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Constructing prediction interval for artificial neural network rainfall runoff models based on ensemble simulations

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SUMMARY

This paper presents a method of constructing prediction interval for artificial neural network (ANN) rainfall runoff models during calibration with a consideration of generating ensemble predictions. A two stage optimization procedure is envisaged in this study for construction of prediction interval for the ANN output. In Stage 1, ANN model is trained with genetic algorithm (GA) to obtain optimal set of weights and biases vector. In Stage 2, possible variability of ANN parameters (obtained in Stage 1) is optimized so as to create an ensemble of models with the consideration of minimum residual variance for the ensemble mean, while ensuring a maximum of the measured data to fall within the estimated prediction interval. The width of the prediction interval is also minimized simultaneously. The method is demonstrated using a real world case study of rainfall runoff data for an Indian basin. The method was able to produce ensembles with a prediction interval (average width) of 26.49 m^3/s with 97.17% of the total observed data points lying within the interval in validation. One specific advantage of the method is that when ensemble mean value is considered as a forecast, the peak flows are predicted with improved accuracy by this method compared to traditional single point forecasted ANNs.

1. Introduction

Application of artificial neural network (ANN) technique for predictive purpose has been one of the most existing recent developments in hydrology. Theoretically, ANNs are considered to be universal approximators that have a capability of approximating any nonlinear mapping to an arbitrary degree of accuracy. The computational efficiency of ANNs, without the requirement of a detailed knowledge and description about the relevant physical process, has provided many promising results in the field of hydrology and water resources engineering. This interest has been motivated by the complex nature of hydrological systems (Maier et al., 2010). Despite this popularity, ANNs still suffer from limitations. In addition to the major criticism that ANNs lack transparency (Abrahart et al., 2010), many researchers have mentioned that ANN development is stochastic in nature, and unless carefully designed no identical results can be reproduced on different occasions (Elshorbagy et al., 2010a,b). This is a significant weakness, and therefore it is hard to trust the reliability of ANNs addressing real-world problems. Therefore, a significant research effort is needed to address this deficiency of ANNs (Maier et al., 2010). In fact, there is a belief that point predictions from hydrologic models are of limited value where there is uncertainty in the data or variability in the underlying system. To improve the decision making and operational planning, the modeler should be aware of the uncertainties associated to the point forecasts. A reasonable estimate of prediction interval for the hydrologic variables provides valuable information in water resources problems (Liu and Gupta, 2007).

It is well known that model error is the mismatch between observed and simulated values due to inherent uncertainty in process (Shrestha and Solomatine, 2008). These uncertainties mainly arise from input, parameter and model structure. The input (measured/forecasted precipitation in case of hydrologic models) uncertainty is mainly due to measurement and sampling error. The parametric uncertainty lies in inability to identify unique set of best parameters. The simplification, inadequacy and ambiguity in description of real world process through mathematical equation leads a model structure uncertainty. While all these uncertainties are important, the current study is focusing on the parametric uncertainty and its effect on the output uncertainty.

In the literature, several methods have been proposed for construction of prediction intervals and assessment of the ANN output uncertainty (Khosravi et al., 2011). While they differ in the way of implementation, the methodology applied is generally common: train an ANN through minimization of an error based

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function such as sum of squared errors; and subsequently constructs the prediction interval for the ANN outputs. For instance, the delta technique introduced by Chryssolouris et al. (1996) considers linearizing the ANN model around a set of parameters, and constructing the prediction interval by application of standard asymptotic theory to the linearized model. However this method is based on the assumption that noise is homogenous and normally distributed which may not be true in many real world problems (Ding and He, 2003). The Bayesian technique is another method for construction of prediction intervals (MacKay, 1992). Despite the strength of the supporting theories, the method suffers from massive computational burden, and requires calculation of the Hessian matrix of the cost function for construction of prediction intervals (Papadopoulos et al., 2001). A mean–variance estimation-based method for prediction interval construction has also been proposed by Nix and Weigend (1994). The method uses an ANN to estimate the characteristics of the conditional target distribution. Additive Gaussian noise with non-constant variance is the key assumption of the method for predictive interval construction. However, this method underestimates the variance of data, leading to a low empirical coverage probability, as discussed in Ding and He (2003). Bootstrap is one of the most frequently used techniques in the literature for construction of prediction intervals for ANN forecasts (Srivastav et al., 2007; Tiwari and Chatterjee, 2010). The main advantage of this method is its simplicity and ease of implementation. It does not require calculation of complex derivatives and the Hessian matrix involved in the delta and Bayesian techniques.

The challenge for performing an uncertainty analysis of ANN outputs lies in the fact that the ANNs have large degrees of freedom in their development. Consequently, the hydrologic applications have received little attention in assessing the uncertainty in ANN model predictions, with the exception of a few. Ensemble based prediction is a technique to predict hydrologic variables which requires a detailed information of model structure, parameter, input forcing error for the explicit quantification of uncertainty (Pagano et al., 2013). In case of neural network hydrologic prediction, probably the first attempt was by Dawson et al. (2000) who reported a six member ensemble mean of radial basis function neural network. The ensembles were created by varying the internal transfer function, and the corresponding variation in model output was considered as a measure of uncertainty. Ensemble modeling approach was also explored by Boucher et al. (2010) and Araghinejad et al. (2011). They demonstrated the potential of probabilistic combining of ensemble simulations of ANN models. Kingston et al. (2005) applied Bayesian training method to assess the parametric uncertainty of ANN models, and found that the Bayesian approach produces prediction limits that indicate the level of uncertainty in the predictions. Further the comparison of their results with deterministic ANN showed that Bayesian training of neural network not only improves the quality of prediction, but the prediction interval from the Bayesian network helped in making better decisions when forecasts were made outside the range of the calibration data. Khan and Coulibaly (2006) defined the posterior distribution of network weights through a Gaussian prior distribution and a Gaussian noise model. Their results indicated the predictive distribution of the network outputs by integrating over the posterior distribution with the assumption that posterior of network weights is approximated to Gaussian during prediction. Srivastav et al. (2007) quantified parameter uncertainty through bootstrapping of input examples with deterministic model structure. Sharma and Tiwari (2009) and also Tiwari and Chatterjee (2010) used a similar approach to quantify the variability in ANN predictions to estimate prediction intervals. Han and Kwong (2007) proposed a method to understand the uncertainty in ANN hydrologic models with the heuristic that the distance between the input vector at prediction and all the training data provide a valuable indication on how well the prediction would be. However, their method did not quantify the uncertainty of the model parameters or the predictions. Shrestha and Nestmann (2009) investigated the uncertainty in the case of a stage–discharge relationship by defining fuzzy uncertainty bounds for the relationship curve. Alvisi and Franchini (2011) considered the ANN parameters as fuzzy numbers, and estimated the prediction intervals of stream flow predictions. While most of the above studies have considered parametric uncertainty, there are a few studies which considered the structural uncertainty also. For instance, Zhang et al. (2009) applied Bayesian Neural Network (BNN) to predict the uncertainty and their results showed that BNN based models give reasonable estimate of uncertainty in stream flow simulation. Zhang et al. (2011) proposed a method to quantify the combined effect of input and structural uncertainty.

It is to be noted that there is no clear evidence in literature to show that one method outperforms another in terms of accuracy of estimated prediction interval of model output, and also that each of these methods vary in assumption, principle, complexity and computational cost (Wagener and Gupta, 2005; Khosravi et al., 2011). Since neural network calibrates its parameters based on parallel computing, quantification of uncertainty along with calibration is a difficult task, plausibly due to the complexity in computations. Therefore the quantification of uncertainty generally is carried out after the model calibration. This paper presents a method of constructing prediction interval of the ANN rainfall runoff models during calibration itself with a consideration of generating ensemble of predictions. A two stage optimization procedure is proposed in this study for construction of prediction interval for the ANN. In the first stage of optimization, the optimal weights of an ANN are obtained. In the second stage, optimal variability of these weights are identified that help generate ensembles with minimum residual variance for the ensemble mean, while ensuring a maximum of the measured data to fall within the estimated prediction interval, whose width also is minimized simultaneously.

2. Methodology

2.1. Stage 1: ANN architecture identification and Initial training

In Stage 1 of the proposed method, an ANN model is developed for the process being modeled. While a general procedure for developing ANN is available in many published papers, a brief description of the methodology followed in this study is discussed here. Since the focus of the study is to develop rainfall runoff model, the output from the ANN is considered to be the stream flow. Identification of most significant influencing variables (inputs) that can be used for estimating stream flow is the first step in the ANN hydrologic model development process (Bowden et al., 2004a,b). When *a priori* knowledge about the process being modeled is available, that can be used to specify plausible inputs (Campolo et al., 1999; Thirumalaiah and Deo, 2000). On the other hand, if the process is not clearly understood, often analytical or statistical techniques are employed (Sajikumar and Thandaveswara, 1999; Luk et al., 2000; Silverman and Dracup, 2000; Sudheer et al., 2002). The current study employed a statistical approach suggested by Sudheer et al. (2002) to identify the appropriate input vector. The method consists of statistical analysis of the data series that uses cross-, auto-, and partial-auto correlations among the variables in question. The major disadvantage associated with using correlation measures is that it is only able to detect linear dependence between two variables, while the modeled relationship may be highly nonlinear. Nonetheless, the cross-correlation