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Uncertainty analysis of a semi-distributed hydrologic model based on a Gaussian Process emulator

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ABSTRACT

Despite various criticisms of GLUE (Generalized Likelihood Uncertainty Estimation), it is still a widely-used uncertainty analysis technique in hydrologic modelling that can give an appreciation of the level and sources of uncertainty. We introduce an augmented GLUE approach based on a Gaussian Process (GP) emulator, involving GP to conduct a Bayesian sensitivity analysis to narrow down the influential factor space, and then performing a standard GLUE uncertainty analysis. This approach is demonstrated for a SWAT (Soil and Water Assessment Tool) application in a watershed in China using a calibration and two validation periods. Results show: 1) the augmented approach led to the screening out of 14–18 unimportant factors, effectively narrowing factor space; 2) compared to the more standard GLUE, it substantially improved the sampling efficiency, and located the optimal factor region at lower computational cost. This approach can be used for other uncertainty analysis techniques in hydrologic and non-hydrologic models.

1. Introduction

Distributed hydrological modelling is a way to understand site-specific hydrology and support operational management, planning and decision making in water resources under various scenarios (e.g., water use, land use change, or climate change) (Arnold et al., 2015). Prior to its application, models generally go through a so-called calibration process. Although the hydrologic and other environmental modeling communities have generally promoted the concept and desirability of uncertainty analysis (UA) (e.g. Beven and Freer, 2001; Todini, 2007; Jakeman et al., 2006), there is still a need for its more widespread general practice, especially for distributed hydrologic modelling (Muleta and Nicklow, 2005; Yen et al., 2015). For example, most applications are still based on reporting a single optimum parameter set (Fang et al., 2015; Liu et al., 2011; Luo et al., 2012). The reasons are multifold; for example, some uncertainty analysis techniques are difficult to apply (e.g. the need for testing statistical assumptions in Bayesian inference; see Yang et al., 2008 for a discussion), or only one parameter set is intended or sought for decision making (Song et al., 2015). For complex environmental models, as occur in distributed hydrologic modelling, a restriction would often be the number of model runs required for the UA, which can be a burden, even with the ongoing advances in information technology (e.g. increase of CPU speed and parallel computation technology).

Various quantitative UA techniques have been developed or applied in the literature (Matott et al., 2009) and there are now many societies and journals that promote UA. In the hydrologic modelling literature, such techniques include Generalized Likelihood Uncertainty Estimation or GLUE for short (Beven and Binley, 1992), SUFI (Abbaspour et al., 2007), first-order approximation (Vrugt and Bouten, 2002), and Bayesian inference (Kuczera and Parent, 1998; Kavetski et al., 2006; Yang et al., 2007). Among all these techniques, GLUE is still by far the most widely applied technique in hydrology (Shen et al., 2012; Stedinger et al., 2008) due to its simplicity and practicality, though it has been criticized for several reasons including its informal statistical basis, sampling inefficiency and flat response surface (Mantovan and Todini, 2006; Yang et al., 2008; Beven and Binley, 2014). On the other hand, it can be argued that GLUE warrants use as a guide at least to appreciating the level of various sources of uncertainty. When applying GLUE, however, one might face a substantial computational burden as

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captured in Beven and Binley (2014; Page 5905) who state "it remains an issue, either because of a model that is particularly slow to run so that it is still not possible to sample sufficient realizations or because of a high number of parameter dimensions". This often arises in spite of suggestions (e.g. McMillan and Clark, 2009) to seek increases in the efficiency of finding behavioral models. It has been noted that the sample efficiency (i.e., number of behavioral sets over number of sampling sets) of some applications can be lower than 10^{-4} (Iorgulescu et al., 2005, 2007; Yang et al., 2008).

Over recent decades, emulators (or in some literature meta-models or surrogate models) have been widely applied as a surrogate to deterministic models, partly to overcome the high computational cost of the latter. But certain types of surrogates like Gaussian Processes can also be used to assess properties of the model response surface (e.g. see Asher et al., 2015 for a review in the groundwater domain). These emulators include polynomial regression (Jones, 2001), multivariate adaptive regression splines (Friedman, 1991), radial basis functions (Dyn et al., 1986), polynomials chaos (Wiener, 1938; Xiu and Karniadakis, 2002) and Gaussian Processes (Kennedy and O'Hagan, 2001; Sacks et al., 1989). Most of these applications (especially in hydrologic modelling) have been for optimization (Emmerich et al., 2006; Jones, 2001) and global sensitivity analysis (Oakley and O'Hagan, 2004; Ratto et al., 2007).

In this paper, we propose an emulation-augmented GLUE, using Gaussian Process (GP) emulation of the original model, to help conduct uncertainty analysis. This GLUE-GP uses global and local sensitivity analysis arising as a natural byproduct of the GP emulation to screen out unimportant parameters and reduce the ranges of more sensitive ones, implemented in the software GEM-SA (www.tonyohagan.co.uk/academic/GEM/), before application of GLUE. The GP also allows improvement in the sampling efficiency and location of the optimal region for GLUE sampling at a much lower computational cost than the standard GLUE. The GLUE-GP method is thus akin to GLUE in the sense that it is an augmentation that applies a GLUE procedure but only to those factors and their ranges as informed by the initial GP emulation and its inherent sensitivity analysis. Thus it is an approximation of GLUE whose differences are numerically investigated here in both calibration and validation modes. This approach is demonstrated on the semi-distributed hydrologic model SWAT (Soil and Water Assessment Tool; Arnold et al., 1998) with an application to the Kaidu River Basin in Xinjiang, China, which is an important water source for human activity and ecological function in the oasis downstream.

The remainder of this paper is structured as follows: section 2 gives a brief introduction to GLUE and the GP emulator, and then focuses on the proposed emulation-based GLUE approach (GLUE-GP) and case study; section 3 introduces the SWAT model and case study area; section 4 presents and discusses results; and finally conclusions are summarized in section 5.

2. Methodology

A large class of hydrologic and environmental models can be formulated as $y = f(\boldsymbol{x})$, where $\boldsymbol{x} = (x_1, x_2, \ldots, x_m)$ is a vector of m factors and y is either scalar or vector model output (e.g., flow rate time series) or objective function (e.g., root mean square error between simulated and observed flows), and the notation x_i^j to indicate the jth realization of the ith factor of $\boldsymbol{x}$. Here, we distinguish factors from model parameters in that a factor could be a model parameter or a modification to a distributed parameter either in a relative way or with a replacement to their initial values (examples are given in Table 1 and section 3.2). Thus we use the terminology factors instead of model parameters for the GP and uncertainty analyses below.

2.1. GLUE

GLUE (Beven and Binley, 1992, 2014) is an uncertainty analysis technique inspired by the regional sensitivity analysis of Hornberger and Spear (1981). In contrast to assuming that there is a single "optimal" factor set for a model, it is based on the concept of "equifinality" in which different "behavioral" factor sets lead to similarly good model results in some sense. It recognizes that most environmental models used for prediction are non-identifiable due largely, but not only, to the over-parameterised structure of the model (see Shin et al., 2015 for an overview of methods to check structural identifiability). Fig. 1(a) shows a typical procedure for uncertainty analysis based on GLUE.

When applying GLUE, one needs to define an objective function $L(.)$ (or "generalized likelihood measure"), and a given threshold value which is used to assess if a sampled factor set is "behavioral" or "non-behavioral" through a comparison: if the corresponding "likelihood measure" is better or worse than the given threshold value. Each behavioral factor is then given a "likelihood weight" according to:

$$w_i = \frac{L(x^i)}{\sum_{k=1}^{N} L(x^k)} \tag{1}$$

where $L(x^i)$ is the objective function value of factor set x^i, and N is the number of behavioral factor sets from N_T total samples. Then the model predictive uncertainty is described as a prediction band from the cumulative distribution of the model output realized from the weighted behavioral factor sets.

Based on these behavioral and non-behavioral factor sets, factor sensitivity can also be studied with Regionalized Sensitivity Analysis (RSA; Spear and Hornberger, 1980) which inspired GLUE but is not generally part of GLUE. The idea of RSA is: if the distributions of a factor in the behavioral and non-behavioral factor sets are dissimilar then this factor is considered influential. In practice, this is performed with the Kolmogorov-Smirnov test to obtain a distance measure (D) which is the maximum distance between the two empirical cumulative distributions (i.e. behavioral and non-behavioral).

2.2. Gaussian Process emulator

The emulator we invoke is the Gaussian Process emulator, although other emulators such as those based on Polynomial Chaos (Wiener, 1938; Xiu and Karniadakis, 2002) have similar advantages, mainly sampling efficiency improvements and global and local sensitivity measures as byproducts of the emulation (largely because such emulators and their response surfaces are continuous functions which can be differentiated). The idea is to construct a simpler and computationally efficient model as a surrogate for the complicated (more physically based) and less computationally efficient model. When applying a GP emulator to a hydrologic model $y = f(\boldsymbol{x})$, it approximates $f(\boldsymbol{x})$ as a Gaussian process (Kennedy and O'Hagan, 2001)

$$\widehat{f}(\boldsymbol{x}) = m(\boldsymbol{x}) + e(\boldsymbol{x}) = h(\boldsymbol{x})^T\boldsymbol{\beta} + e(\boldsymbol{x}) \tag{2}$$

where $\boldsymbol{x}$ *is* a vector of factors, $m(\boldsymbol{x})$ is the mean function, $h(\boldsymbol{x})$ a known regression function, and $e(\boldsymbol{x})$ a zero mean Gaussian process with correlation given by $cov[f(\boldsymbol{x}), f(\boldsymbol{x}')] = \sigma^2 c(\boldsymbol{x}, \boldsymbol{x}')$. In this study $c(\boldsymbol{x}, \boldsymbol{x}')$ is a correlation function between two points $\boldsymbol{x}$ and $\boldsymbol{x}'$ that takes the form $\exp[-(\boldsymbol{x} - \boldsymbol{x}')\boldsymbol{\theta}(\boldsymbol{x} - \boldsymbol{x}')]$.