**Prediction and Structural Uncertainty Analyses of Artificial Neural Networks Using
Hierarchical Bayesian Model Averaging**

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Abstract

This study adopts a hierarchical Bayesian model averaging (HBMA) method to analyze prediction uncertainty resulted from uncertain components in artificial neural networks (ANNs). The HBMA is an ensemble method for prediction and is used to segregate the sources of model structure uncertainty in ANNs and investigate their variance contributions to total prediction variance. Specific sources of uncertainty considered in ANNs include the uncertainty in neural network weights and biases (model parameters), uncertainty of selecting an activation function for the hidden layer, and uncertainty of selecting a number of hidden layer nodes (model structure). Prediction uncertainties due to uncertain inputs and ANN model parameters are represented by within-model variance. Prediction uncertainties due to uncertain activation function and uncertain number of nodes for the hidden layer are represented by between-model variance. The method is demonstrated through a study that employs ANNs to predict fluoride concentration in the aquifers of the Maku area, Azarbaijan, Iran. The results show that uncertain inputs and ANN model parameters produces the most prediction variance, followed by prediction variances from uncertain number of hidden layer nodes and uncertain activation function.

Keywords: Bayesian model averaging, artificial neural network, uncertainty, ensemble method

1. Introduction

Artificial neural networks (ANNs) are mathematical approximators with strong ability to find the non-linear correlation between input and output data without requiring a comprehensive knowledge about the physical system (Zhang et al., 2009). ANNs have been applied to various hydrologic problems (Govindaraju, 2000a; b; Dawson and Wilby, 2001), for example river flood forecasting (Sudheer et al., 2003; Wei et al., 2012), rainfall forecasting (Hsu et al., 1995; Kumar et al., 2005; Valverde Ramírez et al., 2005), evaporation modeling (Sudheer et al., 2002), groundwater level modeling (Coppola et al., 2005; Daliakopoulos et al., 2005; Nourani et al., 2008a,b; Jha and Sahoo, 2015), and groundwater remediation optimization (Rogers and Dowla, 1994). Despite wide applications of ANNs in the field of hydrology, over-parameterization in weights and biases and consequently overfitting to “in-sample” data is a major limitation of ANNs, which may occur in the process of maximizing likelihood functions or alternatively minimizing fitting errors (Kingston et al., 2008). This may reduce prediction accuracy for “out-sample” data that are not used for training ANNs (Tetko et al., 1995; Maier and Dandy, 2000). In other words, overfitting can reduce the “generalization” ability of ANN models. Generalization is the ability of an ANN model to represent an underlying system for an “out-sample” data that are not used in the training procedure. Therefore, it is crucial to select an ANN structure based on the parsimony principle (Box, 1976; Stone, 1981) to balance fitting errors and the number of unknown parameters. To address this issue, Franses and Draisma, (1997) proposed the use of information criteria to choose the best ANN structure. Information criteria tend to select a simpler ANN structure unless a more complicated structure provides a better understanding of the underlying system. However, Qi and Zhang (2001) empirically showed that the selected ANN based on information criteria does not necessarily have an acceptable performance for

fitting “out-sample” data. They concluded that “to improve generalization performance of neural network models, one may need to go beyond the model selection methods”.

An alternative to the model selection approach is the artificial neural network ensemble (Shu and Burn, 2004). In this approach, outputs from several ANN models, which are trained by the same data, are combined to generate an ensemble output. Several methods for combining the outputs of multiple artificial intelligence models are proposed in the literature (Ahmad and Zhang, 2002; Shu and Burn, 2004), such as the committee machine (CM) (Perrone and Cooper, 1993; Wong et al., 2000; Chen and Lin, 2006; Kadkhodaie-Ilkhchi et al. 2009; Labani et al. 2010), the supervised committee machine (SCM) (Drucker, 1997; Hu and Tsoukalas, 2003; Nadiri et al., 2013), and the Bayesian model averaging (BMA) (Nadiri et al., 2014). Although the committee machine methods are shown to improve the generalization ability of ANNs (Shu and Burn, 2004), they are subjected to two major shortcomings. First, they are not able to quantify the prediction uncertainty. Second, they do not consider the parsimony principle in evaluating the combination of individual ANN models.

ANN prediction uncertainty stems from two main sources: (1) the uncertainty in ANN inputs, weights and biases and (2) the uncertainty in ANN structures. Bayesian neural networks (BNNs) (Bishop, 1995; Neal, 1995; Müller and Insua, 1998) were used to train ANN models and to quantify uncertainties from ANN weights and biases (Kingston et al., 2005; Khan and Coulibaly, 2006) as well as uncertainties from model structures (Zhang et al., 2009). The BNN approach prescribes ANN parameters by relatively broad prior probability distributions. Then, during the calibration (training) period, prior distributions are sampled by Markov chain Monte Carlo (MCMC) (Geyer, 1992) or Metropolis algorithm (Haario et al., 2001) to update to posterior distributions given observation data. Finally, the posterior distributions of ANN

parameters are used to evaluate prediction means and variances. However, the BNN method can be overwhelmed by a high number of ANN parameters. In addition, it is crucial to identify the contribution of individual sources of uncertainty to total prediction uncertainty (Wagener and Gupta, 2005).

In this study, we adopt the hierarchical Bayesian model averaging (HBMA) (Chitsazan and Tsai 2015a; Tsai and Elshall, 2013) to analyze the contribution of individual sources of uncertainty to ANN predictions. Bayesian model averaging (Draper, 1995; Hoeting et al., 1999) is a well-known ensemble approach based on the law of total probability and Bayes' theorem. BMA derives overall prediction mean and variance by averaging all models at once (Nadiri et al. 2014). However, it does not quantify contributions of individual uncertain model elements to total estimated variance. The HBMA extends the Bayesian model averaging method by segregating multiple sources of conceptual model structure uncertainty in a hierarchical order (Chitsazan and Tsai, 2015b). The HBMA derives BMA prediction mean and variance by averaging subset models that are developed by an uncertainty source. By doing so, the HBMA is able to identify the contribution of each source of uncertainty to total prediction variance. This study adopts the HBMA to analyze the structural uncertainty as well as parameter uncertainty in the ANNs. The advantages of the HBMA in comparison to other neural network ensemble methods are investigated via the study of predicting fluoride concentration in aquifers of the Maku area, Azarbaijan, Iran.

2. Methodology

2.1 Artificial Neural Network (ANN)

Artificial Neural Networks (ANNs) have been applied to various large-scale problems, including pattern recognition, classification, parameter estimation and prediction (Anderson and

McNeill, 1992; Ablameyko, 2003). The most widely used ANNs to simulate hydrological systems are the multilayer perceptron (MLP), a three-layer feedforward neural network (Govindaraju, 2000 a,b; Sharma et al., 2003). The MLP consists of an input layer, a hidden layer, and an output layer. Figure 1 shows a schematic of a typical multilayer perceptron ANN structure. This study uses four types of input data (Na^+ , K^+ , Ca^{2+} , HCO_3^-). The processing elements in each layer are called neurons or nodes. The input layer consists of input variables for the network. The output layer sends out predictions (outputs) of the network. The output function of the output layer is a linear function that aggregates the input signals of the output layer. The hidden layers are placed between the input layer and the output layer to transform and deliver signals. A vital part of the hidden layer which has a main role in transferring the network inputs to output is an activation function, which is typically a continuous and bounded nonlinear function such as hyperbolic-tangent-sigmoid (Tansig) or logarithm-sigmoid (Logsig) functions (Cybenko, 1989).

Training algorithms are needed in order to train ANNs to behave similar to the system of interest. Data used for training ANNs are referred to as “in-sample” data. Data that are not used in the training procedure is referred to as “out-sample” data. A brief overview of the MLP, including its mathematical aspects and implementation details, can be found in Govindaraju (2000a). The mathematical expression of a three-layer feedforward ANN for prediction is

$$O_{jk} = f_1 \left(b_j + \sum_i W_{ij} I_{ik} \right) \quad (1)$$

$$O_k = b + \sum_j W_j O_{jk} \quad (2)$$

where f_1 is the activation function for the hidden layer, I_{ik} is the i^{th} input for the k^{th} sample point, O_{jk} is the output of j^{th} node of the hidden layer, W_{ij} and W_j are the weights that control the

strength of connections between layers and b_j and b are the biases that are used to adjust the mean value for the hidden layer and the output layer, respectively. The ANN output O_k is the k^{th} predicted fluoride concentration. In the ANN training step, we use the Levenberg-Marquardt (LM) algorithm (Sahoo and Ray, 2006; Sahoo et al., 2006) as a supervised learning algorithm to estimate the weights (W_{ij} and W_j) and the biases (b_j and b) (Daliakopoulos et al., 2005).

There are two common sources of uncertainty in the three-layer feedforward ANN structure: (1) which activation function should be used for the hidden layer? (2) how many nodes are needed in the hidden layer? This study considers Tansig and Logsig activation functions and two to nine nodes in the hidden layer, combinations of which result in $2 \times 8 = 16$ ANN structures for fluoride concentration prediction.

2.2 Hierarchical Bayesian Model Averaging for Neural Networks

To segregate and prioritize the sources of structural uncertainty in ANNs, this study introduces the Hierarchical Bayesian Model Averaging (HBMA) for prediction and uncertainty analysis. Consider p sources of uncertainty in a hierarchical order. Each uncertainty source may suggest a number of propositions (or alternatives). For example, in this study the uncertainty in choosing an activation function for the hidden layer suggests two propositions: Tansig function and Logsig function. The uncertainty in choosing the number of nodes in the hidden layer suggests eight propositions: from two nodes to nine nodes. The combinations of all considered sources of structural uncertainty form the base models for fluoride concentration prediction.

We segregate and prioritize the sources of uncertainty in a hierarchical order and denote the base models at level p and name this level as base level. Aggregation of base models through the BMA over different propositions under the same source of uncertainty forms BMA models at one level up, named level $p-1$. Aggregation of BMA models at level $p-1$ through the BMA over

different propositions under the same source of uncertainty forms another BMA models at one level up, named level p-2. Aggregating models continues until the final BMA model, named the hierarch model, is obtained at level 0, which is named the hierarch level. As a result, a BMA tree structured by the base models and the BMA models is developed. In the BMA tree, a parent model is a model in a level with respect to its child models immediately one level below.

Using the law of total probability (Yates and Goodman, 1999), given a set of data $\mathbf{D}$ the posterior probability of estimated fluoride concentration F at level n can be obtained as follows (Chitsazan and Tsai, 2015a,b)

$$\begin{aligned} \Pr(F | \mathbf{D}, \mathbf{M}_n) &= E_{\mathbf{M}_{n+1}} \left[\Pr(F | \mathbf{D}, \mathbf{M}_{n+1}) \right] \\ &= \sum_q E \left(\Pr(F | \mathbf{D}, \mathbf{M}_{n+1}^{(q)}) \Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D}, \mathbf{M}_n) \right) \end{aligned} \quad (3)$$

where $E_{\mathbf{M}_{n+1}}$ is the expectation operator over child models $\mathbf{M}_{n+1}^{(q)}$ at level n+1 under their parent model $\mathbf{M}_n$, $\Pr(F | \mathbf{D}, \mathbf{M}_{n+1})$ is the posterior probability of the fluoride concentration prediction F given data $\mathbf{D}$ and base models $\mathbf{M}_{n+1}$ at level n+1, and $\Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D}, \mathbf{M}_n)$ is the conditional posterior probability for model $\mathbf{M}_{n+1}^{(q)}$ under their parent models $\mathbf{M}_n$ given data $\mathbf{D}$. It is important to recognize that $\mathbf{M}_{n+1}^{(q)}$ is a child model of $\mathbf{M}_n$ in $\Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D}, \mathbf{M}_n)$.

When $n=p$, $\mathbf{M}_p$ is the set of the ANN models, the base models. Using equation (3) as a recursive equation, the posterior probability of estimated fluoride concentration prediction at level n is

$$\Pr(F | \mathbf{D}, \mathbf{M}_n) = E_{\mathbf{M}_{n+1}} E_{\mathbf{M}_{n+2}} \cdots E_{\mathbf{M}_p} \left[\Pr(F | \mathbf{D}, \mathbf{M}_p) \right] \quad (4)$$

where $E_{\mathbf{M}_{n+1}} E_{\mathbf{M}_{n+2}} \cdots E_{\mathbf{M}_p}$ represents a series of averaging operations over the models from level p up to level n+1.

According to the law of total expectation, the expectation of fluoride concentration prediction at level n is

$$E(F | \mathbf{D}, \mathbf{M}_n) = E_{\mathbf{M}_{n+1}} [E(F | \mathbf{D}, \mathbf{M}_{n+1})], \quad (5)$$

where $E(F | \mathbf{D}, \mathbf{M}_{n+1})$ is the expected value of prediction for given data $\mathbf{D}$ and models at level $n+1$. According to the law of total variance, the variance of fluoride concentration prediction at level $n < p$ is

$$\text{Var}(F | \mathbf{D}, \mathbf{M}_n) = E_{\mathbf{M}_{n+1}} [\text{Var}(F | \mathbf{D}, \mathbf{M}_{n+1})] + \text{Var}_{\mathbf{M}_{n+1}} [E(F | \mathbf{D}, \mathbf{M}_{n+1})], \quad (6)$$

where $E_{\mathbf{M}_{n+1}} [\text{Var}(F | \mathbf{D}, \mathbf{M}_{n+1})]$ is the within-model variance of fluoride concentration prediction using models at level $n+1$ calculated by

$$E_{\mathbf{M}_{n+1}} [\text{Var}(F | \mathbf{D}, \mathbf{M}_{n+1})] = \sum_q \text{Var}(F | \mathbf{D}, \mathbf{M}_{n+1}^{(q)}) \Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D}, \mathbf{M}_n). \quad (7)$$

$\text{Var}_{\mathbf{M}_{n+1}} [E(F | \mathbf{D}, \mathbf{M}_{n+1})]$ is the between-model variance using models at level $n+1$ calculated by

$$\begin{aligned} \text{Var}_{\mathbf{M}_{n+1}} [E(F | \mathbf{D}, \mathbf{M}_{n+1})] &= E_{\mathbf{M}_{n+1}} \left[\left(E(F | \mathbf{D}, \mathbf{M}_{n+1}) - E(F | \mathbf{D}, \mathbf{M}_n) \right)^2 \right] \\ &= \sum_q \left[E(F | \mathbf{D}, \mathbf{M}_{n+1}^{(q)}) - E(F | \mathbf{D}, \mathbf{M}_n) \right]^2 \Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D}, \mathbf{M}_n) \end{aligned} \quad (8)$$

$\text{Var}_{\mathbf{M}_{n+1}}$ is the variance operator with respect to models $\mathbf{M}_{n+1}$.

The conditional posterior probability for a child model $\mathbf{M}_{n+1}^{(q)}$ at level $n+1$ under its parent model $\mathbf{M}_n$ at level n is (Chitsazan and Tsai, 2015a,b)

$$\Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D}, \mathbf{M}_n) = \frac{\Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D})}{\Pr(\mathbf{M}_n | \mathbf{D})}. \quad (9)$$

188 where $\Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D})$ is the posterior model probability for model $\mathbf{M}_{n+1}^{(q)}$. Since $\mathbf{M}_{n+1}^{(q)}$ is a child
189 model of its parent model $\mathbf{M}_n$, $\Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D})$ also represents the joint probability of $\mathbf{M}_{n+1}^{(q)}$ and
190 $\mathbf{M}_n$. $\Pr(\mathbf{M}_n | \mathbf{D})$ is the posterior model probability for model $\mathbf{M}_n$. $\Pr(\mathbf{M}_n | \mathbf{D})$ is calculated by
191 $\Pr(\mathbf{M}_n | \mathbf{D}) = \sum_q \Pr(\mathbf{M}_{n+1}^{(q)} | \mathbf{D})$. (10)

192 2.3 Between Model Uncertainty Analysis for Two Sources of Model Structure Uncertainty

193 This study considers two sources of model structure uncertainty in two level as between
194 model uncertainty. The first level source of uncertainty is from the choice of an activation
195 function for the hidden layer. A BMA model at level 1 is denoted as $\mathbf{M}_1^{(p)}$. The second level
196 considers the source of uncertainty from the choice of the number of hidden layer nodes. Under
197 an activation function, an ANN model at level 2 (base level) is denoted as $\mathbf{M}_2^{(q)}$, which is a child
198 model of $\mathbf{M}_1^{(p)}$. We denote the set of ANN models as $\mathbf{M}_2^{(q)} = \{ANN_{p,q}\}$.

199 Based on Bayes' theorem (Shafer, 1976), the posterior model probability of an ANN
200 model given an activation function and a number of hidden layer nodes is

$$201 \Pr(ANN_{p,q} | \mathbf{D}) = \Pr(\mathbf{M}_2^{(q)} | \mathbf{D}) = \frac{\Pr(\mathbf{D} | \mathbf{M}_1^{(p)}, \mathbf{M}_2^{(q)}) \times \Pr(\mathbf{M}_2^{(q)} | \mathbf{M}_1^{(p)}) \times \Pr(\mathbf{M}_1^{(p)})}{\sum_p \sum_q \Pr(\mathbf{D} | \mathbf{M}_1^{(p)}, \mathbf{M}_2^{(q)}) \times \Pr(\mathbf{M}_2^{(q)} | \mathbf{M}_1^{(p)}) \times \Pr(\mathbf{M}_1^{(p)})} \quad (11)$$

202 where $\Pr(\mathbf{D} | \mathbf{M}_1^{(p)}, \mathbf{M}_2^{(q)})$ is the marginal likelihood function of a base model given an
203 activation function and a number of hidden layer nodes, $\Pr(\mathbf{M}_2^{(q)} | \mathbf{M}_1^{(p)})$ is the conditional prior
204 probability of a base model that uses a number of hidden layer nodes given an activation
205 function. And $\Pr(\mathbf{M}_1^{(p)})$ is the prior probability of a BMA model that uses an activation
206 function.

From equation (10), the posterior model probability of a BMA model at level 1 that uses an activation function and all proposed numbers of hidden layer nodes is

$$\Pr(\mathbf{M}_1 | \mathbf{D}) = \sum_q \Pr(\mathbf{M}_2^{(q)} | \mathbf{D}) \quad (12)$$

The conditional posterior probability of an ANN model that uses a proposed number of hidden layer nodes given an activation function is

$$\Pr(\mathbf{M}_2^{(q)} | \mathbf{M}_1, \mathbf{D}) = \frac{\Pr(\mathbf{M}_2^{(q)} | \mathbf{D})}{\Pr(\mathbf{M}_1 | \mathbf{D})} \quad (13)$$

Using the Laplace approximation (Tierney and Kadane, 1986), the marginal likelihood function $\Pr(\mathbf{D} | \mathbf{M}_2^{(q)})$ can be approximated by the Bayesian information criterion (BIC) (Li and Tsai, 2009) as

$$\Pr(\mathbf{D} | \mathbf{M}_1^{(p)}, \mathbf{M}_2^{(q)}) \approx \exp \left[-\frac{1}{2} \text{BIC}_{p,q} \right] \quad (14)$$

where

$$\text{BIC}_{p,q} = Q_{p,q}(\boldsymbol{\beta}_{p,q}) + n \ln 2\pi + m_{p,q} \ln n \quad (15)$$

where $Q_{p,q}$ is the sum of the weighted square errors, $\boldsymbol{\beta}_{p,q}$ is the maximum-likelihood estimated parameters (weights and biases) for an ANN model. n is the size of “in-sample” data, and $m_{p,q}$ is the size of $\boldsymbol{\beta}_{p,q}$.

This study assumes equal prior probability for $\Pr(\mathbf{M}_1^{(p)})$ and equal conditional prior probability for $\Pr(\mathbf{M}_2^{(q)} | \mathbf{M}_1^{(p)})$. By substituting equation (14) to equation (11) and using the variance window (Tsai and Li, 2008a,b; Singh et al., 2010) to enlarge the acceptance window size, the ANN posterior model probabilities can be obtained as follows

$$\Pr(ANN_{p,q} | \mathbf{D}) = \Pr(\mathbf{M}_2^{(q)} | \mathbf{D}) = \frac{\exp\left[-\frac{1}{2}\alpha\Delta\text{BIC}_{p,q}\right]}{\sum_p \sum_q \exp\left[-\frac{1}{2}\alpha\Delta\text{BIC}_{p,q}\right]} \quad (16)$$

where $\Delta\text{BIC}_{p,q} = \text{BIC}_{p,q} - \text{BIC}_{\min}$. $\text{BIC}_{\min}$ is the smallest BIC value among the ANN models. α is the scaling. The readers are referred to Tsai and Li (2008a) for choosing an α value.

2.4 Fluoride Concentration Prediction and Uncertainty by HBMA

Using equation (4), fluoride concentration prediction by the hierarch model, which uses all of the propositions of the activation functions and the numbers of hidden layers, is

$$E(F | \mathbf{D}) = E_{\mathbf{M}_1} E_{\mathbf{M}_2} [E(F | \mathbf{D}, \mathbf{M}_2)] \quad (17)$$

where $E(F | \mathbf{D}, \mathbf{M}_2)$ is the mean fluoride concentration predicted by an ANN model at the base level. The mean fluoride concentration predicted by BMA at level 1 is

$$E(F | \mathbf{D}, \mathbf{M}_1^{(p)}) = E_{\mathbf{M}_2} [E(F | \mathbf{D}, \mathbf{M}_2)] \quad (18)$$

The total variance of the fluoride prediction using the hierarch model is

$$\text{Var}(F | \mathbf{D}) = E_{\mathbf{M}_1} E_{\mathbf{M}_2} \text{Var}(F | \mathbf{D}, \mathbf{M}_2) + E_{\mathbf{M}_1} \text{Var}_{\mathbf{M}_2} E(F | \mathbf{D}, \mathbf{M}_2) + \text{Var}_{\mathbf{M}_1} E_{\mathbf{M}_2} E(F | \mathbf{D}, \mathbf{M}_2) \quad (19)$$

where $\text{Var}(F | \mathbf{D}, \mathbf{M}_2)$ is the variance of predicted fluoride concentration by an ANN model at the base level.

The total variance consists of three variance terms. The first term in equation (19) is the within-model variance of the prediction, which stems from the uncertain inputs and uncertain parameters. The second and the third terms in equation (19) stem from the uncertainty in the number of hidden layer nodes and the uncertainty in the hidden layer activation function, respectively.

The variance of fluoride concentration prediction using a BMA model at level 1 is

$$\text{Var}(F | \mathbf{D}, \mathbf{M}_1) = \mathbb{E}_{\mathbf{M}_2} [\text{Var}(F | \mathbf{D}, \mathbf{M}_2)] + \text{Var}_{\mathbf{M}_2} [\mathbb{E}(F | \mathbf{D}, \mathbf{M}_2)] \quad (20)$$

Equations (19)-(20) enable us to explicitly evaluate the contribution of individual sources of uncertainty in the total prediction variance.

2.5 Within-Model Variance Derivation

Given an ANN structure, the within-model variance of prediction $\text{Var}(F | \mathbf{D}, \mathbf{M}_2)$ can be estimated through Monte Carlo (MC) simulation as long as the variance of the ANN inputs and ANN parameters are known. In this study, the variance of the input data at unsampled location is estimated by the kriging variance that stems from using the kriging algorithm to interpolate the input data to unsampled location. To quantify the variance of ANN parameters, we follow Yeh and Yoon (1976, 1981) that the covariance matrix of estimated model parameters $\boldsymbol{\beta}_{p,q}$ is

$$\text{Cov}_F(\boldsymbol{\beta}_{p,q}) = \hat{\sigma}_F^2 (\mathbf{J}_F^T \mathbf{J}_F)^{-1} \quad (21)$$

where $\hat{\sigma}_F^2$ is the estimated variance of fluoride concentration, which is

$$\hat{\sigma}_F^2 = \frac{\sum_{k=1}^n [F_k(\text{ANN}_{p,q}, \boldsymbol{\beta}_{p,q}) - F_k^{obs}]^2}{n - m_{p,q}} \quad (22)$$

where $F_k(\text{ANN}_{p,q}, \boldsymbol{\beta}_{p,q})$ is the predicted fluoride concentration by $\text{ANN}_{p,q}$ using the model parameters $\boldsymbol{\beta}_{p,q}$ and F_k^{obs} is the measured fluoride concentration. $\mathbf{J}_F = \partial F / \partial \hat{\boldsymbol{\beta}}_{p,q}$ is the Jacobian matrix of the fluoride concentration to model parameters, which is

$$\mathbf{J}_F = \begin{bmatrix} \frac{\partial F}{\partial W_{i,j}} & \frac{\partial F}{\partial b_j} & \frac{\partial F}{\partial W_j} & \frac{\partial F}{\partial b} \end{bmatrix} \quad (23)$$

According to equations (1) and (2), the derivatives of fluoride concentration F_k to the ANN weights $W_{i,j}$ and biases b_j are

$$\frac{\partial F_k}{\partial W_{ij}} = \frac{\partial f_1(L_{jk})}{\partial L_{jk}} W_j I_{ik} \quad (24)$$

$$\frac{\partial F_k}{\partial b_j} = \frac{\partial f_1(L_{jk})}{\partial L_{jk}} W_j \quad (25)$$

where $L_{jk} = b_j + \sum_i W_{ij} I_{ik}$. The derivatives of fluoride concentration F_k to the ANN weights W_j and biases b are

$$\frac{\partial F_k}{\partial W_j} = f_1'(L_{jk}) \quad (26)$$

$$\frac{\partial F_k}{\partial b} = 1 \quad (27)$$

Using the covariance matrix of estimated parameters in equation (23) and the kriging variances of the input data, Monte Carlo simulation was conducted to determine the within-model variance of the fluoride concentration for each ANN model.

3. Study Area

The Maku area shown in Figure 2 is located in the West Azarbaijan province, northwest of Iran. The total study area is about 1595 Km², where up to 397 Km² is covered by basaltic lavas bounded on the west by Turkey and on the east by Aras River. The main residential areas in the region are Maku and Poldasht. The climate in the area is cold and arid with annual-mean temperature 11.2 °C (1985-2012). The annual-mean precipitation is about 286.6 mm (1992-2012). The maximum and minimum precipitations occur in May and September, respectively. Total evaporation is 1500 mm per year, three times more than annual precipitations (Asghari Moghaddam and Fijani, 2008). The main rivers in the study area are Sari Su and Zangmar, which flow from west to east. The main source of water is groundwater to meet the demands for different purposes such as drinking, agriculture and industry. Groundwater discharges at 12

large-scale springs ranging from 20 to 4000 Ls⁻¹ and at several withdrawal wells (Asghari Moghaddam and Fijani 2009).

The study area is covered by two major geological formations: (a) the basaltic area, where the aquifer mainly consists of basaltic rocks and covered by alluvium (basalt-alluvium aquifer), and (b) the non-basaltic area, where the aquifer consists of limestones of Qom formation (Oligo-Miocene age) and massive limestone and dolomites of Ruteh formation (Permian). Other formations, such as shale, marl and conglomerate, are present in small areas. Prior studies (Asghari Moghaddam and Fijani 2008) showed that ion concentration, electrical conductivity (EC), total dissolved solid (TDS) and alkalinity in the basaltic aquifer are higher than those in the non-basaltic aquifer and in the mixing zones where non-basaltic water and basaltic water mix (Asghari Moghaddam and Fijani 2009).

4. Data Analysis

To estimate the fluoride concentration in the study area, 129 water samples were collected over water sources (wells, springs, ganats, etc.) in a five-year period 2004-2008. The sample locations are shown in Figure 2. The samples were analyzed in a hydrogeological laboratory in the University of Tabriz using the standard procedure of APHA (1998) for fluoride and other 11 hydrochemical parameters. The observed precision of ion analysis was within the range of acceptability ($\pm 5\%$) used in most of chemical analysis. After the correlation matrix and factor analyses (Nadiri et al., 2013), four highly correlated parameters (Na^+ , K^+ , HCO_3^- , and Ca^{2+}) to fluoride concentration are chosen as input data for the ANN models. 110 samples were used in the training step (“in-sample” data set) and 19 samples were used in the test step (“out-sample” data set). The training and test data sets have similar statistical characteristics. Different

types of the input data were scaled to have a range between 0 and 1 and the samples were selected to cover the entire area.

5. Results and Discussion

5.1 Model Selection

For simplicity, we use the activation function name followed by the number of hidden layer nodes to denote an ANN model. For example “Tansig-6” represents an ANN model that uses the Tansig activation function and six nodes in the hidden layer. Figure 3 shows the BIC values and posterior model probabilities for the 16 trained ANNs. From left to right, the first eight super columns represent the ANNs using Logsig activation function. The second eight super columns represent ANNs using Tansig activation function. Each super column in Figure 3 consists of two sub-columns showing the weighted sum of squared errors ($Q_{p,q}$) and the BIC complexity term ($N \ln 2\pi + m_p \ln N$). By increasing the number of nodes in the hidden layer, the complexity of the ANNs increases, which decreases the Q_p value, but risks the increase in BIC value. For example, given the Tansig activation function, BIC value decreases by increasing the number of the hidden layer nodes from two to six. However, BIC starts to increase for more than six nodes because the reduction in Q_p is not sufficient to compensate the increase of the complexity term. From the model selection perspective, the best neural network is Tansig-6 with the minimum $BIC = 447.33$. The coefficient of determination (R^2) and the root mean squared errors (RMSE) of Tansig-6 model are $R^2 = 0.9608$ and $RMSE = 0.0413$ for the “in-sample” data and $R^2 = 0.4946$ and $RMSE = 0.0582$ for the “out-sample” data, respectively. This result indicates that although BIC is a sound criterion for model selection, the best model does not perform well for the “out-sample” data. In the following discussion, we apply the HBMA to address this problem.

5.2 HBMA Results

Figure 3 shows the posterior model probabilities for the ANN models using Occam's window ($\alpha=1$) and variance window ($\alpha=0.404, 0.202$ and 0.101) with 5% significant level and two, three and four standard deviations of errors. Occam's window only accepts the best model "Tansig-6" and the second best model "Logsig-4" with 92.56% and 7.44% posterior model probabilities, respectively. Tsai and Li, (2008a, b) noted that when the number of observation data increases, Occam's window tends to single out the best model. By introducing the scaling factor that considers the factor of data size, variance window includes more models as shown in Figure 3 for analysis.

Figure 4 shows the comparisons of the "out-sample" data against the mean fluoride concentration predicted by the hierarch model given Occam's window and three variance window sizes. Using Occam's window, R^2 and RMSE are 0.5593 and 0.0543, respectively, which performs better than Tansig-6 model. However, the improvement is smaller than those using variance windows because Occam's window only accepts the best two ANN models. The $4-\sigma$ variance window size has the highest $R^2=0.7862$ and lowest RMSE=0.0378. This result supports the Ahmad and Zhang, (2002) conclusion that combining the neural networks improves the robustness of predictions by sharing and averaging the prediction errors. In this study, we choose 4σ variance window with 5% significance level for further analysis.

Figure 5 shows the BMA tree of conditional posterior model probabilities and posterior model probabilities. Tansig-6 and Logsig-4 at level 2 are the best ANN model and the second best ANN model with 24.20% and 18.67% posterior model probabilities, respectively. Tansig and Logsig models at level 1 have similar conditional model posterior probability close to 50%, which indicates that both activation functions are equally important in producing the outcome.

Given the Logsig activation function, the ANN model with four nodes in the hidden layer has the highest conditional posterior model probability 36.51% followed by the model with three nodes in the hidden layer with 28.69% posterior model probability. However, given the Tansig activation function, the ANN models with six and seven nodes in the hidden layer are the best and second best models with 49.53% and 18.68% posterior model probability, respectively. This result indicates that the optimal number of hidden layer nodes for an ANN model depends on the hidden layer activation function.

5.3 Comparison between Ensemble Methods

In this section, we compare the performance of the best neural network (Tansig-6), the hierarch model, the committee machines (CM) (Perrone and Cooper, 1993; Wong et al., 2000; Chen and Lin, 2006; Kadkhodaie-Ilkhchi et al. 2009; Labani et al. 2010), and the supervised committee machines (SCM) (Drucker, 1997; Hu and Tsoukalas, 2003; Nadiri et al., 2013) for fluoride concentration prediction. Table 1 summarizes the formulation of the compared ANN ensemble methods. The CM outputs are the simple averaged or the weighted averaged of the predictions of individual ANNs. The SCM outputs are the nonlinear combination of the predictions of individual ANNs, provided by a supervised ANN model. In other words, SCM receives the predictions of individual ANNs as input, and provides new predictions with reduced fitting error to the “in-sample” data set.

Table 2 lists the maximum error, RMSE and the R^2 of the estimated fluoride concentrations for the “in-sample” and “out-sample” data sets. All ensemble methods show less errors and better fitting than the best model Tansig-6. This demonstrates the potential risk of using a single ANN model and the importance of using multiple models for prediction. Ensemble

methods significantly reduce the maximum error by averaging the errors from different neural networks.

For the “in-sample” data set, the supervised committee machines has the best fitting error, followed by the weighted averaging committee machines, the hierarch model, and the simple averaging committee machine. However, the supervised committee machines and the weighted averaging committee machines performed poor to the “out-sample” data set because both methods do not consider the complexity of the ANN models in combining the predictions of ANN models. The hierarch model has the best fitting to the “out-sample” data set. Also, the simple averaging committee machine performs better than SCM and CM for the “out-sample” data set. This draws an important remark that methods with less fitting errors for the “in-sample” data set do not necessarily have better performance for the “out-sample” data set. The parsimony principle should be taken into account to sensibly determine the combination of ANN predictions.

Moreover, using the weighted averaging committee machine, the ANNs with less than six nodes in the hidden layer are virtually ignored. However, the posterior model probabilities in Figure 5 suggest models with less than six nodes in the hidden layer can be important. The result supports the HBMA method since the posterior model probabilities are more meaningful than either the optimized model weights or equal model weights in the committee machines.

5.4 Fluoride Estimation Variances

Figure 6 shows the prediction variances for the “out-sample” data set. Each super-column consists of three sub-columns from bottom to top showing the variances from uncertainty in ANN weights and biases (within-model variance), the variances from uncertainty in the number

of hidden layer nodes and the variances from uncertainty in the hidden layer activation function. The sum of the second and third sub-columns shows the between-model variance.

To calculate the within-model variance of each ANN model, we used the equations (21)-(27) to calculate the variance of the neural network weights and biases. Then, realizations of the weights and biases are generated by Monte-Carlo simulation and are used in the neural network to generate ensemble variance of fluoride concentration.

We use the result in Figure 6 to calculate the variance contributions of individual sources of uncertainty to the total prediction variance. The within-model variance contributes from 98.24% to 54.09% to the total variances and is the most important source of uncertainty. It indicates that reducing uncertainty in the ANN parameters is more important than ANN structures. The hidden layer node uncertainty contributes from 43.19% to 1.74% and the activation function uncertainty contributes 18.03% to 0.01% to the total variances. The low variance contribution in the activation function shows that the neural networks with different activation functions can have similar performance. In other words, given an “in-sample” data set, for different activation functions, neural networks adjust their parameters in a way that lead to similar performance. The total between model variance contributes from 45.90% to 1.76%, respectively. This result indicates that although the within-model variances are more important the between-model variances are also significant and cannot be ignored.

Figure 7 shows, using the best neural network (Tansig-6), three out of the 19 “out-sample” fluoride measurements has higher than one standard deviation estimation error. However, using the hierarch model, all of 19 measurements have less than one standard deviation error. The reason is that the best neural network underestimates the prediction variances by ignoring the between-model variances.

5.5 Spatial Fluoride Prediction and Prediction Variances in Maku Area

Figure 8(a) shows the estimated mean fluoride concentration map for the Maku area by the hierarch model. The fluoride concentration is high in the south area between the Maku and Poldasht rivers, where the aquifer is mainly consist of basaltic rocks and covered by alluvium (basalt-alluvium aquifer). This result shows a significant correlation between the basaltic formation and the presence of fluoride in the aquifer system. Figure 8(b) shows the standard deviation map of the estimated fluoride concentration that stems from the kriging variance of the input data, the variance of the ANN model parameters and the uncertainty of ANN model structures. It is observed that the estimation standard deviations are less in the basaltic area. This observation shows that different ANN models predict similar high fluoride concentration in the basaltic area.

6. Conclusion

This study introduces the hierarchical Bayesian model averaging (HBMA) to combine the predictions of multiple artificial neural networks (ANNs) and assess the uncertainty of the predictions. The HBMA is able to segregate the variances from different sources in order to explicitly evaluate the contribution of each source to the total uncertainty. The HBMA prediction results are found better than using a single ANN model.

This study shows that combining the ANN predictions can reduce the prediction errors by averaging the errors of individual models. The results also illustrate that the ensemble methods with less fitting errors for the “in-sample” data set do not necessarily have better performance for the “out-sample” data set. This study found that the BMA outperforms the committee machines

because BMA considers the parsimony principle in determining the posterior model probabilities.

The prediction variances are also quantified by using the HBMA approach. It was found that the high predicted fluoride concentration in the basaltic area is attributed to small variance, which shows strong correlation between the basaltic formations and the presence of fluoride in the groundwater system. In addition, by segregating the sources of uncertainty HBMA can calculate the contribution of each sources of uncertainty in the total prediction variance. The results show that the variances from ANN uncertain inputs and parameters are the most important prediction variances followed by the prediction variances from uncertain number of hidden layer nodes and uncertain activation function. The contribution of between-model variance in the total prediction variance is smaller than the within-model variances. However, they are in the same order of magnitude; therefore, ignoring the between-model variances might lead to underestimating the prediction variances.

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613 **Table Captions:**

614 Table 1: ANN ensemble methods for prediction

615 Table 2: Maximum error and the coefficient of determination (R^2) for “in-sample” and “out-
616 sample” data sets, using the Best ANN (Tansig-6) and four ANN combination methods.

Figure Captions:

Figure 1: A schematic of a typical multilayer perceptron ANN structure.

Figure 2: Map of the Maku area. The x and y coordinates are the UTM (meter) zone 83.

Figure 3: BIC, $Q_{p,q}$ and model weights using Occam's window and variance window using 18 ANN models.

Figure 4: Comparison between different variance window sizes in predicting "out-sample" fluoride concentrations: (a) Occam's window ($\alpha = 1.0$), (b) 1σ variance window with ($\alpha = 0.404$), (c) 2σ variance window ($\alpha = 0.202$) and (d) 4σ variance window with ($\alpha = 0.101$).

Figure 5: BMA tree of posterior model probabilities and conditional posterior model probabilities.

Figure 6: Fluoride estimation variances for the "out-sample" data set. The variances from bottom to top are from uncertainty in ANN weights and biases, from uncertainty in the number of hidden layer nodes and from uncertainty in the hidden layer activation function.

Figure 7: One standard deviation error of the "out-sample" data set for (a) the best ANN (Tansig-6) and (b) the hierarch model.

Figure 8: (a) The estimated mean fluoride concentration map and (b) the standard deviation map of the estimated fluoride concentration by the hierarch model.

Figure 1

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Figure 4

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Figure 8

652 Table 1: ANN ensemble methods for prediction

Ensemble method	Ensemble prediction equation	Ensemble weights	References
HBMA-NN	Equation (17)	Equation (16)	This study
CM (simple averaging)	$F = \sum_{i=1}^N W_i \times F_i$	$W_1 = \dots = W_N = \frac{1}{N}$	(Perrone and Cooper, 1993; Wong et al., 2000)
CM (weighted averaging)	$F = \sum_{i=1}^N W_i \times F_i$	$W_1, W_2, \dots, W_N$ are optimized to provide the best fit to the “in-sample” data set.	(Chen and Lin, 2006; Kadkhodaie-Ilkhchi et al., 2009; Labani et al., 2010)
SCM	$F = b + \sum_j W_j \times f_1 \left(b_j + \sum_{i=1}^N W_{ij} F_i \right)$	b, b_j, W_j and W_{ij} are optimized by a supervised ANN to provide the best fit to the “in-sample” data set.	(Drucker, 1997; Hu and Tsoukalas, 2003; Nadiri et al., 2013)

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655 Table 2: Maximum error and the coefficient of determination (R^2) for “in-sample” and “out-
656 sample” data sets, using the Best ANN (Tansig-6) and four ANN combination methods.

Model	“In-sample”			“Out-sample”		
	Max Error	RMSE	R^2	Max Error	RMSE	R^2
Tansig-6	0.0596	0.0413	0.9608	0.1326	0.0582	0.4946
Hierarch	0.0370	0.0349	0.9720	0.0968	0.0378	0.7862
CM (simple averaging)	0.0472	0.0390	0.9650	0.0983	0.0391	0.7656
CM (weighted averaging)	0.0247	0.0200	0.9908	0.1179	0.0525	0.5885
SCM	0.0237	0.018	0.9926	0.1007	0.0511	0.6094

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