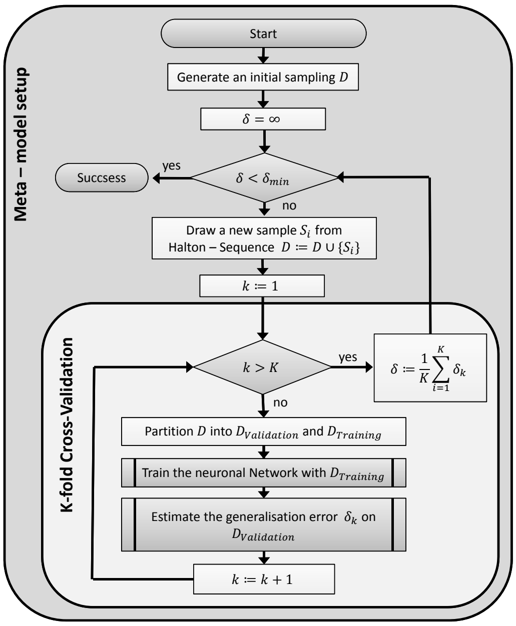


Figure 2: Flowchart of the sampling process: δ denotes the mean generalisation error of the ANN, K the iterations of the crossvalidation routine and D the current set of samples.

2.2 Sensitivity Methods

The ***Regional Sensitivity Analysis*** of Hornberger and Spear [1981] is frequently used for environmental modeling. It apportions the sample into acceptable (*behavioral*) and unacceptable (*non-behavioral*) simulations. For both sets the cumulative distribution function of the input factor under analysis is calculated. If the distributions differ significantly from each other, the input factor is influential. The opposite statement is not always true. However, if the distributions are similar, the input factor can be suspected to be non-influential. To quantify the sensitivity objectively, the *Kolmogorov-Smirnoff-Test* ([Kendall et al., 1987] is usually applied, whose null hypothesis supposes both distributions to be identical.

The Morris Method [Morris, 1991] is based on *Elementary Effects:*

$$E_i = \left(f\left(x + h \cdot e_i\right) - f\left(x\right)\right)/h,$$

which is a local measure of sensitivity. In this definition, the step length $h \in \mathbb{R}^+$ is usually small and e_i the i-th unit vector. Thus, the effect E_i can non-ambiguously be assigned

[1] `http://www.heatonresearch.com/encog`

to the factor i. To calculate the Elementary Effects for each factor, $n + 1$ samples are taken along a trajectory. Morris' method calculates this measure at numerous points in the parameter space, producing a set of Elementary Effects which is then statistically evaluated. The mean (eqn. 1), absolute mean (eqn. 2), and variance (eqn. 3)

$$\mu_i = \frac{1}{k} \sum_{j=1}^{k} E_i^j \tag{1}$$

$$\mu_i^* = \frac{1}{k} \sum_{j=1}^{k} \left| E_i^j \right| \tag{2}$$

$$\sigma^2 = \frac{1}{k} \sum_{j=1}^{k} \left(E_i^j - \mu_i \right)^2 \tag{3}$$

give information about the sensitivity, monotonicity, and linearity of the input factors with respect to the model output [Norton, 2009].

Sobols method [Sobol, 1993] is recommended by Saltelli et al. [2008] because it is model-independent, can estimate the influence of input factors over the whole range of variation, tolerate effects of interaction between parameters, and can estimate the combined effect of groups of parameters. The key idea is to decompose the total variance of the model output into

$$V_f(x) = \sum_i V_{x_i} + \sum_{i,j} V_{x_{i,j}} + \sum_{i,j,k} V_{x_{i,j,k}} + \cdots + V_{x_{1\ldots n}}.$$

In this formula, the term $V_{x_i} = V_{x_i}\left(E_{x_{\bar{i}}}(f(x)\,|x_i)\right)$ denotes the conditional variance of the model output if the i-th parameter is fixed and all other parameters can vary freely. This is a natural way to define the *main effect* of an input factor

$$S_i = \frac{V_{x_i}}{V_x(f(x))}.$$

In the same way, groups of parameters can be handled, e.g. the combined effect of x_i and x_j is simply defined as $S_i = V_{x_{i,j}}/V_x(f(x))$, allowing the identification of interactions between parameters. Finally, the *total effect*

$$S_{T_i} = 1 - \frac{V_{x_{\neg i}}}{V_x(f(x))}$$

accounts for the main effect and all interactions of a factor (the meaning of $\neg i$ is 'all but i').

2.3 The Hydrological Model J2000

The distributed, process-oriented model J2000 was developed for hydrological simulation of the upper meso- and macro scale [Krause, 2001]. It is implemented in the Jena Adaptable Modeling System (JAMS[2] Kralisch and Krause [2006]), which is a software framework for component-based development and application of environmental models. The model describes the hydrological processes as encapsulated process modules. In addition to the simulation of the runoff generation and runoff concentration processes, J2000 also offers routines for regionalization and correction of climate and precipitation input data, model calibration, and visualization [Kralisch et al., 2007].

[2] http://jams.uni-jena.de/

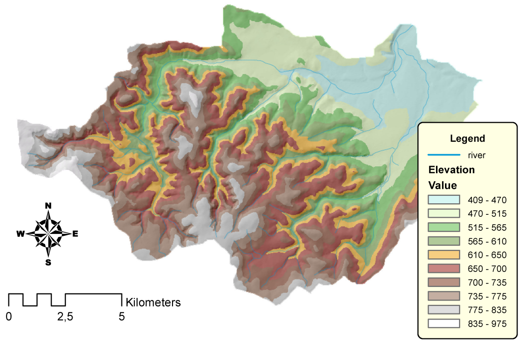


Figure 3: Topography of the Ilm catchment

In J2000, the spatial representation of a catchment is based on the concept of Hydrological Response Units (HRUs). HRUs are homogenous regarding their physiography (e.g. topographic features, land use, soil properties). Therefore, it is possible to assign a characteristic hydrological process response to each HRU [Flügel, 1996]. They are connected by a lateral routing scheme to simulate lateral water transport processes either with their downhill successor HRU or with a river reach they are drain in. River reaches themelves are always connected with their downstream reach. The model simulates relevant hydrological processes, such as evapotranspiration, snow accumulation and melt, soil-water balance and groundwater processes, for each HRU separately.

3 Study area

The well-investigated catchment of the *Ilm* is selected to demonstrate the described methods using the model J2000. The Ilm has its source in the central part of the Thuringian Forest, which is located in central Germany. The catchment has a size of 155 km^2 and an elevation range of 500m. The dominating land use of the catchment is coniferous forest (60%), grassland (12%), and settlement (10%). The hydrological system is influenced mainly by lateral flow processes and snow melt. The average annual temperatures in the catchment are around $6 - 7\,^{\circ}\mathrm{C}$. In the higher parts, annual precipitation is larger than 1,400 mm.

4 Application

Validation of the meta-model

The sensitivity analysis was carried out for the full set of 34 parameters of the model J2000, so that the effect of these parameters on the Nash-Sutcliffe efficiency between the simulated and observed catchment discharge is assessed. For reasons of clarity and comprehensibility only a subset of seven parameters is discussed here. Those parameters are *a_rain* and *a_snow* parameterizing the interception of rain and snow on the vegetation of the catchment. *soilConcRD1* and *soilConcRD2* influence the dynamics of the surface runoff and interflow. *initRG1* defines the initial storage of one of the two groundwater storages. *ACAdaptation* controls the capacity of the large pore storage of the soil and *baseTemp* influences the snow melt process.

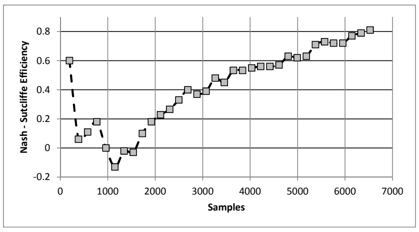


Figure 4: Progress of the learning process

The ANN was able to imitate the model, well. Only 6,528 samples were required to achieve a Nash-Sutcliffe Efficiency of more than 0.8 between the original model and the meta-model. This estimation is based on a ten-fold cross-validation. Figure 4 shows the progress of the learning process. Shortly after the start of the procedure, the similarity between the model and the meta-model is quite high, but it drops rapidly to a minimum of -0.13 at 1152 samples. Afterwards, the quality of the meta-model improves continuously. The reason for this non-monotonic behavior is not fully understood right now. The learning process will also stagnate eventually. It seems plausible that the complexity of the

Artificial Neuronal Network is not sufficient to learn every detail of the model's behaviour. For the scope of this article, the quality is sufficient but if a higher quality is required, the complexity of the ANN could be enlarged. To dig deeper into detail, the original sampling

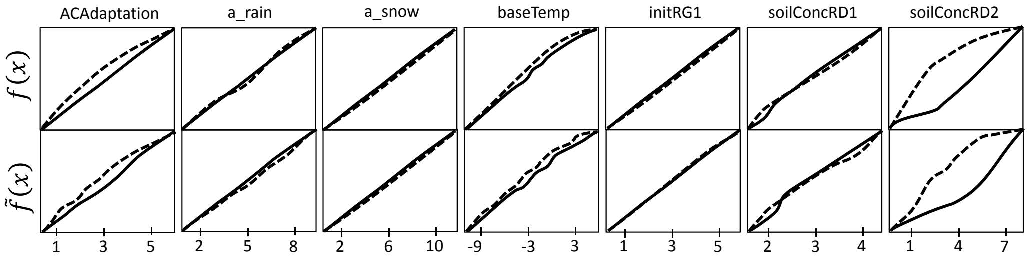


Figure 5: Regional Sensitivity Analysis calculated from the original sampling (upper row) and from a sampling of the meta-model (lower row). The dotted line shows the cumulative distribution function of the behavioral parameter set and the solid black line that of the non-behavioral set.

and a sampling generated by the meta-model (with 6.000 samples) are used to apply the Regional Sensitivity Analysis. The RSA method does not demand any special requirements of the sampling, so that a comparison is easily possible. Figure 5 shows the cumulative distribution functions of the behavioral (solid line) and non-behavioral (dotted line) parameter set for both samplings. At the first glance, the differences between the upper and lower plots are hardly recognizable. The RSA plots of the meta-model tend to be a little bit more noisy and the distance between both distribution functions is smaller. The relative difference between both sensitivity indices varies from 7% to 80% percent, but the absolute difference is always lower than 4%. This verification indicates that the discrepancy between the model and the meta-model is acceptable.

Application 1: Parameter Ranking
RSA, Morris' method and Sobols method provide sensitivity indices, which can be used to create a priority ranking of the input parameters. To make the sensitivity indices comparable, they are linearly normalized. Figure 6 shows the comparison of the several measures. The resulting priority rankings of the three SA methods are not equal, but the same parameters are classified as sensitive. Consistently, soilConcRD2 is the most sensitive parameter by far. The parameters ACAdaptation, baseTemp and soilConcRD1 have some influence, but do not dominate the model response. The other parameters are less or not sensitive. The total effect puts more weight on the sensitive parameter while neglecting the others. Morris' Method and RSA are very similar, but the total effect differs heavily for the parameters ACAdaptation and a_rain.

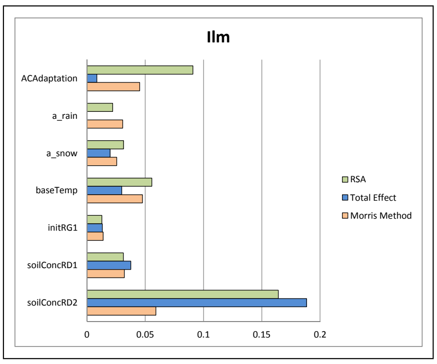


Figure 6: Parameter ranking for the Ilm catchment. The x-axis represents the sensitivity of the parameter.

Application 2: Identifiability
The behavioral cumulative distribution function of the RSA plot can be used to find identifiable model parameters. A steep increase of the distribution function indicates the optimal region of the parameter. In Figure 5, ACAdaptation, baseTemp, and soilConcRD2 seem to be identifiable. The RSA plots indicate that their optimal value is located within the ranges $[0, 3]$, $[-9, 2]$, and $[1, 4]$. The real optimal values are approximately $1.0, 0.3$, and 2.0, which were deter-

mined by calibrating the using the evolutionary optimization method of *Shuffled Complex Evolution* [Duan et al., 1992].

Parameter	a_rain	a_snow	ACAdaptation	baseTemp	soilConcRD1	soilConcRD2	initRG1
Morris Method	4.21	1.35	2.58	0.92	0.52	6.12	9.9
Morris Method*	0.00	0.00	0.02	0.05	0.20	0.07	9.8
Δ	100%	100%	100%	14%	44%	100%	3%
Variability	22%	48%	32%	220%	60%	33%	14%

Table 1: Results of Morris's method

Application 3: Linearity and monotonicity
Morris' Method can be used to determine whether or not an input factor affects the model response in a linear and monotonic way. For this purpose, the mean μ, the absolute mean μ^* and the variance σ^2 of the Elementary Effects are compared among each other. A significant difference between μ and μ^* implies non-monotonic behaviour of the input factor. The variability σ^2/μ is a measure for linearity. The model is linear in the parameters if the variance is zero, while a larger value indicates non-linearity. Since it is unlikely to find linearity and monotony in an efficiency measure, the total amount of the discharge from the catchment is analyzed instead. The results are summarized in Table 1. Except for initRG1 all parameters show non-monotonic behaviour. This seems plausible, because initRG1 controls the initial amount of water in the groundwater storage. The other parameters do not consistently increase the amount of discharge. The variability indicates that the parameter initRG1 and a_rain show mostly linear behaviour. a_snow, ACAdaptation, soilConcRD1, and soilConcRD2 is somehow linear and baseTemp mostly non-linear.

Application 4: Parameter Interaction
Even non-influential input factors could have a strong effect when interacting together with other parameters. While most sensitivity analysis methods are not capable of handling groups of input factors, Sobols method can easily accomplish this task. The difficulty is to find interesting interacting groups because there are as much as 2^n groups. However, this is not in the scope of this article. We demonstrate interaction effects by showing the sensitivity of parameter groups of two, so that direct interactions can be uncovered. Figure 7 indicates that most of the parameters do barely interact directly or the effect is too small to become visible in the analysis (white cells in Fig. 7). baseTemp and a_snow compensate their effects. Positive interactions are observable for the a_rain interacting with a_snow and soilConcRD2 interacting with a_snow.

Parameter	ACAdaptation	a_rain	a_snow	baseTemp	initRG1	soilConcRD1	soilConcRD2	**Ilm**
ACAdaptation		0.06	0.04	0.05	0.07	0.09	0.13	
a_rain			0.09	0.04	0.05	0.05	0.13	
a_snow				0.03	0.07	0.04	0.2	
baseTemp					0.06	0.03	0.17	
initRG1						0.05	0.17	
soilConcRD1							0.16	
soilConcRD2								

Figure 7: Parameter interaction effects: Ilm(upper right triangle)

5 Conclusion

This article presents a toolbox for sensitivity analysis which uses an Artificial Neural Network as a meta model to efficiently apply several sensitivity analysis methods at once. The article shows that the artificial neural network requires less than 10^4 samples generated from a quasi-random sequence to learn the behavior of the complex distributed hydrological model J2000. It becomes clear that the results of the sensitivity analysis from the meta-model do not differ much from the results of the sensitivity analysis based on the original model. In contrast, there is an enormous gain in runtime performance during the sampling. Generating the input data for the ANN took approximately 24 hours on a parallel computer with 48 computing units. As shown in this article, each application, would have required a new sampling and thus additional time each without the ANN. Using the ANN the whole process of setting up the artifical neural network and applying the sensitivity analysis took about one minute on a conventional notebook.

Future work is focusing on applying the presented methodology to other catchments and models. Additional tools for Factor Fixing, Risk Analysis and Tradeoff Analysis will be added to the toolbox.

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