Mathematical & Computational Applications, Vol. 8, No. 2, pp. 209-216, 2003

PREDICTION OF RATIO OF MINERAL SUBSTITUTION IN THE PRODUCTION OF LOW-CLINKER FACTORED CEMENT BY ARTIFICIAL NEURAL NETWORK

Fethullah CANPOLAT[a], Kemalettin YILMAZ[b], Raşit ATA[c], M.Metin KÖSE[a]
[a]Dep. of Civil Eng. Celal Bayar University, 45040 Manisa, Turkey
[b]Dep. of Civil Eng, M.Y.O., Sakarya University, 54188 Adapazarı, Turkey
[c]Dep. of Electrical and Electronics Eng. Celal Bayar University, 45040 Manisa, Turkey

Abstract- Artificial Neural Networks (ANN) has been widely used to solve some of the problems in science and engineering, which requires experimental analysis. Use of ANN in civil engineering applications started in late eighties. One of the important features of the ANN is its ability to learn from experience and examples and then to adapt with changing situations. Engineers often deal with incomplete and noisy data, which is one of the areas where ANN can easily be applied. Dealing with incomplete and noisy data is the conceptual stage of the design process.

This paper shows practical guidelines for designing ANN for civil engineering applications. ANN is in cement industry: in the production of low-clinker factored cement, and in the derivation of composition of natural and artificial puzzolans in the production of high performance cement and concrete. By using ANN, a study to find out the optimum ratio of substitution and compression strengths was carried out.
Keywords- Artificial neural networks; Civil engineering materials design and optimization; blended cement, Mineral admixtures in cement; Natural zeolites, fly ash, coal bottom ash, volcanic ash.

1. INTRODUCTION

As civil engineering and science of structures have progressed, structures become more complex and much bigger. So, need for the high performance and multi-purpose cement becomes high. [1].

Cement, which contains only fly ash, silica fume or natural puzzolon, can not be satisfied the demand for performance and functionality. As a result, recent researches have been concentrated on the cements that have more than two additives [2]. Mineral admixtures in cement reduced bleeding, reduced temperature rise, reduced alkali-aggregate reaction, reduced permeability, reduced volume change reduced creep, improved sulfate resistance, increased ultimate strength and economy[3,4]. It has been expected that production process of cements that have three or four additives will be determined more accurately and this kind of cements will be used more widely in 21st century [2].

Reduction of NOx and COx in the cement reduction will make possible to produce low-clinker factored cement. Use of admixtures which does not produce CO_2 in the cement production will reduce the air pollution and production cost.

2. ARTIFICIAL NEURAL NETWORKS

Artificial neural systems are physical cellular systems, which can acquire, store and utilize knowledge. Currently neural networks can already be of great value in helping to solve many problems. Architectures with a large number of processing units enhanced by extensive interconnectivity provide for concurrent processing as well as parallel distributed information storage.

In this study, a multi-layer, feed-forward, back-propagation ANN architecture is used. The multi-layer perception has an input layer, two hidden layers, and an output layer. The input vector representing the pattern to be recognized is incident on the input layer and is distributed to subsequent hidden layers, and finally to the output layer via weighted connections. Each neuron in the network operates by taking the sum of its weighted inputs and passing the result through a nonlinear activation function (transfer function) [5].

If o_j^m represent the output of the *j*th neuron in the *m*th layer, and W_{ij}^m the weight on connection joining the *i*th neuron in the $(m-1)$th layer to the *j*th neuron in the *m*th layer, then:

$$o_j^m = f\left[\sum_i \left(W_{ij}^m o_j^{m-1}\right)\right], \qquad m \geq 2, \tag{1}$$

where the function *f*(.) can be any differentiable function. In this study the sigmoid function defined below is used as the transfer function.

$$f(x) = \frac{1}{1+e^{-x}} \tag{2}$$

This function limits the outputs o_j^m among 0 and 1. To achieve the required mapping capability, the network is trained by repeatedly presenting a representative set of input/output patterns, with a back-propagation error and weight adjustment calculation to minimize the global error E_P of the network, i.e.

$$E_P = \frac{1}{2}\sum_{j=1}^{n_0}\left(t_{pj} - o_{pj}^m\right)^2 , \tag{9}$$

where t_{pj} is the target output of neuron *j* and o_{pj}^m is the computed output from the neural network corresponding to that neuron. Subscript *p* indicates that the error is considered for all the input patterns.

Minimization of this average sum-squared error is carried out over the entire training patterns. As the outputs o_{pj}^m are functions of the connection weights $\mathbf{w}^m$ and the outputs o_{pj}^{m-1} of the neurons in the layer $m-1$, which are functions of the connection weights $\mathbf{w}^{m-1}$, the global error E_P is a function of $\mathbf{w}^m$ and $\mathbf{w}^{m-1}$. Here, **w** with a superscript refers to the connection matrix. To accomplish this, **w** evaluates the partial derivative, $\partial \mathbf{E}/\partial \mathbf{W}_{ij}$ and supplies a constant of proportionality as follows:

$$\Delta W_{ij} = \varepsilon\, \delta_{pj}\, o_{pi} \tag{3}$$

where ε refers to the learning rate, δ_{pj} refers to error signal at neuron *j* in layer *m*, and o_{pi} refers to the output of neuron *i* in layer $m-1$. δ_{pj} is given by

$$\delta_{pj} = (t_{pj} - o_{pj})o_{pj}(1 - o_{pj}) \quad \text{for output neurons,} \qquad (4)$$

$$\delta_{pj} = o_{pj}(1 - o_{pj})\Sigma_k \delta_{pk} w_{kj} \quad \text{for hidden neurons,} \qquad (5)$$

where o_{pj} refers to layer m, o_{pi} refers to layer $m-1$, and δ_{pj} refers to layer $m+1$. In practice, a momentum term (μ) is frequently added to Eq. (3) as an aid to more rapid convergence in certain problem domains. The weights are adjusted in the presence of momentum by:

$$\Delta W_{ij}(n+1) = \varepsilon\,(\delta_{pj}\, o_{pi}) + \mu \Delta W_{ij}(n). \qquad (6)$$

A backpropagation algorithm is used in the optimization in which the weights are modified [5].

3. ANALYSIS OF MINERAL SUBSTITUTION RATE IN CEMENT PRODUCTION BY ANN

As explained in the introduction, it is known that substituted mineral in cement production affect the performance of the cement and concrete. That's why in practice, the substitution rate of the minerals should be optimized.

In this study, use of Gördes natural zeolite, fly ash from Soma thermal plant and volcanic ash form Kula-Gokçeören as admixtures in the cement production with different combination was investigated. Experiments were carried out in laboratory of CIMENTAS Izmir Cement Plant T.A.S.

Physical and chemical properties of the cement mixtures prepared in the laboratory were determined according to TS 687 and TS 24, respectively. 42 different cement compositions were obtained. 252 cement prisms in the dimensions of 4*4*16 cm were produced. 2, 7, 28 and 90 days compression strength of these prisms were determined. The results were used in ANN program as desired values.

The percent mineral substitution rates are taken as input values and the compressive strength of the concrete at 2, 7, 28 and 90 days are taken as output values in ANN analysis.

The design process includes the following steps:

(i) Preparation of suitable training data

(ii) Selection of a suitable ANN structure

(iii) Training of the ANN

(iv) Evaluation of the trained network

It is important to appreciate that the design process is iterative. It is possible that a particular structure chosen in step (ii) may not train to a designer's satisfaction. In this situation, the structure has to change and the ANN should be retrained. Also, the trained network may not perform satisfactorily on test data. In that situation, network structure and training data should be changed and network retrained and tested.

3.1. Preparation of Training Patterns

The training patterns should contain necessary information to generalize the problem. The preparation of a training set includes three stages. Firstly, system parameters are collected and prepared for a load flow study. Additional information needed at this stage is the maximum & minimum load consumption at each load bus and the maximum & minimum generations at each power plant. Secondly, for different system topologies, a number of load flow studies are carried out, assuming that the state variables take values uniformly distributed in between the lower and upper limits. Finally the obtained load flow patterns are normalized between [0,1]. To produce a testing set consistent to the training set, it is necessary to keep track of the normalization. The same normalizing parameters as used in the training data normalization are also used in processing the test data.

3.2. Structure of the Neural Network

The selection of the structure of the proposed network includes the selection of number of layers, choice of transfer function, number of inputs and number of neurons in each layer. As already mentioned, a three-layer feed-forward network can model complex-mapping functions reasonably well and, therefore, is suggested for this application. A sigmoidal non-linear mapping function helps in modeling functions of arbitrary shape and is employed in this application. The number of neurons in the input layer and hidden layers are decided by experimentation, which involves training and testing different network configurations. The neural network literature [6,7] provides guidelines for selecting the number of neurons for a starting network.

3.3 Training and Evaluation

Training of the selected network is done using training patterns and backpropagation algorithm. To achieve generalization, training and testing are interleaved. Training is stopped when the mean squared error between actual outputs and desired outputs stops improving. However, at that point, if the designer is not satisfied with the training and performance of the ANN, the training data and structure of the ANN are modified and the design process is repeated.

ANN has been used widely in many areas due to its multi input parallel processing ability. Even if there is an increase in number nodes, calculation time of network remains constant. Also, making changes or additions in trained ANN when needed can be performed easily.

As seen in Figure 1, structure of ANN was selected as 5:2:4 system. In another words, number of nodes in input layer, number of nodes in hidden layer and number of nodes in output layer was selected as 5, 2 and 4, respectively. Portland cement clinker (PC), natural zeolite (ZE), volcanic ash (VA), fly ash (FA) and bottom ash (BA) were taken as input parameters and compressive strengths of cement samples at 2^{nd} (W), 7^{th} (X), 28^{th} (Y) and 90^{th} (Z) days were taken output parameters. Change of training error vs. number of nodes in hidden layer was shown in Figure 2. As seen from Figure 2, when number of nodes in hidden layer is between 2 and 5 training error becomes minimum. That's why number of nodes in hidden layer was selected as 2. Enough number of training samples was taken into the consideration to generalize the network when ANN was trained by using training data.

As a result, minimum error of 0.543% was reached when number of iteration is equal to 10,000, training coefficient, ε, is equal to 0.9 and momentum coefficient, α, is equal to 0.9. Error values at number iteration of 10,000 for various training and momentum coefficients were given in Table 1.

Tablo 1. %Error at number iteration of 10,000 for various training,ε, and momentum,α, coefficients

Iteration	ε	α	Hidden nodes	% Error
10.000	0.9	0.9	1	1.44
			2	0.51
			3	0.53
			4	0.58
			5	0.54
			6	12.02
			7	316.8
	0.75	0.1	1	1.44
			2	0.59
			3	0.66
			4	0.70
			5	0.67
			6	12.55
			7	45.45
	0.1	0.1	1	1.49
			2	0.81
			3	0.76
			4	0.77
			5	0.76
			6	3.72
			7	136.0

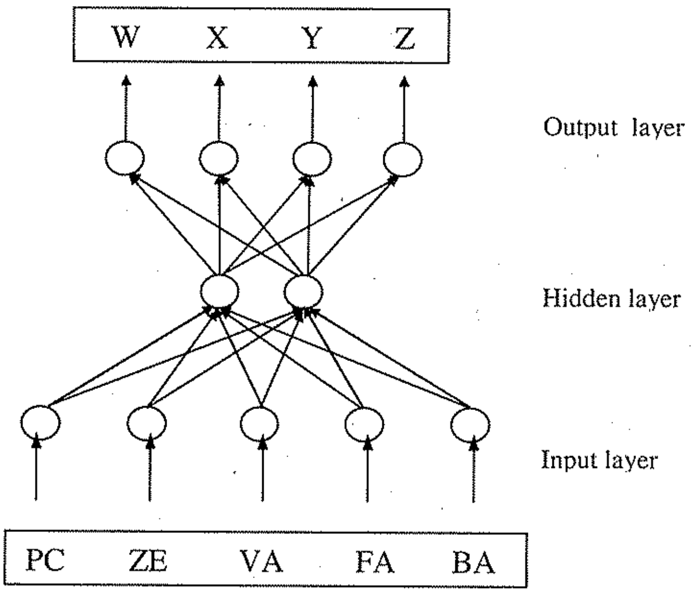

Figure 1. Structure of ANN

This trained ANN was used to obtain the output values for different input values. This was done in testing stage. By testing phase, the results can be obtained about 10^{-3} seconds.

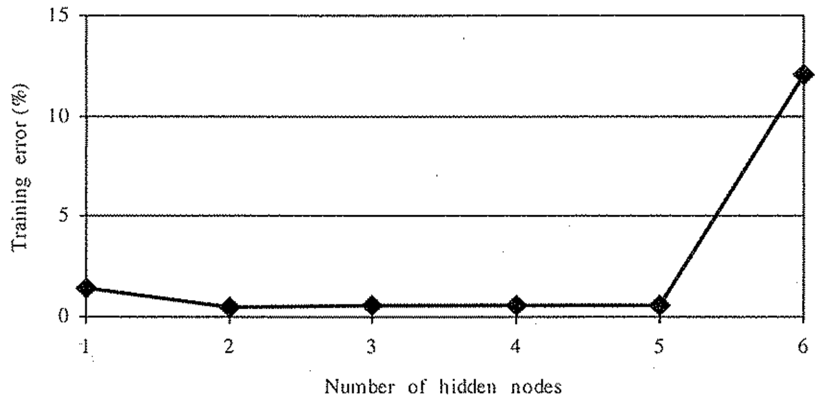

Figure 2. Effect of number hidden nodes to training error.

In this ANN based study, output parameters, 2^{nd}, 7^{th}, 28^{th} and 90^{th} days compressive strengths were estimated with an accuracy of 99.457%. Since the accuracy is very high, ANN can be used in future for the system which has large number of input and output values.

ANN program used in this study was written by authors using Turbo PASCAL programming language and the method of backpropagation. This computer program can be used in PC's and was programmed for a general use in various areas. Number of input neurons, hidden layers, hidden nodes and outputs can be entered easily.

4. APPLICATION EXAMPLE

The different ANN structures, training and momentum coefficient were taken into the account in the training of ANN. Relationship between hidden nodes and training error was shown in Figure 2 for momentum coefficient $\alpha = 0.9$. Also, the relationship between the number of iteration and training error was shown in Figure 3 for ANN structure of 5:2:4 when mometum coefficient $\alpha = 0.9$ and training coefficient $\varepsilon = 0.9$.

In training set of ANN program: input values, ratio of substituted materials in 42 different cement composition, output values and compression strength of cement samples were used.

Relationship between number of hidden nodes and errors is shown in Figure 2 when number of iteration is equal to 10,000. Relationship between number of iteration and errors is Figure 3 when number hidden nodes is equal to 2.

So, at the end of training set, training coefficients were determined as $\alpha=0.9$, $\varepsilon = 0.9$, number of input nodes =5, number of hidden nodes =2 and number of output nodes=4. Experimental results were evaluated in ANN using these coefficients. 10 different cement composition were not used in ANN training phase. These results were used in the ANN testing phase to check reliability of the training coefficients.

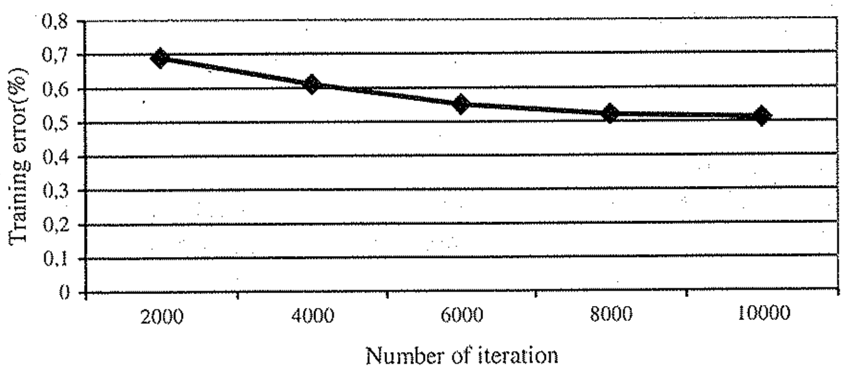

Figure 3. Relationship between number of iteration and training error

Table 2. Input values used in experiments

Test No	INPUT					Total ratio of substituted material (%)
	Ratio of substituted materials (%)					
	Clinker of PÇ	Natural Zeolite	Volcanic ash	Fly ash	Coal Bottom ash	
1	70	30	0	0	0	30
2	75	0	25	0	0	25
3	80	15	0	5	0	20
4	65	30	0	5	0	35
5	80	15	0	0	5	20
6	60	35	0	0	5	40
7	85	5	10	0	0	15
5	70	5	25	0	0	30
9	80	15	5	0	0	20
10	65	30	5	0	0	40

Table3. Comparison of ANN and experimental results

Test No	Real Output				ANN Output			
	Compressive strength (N/mm^2)				Compressive strength (N/mm^2)			
	2 day	7 day	28 day	90 day	2 day	7 day	28 day	90 day
1	13.4	26.8	47.8	58.5	12.7	24.8	48.5	54.8
2	17.5	32.8	42.8	48.3	17.5	28.2	40.4	47.1
3	17.8	28.4	51.0	59.4	17.5	30.5	52.3	58.2
4	11.8	24.2	47.6	54.3	11.8	23.6	47.7	54.0
5	15.5	29.6	52.7	57.9	17.3	30.3	52.3	58.2
6	11.9	21.9	45.6	48.9	9.9	20.9	44.2	50.7
7	17.5	30.3	46.5	53.9	19.8	31.5	46.8	53.1
8	15.0	26.4	39.5	45.0	15.2	25.9	40.0	46.8
9	15.2	28.3	49.0	54.9	17.2	29.6	49.6	55.7
10	11.3	23.0	45.1	51.3	11.2	22.6	44.8	51.3

CONCLUSIONS

In this study, optimization of rates of material substitution was presented by the use of ANN. Due to generalization and parallel information process capacity of ANN, ANN analysis predicted the multi-layer network output value as well as 99.457%.

This study is one of the first step of series of the studies can be made in this field. So, a successful application of ANN in this field is very important. Using ANN in the determination of the different composition of the substituted materials in the production of the low-clinker factored cement, adequate cement compositions, which takes one to three months experimentally, can be determined. Different cement compositions can be obtained using ANN in a very short time (Using the test phase in trained ANN, goal value was reached in 10^{-3} seconds) with a degree of error of 0.543% as shown in Table 3 after training phase is completed. In this study it was shown that ANN could be used in the determination of the ratio of substituted materials. Most important feature of the ANN in engineering problems is that ANN learns and makes the calculations by using experimental results. The other important feature is that ANN can be used in the problems, which have scattered or not enough data and in the problems of which theory has not been completed, and it gives solution closer to the exact solution.

REFERENCES

1. Uchikawa, H and Okamura ,T., Binary and Ternary Components Blended Cement, *Mineral Admixtures in Cement and Concrete ,ed. S.L., Sarkar, ABI Press, N. Delhi,1993, pp. 1-83*
2. ROUMAIN, J.C. and SARKAR, S.L., Cements of the 21st Century, *Second International Symposium on Cement and Concrete Technology in the 2000 s*, Vol.1, pp.29-40, Istanbul, 2000
3. Sobolev K.G.and Soboleva S.V,"High Performance Indegeneous Cement"; *XXIVth World Housing Congress*, pp .189-202, Ankara,1996.
4. Sobolev K.G.and Soboleva S.V,"Complex Admixture and Method of Cement Based Materials Production "; *Patent Application No 97/00426*, Ankara, 1997
5. Karlik B, Ozkaya E, Aydin S, Pakdemirli M. Vibrations of a beam-mass systems using artificial neural networks. Computers & Structures 1998;69: 339-347.
6. R.P. Lippman, "An Introduction to Computing with Neural Nets", *IEEE ASSP Magazine*, April, 4-22, 1987.
7. D. Hammerstrom, "Working with Neural Networks", *IEEE Spectrum*, July, 46-53, 1993.