



A Heuristic Approach for Predicting the Geometrical Packing of Cementitious Paste to Reduce CO₂ Emissions in Reinforced Concrete Production

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ABSTRACT

In recent years, a number of researchers have adopted the wet packing (WP) approach to design different types of concrete mixes. Particle grading is a key to the optimization of the wet compactness density; for that reason, all empty spaces that exist in between large-size particles need to be completely filled with particles of smaller size. Previously-conducted studies in this field have been focused on measuring the particle size distribution's packing density (PD) of the of granular matrices is the purpose of investigating how to increase the PD of cementitious materials. Thus, literature lacks models capable of predicting the optimal PD value. The current study collected and analyzed 216 datasets in order to construct a model for accurate prediction of PD. The main datasets were organized into two categories: modeling datasets and validation datasets. To configure the model in the best way, a hybrid gravitational search algorithm-artificial neural network (GSA-ANN) was also developed in this study. The findings confirmed ANN as an effective alternative for measuring the ultimate PD of cementitious pastes. ANN provided high levels of accuracy, practicality, and effectiveness in the process of predicting the PD value. Based on the final results, the implementation of the hybrid GSA-ANN technique causes a significant decrease in the number of tests conducted on experimental samples, which results in not only saving time and money, but also reducing the CO₂ emission volume

1. Introduction

The recent literature consists of a great deal of research concentrated upon developing eco-friendly mixes of concrete by taking the control of both producing and utilizing processes of Portland cement (PC) in large amounts (Scrivener and Kirkpatrick, 2008; Yıldırım; 2019; Flatt et al., 2012). An earth-friendly building can be constructed through the minimization of the energy consumption in the course of the projects involving the PC and concrete production and also decreasing the CO₂ volume emitted throughout such projects (Proske et al., 2014; Damineli

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et al., 2010). To enhance the PD of aggregates, there is a need for the minimization of the cementitious materials and the cement paste required for the aggregate's surfaces coverage.

The recent century has witnessed a growing interest of researchers and practitioners in the packing density (PD) of particles (Worrell et al., 2001). The environment could be more protected from the concrete impacts by improving the PD of the aggregates through decreasing its structure voids, hence decreasing the unnecessary PC production (Abdulhameed et al. 2021). PD can be properly improved when the utilized aggregate is appropriately graded.

A review of literature revealed a lack of research into the cement paste PD with a focus on constructing a model that can predict the PD of cementitious materials (Kwan and Fung, 2009). Banyhussan et al., 2020 reported the implementation of the optimization techniques for the aim of estimating the PD value. According to the findings of that research, depending on the technique applied to the construction of the model, the coefficient of variation may increase or decrease. As a result, the current study is mainly aimed at configuring a PD model adopting a hybridized method, called Gravitational search algorithm-artificial neural network (GSA-ANN), with a broad range of conventionally-used concrete constituents. The model partially replaces the cementitious materials with fly ash, silica fume, and slag. In addition, the developed PD prediction model is optimized and then evaluated using a soft-computing base-model.

Literature shows that the engineering based-models created through the soft-computing technique have received a great attention from researchers as effective empirical models (Gholami et al., 2013). Note that the soft-computing modeling is typically dependent upon experimental data rather than theoretical concepts as can be observed in other conventional models constructed on the basis of engineering principles. Soft-computing has a sophisticated methodology even in cases involving the formation of explicit mathematical relationships. For that reason, these methods are generally adopted as a part of a computer program as a subroutine, which restricts their efficacy.

When dealing with the solution of the complex classification and pattern recognition problems in various domains (e.g., structural engineering), the most popular technique is the artificial neural network (ANN) (Jiang and Adeli, 2005; Adeli and Jiang, 2006). This soft computing technique (developed in the early 1940s) is principally inspired by biological neural networks (Haykin, 2001; Perlovsky, 2001). ANNs are predictive tools applied to establishing the complex system mathematical models. These networks are offered in different types among which one of the most efficient ones is multilayer perception (MLP) (Cybenko, 1989). MLP-ANNs are normally fed architectures; in addition, they are normally equipped in back propagation algorithms. An MLP network contains one input layer, one output layer, and a minimum of one hidden layer. That layer contains one or more processing units as well as several nodes. In MLP, every unit is completely linked with weighted connections (w_{ij}) to the units that exist in the next layer. The output (Y) is achieved through passing into an activation method the sum of the combinations of input and weight. To enhance the ANN effectiveness, a number of studies have integrated the global optimization algorithms with these networks (Little & Rubin, 2019; Gandomi & Roke, 2015). As a result, nonlinear problems (in certain structural problems) can be solved with the use of the soft-computing methods. ANNs have shown an outstanding capacity in pattern detection processes, which has made it attractive for many researchers. A key issue to be determined properly is the number of hidden nodes to apply to ANN model; this is due to the fact that a complex model will overfit. The upper limit of the number of hiding neurons had been proposed by Hecht-Niselen (Hecht-Niselen, 1987). The Kalmogorov theorem was employed as $n_h \leq 2n_i + 1$. The n_h stands for the numbers of hidden neurons; while, refers to numbers of n_i inputs, respectively. Addition overfitting criteria was suggested by Belman-Flores et al., 2013 in systems within only one hidden layer. They determined a lower bound for the number of training sets as $n_T \geq 4(n_i + 1)n_h$. With taking into consideration the preferences and the number of outputs, this criteria can be stated as follow: $n_T \geq c(n_h(n_i + 1) + n_o(n_h + 1))$, where n_o denotes the number of outputs and c stands for a coefficient greater than or equal to 4. After that, in one hidden layer, the maximum number of hidden neurons can be expressed in the system as

$$n_h \leq \left\lfloor \frac{n_T - cn_o}{c(n_i + n_o + 1)} \right\rfloor.$$

Nonetheless, these methods are confined to the upper values, the number of hidden layers, and certain suppositions such as the coefficient value (c). Consequently, a significant challenge is how to discover the secret neurons in the neural networks (NNs). The problem is that the network has a strong match with the data, which makes it impossible to generalize the test results. Moreover, the parameter of learning rate determines the weight adjustments in size when the weight is altered in the course of the workout. Thus, another problem of ANN is how to predict the value of the learning scale, which varies in the interval between 0 and 1. In this study, a trial

and error approach was adopted for the aim of determining the significance of the learning rate (Attoh-Okine 1999; Kim and Park 2001). As a result, two factors are determined in a random way: 1) the number of hidden neurons to apply to the network, and 2) the significance of the learning rate in the ANN model. For that reason, both of them are normally determined through a trial-and-error process.

In the present study, a hybrid GSA-ANN algorithm is proposed in order to measure the cement PD level. In this model, the gravitational quest algorithm (GSA) is used to estimate the number of neurons that should be put within the hidden layers and also to determine how the learning rate affects the learning algorithm convergence.

To this end, a dataset was collected by doing a review on previously-conducted studies on 216 packing density samples. The main objective is to improve the accuracy and efficiency of PD prediction processes and also to provide reliable solutions to the most important problems that may arise by the use of traditional approaches.

2. Methodologies: Soft-computing techniques

In general, soft computing methods are applied to solving the complex numerical optimization problems (Phoemphon et al., 2018). These methods are applicable to numerous categories of algorithms, including Adaptive Neural Fuzzy Inference System (ANFIS), Fuzzy Logic (FL), Support Vector Machine (SVM), Artificial Neural Network (ANN), and Optimization Algorithms (OA) (Phoemphon et al., 2018). Each classify has a fine grain set like genetic algorithm (GA), Ant Colony optimization (ACO), particle swarm optimization (PSO), Differential Evolution (DE), and Artificial Bee Colony (ABC), which are classified in the category of OA.

The current paper, as mentioned earlier, is aimed at the development of an innovative model for measuring the PD of cementitious pastes with the use of the GSA-ANN algorithm. The five effective input parameters of the hybrid algorithm are as follow:

$$PD=f(W,PC,FA,SL,SF) \quad (1)$$

Where:

PD stands for the packing density of a specific cement paste (which is expected to be estimated thru the proposed model);

W refers to water amount;

PC signifies the amount of cement;

FA represents the amount of fly ash;

SL is slag amount; and

SF signifies the amount of silica fume.

2.1. Artificial Neural Network

Artificial neural network (ANN) refers to a system for processing information, which is indeed a mathematical model of the nervous system that exists in human beings (Gholami et al., 2013). The localization techniques that work based on ANNs are capable of modelling complex mathematical relationships between the independent variables (inputs in this study, which are W,PC,FA,SL,and SF) and the PD value the dependent variable (output). The current research makes use of the backpropagation (BP) neural network and the Levenberg-Marquardt (LM) training algorithm for the purpose of testing, training and validating the suggested model. The latter is used due to not only its capacity of minimizing the localization error (as confirmed by Payal et al.,2014), but also its high speed and efficiency. On the other hand, this algorithm needs a great deal of working memory (Kukolj and Levi, 2004).

In ANN, prior to the training, testing, and validation processes, the user needs to determine the numbers of inputs, hidden layers, and of neurons in each hidden layer in addition to the number of outputs and learning rate. In this paper, three-layer ANN architecture is employed for the purpose of determining the PD capacity on the basis of the W,PC,FA,SL,and SF parameters of the cementitious pastes. The ANN comprises three types of layers, i.e., the input layer, the hidden layer, and the output layer (see Figure 1). The input layer is consisted of five parameters: W,PC,FA,SL,and SF. Each neuron in the hidden layer summed the input parameters after weighting them according to the strengths of individual connections W_{ij} . After that, the inputs of the hidden layer were weighted against the strengths of particular connections, $W_{(ik)}$ and the summated by each neuron with the aim of computing the output y_k in the third layer. Covering all possible input values in the hidden layer with tan-sigmoidal activation functions, and all possible output values in PD with linear activation functions. GSA was

used for the aim of determining the number of neurons within the hidden layer and the learning rate. These parameters are set through a trial-and-error procedure, which unnecessarily result in the best solution. To cope with this problem, GSA determines the optimal number of nodes within the hidden layer and the optimal value of learning the rate of ANN. This way, the ANN interpretation is able to be enhanced. The current project, the algorithm can be integrated with an ANN in a way to construct a different algorithm, called GSA-ANN, which is capable of gaining the lowest amount of errors in the PD prediction process.

In multilayer feed-forward networks, BP is of the highest benefits because of its certain mathematical design that allows it to learn complex nonlinear correlations. BP preserves an efficiency, which is defined as the value with the smallest standard deviation (SSD) (Avci et al., 2021). The error is calculated by SSD as the difference between the value that was measured and the value that was supposed by the methodology. BP is capable of minimizing SSD through the use of an algorithm for gradient descent that tracks an error gradient curve downwards over all possible inputs. Equation (2) expresses the SSD operation:

$$SSD = \frac{1}{n} \sum_{i=1}^{n_s} (t_i - o_i)^2 \quad (2)$$

In this formula, n is the number of training sets, t_i is the target's output, and o_i is the network's output for input i . The application of ANNs often provides two primary advantages: 1) their high diagnosis capacity even in cases they are trained with partially imprecise data, 2) their ability to keep learning and improve their performance when new training data is given to them.

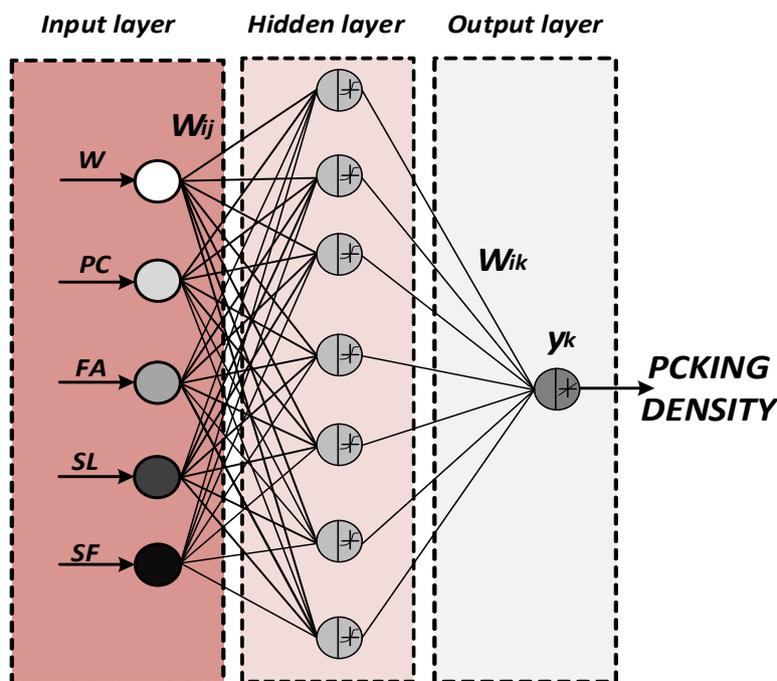


Fig. 1 ANN model

2.2. GS algorithm

Heuristic algorithms are popular due to their capacity of finding an optimum solution at a reasonable computational cost in cases where there is not any possibility for conducting neither optimality nor feasibility research. Additionally, in many cases, these algorithms are employed for the aim of clarifying the closeness to the best prediction (Heidari et al., 2019). In instances where sufficient ANN variables and a large number of input model parameters are accessible, ANNs are capable of properly expressing the relationships between the inputs and outputs. GSA, as a heuristic algorithm, was integrated with ANN in the present paper for the aim of

determining the optimal ANN parameters, namely the number of neurons required to be put in each hidden layer and the learning rate.

GSA developed by Heidari et al., 2019 is known as one of the cutting-edge heuristic algorithms proposed in literature, which has been developed on the basis of the Newtonian laws of gravity and motion. In GSA, agents represent the objects, whose performance quality is assessed considering their masses. In 1687, Newton proposed the law of universal gravitation. In a general definition, gravity is a natural force that exerts its impact on all objects having a mass. Its range is infinite; it always attracts and never shows repulsion; nothing can absorb, transform, or shield it. Lots of natural phenomena can be explained by universal gravitation (Siddique and Adeli, 2016).

All the agents in GSA are in an interaction on the basis of the Newtonian laws of gravity and motion (Visconti, 2016). The gravitational force of attraction causes the movement of all agents towards an object with heavier mass. The notion is illustrated in Figure 2 where F_{1i} stands for the force acting on M_1 because of M_i , and F_1 denotes the resultant force acting upon M_1 due to $M_2, M_3,$ and M_4 . In GSA, the objects performances are measured considering their masses. The heavy masses reflect good solutions and move with a slower pace compared to the lighter masses. This step improves the algorithm exploitation capacity.

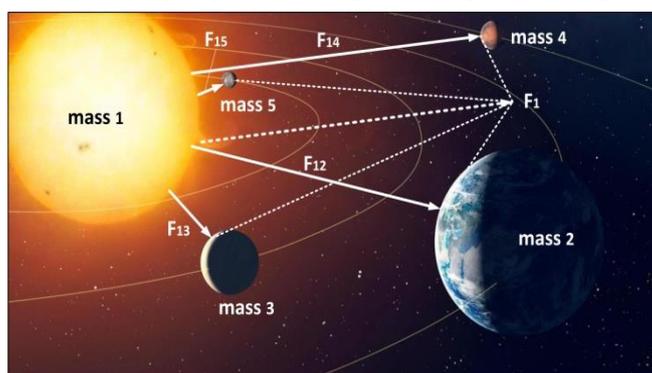


Fig. 2 Mass effect with other masses.

The i th agent position in GSA can be expressed in below:

$$X_i = (x_i^1, x_i^2, \dots, x_i^d, \dots, x_i^n) \quad i = 1, 2, 3, \dots, P \tag{3}$$

where x_i^d signifies the position of the i th agent in the d th dimension, n denotes the search space dimension, and P represents the number of agents. At the t th iteration, the gravitational force that acts upon the i th object due to the j th object can be expressed as follows (Heidari et al., 2019):

$$F_{ij}^d(t) = G(t) \times \left(\frac{M_j(t) \times M_i(t)}{R_{ij}(t) + \varepsilon} \right) \times (x_j^d(t) - x_i^d(t)) \tag{4}$$

where, M_i stands for the mass at the j th agent and $G(t)$ for the gravitational constant at time t , ε denotes an extremely small constant; however, between the i th and j th agents, the Euclidean distance signifies $R_{ij}(t)$, which is calculated using Eq. (5):

$$R_{ij} = \|x_i(t) - x_j(t)\|_2 \tag{5}$$

Pelusi et al. (2018) determined the following value for the gravitational constant $G(t)$, which is set initially high and lowered over the course of the search to set the precision with which results are returned.

$$G(t) = G_0 \times e^{-\alpha t / Iter_{max}} \tag{6}$$

When G_0 is the initial value of the gravitational constant, $Iter_{max}$ is the maximum number of iterations (the age of the system), and is α constant term. The sum of all forces acting on the i th agent can be written as:

$$F_i^d(t) = \sum_{j=1}^{k_{best}} rand_j \times F_{ij}^d(t) \quad j \neq i \tag{7}$$

where $rand_j$ is a random number between 0 and 1, and k_{best} is the first k number of agents with the best fitness (objective function) value; it is assessed since it is reduced continuously over time (Heidari et al., 2019). At the last iteration, its value becomes 2% of the initial number of agents. The acceleration of the i th agent at the t th iteration in the d th direction, according to Newton's law of motion, is given by:

$$a_i^d(t) = \frac{F_i^d(t)}{M_i(t)} \tag{8}$$

Where,

$$M_i(t) = \frac{m_i(t)}{\sum_{j=1}^P m_j(t)} \tag{9}$$

and

$$m_i(t) = \frac{fit_i(t) - worst(t)}{best(t) - worst(t)} \tag{10}$$

Where $fit_i(t)$ represents the efficiency of the i th operator on the t th iteration, and $worst(t)$ and $best(t)$ are found by Eqs. (11) and (12), respectively:

$$best(t) = \min(fit_i(t)) \quad i = 1, 2, \dots, P \tag{11}$$

$$worst(t) = \max(fit_i(t)) \quad i = 1, 2, \dots, P \tag{12}$$

An agent's updated velocity is considered in GSA as a percentage of its current velocity plus its acceleration, as stated by Heidari et al., 2019. This allows us to write down an expression for the i th agent's position and velocity at the t th iteration, in the d th direction:

$$v_i^d(t + 1) = rand_i \times v_i^d(t) + a_i^d(t) \tag{13}$$

$$x_i^d(t + 1) = x_i^d(t) + v_i^d(t + 1) \tag{14}$$

In the following, nine stages involved in the proposed algorithm are explained:

- 1) Randomly initializing all the control variables of the P number of agents in the given search interval with the use of Eq. (7).
- 2) Calculating the agents' fitness values, and then determining the best and worst fitness values of the population set.
- 3) Finding the mass of every i th component, $M_i(t)$.
- 4) At each iteration t , the gravitational constant is calculated using Eq (6).
- 5) Evaluating the total force that acts upon each agent with the use of Eq. (7).
- 6) Modifying the acceleration of each agent by means of Eq. (8).
- 7) Updating each agent velocity and position with the use of Eqs. (13) and (14), respectively.
- 8) Checking each solution set feasibility, and then replacing the infeasible solution by a new solution set that is produced randomly using the following equation:

$$P_{ij} = P_j^{min} + rand \times (P_j^{max} - P_j^{min}) \quad j = 1, 2, \dots, d; i = 1, 2, \dots, N_i \tag{15}$$

The inaccessible solution count is denoted by N_i , while the dependent variable count is indicated by d .

- 9) Inspecting the optimal solution; if it is satisfied GSA is terminated; otherwise, the process starts again from stage 2.

In GSA, the gravitational and inertial masses are considered as identical units; though, different values may be allocated to them. The bigger the inertial mass, the more accurate search operation is performed, because the agents' motions are slow. Whereas, a bigger gravitational mass results in higher agents' attraction, which leads to a convergence rate of a higher speed.

2.3. Model development by means of GSA-ANN

Training of ANNs is performed using the set of data already determined as ‘training set’. The training process optimizes the weights of the network. Two main steps are involved in the training process, i.e., initialization and optimization (Alavi and Gandomi, 2011). During the former, the network weights are allocated with initial values; this is done either randomly or via a global optimization method, e.g., GSA. On the other hand, the process of optimization employs a gradient-based algorithm that is applicable to local search operations. Consequently, to obtain desired results, there is a need to determine a starting point for optimization, which is achieved from a global search. To have a fully reliable training procedure, both the initialization and optimization processes are required to be performed well (Ledesma et al., 2007).

The suggested GSA-ANN model is shown in schematic form in Figure 3. In the first stage, the initial weights are optimized using GSA, and in the second, the MLP is used to find the optimal values.

This research uses the difference between the observed and anticipated PD values as the optimization problem. The mean absolute error (MAE) is applied to this study as the objective function. MAE is computed considering the difference between the observed values and the predicted ones relative to the observed value, as expressed in Eq. (16):

$$MAE = \frac{|\sum(PA_i - PE_i)|}{ns} \tag{16}$$

Where ns signifies the number of test data points, and

PA_i and PE_i stand for the actual value and the predicted value of PD capacity, respectively.

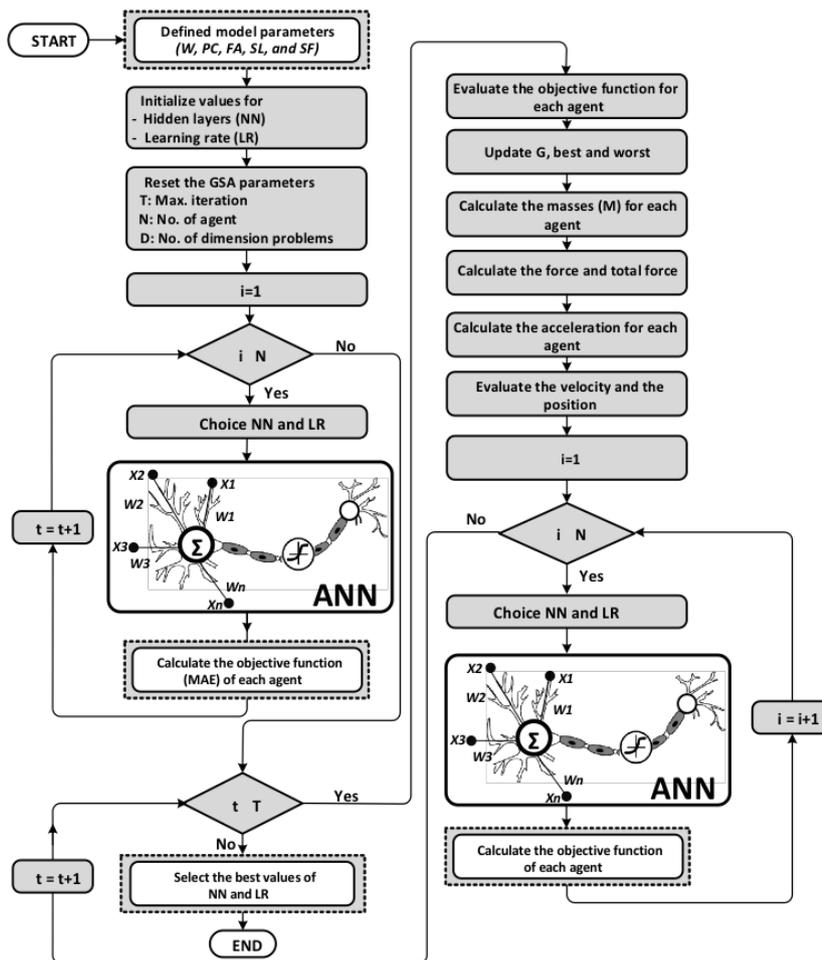


Fig. 3 Schematic representation of the GSA-ANN model

2.4. Experimental data and data pre-processing

A full of 216 experiment data presented in the Banyhussan et al. (2020) study was used to form the database required for the present research. The amount of water, cement, fly ash, slag, and silica fume are the inputs for the learning process, while the PD value is the output.

In general, the models configured with the use of the soft-computing tools show a prediction capacity within the range of data applied to their development process. For that reason, a key issue is the amount of data applied to the modeling process since it significantly affects the reliability degree of the constructed model. In case of the model developed by means of this database, the quality of its performance depends on its variable distributions and also the size samples used. Thus, Figure 4 illustrates the data as histograms. Table 1 demonstrates the descriptive statistics of the samples demonstrated in Figure 4.

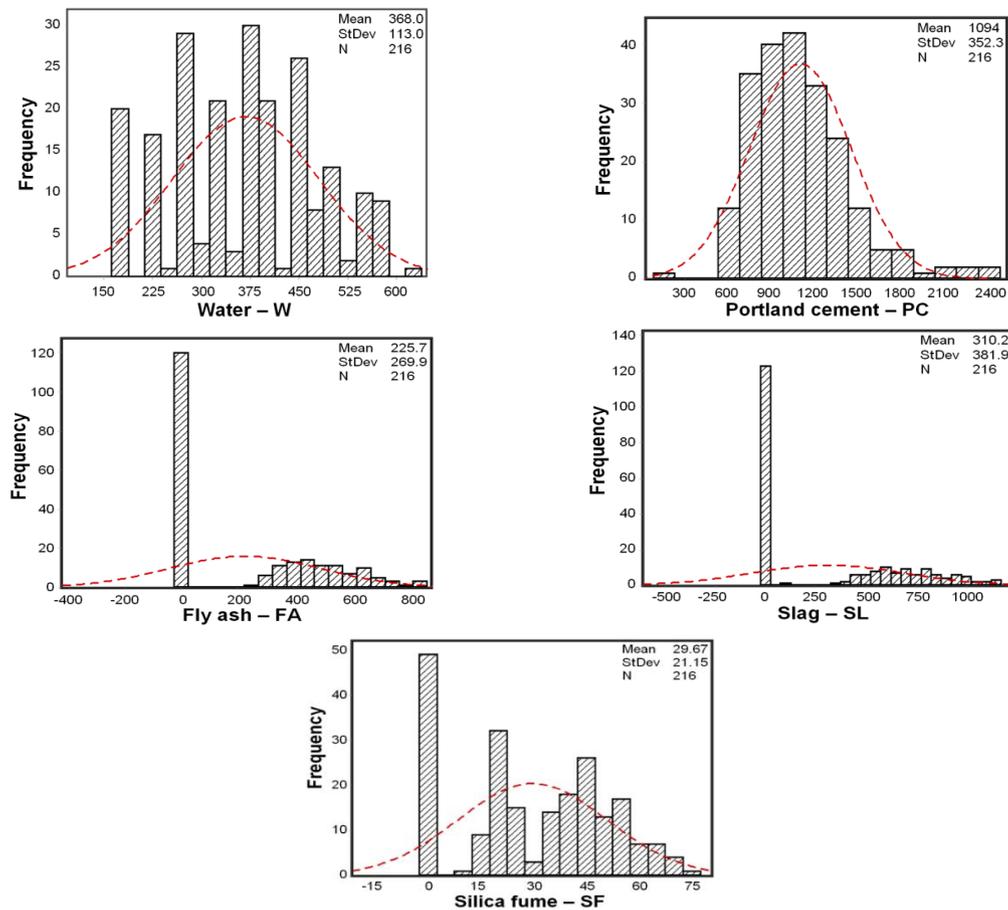


Fig. 4 Independent input variables histograms

Table 1 – GSA parameters

Parameters	Value
Inputs layer number	5.00
Hidden layers number	1.00
Outputs number	1.00
Size of population	10, 20, 30, 40, and 50
Iteration	1000
Target error	1e-05
G_0	1.00
α	0.20

3. Results and discussion

The results obtained by the GSA-ANN developed are discussed regarding to the accuracy of the PD values obtained. First, the results corresponding to GSA-ANN are presented; then, the results of the ANN training and validation processes will be explained. The results achieved by GSA-ANN are then compared with those of other studies in literature.

3.1. Hybrid GSA-ANN Algorithm

GSA was executed with the use of the parameter settings of the heuristic algorithm (see Table 1), and for the population sizes of 10, 20, 30, 40, and 50, the objective function was attained. Numerous researchers, e.g., Gharghan et al. (2016), have applied this range of population sizes. Different population sizes were used in order to help the algorithm choose the appropriate population size that can minimize the objective function and elapsed time. On the other hand, no certain algorithm has provided yet a precise result for all of the optimization problems. In this study, the ANN was trained recurrently (100 iterations) by means of numerous epochs till the minimized error between the actual and the predicted PD values was obtained.

Table 2 presents the neurons of the hidden layer (NN) and the learning rate (LR), which were achieved through the implementation of GSA in MATLAB on the basis of various population sizes. Figure 5 shows the objective functions of the hybrid GSA-ANN for various agents for measuring the PD of the available cementitious pastes.

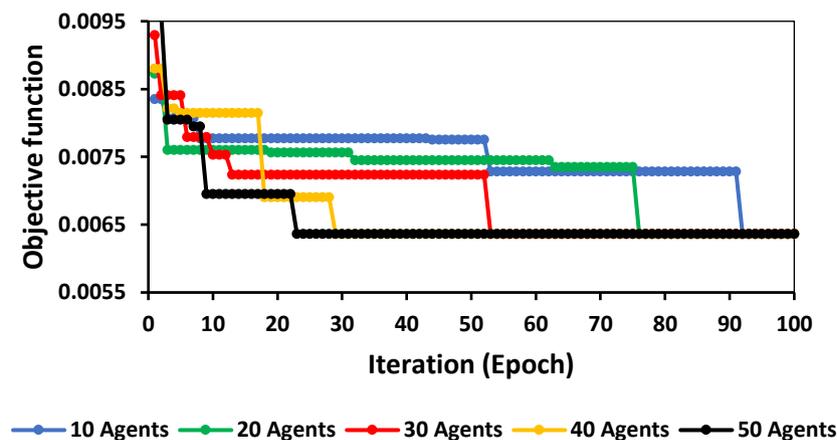


Fig. 5 Objective function (MAE) versus iteration

Table 2 Neurons per hidden layer and the GSA-based learning rate of the ANN at various population sizes.

Population Size	Parameter	Value
10	NN	20
	LR	0.2558
20	NN	19
	LR	0.3776
30	NN	19
	LR	0.5032
40	NN	20
	LR	0.0227
50	NN	16
	LR	0.6078

A rational hypothesis Smith, (1986) maintains that a correlation coefficient greater than 0.8 ($R > 0.8$) indicates that the measured and predicted values are strongly correlated with each other. The regression coefficient of

determination (R) between the measured and the estimated PD confirms that GSA-ANN has a high prediction capacity. Figure 6 shows R values of 0.9851, 0.97917, 0.96337, 0.87552, and 0.75338 in case of 10, 20, 30, 40, and 50 agent sizes, respectively. According to the calculated regression coefficients, the observed and predicted PDs were very similar. As shown in Figures 5 and 6, if assumed that the minimum objective function can be met by a population size of 50, then we may have found the ideal solution for GSA. While the other population sizes examined in this research brought a large number of flaws. In accordance with the GSA-ANN results, training, testing, and validation were performed on ANN with use of the parameters that obtained the minimum objective functions for the population size. Such parameters could increase the ANN process successfully all through the three phases of training, testing, and validation, that finally led to high accuracy in predicting the PD value.

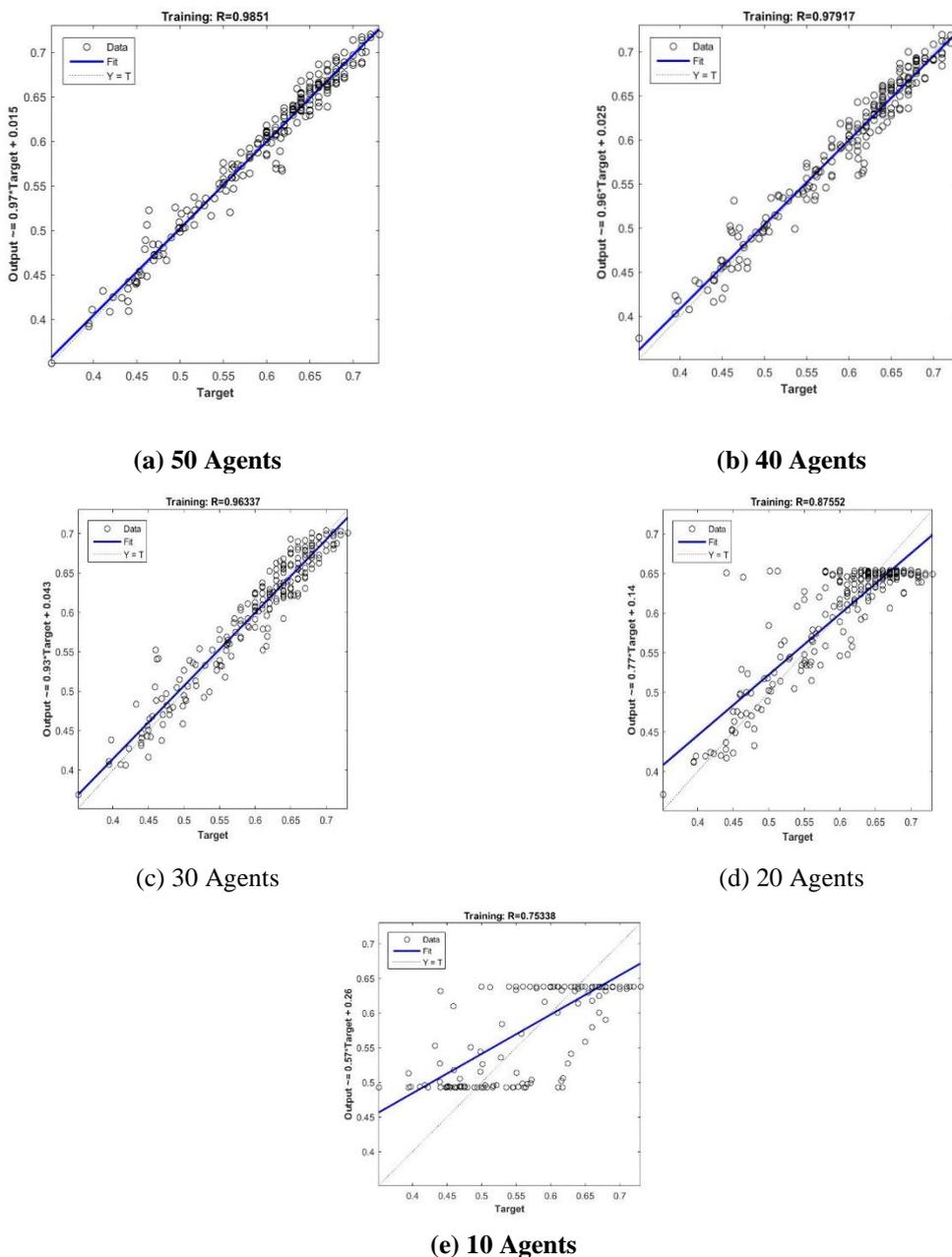


Fig. 6 R values against agent sizes

3.2. Training and validation of the Artificial Neural Network

The performance of ANN was optimized using GSA through choosing the optimal number of neurons within each hidden layer and the best values for the learning rate. ANN was subject to the processes of training, testing, and validating with the use of the measured values of (W, PC, FA, SL, SF) as sources and the genuine PD values as results. The potential of ANN framework, with 5 input parameters (W, PC, FA, SL, SF), 16 neurons in the hidden layer and 1 output parameter for the PD capacity were evaluated in order to determine the best settings for cementitious pastes. Figure 7 displays the ANN model chosen for the current research.

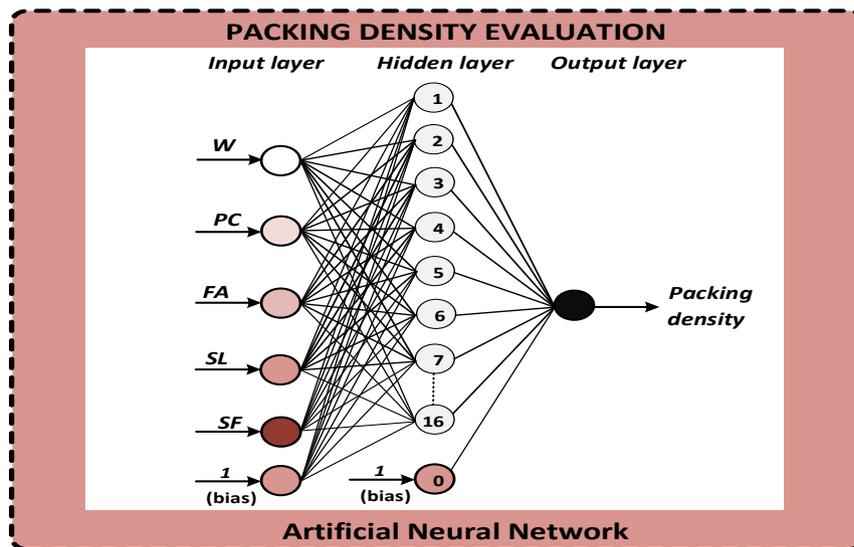
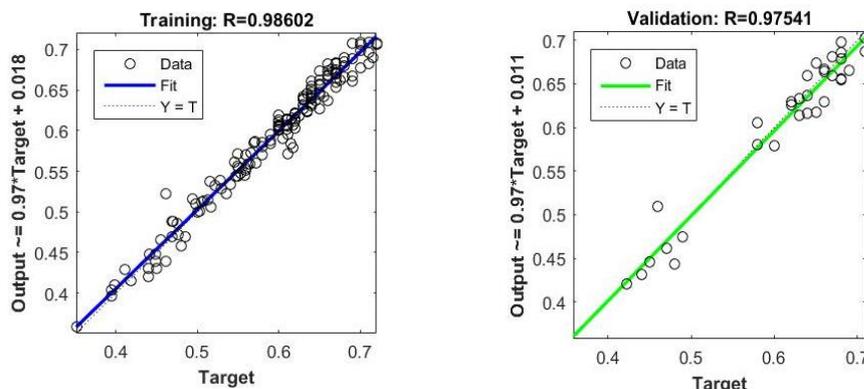


Fig. 7 ANN configuration used to predict the PD value

The experimental and estimated PD values obtained through the training, testing, and validation processes are compared to each other in Figure 8. Based on the results presented, the values estimated are very close to the actual ones since all values fall adjacent to the “ideal fit” line. From the statistical perspective, the results obtained by the training, testing, and validation phases have a high degree of similarity, which normally shows that the developed model has been trained appropriately, which will be clarified in the following sub-section. The regression coefficient of determination (R) between the measured and the estimated PD clearly demonstrates the accuracy of GSA-ANN's ability. Figure 8 demonstrates the R values of 0.98602 for training, 0.9439 for testing, and 0.97541 for validation phases, as well as the value of 0.97737 as the total. The results of the regression coefficient show a close agreement between the measured and the estimated PD value. Figure 9 demonstrates the model error histogram. This histogram shows that most of the experimental values lie close to zero error; in other words, there is a small relative error between the experimentally-measured values and the values estimated by the proposed model.



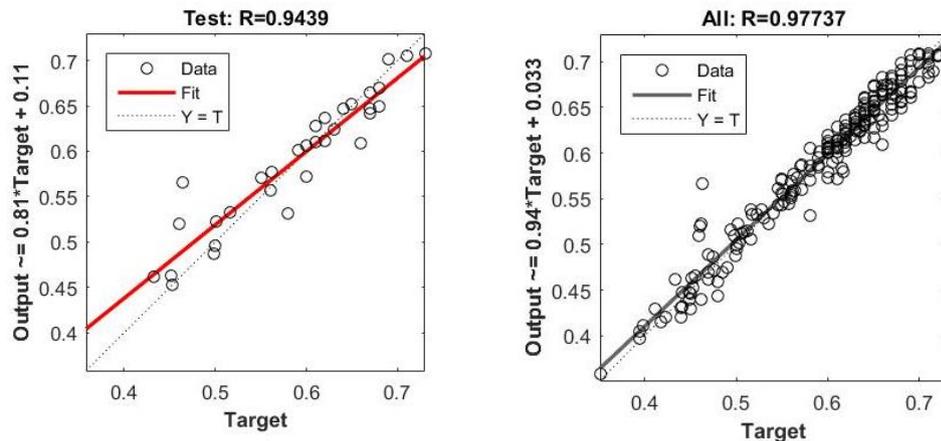


Fig. 8 Schematic depicting the GSA-ANN statistical method

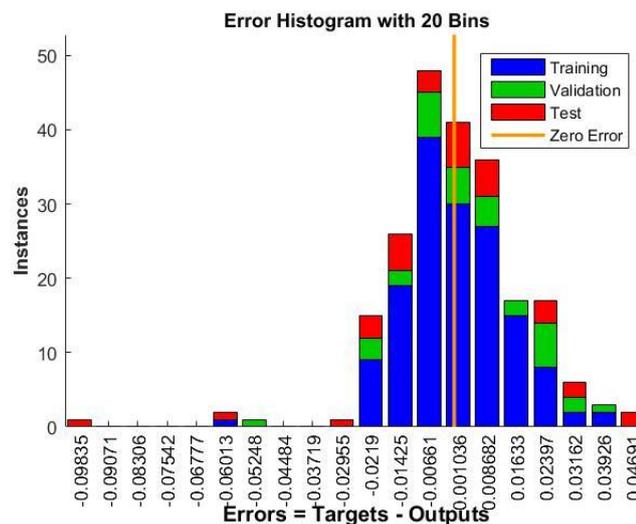


Fig. 9 Distribution of GSA-ANN errors

3.3. Comparative study

A comparison was made between the prediction results of GSA-ANN and ANN considered in the current paper and those of a model introduced by Banyhussan et al (2020). In the present section, the results obtained by the models for the all the datasets are presented. In short, the comparative results clearly confirmed that the proposed GSA-ANN model outperformed the rival.

The proposed model was evaluated using a dataset containing twenty percent of the whole dataset, or 44 experimental samples. These data were not applied to the process of optimization. Based on Table 1, the PD value estimated using the proposed model (PD-ANN- GSA) is of high reliability on the basis of the experimental outcomes (PD-EXP) and in comparison, with the PD-GSA model of Banyhussan et al. (2020).

The predictions of the proposed model led to a CoV of 2.693%, a mean of 0.99, and an SD of 0.027, which confirm that the model is both accurate and consistent. A comparison of the PD between the values obtained through experiments and those predicted the suggested model is shown in Figure 10, which demonstrates the dependability of the proposed model. According to the authors in Gandomi & Roke (2015), the CoV value shows the accuracy of the relationships between the inputs and the goal, where the CoV values of less than 10%, 20–30%, and more than 30%, respectively, denote great accuracy, poor accuracy, and extremely low precision. In

case of the proposed model, the CoV value was obtained as 2.693%, which indicated its high level of accuracy. The proposed model also obtained a value close to 1.0 of the mean (1.03). In addition, the R-value of 0.9676 (as can be observed in Figure 10 and Table 3) and the CoV value of 2.693% show an acceptable agreement between the actual PD and the estimated one. Considering various material properties/proportions, these findings confirm that the suggested model has a high efficiency in the prediction of the PD capacity of cementitious pastes.

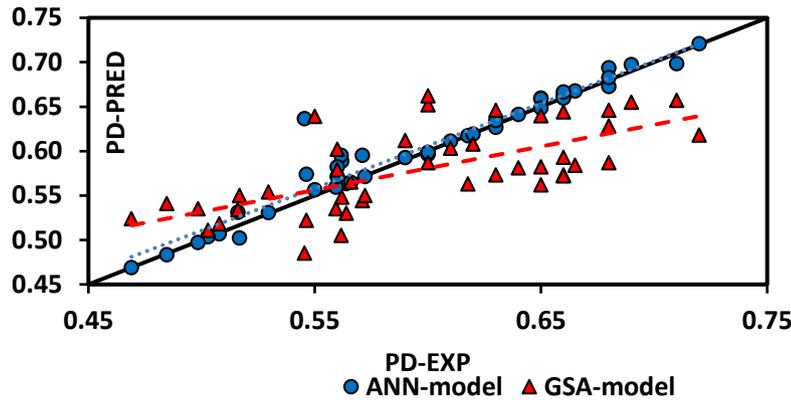


Fig. 10 Comparisons the amongst the estimated and experimental PD values of cementitious pastes allocated to verification process

Table 3 Experimental database and values estimated with the use of the proposed model.

Sample ID	PD-Exp	PD-ANN	PD-Exp/PD-ANN	PD-GSA	PD-Exp./PD-GSA
C100w0.7	0.55	0.64	0.857	0.485	1.134
C70FA30w0.8	0.56	0.56	1.001	0.530	1.057
C70FA30w1.0	0.51	0.51	1.002	0.518	0.983
C60FA40w0.8	0.56	0.59	0.955	0.548	1.022
C60FA40w1.0	0.52	0.53	0.972	0.534	0.973
C50FA50w0.8	0.57	0.56	1.002	0.565	1.009
C50FA50w1.0	0.52	0.50	1.029	0.550	0.945
C95SF5w0.8	0.56	0.60	0.944	0.505	1.108
C90SF10w0.6	0.62	0.62	1.000	0.563	1.102
C90SF10w0.8	0.57	0.60	0.959	0.544	1.047
C85SF15w1.0	0.53	0.53	0.998	0.554	0.956
C85SF15w1.2	0.48	0.48	1.003	0.541	0.888
C70SL30w0.8	0.55	0.57	0.952	0.522	1.050
C70SL30w1.0	0.50	0.50	0.998	0.511	0.978
C60SL40w0.6	0.57	0.57	1.002	0.550	1.037
C60SL40w0.8	0.56	0.56	1.000	0.535	1.047
C50SL50w1.0	0.50	0.50	1.003	0.535	0.934
C50SL50w1.2	0.47	0.47	1.001	0.524	0.896
C65FA30SF5w0.5	0.67	0.671	0.996	0.584	1.148
C65FA30SF5w0.6	0.66	0.66	0.999	0.573	1.151
C55FA40SF5w0.6	0.66	0.66	0.996	0.593	1.114
C55FA40SF5w0.7	0.65	0.66	0.986	0.582	1.116
C45FA50SF5w0.36	0.68	0.67	1.011	0.646	1.052
C45FA50SF5w0.4	0.65	0.66	0.986	0.640	1.016
C60FA30SF10w0.3	0.66	0.66	1.000	0.644	1.024
C60FA30SF10w0.4	0.68	0.69	0.980	0.628	1.083
C60FA30SF10w0.8	0.64	0.64	0.998	0.581	1.101
C60FA30SF10w0.9	0.63	0.63	1.005	0.573	1.100

Sample ID	PD-Exp	PD-ANN	PD-Exp/PD-ANN	PD-GSA	PD-Exp/PD-GSA
C40FA50SF10w0.49	0.71	0.70	1.017	0.657	1.081
C40FA50SF10w0.5	0.69	0.70	0.990	0.655	1.053
C55FA30SF15w1.0	0.60	0.596	1.006	0.587	1.022
C55FA30SF15w1.1	0.56	0.582	0.962	0.579	0.968
C45FA40SF15w0.9	0.59	0.593	0.996	0.612	0.964
C45FA40SF15w1.0	0.56	0.571	0.980	0.602	0.930
C35FA50SF15w0.7	0.60	0.598	1.003	0.652	0.920
C35FA50SF15w0.8	0.55	0.556	0.989	0.639	0.860
C65SL30SF5w0.5	0.61	0.666	0.990	0.572	1.067
C65SL30SF5w0.6	0.62	0.648	1.003	0.562	1.103
C55SL40SF5w0.5	0.64	0.683	0.996	0.587	1.090
C45SL50SF5w0.5	0.61	0.611	0.998	0.603	1.011
C50SL40SF10w0.5	0.72	0.721	0.999	0.618	1.165
C40SL50SF10w0.7	0.62	0.619	1.002	0.608	1.019
C45SL40SF15w0.4	0.60	0.599	1.002	0.662	0.906
C45SL40SF15w0.5	0.63	0.634	0.994	0.646	0.976
		M	0.990		1.027
		SD	0.027		0.078
		CoV%	2.693		7.546

3.4. Model validity

The suggested novel criteria by Golbraikh his fellow (2002) was applied to the GSA external verification on the testing datasets. According to Gandomi and Alavi (2013a), The slope of regression lines (k or k') over the origin must be near to 1 for at least one regression line. A confirmatory index of the external predictability of models, designated R_m by Roy and Roy (2008), was proposed. The condition is satisfied if R_m > 0.5. Over the origin, the squared coefficient of correlation between the estimated values and the experimentally-measured ones (R_o²) needs to be close to 1. Table 4 presents the validation criteria considered in this study and the relevant results of the proposed model. As the table clearly demonstrates, the model could meet the required conditions. Table 4 also presents the external validation criteria results of the models. As it is clearly seen, GSA-ANN could satisfy all the conditions.

Table 4 External validation statistics for the GSA-ANN framework.

Item	Formula	Condition	GSA-ANN	Banyhussan et al. (2020)
1	$R = \frac{\sum_{i=1}^n (EA_i - \overline{EA_i})(EE_i - \overline{EE_i})}{\sqrt{\sum_{i=1}^n (EA_i - \overline{EA_i})^2 \sum_{i=1}^n (EE_i - \overline{EE_i})^2}}$	R > 0.8	0.9676	0.8072
2	$k = \frac{\sum_{i=1}^n (EA_i \times EE_i)}{EA_i^2}$	0.85 < k < 1.15	1.01	1.02
3	$k = \frac{\sum_{i=1}^n (EA_i \times EE_i)}{EE_i^2}$	0.85 < k < 1.15	0.99	0.98
4	$R_m = R^2 \times \left(1 - \sqrt{ R^2 - R_o^2 }\right)$	R _m > 0.5	0.95	0.51
where $R_o^2 = 1 - \frac{\sum_{i=1}^n (EE_i - EA_i^o)^2}{(EE_i - \overline{EE_i})^2}$, $EA_i^o = k \times EE_i$				

Figure 11 illustrates the PD value estimated by the proposed GSA-ANN and those estimated by the model of Banyhussan et al. (2020) in case of 44 datasets. A prediction is considered accurate when the ratio of the experimental to estimated PD is 1. As Figure 10 depicts, in case of the GSA-ANN model, the distribution frequency of the ratio of the experimental to estimated PD offered a more accurate prediction compared to that of the model proposed by Banyhussan et al. (2020).

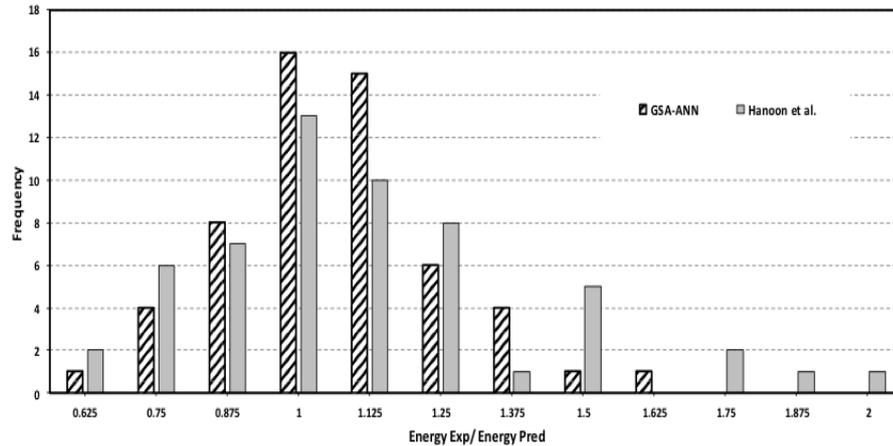


Fig. 11 GSA-ANN predicts and experiments PD capabilities

3.5. Error evaluation

The accuracy of predictions made by a model cannot be evaluated by merely a correlation coefficient since this coefficient is insensitive to the multiplication or addition of output values by a constant. For that reason, along with the correlation coefficient, there is a need for an error function to evaluate the performance quality of the model more reliably. A function was suggested by Gandomi et al. (2011) for the evaluation of the performance quality of a model, which considers the changes to both correlation and error functions. A performance index (PI) was employed in the current research based on the Gandomi et al. (2011) function

To evaluate the model's performance as a function of the corresponding root standard deviation (CRSD) and the correlation coefficient (R), do the following:

$$PI = \frac{CRSD}{R + 1} \tag{18}$$

$$CRSD = \frac{1}{|\overline{PA}_i|} \sqrt{\frac{\sum_{i=1}^n (PA_i - PE_i)^2}{n}} \tag{19}$$

$$R = \frac{\sum_{i=1}^n (PA_i - \overline{PA}_i)(PE_i - \overline{PE}_i)}{\sqrt{\sum_{i=1}^n (PA_i - \overline{PA}_i)^2 \sum_{i=1}^n (PE_i - \overline{PE}_i)^2}} \tag{20}$$

where PA_i and PE_i stand for the i th experimental and the estimated outputs, respectively, \overline{PA}_i and \overline{PE} represent the average values of the experimental and estimated outputs, respectively; and n signifies the number of samples.

Note that lower root smallest standard deviation (RSSD) values and higher R values lead to a lower PI , which shows a higher accuracy of the model in hand. PI values are range between 0 and $+\infty$, where the smaller the value, the better performance is achieved. In the case of the PI proposed in this study, a value close to zero (which is the recommended acceptance threshold) shows that the model has been successful in predicting accurate values.

As explained earlier, a GSA-ANN model was constructed in this study for the aim of predicting the PD of cementitious pastes. Table 5 summarizes the results of the GSA-ANN model and the model of Banyhussan et al. (2020). In comparison, GSA-ANN achieved better (higher) R values and also lower RSSD values than the rival.

This table also demonstrates that GSA-ANN had a PI value lower than the model proposed by Hanoon et al. (2017). Remember that, based on the statistical criteria, the GSA-ANN model showed an acceptable correlation and covariance including a proper PI value.

Based on the recommendation given by Bagheri et al. (2012), the absolute relative error (ARE) percentage was computed using Eq. (21):

$$ARE = \left| \frac{PA_i - PE_i}{PA_i} \right| \times 100 \tag{21}$$

Figure 12 shows the ARE distribution for both the GSA-ANN model and Banyhussan et al. (2020) model. In an ideal condition, the frequency depicted in Figure 12 should be reduced with an increase in ARE. GSA-ANN demonstrated the maximum rate of low absolute relative error (less than 5%) and the minimum rate of high absolute relative error (more than 25%). GSA-ANN had acceptable error distributions and a relatively low frequency of extremely high ARE values when compared to the other model. In addition, between models, the GSA-ANN model had more acceptable error distributions compared to the model of Banyhussan et al. (2020) as displayed previously in Figure 11.

Table 5 Summary of the general model performances for estimating RC beams' PD capacity.

Model	Experimental vs predicted			Experimental/predicted		
	RSSD (%)	R2	PI	Average	SD	CoV (%)
GSA-ANN	0.029	0.9676	0.015	0.990	0.027	2.693
Banyhussan et al. (2020)	0.047	0.8072	0.026	1.030	0.078	7.55

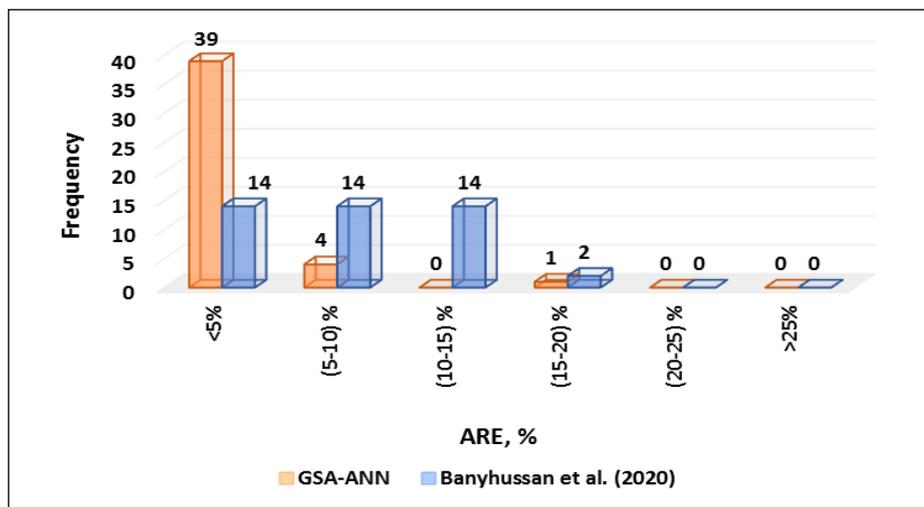


Fig. 12 ARE distribution of GSA-ANN and the model of Banyhussan et al. (2020)

4. Conclusion

The present paper was aimed at developing a novel hybrid method integrating GSA and ANN, called GSA-ANN, for the purpose of predicting the packing density (PD) value of cement pastes. The model introduced in this paper was developed with the help of an extensive database that involved data related to five parameters of water amount (W), the cement amount (PC), the fly ash amount (FA), the slag amount (SL), and the silica fume amount (SF). In the following, the key findings of this study are presented:

The ANN relationships developed in this study were successful in reliably predicting the PD value of cement pastes. The GSA-ANN model effectively met majority of the conditions considered for the external validation.

The model was further verified through comparing its results with the results accessible in the literature. The comparative research confirmed that ANN outperformed the benchmark model (Banyhussan et al., 2020).

The results showed the high accuracy of the ANN technique when dealing with problems arising in the civil engineering field. As a result, it is applicable as an efficient tool to prediction of the PD value of cement pastes.

This study implemented a dataset that consisted of a total of 216 samples for the purpose of assessing the accuracy level of GSA-ANN. In addition, statistical analysis was carried out, which obtained the coefficient of variation (CoV), mean, and correlation coefficient (R) values of 2.35%, 0.999, and 0.9876, respectively. The results showed that estimations provided by the model were highly consistent and accurate. Consequently, GSA-ANN is a reliable tool that is capable of predicting the PD value of cementitious pastes.

Literature lacks adequate research focusing on predicting the PD of cement pastes. Therefore, there is a need for further experimental research to be carried out with the use of additional data to further test and develop the proposed GSA-ANN model and also to analyze a broader range of parameters relevant to the issue.

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