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Artificial Neural Network Application on Estimation of Aquifer Transmissivity

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Abstract

The present study focuses on the unexplored area of application of artificial neural network in groundwater hydrology. Three models, each based on artificial neural networks, are applied for prediction of zonal transmissivity. These techniques can be considered as black box models that can predict output values for given range of input values after establishing an acceptable relation which is obtained by training the system. The study is based on coupling of Finite Element Method (FEM) - Artificial Neural Network (ANN) model, which serve as forward (FEM) and inverse (ANN) models. An inverse technique using ANN is considered for estimating parameters of groundwater system. A synthetic problem is examined for two different scenarios, the first one involving the sink and/or sources terms and the second, without these. Inverse model is applied to estimate transmissivity of various zones (64 data pairs involving nodal head and node coordinates) of aquifer domain. The performance evaluation criteria are shown to have good agreement between true transmissivity and estimated transmissivity, both at training and testing stages.

Keywords: Aquifer Parameter; Feed Forward Back Propagation; Radial Basis Function; Recurrent Artificial Neural Network; Inverse Modeling; Finite Element Method;

1. Introduction

Groundwater resource management is a highly complex issue covering a wide spectrum of activities in the field of assessment, planning, designing, operation and maintenance. Efficient management of groundwater system depends upon many activities such as budget, time, type of modeling and availability data resource. Groundwater modeling primarily depends on adequate knowledge of system hydrogeologic parameters such as transmissivity, hydraulic conductivity, storativity, specific yield and aquifer recharge. These parameters can be determined by experimental and field studies but the entire process is time consuming, very complex and financially demanding. Parameter estimation of aquifer systems is a dynamic process, due to the fact that the state of any hydrological system keeps changing with time. Moreover, scientific techniques involved to evaluate such systems are evolving continuously.

To build a model for a real groundwater system, it is necessary to solve both the forward and inverse problems. So far we have been only dealing with the forward, i.e. simulation problem. In the

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forward problem, the unknown heads are determined by solving the groundwater equation for either steady-state or transient state by assuming that the parameter values, control variables and boundary conditions are known. On the other side an inverse model can find optimal values for the parameters that produce the closest fit between the observed and the simulated aquifer state variables in the flow region. Inverse modeling is applied to estimate the hydraulic conductivity, transmissivity, storage coefficient, specific yield, porosity, and aquifer recharge in various sub regions of a system with adequate reliability.

Stallman (1956) used direct inverse technique to estimate the transmissivity however the technique suffered problems due to solution instability. In the past straightforward trial and error method was used for parameter estimation by selecting different sets of parameter values for the model and the computed model outputs (keidser and Rosbjerg, 1991). Later, extensive research was conducted to study the problem of parameter estimation for groundwater flow models that resulted in the development of number of techniques which employ search methods to find the parameter values that minimize the difference between the observed and the calculated hydraulic head values (Mc Laughlin and Townley, 1996).

During the past four decades, iterative statistical solutions and recursive filtering techniques have been applied as inverse models to calculate transmissivity values for given hydraulic heads. Transmissivity and storage coefficient was estimated using an iterative quadratic programming technique in a heterogeneous porous medium (Yeh 1975), however the method was not able to integrate the known aquifer properties. Cooley (1977, 1982) considered the parameter estimation problem as a nonlinear regression problem and the statistical solutions were based on least squares (Cooley, 1982) or maximum likelihood (Carrera and Neuman, 1986). Ferraresi et al. (1996) used the Kalman filter for a solution to the inverse problem in groundwater hydrology and the technique falls under the class of Bayesian estimators.

Now a day's artificial neural networks have been successfully used to directly map nonlinear complex relations (Flood and Kartam, 1994 a, b).The inversion process thorough an iterative process to estimate missing parameters (Hwang and Chan 1990; Kindermann and Linden 1990). Artificial Neural Network (ANN) has also been used in the field of hydrology research, such as rainfall-runoff modeling, precipitation forecasting and groundwater modeling since the beginning of last decades (ASCE 2000; Maier and Dandy, 2000). Very few works have been done on parameter estimation using ANN (Aziz and Wong, 1992; Balkhair, 2002). Shigidi and Garcia (2003) estimated missing transmissivity value of a cell in confined aquifer using Feed Forward Back Propagation as a inverse model for know head values and the head values were calculated using MODFLOW as a forward model.

Ajmera and Rastogi (2007) demonstrated the importance and compared different training algorithms for aquifer parameter estimation using Feed Forward Back Propagation (FFBP), without source/sink terms. To our knowledge, as yet, no works have been reported in the literature that addresses the estimation of aquifer parameter based on Radial Basis Function (RBF) and Recurrent Artificial Neural Network (RANN). In this paper, an attempt has been made to show the application of different types of neural networks (FFBP, RBF, and RANN) for parameter estimation of an aquifer and the results were compared using different performance evaluation criteria (expand these R, E, and RMSE) for two different scenarios, one with source/sink terms and another without source/sink terms. The present study differs from the previous works reviewed here in that it different methods of parameter estimation in confined aquifer using ANN modeling.

2. The Objectives of the Present Study are

- To develop a flow simulation model based on Galerkin's finite element approach.
- To develop an inverse model for aquifer parameter estimation by coupling FEM with ANN.
- To estimate the optimal transmissivity of a confined aquifer in flow domain by using ANN.

3. Artificial Neural Networks

An artificial neural network consists of a number of interconnected processing element neurons, which are logically arranged in two or more layers and interact with each other through weighted connections. The number of neurons in each layer and the number of layers in the network depend on the nature of the problem. There is no unique guiding theory for the proper selection of the number of neurons and the number of layers. The scalar weights determine the nature and strength of the influence between the interconnected neurons. Each neuron is connected to all the neurons in the next layer. The neural network consists of: 1) an input layer, where data are presented to the network, and 2) an output layer that holds the response of the network to the input. Additional intermediate layers, also termed as hidden layers, enable these networks to represent and compute complicated associations between inputs and outputs. The structure of a typical neural network is shown in Fig.1

3.1 Mathematical operation of a network

The training algorithm of back propagation involves four stages.

Stage 1: Initialization of weights

Step 1. Initialize weight (between 0.5 to -0.5)

Step 2. While stopping condition is false, do step 3-10

Step 3. For each training pair do step 4-9

Stage 2: Feed Forward

Step 4. Each input node receives the input signal x_i (i = 1, 2…, p) and transmits this signal to all nodes in the next layer above i.e. hidden nodes,

Step 5. Each hidden node (h_j, j = 1,…, q) sums its weighted input signals

$$h_{wsj} = b_j + \sum_{i=1}^{p} x_i w_{ij} \tag{1}$$

applying activation function

$$h_j = f_h\left(h_{wsj}\right) \tag{2}$$

and sends this to all nodes in the layer above i.e. output nodes.

Step 6. Each output node (y_k, k=1, 2…., r) sums its weight input signals

$$y_{wsk} = b_k + \sum_{j=1}^{q} h_j w_{jk} \tag{3}$$

and applies its activation function to calculate the output signals.

$$y_k = f_o\left(y_{wsk}\right) \tag{4}$$

Stage 3: Back Propagation of Errors

Step 7. Each output node (y_k, k = 1, 2…, r) receives a target pattern corresponding to an input pattern. Error information term is calculated as

$$\delta_k = \left(t_k - y_k\right) f_o\left(y_{wsk}\right) \tag{5}$$

Step 8. Each hidden node (h_j, j = 1, 2…, q) sums its delta inputs from nodes in the layer above

$$\delta_{dsj} = \sum_{k=1}^{r} \delta_j w_{jk} \tag{6}$$

The error information term is calculated as

$$\delta_j = \delta_{dsj} f_h\left(h_{wsj}\right) \tag{7}$$

Stage 4: Update of Weights and Biases

Step 9. Each output node (y_k, k = 1, 2…, r) updates its bias and weights (j = 1, 2…, p)

The weight correction term is given by

$$\Delta w_{jk} = \alpha \delta_k h_j \tag{8}$$

and the bias correction term is given by

$$\Delta b_k = \alpha \delta_k \tag{9}$$

Therefore, $w_{jk}\left(new\right) = w_{jk}\left(old\right) + \Delta w_{jk}$, $\quad b_k\left(new\right) = b_k\left(old\right) + \Delta b_k$ (10)

Each hidden unit (h_j, j = 1, 2…, q) updates its bias and weights (i = 1, 2…, p)

The weight correction term

$$\Delta w_{ij} = \alpha \delta_j x_i \tag{11}$$

The bias correction term

$$\Delta w_{oj} = \alpha \delta_j \tag{12}$$

Therefore, $w_{ij}(new) = w_{ij}(old) + \Delta w_{ij}$, $b_j(new) = b_j(old) + \Delta b_j$ (13)

Step 10. Test the stopping condition.

The stopping condition may be the minimization of the errors, goal and numbers of epochs.

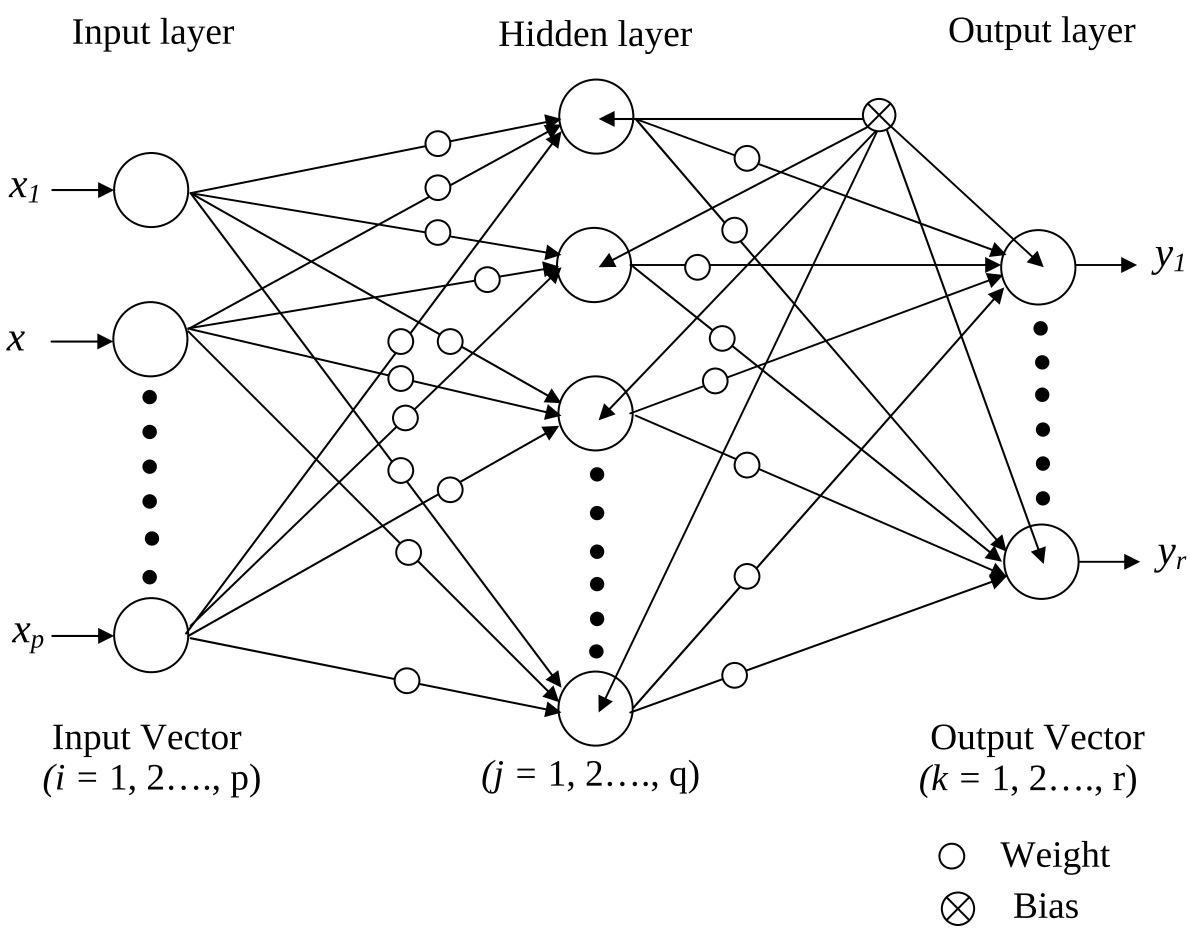

Figure 1 A typical three layer feed forward neural network

3.2 Radial Basis Function (RBF)

Radial Basis Function network is considered a good candidate for approximation problems because of its faster learning capability compared with other feed forward networks. In traditional RBF networks, the Gaussian function and the least squares (Chen et. al., 1991) criterion are selected as the activation function of network and the objective function, respectively. A network adjusts parameters of each node iteratively by minimizing the least squares criterion according to gradient descent algorithm. Since a neural network can accomplish a highly nonlinear mapping from input space to output space.

RBF networks are nonlinear hybrid networks typically containing a single hidden layer of processing elements. This layer uses Gaussian transfer functions, rather than the standard sigmoidal functions employed by FFBP. The centers and widths of the Gaussians are set by unsupervised learning rules, and supervised learning is applied to the output layer. These networks tend to learn much faster than FFBP.

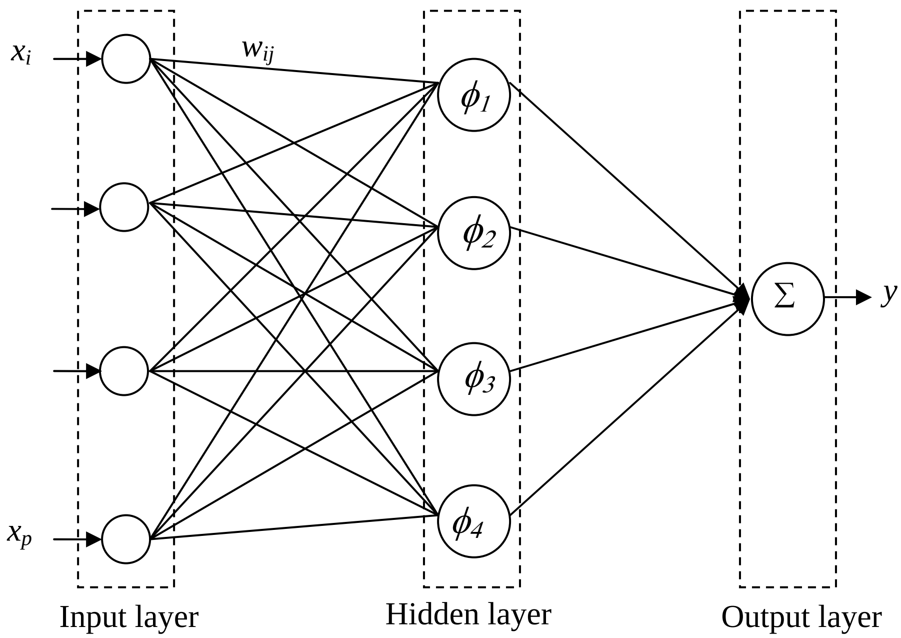

Figure 2 A typical radial basis function network

The number of Gaussians is entered using the Cluster Centers field. It is very difficult to suggest an appropriate number of Gaussians, because it is problem dependent. We know that the number of patterns in the training set affects the number of centers (more patterns imply more Gaussians), but this is mediated by the dispersion of the clusters. If the data is very well clustered, then few Gaussians are needed. On the other hand, if the data is scattered, many more Gaussians are required for good performance. Figure 2 shows a typical radial basis function network which consists of four input nodes, a hidden layer of four nodes and one output node. The output of RBF model is computed by following Eq. (14).

$$y = \sum_{i=1}^{p} w_{ij}\phi_j \left\| x - c_i \right\| + b_j \tag{14}$$

Where w_{ij} = Weight value between i^{th} input node to j^{th} hidden node, b_j = Bias value on j^{th} hidden node, $\phi_j\|x-c_i\|$ indicates a radial basis function which is normally a Gaussian having expression:

$$\phi\|x-c_i\| = -\exp\left[-\sum_{i=1}^{p}\frac{\|x_i-c_i\|^2}{2\sigma_i^2}\right] \tag{15}$$

3.3 Recurrent Artificial Neural Network (RANN)

Recurrent artificial neural networks have been successfully applied to variety of spatial and temporal modeling such as stream flow prediction (Hus et. al., 1995) and groundwater level forecasting (Daliakopoulos et. al., 2004). In RANN, one adds cycles to the feed-forward network structure to produce ANN with a sort of memory. Jordan (1986) proposes a form of RANN in which the network's output at time t is fed into a set of "context" layer. These units, in turn, provide data to hidden units along with that provided by the input units at time t + 1. The recurrent network provides an implicit memory of its previous states, and allows it to model temporal sequences of arbitrary length.

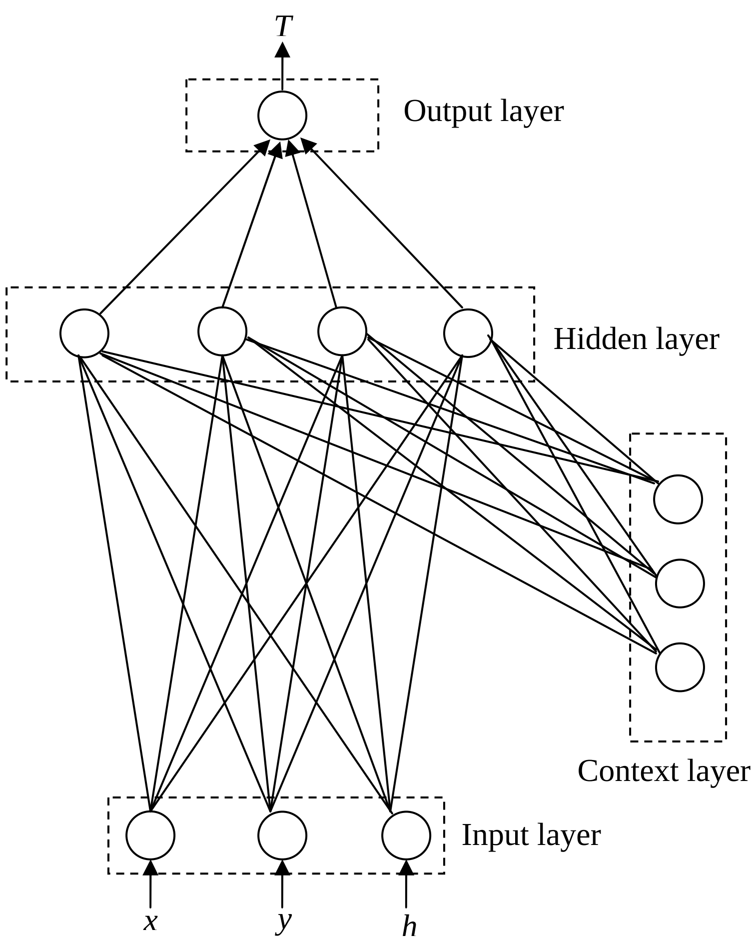

Figure 3 A typical recurrent neural network

Elman (1990) suggests a modification to this approach in which the context units are fed the output of the network's hidden units, rather than the network output. Intuitively, this provides the network with more detailed information about its previous internal states and therefore forces the hidden units to map both the external stimulus and the networks own internal structure at time t−1.The context layer is added to the structure, which retains information between observations. At each timestep, new inputs are fed into the RANN. The previous contents of the hidden layer are passed into the context layer. These are then fed back into the hidden layer in the next time step. Similar backpropagation algorithm has been applied in the RANN. Figure 3 shows a typical recurrent network consisting of three input nodes, a hidden layer with four nodes, one output node and a context layer interconnected with each other.

4. Problem Description

In this study, the developed models are applied to a hypothetical rectangular confined aquifer as shown in fig.4, having an area of 16 sq. km. The flow region is discretized into 128 linear triangular elements involving 81 nodes. This region is bounded by two impervious (Neuman boundary condition) and two prescribed head (Dirichlet boundary condition) boundaries. The heads of northern and southern boundaries are 110 m and 100 m respectively. The aquifer is assumed to have 64 zones of different transmissivity values varying within the range from 200 to 1000 m^2/d. Three wells W_1 (node 21), W_2 (node 52), and W_3 (node 57) pumping at a rate of 2000 m^3/d, 3000 m^3/d and 5000 m^3/d, respectively, are considered within the flow domain. A storativity value of 0.001 is considered for the present aquifer.

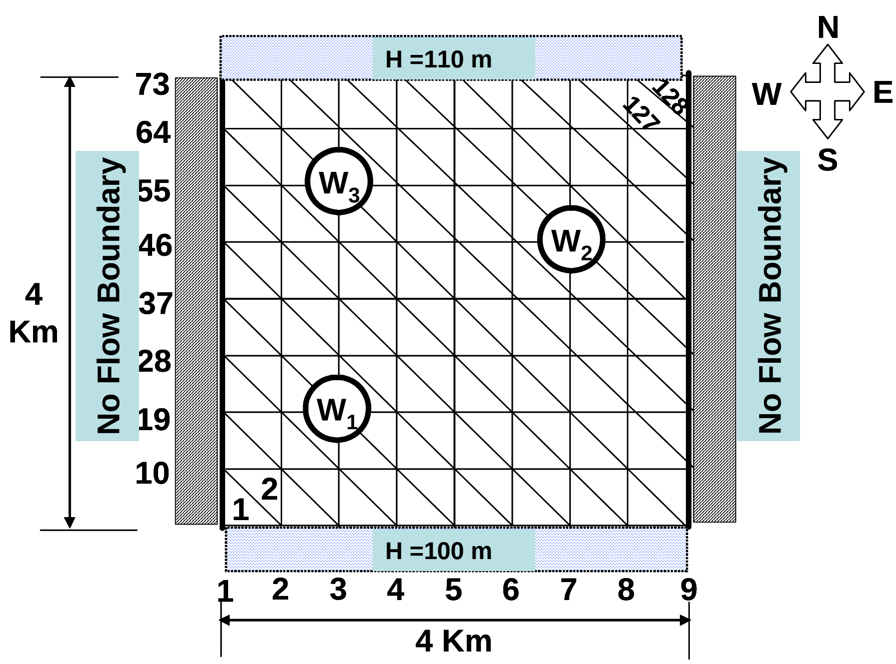

Figure 4 Aquifer domain (No. of nodes: 81, No. of element: 128)

4.1 Governing Flow Equation

The governing equation describing the flow in a two dimensional heterogeneous confined aquifer is given by

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right)=Q+S\frac{\partial h}{\partial t} \qquad (16)$$

Subject to the following boundary conditions

North Boundary: $h(x,y,t)$ = Know head = 110 m

South Boundary: $h(x,y,t)$ = Know head = 100 m

East and West boundaries are impervious (17)

Where, h is piezometric head (m), T is transmissivity (m^2/d), S is storage coefficient, Q is a source or sink function ($-Q$: source and $+Q$: sink) ($m^3/d/m^2$), x, y are the horizontal space variables (m), t is time (d),

The Galerkin's finite element method with linear triangular basis function is used for estimating the hydraulic heads within the aquifer domain for the known distribution of transmissivity. Implicit FDM scheme is applied for the head time derivative. The approximate solution of hydraulic head is expressed in the following Eq.18 which are solved by Gauss Seidel iterative technique.

$$\left\{[G]+\frac{1}{\Delta t}[P]\right\}\left\{h_I^{t+\Delta t}\right\}=\frac{1}{\Delta t}[P]\left\{h_I^{t}\right\}+\left\{F_I\right\} \qquad (18)$$

Where [G] is conductance matrix consisting of transmissivity terms, [P] is storage matrix consisting storativity terms, Δt is the time step size, $[F_I]$ is the nodal recharge or discharge vector, $h_I^{t+\Delta t}$ is the unknown heads vector at time $t+\Delta t$ and h_I^t is the known heads vector at time t.

5. Methodology

In the present study the hydraulic head values at each nodes (h) and the location of the nodes (x, y) are considered as input parameters for finding the unknown parameter the transmissivity (T_E). Initial values of transmissivity (T_A) at nodes are assumed and used in the finite element method (Forward model) in order to find the value of hydraulic head at that node. The hydraulic head values were used in the artificial neural networks (Inverse model) to estimate the value of transmissivity (T_E). For a given study area the detailed methodology for coupling of finite element method and inverse model is given in the flow chart mentioned below (Fig. 5).

The study is based on coupling of forward model and inverse model. In general terms, the parameter estimation process consists of identifying a model that would reverse a complex forward relation. The forward relation between a measurement vector h and an unknown parameter vector T_A can be expressed as

$$h = F\left(T_A\right) + e \qquad (19)$$

Where, *F* is the forward operator that maps T_A to *h,* and e is the measurement error vector. It can be suggested that a generalized inverse model that maps the parameter vector T_A, given the measurement vector *h,* does exist and can be identified (Fig.5). The parameter estimation process can thus be viewed as a process of identifying a universal inverse operator U such that

$$T_E = U(h) = U\left[F\left(T_A\right) + e\right] \qquad (20)$$

The objective of the universal inverse operator is to obtain unknown optimal parameters that are consistent with prior measurements of flow parameter and best reproduce, through the flow equations, the measured heads. In this case, the hydraulic head values are being reproduced through the relevant groundwater flow equation.

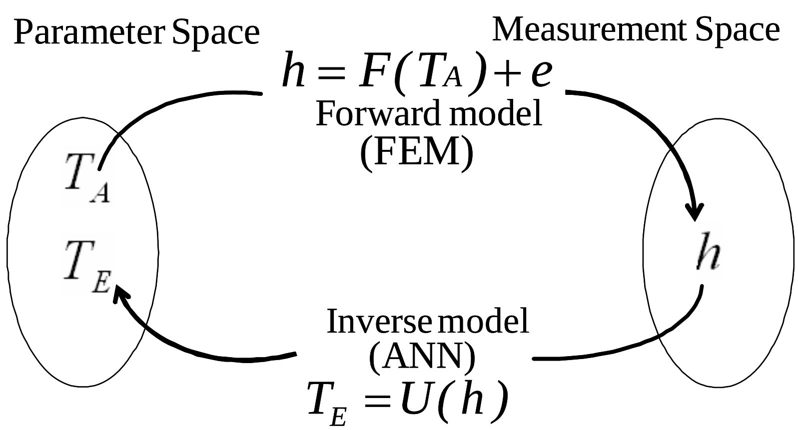

Figure 5 Flowchart of coupled model

6. Performance Evaluation Criteria

The performance of a model can be evaluated in terms of several criteria. The various criteria used in performance evaluation of the hydrological models are given below.

Root Mean Square Error (RMSE): This is determined by calculating the deviations of points from their true position, summing up the measurements, and then taking the square root of the sum.

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(T_{Ai} - T_{Ei}\right)^2} \qquad (21)$$

Coefficient of Efficiency (E): This coefficient is originally proposed by Nash and Sutcliffe (1970). It is analogous to the coefficient of determination in linear regression but not identical.

It is given by
$$E = 1 - \frac{\sum_{i=1}^{N} \left| T_{Ai} - T_{Ei} \right|}{\sum_{i=1}^{N} \left| T_{Ai} - \bar{T}_A \right|} \tag{22}$$

Coefficient of Correlation (R): The coefficient of correlation, normally denoted by R, is a measure of the strength of the linear relationship developed by a particular model. The value of the coefficient of correlation can be computed using the following equation

$$R = \sqrt{\frac{\sum_{i=1}^{N} \left(T_{Ai} - \bar{T}_A \right)^2 - \sum_{i=1}^{N} \left(T_{Ai} - T_{Ei} \right)^2}{\sum_{i=1}^{N} \left(T_{Ai} - \bar{T}_A \right)^2}} \tag{23}$$

A value of R close to 1.0 represents a good model performance while value close to 0.0 represents a poor model performance

$$\bar{T}_A = \frac{1}{N} \sum_{i=1}^{N} T_{Ai} \tag{24}$$

Where, T_{Ai} is the true transmissivity or observed transmissivity of aquifer cell, T_{Ei} is the estimated transmissivity of aquifer cell (by ANN) and $\bar{T}_A$ is the mean of observed transmissivity of aquifer system.

7. Results and Discussion

As the field hydraulic head values are not available, the heads are first generated by solving the direct problem by finite element analysis (Coding in C language) for the known system parameters for a synthetic aquifer. The inverse problem is solved by artificial neural network and the transmissivity parameters are estimated (Coding in Matlab 7.04).

7.1 Development of Artificial Neural Network Architecture

Determining the ANN architecture is the most important part and is determined by trial and error process. The process entails determining the number of input neurons, the number of output neurons, the network's transfer functions, and the error function which monitors the network's performance, the number of hidden layers and the number of neurons in the hidden layers. The numbers of input and output neurons are decided by the nature of the problem. In the present problem, two different scenarios have been considered for all models. For scenario-1, three inputs are considered such as x and y coordinates of the nodal point and the hydraulic head at that node without taking into consideration the sink or source term.

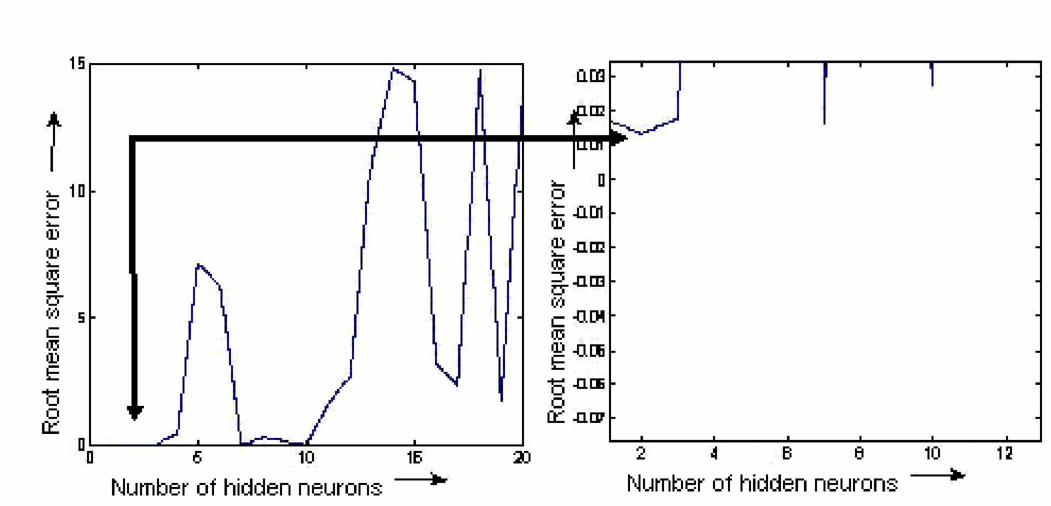

Figure 6 Number of hidden neurons v/s RMSE

Similarly for scenario-2, four inputs are given such as x and y coordinates of the node, hydraulic head and the sink/ source term.Only one hidden layer has been considered based on the recommendation of Goh (1995). The number of neurons in the hidden layer is varied from 1 to 20. Optimum number of hidden neurons in the hidden layer has been calculated using plot curve between numbers of hidden neurons and mean square root error as shows in the Fig.6. Three nodes in hidden layer show minimum error in the Fig.6.

For present study, FFBP (3x2x1) architecture is selected in the model. The logsig transfer function is applied in the hidden layer and the purelin transfer function is applied in the output layer. Fifty nodal pair values are used for training purpose which results the optimal weights values and bias values that are used for testing purpose. Remaining thirty-one nodal outputs are estimated and the percentage errors with respect to the true output are calculated. Table 1 shows following training parameter values are selected in the ANN code.

Table 1 List of Training Parameter

Learning Parameter	Values
Momentum coefficient	0.7
Learning rata	0.5
Delta	0.001
Maximum epoch	5000
Goal (training tolerance)	0.0000055
Minimum grad	1e-15

Figure 7 shows the comparison of true transmissivity and estimated transmissivity and the scatter plot made by the FFBP-scenario-1 network. In this figure all the data lies on exact fit line. This is confirmed by values of the error measures, namely, the correlation coefficient(R) the root mean square error (RMSE), and the correlation of efficiency (E).

It may be noted that each one of these error criterion has usefulness and limitations and hence they should be viewed together while drawing any inference based on their magnitudes. The linear correlation coefficient is a widely accepted measure of the degree of linear association between the target (true) and the network outcome (estimated) but the extreme values heavily affect it. The root mean square error is specially suited for iterative algorithms and is a better measure for high values; however for assessing the fit at moderate values within the range of the given output. The coefficient of efficiency is not very sensitive to systematic model over and under prediction.

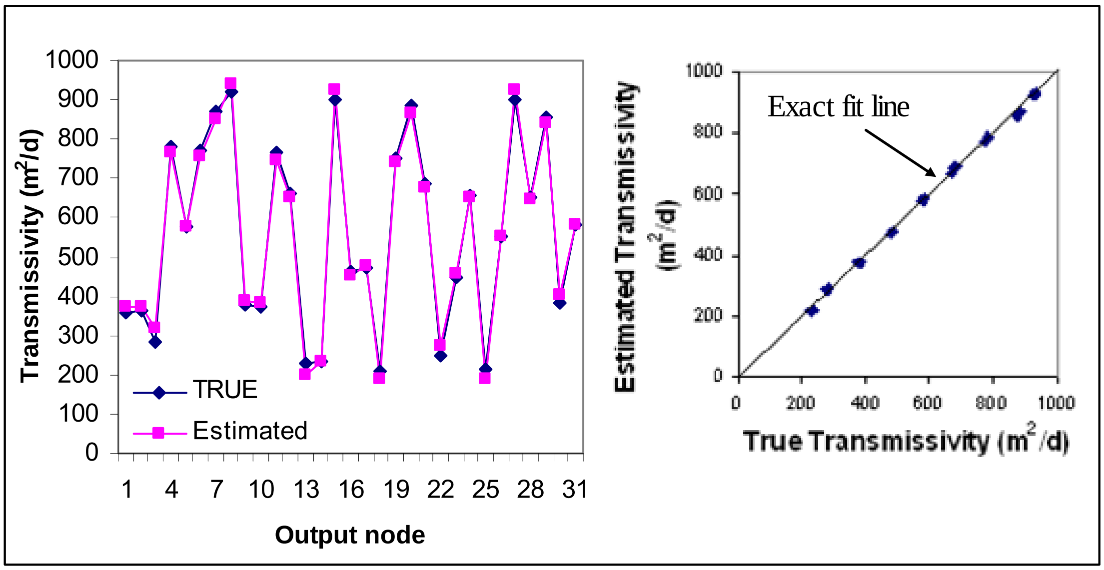

Figure 7 Time series and scatter plot true v/s estimated transmissivity for FFBP-Scenario-1

The magnitude of R and E for the FFBP-secnario-1 - based predictions (Fig. 7) are high as 0.9996 and 0.9720 respectively while the same of RMSE is low as 0.0137, indicating satisfactory working of this scheme.

Table 2 shows performance evaluation criteria for all models. The magnitude of R, and E are very high ranges from 0.9996 to 0.9511, and 0.9720 to 0.8693, respectively, while the same of RMSE are very low ranging from 0.0137 m^2/d to 1.7583 m^2/d, indicates satisfactory working of all models. FFBP-scenario-1 gives relatively better results when compared to other models.

Table 2 Performance evaluation criteria for models

Model	Scenario	R	E	RMSE(m^2/d)
FFBP	Scenario-1	0.9996	0.9720	0.0137
	Scenario-2	0.9973	0.9365	0.0203
RBF	Scenario-1	0.9942	0.9341	0.0232
	Scenario-2	0.9631	0.8845	1.3552
RANN	Scenario-1	0.9653	0.8867	1.2965
	Scenario-2	0.9511	0.8693	1.7583

8. Conclusions and Summary

The present study is based on two models, which are the forward model (finite element method) and the inverse model (artificial neural network). The results obtained for FEM are used as observed hydraulic heads, which are noise free data. It is used as an input in the inverse model (ANN). Errors between the true and estimated transmissivity values are found to be very small, hence it can be said that models are working satisfactorily.

A hypothetical study is used to explore the performance of the proposed methodology. The main reason why a hypothetical study is preferred to a real case study is that, the application of ANN for inverse modeling is at developmental stage and the parameters that are sought in the parameter estimation process are known for a hypothetical study case Therefore a meaningful comparison between estimated and true parameter can be made to suggest the adequacy of ANN for real system application. The hypothetical case thus allows for a better evaluation of the assessment of the technique used to estimate the missing parameter.

The basic problem that arises in solving the inverse problem is how to overcome or avoid the ill-posedness of the inverse solutions. The fundamental way out is to gain sufficient observations, both in quality and quantity. It is also important to incorporate all existing geological and hydrological information into the inverse solution procedure.

The performance evaluation criteria demonstrate that FFBP-scenario-1 gives better results as compared to other models. The present work suggests that ANN can be used after appropriate modification for real groundwater system simulation.

Nomenclature

x_i = Input node (i = 1, 2….., p)

h_j = Hidden node (j = 1, 2….., q)

y_k = Output node (k = 1, 2….., r)

b_j = Bias value on j^{th} hidden node

b_k = Bias value on k^{th} output node

w_{ij} = Weight value between i^{th} input node to j^{th} hidden node

w_{jk} = Weight value between j^{th} hidden node to k^{th} output node

h_{wsj} = Weighted sums at j^{th} hidden node

y_{wsk} = Weighted sums at k^{th} output node

h_j = Output after activation function applied at j^{th} hidden node (hidden ouput)

y_k = Output after activation function applied at k^{th} output node (final output)

f_h = Activation function at hidden layer

f_o = Activation function at output layer

t_k = Target output at k^{th} output node

δ_{dsj} = Delta sums at j^{th} hidden node

δ_j = Error at j^{th} hidden node

δ_k = Error at k^{th} output node

α = Learning rate

Δw_{ij} = Weight correction between i^{th} input node to j^{th} hidden node

Δw_{jk} = Weight correction between j^{th} hidden node to k^{th} output node

Δb_j = Bias correction at j^{th} hidden node

Δb_j = Bias correction at k^{th} output node

h = Piezometric head (m),

T = Transmissivity (m/d),

S = Storage coefficient,

Q = a source or sink function (-Q: source and +Q: sink) ($m^3/d/m^2$),

x, y = Horizontal space variables (m),

$h_I^{t+\Delta t}$ = Unknown heads (m),

h^t = Known heads (m),

t = Time (d),

e = Measurement error,

T_A = Assumed transmissivity (m^2/d),

T_E = Estimated transmissivity (m^2/d),

w = Weight value,

b = Bias value,

U = Universal inverse operator,

R = Coefficient of Correlation,

R^2 = Coefficient of Determination,

E = Coefficient of Efficiency,

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