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ADAPTIVE NEURO-FUZZY INFERENCE SYSTEM AND STEPWISE REGRESSION FOR COMPRESSIVE STRENGTH ASSESSMENT OF CONCRETE CONTAINING METAKAOLIN

Y. Sharifi^{*,†} and M. Hosseinpour Department of Civil Engineering, Vali-e-Asr University of Rafsanjan, Rafsanajn, Iran

ABSTRACT

In the current study two methods are evaluated for predicting the compressive strength of concrete containing metakaolin. Adaptive neuro-fuzzy inference system (ANFIS) model and stepwise regression (SR) model are developed as a reliable modeling method for simulating and predicting the compressive strength of concrete containing metakaolin at the different ages. The required data in training and testing state obtained from a reliable data base. Then, a comparison has been made between proposed ANFIS model and SR model to have an idea about the predictive power of these methods.

Keywords: adaptive neuro-fuzzy inference system (ANFIS); stepwise regression (SR); compressive strength of concrete; reliable modeling method, metakaolin.

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1. INTRODUCTION

It is well known that utilize of pozzolana such as silica fume, fly ash and granulated blast furnace slag can present great variations of properties. During the past decade, calcined clay in the form of metakaolin as a pozzolanic addition for mortar and concrete has recived considerable interest. On the latest advancing of concrete technology the use of pozzolanic materials such as metakaolin is necessary for access to high-performance concrete. Due to its high pozzolanic activity, the addition of metakaolin greatly enhances the mechanical and/or durability properties of concrete. Metakaolin as a thermally activated alumino-silicate material obatained by calcining kaolin clay, this process occur within the temperature range of 700-850 °C. Material availability and durability have been the important reason for use of clay-based pozzolans in the mortar and concrete, however depending on the temperature and

^{*}Corresponding author: Department of Civil Engineering, Vali-e-Asr University of Rafsanjan, Rafsanajn, Iran

[†]E-mail address: yasser_sharifi@yahoo.com (y.sharifi@vru.ac.ir) (Y. Sharifi)

type of clay enhancement in strength particularly during the early stages of curing maybe occur [1-5].

Intelligent methods give a very strong a reliable procedure to develop formulation for comprehensive and explicit functions consisting of several variables [6-13]. In the current research, an intelligent method based ANFIS approach has been developed to present an formulation for predicting the compressive strength of concrete containing metakaolin.

There are many research that indicate increasing of the compressive strength (f_c) of concrete contain *MK* as compared to conventional concrete. These research have indicated clearly, more improvement in f_c , especially at the early stages of curing, can be carried out. Compressive strength of these kind of concrete can be related to the age of specimen (*AS*) and the ratios of metakaolin-binder (*MB*), super plasticizer-binder (*SB*), water-binder (*WB*), binder-aggregate (*BA*) and fine aggregate to coarse aggregate (*FC*). These data using the available experimental results for 469 specimens produced from 13 different technical literatures [3-5, 14-23]. Based on the database initial input and output vectors of the ANN model include respectively six and one components as follows:

 $Input = \{AS, MB, SB, WB, BA, FC\}$

 $Output = \{f_c\}$

It is appear that input variables included AS, MB, SB, WB, BA and FC to be potentially to predicting the f_c of concrete containing metakaolin. The ranges and statistics of the variables involved in these models development are given in Table 1. Also in order to picture the distribution of the variables, the data have been shown by frequency histograms in Fig. 1.

Table 1: Descriptive statistics of the variables used in the model development.								
Parameter	f_c	AS	MB	SB	WB	BA	FC	
Number	469	469	469	469	469	469	469	
Mean	61.7123	50.2473	0.0988	0.0144	0.3868	0.2424	0.7439	
Std. Error of Mean	0.9697	2.6230	0.00374	0.0010	0.0035	0.0026	0.0143	
Median	62.5000	28.0000	0.1000	0.0090	0.4000	0.2400	0.6600	
Mode	67.00	28.00	0.00	0.00	0.45	0.29	1.22	
Std. Deviation	21.0009	56.8039	0.0809	0.0224	.0765	0.0559	0.3105	
Variance	441.038	3226.682	0.007	0.001	0.006	0.003	0.096	
Skewness	-0.025	1.265	0.599	2.303	-0.001	-0.495	0.812	
Std. Error of Skewness	0.113	0.113	0.113	0.113	0.113	0.113	0.113	
Kurtosis	-0.483	0.452	-0.128	5.008	-1.345	0.169	-0.575	
Std. Error of Kurtosis	0.225	0.225	0.225	0.225	0.225	0.225	0.225	
Range	110.00	179.00	0.30	0.09	0.25	0.25	1.14	
Minimum	10.30	1.00	0.00	0.00	0.25	0.10	0.31	
Maximum	120.30	180.00	0.30	0.09	0.50	0.35	1.45	

Table 1: Descriptive statistics of the variables used in the model development













Figure 1. Histograms of the variables used in the model development

2. ADAPTIVE NEURO-FUZZY INFERENCE SYSTEM (ANFIS)

Fuzzy modeling is a strong method which deals with the construction of a fuzzy model that can explain the behavior of an unknown system determined by a set of sample data. Fuzzy inference system (FIS) simulate nonlinear behavior with linguistic fuzzy rules. The components of this system are comprised: fuzzy if-then rules, membership function and inference system that combines the fuzzy rules and produces results of system. There are two methodologies of FIS including Mamdani-type and Sugeno-type. The first fuzzy identification explored by Sugeno et al, has found numerical applications in control and predicting. [24-27]

For example if the FIS had two inputs, x_1 and x_2 , and one output, y, for the zero-order Sugeno-type system, two typical rules are expressed as below:

- Rule-1: If x_1 is A_1 and x_2 is B_1 , then $y_1 = a_1x_1 + b_1x_2 + c_1$
- Rule-2: If x_1 is A_2 and x_2 is B_2 , then $y_2 = a_2 x_1 + b_2 x_2 + c_2$

Where, x_1 and x_2 are the crisp inputs, A_i and B_i are the linguistic labels qualified by membership functions and a_i , b_i and c_i are the result parameters. While y_i is constant instead of linear relationship, we have zero-order Sugeno-type fuzzy system. The adaptive neurofuzzy inference system (ANFIS) mechanism are shown in the Fig. 2, as can be seen form this figure, the ANFIS process includes of six steps, the sequence of ANFIS architecture are given as follow [28-31]:

Layer 1: In this layer, the inputs are distributed to the neurons in the next layer.

Layer 2: In this layer as a fuzzification layer, each neuron *i* produce a member ship grades of a linguistic label. Each node's output O_i^2 , in this layer is calculated as below:

$$O_i^2 = \alpha A_i(x_1); \quad O_i^2 = \alpha B_i(x_2); \quad i = 1, 2$$
 (1)

where, αA_i and αB_i are the membership functions for A_i and B_i fuzzy sets, respectively. To specification of membership grades various membership functions can be used, for example trapezoidal, triangular, Gaussian function, etc.



Figure 2. Corresponding adaptive neuro-fuzzy inference system architecture

Layer 3: This layer is named rule layer. In this layer each node matches to a single fuzzy rule. Each rule neurons receives inputs from respective fuzzification node in previous step and calculates the firing strength of the rule. The firing strength O_i^3 called as w in the below equation:

$$O_i^3 = w_i = \alpha A_i(x_1) \alpha B_i(x_2), \quad i = 1, 2$$
 (2)

Layer 4: Each node of this layer as a normalization layer, receives inputs from neurons of the rule layer and computes the normalized firing strength. Indeed each outputs of this layer is the ratio of the *i* th rule's firing strength to the summation of all rule's firing strength:

$$O_i^4 = \overline{w}_i = \frac{w_i}{\sum w_i}, \quad i = 1, 2$$
 (3)

Layer 5: This layer is the defuzzification layer. Each node in this layer receives initial inputs, x_1 and x_2 , and calculates the output according the follow defined equation:

$$O_i^5 = \overline{w_i} y_i = \overline{w_i} (a_i x_1 + b_i x_2 + c_i), \quad i = 1, 2$$
 (4)

where w_i is the *i* th respective neuron in the layer 4. Also a_i , b_i and c_i are the coefficients of the linear stucture in the Sugeno-type FIS.

Layer 6: Finally a single node of this layer calculates the summation of outputs of all nodes in the previous layer. So the crisp output is obtained from this layer by defuzzification

process using following equation:

$$O_i^6 = y(x_1, x_2) = \sum \overline{w_i} y_i = \frac{\sum w_i y_i}{\sum w_i}$$
(5)

2.1 Development of the ANFIS model

The structure of each ANFIS model includes the issues such as select the inputs, choosing a type of FIS, determining the number of rules, specification of the type and number of membership function, etc. The most crucial step of these models is the determination of the optimum number and form of fuzzy rules. There are various algorithms to automate this process, such as *k*-means clustering, *C*-means clustering and subtractive clustering. In this study we use the subtractive clustering method. This method based on the density of surrounding data points, calculates a measure of the likelihood that each data point would define the cluster center. This algorithm can be defined as follow:

- 1. Select the highest potential data point to be the first cluster center.
- 2. Determine all data point in the vicinity of the first cluster center by the range of influence and remove them.
- 3. Iteration of this process until all data point are within the radii of a cluster center.
 - Also there are four parameters that adjust rate of clustering process:

(1) Range of influence: It specifies the radius of a cluster when space of data is a unit hypercube. This parameter usually are considered between 0.2 and 0.5. It is clearly that smaller radius produces more clusters in the data and it is also resulted more rules. In this study the value of 0.5 was used for all of inputs and output.

(2) Squash factor: This parameter determine the neighborhood of cluster center by multiply the radii values, so the potential of outlying points is squashed to be considered as part of cluster. The factor of 1.25 was used in here.

(3) Accept ratio: This ratio determines the potential of the data points as a fraction of the potential of the first cluster center, each data point with value above which another data point, will be accepted as a cluster center. A ratio of 0.5 was used in this study.

(4) Reject ratio: This ratio determines the potential of the data points as a fraction of the potential of the first cluster center, each data point with value below which a another data point, will be rejected as a cluster center. A ratio of 0.15 was used in this study. [32, 33]



Figure 3. Membership function plots

Optimization of membership function's parameter is another important step. The membership functions (MF) plots of AS (range of 1-180), MB (range of 0-0.3), SB (range of 0-0.09), WB (range of 0.25-0.5), BA (range of 0.1-0.35) and FC (range of 0.31-1.45) are shown in Fig. 3, respectively. To achieve the best fit of input-output data set, two learning rule are used, the back-propagation gradient descent is the basic learning rule of ANFIS. This method calculates errors from output node backward to the input nodes, recursively. Another learning rule is named hybrid-learning, this rule combines the gradient descent and least-squares method to find antecedent and consequent parameter sets. A procedure of this method is shown schematically in Fig. 4. Hybrid-learning was used in this study. Over fitting is one of the problems that occur during ANFIS learning. This problem occurs when the error of training data set is small, but by entering new data to the ANFIS structure, the output error is large. For solving this problem, the data set is divided into three category: training set, checking set and testing set. Accordingly when over fit begins, the error of checking set increases and the learning is stopped. So the checking set are used to prevent over fitting in the ANFIS learning process, which is referred to a case where the error is driven to very small values, yet the ANFIS loses its ability to make accurate predictions for other data than those used in the training set. In this study available data base are randomly divided into three sets, 60% for training, 20% for checking and the last 20% for testing.

Therefore out of 469 experimental data, 329 vectors are used for training, 70 data for checking and 70 data for testing.



Figure 4. Hybrid learning procedure of ANFIS

3. STEPWISE REGRESSION (SR) PROCEDURE

SR is potentially capable of generating statistical models that capture the relationship between independent variables and dependent variable. SR is an iterative process that is used to choose which predictor variables to include in a regression model. SR selects the best combination of independent variables to predict the dependent variable for a system in which no clear relationship is available between inputs and outputs. The best combination of independent variables that best fits the dependent variable are identified sequentially by adding or deleting, depending on the method, the one variable that has the greatest impact on the residual sum of squares. Although it is felt that the investigation of all subsets produces the "best" set, it is not the most widely used method because of its computational cost. The stepwise procedures, which consist of either adding or deleting one explanatory variable at a time, have been the favorite methods throughout. One distinguishes forward selection and backward elimination stepwise procedures, and a combination of both. Forward stepwise selection of variables chooses the subset models by adding one variable at a time to the previously chosen subset. Forward selection starts by choosing as the one-variable subset the independent variable that accounts for the largest amount of variation in the dependent variable. This will be the variable having the highest simple correlation with dependent variable. At each successive step, the variable in the subset of variables not already in the model that causes the largest decrease in the residual sum of squares is added to the subset. Without a termination rule, forward selection continues until all variables are in the model. On the other hand, backward elimination of variables chooses the subset models by starting

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with the full model and then eliminating at each step the one variable whose deletion will cause the residual sum of squares to increase the least. This will be the variable in the current subset model that has the smallest partial sum of squares. Without a termination rule, backward elimination continues until the subset model contains only one variable. It should be kept in mind that neither forward selection nor backward elimination takes into account the effect that the addition or deletion of a variable can have on the contributions of other variables to the model. A variable added early to the model in forward selection can become unimportant after other variables are added, or variables previously dropped in backward elimination can become important after other variables are dropped from the model. The variable selection method commonly labeled SR is a forward selection process that rechecks at each step the importance of all previously included variables. If the partial sums of squares for any previously included variables do not meet a minimum criterion to stay in the model, the selection procedure changes to backward elimination and variables are dropped one at a time until all remaining variables meet the minimum criterion and then forward selection resumes. Stepwise selection of variables requires more computing than forward or backward selection but has an advantage in terms of the number of potential subset models checked before the model for each subset size is decided. It is reasonable to expect stepwise selection to have a greater chance of choosing the best subsets in the sample data, but selection of the best subset for each subset size is not guaranteed. The stopping rule for stepwise selection of variables uses both forward and backward elimination criteria. The variable selection process terminates when all variables in the model meet the criterion to stay and no variables outside the model meet the criterion to enter (except, perhaps, for the variable that was just eliminated). The criterion for a variable to enter the model need not be the same as the criterion for the variable to stay [33].

3.1 Model development

SR was used to predict the compressive strength of concrete containing metakaolin. four different models are developed for this purpose. These models use 80% of the total data for training and the remaining 20% for testing. Possible forms for all combinations of independent variables used for the stepwise selection process are given as follows:

$$X_i, X_i \times X_j, \frac{X_i}{X_j}, X_i^{X_j}$$

Where X_i stands for the independent variables given in {*Input*}. Models considered for the SR process are given in Table 2 for two independent variables (X_1 , X_2) and one dependent variable (y) with possible corresponding equations. All possible combinations of independent variables with models considered and corresponding equation of best subset are given in Table 3. For the analysis, the data sets are divided into training and testing subsets. Out of 469 data for the prediction of f_c of concrete containing metakaolin, 375 data vectors are used for training and 94 data for testing data. The SR analysis was implemented by using the SPSS. As it is obvious a model equation with more parameters gives more accurate formulae. It should be mentioned that using a lengthy model equation lead to a more complicated formulae. Therefore, it is desirable to achieve a practical formula by considerable accuracy. Here we investigate four different models to evaluate the target formulations based SR method. Each model more comprehensive than 4 gives a lengthy and

tedious equation which cannot be recommended for practical usage. Therefore, the equation 4 gives the compressive strength of concrete containing metakaolin with good accuracy for practical considerations.

Table 2: Models considered in SR method.						
Model	Input	Equation				
1	X_1, X_2	$y = a_0 + a_1 X_1 + a_2 X_2$				
2	$X_1, X_2, X_1^2, X_1 \times X_2, X_2^2$	$y = a_0 + a_1 X_1 + a_2 X_2 + a_3 X_1^2 + a_4 (X_1 \times X_2) + a_5 X_2^2$				
3	$X_1, X_2, X_1^2, X_1 \times X_2$, $X_2^2, \frac{X_1}{X_2}, \frac{X_2}{X_1}$	$y = a_0 + a_1 X_1 + a_2 X_2 + a_3 X_1^2 + a_4 (X_1 \times X_2) + a_5 X_2^2 + a_6 \frac{X_1}{X_2} + a_7 \frac{X_2}{X_1}$				
4	$X_{1}, X_{2}, X_{1}^{2}, X_{1} \times X_{2}, X_{2}^{2}, \frac{X_{1}}{X_{2}}, \frac{X_{2}}{X_{1}}, \frac{X_{2}}{X_{1}}, X_{1}^{X_{1}}, X_{1}^{X_{2}}, X_{2}^{X_{1}}, X_{2}^{X_{2}}$	$y = a_0 + a_1 X_1 + a_2 X_2 + a_3 X_1^2 + a_4 (X_1 \times X_2) + a_5 X_2^2 + a_6 \frac{X_1}{X_2} + a_7 \frac{X_2}{X_1} + a_8 X_1^{X_1} + a_9 X_1^{X_2} + a_{10} X_2^{X_1} + a_{11} X_2^{X_2}$				

 Table 3: Equations representing SR generated for estimating compressive strength of concrete containing metakaolin

Model	Equation	R				
	A					
1	$f_c = 30.063 + 69.253AS^{0.1} - 151.502WB - 10.098FC + 16.692MB + 59.645SB $ (6)	0.867				
	$f_{c} = -240.947 - 242.935(WB \times BA) + 411.112AS^{0.1} - 124.725AS^{0.2} - 47.744(WB \times FC) - 277.475(MB \times BA)$					
2	$+110.766 MB - 476.483 MB^{2} + 436.814 BA^{2} + 2488.03 (SB \times FC) - 6255.1 (SB \times BA) + 24.303 (AS^{0.1} \times FC) + 24.303 $					
	$-20.145FC^{2} - 53.623(AS^{0.1} \times WB) + 56.66(AS^{0.1} \times MB) $ (7)	0.948				
	$AS^{0.1}$ WB					
	$f_c = 243.563 + 33.358 \frac{AS^{0.1}}{FC} - 14.217 \frac{WB}{BA} - 1010.52(MB \times BA) - 519.388MB^2 + 1479.215(MB \times WB)$					
	$-170.179 \frac{FC}{AS^{0.1}} - 102.689 \frac{WB}{AS^{0.1}} + 28.822 \frac{FC}{BA} - 3325.94 (WB \times BA) - 243.345 (AS^{0.1} \times MB) + 231.093 \frac{MB}{WB}$					
3	$-28.021\frac{MB}{BA} - 545.45\frac{MB}{AS^{0.1}} + 3550.703(SB \times BA) + 27.661\frac{MB}{FC} - 439.176\frac{BA}{WB} + 2032.934WB^{2}$	0.968				
	$-130.082(AS^{0.1} \times WB) + 641.942 \frac{SB}{BA} - 2287.47 \frac{SB}{FC} - 1395.78WB + 3915.356BA - 133.568 \frac{BA}{FC}$					
	$-363.719(AS^{0.1} \times BA) - 472.876 \frac{BA}{AS^{0.1}} $ (8)					

	$f_c = -268.121 - 322.003AS^{0.1WB} + 112.041SB^{BA} + 28.939AS^{0.1AS^{0.1}} + 216.469(WB \times FC) - 114.466SB^{FC}$					
	$-190.592\frac{BA}{FC} + 8004.884(SB \times WB) + 17.795\frac{FC}{BA} - 79.677\frac{MB}{FC} + 133.231AS^{0.1FC} - 225.105FC^{MB}$					
4	$-592.274(AS^{.01} \times MB) - 489.459 \frac{WB}{AS^{0.1}} - 899.175FC^{BA} + 429.917(BA \times FC) - 201.198(AS^{0.1} \times FC)$					
	$-173.867 SB^{WB} + 998.391 WB^2 - 729.862 MB^{AS^{0.1}} + 1380.058 MB + 67.989 FC^{AS^{0.1}} - 41.187 MB^{FC}$					
	$+3.405SB^{MB} - 1132.85SB^{AS^{0.1}} - 566.081WB - 214.631WB^{AS^{0.1}} + 1819.592\frac{SB}{AS^{0.1}} - 23430.8SB^{2}$					
	$+2288.716(SB \times FC) + 1830.231(SB^{SB}) + 5939.491(SB \times BA) $ (9)					

4. PERFORMANCE ANALYSIS, MODEL VALIDITY, AND COMPARATIVE STUDY

The parameters used to evaluate the performance of the proposed models were absolute percentage error (Err) for the *i*th output, correlation coefficient (R), mean squared error (MSE) and mean absolute error (MAE). *Err*, *R*, *MSE* and *MAE* can be presented in form of formulas as follows:

$$Err_{i} = \frac{\left|y_{i} - t_{i}\right|}{t_{i}} \times 100 \tag{10}$$

$$R = \frac{\sum_{i=1}^{N} (y_i - \overline{y}_i)(t_i - \overline{t}_i)}{\sqrt{\sum_{i=1}^{N} (y_i - \overline{y}_i)^2 \sum_{i=1}^{N} (t_i - \overline{t}_i)^2}}$$
(11)

$$MSE = \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)^2$$
(12)

$$MAE = \frac{1}{N} \sum_{i=1}^{N} |y_i - t_i|$$
(13)

Where t_i and y_i are the actual and predicted output values for the *i*th output, respectively. $\overline{t_i}$ and $\overline{y_i}$ are the average of the actual and predicted outputs, respectively and *N* is the number of samples.

Performance statistics of the ANFIS and SR models in terms of its prediction capabilities is summarized in Table 4. These parameters show that two models are more capable to predict the predict f_c of concrete containing metakaolin. Also the results of predicted f_c values using ANFIS and SR models are illustrated in Fig. 5 and Fig. 6.

Method	Training			checking			Testing		
	R	MSE	MAE	R	MSE	MAE	R	MSE	MAE
ANFIS Model	0.9238	67.1307	5.2161	0.9247	66.1179	4.9662	0.9482	48.5435	4.4715
SR Model	0.9805	17.4023	3.1714	-	-	-	0.9506	39.9959	4.5094

Table 4: Performance statistics of the models for f_c prediction.



Figure 5. Results of predicted strength of concrete containing metakaolin using ANFIS model



Figure 6. Results of predicted strength of concrete containing metakaolin using SR model

In order to show the validation of the developed aforementioned model, it needs to propose an accepted criteria. Gandomi *et al.* [34] introduced a criteria that suggested by Smith [35] for model validity as follow:

1- If a model gives |R| > 0.8, a strong correlation exists between the predicted and measured values.

2- If a model gives 0.2 < |R| < 0.8 a correlation exists between the predicted and measured values.

3- If a model gives |R| < 0.2, a weak correlation exists between the predicted and measured values. It was mentioned by Alavi *et al.* [36] that for a good validation the error values (e.g., *MSE*, *MAE*) should be at the minimum. Therefore, a developed model with high *R* and low *MSE*, *MAE* values gives an acceptable degree of accuracy. Based on the measured

performance values in Table 4, it can be found that the proposed models give reasonable degree of accuracy, and it can be judged as accurate models, however SR model has a more strong correlation between the predicted and measured values. A comparison between the predicted and experimental compressive strength values of concrete are visualized in Fig. 7. It is obvious that a model contains reasonable accuracy as the numerical to predicted values of strength ratio is close to one. It can be seen from Fig. 7 that, the distribution frequency for SR proposed equation gives us a more accuracy than ANFIS model.



Figure 7. A comparison between the predicted and experimental compressive strength values of concrete containing MK

Also the ratios of the $P_{exp} / P_{proposed model}$ with respect to the AS, MB, SB, WB, AB and FC are also shown in Figs. 8, 9, 10, 11, 12 and 13, respectively. Based on the presented graphs, if the scattering increases, the accuracy of the model would be decreased subsequently. It is

evident from the presented figures that the predictions based proposed formula by SR gives more exact results compare to ANFIS model.



Figure 8. The ratio between the predicted and experimental compressive strength values with respect to AS



Figure 9. The ratio between the predicted and experimental compressive strength values with respect to MB





Figure 10. The ratio between the predicted and experimental compressive strength values with respect to SB



Figure 11. The ratio between the predicted and experimental compressive strength values with respect to WB



Figure 12. The ratio between the predicted and experimental compressive strength values with respect to BA





Figure 13. The ratio between the predicted and experimental compressive strength values with respect to FC

5. CONCLUSIONS

In the current study the numerical study was undertaken for 496 data providing from reliable database and proposed two models for predict compressive strength of concrete containing metakaolin. For its sake six input parameters including age of specimen and ratios of metakaolin-binder, super plasticizer-binder, water-binder, binder-aggregate and fine aggregate- coarse aggregate, was undertaken. In the first step, Neuro-fuzzy network was used to model the strength of concrete containing metakaolin and system was trained by dividing dataset into three sets including training, checking and testing dataset and using of hybrid-learning. In the next step, stepwise regression was used for propose the new formulae to predict the compressive strength of concrete containing metakaolin. Finally the comparison was accomplished between two models. The result demonstrated that SR model is accurate than ANFIS model. However the both of models are capable to be employed for assessment of compressive strength of concrete containing metakaolin by practical engineers.

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