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An Interval-Deviation Approach for hydrology and water quality model evaluation within an uncertainty framework

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SUMMARY

Uncertainty assessment is becoming one of the main topics in hydrology and water resources. In this study, an Interval-Deviation Approach (IDA) was designed and incorporated into the process of model evaluation. The proposed IDA was validated in a real application of the Soil and Water Assessment Tool (SWAT) and Generalized Likelihood Uncertainty Estimation (GLUE) in the Three Gorges Reservoir Area (TGRA), China. Compared with the traditional point-to-point comparison between measured and predicted data, the main superiority of the IDA is its innovative theory that models should be evaluated by each absolute distance between the paired uncertainty intervals or probability distribution for each measured and predicted data. In addition, the IDA can be used to quantify the possible range of model performance in a real application of the SWAT. This proposed IDA can be useful for error form indicators and models by providing a substitute method to facilitate enhanced evaluation of watershed models within an uncertainty framework.

1. Introduction

Hydrology and water quality (H/WQ) models are essential tools for developing watershed programs, such as Total Maximum Daily Load (TMDL) and the Water Framework Directive (WFD) (Stow and Borsuk, 2003; Panagopoulos et al., 2012). The confidence that we have in these models depends on how well the models match the real system that they are intended to represent (Mediero et al., 2011). However, the meteorological-, geological-, hydrological-, and ecological processes at basin scale are notably complex and are not always well known (Renard et al., 2010; Beven and Alcock, 2012). Faced with such insufficient knowledge and natural randomness, uncertainty becomes an inherent part of watershed modeling (Beven and Alcock, 2012).

Prediction uncertainty is a major concern and has been routinely incorporated as a key part of TMDL plans (Renard et al., 2010). Many researchers have focused on prediction uncertainty, specifically addressing the sources of uncertainty (Shen et al., 2012a), uncertainty propagation (Naranjo et al., 2012), evaluation methods (Zhang et al., 2011), uncertainty expression (Zheng and Keller, 2007) and the control of uncertainty (Beven et al., 2008). Beck (1987) reported that residual uncertainty exists even with the best model structure and input data. Additionally, measurement uncertainty may stem from errors in flow measurements and water quality sample collection (Harmel and King, 2005; Howden et al., 2011). Given the river discharge data, errors from different sources such as river stage measurement or the interpolation of the rating curve, affect the measured data (Di Baldassarre and Montanari, 2009). In a thorough review (Harmel et al., 2006), several potential errors in the H/WQ measured data were compiled, indicating that appreciable inherent errors exist in the measured data even when following strict quality assurance and quality control (QA/QC) guidelines (Beven et al., 2012).

Model evaluation, in terms of calibration and validation, is a critical step in model application (Guinot et al., 2011). Model calibration is the process of estimating model parameters using a pairwise comparison between the predicted and measured data, while the validation process involves running the well-calibrated model to check its performance. In traditional applications, model evaluation is usually conducted by a regression measure, most commonly the point-to-point comparison of predicted and measured data (Westerberg et al., 2011). The multi-objective functions, which usually considered the variety of hydrological events that may occur in a basin, are also used to calibrate models by the

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(predicted) point-to-(measured) point comparison (Kollat et al., 2012; Naranjo et al., 2012). To acknowledge model uncertainties, Beven (2006) proposed a formal structure for using limits of acceptability based on set theory and the idea of equifinality. In this case, the deviation calculations between the predicted and measured data can be estimated within the framework of Generalized Likelihood Uncertainty Estimation (GLUE) or the Bayesian method (Zhang et al., 2009b; Gong et al., 2011). However, it is important to mention that such point-to-point methods, are not always exact because the predicted and measured data, are typically associated with a certain confidence interval (CI) or probability distribution function (PDF) when subject to random variability (Zhang et al., 2009a; Franz and Hogue, 2011). Borga et al. (2006) suggested that more measured data would fall into the corresponding prediction uncertainty intervals. Haan et al. (1995) demonstrated that the amount of overlap between paired simulated interval and measured interval can be a substitute indicator of model performance. Harmel and Smith (2007) further developed this idea into a correction factor (CF) for each deviation calculation (point-to-interval), which is based on the theory that H/WQ models should be evaluated against the measurement uncertainty. However, this factor is sometimes misleading because this factor is determined by the deviation between the predicted data and the nearest boundary of measurement uncertainty interval. In this sense, a larger value of CF means that more predicted data can be found inside the paired measured intervals at the price of increasing the length of the measured intervals. Therefore, this may lead to greater trust in larger uncertainties because they are more likely to overlap than precise point-to-point deviation. This dilemma also exists in other CFs (interval-to-interval) represented by the overlap of paired probability distribution functions (PDF) about each simulated data and measured value (Harmel et al., 2010).

The primary objective of the present study is to develop an Interval-Deviation Approach (IDA) (interval to interval) to facilitate enhanced evaluation of watershed model within an uncertainty framework. The basis of the IDA was the theory that H/WQ models should not be evaluated against the paired data points, which are uncertain, but against the inherent uncertainty intervals. In this sense, each absolute distance (at least between the nearest boundaries and between the farthest boundaries) should be considered for a given uncertainty interval or probability distribution for each measured and predicted datum. The developed IDA was subsequently validated with simulated and measured data collected in the Three Gorges Reservoir Area (TGRA) in China.

2. Materials and methods

2.1. The Interval-Deviation Approach

In previous papers, the degree of uncertainty is expressed by one or more of the followings: (1) a CI, which is derived by ordering all potential values and later identifying the upper and lower thresholds that act as good estimates of the unknown data sets (Shen et al., 2012a); (2) a probable error range (PER), for which each simulated or measured data point should be determined and the error range (presented as ±% deviations from the data point) is estimated from statistical analysis (Harmel et al., 2006); and (3) a PDF, designed for each data set using statistical estimation of the probability distributions, depending on the distributional properties throughout the data sets (Shen et al., 2012b).

It is evident that the traditional error term ($P_i - O_i$) is determined simply as the difference between predicted and measured data points, but this error term does not account for any prediction uncertainty and measurement uncertainty in model evaluation. Instead, the basic idea of the IDA is that the deviation can be calculated by each absolute distance between the paired uncertainty intervals or probability distributions of each simulated value and measured data. Modification 1 is introduced here when only uncertainty boundary is known. Modification 2, which is applied when the probability distribution is known or assumed for each data, produces a more practical estimate of the deviation. In this sense, the paired predicted and measured intervals (CI, PER or PDF) were firstly designed mathematically as:

$$P_i = [P_i^-, P_i^+] = \{x \in R | P_i^- \leqslant x \leqslant P_i^+\} \quad (1)$$

$$O_i = [O_i^-, O_i^+] = \{x \in R | O_i^- \leqslant x \leqslant O_i^+\} \quad (2)$$

where all of the predicted data values, $p_{i1}, p_{i2}, \ldots, p_{ij}, \ldots, p_{in}$, are located in the interval $[P_i^-, P_i^+]$. Similarly, all of the observed data values, $o_{i1}, o_{i2}, \ldots, o_{ik}, \ldots, o_{in}$, are located in the interval $[O_i^-, O_i^+]$. R is the set of real numbers. The error term of each predicted and observed pair (P_i, O_i) is given by $P_i - O_i$.

2.1.1. Methodology 1

Methodology 1 is applied when only the CI or PER are known or assumed, while no PDF can be assumed. Using Methodology 1, the calculation of deviation is related to the distances between the nearest and farthest boundaries of the paired uncertainty intervals. In this study, a CI or a PER is assumed to be a set of real numbers with the property that any value that lies between the uncertainty boundaries is also included in the set. In the first step, the error term $P_i - O_i$ is derived from the distance between the farthest boundaries (d_{imax}) and the distance between the nearest boundaries (d_{imin}) of each paired intervals. As illustrated in Fig. 1, d_{imin} is set equal to 0 if any interval boundaries fall within the paired intervals. Otherwise, d_{imax} and d_{imin} can be determined by the absolute distance between the paired interval boundaries, which are shown numerically in Eqs. (3) and (4).

$$d_{imax} = Max(d(P_i^-, O_i^-), d(P_i^+, O_i^-), d(P_i^-, O_i^+), d(P_i^+, O_i^+)) \quad (3)$$

$$d_{imin} = Min(d(P^-, O^-), d(P^-, O^+), d(P^+, O^-), d(P^+, O^+)) \quad (4)$$

The error term $P_i - O_i$ is then treated as the deviation calculated by the weighted values of d_{imax} and d_{imin}. The calculation of the error term is shown in Eq. (5).

$$P_i - O_i = x_i * d_{imax} + (1 - x_i) * d_{imin} \quad (5)$$

where weight x_i is used in the case of a weighted linear combination of the farthest and nearest absolute distances between the paired intervals. The value of x_i varies from 0 to 1, and a higher value of x_i indicates the probability of d_{imax} increases for a given uncertainty interval. The concept is undeniably sound, but it leaves for further determination the extent of x_i. This is considerable difficult due to the lack of a prior distribution of the paired intervals. For this reason, the weight (x_i) can be set to 0.5 based on the idea that there was equal faith in the farthest and nearest absolute distances.

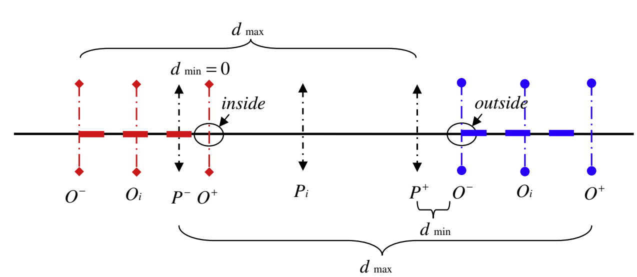

Fig. 1. Graphical representation of the Interval-Deviation Approach to calculate the nearest and farthest distances between the paired intervals.