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Estimating the Saturated Hydraulic Conductivity of Granular Material, Using Artificial Neural Network, Based on Grain Size Distribution Curve

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Abstract

The spatial distribution of saturated hydraulic conductivity based on data measured or observed at well locations is necessary for the numerical simulation of various ground water flow and transport problems. An Artificial Neural Network (ANN) model for estimating of hydraulic conductivity of a saturated granular porous medium from easily measured grain size distribution curve was developed and tested. Five types of porous media are considered in this work: loamy sand, sand, sandy-loam, sand-clay-loam, and silt-clay-loam family. The application of artificial neural network technology for estimating of saturated hydraulic conductivity from grain size distribution curve has been investigated. It has been found that reasonable estimates of this parameter can be obtained with the help of a network that uses the percent finer of the aquifer material as the input neurons, and the logarithm of the hydraulic conductivity value as the output neuron. A better estimate is obtained with a model that takes into account the logarithm of sigmoid function in hidden layer as a transform function. The artificial neural network models are found to give better estimates of saturated hydraulic conductivity of the individual group of soil as input neuron rather than all type of soil groups as input neuron for training step. For the loamy sand soils, the prediction of hydraulic conductivity was the best estimator. A comparison between the measured values of hydraulic conductivity of an unconfined Aquifer in Zahedan by pumping test and predicted value from their grain size distribution curve using the artificial neural network model shows a reasonable estimate of this parameter when using the model which trained by loamy sand data.

Keywords: Hydraulic conductivity; Artificial neural network; Grain size distribution curve

Introduction

It is evident from Darcy experiment that saturated hydraulic conductivity is a function of properties of both the porous medium and the fluid flowing through it. Based on this relationship, during the past century, numerous investigators have studied the correlation between hydraulic conductivity or permeability and

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grain-size distribution of saturated materials to generate practical formulas for the estimation of these quantities. These formulas are useful especially during the initial stages of many aquifers studies, such as designing aquifer pump tests and estimation of some other quantities, if measured hydraulic conductivities under field conditions are not available. However, grain-size distribution data can be available in a relatively cheaper and faster manner.

Particle size is an important parameter in numerous civil, environmental, and petroleum engineering applications. In ground-water flow, the size of individual particles comprising the soil affects the soils pore size distribution and, hence, the important flow characteristics such as hydraulic conductivity and head loss. In addition to affecting the pore size distribution, particle size determines the total surface area available for sorption and other surface reactions affecting the fate and transport of subsurface contaminants. For filters used in water and waste-water treatment, particle size determines the total surface area and pore geometry for solids removal by straining, sedimentation, interception, and diffusion. Additionally, petroleum geologists are concerned with the effect of pore size characteristics on the ability to pump petroleum from an aquifer.

This research is a comparison between neural network model estimates of hydraulic conductivity of granular materials for various groups of soils.

Artificial neural network (ANN) is a relatively new technology based on the processes of the biological brain and has many human-like qualities (Kohonen, 1989). Since a neural computer learns from data, it does not need to be programmed with fixed rules or equations. It provides a radically different way of producing rapid solutions to complex problems. It has the ability to turn data into internally held relationships which can be analyzed and viewed later. The neural approach solves problems in a uniquely different way. Neural computers learn the key relationships in the data and then generalize from those relationships, building their own "rules". These can then automatically produce predictions or estimates based upon their experience.

Artificial neural network (ANN) technology is a relatively recently developed method, where the pattern recognition capability of the brain is simulated in creating a weighted matrix through trial-and-error cycles. The weighted matrix can be used later in identifying a given data pattern, classifying objects, or in estimating a dependent parameter. Details of the principles of the neural networks have been elaborated [11]. An evolutionary history of ANN models and basic principles on which they work have been presented [16].

The basic model of a neural network consists of sets of neurons distributed over input, hidden, and output layers. Each neuron in the input layers represents one of the independent variables, those in the output layers represent dependent variables, and the neurons in the hidden layers act as an associative memory of weights that connect the input neurons to the output neurons.

The first step in the designing a neural network is the identification of the variables that produce patterns that can be associated with certain distinctive outputs. These variables act as input neurons and the answers that are being sought are the output neurons. This is an almost intuitive process aided by trial-and-error procedure.

Relationship between Hydraulic Conductivity and Grain Size

In the following sections, some of the well-known equations as well as the new approaches which have been developed during the past decade are presented. These equations relate the saturated hydraulic Conductivity of granular materials to their Grain Size Distribution Curves are presented.

Hazen Equation

Hazen's approximation, which is a simple relationship, is based on Equation 1 [8]. Freeze and Cherry (1979) give the following empirical relation due to [8] for hydraulic conductivity estimates [7]:

$$K = cd^2 \tag{1}$$

where the units of K and d_{10} are cm/s and mm, respectively, and c = 1.0.

Shepherd Equation

Shepherd (1989) performed statistical power regression analyses on 19 sets of published data on hydraulic conductivity *vs.* grain size using the Equation 2 [14]:

$$K = ad^b \tag{2}$$

where K is hydraulic conductivity, d is grain diameter, a and b are some parameters According to the results of Shepherd, values of the coefficient a ranged from (4.79X10-2 to 9.86 cm/s). The exponent b (dimensionless) ranged from 1.11 to 2.05, with an average of 1.72. The higher values of coefficient a correspond to more texturally mature samples; the lowest values of exponent b correspond to texturally immature sediments.

Kozeny-Carman Equation

One of the most widely accepted derivations of permeability as a function of the characteristics of the medium was proposed by Kozeny (1927) and later modified by Carman (1956) [4,10]. The Kozeny-Carman equation according to [2] is:

$$K = \left(\frac{\rho g}{\mu}\right)\left[\frac{n^3}{(1-n)^2}\right]\left(\frac{d_m^2}{180}\right) \quad (3)$$

where K is hydraulic conductivity, ρ is the density of water, g is the acceleration of gravity, μ is the dynamic viscosity, n is porosity, and d_m is a representative grain size. Equation 3 is dimensionally correct and suitable for application with any consistent set of units.

Fair and Hatch Equation

Based on dimensional considerations and experimental verification, the following equation for the estimation of hydraulic conductivity was [2,5]:

$$K = \left(\frac{\rho g}{\mu}\right)\left[\frac{n^3}{(1-n)^2}\right]\left[\frac{1}{\beta\left(\frac{\alpha}{100}\sum_{m=0}^{N}\frac{P_m}{d_m}\right)^2}\right] \quad (4)$$

where K is hydraulic conductivity; ρ is the density of water; g is the acceleration of gravity μ is the dynamic viscosity; n is porosity; β is a packing factor, found experimentally to be about 5; a is a sand shape factor, varying from 6.0 for spherical grains to 7.7 for angular grains; Pm is percentage of sand held between adjacent sieves; dm is the geometric mean diameter of the adjacent sieves; m is a dummy variable; and N is the number of the percentages held between adjacent sieves.

Alyamani and Sen Equation

The equations presented above, which relate the hydraulic conductivity to grain-size distributions, are based on a single parameter, such as the effective grain diameter for the Hazen equation, representative grain diameter for the Kozeny-Carman equation and the geometric mean diameter for the Fair and Hatch equation. In the equations presented by Shepherd, the grain diameter is a variable. As an alternative, Alyamani and Sen (1993) proposed the following equation based on analysis of 32 samples from Saudi Arabia and Australia that incorporates the initial slope and the intercept of the grain-size distribution curve [1]:

$$K = 1300\left[I_0 + 0.025\left(d_{50} - d_{10}\right)\right]^2 \quad (5)$$

where K (unit m/day) is hydraulic conductivity and I_o (unit mm) is the x intercept of the slope of the line formed by d_{50} and d_{10} of the grain-size distribution curve. Here, d_{50} is the effective grain size where 50% of particles are finer than d (mm). The linear x and y coordinates of the grain-size distribution curve are the "grain size" in mm and "percent finer", respectively. The intercept occurs where the observed straight line crosses the horizontal axis. The value of the x intercept is expected to be very close to zero or to the effective grain diameter. Physically, this means that there is no passing material from the set of sieves. The higher the x-intercept values, the higher the hydraulic conductivities.

Properties of Alyamani and Sen Equation, Equation 5. 1) In general, I_o is very close to the value of d_{10}. 2) From Equation 5, it can be said that the hydraulic conductivity, K, is proportional to d_{10}, which is the base of the Hazen equation as given by Equation 1. In other words, the Hazen equation, Equation 1, is a special case of the Alyamani and Sen equation, Equation 5. 3) The appearance of difference ($d_{50} \sim d_{10}$) in Equation 5 implies that the hydraulic conductivity is proportion to the dispersion of grain size.

Evaluation of the Equations

Sperry and Peirce (1995) performed an evaluation by comparing the measured K values of different porous materials with those determined from their own equations as well as the equations of Hazen, Kozeny-Carman and Alyamani and Sen [15]. Sperry and Peirce (1995) reached the following conclusions for the tested materials [15]: (1) Overall, the Hazen equation provides the best estimate of the hydraulic conductivity of the media studied, except for irregularly shaped particles.

The values determined from the Hazen model are within a factor or two of the experimental values, except for irregularly shaped particles for which the values are within 330% of the experimental values. This reflects the fact that the Hazen equation is not convenient for irregularly shaped particles. (2) The Kozeny-Carman equation estimates are 73% to 83% lower than the measured hydraulic conductivity for the filter pack sands. (3) The Alyamani and Sen equation estimates are 30% to 36% greater for the same media.

Results from this section show the importance of grain size distribution curves for prediction of hydraulic conductivity of porous materials with regular grain shape. Hence the separation of soil types for artificial neural network models will improve the accuracy of predictions.

Development of Backpropagation Neural Networks

The backpropagation neural network (BPN) used in this research is the most widely used feedforward neural network system. The term backpropagation refers to the training method by which the weights of the network connection are adjusted. The calculations procedure is feedforward, from input layer through hidden layers to output layer. During training, the calculated outputs are compared with the desired values, and then the errors are backpropagated to correct all weight factors. The whole calculation procedure (for a three-layer BPN) is summarized as follows:

1. Randomly assign values between 0 and 1 to weights Wi,j (I) for each layer (I). All input-layer thresholds are assigned to zero, *i.e.* Ti,1 = 0 ; all hidden and output-layer thresholds are assigned to one, *i.e.*, Ti,2 = 1, Ti,3 = 1.

2. Introduce the input Ii into the neural network, and calculate the output from the first layer according to the following equations:

$$x_i = I_i + T_{i,1} \tag{6}$$

$$\alpha_{i1} = f(x_i) \tag{7}$$

where f ( ) is the transfer function.

3. Obtaining the output from the first layer, calculate outputs from the second layer, using the equation:

$$\alpha_{i2} = f(\sum_j^l (W_{j,i}(2)\alpha_{j,1} + T_{i,2}) \tag{8}$$

4. Given the output from the second layer, calculate the output from the output-layer, using the following equations:

$$\alpha_{i3} = f(\sum_j^l (W_{j,i}(3)\alpha_{j,2} + T_{i,3}) \tag{9}$$

$$y_i = \alpha_{i3} \tag{10}$$

Steps 1 to 4 represent the forward activation flow; that is, the given input values I_i move forward in the network, activate the nodes, and produce the actual output values y_i based on the initially assumed values of interconnecting weights, $W_{i,j}$(I) and internal threshold, $T_{i,I}$. Obviously, the initial calculation will not produce the desired output values (d_i). The next few steps of the backpropagation algorithm represent the backward error flow in which the errors between the desired output d_i and the actual output y_i flow backward through the network and try to find a new set of network parameters ($W_{i,j}$(I) and T_i).

5. Now backpropagate the error through the network, starting from the output layer and moving backward toward the input layer. Calculate the gradient-descent term ($\delta_{1,3}$) using the following equations:

$$x_{i,3} = \sum_j^l (W_{j,i}(3)\alpha_{j,2}) + T_{i,3} \tag{11}$$

$$\delta_{i,3} = (d_i - y_i)\frac{\partial f(x_i)}{\partial x_i} \tag{12}$$

6. Knowing the output-layer, ($\delta_{1,3}$) calculate ($\delta_{1,2}$) the gradient-descent term for the hidden layer (layer 2) using these equations:

$$x_{i,2} = \sum_j^l (W_{j,i}(2)\alpha_{j,1}) + T_{i,2} \tag{13}$$

$$\delta_{i,2} = \left(\sum_k \delta_{k,3} W_{k,j}(3)\right)\frac{\partial f(x_i)}{\partial x_i} \tag{14}$$

7. Knowing the deltas for the hidden and output layers, calculate the weight changes, $\Delta W_{i,j}$ using the equation:

$$\Delta W_{i,j}(I)_{new} = \eta\delta_{i,j}\alpha_{j,i-1} + \alpha\Delta W_{i,j}(I)_{old} \tag{15}$$

where η is the learning rate, and α is the momentum coefficient. The momentum term is added to speed up the training rate. The momentum coefficient, α, is restricted to $0 < \alpha < 1$.

8. Knowing the weight changes, update the weights as:

$$W_{i,j}(I)_{new} = W_{i,j}(I)_{old} + \Delta W_{i,j}(I)_{new} \tag{16}$$

One iteration is completed so far. This feedforward calculation and error backpropagation procedure is repeated until the sum of errors is less than the specified value. This is the whole learning process for the neural network. The new weight factors are calculated from the old weight factors of the previous training iteration by the following general expression:

$$\begin{aligned}\left[W_{i,j}\right]_{new} &= \left[W_{i,j}\right]_{new} + \begin{bmatrix}Learning\\ rate\end{bmatrix} \times \begin{bmatrix}input\\ term\end{bmatrix}\\ &\times \begin{bmatrix}gradient-descent\\ correlation\ term\end{bmatrix} \times \begin{bmatrix}momentum\\ coefficient\end{bmatrix} \times \begin{bmatrix}previous\\ weight\ change\end{bmatrix}\end{aligned} \tag{17}$$

Number of Hidden Layers = Number of Data Samples/(Input Layers + Output Layers)

Next are several training parameters. These variables impact how the net is trained.

The Learning rate impacts how much weights are changed on each iteration. For this research it was found 0.2. The Momentum Coefficient is a factor that impact how much the weight will be adjusted based on the weight changes in the previous iterations. For this research it was found 0.6.

The last training parameter is the Convergence Criteria. This is the value of the normalized sum of errors. The training will iterate until the Convergence Criteria is reached or the Maximum Iterations is encountered. For this research it was set to 0.02.

A stepwise procedure was followed in investigating the applicability of ANN technology in the estimation of the hydraulic conductivity of the porous media. The available softwares, *Professional II/PLUS, 2000* and *Neuro3, 2002,* were used and compared in creating the neural network. The 168 grain size distribution curve and related saturated hydraulic conductivity values in cm/day derived from the UNSODA database were used for the study [6]. Within the scope of the present work have shown that better correlation of individual soils is obtained with the logarithm of the hydraulic conductivity instead of its raw value, and this has been used as the output variable (neuron). It sets apart 10% of the available input data, as test data and uses the rest as a training dataset. A stepwise process was followed in developing six neural network models with different type of soils as input neurons (variables). The trial and-error method was followed in assigning the degree of tolerance in matching the ANN estimated values with the observed values of the logarithm of hydraulic conductivity and in deciding the percentage of match at which the training of the network can stop. A RMS error value of 0.02 was found to provide a trained network within a reasonable number of runs (<100,000) with an average training error of 5% or less. The performance of the network developed was checked against the test data. For accepting a network, a match of at least 95% of the training and test data were considered.

Figure 1 shows the line plot of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database for all group of soils [6].

After a few preliminary test runs, it was found that one hidden layer with 17 hidden neurons was giving the best overall performance, and these were accepted for all the networks developed. The characteristics of the 6 models developed for five soils type are as follow:

Model-1: Input neurons are the percent finer for particle size in Φ scale (3.3, 2.3, 2, 1.6, 1.3, 1, 0.6, 0.3) of loamy-sand. The number of training data: 23, number of test data: 12. The output neuron is the saturated hydraulic conductivity of loamy-sand (Fig. 2, a and b).

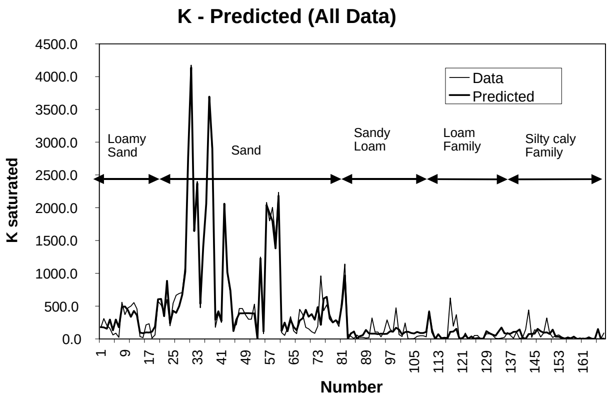


Figure 1. Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database for all group of soils.

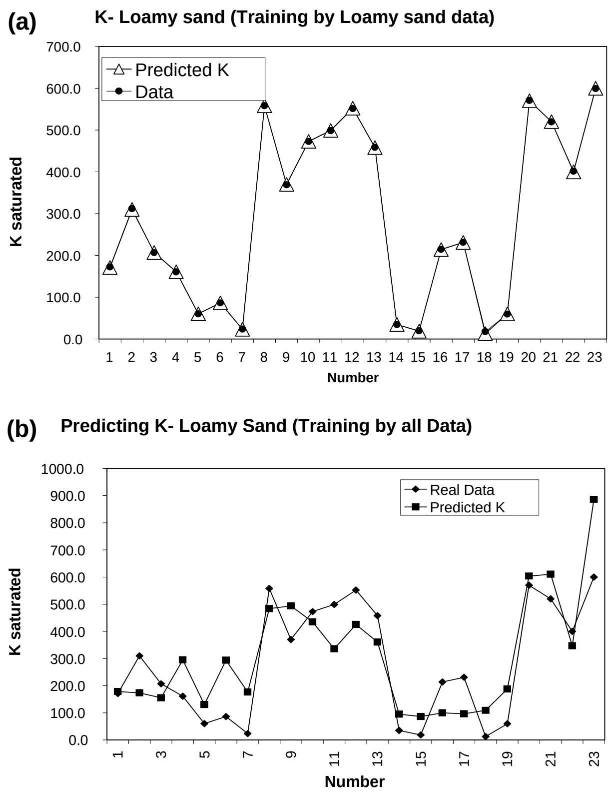


Figure 2. (a) Model-1, Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by loamy sand data; **(b)** Mode-1, Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by all group of soils.

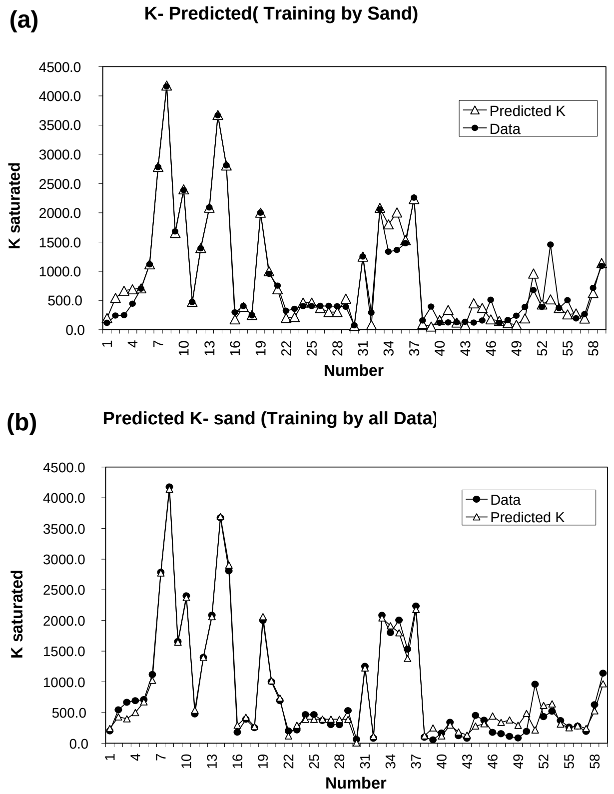


Figure 3. (a) Model-2 Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by sandy soils; **(b)** Model-2 Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by all group of soils.

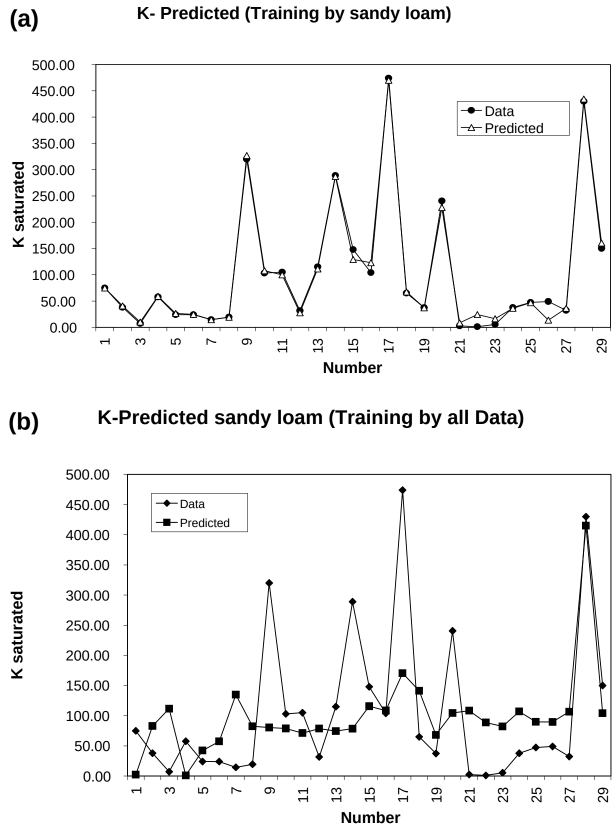


Figure 4. (a) Model-3, Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by sandy loam soils; **(b)** Model-3, Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by all group of soils.

Model-2: Input neurons are the percent finer for particle size in Φ scale (3.3, 2.3, 2, 1.6, 1.3, 1, 0.6, 0.3) of sand. The number of training data: 59, number of test data: 12. The output neuron is the saturated hydraulic conductivity of sand (Fig. 3, a and b).

Model-3: Input neurons are the percent finer for particle size in Φ scale (3.3, 2.3, 2, 1.6, 1.3, 1, 0.6, 0.3) of sandy-loam. The number of training data: 29, number of test data: 10. The output neuron is the saturated hydraulic conductivity of sandy-loam (Fig. 4, a and b).

Model-4: Input neurons are the percent finer for particle size in Φ scale (3.3, 2.3, 2, 1.6, 1.3, 1, 0.6, 0.3) of sandy-clay-loam, clay-loam, clay and loam (sand-clay-loam family). The number of training data: 29, number of test data: 10. The output neuron is the saturated hydraulic conductivity of sandy-clay-loam, clay-loam, clay and loam (Fig. 5, a and b).

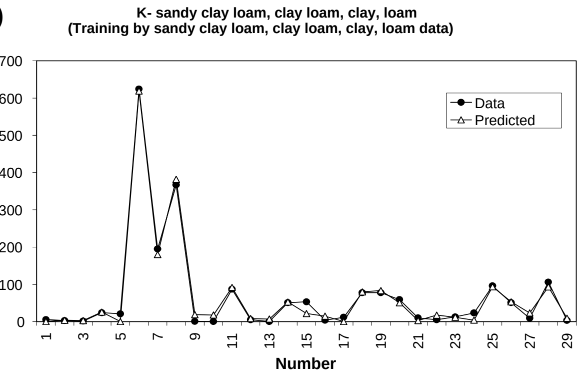
Model-5: Input neurons are the percent finer for particle size in Φ scale (3.3, 2.3, 2, 1.6, 1.3, 1, 0.6, 0.3) of silty-clay-loam, silty-loam, silty-clay and silt (silt-caly-loam family). The number of training data: 28, number of test data: 10. The output neuron is the saturated hydraulic conductivity of silty-clay-loam, silty-loam, silty-clay and silt (Fig. 6, a and b).

Model-6: Input neurons are the percent finer for particle size in Φ scale (3.3, 2.3, 2, 1.6, 1.3, 1, 0.6, 0.3) of all soils in Model-1 to Model-5. The number of training data: 168, number of test data: 50. The output neuron is the saturated hydraulic conductivity of all soils in Model-1 to Model-5 (Fig. 1).

The training and testing tolerances for the first five models were set at 5% and those of model-6 were 10%. The stop training criterion for model-1 to model-5 was 95% and for model-6 this parameter was set at 85% of the training data.

Finally for testing the application of artificial neural network technology for an aquifer, the predicted hydraulic conductivity was checked against the measured values of pumping test data. For this purpose 14 measured hydraulic conductivity values measured by pumping test analysis in an unconfined Aquifer in Zahedan (City of Zahedan in Iran) has been investigated by their grain size distribution curve obtained in the laboratory using the artificial neural network model. It has been found that reasonable estimate of this parameter can be obtained with the help of a network that trained using the only grain size distribution curve for relatively fine grained medium. A better estimate was obtained with a model that uses the special group of soil for training the network. Figure 7 shows the line plot of the measured values of hydraulic conductivity of an unconfined Aquifer in Zahedan measured by pumping test analysis and predicted value by their grain size distribution curve using the artificial neural network Mode-l, trained by loamy sand data.

(a)



(b)

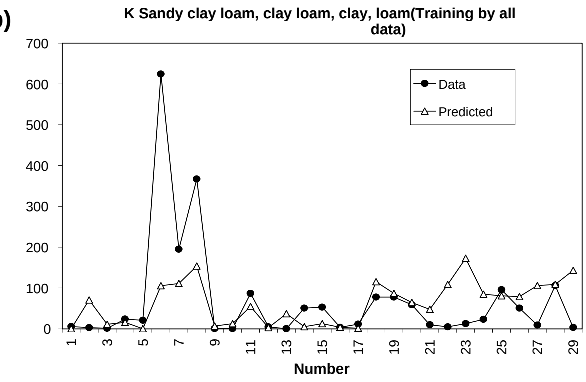
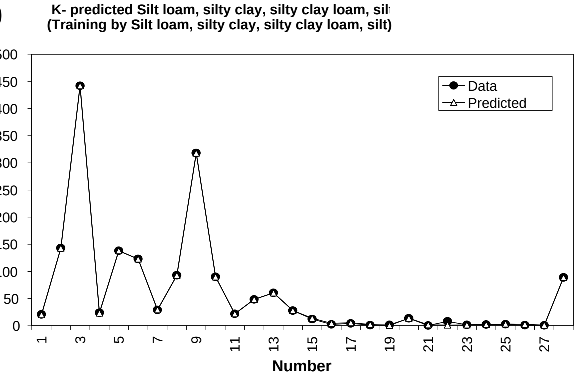


Figure 5. **(a)** Model-4 Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by sandy caly loam family; **(b)** Model-4, Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by all data.

(a)



(b)

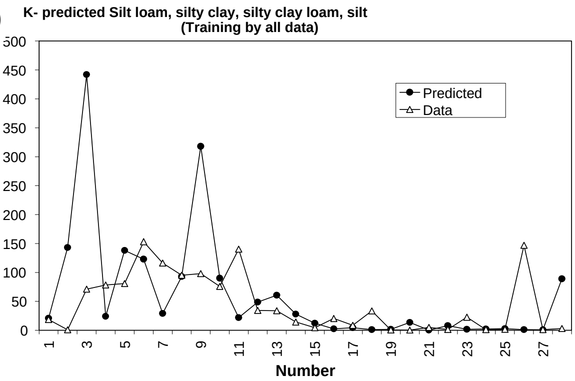


Figure 6. **(a)** Model-5, Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by silt-clay-loam family; **(b)** Model-5 Crossplots of neural network estimated hydraulic conductivity (cm/d) and measured hydraulic conductivity (cm/d) from UNSUDA database training by all data.

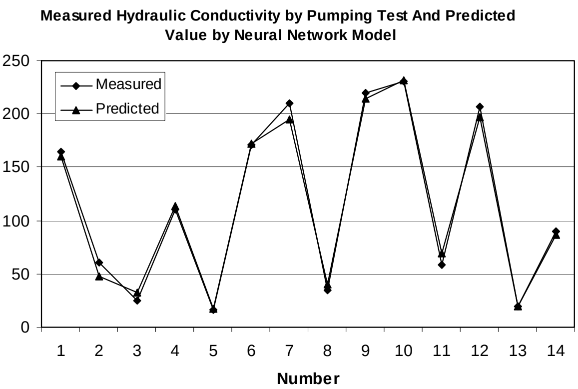


Figure 7. Crossplots of neural network estimated hydraulic conductivity (cm/d) from grain size distribution curve using Model-1 and measured hydraulic conductivity (cm/d) for an unconfined aquifer in Zahedan.

Comparative Assessment of the Networks Developed for Individual Groups of Soils

The comparisons of the neural network predicted values with the measured values of five soil group (including loamy-sand, sand, sandy-loam, sand-clay-loam, silt-caly-loam) from UNSUDA database are shown in Figures 2-6 [6]. It is apparent from the figures that the prediction of neural network was improving through training the network with different group of soils (Models), and the majority of the predicted values were within the 95% confidence limits in all the cases. The Model-6 in which uses all types of soils, however was unable to predict very high (more than 1000 cm/d) and very low (less than 10 cm/d) values of hydraulic conductivity adequately.

Conclusion

The artificial neural network technique can be the best alternative method for estimating aquifer hydraulic conductivity from grain size distribution curve.

The results of the present study suggest that reasonable and acceptable estimates of hydraulic conductivity are obtainable using this technique, provided enough training data covering the whole spectrum of soils type. Some trial-and-error runs need to be made to select an optimum combination of input neurons, number of hidden layers and the hidden neurons, and to decide when to stop training and to accept the network as trained. It was realized that the model that uses only one special type of porous media provides better predicted value. Results show that there is a reasonable estimate of hydraulic conductivity of Zahedan unconfined Aquifer from grain size distribution curve data using the artificial neural network Mode-l, trained by loamy sand data.

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