Neural network architecture optimization by analyse the mechanical characteristics of civil engineering materials

C I Alecu¹, L Judele², M Movila², D Lepadatu³

¹Senior scientific researcher at Institute of Economic and Social Research Gh. Zane - Iasi, Romanian Academy Branch
²Senior Lecturer at Technical University “Gh. Asachi” Iaşi, Faculty of Civil Engineering and Building Services, Romania
³Associate Professor at Technical University “Gh. Asachi” Iaşi, Faculty of Civil Engineering and Building Services, Romania
daniel.lepadatu@gmail.com

Abstract. Our proposal for this paper is to diversify the architecture of neural networks in order to optimize it and to obtain the best performing configurations that minimize errors of predictive mechanical properties of polymeric concrete. In this paper different architectures of artificial neural networks will be used for investigating the flexural strength of polymer concrete with fly ash and fibres. In the present study the epoxy resin was used for binding the aggregates. In the composition were introduced near the fly ash, used as filler, the cellulose fibres for improving the properties. The characteristics of these artificial neural networks architectures will be presented and analysed in order to choose the one that minimizes the prediction errors of the mechanical characteristics of polymer concrete and presents an optimal configuration that allows a high working speed that can adapt to this type of approaching the problem with a strong nonlinear character. By using this modern predictive methods, it was attempted to highlight its basic character - learning by examples specific to the human brain but much more efficient due to the mathematical models of the activation functions and the interconnection between the layers of neurons that exponentially increase their ability to adapt to strong nonlinear phenomena. Thus one can say that such a prediction helps to reduce the number of real experiences and can greatly contribute to obtaining the optimal configuration of parameters necessary to obtain a desired mechanical characteristic of the analysed concrete.

1. Introduction

The present paper proposes a modern approach to the prediction concept for phenomena with a strong non-linear character using artificial neural networks. The precision of such predictions is the ability of the user experience to find the optimal network configuration that approximates the numerical results obtained by artificial intelligence from the experimental tests. This method is used by many researchers in different domains [1-5] because of its adaptability and prediction power which, through a process similar to that of the human neuron, brings consistency, rigor and speed to phenomena of black box type that involves far more resources to achieve the same results. From vocal recognition [1] to bioengineering [2], medicine [3, 4] or civil engineering [5-7], ANN use is an increasingly common option for analyzing and predicting complex phenomena.
To illustrate this phenomenon, we considered the choice of experimental testing in the area of concern of authors and the need to show that experimental design and optimization require modern methods of investigation and analysis. To highlight what has been said the aim in the paper is to study the polymer concrete with epoxy resin, fly ash and cellulose fibers, all composition with different dosage of components. The experimental results obtained for mechanical characteristics were compared with that obtained by using ANN model.

2. Materials and methods

2.1 Materials

The experimental researches on polymer concrete were made by using the following materials: polymer (X₁), fly ash as filler (X₂), crushed aggregates and fiber type ARBOCEL. The polymer was type epoxy resin, called ROPOXID, made in Romania by POLICOLOR București [8, 9]. The fly ash (FA) from the power plant CET Holboca Iasi was added to the fine aggregates. The principal characteristics of FA are: colour gray to black function of carbon unburned, particles sizes between 0.01 to 100 μm; the shape of particles is spherical, specific surface is between 4800-5200, the density is between 2400 and 2550 kg/m³ [2]. The aggregates were used in two sorts: 0-4 mm (X₃) and 4-8 mm (X₄), with continuous granulosity, obtained from crushed river gravel. The ARBOCEL fibers are natural cellulose fibers, produced by J. Rettenmaier and Sohne GMBH. ARBOCEL is produced from cellulose in a various qualities (fiber lengths, thicknesses, purities, etc.) The properties of ARBOCEL cellulose fibers are: mean fiber length of 10 μm, completely safe, insoluble in water and organic solvents, resistant to dilute acids and bases. The fiber was used in proportion of 3% from the mass of resin plus the hardener. For the study of polymer concrete properties nine compositions were prepared in the experimental program (Table 1) using Design of Experiment Method [10-13].

| Mix | Resin (%) | FA (%) | Aggregate (%) Sort I | Aggregate (%) Sort II | Response Y₁ |
|-----|-----------|--------|----------------------|----------------------|-------------|
| 1   | 12.4      | 12.8   | 37.4                 | 37.4                 | 14.69       |
| 2   | 12.4      | 6.4    | 43.8                 | 37.4                 | 14.18       |
| 3   | 15.6      | 9.6    | 37.4                 | 37.4                 | 17.09       |
| 4   | 15.6      | 6.4    | 40.6                 | 37.4                 | 14.09       |
| 5   | 12.4      | 9.6    | 40.6                 | 37.4                 | 14.60       |
| 6   | 16.4      | 7.2    | 38.2                 | 38.2                 | 17.03       |
| 7   | 13.2      | 10.4   | 38.2                 | 38.2                 | 15.35       |
| 8   | 13.2      | 7.2    | 41.4                 | 38.2                 | 13.55       |
| 9   | 14.0      | 8.0    | 39.0                 | 39.0                 | 17.57       |

2.2 Methods

This paper approach a field of high interest in research eco-concrete or ecological concrete with the possibilities of optimizing the additions of different recyclable wastes (ash, glass fiber for the present study), while maintaining its mechanical performances using a modern experimental planning methodology - Design of Experiment Method – DoE [10-12] specifies the investigation of new materials, supplemented by the power of analysis and optimization given by Artificial Neural Networks - ANN [1-7]. Concrete in combination with recyclable materials [8-11] such as ash and ultra-fine silica has unpredictable effects on concrete properties and therefore we have chosen to use these methods of investigation, since statistics and mathematics can capture the non-linear behaviour of this new additive material with the addition of recyclable materials. These additions can, in certain configurations of the recipe, greatly improve its mechanical behaviour doubled at the same time as the effective and
sustainable take-over of the effects of waste [13-15] on society and the environment. Based on learning from the examples, neural networks are able to predict the mechanical characteristics of ecological concrete with very high precision within the field of study, and sometimes even outside, so that to achieve superior performance of these features, it only takes their experimental validation, and therefore a substantial reduction in the cost of testing for the necessary mix formulas.

2.3 Artificial neural network (ANN) architecture

The ANN modelling approach is a computer methodology with artificial neurons that attempts to be similarly with the human nervous system. ANN has ability to solve new problems by applying information learned from past experience, as human brain [7, 12, 16]. Multi Layer Perceptrons (MLP) have been applied successfully to solve some difficult and diverse problems by training them in a supervised manner with a highly popular algorithm known as the error back-propagation algorithms. The most frequent structure for neural networks in investigations specific to engineering is MLP type. A back propagation algorithm can be used to train these multilayer feed-forward networks with differentiable transfer functions to perform function approximation, pattern association, and pattern classification. The training of ANNs by back propagation involves three stages:

1. feed-forward of the input training pattern,
2. calculation and back propagation of the associated error
3. adjustment of the weights.

This process can be used with a number of different optimization strategies [2, 7, 16]. Once the network is trained, it can be tested on a different set of data than that used for training. It is a good approach to divide the given input/output data into two parts: one part (about 70%) is used for training, whereas the other part, usually smaller, is used for testing the neural network model. The testing data set is reserved to validate the trained network. The training and testing of the networks were performed by means of the Matlab software. In this study, the performance of the ANNs were compared with respect to: mean squared error (MSE), mean absolute error (MAE), linear correlation coefficient (r). These performance measures are defined in the following equations (Eq. 1).

\[
MSE = \frac{1}{N} \sum_{i=0}^{N} (d_i - y_i)^2, \quad MAE = \frac{\sum_{i=0}^{N} |d_i - y_i|}{N}, \quad r = \frac{\sum_i (x_i - \bar{x})(d_i - \bar{d})}{\sqrt{\sum_i (x_i - \bar{x})^2} \sqrt{\sum_i (d_i - \bar{d})^2}}
\]

where: \(N\) is the total of training or testing exemplars, \(y_i\) is network output for exemplar \(i\), \(d_i\) is desired output for exemplar \(i\), \(x_i\) is network output, \(\bar{x}\) is average network output and \(\bar{d}\) is average desired output.

3. Results and Discussion

According to EN 12390 (2001) [17] the mechanical characteristic of polymer concrete with cellulose fiber experimentally determined: flexural strength (N/mm²) – \(Y_1\) are given in Table 1. The epoxy resin, fly ash and aggregate were considered as input variables, while \(Y_1\) were considered as the output value. Thus, each ANN presents three input variables and three output variable. In this study, the MLP (Fig. 2) was used for the modelling of the flexural properties of polymer concrete. In the present study, ANN network was trained using 6 data sets, they were then tested using 3 test data sets for verification of result. For neural modelling the following parameters have been used: the ANN is trained using the Backpropagation algorithm and the Conjugate Gradient method, maximum epochs of 20,000 and 0.001 learning rate. In our case in the process of learning, training and testing with several types of neural networks (100000) have chosen those configurations that approximates as closely as mechanical characteristic considered (Table 2).
So was kept three network architectures marked ANN 1 to 3 which have 4 input neurons and one output neuron or two hidden layers with variable number of neurons from any neuron in the second layer of the first type ANN - 1 to 10 neurons in the first hidden layer (Fig. 2) for the other two types of ANN - 2 and ANN - 3.

### Table 2. ANN architectures for polymer concrete mixtures

| Type      | Profile          | Inputs neurons | Haiden 1 | Haiden 2 | Outputs neurons |
|-----------|------------------|----------------|----------|----------|-----------------|
| ANN - 1   | MLP 4:4-6-1:1    | 4              | 6        | 0        | 1               |
| ANN - 2   | MLP 4:4-10-7-1:1| 4              | 10       | 7        | 1               |
| ANN - 3   | MLP 4:4-10-6-1:1| 4              | 10       | 6        | 1               |

In Table 3 you can see the determined response values using three neural networks and residual error values for each.

### Table 3. ANN prediction for flexural strength – Y₁ of polymer concrete

| EXP | EXP | Network 1 | Residual | Network 2 | Residual | Network 3 | Residual |
|-----|-----|-----------|----------|-----------|----------|-----------|----------|
| 1   | 14.69 | 13.75 | -0.94   | 14.68 | -0.01 | 15.10 | 0.41 |
| 2   | 14.18 | 14.17 | -0.01   | 13.64 | -0.54 | 14.22 | 0.04 |
| 3   | 17.09 | 17.09 | 0.00    | 17.05 | -0.04 | 17.07 | -0.02 |
| 4   | 14.09 | 14.06 | -0.03   | 14.27 | 0.18  | 14.25 | 0.16 |
| 5   | 14.6  | 14.91 | 0.31    | 14.57 | -0.03 | 14.58 | -0.02 |
| 6   | 17.03 | 16.75 | -0.28   | 17.04 | 0.01  | 17.02 | -0.01 |
| 7   | 15.35 | 15.35 | 0.00    | 15.66 | 0.31  | 15.34 | -0.01 |
| 8   | 13.55 | 13.57 | 0.02    | 14.10 | 0.55  | 13.46 | 0.09 |
| 9   | 17.57 | 17.56 | -0.01   | 17.57 | 0.00  | 17.58 | 0.01 |

In Table 4 is presented some statistical data corresponding to the three types of neural architectures and could see that the coefficient of correlation - R is between 0.97 and 0.99 for all network architecture which shows a strong correlation of type 3 network. Standard error is a measure of degree of impedance in flexural strength data vs. mean. If we look at this (Table 4) we notice that its highest value is 0.33 for the Y1.1 network, which can also induce a greater error probability with half its decrease for the higher-precision network Y1.3. Standard deviation is a measure of variability or diversity in flexural strength data. This means that Standard Deviation keeps the same trend. While mean has the same value for all three networks, which implies a relatively small difference in processed data with almost identical scattering around the centre value.

In the figure above are the four datasets - experimental and those obtained by using artificial neural networks. Note that network no.3 provided the data closest to the experimental (Fig. 3). The residual errors are very small in value, all subunit and ANN-3 network errors are between 0.4 and 0.01 which confirms a good approximation obtained through this network (Fig. 4).
Table 4. Statistical data of three ANN architecture prediction

|                | Y1.1 | Y1.2 | Y1.3 |
|----------------|------|------|------|
| Data Mean      | 15.35| 15.35| 15.35|
| Data S.D.      | 1.41 | 1.41 | 1.41 |
| Error Mean     | 0.10 | 0.05 | 0.05 |
| Error S.D.     | 0.33 | 0.28 | 0.14 |
| Abs E. Mean    | 0.18 | 0.18 | 0.08 |
| S.D. Ratio     | 0.23 | 0.20 | 0.10 |
| Correlation – R| 0.97 | 0.98 | 0.99 |

Figure 3. Experimental flexural strength versus three ANN architecture

Figure 4. Residual errors for the three ANN architecture

4. Conclusions

The purpose of the study was to point out that compared to the traditional methods of predicting some mechanical characteristics of new materials that required multiple experimental testing and were very costly depending on the complexity of the prescription and the number of controlled parameters, the proposed method uses only the experimental data set existing for training. The prediction can then be done with great precision on desired configurations, leaving only validation to be done under experimental conditions. Artificial neural networks prove to be a powerful and modern interdisciplinary subject that helps solving various different engineering problems that cannot be solved by traditional modeling and statistical methods.

The power of these networks consists in their ability to adapt and learn in particular processes with a non-linear character. It was also stressed the need to use in the experimental process and the DoE the significant reduction of the required number of tests to obtain results with maximum scientific reliability using experimental matrices adapted to each study but capable of capturing the complex behaviour of chemistry in the process of reaction hardening of the polymer concrete studied. Flexural strengths of polymer concrete with fly ash and cellulose fibre were analysed using a different ANN architecture. Thus we tested several configurations of neural architectures in order to choose the one that gives us the best accuracy of the results and minimal residual errors. Were tested over 100,000 networks to find the optimal configuration that ensures great precision of predictive analysed response by an optimal neural network architecture. The results of this study indicate that the appropriate selection of training algorithm is essential for successful data modelling by ANN and it depends on the number of experimental results which are used.
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