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On the metaheuristic models for the prediction of cement-metakaolin mortars compressive strength

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Abstract. In recent years, metakaolin, as a highly reactive pozzolan, has been in the center of research concerning mortar-based materials. Metakaolin is used as an addition in cement-mortars, substituting the cement fraction to a certain extent, in order to enhance sustainability of cement mortars, both in terms of environmental impact of raw materials production, as well as in terms of improving cement-based mortars durability under environmental actions. However, as metakaolin affects the mechanical performance of cement-based mortars, it is important to know the compressive strength that these blended mortars achieve at 28-days, in terms of structural design. Toward this direction, metaheuristic models such as ANN and Genetic Programming (GP) models have been developed and trained through the use of a database, compiled by available, in the literature, experimental works related to cement and blended cement-metakaolin mortars. In the model development phase, the most important parameters affecting the strength of concrete-based mortars, were investigated and selected. In addition, the effect of the selected transfer functions, as well as the initial values of weights and biases on the performance of ANN models, were also investigated. Based on this analysis, it was shown that ANNs with selected transfer functions (such as the Radial

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Basis transfer function, the Soft-Max transfer function, and the Normalized Radial Basis transfer function) were, able to reliably simulate the 28-days compressive strength of the cement-based mortars. In addition, it was shown that parameters such as the cement grade and the maximum diameter of aggregates, are very important in determining compressive strength of the cement-based mortars; this is an important finding, because these parameters are usually not taken into account in the research studies concerned in the prediction of compressive strength through computational models.

Keywords: artificial neural networks (ANNs); cement; compressive strength; Genetic Programming (GP); metakaolin; mortar; metaheuristic algorithms; surrogate models

1. Introduction

Mortar is an important constituent of masonry structures, as it is the material used to join stone and/or brick units comprising masonry. Mortars consist of binder materials, aggregates and, in some cases, additives. The choice today in relation to contemporary construction is the use of cement as binding material, however, efforts are being made to substitute cement in the mortar mix in current constructions, aiming to minimize the environmental impact of the cement industry and in an effort to improve the life cycle assessment of the mortars used in construction. A material which has been used in this context, with the added effect of improving cement mortar characteristics, is metakaolin. Although much research has been conducted regarding these materials, no tool yet exists that can assist in a quantitative manner in the optimum design of cement-based mortars. This is attributed to the fact that the mechanical properties of mortar materials exhibit a strong nonlinear nature derived from the parameters involved in their composition; it is this nonlinear behavior that makes the development of an analytical formula for the prediction of the mechanical properties using deterministic methods rather difficult.

Artificial neural networks (ANNs) have emerged over the last decades as an attractive meta-modelling technique applicable to a vast number of scientific fields including material science among others. In particular, such surrogate models can be constructed after a training process with only a few available data, which can be used to predict pre-selected model parameters, reducing the need for time- and money-consuming experiments. Thus far, the literature includes studies in which ANNs were used for predicting the mechanical properties of concrete materials (Dias and Pooliyadda 2001, Lee 2003, Topçu and Saridemir 2008, Trtnik *et al*. 2009, Waszczyszyn and Ziemiański 2001, Belalia Douma *et al*. 2016, Mashhadban *et al*. 2016, Açikgenç *et al*. 2015, Asteris *et al*. 2016a and Apostolopoulou *et al*. 2020). In their study, Asteris *et al*. (2016a) used ANNs to estimate the compressive strength of self-compacting concrete through a training process involving as input parameters the eleven parameters of synthesis and with output parameter the value of the compressive strength. Moreover, similar methods, such as fuzzy logic and genetic algorithms, have also been used for modelling the compressive strength of concrete materials (Baykasoğlu *et al*. 2004, Akkurt *et al*. 2004, Özcan *et al*. 2009, Saridemir 2009, Eskandari-Naddaf and Kazemi 2017, Oh *et al*. 2017, Khademi *et al*. 2017, Türkmen *et al*. 2017, Nikoo *et al*. 2015). A detailed state-of-the-art report can be found in (Adeli 2001, Asteris and Nikoo 2019, Asteris *et al*. 2019, Safiuddin *et al*. 2016, Mansouri and Kisi 2015, Mansouri *et al*. 2016, Reddy 2017, Salehi and Burgueño 2018, Pham *et al*. 2018, Nguyen and Bui 2019, Duan *et al*. 2020, Apostolopoulou *et al*. 2020, Ly *et al*. 2020 and Armaghani and Asteris 2020). Recently, in the study by Apostolopoulou *et al*. 2019, ANNs were successfully employed for the prediction of natural hydraulic lime mortars compressive strength.

ANNs have already proved successful in predicting the compressive strength of cement mortars at different specimen ages, taking into account (as input parameters) the percentage of metakaolin in relation to the total binder materials (MK/B), the water-to-binder ratio (W/B), the superplasticizer (SP) addition, and the binder-to-sand ratio.

In this context, in the work presented herein, the modelling of the 28-day compressive strength of mortar materials has been investigated in-depth using soft-computing techniques, such as surrogate models. In particular, this study investigates the application of Artificial Neural Networks (ANNs) and Genetic Programming models for the prediction of the 28-day compressive strength of cement-based mortars. Specifically, for the development and the training of NN models a database consisting of 186 specimens, taken from the literature, was utilized. Based on this database, the maximum diameter of aggregates (MDA) and the cement grade (CG) as well as four parameters of synthesis (Metakaolin to total binder (MK/B) ratio, Water to Binder (W/B) ratio, Superplasticizer (SP), and Binder to Sand (B/S) ratio) were used as input parameters, while the value of the 28-day compressive strength was used as output parameter.

It is also worth noting that, to the knowledge of the authors, the cement grade (CG) as well as the maximum diameter of aggregates (MDA) have not been used for the modeling of cement based mortars until now.

2. Research significance

Much research has been conducted internationally regarding the addition of metakaolin in cement mortars, substituting a percentage of cement content in the mortar mix in order to achieve a mortar of enhanced characteristics. Due to the non-linear interaction between mixed components and mortar characteristics, it is difficult to predict the compressive strength of a mortar mix. This difficulty necessitates costly and time consuming experiments which are based on empirical or semi-empirical calculations of the appropriate mortar mix synthesis parameters.

To this end, soft-computing techniques, such as Artificial Neural Networks (ANN), can contribute, as a feasible tool, towards the estimation of the mechanical properties of cement-based materials (Saridemir 2009, Ince 2004, Adhikary and Mutsuyoshi 2006, Kewalramani and Gupta 2006, Pala *et al*. 2007, Topçu and Saridemir 2007, Demir 2008, Altun *et al*. 2008, Gazder *et al*. 2017, Onyari and Ikotun 2018, Naderpour and Mirrashid 2018).

In this study, Artificial Neural Networks have been developed for the prediction of the 28-day compressive strength of mortars.

3. Materials and methods

3.1 Metaheuristic models

In this section, the basic principles and the constitutive rules obeyed by Artificial Neural Networks (ANNs) will be presented, focusing on the specific ANNs type known as back-propagation neural networks (BPNNs), as well as on the Genetic Programming method.

3.1.1 Artificial neural networks

Before presenting the basic aspects, principles and constitutive rules related to Artificial neural networks, a comment must be made regarding their name. ANNs were named in order to imply the fact that they derive from, or rather are related to, biological neural networks. Their ambition is to mimic the biological neurons and in fact to mimic the process of biological learning and knowledge storage. However, this ambition, is yet to be achieved and artificial neural networks are, in reality, based on coarse elements of the biological neurons networks, especially taking into account, that science still knows very little about the true and in depth function of biological neurons.

Artificial Neural Networks (ANNs) are information-processing models that are configured to learn and perform several tasks, such as classification, prediction, and decision-making. A trained ANN maps a given input onto a specific output, and therefore it is considered to be similar to a response surface method. The main advantage of a trained ANN over conventional numerical analysis procedures (e.g., regression analysis) is that the results are more reliable and can be produced with much less computational effort (Samui 2008, Das *et al.* 2011, Samui and Kothari 2011, Asteris *et al.* 2016b, Hornik *et al.* 1989, Plevris and Asteris 2014a, Sadowski and Nikoo 2014, Plevris and Asteris 2014b, Sadowski *et al.* 2015, Plevris and Asteris 2015, Asteris and Plevris 2013, Nikou *et al.* 2016, 2017 and 2018, Asteris and Plevris 2016, Cavaleri *et al.* 2017, Asteris *et al.* 2017 and 2018, Asteris and Kolovos 2017, Apostolopoulou *et al.* 2018, Kechagias *et al.* 2018, Apostolopoulou *et al*. 2019, Asteris and Mokos 2019, Armaghani *et al*. 2019, Cavaleri *et al.* 2019, Xu *et al*. 2019, Chen *et al*. 2019).

In the work presented herein, a specific ANNs type has been used, namely the back-propagation neural networks (BPNNs). A BPNN is a feed-forward, multilayer network (Hornik *et al.* 1989), meaning that information flows only from the input towards the output with no feedback loops, and the neurons of the same layer are not connected to each other, but they are connected with all the neurons of the previous and subsequent layer. A BPNN has a standard structure that can be written as

$$\mathrm{N} - \mathrm{H}_1 - \mathrm{H}_2 - \cdots - \mathrm{H}_{\mathrm{NHL}} - \mathrm{M} \tag{1}$$

where N is the number of input neurons (input parameters), $\mathrm{H_i}$ is the number of neurons in the i^{th} hidden layer for i =1, … ,NHL, NHL is the number of hidden layers and M is the number of output neurons (output parameters).

Despite the fact that the majority of researchers dealing with ANN techniques use multilayer NN models, ANN models with only one hidden layer can predict any forecast problem in a reliable and robust manner.

A notation for a single node (with the corresponding R-element input vector) of a hidden layer is presented in Fig. 1.

For each neuron i, the individual element inputs $\mathrm{p_1, \dots, p_R}$ are multiplied by the corresponding weights $\mathrm{w_{i,1}, \dots, w_{i,R}}$ and the weighted values are fed to the junction of the summation function, in which the dot product $(\mathrm{W \cdot p})$ of the weight vector $\mathrm{W} = [\mathrm{w_{i,1}, \dots, w_{i,R}}]$ and the input vector $\mathrm{p} = [\mathrm{p_1, \dots, p_R}]^{\mathrm{T}}$ is generated. The threshold b (bias) is added to the dot-product forming the net input n, which is the argument of the transfer function *f*

$$n = W \cdot p = w_{i,1}p_1 + w_{i,2}p_2 + \dots + w_{i,R}p_R + b \tag{2}$$

The choice of the transfer (or activation) function *f* may strongly influence the complexity and performance of the ANN. Although sigmoidal transfer functions are the most commonly used, one may use different type of functions. Previous studies (Bartlett 1998, Karlik and Olgac 2011) have proposed a large number of alternative transfer functions. In the present study, the Logistic

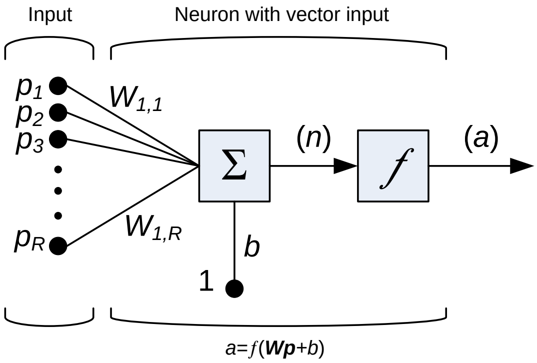

Fig. 1 A neuron with a single R-element input vector

Sigmoid and the Hyperbolic Tangent transfer functions were found to be appropriate for theproblem investigated. During the training phase, the training data are fed into the network which tries to create a mapping between the input and the output values. This mapping is achieved by adjusting the weights in order to minimize the following error function

$$E = \sum (x_i - y_i)^2 \tag{3}$$

where x_i and y_i are the measured value and the prediction of the network, respectively, within an optimization framework. The training algorithm used for the optimization plays a crucial role in building a quality mapping, thus an exhaustive investigation was performed in order to find the most suitable for this problem. The most common method used in the literature is the back-propagation technique, in which, as stated by its name, the information propagates to the network in a backward manner in order to adjust the weights and minimize the error function. To adjust the weights properly, a general method called gradient descent is applied, in which the gradients of the error function with respect to the network weights is calculated. Further discussion on the training algorithms, as well as on the activation functions, is given in the numerical example section.

In the present work, an in-depth investigation was carried out based on (i) a plethora of different architectures and (ii) ten different activation functions. This resulted in 100 (10^2) different combinations being applied during the training and development process of the BPNNs.

3.1.2 Genetic programming

Genetic programming (GP) is a soft computing technique that automatically solves problems without giving any instructions. It is the extension of the Genetic Algorithm (GA) developed by (Koza 1992). The principle of Genetic programming is Darwinian natural selection and genetic recombination where the individuals in the population are computer programs. GP computing itself by randomly generating a population of computer programs and generate a new population. Mutation, crossover, and reproduction take place during computation. Generation by generation GP iteratively transforms populations of programs into other populations of programs. During the course of its processes, GP builds new programs by spreading different specialized genetic exercises to fit it on computer programs.

In this soft computing technique, a random population of each individual (i.e., computer programs) is generated to reach high multiplicity. A member (a tree-like structure) is formed hierarchically by trial and error optimization of several functions. These functions are selected randomly or one by one or a set of functions. There are several functions available such as Boolean logic functions (OR, NOT, AND, etc.), arithmetic operations (sum, divide, multiplication, substation, etc.), trigonometric functions (sin, cos, tanh, etc.), other mathematical functions, etc. All these functions performed three-dimensionally in the concept of genetic operators such as reproduction, recombination (crossover) and mutation. Reproduction is carried out by copying an individual without affecting it. Recombination is carried out by changing genes between two individuals and mutation is carried out by exchanging a part of randomly selected genes.

In order to obtain better accuracy, a series of runs to be processed by changing and altering the main functions and terminating criterion. The terminating criteria used for this model are maximum population size, maximum number of generations, maximum tournament size, elite fraction, maximum number of genes, maximum tree depth and fitness value. Details of these criteria are discussed below in the results and discussion section. However, each criterion should be optimized carefully to deal with the local optima and global optima cases.

3.2 Cement-based mortars database

As a general trend, it is noticed that, during the process of developing a forecast model, researchers pay particular attention to the computational model itself, while at the same time, not giving the same amount of attention to the database that is used for the development, training and validation of the model. Although research related to new computational models is of course of high importance and added value for the international scientific community, the authors believe that, since the ultimate goal is a reliable forecast, the reliability of the database should be of utmost importance and should be thoroughly investigated in this regard. In fact, a reliable database must comprise of not only reliable data, but also of a sufficient amount of data, that covers the full range of parameter values, regarding the parameters which influence the problem investigated. Aiming to avoid misinterpretation of the term “sufficient”, it is highlighted that a sufficient amount of data is not necessarily a high amount of data, but rather datasets that cover a wide range of combinations of input parameter values, thus assisting in the model’s ability to simulate the problem. The demand for a reliable and capable database is especially crucial in the case of experimental databases, that is databases which are compiled using experimental results. In this case, high deviation between experimental values is frequently noticed, not only between experiments conducted by different research teams and laboratories, but even between datasets that derive from experiments conducted on specimens of the same synthesis, produced by the same technicians, cured under the same conditions and tested implementing the same standards and the same testing instruments.

Thus, a reliable database, that also covers the full range of parameter values and combinations of parameter values, in addition to contributing to the development of reliable mathematical models, will also decisively contribute to the reliable comparison between different forecast computational models.

In light of the above discussion, a large database has been composed. Specifically, the database used herein for the development and training of the computational models regarding the prediction of cement-based mortars’ 28-day compressive strength, consists of 186 experimental datasets that have been obtained from twenty-one well known and reliable published experimental works, available in the literature (Table 1). All the datasets used, are based on specimens that have been prepared and tested following the same international standards. The experimental data selected

Table 1 Data from experiments published in literature

No.	Reference	Number of Samples	Parameters		Compressive Strength (MPa)
			MK	SP	
1	Vu *et al.* 2001	36			22.48 - 49.00
2	Courard *et al.* 2003	5			57.00 - 71.20
3	Sumasree and Sajja 2016	7			26.39 - 34.24
4	Batis *et al.* 2005	4			57.5 - 69.7
5	Kadri *et al.* 2011	3			80.42 - 97.29
6	Mardani-Aghabaglou *et al.* 2014	2			48.9 - 50.05
7	Potgieter-Vermaak and Potgieter 2006	4			50.9 - 92.8
8	Cizer *et al.* 2008	1			66.23 - 66.23
9	Al-Chaar *et al.* 2013	1			10.48 - 10.48
10	Curcio *et al.* 1998	5			94.3 - 111.28
11	Cyr *et al.* 2007	2			59.8 - 62.8
12	Saidat *et al.* 2012	8			51.6 - 64.5
13	Ashok *et al.* 2017	1			43.13 - 43.13
14	Geng and Li 2017	5			68.65 - 78.53
15	Pavlikova *et al.* 2009	27			44.98 - 83.16
16	Khater 2010	6			9.75 - 11.78
17	Parande *et al.* 2008	5			40 - 60
18	Mansour *et al.* 2012	2			78.74 - 83.05
19	Lee *et al.* 2005	4			46.3 - 51.2
20	Eskandari-Naddaf and Kazemi 2017	54			12.2 - 64.89
21	Khatib *et al.* 2012	4			34.79 - 50.95
	Total	186	20	7	9.75 - 111.28

from the literature, was related only to cement mortars with or without the addition of high quality metakaolin, in different percentages, in order to ensure the consistency of the experimental data. More specifically, experimental data from only one experimental work (Eskandari-Naddaf and Kazemi 2017) without the use of metakaolin have been included in the database, while all other research works included, investigated the addition of metakaolin in different percentages. Furthermore, in 7 of the 21 experimental works, the effect of superplasticizer on the compressive strength of mortars has also been investigated (Vu *et al.* 2001, Kadri *et al.* 2011, Curcio *et al.* 1998, Pavlikova *et al.* 2009, Mansour *et al.* 2012, Lee *et al.* 2005 and Eskandari-Naddaf and Kazemi 2017).

In the framework of the principles described above, during the preparation process of the database, the following steps were followed:

- Each specimens' compressive strength value was collected from the respective paper. In the case where the values were not stated in numerical form, but in graphical form, they were extracted in numerical form from the figures, with the aid of appropriate software, the so-called graph digitizers.
- The papers taken into consideration were carefully chosen, as to contain mixes that did not

include mix design parameters other than: cement, metakaolin, sand, water and superplasticizer.

- It was decided to only include experimental results related to specimens produced with sand presenting a maximum particle diameter of up to 5.00 mm. In the case where the sand used for the production of the specimen presented a maximum particle diameter higher than 5.00mm, the specimens were not included.
- In the case where any of the influencing parameters was not presented in a distinct manner within the paper, clarifications were requested from their respective researchers. Parameters that appeared to be mostly ambiguous, were sand's maximum particle diameter and the cement's grade. Regrettably, there was a large number of papers, containing many experimental data, without distinctive cement classification for the specimens used, while it was not possible to identify the cement grade by contacting the researchers themselves, and the related data was thus not included or utilized. Not including ambiguous data allows for a more reliable model, even though the amount of data may be less.
- Many researchers use datasets with different values of compressive strength, even though they correspond to the same mix parameters. In the database presented herein, after appropriate filtering, the data included was related to specimens that presented different combinations of input parameter values. In only one dataset, as the input parameter values were identical, the compressive strength value was averaged.
- Additionally to the filtering of the database above, when specimens from different researchers presented the same parameter values, only one of the datasets was included.

The experimental data selected from the literature was that of mortars with OPC (ordinary portland cement) as main binding material and the addition of high quality metakaolin in different percentages in order to ensure the consistency of the experimental data and the data was compiled abiding to the above framework. Namely, Vu *et al*. 2001 prepared 36 cement mortar samples using OPC, metakaolin, sand, and superplasticizer. A ratio by weight of 1 part binder and 2.75 parts of sand was used, along with a water to binder ratio varying from 0.40 to 0.53. Metakaolin was used to partially replace cement with different percentages, ranging from 0% to 30% with a 5% step increment. The superplasticizer was added with three percentages, 0%, 0.5% and 1.4%. Compressive strength was measured in accordance to ASTM C109 (1983) on six cubic samples.

Courard *et al.* (2003) produced cement mortar samples using OPC, sand, and metakaolin with various percentages (0-20% with a 5% increment). The weight ratio of binder to sand was 1/3. Compressive strength was measured in accordance with NBN B12-208 (1969) on six samples of 4cm x 4cm x 4cm.

Sumasree and Sajja (2016) prepared OPC and OPC-metakaolin mortars. Metakaolin replaced cement at different percentages, from 0% to 30%, with a 5% increment. The binder to sand ratio was 0.50 by weight, and the water/binder ratio was kept constant at 0.46. Compressive strength measurements were conducted on specimens 4cm x 4cm x 4cm.

Batis *et al.* (2005) produced mortar samples with OPC and sand, and metakaolin was added in various cement substitution ratios (i.e., 0%, 10%, 20%). The water to binder was kept constant at 0.6, and the binder to aggregates ratio was kept at 0.33 by weight. The compressive strength was measured in accordance with EN 196-1 (1994).

Kadri *et al.* (2011) produced samples with the use of OPC, metakaolin in two substitution percentages (0% and 10% of total binder), and sand. The superplasticizer was added with three percentages, 1.4%, 2%, and 2.3%. The water-to-binder ratio was maintained at 0.36. The compressive strength measurements were conducted on 4 cm x 4 cm x 4 cm specimens, abiding by

EN 196-1 (1994).

Mardani-Aghabaglou *et al.* (2014) prepared mortar mixes using OPC and standard sand conforming to EN 196-1 (1994) standard. Metakaolin was also added in one mix, substituting cement in a percentage of 10% per weight concerning total binder. The binder-to-sand ratio was kept constant (with and without metakaolin), at 0.37 by weight, whereas the water to binder ratio was kept constant at 0.485. Compressive strength was measured on cubic samples 5cm x 5cm x 5cm in accordance with ASTM C 109 (1983).

Potgieter-Vermaak and Potgieter (2006) produced mortars with OPC, local metakaolin heated at different temperatures, and sand. The mortar samples were produced with different metakaolin percentages in relation to total binder (0% to 30% with an increment of 10%). The water-to-binder and the binder-to-sand ratios were kept constant at 0.38 and 0.33 (by weight), respectively. The measurements were conducted on specimens with dimensions of 4 cm x 4 cm x 4 cm.

Cizer *et al.* (2008) examined the compressive strength of blended cement-lime mortars. In the database presented herein, only the control cement mortar was incorporated, where the binder-to-sand ratio was 1/3 by weight, and the water-to-binder ratio was 0.45. The compressive strength was measured at 66.23 (MPa).

Al-Chaar *et al.* (2013) examined the use of natural pozzolans as a partial substitution of cement in mortars. In the present database, only the reference mortar characteristics were incorporated. The water to binder ratio was 0.48, while the binder to sand ratio was 0.36. The experimental procedure was conducted in accordance with ASTM C109 (1983) and cubic specimens 5cm x 5cm x 5cm, where the compressive strength measured was 10.48 MPa.

Curcio *et al.* (1998) studied the 15% replacement of cement by four commercially available super-plasticized mortars containing metakaolin. The water/binder ratio was 0.33. The compressive strength at 28 days varied from 94.3 to 111.28 MPa.

Cyr *et al.* (2007) investigated the possibility of using two industrial by-products (municipal solid waste incineration fly ash, MSWIFA, and sewage sludge ash, SSA) in cement-based materials containing metakaolin. The analyzed binders composed of 75% cement, 22.5% metakaolin, and 2.5% residue. The measured values of 28 days compressive strength were in the range of 59.80 - 62.80 MPa.

Saidat *et al.* (2012) tested different chemical activators for metakaolin to obtain short-term strength similar to that obtained without metakaolin. A number of 12 activators were selected and tested in mortars at different concentrations along with 4 types of cement. The measured values of compressive strength at 28 days were in the range of 51.60 - 64.50 MPa.

Ashok *et al.* (2017) studied the possibility of combining two nanomaterials, namely nano-silica (NS) and nano clay metakaolin (NMK), with OPC. Mortar cube specimens of 5 cm x 5 cm x 5 cm were cast using partial replacement of the OPC with the various levels of NS, and NMK varied from 0.5% - 2.0% by the weight of cement, with a mix ratio of 1/3 and water-cement ratio as 0.4. Only one sample was taken into account in the database, and the measured compressive strength was 43.13 MPa.

Geng and Li (2017) studied the effect of metakaolin addition on cement mortar compressive strength. The mix design of the mortar included 450 kg/m^3 of cementitious materials and 1350 kg/m^3 of sand, with a ratio w/c of 0.45. Mortar specimens of 4 cm x 4 cm x 4 cm were used for compressive strength tests at 1, 3, 7 and 28 days following the standard EN 12390. The measured compressive strength at 28 days ranged from 68.65 to 78.53 MPa.

Pavlikova *et al.* (2009) studied the effect of metakaolin as a pozzolanic addition in high-performance cement mortars using water-to-cement ratios of 0.33, 0.45, and 0.55, respectively.

The 28-days compressive strength of the mortars were found in the 9.61 - 48.08 MPa range.

Khater (2010) performed an experimental study on the resistance of mortar specimens, incorporating 0%, 5%, 10%, 15%, 20%, 25%, and 30% metakaolin, to the magnesium chloride solution. The water-binder ratio was 0.60 by weight, whereas the cementitious material/fine sand ratio was 1:3 for all mortar mixtures. A range 9.75 - 11.78 MPa of compressive strength was achieved.

Parande *et al.* (2008) used OPC with aggregates and metakaolin (i.e., 0% to 20% with a 5% increment) to produce blended MK-cement mortars. The binder to sand ratio was constant at 1/3 by weight, and the water binder ratio was constant at 0.40. Cube mortar specimens were produced (10cmx10cmx10cm) and measured at different ages. A range of 40 to 60 MPa of compressive strength at 28 days was achieved.

Mansour *et al.* (2012) prepared 2 samples with 10% metakaolin, containing the same weight proportions of sand, binder (cement and metakaolin) and water, while the ratio of water to cement was 0.30. The 28 days compressive strength was 78.74 and 83.05 MPa.

Lee *et al.* (2005) reported an experimental study of mortar specimens incorporating 0%, 5%, 10% and 15% of metakaolin. The water to cement ratio (w/c) was fixed at 0.45 by weight. The cement to fine aggregate was 2.0. Four samples were collected, with the 28 days compressive strength varying from 46.3 to 51.2 MPa.

Eskandari-Naddaf and Kazemi 2017 reported 54 samples containing different cement strength classes of CME 32.5, 42.5, and 52.5 MPa. Six water to cement ratios of 0.25, 0.3, 0.35, 0.4, 0.45, 0.5, along with three sand to cement ratios of 2.5, 2.75, 3, and three types of cement were used. The 28 days compressive strength varied from 12.2 to 64.89 MPa.

Khatib *et al.* (2012) investigated mortars containing high volume of metakaolin as partial substitution of cement. The replacement of metakaolin was varied up to 50% with an increment of 10%. The water to binder ratio was 0.5, and the compressive strength tests were conducted using cube specimens of dimensions 5cm x 5cm x 5cm. The range of obtained compressive strength at 28 days varied between 34.79 and 50.95 MPa.

Based on the above database, each input training vector p (input parameters) is of dimension 1×7 and consists of the value of the max diameter of aggregate (MDA), the cement grade (CG) and the values of the four parameters of synthesis, namely the percentage of metakaolin in relation to the total binder materials (MK/B, w/w%), the water-to-binder ratio (W/B), calculated as the weight of water divided by the weight of total binder materials (w/w), the superplasticizer (SP), meaning the percentage of the addition of superplasticizer in relation to the total binder (%w/w), and the binder-to-sand ratio (B/S), meaning the w/w of binder materials to aggregate materials. The corresponding output training vector (output parameter) is of dimension 1×1 and consist of the value of the compressive strength of the cement-based mortar specimens.

The mean values of the parameters included in the database, together with the minimum, maximum values, as well standard deviation (STD) values, are listed in Table 2. It should be noted that some of the cement metakaolin mortars variables could be dependent on each other. Subsequently, the correlation coefficients between all possible variables have been specified and presented in Table 3, as well as in Fig. 2. High negative or positive values of the correlation coefficient between the input variables may result in poor efficiency of the methods and to the difficulty in construing the effects of the expository variables on the response. As can be seen, there are not significant correlations between the independent input variables. On the other hand, in order to develop a reliable, robust and optimum NN model, the correlation coefficients between the input variables (parameters) and the output parameter of compressive strength (CS), last line in

Table 2 The input and output parameters used in the development of BPNNs (All Datasets)

No.	Variable	Symbol	Units	Category	Statistics			
					Min	Average	Max	STD
1	Max diameter of aggregate	MDA	mm	Input	0.60	2.99	5.00	9.72
2	Cement Grade	CG	MPa	Input	32.00	42.76	53.50	8.41
3	Metakaolin percentage in relation to total binder	MK/B	(%w/w)	Input	0.00	8.42	30.00	9.72
4	Water to Binder Ratio	W/B	w/w	Input	0.25	0.43	0.60	0.09
5	Superplasticizer	SP	(%w/w)	Input	0.00	0.47	3.91	0.84
6	Binder-to-sand ratio	B/S	w/w	Input	0.33	0.39	0.51	0.07
7	Compressive Strength	CS	MPa	Output	9.75	50.10	111.28	20.67

Table 3 Correlation matrix of the variables

		Input						Output
		MDA	CG	MK/B	W/B	SP	B/S	CS
Input	MDA	1.00						
	CG	0.28	1.00					
	MK/B	-0.46	-0.11	1.00				
	W/B	-0.44	-0.11	0.33	1.00			
	SP	0.18	-0.05	-0.23	-0.72	1.00		
	B/S	-0.25	-0.29	0.29	-0.01	-0.02	1.00	
Output	CS	0.01	0.48	0.07	-0.27	-0.04	-0.06	1.00

Table 3, need to be high. Based on these values, it is clearly shown that there is a strong relation between the mortar compressive strength (CS) and the input parameter of the cement grade (CG).

Moreover, Fig. 3 demonstrates the frequency histograms of the parameters used for the modelling of cement mortars 28-day compressive strength. These figures are extremely useful, as they determine the ranges of parameter values, where data is insufficient. When sufficient data exists, covering a wide range of parameter values, then the model can lead to a reliable forecast; when however, a certain range of an input parameter is deficient or even lacking in data, the opposite usually occurs, as the model does not have enough data to be trained. Furthermore, these figures can highlight areas where experimental data is lacking and can thus guide mortar mix design in order to investigate the aforementioned synthesis, thus, not only leading to new experimental results, but also to enhancing the database.

It is obvious that most datasets are in the range of parameters, as dictated by the standard for the mortar mix: sand with max diameter 2 mm, B/S ratio of 0.33 and W/B ratio of 0.50 (EN 196-1, 1994).

There is a lack of data for mortars produced with 4 mm MDA, even though sand of such gradation is quite usual in practice. Furthermore, there seems to be a lack in data related to superplasticizer addition higher than 2% in relation to binder, which however can be explained by the fact that only low amounts are necessary to obtain the desired fluidity. Overall, the database covers a wide range of input parameter values and is thus considered as adequate for the

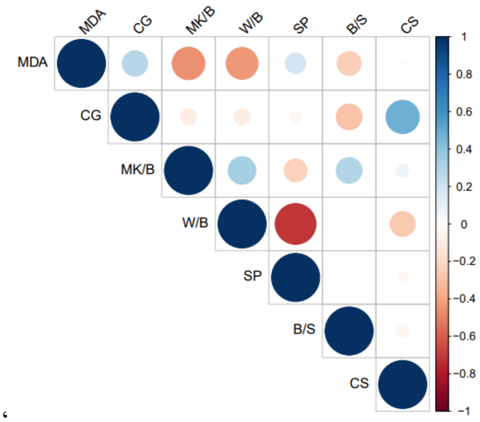

Fig. 2 Correlogram of the variables (Input and Output parameters)

development and training of the ANNs in question.

3.3 Short review on the behavior of cement-based mortars

Most of the published works in the literature focused on the possibility of using metakaolin as cement replacement, as well as investigating the most appropriate cement replacement ratio. For example, in the work of Vu *et al*. (2001), it was found that compressive strength can be improved with a replacement level of 15-20% of cement, regarding 7 to 28 days compressive strength values, whereas a higher replacement ratio can enhance compressive strength at higher ages. Other researchers concluded that the optimum admixture of metakaolin is in the range of 10% to 15%, in order to obtain the best mechanical performance (Courard *et al.* 2003, Batis *et al.* 2005). Curcio *et al.* (1998) confirmed that the replacement of 15% cement by metakaolin produced a higher rate of compressive strength development at 28 days. In Sumasree and Sajja (2016), the highest compressive strength at 28 days was found with a replacement of 25% of cement by metakaolin, however, the binder/sand and water/binder ratios remained constant in the experiments. Saidat *et al.* (2012) confirmed such an observation while using a ratio of binder to sand to water of 1/3/0.5. It is reported that finer metakaolin enhances the strength of mortar compared with coarser metakaolin (Kadri *et al.* 2011). With a ratio of W/C = 0.33, the effect of metakaolin replacement was reported as not important (Pavlikova *et al.* 2009), whereas for other ratios, the replacement of 10% was considered as a safe solution. Besides, the effect of a higher amount of superplasticizer (more than 1%) was not significant. The cement grade was concluded as a significant and effective parameter in predicting the strength of cement-based mortar (Eskandari-Naddaf and Kazemi 2017).

3.4 Sensitivity analysis of the parameters affecting the compressive strength of mortars based on experimental database

In general, sensitivity analysis of a numerical model is a technique used to determine if the output of the model is affected by changes in the input parameters. This will provide feedback as

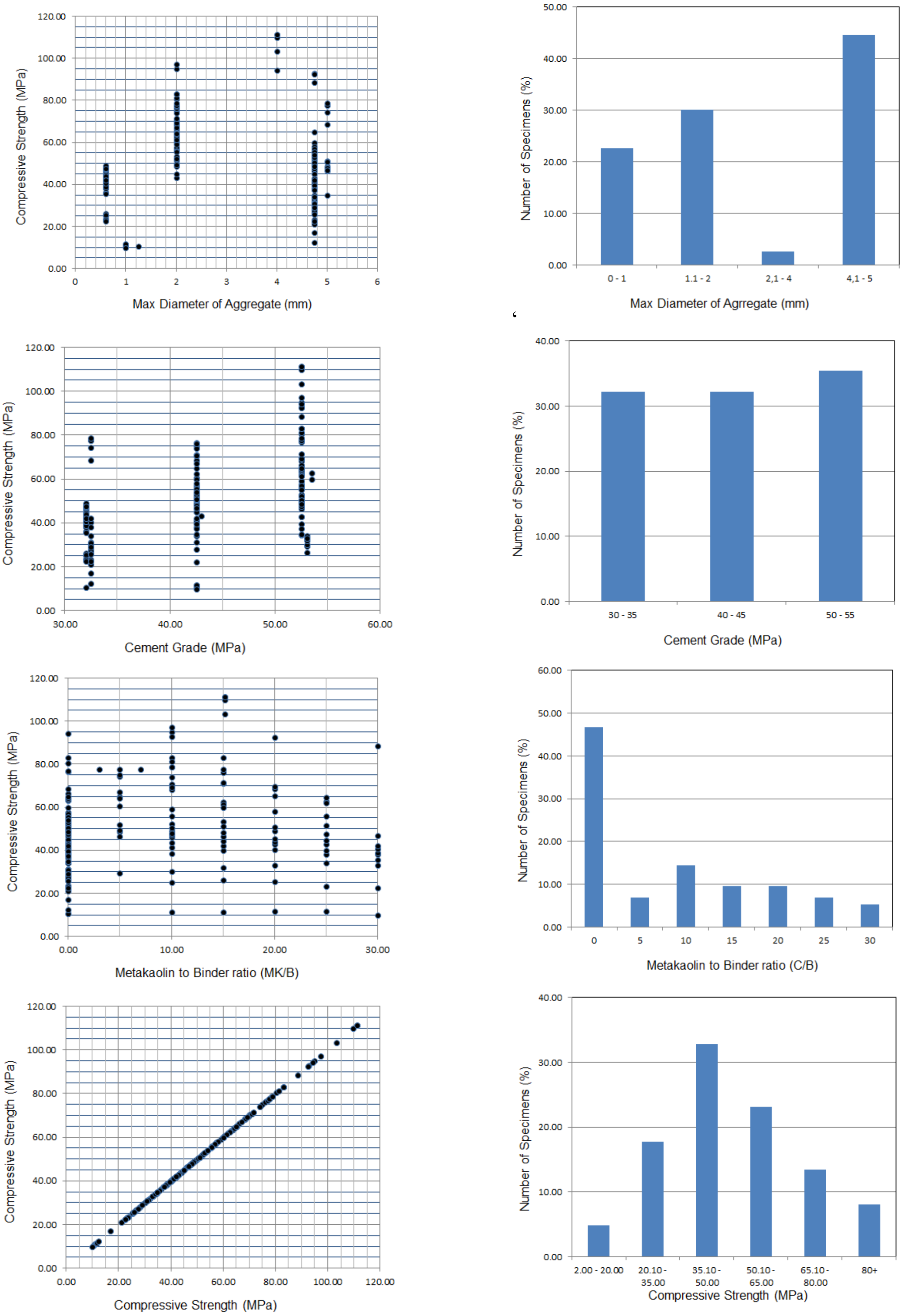

Fig. 3 Histograms of the parameters

to which input parameters are the most significant, and thus, by removing the insignificant ones, the input space will be reduced and subsequently the complexity of the model as well as the training times required for its training will be also reduced. In order to identify the effects of model inputs on the output, the sensitivity analysis (SA) can be conducted on the database. Sometimes, the results of SA could help the researchers/designers to remove one or more input parameters from the database to obtain better analyses with a higher level of performance prediction. To perform the SA, the cosine amplitude method (CAM), which has been used by many researchers (Armaghani *et al.* 2015, Momeni *et al.* 2015 and Khandelwal *et al.* 2016) was selected and implemented. In CAM, data pairs will be used to construct a data array, X, as follows

$$X = \{x_1, x_2, x_3, \dots, x_i, \dots, x_n\} \tag{4}$$

Variable $\mathrm{x_i}$ in array, X, is a length vector of m as

$$\mathrm{x_i} = \{\mathrm{x_{i1}}, \mathrm{x_{i2}}, \mathrm{x_{i3}}, \dots, \mathrm{x_{im}}\} \tag{5}$$

The relationship between $\mathrm{R_{ij}}$ (strength of the relation) and datasets of $\mathrm{X_i}$ and $\mathrm{X_j}$ is presented by the following equation

$$\mathrm{R_{ij}} = \frac{\sum_{\mathrm{k=1}}^{\mathrm{m}} \mathrm{x_{ik}x_{jk}}}{\sqrt{\sum_{\mathrm{k=1}}^{\mathrm{m}} \mathrm{x^2{}_{ik}} \sum_{\mathrm{k=1}}^{\mathrm{m}} \mathrm{x^2{}_{ik}}}} \tag{6}$$

The $\mathrm{R_{ij}}$ values between the compressive strength and the input parameters are shown in Fig. 4. This analysis reveals that, the cement grade has the greatest influence on compressive strength values, with a strength value of 0.9429, followed by binder to sand ratio (0.9061), water to binder ratio (0.8858), maximum diameter of aggregate (0.8023), metakaolin percentage in relation to total binder (0.6273) and, the parameter with the lowest influence on compressive strength seems to be the Superplasticizer in relation to the total binder (0.4386).

3.5 Performance indices

Three different statistical parameters were employed to evaluate the performance of the derived FF-ABC-NN model as well as the available in the literature formulae, including the root mean square error (RMSE), the mean absolute percentage error (MAPE), and the Pearson Correlation Coefficient R^2. The lower RMSE and MAPE values represent the more accurate prediction results. The higher R^2 values represent the greater fit between the analytical and predicted values. The aforementioned statistical parameters have been calculated by the following expressions (Alavi and Gandomi 2012)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2} \tag{6}$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{x_i - y_i}{x_i}\right| \tag{7}$$

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{n}(x_i - y_i)^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right) \tag{8}$$

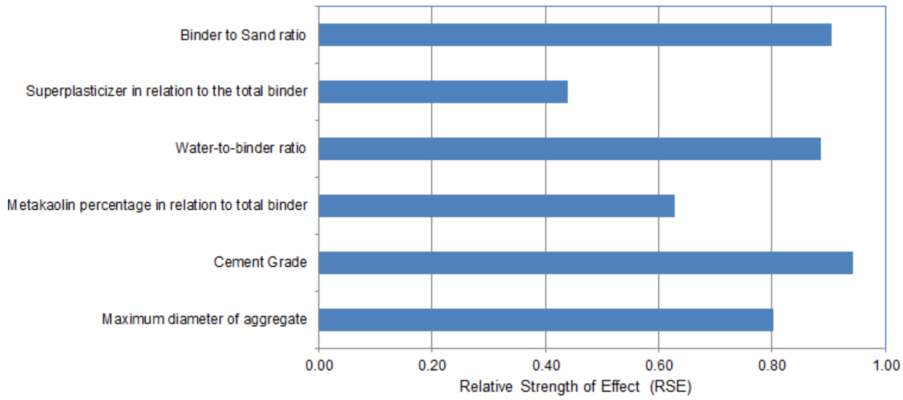

Fig. 4 Sensitivity analysis of cement-metakaolin mortars compressive strength

where n denotes the total number of datasets, and x_i and y_i represent the predicted and target values, respectively.

The reliability and accuracy of the developed neural networks were evaluated using Pearson's correlation coefficient R and the root mean square error (RMSE). RMSE presents information on the short term efficiency which is a benchmark of the difference of predicated values in relation to the experimental values. The lower the RMSE, the more accurate is the evaluation. The Pearson's correlation coefficient R measures the variance that is interpreted by the model, which is the reduction of variance when using the model. R values ranges from 0 to 1 while the model has healthy predictive ability when it is near to 1 and is not analyzing whatever when it is near to 0. These performance metrics are a good measure of the overall predictive accuracy.

Recently, the following new engineering index, the a20-index, has been recently proposed (Apostolopoulou *et al*. 2018) for the reliability assessment of the developed ANN models

$$a20 - index = \frac{m20}{M} \tag{9}$$

where M is the number of dataset sample and m20 is the number of samples with value of rate Experimental value/Predicted value between 0.80 and 1.20. Note that for a perfect predictive model, the values of a20-index values are expected to be equal to 1. The proposed a20-index has the advantage that its value has a physical engineering meaning. It declares the amount of the samples that satisfies predicted values with a deviation ±20% compared to experimental values.

4. Methodology

As already mentioned in a previous section, artificial neural networks, as well as an analytical expression deriving through genetic programming, will be utilized for the prediction of compressive strength of cement-based mortars. Aiming to minimize the space-dimensions of the issue under examination, in the first stage, neural networks will be implemented and the optimum simulation of compressive strength will be sought out and selected in relation to the parameters affecting compressive strength. Simplicity of the proposed model is also included within the term optimum. This means that amongst two models with small differences between their performance indices, namely the a20-index, R2, RMSE and MAPE, as presented above, the model with the simplest architecture will be selected.

At this point it is worth noting that the majority of researchers involved with the simulation of compressive strength of cement-based materials, such as mortars and concrete, do not take important influencing parameters into consideration. Specifically, it is noticed that the gradation of the sand is usually not stated; moreover, it is noticed that researchers do not even take the crucial information regarding the cement grade, which highly influences the compressive strength of the mortar, into consideration.

In order to obtain the aim of this research, different cases are examined regarding the parameters which will be taken into account as influencing for the development of mortar compressive strength.

During this investigation to reveal the optimum forecast of compressive strength, the effect of normalization of the parameters will also be studied and evaluated, as well as the effect of the transfer functions, in relation to the optimum prediction of compressive strength. That is, the influence of the above parameters on the prediction capacity of the artificial neural networks.

When obtaining the optimum solution in regards to the parameters which influence compressive strength, and must, thus, serve as input parameters for the reliable prediction of compressive strength, the genetic programming method will be implemented in order to reveal an analytical formula, capable of predicting the compressive strength of mortars.

5. Results and discussions

5.1 Development of ANN models

Based on the above, different architecture ANNs were developed and trained. More specifically, during the development and training of the ANN models the following steps (which are summarized in Table 4) were followed:

- Four databases, each containing 186 datasets were used, however with varying input parameters, important for the simulation of cement-based mortar compressive strength (Table 5).
- The 186 datasets comprising each database were divided into three separate sets. Specifically, 124 of 186 (66.6%) datasets were designated as Training datasets, 31 (16.7%) as Validation datasets, while 31 (16.7%) datasets were used as Testing datasets.
- During the training phase of the ANNs, the above datasets were used with and without normalization. In the case were normalization of the data was conducted, the minmax normalization technique in the range [0.10, 0.90] was implemented.
- The Levenberg–Marquardt algorithm was used for the training of the ANNs (Lourakis 2005).
- 10 different initial values of weights and biases were applied for each architecture.
- ANNs with only one hidden layer were developed and trained.
- The Number of Neurons per Hidden Layer ranged from 1 to 50 by an increment step of 1.
- Two functions, the Mean Square Error (MSE) and Sum Square Error (SSE) functions, were used as cost function during the training and validation process.
- 10 functions, as presented in Table 4, were used as transfer or activation functions.

Table 4 Training parameters of ANN models

Parameter	Value
Training Algorithm	Levenberg-Marquardt Algorithm
Normalization	Minmax in the range 0.10 – 0.90
Number of Hidden Layers	1
Number of Neurons per Hidden Layer	1 to 50 by step 1
Control random number generation	Rand (seed, generator) where generator range from 1 to 10 by step 1
Training Goal	0
Epochs	250
Cost Function	Mean Square Error (MSE) Sum Square Error (SSE)
Transfer Functions	Hyperbolic Tangent Sigmoid transfer function (HTS) Log-sigmoid transfer function (LS) Linear transfer function (Li) Positive linear transfer function (PL) Symmetric saturating linear transfer function (SSL) Soft max transfer function (SM) Competitive transfer function (Co) Triangular basis transfer function (TB) Radial basis transfer function (RB) Normalized radial basis transfer function (NRB)

The above steps resulted in the development of 240.000 different ANNs. It is worth noting that only the use of 10 different transfer function results in 100 different ANNs, for each architecture with the same number of neurons, as a result of 100 (=10^2) different dual combinations of the 10 transfer functions investigated.

5.2 Optimum parameters for modelling mortar compressive strength

Regarding the simulation of mortar compressive strength it is particularly important to select the main parameters which affect the obtained value of compressive strength. Researchers involved in the prediction of cement-based mortars, as well as for the general case of cement-based materials such as concrete materials, use four common input parameters. These common parameters are (i) the metakaolin percentage in relation to total binder, (ii) the water to binder ratio, (iii) the binder-to-sand ratio and (iv) the superplasticizer percentage.

Despite the fact that the importance of sand gradation and cement grade for compressive strength development has been highlighted in many experimental researches related to cement based mortars (Vu *et al.* 2001, Pavlikova *et al.* 2009, Eskandari-Naddaf and Kazemi 2017), it seems that these two parameters have been greatly overlooked and usually not taken into consideration during the development of computational models, with the sole exception of the work of Eskandari-Naddaf and Kazemi 2017, who took the cement grade into consideration, however did not take into consideration either the gradation of the sand (here expressed as the maximum sand diameter) or the metakaolin percentage in relation to total binder in their

Table 5 Cases of variables used for the estimation of cement-based mortars compressive strength

Case	Variables – Input Parameters					
	MDA	CG	MK/B	W/B	SP	B/S
I			√	√	√	√
II		√	√	√	√	√
III	√		√	√	√	√
IV	√	√	√	√	√	√

Table 6 Optimum architectures for the four cases of variables investigated for the estimation of cement-based mortars compressive strength

Case	Normalization	Cost Function	Transfer Function		Random Number	Architecture	Epochs	RMSE
			Hidden Layer	Output Layer				Testing
I	√	MSE	HTS	HTS	2	4-30-1	5	14.9847
		MSE	TB	Li	7	4-13-1	9	14.6032
II	√	SSE	SSL	HTS	3	5-23-1	6	10.1948
		MSE	HTS	HTS	1	5-16-1	15	8.9312
III	√	SSE	HTS	SSL	1	5-20-1	6	10.3953
		SSE	RB	HTS	9	5-7-1	8	9.3732
IV	√	SSE	NRB	HTS	3	6-6-1	50	8.0239
		SSE	NRB	SSL	10	6-7-1	21	**7.5098**

HTS: Hyperbolic Tangent Sigmoid transfer function; Li : Linear transfer function; SSL : Symmetric saturating linear transfer function
TB : Triangular basis transfer function; RB : Radial basis transfer function; NRB : Normalized radial basis transfer function

computational model.

In the present section, four different cases are examined (Table 5) regarding the parameters which will be taken into account as influencing for the development of mortar compressive strength.

As stated in Table 5, case scenario I is the reference scenario, where the four basic mix design parameters, influencing compressive strength, are taken into consideration. Namely, the parameters: Metakaolin percentage in relation to total binder, the Water to Binder Ratio, the Superplasticizer percentage in relation to total binder and the Binder-to-sand ratio (per weight). In case scenario II, the input parameters are increased to five, in order to also include the Cement Grade. In case scenario III, instead of including the Cement Grade, as the fifth parameter, the Max diameter of aggregate is considered. Case scenario IV includes all six mix design parameters.

In order to evaluate which of the four above cases is the most appropriate for the most accurate prediction of cement mortar compressive strength, and taking into account the steps described in the previous section, 60.000 ANNs were developed, trained and evaluated. The optimum architectures are presented in Table 6.

Based on the results presented in Table 6, the important effect of sand gradation (MDA), as

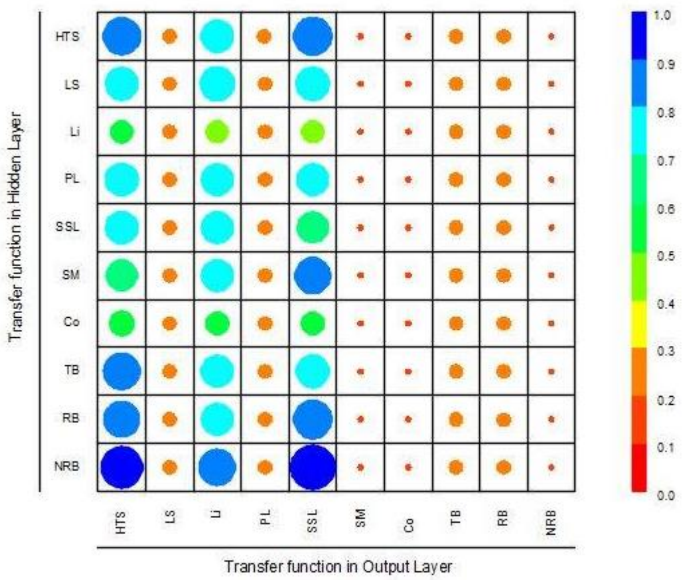

Fig. 5 Best Min RMSE to Min RMSE for each transfer functions combinations

well as cement grade, is highlighted. At this point it is worth noting that for all four cases examined, the best results were obtained without normalization of the data. Regarding the maximum diameter of aggregate and the cement grade, it is noted that both parameters increase the prediction capacity and simulation, regarding compressive strength of cement-based mortars. In fact, in agreement with the results of the sensitivity analysis conducted in a previous section (Fig. 4), the cement grade has a greater effect on compressive strength (RMSE=8.93) in relation to the maximum diameter of the sand used (RMSE=9.37). Furthermore, by including both parameters, compressive strength is simulated with an even higher degree of accuracy (RMSE=7.51).

5.3 The effect of transfer functions on the performance of ANN models

In the present section, with the advantage of having four different databases corresponding to the four compressive strength simulation scenarios examined in the previous section, ´the effect of transfer functions on the performance of ANN models is investigated. Specifically, for each ANNs architecture, ten different transfer functions are employed, as presented in Table 4. It is worth noting that the majority of researchers use only three of the ten above transfer functions, and without examining all of their nine combinations. More specifically, usually the Hyperbolic Tangent Sigmoid transfer function (HTS), the Linear transfer function (Li) and the Log-sigmoid transfer function (LS) are employed. In the case were the ANN presents a one hidden layer architecture, two transfer functions are required, one for the hidden layer and one for the output layer. This demand, when examining ten transfer functions, leads to the investigation of 100 ($=10^2$) different combinations for each ANN architecture case.

In Fig. 5 the ratio of the minimum RMSE of all investigated ANNs towards the minimum RMSE of each of the 100 combinations resulting from different combinations of the 10 different transfer functions, is graphically represented. Unity corresponds to the optimum combination of

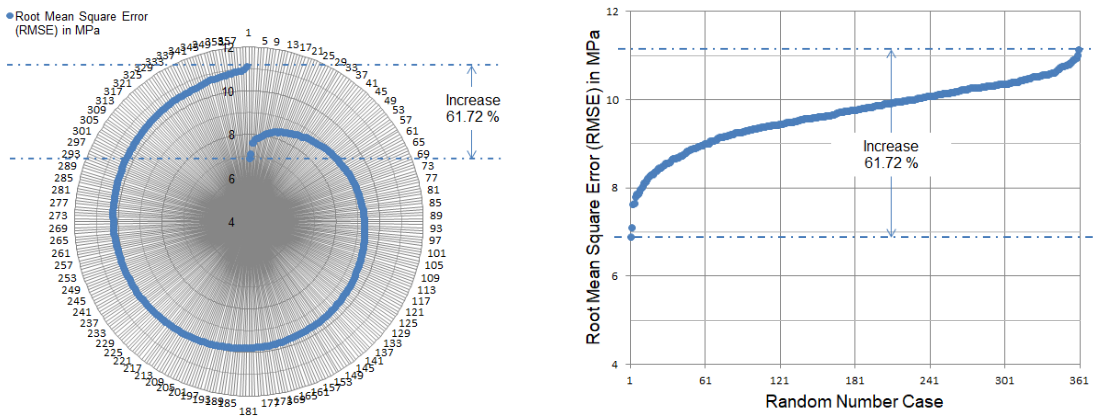

Fig. 6 Root mean square error (RMSE) in regard to initial values of ANNs' weights and biases

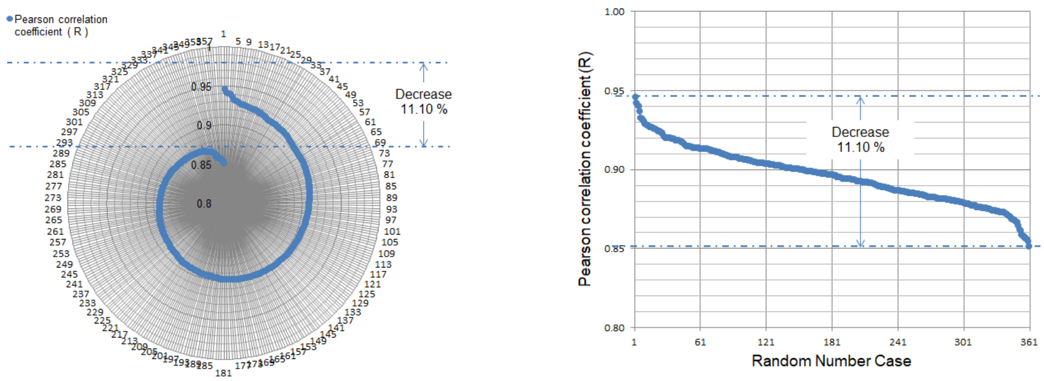

Fig. 7 Pearson correlation coefficient (R) in regard to initial values of ANNs' weights and biases

transfer functions (Normalized radial basis transfer function in the hidden layer and Symmetric saturating linear transfer function). To the authors' best knowledge this combination of transfer functions has not as yet been used in the literature. Based on this figure, it is highlighted that

- Regarding the hidden layer, among the ten transfer functions investigated, only two are considered as inappropriate, namely the Linear transfer function (Li) and the Competitive transfer function (Co) and
- Regarding the output layer only three transfer functions are assessed as appropriate, the Hyperbolic Tangent Sigmoid transfer function (HTS), the Linear transfer function (Li) and the Symmetric saturating linear transfer function (SSL)

These findings result in a decrease of the combination of transfer functions, from 100(10×10) to 24 (8×3). It is also worth noting that, to the knowledge of the authors, Symmetric saturating linear transfer function (SSL) has never up to now been proposed as transfer function for the output layer of ANNs simulating material engineering issues.

5.4 The effect of Initial values of weights and biases on Optimum ANN model

Another important parameter which affects the performance of ANNs is related to the initial

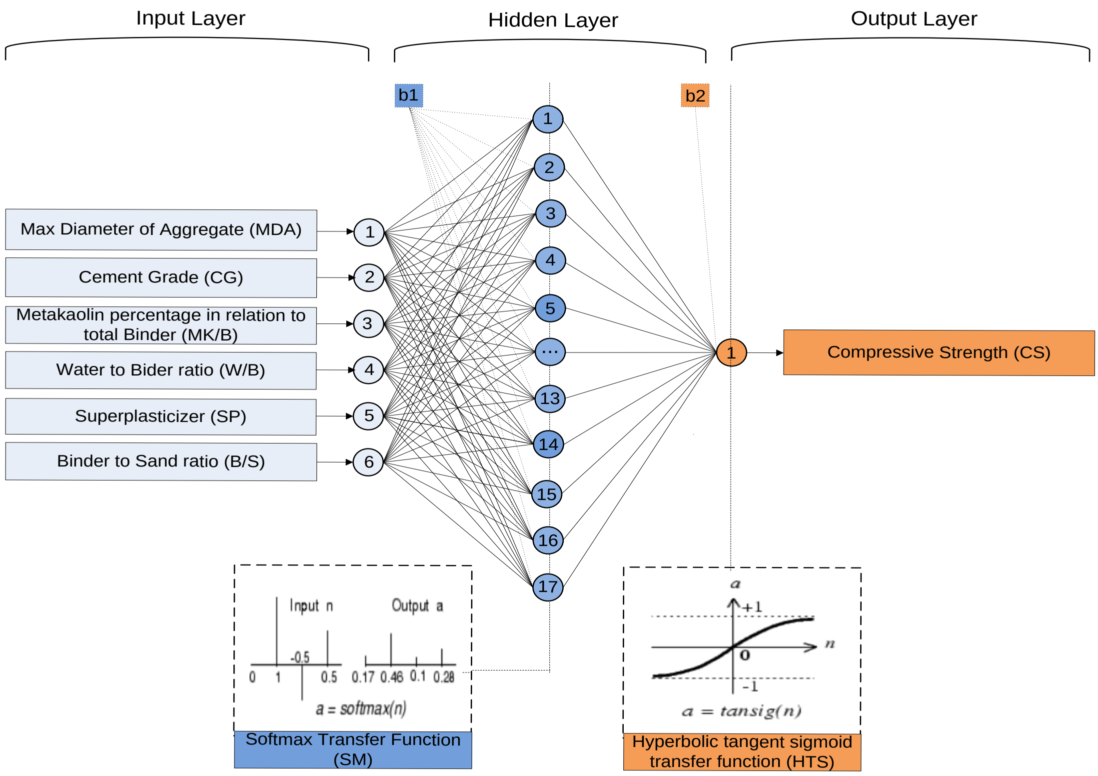

Table 7 Architectures of Top Ten ANNs based on Testing Datasets Root Mean square error (RMSE)

No.	Architecture	Cost Function	Transfer Functions		Performance Indices					
					Testing Datasets		Training Datasets		All Datasets	
			Hidden Layer	Output Layer	R	RMSE	R	RMSE	R	RMSE
1	6-17-1	SSE	SM	HTS	0.94621	6.8948	0.9865	3.1663	0.9719	4.8872
2	6-5-1	MSE	NRB	Li	0.94236	7.1122	0.9683	4.8302	0.9575	5.9548
3	6-9-1	SSE	NRB	HTS	0.94181	7.6425	0.9856	3.2729	0.9560	6.2339
4	6-15-1	MSE	RB	HTS	0.94034	7.6508	0.9950	1.9346	0.9739	4.9753
5	6-5-1	MSE	NRB	HTS	0.93736	7.8069	0.9763	4.1919	0.9652	5.4076
6	6-31-1	SSE	RB	HTS	0.9293	7.8655	0.9166	7.8779	0.9099	8.6795
7	6-4-1	MSE	NRB	SSL	0.9284	7.8689	0.9478	6.1572	0.9458	6.7028
8	6-5-1	MSE	NRB	HTS	0.92716	7.9115	0.9717	4.5647	0.9584	5.9022
9	6-24-1	SSE	RB	HTS	0.92625	7.9707	0.9512	6.0315	0.9423	6.9757
10	6-7-1	SSE	NRB	HTS	0.92733	8.0091	0.9840	3.4373	0.9672	5.2638

HTS : Hyperbolic Tangent Sigmoid transfer function; Li : Linear transfer function; RB : Radial basis transfer function;
SM : Soft max transfer function; SSL : Symmetric saturating linear transfer function; NRB : Normalized radial basis transfer function

Table 8 Parameters used for the development of GP model

Parameter/Variable	Value
Population size	800
Number of generations	100
Tournament size	25
Lexicographic selection	True
Max tree depth	5
Max nodes per tree	Inf
Using function set	TIMES MINUS PLUS TANH SQUARE SIN COS EXP
Number of inputs	6
Max genes	5
Constants range	[-10 10]
Using fitness function	regressmulti_fitfun.m

values of weights and biases. In this section, the results of a thorough investigation are presented, related to the effect of these issues. Specifically, for the 24 optimum combination of Transfer functions presented above, the effect of the initial values of weights on the Root Mean square error value (RMSE), as well as on the value of the Pearson correlation coefficient (R) is investigated. For this purpose, one hidden layer ANN models were developed, with a number of neurons ranging from 1 to 50. Regarding the 360 different initial conditions, the rand MATLAB function of rand values was implemented, using as random generator seed parameter from 1 to 360. Each one of the models was trained for 360 different initial conditions and the results are presented in Figs. 6 and 7.

Based on the figures, it is concluded that the initial values of weights and biases highly affect the performance of the ANNs. More specifically, the values of Root Mean square error (RMSE) is increased by 61.7% (Fig. 6), while the Pearson correlation coefficient (R) value presents a 11.1% decrease (Fig. 7).

It is worth noting the above differences are in reference to the total of 24 combinations of transfer functions. It is within the future goals of the authors to investigate the effect of the initial values of weights and biases separately for each of the 24 combinations of Transfer functions.

5.5 Optimum ANN models

Following the investigation implemented in the previous sections, in the current section the 10 optimum architectures, among the 3.600.000 different architectures investigated, are presented. More specifically, in Table 7 the 10 optimum models are presented, assessed in relation to their Root Mean square error (RMSE) values and regarding Testing Datasets. Based on the results presented in the Table the following key findings have been revealed:

- The most appropriate transfer functions for the hidden layer, are the Soft max transfer function (SM), the Normalized radial basis transfer function (NRB) and the Radial basis transfer function (RB)
- Regarding the output layers, the most appropriate functions seem to be the Hyperbolic

Tangent Sigmoid transfer function (HTS), the Linear transfer function (Li) and the Symmetric saturating linear transfer function (SSL)

- Based on the results presented in the Table, the 6-17-1 ANN model seems to be the most appropriate (Fig. 8); however, the authors feel that the 6-5-1 is the optimum model, as, while it presents slightly lower performance indices, it is superior in terms of simplicity, as the hidden layer contains only 5 neurons in contrast to the 17 neurons of the (statistically) optimum ANN.

Even though it is common practice for authors to present the architecture of an optimum ANN model, without any information related to the final values of ANN weights and biases, it must be stressed that any architecture which does not present these values is of limited assistance to others researchers and practicing engineers. If, on the other hand, a proposed ANN architecture is accompanied by the (quantitative) values of weights, it can be of great use, making it possible for the ANN model to be readily implemented in a MS-Excel file, thus available to anyone interested in modeling issues. With this in mind, in Table A1 of the Appendix, the final values of ANN weights and biases are stated.

At this point it is worth noting that the selection of the optimum ANN, should not be conducted based solely on statistical indices, but rather should be evaluated by experts of the issue under investigation, who can select the optimum model among a list of the best performing ones, as presented in Table 7, which have been evaluated through the use of statistical indices. This applies for prediction problems where a high degree of uncertainty exists, where a high degree of interdisciplinarity is necessary and beneficial for the selection of the optimum solution.

5.6 ANN-based predictive formula

In the previous section, the optimum ANN model was proposed, based on statistical indices, while the 6-5-1 ANN was also proposed as the most appropriate computational model for the prediction of 28 day compressive strength. In fact, this model was proposed because, even though it presents slightly lower values regarding statistical performance indices, it is superior in term of simplicity, on behalf of the fact that the hidden layer contains only 5 neurons in contrast to 17 neurons, presented in the 6-17-1 ANN, which scored slightly higher in relation to the performance indices. The small number of neurons facilitates the expression of an analytical equation, which can be easily employed by engineers, without necessitating knowledge in computational mechanics.

Based on the constitutive laws that govern ANNs, the 6-6-1 model, using the final values of weights and biases, can be expressed by the following equation

$$\mathrm{CS} \;=\; 0.4708\times \mathrm{R1} + 0.2838\times \mathrm{R2} - 7114\times \mathrm{R3} - 0.2438\times \mathrm{R4} + 0.3935\times \mathrm{R5} - 0.4782 \tag{10}$$

where

$$\begin{pmatrix} \mathrm{R1} \\ R2 \\ R3 \\ R4 \\ R5 \end{pmatrix} = NRB\left(\begin{bmatrix} -0.4030 & -0.2545 & 0.9321 & -0.7805 & -0.8375 & -0.9722 \\ 1.0076 & 0.5010 & 0.9561 & -0.8144 & 0.6996 & -0.1357 \\ 0.8699 & 0.3752 & 0.4300 & -1.0621 & 1.0554 & 0.1655 \\ -0.7086 & 1.0589 & -0.8848 & 0.1066 & 0.3675 & 0.8938 \\ 0.8646 & -0.4379 & -0.6568 & -0.9838 & -0.6235 & -0.7902 \end{bmatrix} \times \begin{bmatrix} MDA \\ CG \\ MK/B \\ W/B \\ SP \\ B/S \end{bmatrix} + \begin{bmatrix} 1.8307 \\ -0.9154 \\ 0.000 \\ -0.9154 \\ 1.8307 \end{bmatrix}\right) \tag{11}$$

5.7 GP analytical predictive formula

In continuation of the previous section, and under the framework of expressing an analytical formula for the prediction of mortar compressive strength, Genetic Programming (GP) is used next.

During this process, aiming to express an analytical formula through Genetic Programming (GP), the parameters presented in Table 8 were implemented.

Table 8 Parameters used for the development of GP model

Following an exhaustive investigation of a plethora of parameter combinations, the following equation emerged as the optimum analytical formula simulating compressive strength of cement-based mortars

$$\begin{aligned}\mathrm{CS} = {} & 460.1 + 1.202\exp(\mathrm{MDA}) - 1.202\exp(\cos(\mathrm{MKB})) - 1.202\ \sin(\mathrm{MKB} + 2.088) - 77.45\cos(\mathrm{MDA} + \mathrm{BS}) \\ & - 526.6\cos(\cos(\cos(\cos(\mathrm{MDA})))) + 1.202\sin(\mathrm{CG}) \\ & - 3.864\mathrm{WB}(2\mathrm{MDA} + \cos(\mathrm{CG}))(\mathrm{MDA} + \mathrm{WB} + \mathrm{BS} + \sin(\mathrm{MDA} + \mathrm{WB})) \\ & - 0.7802\mathrm{MDA}\,(\sin(\mathrm{BS} + \sin(\mathrm{MDA})))\,(\mathrm{WB} - \mathrm{SP})(2\mathrm{MDA} + \mathrm{WB} - \mathrm{SP})\end{aligned} \tag{11}$$

5.8 Comparisons of derived models

Aiming to compare the three mathematical computational models, regarding their performance in simulating mortars' 28 day compressive strength, performance indices were employed. Specifically, in addition to the well-known R and RMSE indices, the a20-index was also employed. The a-20 index is related to the percentage of datasets where the values predicted presents a deviation od less than 20% in relation to the experimental value, which is considered as true value. The results are presented in Table 9, as well as in Table 10, where the ratio of experimental/predicted values is presented in detail, for each model, in columns from 9 to 11, for all datasets used as Testing Datasets.

Furthermore, in Fig. 9 the predicted values of compressive strength are presented in comparison to the experimental values, for all three models.

Based on the results (Table 9), it seems that the two neural networks outperform the GP model, however it is difficult to select the optimum among the two ANN models, as the ANN 6-17-1 presents higher R and RMSE indices, while the ANN 6-5-1 presents a higher a20-index. At this point it is worth noting the importance of evaluating the optimum computational model, not only based on statistical indices, but also through a verification implementing the available experimental results.

5.9 Experimental verification of developed models

In addition to the evaluation of the three computational models, developed and trained to predict the compressive strength of mortars, through performance indices, as presented in the previous section, in the current section an additional evaluation of the three models is performed. More specifically, the three models are assessed in relation to their capability to successfully simulate the experimental behavior of these materials.

In order to achieve this aim, and on account of the large amount of parameters which are involved in the issue under investigation, experimental results, which can adequately reveal the behavior of the material, are necessary. Meaning that experimental results must be available, where all input parameters remain constant, except from one, whose value alters. Such a case are the experimental results of Pavlikova *et al.* 2009. In the aforementioned study, the effect of

Table 9 Performance of the development of models

Model	Datasets	Performance Indices		
		a20-index	R	RMSE
ANN 6-17-1	Training	0.9839	0.9865	3.1663
ANN 6-5-1		0.9355	0.9683	4.8302
GP		0.7984	0.9331	6.9449
ANN 6-17-1	Testing	0.7097	0.9462	6.8948
ANN 6-5-1		0.7742	0.9424	7.1122
GP		0.6452	0.9049	9.6588

metakaolin addition on 28-day compressive strength is investigated, for two different cement grades 42.5 MPa and 52.5 MPa. In Figures 10 and 11, the experimental values are plotted in addition to the respective values, as predicted by the models. More specifically, these figures reveal the effect of varying metakaolin addition on compressive strength for mixes were the sand used presents a maximum diameter of aggregates (MDA) 2 mm, Water to binder ratio (W/B) 0.45, without Superplasticizer (SP) and a Binder to Sand (B/S) ratio of 0.33 The effect is shown for two different cement grades, 42.5 MPa (Fig. 10) and 52.5 MPa (Fig. 11).

These figures emerge as particularly useful for the experimental verification of mathematical computational forecast models. That is, they can contribute to answer the question of which model should be selected among the proposed ones, and in fact may highlight the optimum model. From these figures, it is obvious that the Genetic Programming based model is unfit in terms of successfully simulating the problem due to the fact that (i) a large amount of variance of curvature is noticed with varying metakaolin, something that has not been experimentally verified or implied, and (ii) based on the waveform of the curve, which presents abrupt change of curvature, it is revealed that Genetic Programming model achieves overfitting of the data and thus, while it presents adequate forecasting results for the database data parameters, does not in fact successfully simulate the development of compressive strength.

Regarding the two other models, it is noticed that (i) based on the smoothness of the curves, no overfitting phenomena have occurred, something that must be ensured for every forecast model, (ii) between the two models, the 6-17-1 ANN model is the optimum for the prediction and simulation of blended cement - metakaolin mortars 28-day compressive strength.

5.10 Possibilities and limitations of the developed optimum ANN model

Based on the proposed 6-17-1 ANN model, the behavior of mortars was investigated for the range of parameter values that have not been sufficiently experimentally investigated. More specifically, the effect of metakaolin on the 28 day compressive strength of mortars was investigated. In Figs. 12 & 13 the results are presented for a range of metakaolin percentages, from 0 to 20 % revealing its effect on the value of compressive strength for two different binder to sand ratios (0.42 or 0.45) and for two different water to binder ratios. In Fig. 12 the results for w/b=0.45 are presented, while in Fig. 13 the results for w/b=050 are presented.

Based on these figures, it is evident that ANNs can be implemented as a useful tool for revealing the mechanical behavior of these blended materials, as well as a teaching tool for university students.

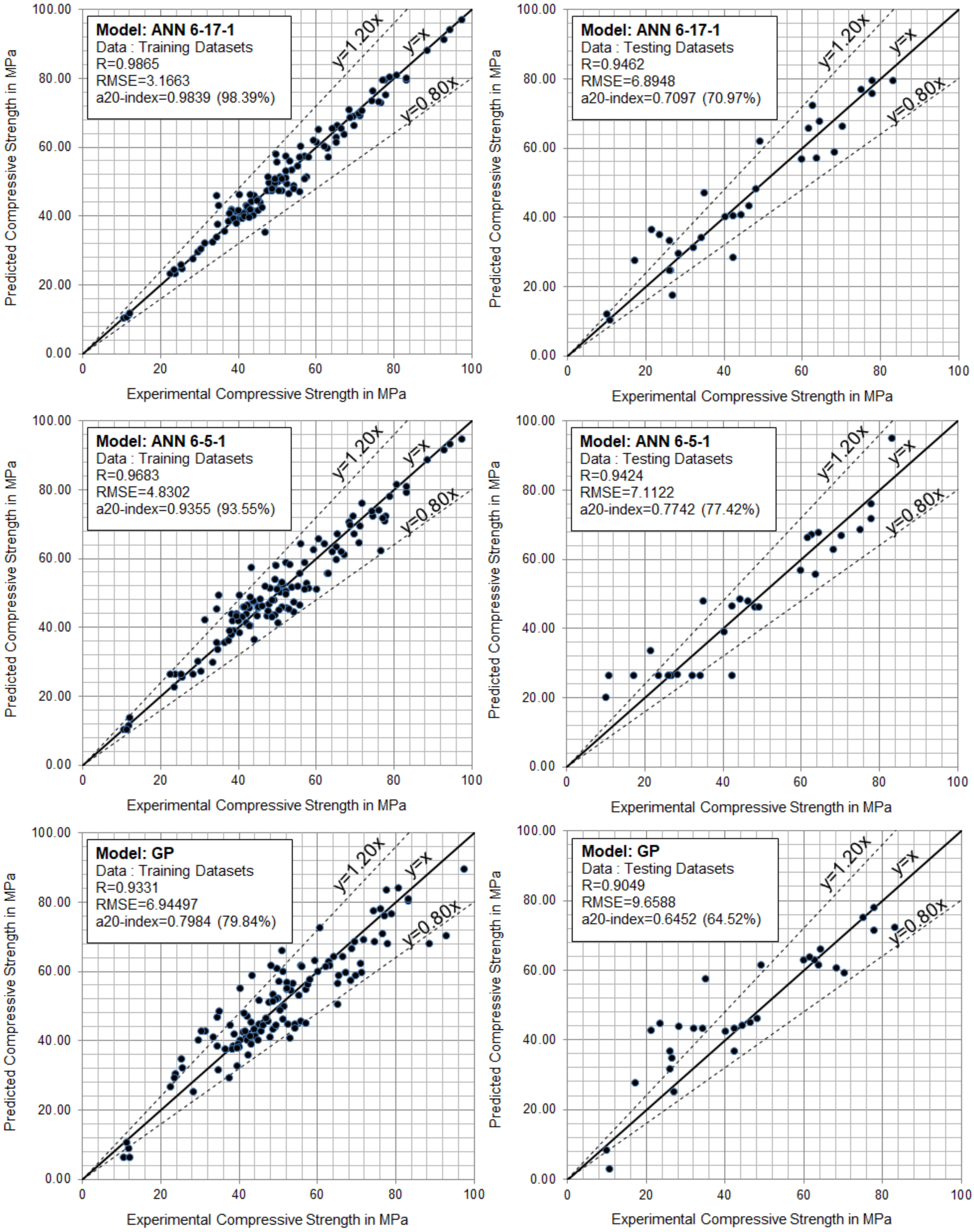

Fig. 9 Experimental vs Predicted values of compressive strength for the three developed models

Table 10 Experimental and Predicted values of the compressive strength of cement-based mortars for the case of testing datasets

No.	Sample Code	MDA	CG	MK/B	W/B	SP	B/S	Experimental to Predicted Compressive Strength		
								BPNN6-17-1	BPNN 6-5-1	GP
		mm	MPa	(%w/w)	(w/w)	(%w/w)	(w/w)			
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)
3	M3	0.60	32.00	15.00	0.50	0.00	0.36	1.05	0.99	0.75
9	M9	0.60	32.00	15.00	0.53	0.00	0.50	0.99	1.02	0.94
15	M15	0.60	32.00	15.00	0.50	0.00	0.50	1.03	0.90	0.97
21	M21	0.60	32.00	15.00	0.47	0.00	0.50	1.08	0.91	1.00
27	M27	0.60	32.00	15.00	0.44	0.50	0.50	1.07	0.96	1.02
33	M33	0.60	32.00	15.00	0.40	1.30	0.50	1.00	1.04	1.04
39	10MK	2.00	42.50	10.00	0.50	0.00	0.33	1.06	1.05	1.18
45	15MK	4.75	53.00	15.00	0.46	0.00	0.50	1.01	1.19	0.73
51	MK-10	2.00	52.50	10.00	0.60	0.00	0.33	1.16	1.08	1.12
57	MK10%	2.00	42.50	10.00	0.49	0.00	0.36	0.79	1.05	0.79
63	REF	1.25	32.00	0.00	0.48	0.00	0.36	1.01	0.39	3.27
69	Mref	2.00	53.50	0.00	0.50	0.00	0.33	1.05	1.05	0.95
75	Bi	2.00	52.50	0.00	0.50	0.00	0.33	1.11	1.14	1.03
81	MK3 28	5.00	32.50	3.00	0.45	0.00	0.33	1.02	1.08	1.08
87	CM16 B	2.00	42.50	5.00	0.33	2.00	0.33	0.97	1.09	1.00
93	CM9	2.00	42.50	15.00	0.45	0.00	0.33	0.86	0.93	0.99
99	CM13	2.00	52.50	5.00	0.33	1.00	0.33	0.97	1.02	0.99
105	CM1	2.00	52.50	5.00	0.45	0.00	0.33	0.95	0.95	0.97
111	CM6	2.00	52.50	15.00	0.55	0.00	0.33	0.93	0.93	0.96
117	30	1.00	42.50	30.00	0.60	0.00	0.33	0.80	0.48	1.13
123	MR28	2.00	52.50	0.00	0.30	0.01	0.33	1.04	0.87	1.15
129	1	4.75	32.50	0.00	0.25	3.25	0.4	0.61	0.64	0.61
135	7	4.75	32.50	0.00	0.25	3.91	0.33	1.50	1.00	1.06
141	13	4.75	32.50	0.00	0.3	1.74	0.36	1.47	1.58	1.14
147	19	4.75	32.50	0.00	0.35	0.61	0.4	0.66	0.88	0.52
153	25	4.75	32.50	0.00	0.35	0.91	0.33	0.94	1.04	0.64
159	31	4.75	32.50	0.00	0.4	0.39	0.36	0.99	1.28	0.79
165	37	4.75	32.50	0.00	0.45	0.11	0.4	1.05	0.97	0.70
171	43	4.75	32.50	0.00	0.45	0.12	0.33	0.58	0.63	0.49
177	49	4.75	32.50	0.00	0.5	0.08	0.36	0.77	0.97	0.81
183	M1	5.00	42.50	0.00	0.50	0.00	0.33	0.74	0.72	0.60

MDA: Max diameter of aggregate; CG: Cement Grade; MK/B: Metakaolin percentage in relation to total binder
W/B: Water to Binder Ratio; SP: Superplasticizer; B/S: Binder-to-sand ratio; CS: Cement based mortar Compressive Strength

It was decided not to illustrate further examples herein, as such an effort would demand an even more extensive database. In fact, the proposed neural network can be used for mortar mix forecasting, within the range of parameters of the database (min and max values) used for its development and training (Table 9). Furthermore, the reliability of the proposed neural network is

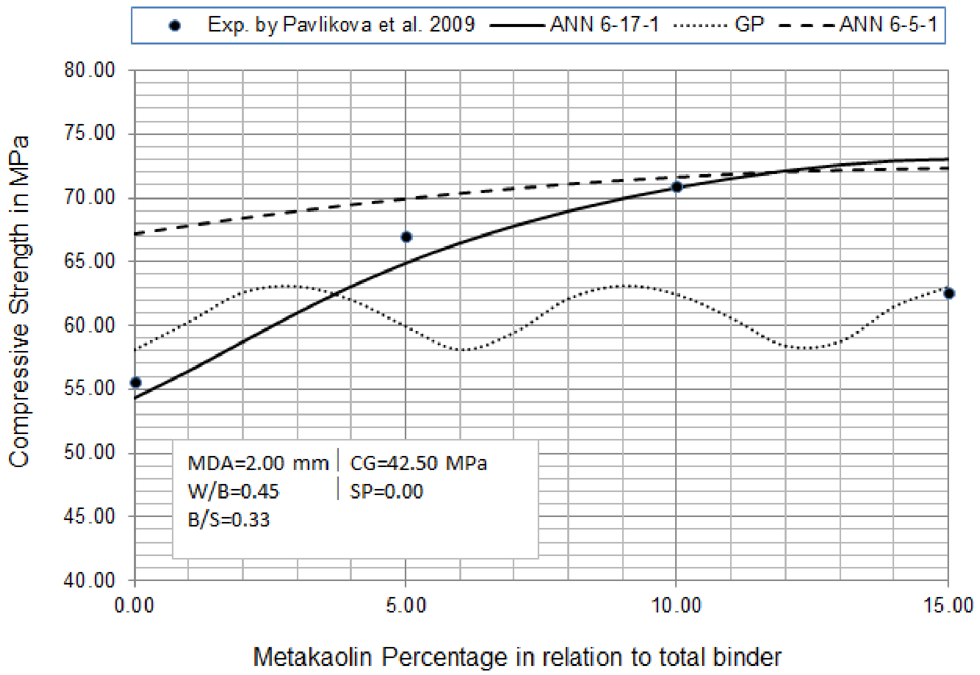

Fig. 10 Experimental verification of the developed models using experimental data by Pavlikova *et al.* 2009, for cement grade 42.5 MPa

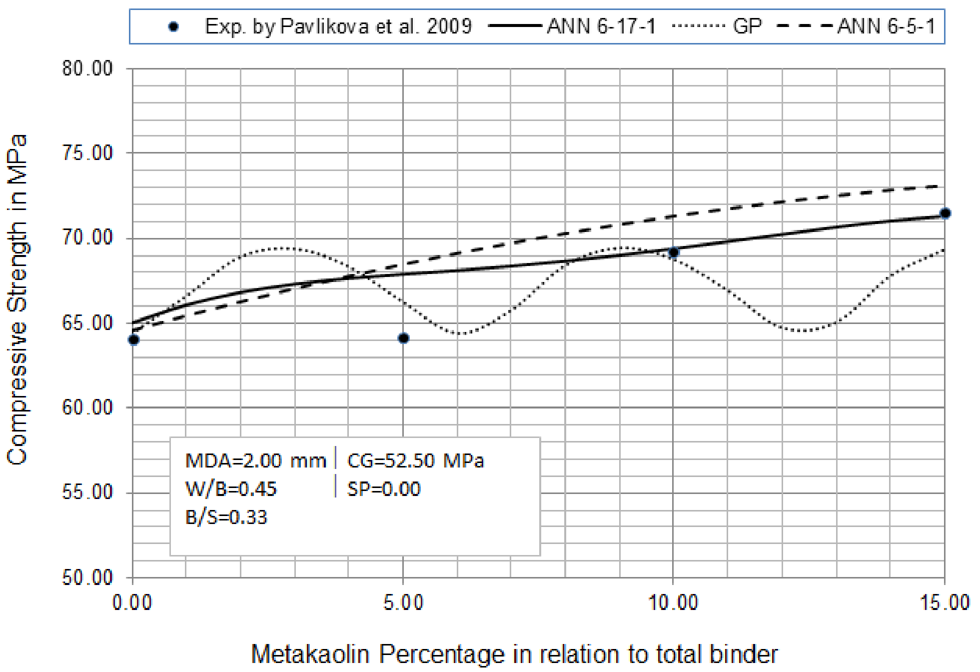

Fig. 11 Experimental verification of the developed models using experimental data by Pavlikova *et al.* 2009. for cement grade 52.5 MPa

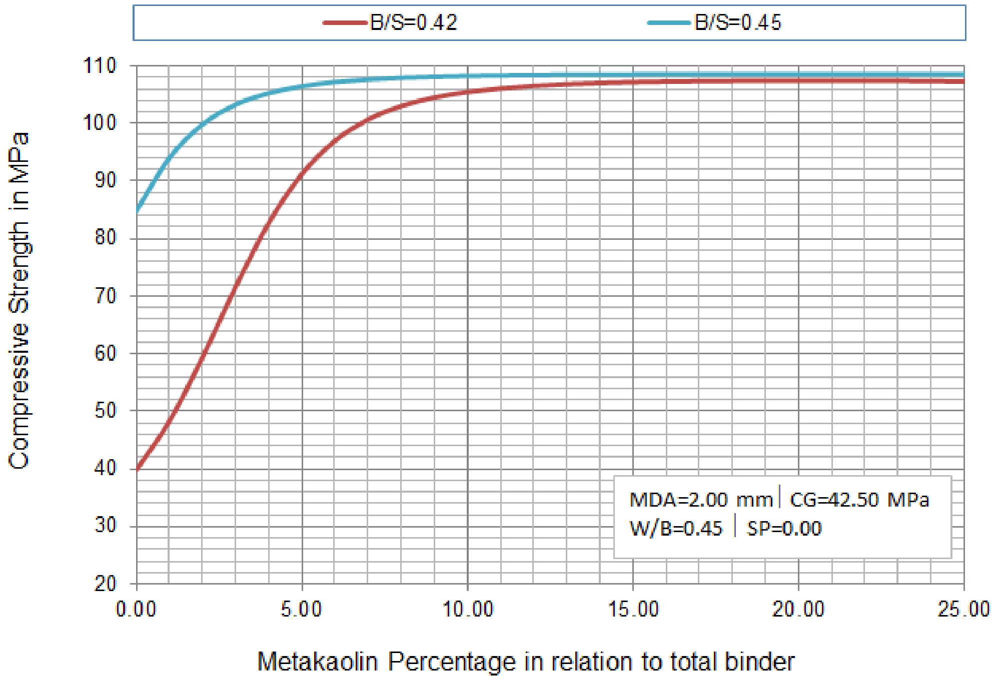

Fig. 12 Mortar Compressive Strength vs Metakaolin to total Binder (MK/B) ratio at various binder to sand ratio (MDA=2.00 mm, CG=42.50, W/B=0.45 and SP=0.00) based on the proposed 6-17-1 ANN model

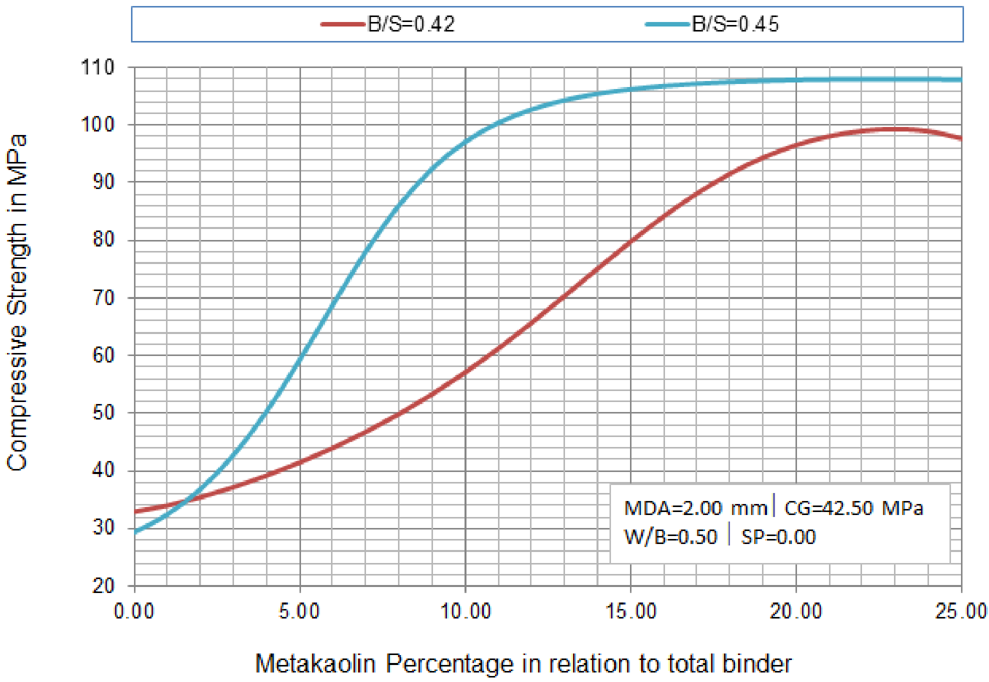

Fig. 13 Mortar Compressive Strength vs Metakaolin to total Binder (MK/B) ratio at various binder to sand ratio (MDA=2.00 mm, CG=42.50, W/B=0.50 and SP=0.00) based on the proposed 6-17-1 ANN model

limited by a number of limitations, related to the database, and the most basic of which are the following:

- Insufficient number of datasets with MDA 2.1-4.0 mm (Fig. 3) and must thus not be used when MDA is within this range,
- For superplasticizer values higher than 2.0%, its reliability is also limited,
- It is proposed to use the model for binder to sand ratios from 0.30 to 0.35 and 0.40 to 0.50, where it presents the highest reliability.

6. Conclusions

As cement-based mortars are considered as main building materials, there is great need for reliable and robust estimation of their 28-day compressive strength. Such a robust and reliable estimation will greatly enhance the successful use of the cement-based materials in the design of modern structures as well as for their use as conservation materials in existing masonry structures, built in the previous century with cement mortars. To this end, as presented in this study, metaheuristic models such as ANN and GP models have been developed and trained for the estimation of their 28-day compressive strength. Based on detailed and in-depth comparisons, the following key findings have been revealed by the experimental and computational results:

- For the successful development of an optimum metaheuristic model, the interdisciplinary nature of the research team is a prerequisite condition. Furthermore, the research teams should cover all the key aspects of the case investigated.
- The selection of the optimum model, among a plethora of predictive computational models, should be based not only on statistical indices but also on human experts' knowledge.
- The maximum diameter of aggregates and the cement grade (which, to the knowledge of the authors, have never up to now, both been used for the modeling of cement based mortars) were revealed to be the most crucial parameters affecting the compressive strength of cement-based mortars.
- The transfer functions employed for the development of the ANN models also play a crucial role to their performance. Specifically, ten different activation functions were used, resulting in 100 (102) different combinations being applied during the training and development process of the BPNNs. Among the ten transfer functions investigated, only two are considered as inappropriate, namely the Linear transfer function (Li) and the Competitive transfer function (Co) for the hidden layer. Regarding the output layer, only three transfer functions are assessed as appropriate, namely the Hyperbolic Tangent Sigmoid transfer function (HTS), the Linear transfer function (Li), and the Symmetric saturating linear transfer function (SSL).
- The initial values of weights and biases highly affect the performance of the Levenberg–Marquardt training algorithm-based BPNNs. Specifically, the values of Root Mean Square Error (RMSE) can increase by 61.7%, while the Pearson correlation coefficient (R) value shows a 11.1% decrease.
- All the proposed models must be checked whether the overfitting problem is avoided (and not be based only on statistical indices as was commented above).
- Based on detailed and in-depth comparisons (including experimental verifications) the proposed ANN model has proved to be a useful tool for the reliable and robust prediction of the 28-day compressive strength of cement-based mortars.

- Using the architecture of the proposed optimum neural network and the resulting values of final weights of the parameters, a useful tool is developed for researchers and engineers, as well as for supporting the teaching and interpretation of the behavior of blended cement, metakaolin-based mortars.
- Although research related to new computational models is, of course, of high importance and adds value for the international scientific community, the authors believe that, since the ultimate goal is a reliable forecast, the reliability of the database should be of utmost importance and should be thoroughly investigated in this regard. In fact, a reliable database must comprise of not only reliable data, but also a sufficient amount of data covering the full range of parameter values (regarding the parameters which influence the problem investigated).
- It is within the future goals of the authors to update the experimental database used herein, including data from future publications as well as conducting further experiments, in order to compose a more reliable experimental database to be used for the development of more reliable, robust and global computational models for the prediction of the 28-day compressive strength of cement-based mortars.

References

Açikgenç, M., Ulaş, M. and Alyamaç, K.E. (2015), "Using an artificial neural network to predict mix compositions of steel fiber-reinforced concrete", *Arab. J. Sci. Eng.*, **40**(2), 407-419. https://doi.org/10.1007/s13369-014-1549-x.

Adeli, H. (2001), "Neural networks in civil engineering: 1989-2000", *Comput. Aided Civ. Infrastruct. Eng.*, **16**(2), 126-142. https://doi.org/10.1111/0885-9507.00219.

Adhikary, B.B. and Mutsuyoshi, H. (2006), "Prediction of shear strength of steel fiber RC beams using neural networks", *Constt. Build. Mater.*, **20**(9), 801-811. https://doi.org/10.1016/j.conbuildmat.2005.01.047.

Akkurt, S., Tayfur, G. and Can, S. (2004), "Fuzzy logic model for the prediction of cement compressive strength", *Cem. Concr. Res.*, **34**(8), 1429-1433. https://doi.org/10.1016/j.cemconres.2004.01.020.

Al-Chaar, G.K., Alkadi, M. and Asteris, P.G. (2013), "Natural pozzolan as a partial substitute for cement in concrete", *Open Construct. Build. Technol. J.*, **7**(1), 33-42. http://dx.doi.org/10.2174/1874836801307010033.

Alavi, A.H. and Gandomi, A.H. (2012), "Energy-based numerical models for assessment of soil liquefaction", *Geosci. Front.*, **3**(4), 541-555. https://doi.org/10.1016/j.gsf.2011.12.008.

Alexandridis, A. (2013), "Evolving RBF neural networks for adaptive soft-sensor design", *Int. J. Neural Syst.*, **23**(6), 1350029. https://doi.org/10.1142/S0129065713500299.

Altun, F., Kişi, O. and Aydin, K. (2008), "Predicting the compressive strength of steel fiber added lightweight concrete using neural network", *Comput. Mat. Sci.*, **42**(2), 259-265. https://doi.org/10.1016/j.commatsci.2007.07.011.

Apostolopoulou, M., Armaghani, D.J., Bakolas, A., Douvika, M.G., Moropoulou, A. and Asteris, P.G. (2019), "Compressive strength of natural hydraulic lime mortars using soft computing techniques", *Procedia Structural Integrity*, **17**, 914-923. https://doi.org/10.1016/j.prostr.2019.08.122.

Apostolopoulou, M., Asteris, P.G., Armaghani, D.J., Douvika, MG., Lourenço, P.B., Cavaleri, L., Bakolas, A. and Moropoulou, A. (2020), "Mapping and holistic design of natural hydraulic lime mortars", *Cement Concrete Res.*, **136**, 106167, https://doi.org/10.1016/j.cemconres.2020.106167.

Apostolopoulou, M., Asteris, P.G., Armaghani, D.J., Douvika, MG., Lourenço, P.B., Cavaleri, L., Bakolas, A. and Moropoulou, A. (2020), "Mapping and holistic design of natural hydraulic lime mortars", *Cem. Concr. Res.*, **136**, 106167. https://doi.org/10.1016/j.cemconres.2020.106167.

Apostolopoulou, M., Douvika, M.G., Kanellopoulos, I.N., Moropoulou, A. and Asteris, P.G. (2018), “Prediction of compressive strength of mortars using artificial neural networks”, *The 1st International Conference TMM_CH, Transdisciplinary Multispectral Modelling and Cooperation for the Preservation of Cultural Heritage*”, Athens, Greece, 10-13 October.

Armaghani, D.J., Hajihassani, M., Sohaei, H., Mohamad, E.T., Marto, A., Motaghedi, H. and Moghaddam, M.R. (2015), “Neuro-fuzzy technique to predict air-overpressure induced by blasting”, *Arab. J. Geosci*., **8**(12), 10937-10950. https://doi.org/10.1007/s12517-015-1984-3.

Armaghani, D.J., Hatzigeorgiou, G.D., Karamani, Ch., Skentou, A., Zoumpoulaki, I. and Asteris, P.G. (2019), “Soft computing-based techniques for concrete beams shear strength”, *Procedia Struct. Integrity*, **17**(2019) 924-933. https://doi.org/10.1016/j.prostr.2019.08.123.

Ashok, M., Parande, A.K. and Jayabalan, P. (2017), “Strength and durability study on cement mortar containing nano materials”, *Advan. Nano Res*., **5**(2), 99-111.

Asteris, P.G. and Kolovos, K.G. (2019), “Self-compacting concrete strength prediction using surrogate models”, *Neural Comput. Appl*., **31**(1), 409-424. https://doi.org/10.1007/s00521-017-3007-7.

Asteris, P.G. and Mokos, V.G. (2019), “Concrete compressive strength using artificial neural networks”, *Neural Comput. Appl*., 1-20. https://doi.org/10.1007/s00521-019-04663-2

Asteris, P.G. and Nikoo, M. (2019), “Artificial bee colony-based neural network for the prediction of the fundamental period of infilled frame structures”, *Neural Comput. Appl*., **31**(9), 4837-4847. https://doi.org/10.1007/s00521-018-03965-1.

Asteris, P.G. and Plevris, V. (2013), “Neural network approximation of the masonry failure under biaxial compressive stress”, *Proceedings of the 3rd South-East European Conference on Computational Mechanics (SEECCM III), an ECCOMAS and IACM Special Interest Conference*, Kos Island, Greece, June.

Asteris, P.G. and Plevris, V. (2016), “Anisotropic masonry failure criterion using artificial neural networks”, *Neural Comput. Appl*., **28**(8), 1-23. https://doi.org/10.1007/s00521-016-2181-3.

Asteris, P.G., Argyropoulos, I., Cavaleri, L., Rodrigues, H., Varum, H., Thomas, J., Paulo B. and Lourenço, P.B. (2018), “Masonry compressive strength prediction using artificial neural networks”, *The 1st International Conference TMM_CH, Transdisciplinary Multispectral Modelling and Cooperation for the Preservation of Cultural Heritage*, Athens, Greece, October.

Asteris, P.G., Kolovos, K.G., Douvika, M.G. and Roinos, K. (2016), “Prediction of self-compacting concrete strength using artificial neural networks”, *Eur. J. Environ. Civ. Eng*., **20**, 102-122. https://doi.org/10.1080/19648189.2016.1246693.

Asteris, P.G., Nozhati, S., Nikoo, M., Cavaleri, L. and Nikoo, M. (2019), “Krill herd algorithm-based neural network in structural seismic reliability evaluation”, *Mech. Advan. Mat. Struct*., **26**(13), 1146-1153. https://doi.org/10.1080/15376494.2018.1430874.

Asteris, P.G., Roussis, P.C. and Douvika, M.G. (2017), “Feed-forward neural network prediction of the mechanical properties of sandcrete materials”, *Sensors*, **17**(6), 1344. https://doi.org/10.3390/s17061344.

Asteris, P.G., Tsaris, A.K., Cavaleri, L., Repapis, C.C., Papalou, A., Di Trapani, F. and Karypidis, D.F. (2016), “Prediction of the fundamental period of infilled rc frame structures using artificial neural networks”, *Comput. Intell. Neurosci*., 5104907. https://doi.org/10.1155/2016/5104907.

ASTM Standards (1983), *ASTM Designation: C 109-80 Standard Test Method for Compressive Strength of Hydraulic Cement Mortars*.

Bartlett, P.L. (1998), “The sample complexity of pattern classification with neural networks: The size of the weights is more important than the size of the network”, *IEEE Trans. Inf. Theory*, **44**(2), 525-536.

Batis, G., Pantazopoulou, P., Tsivilis, S. and Badogiannis, E. (2005), “The effect of metakaolin on the corrosion behavior of cement mortars”, *Cem. Concr. Compos*., **27**(1), 125-130. https://doi.org/10.1016/j.cemconcomp.2004.02.041.

Baykasoğlu, A., Dereli, T.U. and Taniş, S. (2004), “Prediction of cement strength using soft computing techniques”, *Cem. Concr. Res*., **34**, 2083-2090. https://doi.org/10.1016/j.cemconres.2004.03.028.

Belalia Douma, O., Boukhatem, B., Ghrici, M. and Tagnit-Hamou, A. (2016), “Prediction of properties of self-compacting concrete containing fly ash using artificial neural network”, *Neural Comput. Appl*.,

34(11), 1-12. https://doi.org/10.1016/j.cemconres.2004.03.028.

Cavaleri, L., Asteris, P.G., Psyllaki, P.P., Douvika, M.G., Skentou, A.D. and Vaxevanidis, N.M. (2019), “Prediction of surface treatment effects on the tribological performance of tool steels using artificial neural networks”, *Appl. Sci*., **9**(14), 2788. https://doi.org/10.3390/app9142788.

Cavaleri, L., Chatzarakis, G.E., Di Trapani, F.D., Douvika, M.G., Roinos, K., Vaxevanidis, N.M. and Asteris, P.G. (2017), “Modeling of surface roughness in electro-discharge machining using artificial neural networks”, *Ad. Mat. Re*., **6**(2), 169-184. http://dx.doi.org/10.12989/amr.2017.6.2.169.

Chen, H., Asteris, P.G., Armaghani, D.J., Gordan, B. and Pham, B.T. (2019), “Assessing dynamic conditions of the retaining wall using two hybrid intelligent models”, *Appl. Sci*., **9**(6), 1042. https://doi.org/10.3390/app9061042.

Cizer, O., Van Balen, K., Van Gemert, D. and Elsen, J. (2008), “Blended lime-cement mortars for conservation purposes: Microstructure and strength development”, *Structural Analysis of Historic Construction: Preserving Safety and Significance - Proceedings of the 6th International Conference on Structural Analysis of Historic Construction*, 965-972.

Courard, L., Darimont, A., Schouterden, M., Ferauche, F., Willem, X. and Degeimbre, R. (2003), “Durability of mortars modified with metakaolin”, *Cem. Concr. Res*., **33**(9), 1473-1479. https://doi.org/10.1016/S0008-8846(03)00090-5.

Curcio, F., DeAngelis, B.A. and Pagliolico, S. (1998), “Metakaolin as a pozzolanic microfiller for high-performance mortars”, *Cem. Concr. Res*., **28**(6), 803-809. https://doi.org/10.1016/S0008-8846(98)00045-3.

Cyr, M., Idir, R., Escadeillas, G., Julien, S. and Menchon, N. (2007), “Stabilization of industrial by-products in mortars containing metakaolin”, American Concrete Institute, ACI Special Publication, 51-62.

Das, S.K., Samui, P. and Sabat, A.K. (2011), “Application of artificial intelligence to maximum dry density and unconfined compressive strength of cement stabilized soil”, *Geotech. Geolog. Eng*., **29**(3), 329-342. https://doi.org/10.1007/s10706-010-9379-4.

Demir, F. (2008), “Prediction of elastic modulus of normal and high strength concrete by artificial neural networks”, *Construct. Build. Mat*., **22**(7), 1428-1435. https://doi.org/10.1016/j.conbuildmat.2007.04.004.

Dias, W.P.S. and Pooliyadda, S.P. (2001), “Neural networks for predicting properties of concretes with admixtures”, *Constr. Build. Mater*., **15**(7), 371-379. https://doi.org/10.1016/S0950-0618(01)00006-X.

Duan, J., Asteris, P.G., Nguyen, H. Bui, X.-N. and Moayedi, H. (2020), “A novel artificial intelligence technique to predict compressive strength of recycled aggregate concrete using ICA-XGBoost model”, *Eng. Comput*., 1-18. https://doi.org/10.1007/s00366-020-01003-0

SABS, E. (1994), *196-1: 1994 Methods of testing cement. Part 1: Determination of strength*, Pretoria: South African Bureau of Standards.

Eskandari-Naddaf, H. and Kazemi, R. (2017), “ANN prediction of cement mortar compressive strength, influence of cement strength class”, *Constr. Build. Mater*., **138**(1), 1-11. https://doi.org/10.1016/j.conbuildmat.2017.01.132.

Gazder, U., Al-Amoudi, O.S.B., Saad Khan, S.M. and Maslehuddin, M. (2017), “Predicting compressive strength of blended cement concrete with ANNs”, *Comput. Concr*., **20**(6), 627-634. https://doi.org/10.12989/cac.2017.20.6.627.

Geng, H.N. and Li, Q. (2017), “Water absorption and hydration products of metakaolin modified mortar”, *Key Eng. Mat*., 26, 505-509. https://doi.org/10.4028/www.scientific.net/KEM.726.505.

Hornik, K., Stinchcombe, M. and White, H. (1989), “Multilayer feedforward networks are universal approximators”, *Neural Netw*., **2**(5), 359-366.

Ince, R. (2004), “Prediction of fracture parameters of concrete by Artificial Neural Networks”, *Eng. Fracture Mech*., **71**(15), 2143-2159. https://doi.org/10.1016/j.engfracmech.2003.12.004.

Kadri, E.H., Kenai, S., Ezziane, K., Siddique, R. and De Schutter, G. (2011), “Influence of metakaolin and silica fume on the heat of hydration and compressive strength development of mortar”, *Appl. Clay Sci*., **53**(4), 704-708. https://doi.org/10.1016/j.clay.2011.06.008.

Karlik, B. and Olgac, A.V. (2011), “Performance analysis of various activation functions in generalized MLP architectures of neural networks”, *Int. J. Artif. Intell. Expert Syst*., **1**(4), 111-122.

Kechagias, J., Tsiolikas, A., Asteris, P. and Vaxevanidis, N. (2018), “Optimizing ANN performance using DOE: Application on turning of a titanium alloy”, MATEC Web of Conferences, 178,01017.

Kewalramani, M.A. and Gupta, R. (2006), “Concrete compressive strength prediction using ultrasonic pulse velocity through artificial neural networks”, *Automat. Construct.*, **15**(3), 374-379. https://doi.org/10.1016/j.autcon.2005.07.003.

Khademi, F., Akbari, M., Jamal, S.M. and Nikoo, M. (2017), “Multiple linear regression, artificial neural network, and fuzzy logic prediction of 28 days compressive strength of concrete”, *Front. Struct. Civ. Eng*., **11**(1), 90-99. https://doi.org/10.1007/s11709-016-0363-9.

Khater, H.M. (2010), “Influence of metakaolin on resistivity of cement mortar to magnesium chloride solution”, *Ceramics - Silikaty*, **54**(4), 325-333.

Khatib, J.M., Negim, E.M. and E. Gjonbalaj, E. (2012), “High volume metakaolin as cement replacement in mortar”, *World J. Chemistry*, **7**(1), 7-10. http://10.5829/idosi.wjc.2012.7.1.251.

Koza, J.R. (1992), “Genetic programming: on the programming of computers by means of natural selection”, MIT Press, Cambridge, U.S.A.

Lee, S.C. (2003), “Prediction of concrete strength using artificial neural networks”, *Eng. Struct*., **25**(7), 849-857. https://doi.org/10.1016/S0141-0296(03)00004-X.

Lee, S.T., Moon, H.Y., Hooton, R.D. and Kim, J.P. (2005), “Effect of solution concentrations and replacement levels of metakaolin on the resistance of mortars exposed to magnesium sulfate solutions”, *Cem. Concr. Res*., **35**(7), 1314-1323.

Lourakis, M.I.A. (2005), “A brief description of the Levenberg-Marquardt algorithm implemented by levmar”, Hellas (FORTH), *Found. Res.Technol*., **4**(1), 1-6.

Ly, H.B., Pham, B.T., Le, L.M., Le, T.T., Le, V.M. and Asteris, P.G. (2020), “Estimation of axial load-carrying capacity of concrete-filled steel tubes using surrogate models”, *Neural Comput. Applic*., 14-22. https://doi.org/10.1007/s00521-020-05214-w.

Mansour, M.S., Abadlia, M.T., Jauberthie, R. and Messaoudene, I. (2012), “Metakaolin as a pozzolan for high-performance mortar”, *Cement Wapno Beton*, **17**(2), 102-108.

Mansouri, I. and Kisi, O. (2015), “Prediction of debonding strength for masonry elements retrofitted with FRP composites using neuro fuzzy and neural network approaches”, *Compos. Part B Eng*., **70**, 247-255. https://doi.org/10.1016/j.compositesb.2014.11.023.

Mansouri, I., Gholampour, A., Kisi, O. and Ozbakkaloglu, T. (2016), “Evaluation of peak and residual conditions of actively confined concrete using neuro-fuzzy and neural computing techniques”, *Neural Comput. Appl*., **29**(3), 873-888. https://doi.org/10.1007/s00521-016-2492-4.

Mardani-Aghabaglou, A., Sezer, G.İ. and Ramyar, K. (2014), “Comparison of fly ash, silica fume and metakaolin from mechanical properties and durability performance of mortar mixtures view point”, *Construct. Build. Mat*., **70**(15), 17-25. https://doi.org/10.1016/j.conbuildmat.2014.07.089.

Mashhadban, H., Kutanaei, S.S. and Sayarinejad, M.A. (2016), “Prediction and modeling of mechanical properties in fiber reinforced self-compacting concrete using particle swarm optimization algorithm and artificial neural network”, *Constr. Build. Mater*., **119**, 277-287. https://doi.org/10.1016/j.conbuildmat.2016.05.034.

Naderpour, H. and Mirrashid, M. (2018), “An innovative approach for compressive strength estimation of mortars having calcium inosilicate minerals”, *J. Build. Eng*., **19**, 205-215. https://doi.org/10.1016/j.jobe.2018.05.012.

Nguyen, H. and Bui, X.N. (2019), “Predicting blast-induced air overpressure: a robust artificial intelligence system based on artificial neural networks and random forest”, *Nat. Resources Res*., **28**(3), 893-907. https://doi.org/10.1007/s11053-018-9424-1.

Nikoo, M., Hadzima-Nyarko, M., KarloNyarko, E. and Nikoo, M. (2018), “Determining the natural frequency of cantilever beams using ANN and heuristic search”, *Appl. Artificial Intell*., **32**(3), 309-334.

Nikoo, M., Ramezani, F., Hadzima-Nyarko, M., Nyarko, E.K. and Nikoo, M. (2016), “Flood-routing modeling with neural network optimized by social-based algorithm”, *Nat. Haz*., **82**(1). https://doi.org/10.1007/s11069-016-2176-5.

Nikoo, M., Sadowski, L., Khademi, F. and Nikoo, M. (2017), “Determination of damage in reinforced concrete frames with shear walls using self-organizing feature map", *Appl. Comput. Intell. Soft Comput.*, 3508189. https://doi.org/10.1155/2017/3508189.

Nikoo, M., Zarfam, P. and Sayahpour, H. (2015), "Determination of compressive strength of concrete using Self Organization Feature Map (SOFM)", *Eng. Comput.*, **31**(1), 113-121. https://doi.org/10.1007/s00366-013-0334-x.

Oh, T.K., Kim, J., Lee, C. and Park, S. (2017), "Nondestructive concrete strength estimation based on electro-mechanical impedance with artificial neural network", *J. Adv. Concr. Technol.*, **15**(3), 94-102. https://doi.org/10.3151/jact.15.94.

Onyari, E.K. and Ikotun, B.D. (2018), "Prediction of compressive and flexural strengths of a modified zeolite additive mortar using artificial neural network", *Construct. Build. Mater.*, **187**, 1232-1241. https://doi.org/10.1016/j.conbuildmat.2018.08.079.

Özcan, F., Atiş, C.D., Karahan, O., Uncuoğlu, E. and Tanyildizi, H. (2009), "Comparison of artificial neural network and fuzzy logic models for prediction of long-term compressive strength of silica fume concrete", *Adv. Eng. Softw.*, **40**(9), 856-863. https://doi.org/10.1016/j.advengsoft.2009.01.005.

Pala, M., Özbay, E., Öztaş, A. and Yuce, M.I. (2007), "Appraisal of long-term effects of fly ash and silica fume on compressive strength of concrete by neural networks", *Construct. Build. Mater.*, **21**(2), 384-394. https://doi.org/10.1016/j.conbuildmat.2005.08.009.

Parande, A.K., Ramesh Babu, B., AswinKarthik, M., Deepak Kumaar, K.K. and Palaniswamy, N. (2008), "Study on strength and corrosion performance for steel embedded in metakaolin blended concrete/mortar", *Construct. Build. Mater.*, **22**(3), 127-134. https://doi.org/10.1016/j.conbuildmat.2006.10.003.

Pavlikova, M. Brtnik, T., Keppert, M. and Cerny, R. (2009), "Effect of metakaolin as partial Portland-cement replacement on properties of high performance mortars", *Cement Wapno Beton*, **29**(3), 113-122.

Pham, B.T., Hoang,T.A, Nguyen, D.M. and Bui, D.T. (2018), "Prediction of shear strength of soft soil using machine learning methods", *Catena*, **166**, 181-191. https://doi.org/10.1016/j.catena.2018.04.004.

Plevris, V. and Asteris, P. (2015), "Anisotropic failure criterion for brittle materials using Artificial Neural Networks", *The Proceedings of the COMPDYN 2015-5th ECCOMAS Thematic Conference on Computational Methods in Structural Dynamics and Earthquake Engineering, Crete Island*, Greece, May.

Plevris, V. and Asteris, P.G. (2014), "Modeling of masonry compressive failure using Neural Networks", *Proceedings of the OPT-i 2014-1st International Conference on Engineering and Applied Sciences Optimization, Kos*, Greece, June.

Plevris, V. and Asteris, P.G. (2014), "Modeling of masonry failure surface under biaxial compressive stress using Neural Networks", *Constr. Build. Mater.*, **55**, 447-461. https://doi.org/10.1016/j.conbuildmat.2014.01.041.

Potgieter-Vermaak, S.S. and Potgieter, J.H. (2006), "Metakaolin as an extender in South African cement", *J. Mater. Civil Eng.*, **18**(4), 619-623. https://doi.org/10.1061/(ASCE)0899-1561(2006)18:4(619).

Reddy, T.C.S. (2017), "Predicting the strength properties of slurry infiltrated fibrous concrete using artificial neural network", *Front. Struct. Civil Eng.*, **12**(4), 490-503. https://doi.org/10.1007/s11709-017-0445-3.

Sadowski, L. and Nikoo, M. (2014), "Corrosion current density prediction in reinforced concrete by imperialist competitive algorithm", *Neural Comput. Appl.*, **25**(7-8), 1627-1638. https://doi.org/10.1007/s00521-014-1645-6.

Sadowski, L., Nikoo, M. and Nikoo, M. (2015), "Principal component analysis combined with a self organization feature map to determine the pull-off adhesion between concrete layers", *Construct. Build. Mater.*, **78**, 386-396. https://doi.org/10.1016/j.conbuildmat.2015.01.034.

Safiuddin, M., Raman, S.N., Salam, M.A. and Jumaat, M.Z. (2016), "Modeling of compressive strength for self-consolidating high-strength concrete incorporating palm oil fuel ash", *Mater.*, **9**(5), 396. https://doi.org/10.3390/ma9050396.

Saidat, F., Mouret, M. and Cyr, M. (2012), "Chemical activation of metakaolin in cement-based materials. *Special Publication*, **288**, 1-15.

Salehi, H. and Burgueño, R. (2018), "Emerging artificial intelligence methods in structural engineering", *Eng. Struct.*, **171**, 170-189. https://doi.org/10.1016/j.engstruct.2018.05.084.

Samui, P. (2008), “Support vector machine applied to settlement of shallow foundations on cohesionless soils”, *Comput. Geotech*., **35**(3), 419-427. https://doi.org/10.1016/j.compgeo.2007.06.014.

Samui, P. and Kothari, D.P. (2011), “Utilization of a least square support vector machine (LSSVM) for slope stability analysis”, *Scientia Iranica*, **18**(1), 53-58. https://doi.org/10.1016/j.scient.2011.03.007.

Saridemir, M. (2009), “Predicting the compressive strength of mortars containing metakaolin by artificial neural networks and fuzzy logic”, *Adv. Eng. Softw*., **40**(9), 920-927. https://doi.org/10.1016/j.advengsoft.2008.12.008.

Sumasree, C. and Sajja, S. (2016), “Effect of metakaolin and cerafibermix on mechanical and durability properties of mortars”, *Int. J. Sci. Eng.Technol*., **4**(3), 501-506.

Topçu, I.B. and Saridemir, M. (2007), “Prediction of properties of waste AAC aggregate concrete using artificial neural network”, *Comput. Mater. Sci*., **41**(1), 117-125. https://doi.org/10.1016/j.commatsci.2007.03.010.

Topçu, I.B. and Saridemir, M. (2008), “Prediction of compressive strength of concrete containing fly ash using artificial neural networks and fuzzy logic”, *Comput. Mater. Sci*., **41**(3), 305-311. https://doi.org/10.1016/j.commatsci.2007.04.009.

Trtnik, G., Kavčič, F. and Turk, G. (2009), “Prediction of concrete strength using ultrasonic pulse velocity and artificial neural networks”, *Ultrasonics*, **49,** 53-60.

Türkmen, İ., Bingöl, A.F., Tortum, A., Demirboğa, R. and Gül, R. (2017), “Properties of pumice aggregate concretes at elevated temperatures and comparison with ANN models”, *Fire Mater*., **41**, 142-153. https://doi.org/10.1016/j.commatsci.2007.04.009.

Vu, D.D., Stroeven, P. and Bui, V.B. (2001), “Strength and durability aspects of calcined kaolin-blended Portland cement mortar and concrete”, *Cem. Concr. Compos*., **23**(6), 471-478. https://doi.org/10.1016/S0958-9465(00)00091-3.

Waszczyszyn, Z. and Ziemiański, L. (2001), “Neural networks in mechanics of structures and materials - New results and prospects of applications”, *Comput. Struct*., **79**(22-25), 2261-2276. https://doi.org/10.1016/S0045-7949(01)00083-9.

Xu, H., Zhou, J., Asteris, P.G., Armaghani, D.J. and Tahir, M.Md. (2019), “Supervised machine learning techniques to the prediction of tunnel boring machine penetration rate”, *Appl. Sci*., **9**(18), 3715. https://doi.org/10.3390/app9183715.

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Appendix

Table A1.Final values of weights and biases of the optimum ANN 6-17-1 model

Weights							Biases	
IW{1,1}						$LW\{2,1\}^T$	B{1,1}	B{2,1}
(17×6)						(1×17)	(17×1)	(1×1)
-0.4918	-0.6090	-0.8824	0.1767	-0.3170	-0.0582	-1.05483	-0.3292	1.0669
0.6295	0.6399	0.2087	0.3151	0.1848	-0.3124	-1.04919	0.7191	
-0.4422	0.0316	0.2973	-0.8353	0.6651	-0.9850	-0.78649	-0.4655	
-0.4455	-0.2745	0.7342	-0.0604	-0.0640	-0.1778	-0.28556	0.3452	
0.4837	0.8686	0.0833	-0.9770	0.6566	0.9759	0.8024	-0.7606	
-0.8964	0.2693	-0.3382	-0.3749	-0.1685	0.7004	0.522013	-0.8455	
0.3392	-0.0813	-0.4364	-0.6998	-0.6934	-0.5072	0.733269	-0.8395	
0.7458	0.9654	-0.7952	0.6877	0.6556	0.1674	-0.34748	-0.2185	
0.6550	-0.0463	-0.6953	0.4505	0.0638	0.0317	0.592561	0.5055	
0.1374	0.2220	0.7131	0.8826	0.0108	-0.9868	-0.60052	-0.6832	
-0.7859	0.9745	-0.6863	-0.0043	-0.7263	0.7809	-0.70911	-0.5397	
-0.6021	-0.9669	-0.4840	-0.0929	-0.1425	0.0129	-0.41536	-0.7849	
-0.0297	-0.3031	0.1291	0.5345	0.7799	-0.3751	-0.5705	0.5310	
0.2407	-0.0623	0.0479	0.1060	-0.8777	-0.8410	0.081294	-0.0808	
-0.5067	0.7695	-0.6157	-0.5776	-0.3357	-0.6914	-0.44697	-0.3682	
-0.2456	0.5110	-0.2098	0.8147	0.3760	0.4727	0.225178	-0.5704	
0.6051	-0.9949	-0.6447	-0.0843	0.6842	0.5864	1.175572	-0.8478	

IW{1,1}= Matrix of weights values for between input layer and the hidden Layer, LW{2,1}= Matrix of weights values between the hidden Layer and the output Layer

B{1,1}= Bias values for hidden layer , B{2,1}= Bias values for output layer