Evolutionary Regression Modeling with Active Learning: An Application to Rainfall Runoff Modeling

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Abstract. Many complex, real world phenomena are difficult to study directly using controlled experiments. Instead, the use of computer simulations has become commonplace as a feasible alternative. However, due to the computational cost of these high fidelity simulations, the use of neural networks, kernel methods, and other surrogate modeling techniques has become indispensable. Surrogate models are compact and cheap to evaluate, and have proven very useful for tasks such as optimization, design space exploration, visualization, prototyping, and sensitivity analysis. Consequently, there is great interest in techniques that facilitate the construction of such regression models, while minimizing the computational cost and maximizing model accuracy. The model calibration problem in rainfall runoff modeling is an important problem from hydrology that can benefit from advances in surrogate modeling and machine learning in general. This paper presents a novel, fully automated approach to tackling this problem. Drawing upon advances in machine learning, hyperparameter optimization, model type selection, and sample selection (active learning) are all handled automatically. Increasing the utility of such methods for the domain expert.

1 Introduction

For many problems from science and engineering it is impractical to perform experiments on the physical world directly (e.g. airfoil design, earthquake propagation). Instead, complex, physics-based simulation codes are used to run experiments on computer hardware. This allows scientists more flexibility to study phenomena under controlled conditions. However computer experiments still require a substantial investment of computation time. This is especially evident for routine tasks such as prototyping, high dimensional visualization, optimization, sensitivity analysis and design space exploration [1].

As a result researchers have turned to various approximation methods that mimic the behavior of the simulation model as closely as possible while being computationally cheap(er) to evaluate. Different types of approximation methods exist, each with

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their relative strengths. This work concentrates on the use of data-driven, global approximations using compact surrogate models (also known as emulators, metamodels or response surface models (RSM)) in the context of computer experiments. Examples of metamodels include: Artificial Neural Networks (ANN), rational functions, Gaussian Process (GP) models, Radial Basis Function (RBF) models, and Support Vector Machines (SVM).

It is important that we stress the difference between local and global surrogate models as the two are often confused. Local surrogates are by far the most popular and involve building small, relatively low fidelity surrogates for use in optimization. Local surrogates are used as rough approximators of the (costly) optimization surface and guide the optimization algorithm towards good extrema while minimizing the number of simulations. Once the optimum is found the surrogate is discarded. Many advanced methods for constructing and managing these local surrogates have been designed (e.g., [2]).

In contrast, with global surrogate modeling the surrogate model *itself* is the goal. The objective is to construct a high fidelity approximation model that is as accurate as possible over the *complete* design space of interest using as few simulation points as possible. Once constructed, the global surrogate model (also referred to as a replacement metamodel[1]) is reused in other stages of the computational science and engineering pipeline. So optimization is not the goal, but rather a useful post-processing step.

However, constructing accurate surrogate models as efficiently as possible is an entire research domain in itself. In order to come to an acceptable approximation, numerous problems and design choices need to be overcome: what data collection strategy to use (active learning), what model type is most applicable (model selection), how should model parameters be tuned (hyperparameter optimization), how to optimize the accuracy vs. computational cost trade-off, etc. This work draws upon advances in these domains, integrating them in a coherent platform in order to better tackle the model calibration problem in hydrology.

2 Surrogate Modeling

As stated in the introduction, the principal reason driving the use of surrogate models is that the simulator is too time consuming to run for a large number of simulations. One model evaluation may take many minutes, hours, days or even weeks [1]. A simpler approximation of the simulator is needed to make optimization, design space exploration, etc. feasible. A second reason is when simulating large scale systems [3].

There are many methods involved and various choices to be made when generating surrogate models. Consequently, practical implementation leaves many options open to the designer: different model types, different experimental designs, different model selection criteria, different active learning strategies, etc. However, in practice it turns out that the designer rarely tries out more than one subset of options. All too often, surrogate model construction is done in a one-shot manner. Iterative and adaptive methods, on the other hand, have the potential of producing a much more accurate surrogate at a considerably lower cost (less data points). E.g., by applying iterative sample selection

[1] The terms surrogate model and metamodel are used interchangeably.

(also known as active learning and adaptive sampling) an accurate surrogate model can be constructed while minimizing the computational cost. See [4] for a good discussion on this issue. For the application in this paper we will utilize a fully featured toolbox for adaptive surrogate model generation , the SUMO toolbox [5].

3 Application

A task which is often central to hydrological modeling is the identification of suitable parameters for a given set of modeling objectives, catchment characteristics and data. However, this identification process is difficult because conceptual rainfall runoff models generally have a large number of parameters and the accuracy of their calculations depends on how the relevant parameters are defined. Additionally, because of their conceptual nature, these parameters cannot be measured directly and are therefore estimated on the basis of a calibration process, i.e., minimizing an objective function (OF).

We illustrate the strength of global surrogate modeling in improving the process of estimating the right parameters of a rainfall runoff model. The SWAT (Soil Water Assessment Tool) is an operational model that was developed to assist water resource managers in assessing water supplies and non-point source pollution at river basin scale. The model is able to assess the impact of changes in climate, landuse and management, and to simulate the transport and fate of chemicals and water quality loadings. The model is designed so that use can be made of readily available inputs. Upland components include hydrology, weather, erosion/sedimentation, soil temperature, plant growth, nutrients, pesticides, and land and water management. Stream processes include channel flood routing, channel sediment routing, nutrient and pesticide routing and transformation. The ponds and reservoirs component contains water balance, routing, sediment settling, and simplified nutrient and pesticide transformation routines. Water diversions into, out of, or within the basin can be simulated to represent irrigation and other withdrawals from the system. However, one should be aware that every process in the model is a simplification of reality.

In SWAT, a watershed is divided into multiple subwatersheds, which are then further subdivided into *hydrologic response units* (HRUs) that consist of homogeneous landuse, management, and soil characteristics. The HRUs represent percentages of the subwatershed area and are not identified spatially. The model operates in a continuous mode and has been widely used to estimate catchment runoff, nutrient and sediment loads. The SWAT model development, operation, limitations, and assumptions are extensively discussed by [6]. One of the practical problems in applying the SWAT is determining proper values for the more than 30 parameters that control the fidelity of its prediction. While many parameters can be estimated empirically a direct expensive optimization procedure is still routinely used to determine optimal settings [7], requiring many expensive simulations.

We propose to take global surrogate modeling methods routinely used in Electro-Magnetics (EM) and engineering design, and apply them to the setting of rainfall runoff modeling. Through the use of sequential modeling and active learning methods, a replacement metamodel can be generated that captures the relationship between the different SWAT parameters and provides insight in their influence on the prediction quality

of the SWAT. While at the same time minimizing the number of computationally expensive simulations. Optimization can still be performed as a postprocessing step.

4 Related Work

A few studies have been reported in recent years in the field of water resources related to surrogate modeling. Savic et al. [8] applied 2 data-driven models (genetic programming and ANN) to flow prediction, results show that both are able to match up against conceptual models. Khu et al. (2003) [9] reduced the number of simulation runs required by Monte Carlo (MC). This was achieved by using an ANN and hybrid GA to respectively approximate and explore the shape of the objective function. This significantly reduces the computational effort involved in investigating hydrological model parameter uncertainty. Later on, an evolutionary-based metamodel calibration methodology was developed using a coupled genetic algorithm-RBF ANN [10]. Regis and Shoemaker (2004) [11] proposed an approach for costly black box optimization that uses space-filling experimental designs and k-nearest neighbor local function approximations to improve the performance of an EA in twelve-dimensional groundwater bioremediation problem. Broad et al., (2006) [12] evaluated six local search algorithms for purpose of improving the performance of ANN surrogate model-based optimization of water distribution systems. The results show a significant improvement in the value of the objective function by using a local search as a complementary stage of surrogate model-based optimization of water distribution systems. Kamali et al. (2007) [13] evaluate the performance of the design and analysis of computer experiments (DACE) surrogate function along with Latin Hypercube Sampling (LHS) and MC Sampling for hydrological model calibration. The results indicate that DACE along with LHS reduced the computational cost of calibration process. Recent research by Garote et al. [14] advocate the use of Bayesian networks to learn the behaviour of a rainfall runoff model.

5 Experimental Setup

5.1 SWAT

The SWAT requires spatial information about topography, river/stream reaches, landuse, soil and climate to accurately simulate the streamflow. The study basin is that of the Grote Nete (383 km^2), located in the north-eastern part of Belgium. A detailed description of the study basin is given in [15]. Daily observations of precipitation, air temperature, evaporation, and daily streamflow data were obtained from the Royal Meteorological Institute and the Flemish Administration for Land and Water, Belgium. The soil map was available at a scale of 1:25.000; the soil physical data was derived from the Aardewerk-SIBIS Soil Information System and land use was derived from the multi-temporal LANDSAT 5 TM image of 18 July 1997.

The climatic inputs in SWAT include daily precipitation measured in 5 stations scattered in and outside the study area, and the potential evapotranspiration and min/max temperature collected in a station at the northern boundary of the catchment. Details of input data are given in [15]. The catchment was subdivided in 8 subcatchments and 65

HRUs. The flow separation program of [16] was used in this research as to determine the relative contribution of surface runoff and groundwater to total streamflow. The latter were created based on the various combinations of land use and soil types present in the catchment. Climate data were assigned to each HRU using the centroid method. The daily streamflows in the Varendonk outlet station were used for model calibration and verification.

Parameter sensitivity analysis was applied to identify the parameters of the SWAT model that contribute most to the variability of component flows. It is important to have an understanding of catchment characteristics and the hydrological processes involved before 'blindly' applying surrogate modeling to the available data. Based on a critical analysis of the SWAT modules to the hydrology of the study area, the parameters to calibrate were reduced to 18. Although this number of parameters is considerably smaller, to further reduce the number of parameters in the surrogate process, a sensitivity analysis was conducted to determine the most sensitive parameters of the hydrological module simulating streamflow. This analysis (through Latin Hypercube and One-factor-at-a-time) yielded the 4 most sensitive parameters.

The first parameter is p, the percentage by which CN_2 (the SCS curve number) is changed from the initial values. Thus, p, a parameter in the approximation model, is converted to CN_2, the actual parameter of the SWAT, using the following formula: $CN_2 = initial\,CN_2 + \frac{initial\,CN_2 \cdot p}{100}$. Secondly, *RCHRG_DP* stands for the deep aquifer percolation ratio and is a measure for the transfer between the shallow and deep aquifer system. Thirdly, *REVAPMN* is the amount of water (mm) that must be present in the shallow aquifer store before water can move to the unsaturated zone. Finally, *ESCO* is the soil evaporation compensation coefficient. The domains of the 4 parameters are [-40,40] (ensuring absolute bounds of [35 90] for CN_2), [0 3], [0 1] and [0 1] respectively. When the SWAT model is run it generates a time series of predicted flow during the period 1998-2002. This time series is then separated into 3 components useful for runoff prediction: *low flow* (values $\leq$2), *high flow* (values $\geq$5), and *total flow* (all values). On each of these components the Mean Square Error (*MSE*) is then calculated with the true observations during that period, and that is the final output of the simulation code. Separating the total flow in more fine-grained components allows the SWAT to be calibrated for different types of flows. Thus, in sum, the SWAT simulator has 4 inputs (CN_2, *RCHRG_DP*, *REVAPMN*, *ESCO*), and 3 outputs ($MSE_{low}, MSE_{high}, MSE_{total}$).

5.2 SUMO Toolbox

The active learning settings were set as follows: an initial optimized Latin hypercube design of size 50 is used augmented with the corner points. Modeling is allowed to commence once at least 20 of the initial samples are available. Each iteration a maximum of 50 new samples (over all outputs) are selected using the *gradient* adaptive sampling algorithm up to a maximum of 500. A full discussion of the algorithm is out of scope for this paper, details can be found in [17].

There are many surrogate modeling methods available to fit the data and many options implemented in the SUMO Toolbox. However, from the application it is not

immediately clear which surrogate model type or hyperparameter optimization algorithm should be used (ANN, SVM, RBF models, ...). For this reason we shall use an automatic surrogate model type selection algorithm. The algorithm utilizes a genetic algorithm (using the island model) to simultaneously select the model type and model parameters (hyperparameter optimization). The surrogate model types included in the evolution are: single layer feed forward ANNs (using [18]), Kriging models (using [19]), rational functions and LS-SVMs (using [20]). Together with hybrid models (ensembles, that arise as a result of a crossover between two models of different type) this means that 5 model types will compete to fit the data. The population size for each model type is 10 and the maximum number of generations between each sampling iteration is 15. The final population of the previous model type selection run is used as the initial population for the next run. An extinction prevention algorithm is used to ensure no model type goes completely extinct. A full description of the algorithm, model types, and genetic operators is out of scope for this paper. Such settings can be found in [5]. Given the correlation between the outputs, they are not modeled separately (by separate models) but together in a single model with multiple outputs.

Note that this approach relieves the domain expert from technical choices related to the model generation. Besides a few high level options (which model types are of interest) and termination criteria (time limit, sample budget) no further input is required. The hyperparameter optimization, model selection, and sample selection are performed fully automatically, allowing the domain expert to concentrate on the application and not have to deal with modeling technicalities.

In order to drive the hyperparameter optimization a max-min validation set of 20% is used. Since not all data points are available at once but are chosen incrementally, the validation set grows as more data arrives. Validation points are not selected randomly but by maximizing the minimum distance between them, thus ensuring a good coverage of the domain. Note, though, that models are always trained on all the data, it is only when the error is calculated that they are temporarily re-trained on 80% of the available data. The error function that is minimized is the Average Relative Error (*ARE*):

$$ARE(y,\tilde{y}) = \frac{1}{n}\sum_{i=1}^{n}\frac{|y_i-\tilde{y}_i|}{|y_i|},$$

where y_i, $\tilde{y}_i$ are the true and predicted response values respectively. Since we are dealing with multiple outputs per model, a weighted sum over the *ARE* values for each output is taken. Since we wish to treat all outputs equally, all weights were set to 1[2].

The SUMO Toolbox was configured to use the remote Sun Grid Engine (SGE) sample evaluation backend. This means that the toolbox will run simulations in parallel by transparently submitting them to a remote cluster. The cluster in question is the CalcUA cluster which consists of 256 nodes. Thus the SUMO Toolbox (v5.1) is running on a local machine, while the SWAT simulations are scheduled on the cluster. The number of data points selected each iteration is chosen dynamically (but never exceeding the user defined limit of 50) based on the average time needed for modeling, the average duration of a single simulation, and the number of compute nodes available at that point in time. The average time for one simulation is quite short, 4-10 minutes depending on

[2] Alternatively, a multiobjective approach as discussed in [21] could also have been used.

cluster availability. Finally it should be noted that all the algorithms described here are available for download at `http://www.sumo.intec.ugent.be`.

6 Results

Figure 1 shows the evolution of the population as the modeling progresses. Some interesting dynamics can be observed. As soon as migration between the different subpopulations is allowed to take place, Kriging models quickly take over the population resulting in very smooth approximation surfaces. As the number of datapoints increases, the quality of the rational functions increases and they overtake Kriging as the most popular model type. However, the problem with the rational functions is that they are very prone to producing asymptotes in their response due to the increasing existence of poles. The implementation in the toolbox is best suited to low dimensional cases with sufficient data per dimension, in other cases the orders of the polynomials involved grow too quickly, increasing the risk of overfitting. Therefore, it is no surprise that they are finally overtaken by ANN models that, thanks to the pruning functions implemented as part of the mutation and crossover operators, are able to produce smoother responses.

Of course nothing prevents this process from recurring. The fact that the optimal solution changes with time is not necessarily a bad thing and should actually be expected since the hyperparameter optimization landscape is dynamic (due to the active learning). Note that it is the extinction prevention (EP) algorithm that makes these oscillations possible (it ensures a model type never goes completely extinct but that at least 2 individuals of each type are preserved). Without EP these dynamics are impossible and everything depends on the initial conditions. As a result the danger of converging to a poor local optimum (poorly fitted regression model) is significantly larger. Ideally these tests should be repeated many times to conclusively confirm the final outcome. However, naturally, in situations where simulations are costly such repetitions are impossible. In addition, previous work on a wide variety of benchmark problems has shown that the algorithms used here are robust across many repetitions and always perform better or equal than a set of single model type runs.

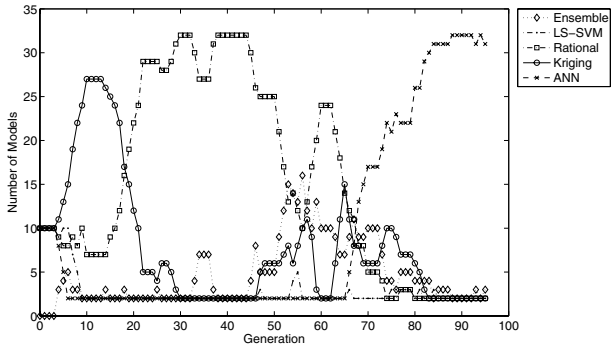

Fig. 1. Population evolution

Table 1. Errors of final ANN model (4-14-3 network)

$\|X\|$	***Output***	ARE_{TR}	ARE_V	CV	minimum x^*	$f(x^*)$
500	MSE_{low}	0.08320	0.1084	0.1036	(-39.9939, 0.6907, 0.9999, 0.6549)	0.8311
	MSE_{high}	0.02491	0.03570	0.02760	(-37.0391, 0.0000, 0.0000, 1.0000)	15.6302
	MSE_{total}	0.02336	0.03809	0.02790	(-39.6159, 0.3025, 0.9998, 0.6660)	10.3791

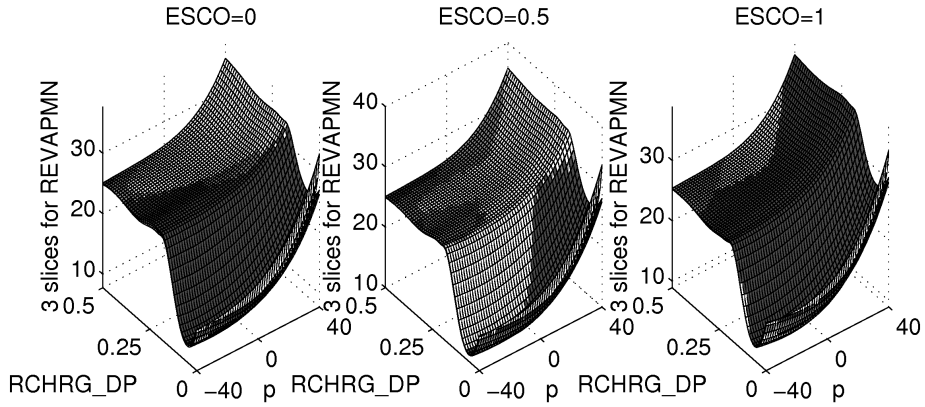

Fig. 2. Final ANN model for MSE_{total}

Table 1 shows the final average relative errors (ARE) for each of the outputs on the training (TR) and validation (V) data. In addition a 10-fold cross validation error (CV) was calculated as well. $|X|$ is the number of samples used to train the ANN model while x^* and $f(x^*)$ denote the minimum and corresponding function value of the ANN model respectively. For the MSE_{high} and MSE_{total} an error of less than 5% (acceptable for the application) is easily reached. The MSE_{low} output appears more difficult, reaching only a final *ARE* of 10%. Thus future runs should take this into account, placing more emphasis on the first output instead of treating all outputs equally. On the other hand, this can also be an indication that the hydrologic model parameters selected are not good enough to capture the trend to simulate base flow. Therefore incorporating more parameters like available water capacity of soils (SOL_AWC) will improve not only low flow simulated values but also high flow simulated values. This is the topic of a follow-up publication.

For space considerations plots of the MSE_{low} and MSE_{high}outputs are omitted in this paper. Figure 2 shows the plot of the final best model (a $4-14-3$ ANN) for MSE_{total}. In the figure *REVAPMN* and *ESCO* have been clamped at 3 values: 0, 1 and 3 for *REVAPMN* and 0, 0.5 and 1 for *ESCO*. The remaining 2 parameters, p and *RCHRG_DP*, are shown along the x-axis and y-axis respectively.

From the figure it is immediately clear that the 3rd and 4th parameters have virtually no influence on the quality of the SWAT prediction: the three slices of each subplot

coincide and the three subplots for each output show little or no differences. This was confirmed by using the model browser of the SUMO Toolbox to browse through each of the 4 dimensions. This is an unexpected result, a further study of the study basin and HRU settings is underway to shed more light on this issue. Though, a preliminary explanation can be given as follows. The 3rd variable, *REVAPMN*, affects when and to what degree subsurface flow occurs, and therefore indirectly govern the contribution of subsurface flow to the total stream flow of the watershed of interest. These two parameters (*ESCO* and *REVAPMN*) have more influence in evapotranspiration simulated by the model. Since we just analyze flow simulated by the model, these values cause a non-noticeable change in the water yield calculations, and therefore adjustments to these values can be left out.

Interesting is also the breakpoint $RCHRG\_DP = 0$, below which the quality of the SWAT prediction markedly improves, reaching a minimum of 0.8 (MSE_{low}), 16 (MSE_{high}), and 10 (MSE_{total}) respectively. The models also clearly show that the SWAT has more trouble predicting high flows than low flows (as can be seen from the higher MSE_{total} value). Peak flow predictions were generally appreciable for low events and poor for higher flow rates because SWAT uses a modified formulation of the Soil Conservation Service (SCS) curve number (CN) technique [22] to calculate surface runoff. This result is consistent with earlier findings that the SWAT tends to overestimate peak flows [23]. In sum, the model captures the relationships between the different parameters in a smooth and intuitive manner.

7 Conclusion

Global surrogate modeling is a powerful approach to facilitate the analysis of computational expensive simulation codes. However, all too often the designer only tries out a small set of techniques for a particular application.

In this paper the computationally expensive problem of parameter setting in rainfall runoff modeling was investigated (calibrating the SWAT). Therefore a replacement metamodel is generated through the use of sequential modeling and active learning methods requiring little or no knowledge about surrogate modeling. The model type and complexity was determined automatically, data points were selected iteratively, and simulations were transparently scheduled on a shared cluster. The final surrogate model produced by the SUMO Toolbox provided insight into the relationship between the different parameters (including identification of the optima) and can be used to improve the prediction quality in other settings (e.g., as part of a wider Geographic Information System (GIS) tool).

Future work will consist of increasing the number of input parameters, generalizing to other study basins, and further investigating the correlation between the different outputs. In addition the effect of applying a multiobjective optimization algorithm (such as NSGA-II) to drive the hyperparameter selection will also be explored to further improve the model quality.

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