Oriental Journal of Chemistry Vol. **26**(4), 1271-1280 (2010)

Estimation of hardgrove grindability index (HGI) based on the coal chemical properties using artifical neural networks

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(Received: October 15, 2010; Accepted: November 17, 2010)

ABSTRACT

In this research, the effect of different parameters of coal composition (coal chemical properties) were studied, to estimate the coal HGI values index. To estimate the HGI values artificial neural networks (ANNs) and linear multivariable regression methods were used for 400 data. In this work, ten input parameters, such as moisture, volatile matter (dry), fixed carbon (dry), ash (dry), total sulfur (organic & pyretic) (dry), Btu/lb (dry), carbon (dry), hydrogen (dry), nitrogen (dry) as well as oxygen (dry), were used. For selecting the best method to predict HGI values, the responses of aforementioned methods were compared. The results of ANNs, show that the training and test data's square correlation coefficients (R^2) achieved at 0.962 and 0.82 respectively. The equation of linear multivariable regression for HGI values were produced. Square correlation coefficients, (R^2), from regression achieved at 0.76. Sensitivity analysis showed that volatile matter (dry), Btu/lb (dry), carbon (dry), hydrogen (dry), fixd carbon (dry), nitrogen (dry) and oxygen (dry) are the most effective parameters on the HGI.

Key words: Coal, HGI, Artificial neural network, Linear multivariable regression, Coal chemical properties

INTRODUCTION

Coal is a heterogeneous substance which consists of the combustible (organic matter) and non-combustible (moisture and mineral matter) materials. Coal grindability, usually measured by the Hardgrove Grindability Index (HGI), is of great interest since it is an important practical and economic property for the coal handling and utilization, particularly for pulverized-coal-fired boilers.

Grindability index of coal is an important technological parameter to understand the behaviour and assess the relative hardness of coals, from the varying ranks and grades during the comminution. Comminution behavior or grindability of coal which is a measure of its resistance to crushing and grinding is related to its physical properties, chemical and petrographical compositions[1]. The examination of the grindability of coal is important for any kind of utilizations such as coal beneficiation, carbonization and many others. The energy cost of grinding is significant at 5 to 15 kWh/ton[2].

Sengupta developed an equation derived by the regression of proximate analysis data with all the components, e.g. moisture, ash, volatile matter, and fixed carbon percent on air-dried basis, to find out the grindability index termed as Statistical Grindability Index (SGI) from that equation correlation coefficient of this relationship achived 0.93 [3]. Ural. *et al,* E. Jorjani et al and H.B. Vuthaluru studied the effects of mineral matter content and elemental analysis of coal on HGI Turkish, Kentucky and Australia coals, respectivly[4,5,6]. They found that water, moistuer, coal blending, acid-soluble mineral matter content, Na_2O, Fe_2O_3, Al_2O_3, SO_3, K_2O and SiO2 positively contribute to the grindability of the coals. High ash and water- and acid-soluble content samples present higher HGI values, whereas, high

ash, high TiO_2, MgO and low water- and acid-soluble content samples have lower-HGI value[4,5,6]. The relationships between grindability, mechanical properties, and cuttability of coal were investigated by many researchers through studies that came up with close correlations between HGI and some coal properties[7]. B. Tiryaki showed that there are strong relationships between HGI of coal and the hardness characteristics[7].

In order to determin the comminution behavior of coal for size reduction, it is necessary to use the tests based on size reduction. One of usual methods for determining the grindability of coal is Hardgrove index method. Soft or hard coals were evaluated for the grindability - toward 100. Coal HGI depends on the coalification, moisture, volatile matter (dry), fixed carbon (dry), ash (dry), otal sulfur (organic & pyretic) (dry), Btu/lb (dry), carbon (dry), hydrogen, nitrogen (dry) and oxygen(dry) parameters. These parameters are effective on the HGI values, for example if carbon contents in coal is more than 60%, HGI moves to maximum range[8]. In this investigation, neural network in mathematic software package MATLAB for the estimation of the HGI of coals was used.

MATERIAL AND METHODS

Artificial Neural Networks (ANNs)

Neural networks are simplified models of the biological structure found in human brains[1]. Derived from their biological counterparts, ANNs are based on the concept that a highly interconnected system of simple processing elements (also called “nodes” or “neurons”) can learn complex nonlinear interrelationships existing between the input and output variables of a data set[9]. Neural networks are powerful tools that have the ability to identify the underlying highly complex relationships from input–output data only[10]. Over the last 11 years, artificial neural networks (ANNs), and particularly feed-forward artificial neural networks (FANNs), have been extensively studied to present process models, and their use in industry has been rapidly growing[11]. The main advantages of the ANN models are: (1) no particular knowledge is needed about the system being modeled, unknown effects could be involved through a proper design of the input–output patterns; (2) the relative simplicity of neural network architecture[12].

The ANNs can be applied successfully in learning, relating, classifying, generalizing, characterizing and optimizing functions[13]. These application processes of an ANN model design include the steps below:

1. Collecting the whole data in one place
2. Determining the train and test sets.
3. Converting the data into the ANN inputs.
4. Determining, training and testing the network topology.
5. Repeating the 1st, 2nd, 3rd and the 4th steps as long as required to determine the optimal model, and.
6. The application of the optimal ANN model.

For developing ANN model of a system, a feed-forward architecture namely MLP[1] is most commonly used. This network usually consists of a hierarchical structure of three layers described as input, hidden, and output layers, comprising I, J, and L number of processing nodes, respectively[14]. General MLP architecture with two hidden layers is shown in Figure 1. When an input pattern is introduced to the neural network, the synaptic weights between the neurons are stimulated and these signals propagate through the layers and an output pattern is formed. Depending on how close the formed output pattern is to the expected output pattern, the weights between the layers and the neurons are modified in such a way that if next time the same input pattern is introduced, the neural network will provide an output pattern, closer to the expected response[1].

Data Set

One of the most important stages in the ANN technique is data collection. The data was divided into training and testing datasets using the sorting method to maintain the statistical consistency. Datasets for testing were extracted at regular intervals from the sorted database and the remaining datasets were used for training. The same datasets were used for all networks to make a comparable analysis of different architecture. In the present study, 400 datasets were collected among which 20% were chosen for testing and validating. Our data collected from Illinois State Geological Survey web site (http://www.isgs.illinois.edu/maps-

data-pub/coal-maps/nonconf_masterfile.xls). These data were collected from Illinois state coal mines and geological database.

Input Parameters

In the current study, input parameters include moisture, ash (dry), volatile matter (dry), Fixed carbon (dry), total sulfur (dry), Btu/lb (dry), carbon (dry), hydrogen (dry), nitrogen (dry) and oxygen (dry) for predicting the HGI. The ranges of input variables to HGI prediction for the 400 samples are shown in Table 1.

RESULTS AND DISCUSSION

Prediction of the HGI Using Linear Multivariable Regression

Multiple regression is an extension of the regression analysis that incorporates additional independent variables into the predictive equation. However, the previous empirical studies provide the guidelines for selecting the dependent variables which are to be used in the predictor development[15]. Here, a multivariate relation was established using the same input variables as the neural network model. The linear multivariable regression equation resulted in the following equation:

HGI=67- 3.16 oxygen- 3.02 nitrogen- 0.23 hydrogen -2.37carbon -0.00585Btu/lb -1.53total S +3fixed carbon -1ash +3volatile matter +1.13moisture ...(1)

Fig. 2 shows the correlation between the experimental HGI data and predicted HGI from the linear multivariable regression. As shown in the Figure 2, the square correlation coefficient (R^2) is 0.76.

Relation of HGI and Individual Constituents

Li *et al.,* and Sengupta *et al*., examined the relation between the coal properties with HGI using a second order regression equation and found that the correlation coefficients of moisture and ash with HGI were -0.45 and 0.31, respectively[16]. Sengupta, using a second-order regression equation (correlation coefficient of 0.93), found that the correlation between the HGI and coal properties should be non-linear[3]. In a recent study, linear multivariable regression was used for the determination of the coefficient between some important coal properties and HGI. Figure 4 and Table II shows the coefficient between some important coal properties (moisture, volatile matter (dry), fixed carbon (dry), ash (dry), total sulfur (organic & pyretic) (dry), Btu/lb (dry), carbon (dry), hydrogen (dry), nitrogen (dry) and oxygen (dry)) and HGI. As shown in Figure 4 and Table II, moisture, volatile matter (dry), fixed carbon (dry), total sulfur (dry), Btu/lb (dry), carbon (dry), hydrogen (dry) and oxygen (dry) had a positive coefficient with HGI, also ash (dry) and nitrogen (dry) had a negative coefficient with HGI.

Table 1: The ranges of variables in coal samples (as determined)

Coal chemical properties	Max	Min	Mean	St.Dev.
Moisture (%)	15,94	6,03	10,32	2,21224
Volatile matter (dry) (%)	45,10	25,49	36,87	2,458445
Fixed carbon (dry) (%)	60,39	30,70	50,58	4,152964
Ash (dry) (%)	43,81	4,41	12,56	4,861197
Total sulfur (organic & pyretic) (dry) (%)	9,07	0,62	3,00	2,018264
Btu/lb (dry)	14076,00	8025,00	12631,08	841,5436
Carbon (dry) (%)	79,32	44,03	70,43	5,026348
Hydrogen (dry) (%)	5,36	3,39	4,78	0,310245
Nitrogen (dry) (%)	3,03	0,35	1,40	0,290988
Oxygen (dry) (%)	12,57	2,16	7,53	1,660288
HGI	72,00	30,00	58,80	5,710457

Network Design and Development

Various algorithms are available for training neural networks. Feed forward back-propagation algorithm is the most versatile and robust technique, which provides the most efficient learning procedure for the multilayer perception (MLP) neural networks. Also, the fact that the back-propagation algorithm is especially capable of solving the predictive problems makes it so popular. The network[1] model presented in this article is a supervised back-propagation neural network, making use of the Levenberg-Marquardt approximation.

This algorithm is more powerful than the commonly used gradient descent methods, because the Levenberg-Marquardt approximation makes training more accurate and faster near minima on the error surface[17].

The method is as follows:

$$\Delta W = \left(J^T J + \mu I\right)^{-1} J^T e \qquad ...(2)$$

In Eq. (2) the adjusted weight matrix ΔW is calculated using a Jacobian matrix J, a transposed Jacobian matrix J^T, a constant multiplier μ, a unity matrix I and an error vector e. The Jacobian matrix contains the weights derivatives of the errors:

$$J = \begin{vmatrix} \frac{\partial E}{\partial w_{11}} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{\partial E}{\partial w_{nn}} \end{vmatrix} \qquad ...(3)$$

If the scalar μ is very large, the Levenberg-Marquardt algorithm will approximate the normal gradient descent method; whereas if it is small, the expression will transform into the Gauss-Newton method (Haykin S. 1994). For more detailed information, the readers refer to Lines and Treitel[18].

After each successful step (lower errors) the constant m is decreased, forcing the adjusted weight matrix to transform as quickly as possible to the Gauss-Newton solution. After a step, if the errors increase, the constant m increases subsequently. The weights of the adjusted weight matrix (Eq. (2)) are used in the forward pass. The mathematics of both the forward and backward pass are briefly explained follows. The net input (net_{pj}) of neuron j in a layer L and the output (o_{pj}) of the same neuron of the pth training pair (i.e. the inputs and the corresponding HGI value of sample) are calculated through:

$$net_{pj} = \sum_{n=1}^{last} w_{jn} o_{pn} \qquad ...(4)$$

where, the number of neurons in the previous layer (L -1) are defined by n =1 to the last neuron and the weights between the neurons of layer L and L -1 by w_{jn}. The output (o_{pj}) is calculated using the logarithmic sigmoid transfer function:

$$O_{pj} = f_{pj}(net_{pj}) = \frac{1}{1+e^{-(net_{pj}+\theta_j)}} \qquad ...(5)$$

where, θ_j is the bias of neuron j.

In general, the output vector, containing all o_{pj} of the neurons of the output layer, is not the same as the true output vector (i.e. the measured HGI value). This true output vector is composed of the summation of t_{pj}. The error between these vectors is the error made while processing the input-output vector pair and is calculated as follows:

$$E_p = \frac{1}{2}\sum (t_{pj} - o_{pj})^2 \qquad ...(6)$$

Table 2: Coefficients of input variable with HGI

Input variable	Coefficient with HGI
Moisture	+1.13
Volatile matter (dry)	+3
Fixed carbon (dry)	+3
Ash (dry)	-1
Total sulfur (dry)	-1.53
Btu/lb (dry)	-0.00585
Carbon (dry)	-2.37
Hydrogen (dry)	-0.23
Nitrogen (dry)	-3.02
Oxygen (dry)	-3.16

When a network is trained with a database containing a substantial amount of input and output vector pairs, the total error E, (sum of the training errors E_p) can be calculated[17].

$$E_t = \sum E_p \qquad ...(7)$$

To reduce the training error, the connection weights are changed during a completion of a forward and backward pass by adjustments (ΔW) of all the connections' weights w. Eqs. (2) and (3) calculate those adjustments. This process will continue until the training error reaches a predefined target threshold error.

Designing a network architecture requires more than selecting a certain number of neurons, followed by training only. Especially phenomena such as overfitting and underfitting should be recognized and avoided in order to create a reliable network. Those two aspects - overfitting and underfitting - determine to a large extent the final configuration and training constraints of the network[17].

The number of input and output neurons is the same as the number of input and output variables. For this research, multilayer network architecture with two hidden layers between the input and output units is applied. During the design and development of

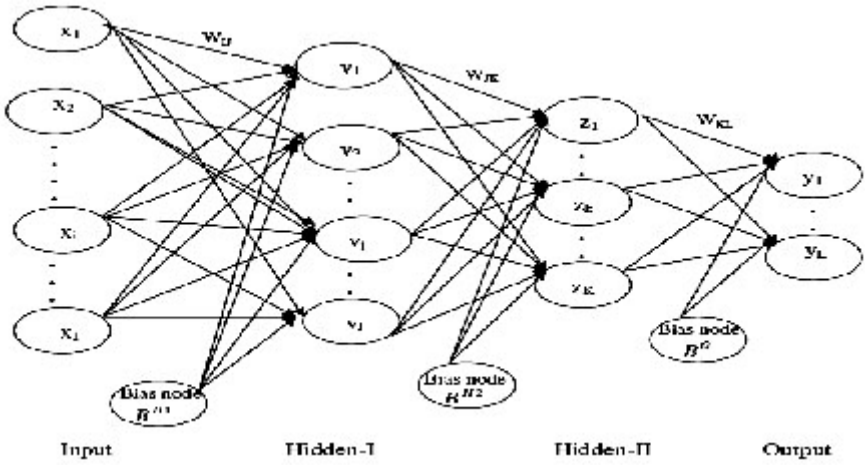

Fig. 1: MLP architecture with two hidden layers [14]

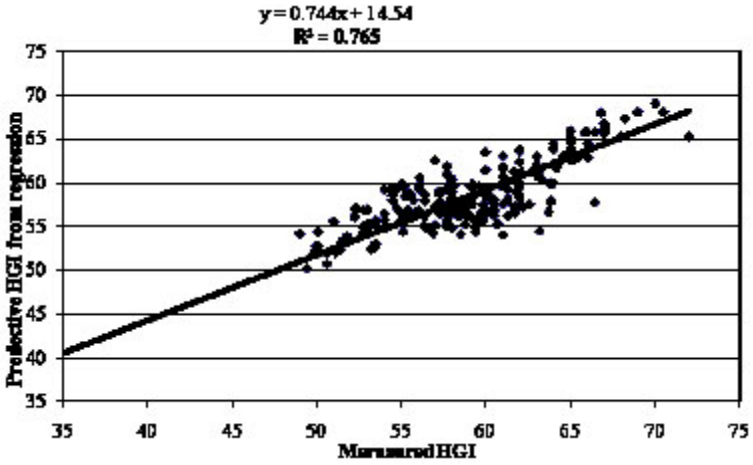

Fig. 2: Relation between measured HGI and predicted HGI from linear multivariable regression

the neural network for this study, it was determined that a Four-layer network with 10 neurons in the hidden layers (two layers) would be the most appropriate. Artificial neural network (ANN) architecture for predicting the HGI is shown in Fig. 5

The learning rate of the network was adjusted so that training time was minimized. During the training, several parameters had to be closely watched. It was important to train the network long enough so it would learn all the examples that were provided. It was also equally important to avoid overtraining, which would cause the memorization of the input data by the network. During the course of training, the network is continuously trying to correct itself and achieve the lowest possible error (global minimum) for every example to which it is exposed. The network performance during the

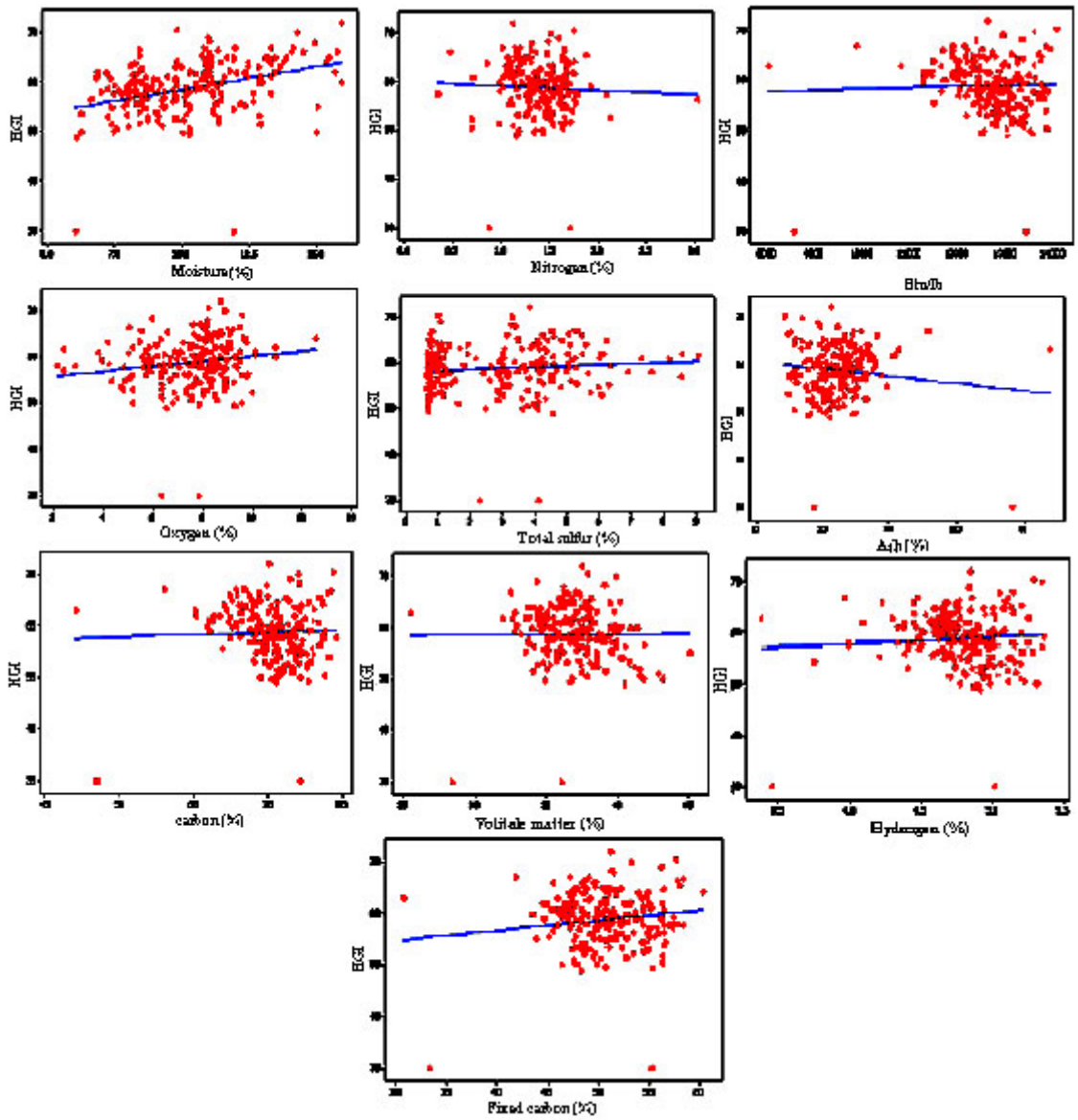

Fig. 3: Relationship between hydrogen (dry), volatile matter (dry), ash (dry), oxygen (dry), total sulfur (dry), nitrogen (dry), moisture, Btu/lb (dry), carbon (dry) and fixed carbon (dry) with HGI

training process is shown in Figure 6., As shown, the optimum epochs of train achieved at about 200 epochs.

For the evaluation of a model, a comparison between the predicted and measured values of HGI can be fulfilled. For this purpose, MAE (E_a) and mean relative error (E_r) can be used. Ea and E_r are computed as follows [17]:

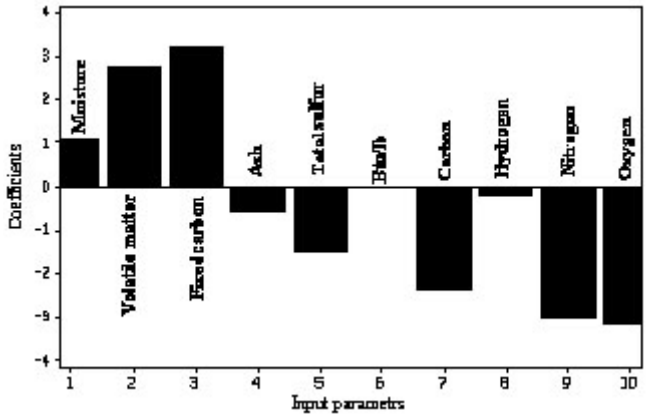

Fig. 4: Coefficients of input parameters (coal chemical properties) with HGI

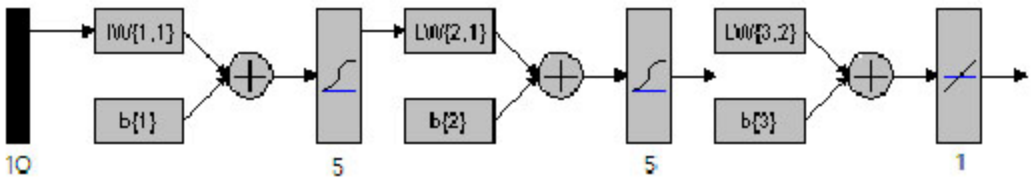

Fig. 5: ANN architecture for predict the HGI

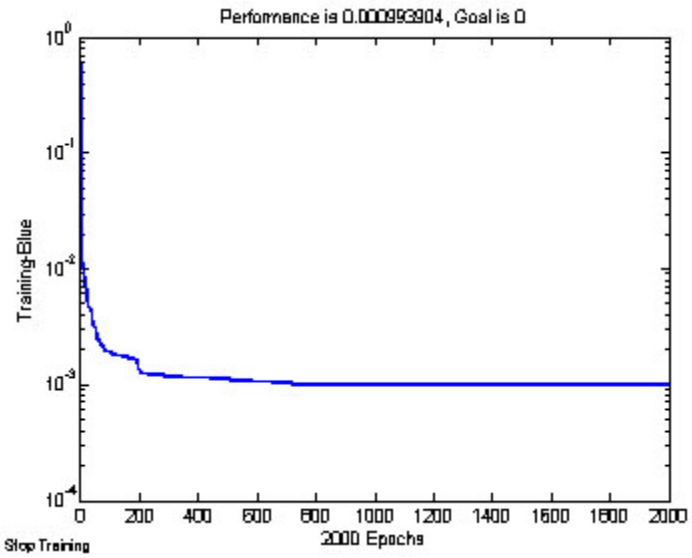

Fig. 6: Network performance during the training process

$$E_a = |T_i - O_i| \quad ...(8)$$

where T_i, O_i and represent the measured and predicted output.

$$E_r = \left(\frac{|T_i - O_i|}{T_i} \right) \quad ...(9)$$

For the optimum model, E_a and E_r were equal to 0.503 and 0.0125 respectively. Also, a correlation between the measured and predicted

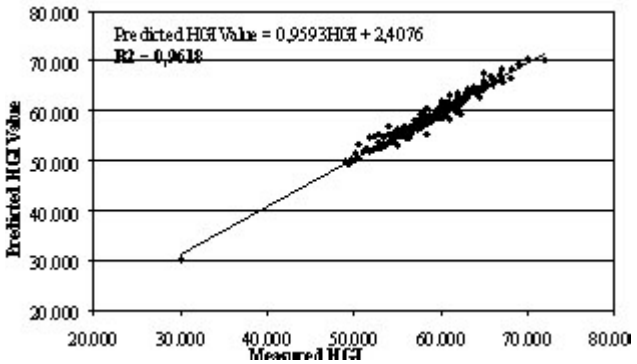

Fig. 7: Correlation between measured and predicted HGI for training data

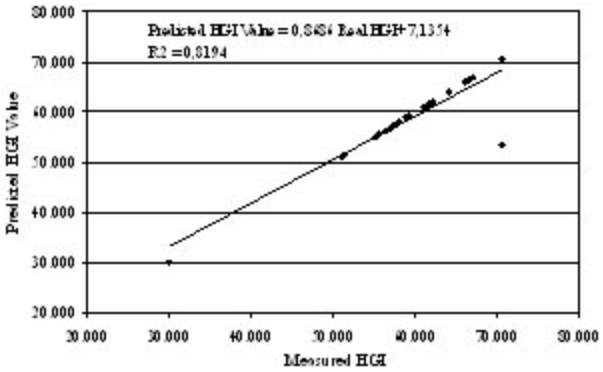

Fig. 8: Correlation between measured and predicted HGI for testing data

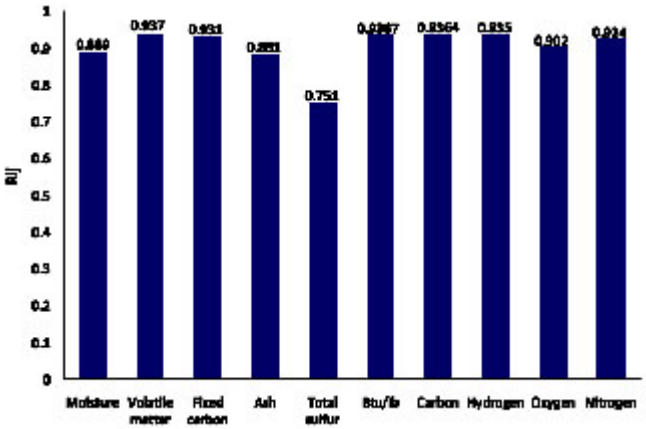

Fig. 9: Strengths of relation (r_{ij}) between HGI and each input parameter

HGI for training an testing data is shown in Figures 7 and 8, respectively. From these figures, it is seen that the coefficient of correlation in both two processes is very good.

Sensitivity Analysis

To analyze the strength of the relationship between the backbreak and the input parameters, the Cosine Amplitude Method (CAM) was utilized. The CAM was used to obtain the express similarity relations between the related parameters. To apply this method, all of the data pairs were expressed in common X-space. The data pairs used to construct a data array X were defined as [19]:

$$X = \{X_1, X_2, X_3, \ldots X_m\} \quad \ldots(10)$$

Each of the elements, Xi, in the data array, X, is a vector of lengths of m, that is:

$$X_i = \{x_{i1}, x_{i2}, x_{i3}, \ldots, x_{im}\}_1 \quad \ldots(11)$$

Thus, each of the data pairs can be thought of as a point in m-dimensional space, where each point requires m-coordinates for a full description. Each element of a relation, rij, results in a pairwise comparison of two data pairs. The strength of the relation between the data pairs, xi and xj, is given by the membership value expressing the strength:

$$r_{ij} = \sum_{k=1}^{m} x_{ik} x_{jk} / \sqrt{\sum_{k=1}^{m} x_{ik}^2 \sum_{k=1}^{m} x_{jk}^2} \quad ..(12)$$

The strengths of the relations (rij values) between HGI and input parameters (coal chemical properties) are shown in Figure 9. As can be seen, the effective parameters on HGI include the volatile matter (dry), Btu/lb (dry), carbon (dry), hydrogen (dry), fixed carbon (dry), nitrogen (dry), oxygen (dry), moisture, ash (dry), and total sulfur (dry), respectively. It is possible to consider and examine the effective parameters in the coal HGI and modification was also applied by changing the further effective parameter.

CONCLUSION

Neural networks are particularly useful in cases where the mathematical or statistical methods, such as linear, non-linear regression, curve fitting, etc. cannot provide a satisfactory solution, i.e. the solution can be too general, or too specific that the model cannot react well to new data points. A network that has memorized all of its training data will perform poorly when exposed to a new set of data for testing. Another important factor is local minima.

In this study, linear multivariable regression and artificial neural network approaches were employed to predict HGI. Input parameters are moisture, volatile matter (dry), fixed carbon (dry), ash (dry), total sulfur (organic & pyretic) (dry), Btu/lb (dry), carbon (dry), hydrogen (dry), nitrogen (dry) and oxygen (dry). In linear multivariable regression analysis method the best equation used the variable HGI and R^2 of 0.76. In ANNs method, the results of ANN shows that training and test data's square correlation coefficients (R^2) achieved at 0.962 and 0.82, respectively.

The results of linear mltivariable regression shows that moisture, volitale matter (dry) and fixed carbon (dry) - positively contribute to the HGI of the coals, and the ash (dry), total sulfur (dry), Btu (dry), carbon (dry), hydrogen (dry), nitrogen (dry) and oxygen (dry) has a negative coefficient with HGI of coals. Comparing of the square coeficient correlations ANNs with the linner multivariable regression shows that ANNs have the best results for predicting HGI. As for network training performance, when the number of epochs is 200, the error of training network minimized and after this point best performance achived for the network. E_a and E_r from ANNs achived at 0.503 and 0.0125, repsectively.

Sensitivity analysis of network shows that the most effective parameters on HGI were volatile matter (dry), Btu/lb (dry), carbon (dry), hydrogen (dry), fixed carbon (dry), nitrogen (dry) and oxygen (dry), respectively, and the low effect parameters on the HGI were moisture, ash (dry), and total sulfur (dry), respectively (Figure 9).

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