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Application of artificial neural networks for the prediction of the compressive strength of cement-based mortars

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Abstract. Despite the extensive use of mortar materials in constructions over the last decades, there is not yet a robust quantitative method, available in the literature, which can reliably predict mortar strength based on its mix components. This limitation is due to the highly nonlinear relation between the mortar's compressive strength and the mixed components. In this paper, the application of artificial neural networks for predicting the compressive strength of mortars has been investigated. Specifically, surrogate models (such as artificial neural network models) have been used for the prediction of the compressive strength of mortars (based on experimental data available in the literature). Furthermore, compressive strength maps are presented for the first time, aiming to facilitate mortar mix design. The comparison of the derived results with the experimental findings demonstrates the ability of artificial neural networks to approximate the compressive strength of mortars in a reliable and robust manner.

Keywords: artificial neural networks (ANNs); cement; compressive strength; metakaolin; mortar; soft computing techniques

1. Introduction

Mortars are important elements of masonry structures, as they are the material used to join stone and/or brick elements comprising a 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 within this framework, with the additional benefit 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 behaviour that makes the development of an analytical formula for the prediction of the mechanical properties using deterministic methods a rather difficult task.

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. An important characteristic of ANNs is that they can be used to build soft-sensors, i.e., models with the ability to estimate critical quantities without having to measure them (Alexandridis 2013). In particular, such surrogate models can be developed 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 cost-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, Peng *et al*. 2009, Waszczyszyn and Ziemiański 2001, Belalia Douma *et al*. 2017, Mashhadban *et al*. 2016, Açikgenç *et al*. 2015, Asteris *et al*. 2016). In their study Asteris *et al*. (2016) 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 as output parameter the value of 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, Bilgehan and Turgut 2010, Boukhatem *et al*. 2012, 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, Mazloom and Yoosefi 2013, Abdollahzadeh *et al*. 2016, Asteris and Nikoo (2019), Safiuddin *et al*. 2016, Mansouri and Kisi 2015, Hoła and Sadowski 2019, Mansouri *et al*. 2016, Reddy 2017, Salehi and Burgueño 2018, Sadowski *et al*. 2015 and

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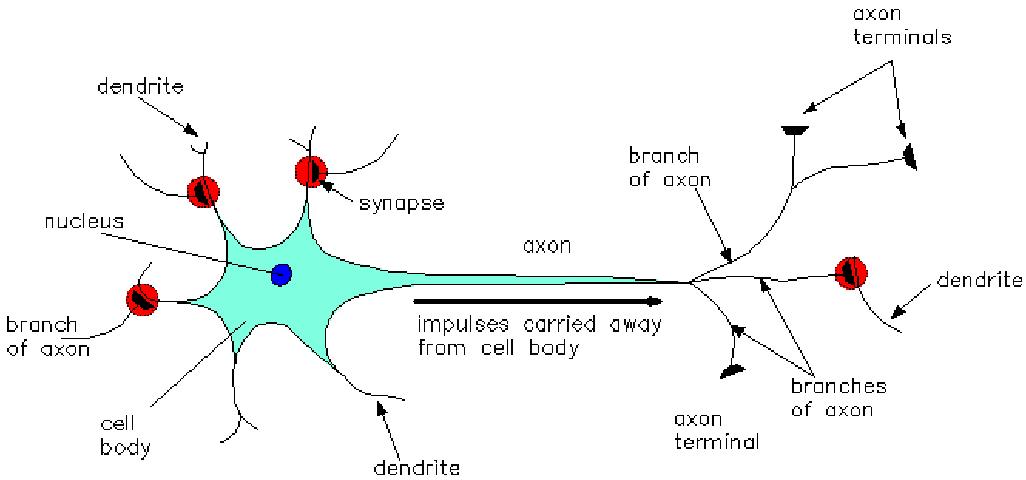

Fig. 1 Schematic representation of biological neuron structure

2019, Kao *et al*. 2017, Castelli, *et al*. 2017, Ongpeng *et al*. 2017, Saha *et al*. 2017, Rashid and Rashid 2017, Camões and Martins 2017, Golafshani and Pazouki 2018, Dutta *et al*. 2018, Erdal *et al*. 2018, Xue 2018, Asteris *et al*. 2019a, Tsai and Liao 2019, Bui *et al*. 2019).

In this context, in the work presented herein, the modelling of the mechanical characteristics 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) models for the prediction of the compressive strength of cement-based mortars. Specifically, for the development and the training of NN models, a database consisting of 268 specimens taken from the literature, was utilized. Namely, based on this database, the age of the specimen (AS) as well as four parameters of synthesis, (Metakaolin to total binder (MK/B) percentage, Water to Binder (W/B) ratio, Superplasticizer (SP), Binder to Sand (B/S) ratio) were used as input parameters, while the value of compressive strength was used as output parameter. The optimum developed NN model has proven to be very successful, exhibiting very reliable predictions. Furthermore, compressive strength maps have been developed and are presented, revealing the compressive strength of mortars in relation to the mortar mix parameters. The developed ANN has the ability to develop many such compressive strength maps, which assist in the visualization of the effect of the different mix parameters on mortar compressive strength and can serve as a tool for educational purposes.

2. Significance of the subject

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 behavior between mixed components and mortar characteristics, it is difficult to predict the compressive strength of a mortar mix, and thus, this difficulty leads to the need for costly and time consuming experiments based on empirical calculations of the appropriate mortar synthesis parameters.

To this end, soft-computing techniques, such as Artificial Neural Networks (ANN), can contribute as a feasible tool for the estimation of the mechanical properties of concrete (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, Kaveh *et al*. 2018, Hoang and Bui 2018, Dao *et al*. 2019, Chen *et al*. 2019). In this study, Artificial Neural Networks have been developed for the prediction of the compressive strength of mortars, using the age and the mix composition parameters of mortar specimens as input parameters and, as output parameter, the value of compressive strength.

3. Artificial neural networks

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 (Asteris *et al*. 2016, Hornik *et al*. 1989, Plevris and Asteris 2014, Plevris and Asteris 2015, Giovanis and Papadopoulos 2015, Asteris and Plevris 2013, Asteris and Plevris 2017, Asteris and Kolovos 2019, Alkayem *et al*. 2018, Alavi Nezhad Khalil Abad *et al*. 2018, Sarir *et al*. 2019, Cavaleri *et al*. 2019, Moayedi *et al*. 2019, Armaghani *et al*. 2018, Nguyen *et al*. 2019, Ly *et al*. 2019, Le *et al*. 2019).

3.1 General

The concept of an artificial neural network is based on the concept of the biological neural network of the human brain. The basic building block of the ANN is the artificial neuron, which is a mathematical model aiming to mimic the behaviour of the biological neuron.

Information is passed into the artificial neuron as input and processed with a mathematical function leading to an output that determines the behaviour of the neuron (similar to fire-or-not situation for the biological neuron). Before the information enters the neuron, it is weighted in order to approximate the random nature of the biological neuron. A group of such neurons consists of an ANN in a manner similar to biological neural networks. In order to set up an ANN, one needs to define: (i) the architecture of the ANN; (ii) the training algorithm, which will be used for the ANN learning phase; and (iii) the mathematical functions describing the mathematical model.

The architecture or topology of the ANN describes the manner in which the artificial neurons are organized in the group and how information flows within the network. For example, if the neurons are organized in more than one layers, then the network is called a multilayer ANN. Regarding the training phase of the ANN, it can be considered as a function minimization problem, in which the optimum value of weights need to be determined by minimizing an error function. Depending on the optimization algorithms used for this purpose, different types of ANNs exist. Finally, the two mathematical functions that define the behaviour of each neuron are the summation function and the activation function. In the present study, we use a back-propagation neural network (BPNN), which is described in section 3.3.

3.2 The History behind ANNs

It can be said that the research on artificial neural networks started back in 1940, when scientists initially attempted to understand and then decode neurons. An extensive activity was followed by several researchers in the 1960s and 1980s, while by the end of the 20th century the foundations were laid for the development of the ANNs that are still deployed nowadays.

In particular, McCulloch and Pitts (1943) were the first to show that neurons can be combined to construct a Turing machine (using ANDs, ORs, & NOTs) (McCulloch and Pitts 1943). Following, Rosenblatt (1958) showed that perceptrons will converge if what they are trying to learn can be represented. Minsky and Papert (1969) showed the limitations of perceptron's, thus pausing research in neural networks for a decade, until in 1985 the backpropagation algorithm by Geoffrey Hinton *et al*. (Ackley *et al*. 1985) revitalized the field. In 1988, Neocognitron developed a hierarchical neural network, capable of visual pattern recognition (Fukushima 1998). CNNs with Backpropagation were developed and utilized for document analysis by LeCun *et al*. (1998). In 2006, the Hinton lab solved the existing training problem for DNNs, which was a turning point in the field (Hinton *et al*. 2006, Hinton and Salakhutdinov 2006). Detailed and in-depth state-of-the-art reports can be found in the works of Widrow and Lehr, (1990), Cheng and Titterington (1994), Ripley (1996), Zhang *et al*. (1998), Schmidhuber (2015), LeCun *et al*. (2015) and Cao *et al*. (2016).

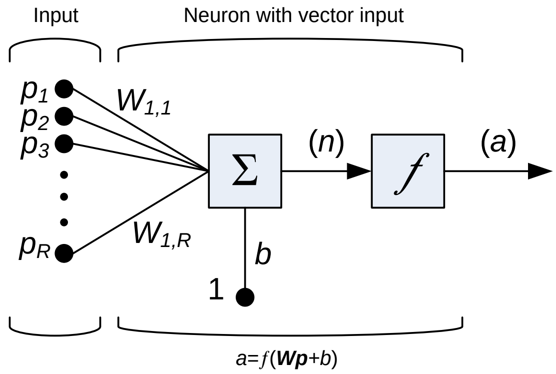

Fig. 2 A neuron with a single R-element input vector

3.3 Architecture of BPNN

A BPNN is a feed-forward, multilayer network (Hornik *et al*. 1989). Thus, 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 parameters, H_v coresponds to the number of neurons in N-hidden level for v=1, … , NHL where, NHL is the number of the hidden layers, and M the number of output parameters.

Based on the above a BPNN with a 5 entry neurons, two hidden levels of 24 and 7 neurons, respectively, and 1 output neuron is encoded as 5-24-7-1 BPNN.

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. 2.

For each neuron i, the individual element inputs $p_1, \ldots, p_R$ are multiplied by the corresponding weights $w_{\mathrm{i},1}, \ldots, w_{i,R}$ and the weighted values are fed to the junction of the summation function, in which the dot product $(W \cdot p)$ of the weight vector $W = [\mathrm{w}_{\mathrm{i},1}, \ldots, w_{i,R}]$ and the input vector $p = [p_1, \ldots, p_R]^T$ 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

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

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 types 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 Sigmoid and the Hyperbolic Tangent transfer functions were found to be appropriate for the problem 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 minimise the following error function

$$E = \sum (x_i - y_i)^2 \quad (3)$$

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 the investigated problem. The most common method used in the literature is the back-propagation technique mentioned above. 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.

4. Materials and methods

This section presents the process for tuning optimum ANNs used for the prediction of the compressive strength of mortar materials, based on experimental data available in the literature.

4.1 Experimental-Database

A prerequisite for the successful function of artificial neuron networks is the use of an extended and reliable database, capable of training the system. In the case of mortars this poses an issue due to many factors.

For one, mortars are composite materials, consisting of binder material and aggregates, while in most cases additives are used, either natural or manufactured or both. Thus, mortars are produced through the mix of water with different natural and manufactured raw materials. During the configuration of the database it is important to distinguish the necessary mix parameters; furthermore, it is crucial to be accurate regarding the type of raw materials used, in order to train the system appropriately. For example, the use of Ordinary Portland cement (OPC) in the mortar mix will have a different effect on the final compressive strength values than the use of white cement or high alumina cement; thus, if different types of cement were used in the different mortars included in the database, it must be appropriately described to the ANN in order to optimize the results.

Another issue is related to the difficulty of one researcher obtaining a large enough amount of experimental data capable of adequately training the ANN. Mortars are produced, casted into steel molds in order to set (dimensions of molds and mortar curing conditions related on standard used and on mortar type produced) and then removed from molds and preserved in specific environmental conditions until the testing date, when the mortar specimen has reached the desired age. It is obvious, that the production of a very large amount of specimens is problematic and costly, while compressive strength measurements are time consuming, not so much in terms of experimental procedure, but in terms of real time between the production of the specimen and its actual measurement; during this time, it must be stored, and this demands space of specific requirements and the subsequent cost. This is an additional reason that many researchers study mortar characteristics up to 28 or 90 days; of course in the literature, there is available data of compressive strength obtained from specimens of larger ages, however data at these higher ages is relatively scarce, with the consequent problems incurred on the ANN prediction.

Thus, the compiling of an adequate experimental database is achieved through the accumulation of smaller databases acquired by different researchers and available in the relevant literature. During the compiling of the database, the reliability of each individual database must be examined. In particular, the raw materials used must be adequately described; the type of cement and metakaolin is of the utmost importance, as different types must be discerned due to their different effect on compressive strength. Furthermore, it is important that the same standards have been followed during the experimental procedure, in order for the results to be comparable and the comparison to be meaningful. An adequate number of specimens must have been tested in order for the values to be statistically acceptable; a small amount of tested specimens, regardless of credibility, cannot give a result that can be considered reliable. When training an ANN, in addition to the reliability of the database, it is crucial that the values of the input parameters (mortar mix synthesis parameters and specimen age) cover all possible value ranges of the parameters. It is no exaggeration to state that the reliability of the optimum developed neural network is crucially dependent on the reliability of the experimental data, thus confirming the famous expression in the field of informatics Garbage In, Garbage Out (GIGO). Predictive analytics begins with good data; more data doesn't necessarily mean better data. A successful predictive analytics project requires, first and foremost, relevant and accurate data. It is obvious from the above that mortars present certain difficulties in predicting their compressive strength. This complexity of course, is the reason that the use of ANN is intriguing in relation to predicting the final characteristics of the mortar after setting and hardening, as no linear approach can be successfully applied.

In light of the above, a large database has been composed. Specifically, the database used herein consists of 268 experimental data sets that have been obtained from eight experimental works available in literature (Table 1). The experimental data selected from the literature was that of mortars with OPC (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. Namely, Vu *et al.* (2001) produced cement mortars, using Portland cement, metakaolin, sand and superplastisizer. Mortar mixes consisted of 1 part binder and 2.75 parts sand by weight. They managed to measure compressive strength of 144 samples, at four different ages (7 days to 3 months), with varying water to binder ratio (0.40 to 0.53), and also with partial replacement of cement with metakaolin in various percentages (ranging from 0% to 30% with a 5% step increment). The superplasticizer (naphthalene sulfonate-based type TM OFT-3) was added in varying percentages (0%, 0.5% and 1.4%). The specimens were cast in steel molds of dimensions 10cmx40cmx40cm. Compressive strength was measured in accordance to ASTM C109-80 (1983) on six cubic samples 10cmx10cmx10cm. Courard *et al.* (2003) produced cement mortar specimens, using ordinary portland cement, metakaolin in different percentages (0-20% with a 5% increment) and sand. The binder to sand ratio was constant at 1/3 by weight. The mortars were cast into 4cmx4cmx16 cm steel molds and tested at different ages, ranging from 3 days to 28 days. Compressive strength was measured in accordance to NBN B12-208 (1969) on six samples (dimensions 4 cm×4 cm×4 cm). In the study of Parande *et al*. (2008) ordinary Portland cement is used with aggregates and metakaolin (0%-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 ration was constant at 0.40. Cube mortar specimens were produced (10 cm×10 cm×10 cm) and measured at different ages (3 days to 90 days). Sumasree and Sajja (2016) studied the compressive strength of OPC/OPC-metakaolin mortars at five different ages, ranging from 3 days to 56 days. Metakaolin replaced cement in the mix at different percentages, ranging from 0% to 30% with a 5% increment. Binder to sand remained at 0.50 by weight and water/binder ratio remained constant at 0.46. Compressive strength measurements were conducted on specimens 4cmx4cmx4cm. Batis *et al*. (2005) also studied the effect of metakaolin on the compressive strength of cement mortars, produced through mixing Ordinary Portland Cement with sand, while metakaolin was added in various cement substitution ratio (0%, 10%, 20%). Water to binder remained constant for all specimens at 0.6, as well as the binder to aggregates ratio, which was kept at 0.33 by weight. Compressive strength was measured at four ages (varying from 1 day to 28 days) and was performed in accordance to EN 196-1 (1994). The blended cement-metakaolin mortars presented compressive strength values ranging from 17.6 to 69.70 MPa taking into account all measured ages.

Kadri *et al*. (2011) studied the influence of metakaolin on the development of compressive strength in cement-mortar systems, produced with the use of ordinary Portland cement, metakaolin in two different substitution percentages (0% and 10% of total binder) and sand. Superplasticizer was added in three different percentages in relation to the binder material (1.4%, 2.3% and 2%), while the mater to binder ratio was kept constant for all mortar mixes at 0.36. The binder to sand ration (by weight) was also kept constant at 0.5. The mortars were studied at 1, 7, 28 and 56 days in relation to their compressive strength, while the compressive strength measurements were conducted on 4cmx4cmx4cm specimens, abiding by EN 196-1 (1994).

Mardani-Aghabaglou *et al.* (2014) studied the mechanical performance of cement mortar mixes, using a CEM I 42.5 R type cement conforming to EN 197-1 (2011) standard 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 in relation to total binder materias. The binder to sand ration was kept constant in the two mixes (with and without metakaolin), at 0.37 by weight, while the water to binder ration was also kept constant at 0.485 by weight. Superplasticizer was not added in any mix. Compressive strength was measured on cubic samples (50 cm×50 cm×50 cm) in accordance to ASTM C 109 at three different ages (7, 28 and 90 days), with values ranging from 37.27 to 56.76 MPa.

Potgieter-Vermaak and Potgieter (2006) examined the use of metakaolin as an extender of South African cement. They produced cement mortars, using a local ordinary Portland cement, local metakaolin, heated at different temperatures and with different activation times, and sand. For the database herein compiled, the mortar mixes where metakaolin was heated at 750°C were taken into account, as to be in accordance with the metakaolin used by the other researchers as well. The mortar mixes were produced with different metakaolin percentages in relation to total binder (0%-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 specimens (dimensions 4 cm×4 cm×4 cm) were crushed to failure on a Farnell cube press in order to obtain the compressive strength value (mean of six specimens). Measurements were conducted at 1, 2, 14 and 28 days, yielding compressive strength values ranging from 23.4 to 92.8 MPa.

Based on the above database, each input training vector p is of dimension 1×5 and consists of the value of the age 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 addition of superplasticizer in relation to the total binder by weight (%w/w), and the binder-to-sand ratio (B/S), meaning the w/w of binder materials to aggregate materials. The corresponding output training vectors are of dimension 1×1 and consist of the value of the compressive strength of the mortar specimens. Their mean values together with the minimum, maximum values as well standard deviation (STD) values are listed in Table 2. Moreover, Fig. 3 demonstrates the frequency histograms of the parameters. Basically, some of the cement metakaolin mortars variables could be dependent on each other. High negative or positive values of the correlation coefficient between the input variables may result in poor efficiency of the methods and difficulty in construing the effects of the expository variables on the respond. Subsequently, the correlation coefficients between all possible variables have been specified and are presented in Table 3. As can be seen in the table, there are not significant correlations between the independent input variables. To the contrary, 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 highlighted line in Table 3- are required to be as high as possible. Based on these values it is clearly

Table 1 Data from experiments published in literature

No	Reference	Number of Samples	Parameters MK	Parameters SP	Compressive Strength (MPa)
1	Vu *et al*. (2001)	144	√	√	15.45-54.90
2	Courard *et al*. (2003)	15	√		27.40-71.20
3	Parande *et al*. (2008)	20	√		22.00-67.00
4	Sumasree and Sajja (2016)	35	√		24.93-35.71
5	Batis *et al*. (2005)	16	√		17.60-69.70
6	Kadri *et al*. (2011)	12	√	√	35.21-99.17
7	Ali Mardani-Aghabaglou *et al*. (2014)	6	√		37.27-56.76
8	Potgieter-Vermaak and Potgieter (2006)	20	√		23.40-92.80
	Total	268			15.45-99.17

Table 2 The input and output parameters used in the development of BPNNs

Variable	Units	Type	Data Used in NN Models				
			Min	Average	Max	Range	STD
Age of Specimen (AS)	Days	Input	2.00	47.77	360.00	2-360	54.75
Metakaolin percentage in relation to total binder (MK/B)	(%w/w)	Input	0.00	16.07	50.00	0-50	11.63
Water-to-binder ratio (W/B)	(w/w)	Input	0.40	0.63	2.60	0.4-2.6	0.38
Superplasticizer (SP)	(%w/w)	Input	0.00	0.16	1.30	0-1.3	0.37
Binder-to-sand ratio (B/S)	(w/w)	Input	0.09	0.41	0.50	0.09-0.5	0.12
Compressive Strength	MPa	Output	0.15	33.38	91.40	0.15-91.40	18.86

shown that there is a strong relation between the mortar compressive strength (CS) and the input parameters of the age of the specimen (AS), the water-to-binder ratio (W/B) and the value of superplasticizer (SP)), at least in the range of parameter values examined.

4.2 Training algorithms

For the training of the BPNN models the use of a large set of training function such as quasi-Newton, Resilient, One-step secant, Gradient descent with momentum and adaptive learning rate and Levenberg-Marquardt back propagation algorithms has been investigated. From all these algorithms the best prediction for the non-linear behaviour of the mortar compressive strength is achieved, by a significant margin with respect to the rest, by the Levenberg-Marquardt implemented by levmar (Lourakis 2005). This algorithm appears to be the fastest method for training moderate-sized feedforward neural networks (up to several hundred weights) as well as non-linear problems. It also has an efficient implementation in MATLAB® software, because the solution of the matrix equation is a built-in function, so its attributes become even more pronounced in a MATLAB environment.

Table 3 Correlation matrix of the input variables

Variable		Input AS	Input MK/B	Input W/B	Input SP	Input B/S	Output CS
Input	AS	1.00					
	MK/B	0.08	1.00			[Symmetric]	
	W/B	0.03	0.09	1.00			
	SP	0.06	-0.05	-0.54	1.00		
	B/S	0.25	0.15	-0.08	0.36	1.00	
Ouput	CS	0.21	-0.02	-0.45	0.39	-0.11	1.00

4.3 Normalization of data

The normalization of data is a pre-processing phase which has proved to be the most crucial step for any type of problem in the field of soft computing techniques, such as artificial neural networks techniques. In the present study, during the pre-processing stage, the Min-Max (Delen *et al*. 2006) and the ZScore normalization methods have been used. In particular, the five input parameters (Table 2), as well as the single output parameter, have been normalized using the Min-Max normalization method. As stated by Iruansi *et al*. (2010), in order to avoid problems associated with low learning rates of the ANN, the normalization of the data should be made within a range defined by appropriate upper and lower limit values of the corresponding parameter. In this work, the input and output parameters have been normalized in the range [0.10, 0.90].

4.4 BPNN model development

In this work, a large number of different BPNN models have been developed and implemented. Each one of these ANN models was trained with over 199 data-points out of the total of 298 data-points, (66.78% of the total number) and the validation and testing of the trained ANN were performed with the remaining 99 data-points. More specifically, 50 data-points (16.78%) were used for the validation of the trained ANN and 49 (16.44%) data-points were used for the testing.

The development and training of the ANNs occurs with a number of hidden layers ranging from 1 to 2 and with a number of neurons ranging from 1 to 30 for each hidden layer. Each one of the ANNs is developed and trained for a number of different activation functions, such as the Log-sigmoid transfer function (logsig), the Linear transfer function (purelin) and the Hyperbolic tangent sigmoid transfer function (tansig) (Asteris *et al*. 2019b, Asteris *et al*. 2017, Cavaleri *et al*. 2017, Asteris *et al*. 2016, Apostolopoulou *et al*. 2018, Asteris *et al*. 2018b, Nikoo *et al*. 2017, Nikoo *et al*. 2018, Nikoo *et al*. 2016).

The parameters used for the ANN training are summarized in Table 4. In order to have a fair comparison of the various ANNs, the datasets used for their training are manually divided by the user into training, validation and testing sets using appropriate indices to state whether the data belongs to the training, validation or testing set. In the general case, the division of the datasets into the three groups is made randomly.

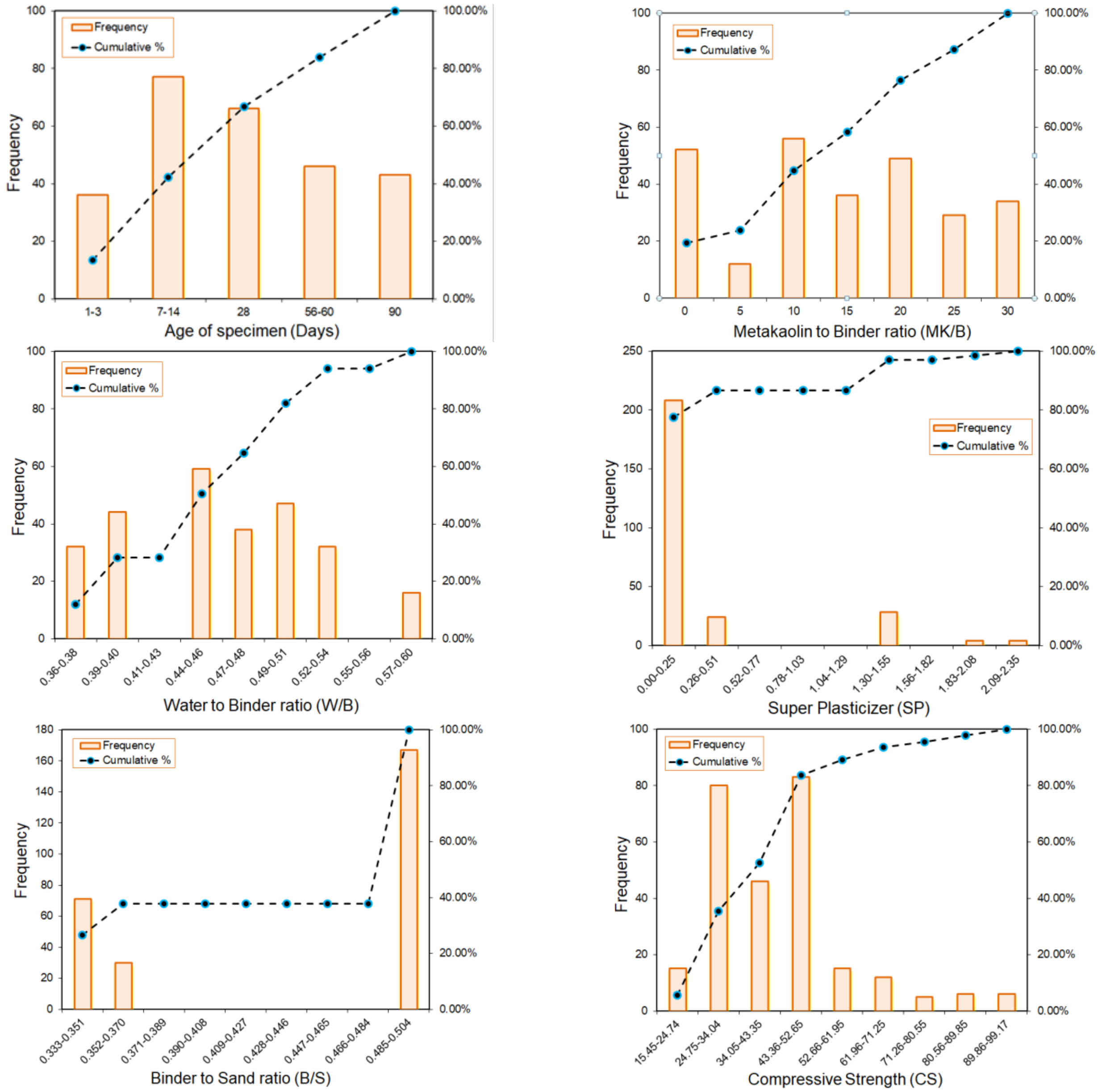

Fig. 3 Histograms of the parameters

Table 4 Training parameters of BBNN models

Parameter	Value
Training Algorithm	Levenberg-Marquardt Algorithm
Normalization	Minmax in the range 0.10 - 0.90
Number of Hidden Layers	1; 2
Number of Neurons per Hidden Layer	1 to 30 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	MSE; SSE
Transfer Functions	Tansig (T); Logsig (L); Purelin (P)

Note:
MSE: Mean Square Error; SSE: Sum Square Error
Tansig (T): Hyperbolic Tangent Sigmoid transfer function
Logsig (L): Log-sigmoid transfer function
Purelin (P): Linear transfer function

4.5 Model validation

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 are calculated by the following expressions (Alavi and Gandomi 2012)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2} \tag{4}$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{x_i - y_i}{x_i}\right| \tag{5}$$

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{n}(x_i - y_i)^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right) \tag{6}$$

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^2 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.

Furthermore, the following new engineering index, the a20-inex, has been recently proposed (Apostolopoulou *et al*. 2019, Armaghani *et al*. 2019, Xu *et al*. 2019) for the reliability assessment of the developed ANN models

$$a20 - index = \frac{m20}{M} \tag{7}$$

where M is the number of dataset samples 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 unity. 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 of ±20% compared to experimental values.

Table 5 Cases of developed ANN architectures

Case	Normalization	Hidden Layers	Neurons per Hidden Layer	Cost Functions	Activation Functions	Random Number Generation	NN Architectures
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8) $=30^{(3)}*(5)*(6)^{((3)+1)}*(7)$
1		1	1-30	2	3	10	5400
2		2					486000
3		1					5400
4	√	2					486000
				Total			982800

Table 6 Statistical indexes of the optimum BPNN models

Data Set	BPNN model		Statistical Indices			
			a20-index	R	RMSE	MAPE
Test	No Preprocess	5-18-1	1.0000	0.9879	2.5492	0.0425
		5-21-14-1	1.0000	0.9879	2.5458	0.0454
	MinMax [0.10, 0.90]	5-13-1	1.0000	0.9870	2.7159	0.0474
		5-6-25-1	1.0000	0.9920	2.0698	0.0420
All	No Preprocess	5-18-1	0.9888	0.9939	1.7781	0.0237
		5-21-14-1	0.9888	0.9944	1.7079	0.0275
	MinMax [0.10, 0.90]	5-13-1	0.9813	0.9922	2.0219	0.0282
		5-6-25-1	0.9963	0.9952	1.5850	0.0197
Training	No Preprocess	5-18-1	1.0000	0.9992	0.5330	0.0085
		5-21-14-1	1.0000	0.9981	0.8090	0.0131
	MinMax [0.10, 0.90]	5-13-1	1.0000	0.9985	0.7174	0.0112
		5-6-25-1	1.0000	0.9997	0.3169	0.0051
Validation	No Preprocess	5-18-1	0.9333	0.9814	1.3455	0.0083
		5-21-14-1	0.9333	0.9875	1.0947	0.0070
	MinMax [0.10, 0.90]	5-13-1	0.8889	0.9754	1.5370	0.0092
		5-6-25-1	0.9778	0.9834	1.3071	0.0077

5. Results and discussion

Based on the above, a total of 982,800 different BPNN models have been developed and investigated in order to find the optimum NN model for the prediction of the compressive strength of mortar materials. Namely for cases based on the combinations of the use or not of normalization technique and the use of one or two hidden layers have been investigated, as stated in Table 5.

The developed ANN models were sorted in a decreasing order based on the RMSE value. Based on this ranking, the optimum BPNN model for the prediction of the compressive strength is that of 5-6-25-1with two hidden layers and the use of normalization technique (Fig. 4). As presented in Fig. 4, the transfer functions are the Linear transfer function (purelin) for the first hidden layer, the Log-sigmoid transfer function (logsig) for the second hidden layer and the Linear transfer function (purelin) for the output layer. In Table 6 the values of statistical indexes R, RMSE and the value of the engineering index a20-index, are presented. Fig. 5 to Fig. 8 depict the comparison of the exact experimental values with the predicted values of the optimum BPNN model for the case of training, validation, testing and all data. It is clearly shown that the proposed optimum 5-6-25-1 BPNN reliably predicts the compressive strength of mortar materials. Also, Fig. 9 and Fig. 10 present a comparison between the exact experimental values with the predicted values of the optimum BPNN model. Furthermore, in Fig. 11 the ratio of the experimental values in relation to the predicted values is depicted, for the datasets which were used in order to test the reliability of the optimum neural network in terms of compressive strength prediction. The values of the input parameters (Age of specimen (AS), Metakaolin to total Binder (MK/B) percentage, Water to Binder (W/B) ratio, Superplasticizer (SP) percentage in relation to total binder, Binder to Sand (B/S) ratio), as well as the predicted value of compressive strength (output parameter) used for this test are stated in Table 7. It is worth noting that all samples used for the testing process have a deviation less than ±20% (points between the two dotted lines in Fig. 5 to Fig. 7). In fact, to

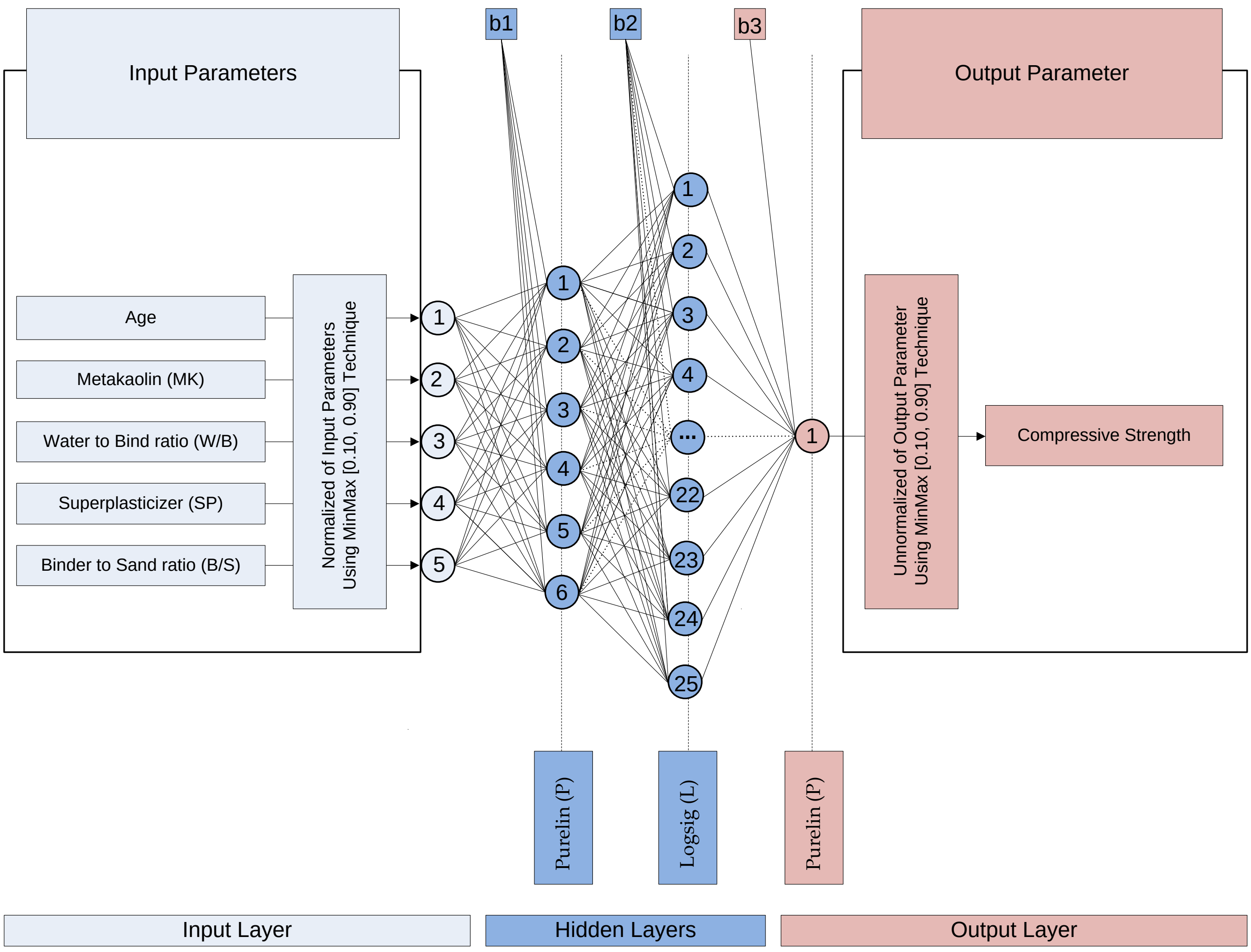

Fig. 4 Architecture of the optimum with two hidden layers 5-6-25-1 BPNN model

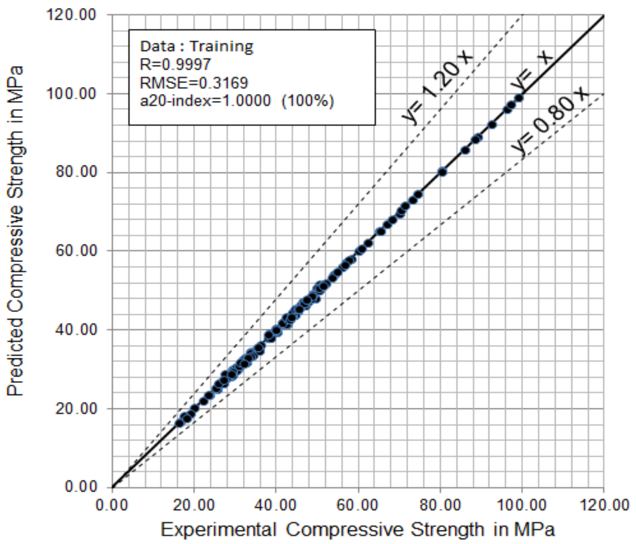

Fig. 5 Experimental vs predicted values of compressive strength for the training process

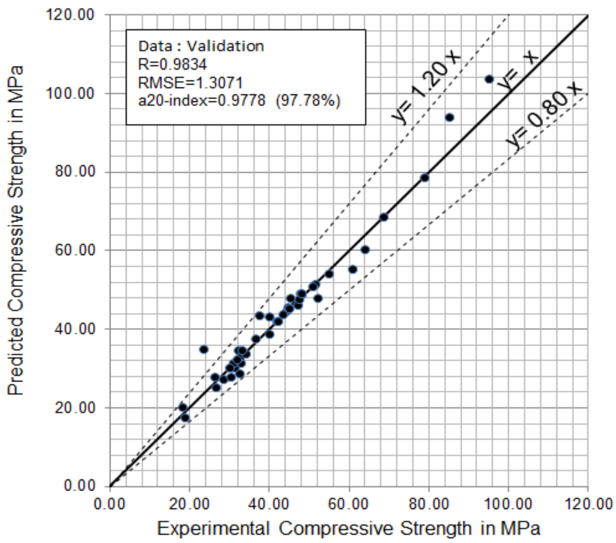

Fig. 6 Experimental vs predicted values of compressive strength for the Validation Process

be more precise, the data used for this test present a deviation of less than ±13% between predicted and experimental values.

At this point it should be noted, that, amongst all the data tested, only one dataset presents deviation higher than 20%. This dataset is related to a mortar which was tested at

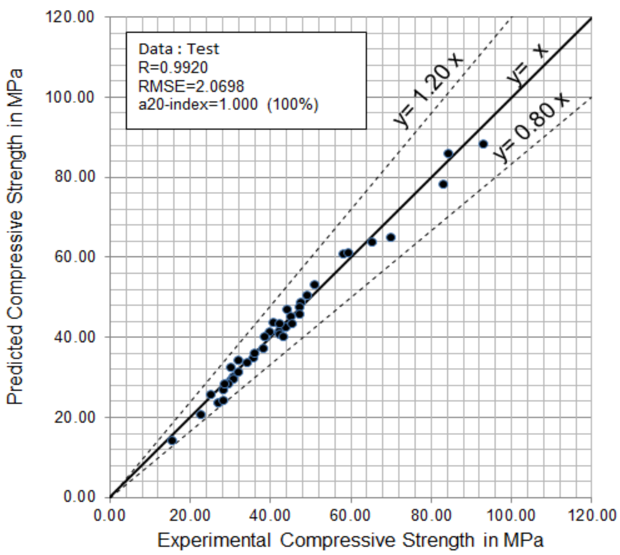

Fig. 7 Experimental vs predicted values of compressive strength for the test process

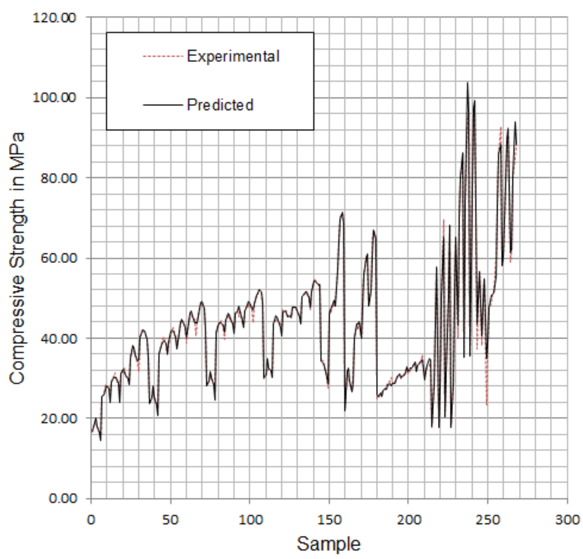

Fig. 9 Experimental vs predicted values of compressive strength for all data

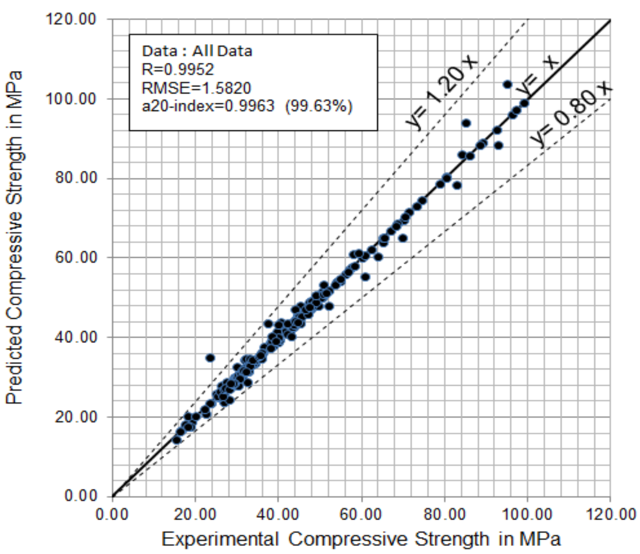

Fig. 8 Experimental vs predicted values of compressive strength of all data

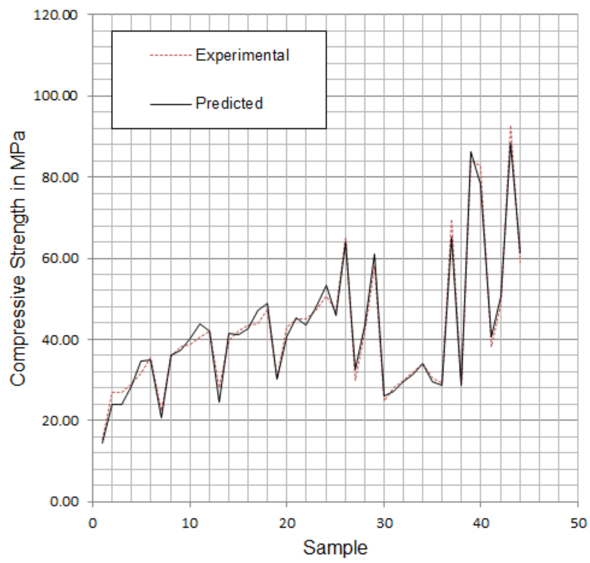

Fig. 10 Experimental vs predicted values of compressive strength for test data

one days of curing, that is one day after its production. Taking into account the early acquirement of compressive strength of cement mortars and the intense alteration of compressive strength during the first hours and days of hardening, this deviation could perhaps be related to the time at which the specimen was tested; if the specimen was tested after 36 hours instead of 24, this could affect the compressive strength value considerably. Other reasons for this deviation could be related to an incorrect measurement of compressive strength, or to an inadequate number of specimens at this age, which could have trained the NN insufficiently for this age. As already mentioned earlier, the reliability of the database as well as a sufficient amount of training datasets, are the most crucial parameters during the design and development of an ANN.

Based on the proposed optimum neural network, a sensitivity analysis was performed in order to reveal the dependence of compressive strength values on the different mix parameters of cement and cement-metakaolin mortars. The results are depicted in Fig. 12. In order to reveal the dependence of compressive strength on each parameter, four different variations on each of the involved mix parameters was undertaken, altering the input parameter by 5% and 10%. During the sensitivity analysis of each parameter, the values of the four others parameters were kept constant. This resulted in the creation of 5360 data (=4×5×268), through which it was possible to examine how the alteration of each parameter affects the value of compressive strength of the mortar, meaning, how compressive strength values are modified. This analysis reveals that, among the parameters examined, the water to binder ratio (W/B) has the greatest influence on compressive strength values, with 163.53%, followed by the binder to sand ration (B/S), with 129.29% and the

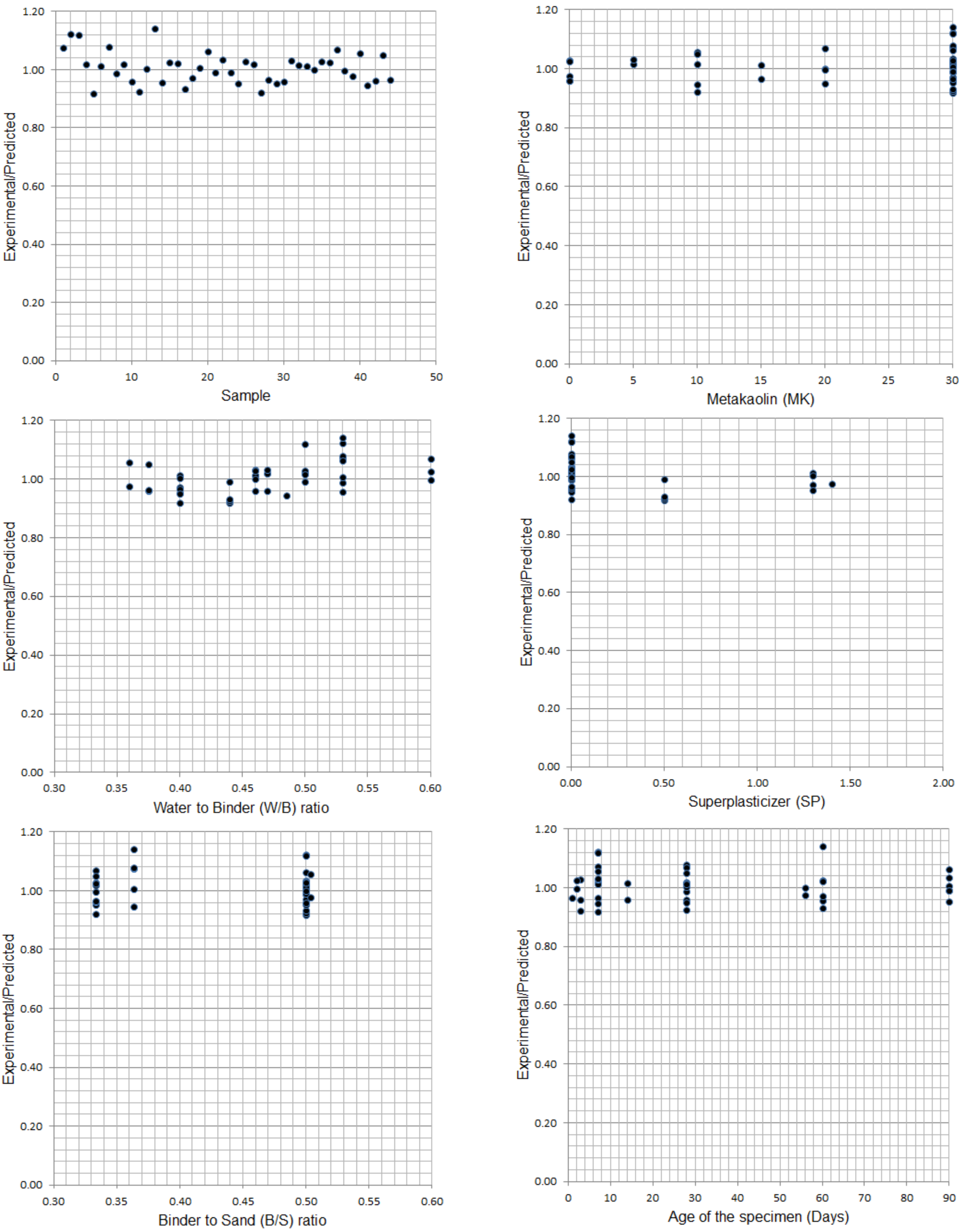

Fig. 11 Experimental vs predicted values of compressive strength for test data

percentage of superplasticizer in relation to binder materials (SP) with 91.85%.

6. Compressive strength maps

From the analysis presented herein, it is highlighted how neural networks can assist in the design of cement mortars. In addition to a reliable prediction of compressive strength, as illustrated in the respective figures (Fig. 5-Fig. 11), neural networks can also assist in the creation of

Table 7 Testing data sets for comparison of observation and predicted results

Sample	AS	MK/B	W/B	SP	B/S	Compressive Strength Exp.	Compressive Strength Pred.	Compressive Strength Exp/Pred	Reference
M6	7.00	30.00	0.53	0.00	0.36	15.45	13.31	1.00	Vu *et al.* (2001)
M12	7.00	30.00	0.53	0.00	0.50	26.80	25.11	1.14	
M18	7.00	30.00	0.50	0.00	0.50	26.80	26.54	0.96	
M24	7.00	30.00	0.47	0.00	0.50	29.00	27.24	1.02	
M30	7.00	30.00	0.44	0.50	0.50	31.70	31.77	1.02	
M36	7.00	30.00	0.40	1.30	0.50	35.50	35.91	0.93	
M6	28.00	30.00	0.53	0.00	0.36	22.48	20.46	0.97	
M12	28.00	30.00	0.53	0.00	0.50	35.70	36.60	1.01	
M18	28.00	30.00	0.50	0.00	0.50	38.10	39.26	1.06	
M24	28.00	30.00	0.47	0.00	0.50	38.70	39.98	0.99	
M30	28.00	30.00	0.44	0.50	0.50	40.60	43.46	1.03	
M36	28.00	30.00	0.40	1.30	0.50	42.10	47.95	0.99	
M6	60.00	30.00	0.53	0.00	0.36	27.97	26.05	0.95	
M12	60.00	30.00	0.53	0.00	0.50	39.60	42.98	1.03	
M18	60.00	30.00	0.50	0.00	0.50	42.10	43.44	1.02	
M24	60.00	30.00	0.47	0.00	0.50	43.60	41.06	0.92	
M30	60.00	30.00	0.44	0.50	0.50	43.90	47.81	0.97	
M36	60.00	30.00	0.40	1.30	0.50	47.50	51.25	0.95	
M6	90.00	30.00	0.53	0.00	0.36	30.40	34.08	0.96	
M12	90.00	30.00	0.53	0.00	0.50	43.00	42.81	1.03	
M18	90.00	30.00	0.50	0.00	0.50	44.90	42.69	1.01	
M24	90.00	30.00	0.47	0.00	0.50	45.10	40.68	1.01	
M30	90.00	30.00	0.44	0.50	0.50	47.10	49.64	1.00	
M36	90.00	30.00	0.40	1.30	0.50	50.80	53.16	1.03	
N	7.00	0.00	0.50	0.00	0.33	47.10	45.76	1.02	Courard *et al.* (2003)
5MK	28.00	5.00	0.50	0.00	0.33	65.10	57.91	1.07	
C+ 10MK	3.00	10.00	0.40	0.00	0.33	30.00	28.35	1.00	Parande *et al.* (2008)
C+ 15MK	7.00	15.00	0.40	0.00	0.33	42.10	44.29	0.98	
C+ 20MK	28.00	20.00	0.40	0.00	0.33	58.00	61.40	1.06	
Control	3.00	0.00	0.46	0.00	0.50	24.93	24.53	0.95	Sumasree and Sajja (2016)
5MK	7.00	5.00	0.46	0.00	0.50	28.01	27.47	0.96	
10MK	14.00	10.00	0.46	0.00	0.50	29.97	29.69	1.05	
15MK	28.00	15.00	0.46	0.00	0.50	31.90	32.25	0.96	
20MK	56.00	20.00	0.46	0.00	0.50	33.99	34.43	1.00	
30MK	3.00	30.00	0.46	0.00	0.50	30.41	30.61	1.14	
PC	2.00	0.00	0.60	0.00	0.33	29.40	26.89	0.96	Batis *et al.* (2005)
MKC -20	28.00	20.00	0.60	0.00	0.33	69.70	65.30	1.02	
MK-20	2.00	20.00	0.60	0.00	0.33	28.50	28.93	1.02	
OPC	56.00	0.00	0.36	1.40	0.50	84.17	81.01	0.93	Kadri *et al.* (2011)
MK2	7.00	10.00	0.36	2.04	0.50	82.71	78.91	0.97	
MK10%	7.00	10.00	0.49	0.00	0.36	38.22	44.05	1.01	Mardani-Aghabaglou *et al.* (2014)
0	14.00	0.00	0.38	0.00	0.33	48.80	52.40	1.06	Potgieter-Vermaak and Potgieter (2006)
0.1	28.00	10.00	0.38	0.00	0.33	92.80	93.71	0.99	
0.3	1.00	30.00	0.38	0.00	0.33	59.10	56.47	1.03	

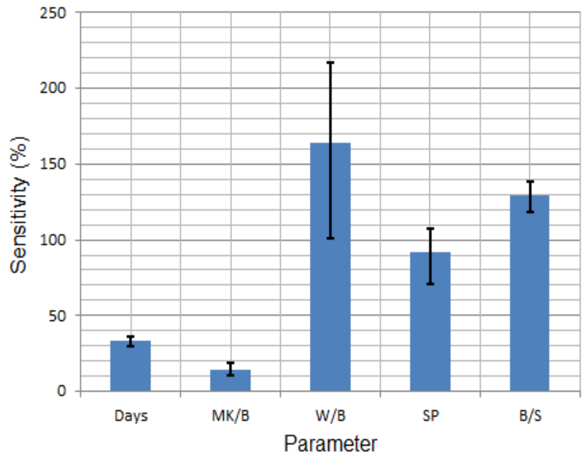

Fig. 12. Sensitivity analysis of the compressive strength to the composition parameters of cement mortar

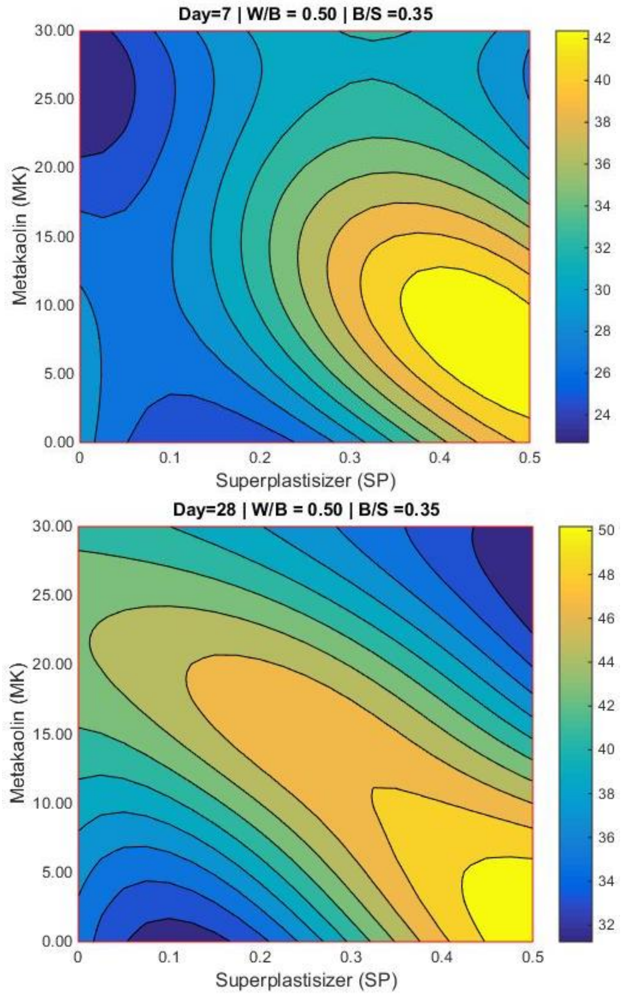

Fig. 13 Compressive strength maps based on optimum BPNN 5-6-25-1 model

compressive strength maps, as illustrated in Fig. 13. In particular, three input values are kept constant and a performance map is created, which depicts the influence of the other two input parameters on compressive strength, through predicting compressive strength for all intermediate values of the two input parameters; thus the proposed artificial neural network, can create a great number of maps, by selecting each time the parameters that will be kept constant in order to examine the influence of the other two parameters on compressive strength. These maps reveal areas and the influence of the input parameters on the output parameter, which is compressive strength. In Fig. 13, two maps are presented. In the upper map, the age of the specimen is kept constant at 7 days, the water to binder ratio is kept constant at 0.5 and the binder to sand ratio is kept constant at 0.35. The percentage of metakaolin in relation to binder ranges between 0% and 30%, while the addition of superplasticizer ranges between 0% and 0.5% in relation to total binder materials. The different colors characterize different values of compressive strength, in accordance to the color bar on the right. Thus, through this map, for a mortar with W/B=0.5 and B/S=0.35, one can examine the development of compressive strength at 7 days of curing in relation to MK and SP. This can reveal the trend of compressive strength development in relation to these two parameters together. Thus, one is allowed to select the mortar mix with the desired value of compressive strength, at the same time, enabling him to understand the combined effect of these two parameters on compressive strength. In the lower map of Fig. 13, the values of W/B and B/S are again kept constant at 0.5 and 0.35 respectively, the same as in the upper figure, however the third input parameter kept stable in this example, the age of the specimen, is kept constant not at 7 days curing, but at 28 days curing. Comparing the two maps, one can see how the input parameters affect the development of compressive strength in a different manner at different curing ages. Thus, although at 7 days ageing for small percentages of SP, compressive strength decreases with the increase of metakaolin, at 28 days curing, compressive strength increases with the increase of metakaolin up to ~28% and then decreases. By creating a series of such maps, the combined influence of all parameters on the development of compressive strength can be revealed.

7. Future research

At this point it must be stressed, that in certain areas, more data is needed, in order to achieve the optimum fitting of the proposed neural network to the data. For example, there is relatively scarce data regarding the use of 5% metakaolin in relation to total binder materials (MK/B%), in comparison with the other percentages. No data exists regarding the production of mortars with water/binder rations (W/B) between 0.41-0.43 and 0.55-0.56. The addition of superplasticizer (SP) is a great issue, as data exists mostly for low additions (0-0.25% in relation to binder materials), while some data was found for percentages 0.26-0.51, 1.30-1.55 and 1.83-2.35. This is attributed to the fact that superplasticizer is usually added in small percentages, however any prediction regarding intermediate percentages is accompanied by high uncertainty in regards to the development of compressive strength. The same is true regarding the binder to sand (B/S) ration, where most researchers select ratios between 0.485 and 0.504, some researchers select much lower ratios (0.333-0.370), while there is no data regarding intermediate relative quantities. Mortar mixes should in the future be designed and studied, aiming to reveal the development of compressive strength of mortars whose mix parameters obtain intermediate values, not included in the database presented herein. Through this optimization process, the influence of each parameter on compressive strength will be further elaborated, and the neural network, having been trained for all ranges of mortar mix parameters, will be able to predict intermediate values more accurately.

8. Conclusions

This study investigated the application of Artificial Neural Networks (ANNs) models for the prediction of the mechanical properties of cement-based mortar materials. The comparison of the derived results with the experimental findings demonstrates the effectiveness of ANNs to build soft sensors with the ability to predict the compressive strength of mortar materials in a reliable manner. Among the five mix design parameters examined, this analysis reveals that the water to binder ratio (W/B) has the greatest influence on compressive strength values, followed by the binder to sand ration (B/S), and the percentage of superplasticizer in relation to binder materials (SP), while specimen age and the percentage of metakaolin in relation to total binder materials have a less pronounced influence.

Thus, through the use of ANNs researchers can be assisted in designing mortar mixes aiming to optimize the compressive strength of mortars containing metakaolin, while minimizing time and resources. Furthermore, the use of ANNs, as illustrated in this research, can greatly assist in revealing the influence of each mix design parameter on compressive strength at different ages. The extension of the database used in this project with more entries will increase accuracy further.

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