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Prediction of the yield stress of printing mortar ink

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Abstract. The development of printable cement-based material is a high priority in the field of 3D printing for construction. There are many admixtures available for the design of the printing mortar ink which can influence the wet and final properties of the mortar. In this work, artificial intelligence has been utilized to predict those properties and guide the dosage of each admixture. The algorithms were developed from a factorial experimental plan. The mortar investigated consists of cement blended with silica fume to reduce the embodied carbon of the mixture. The selected admixtures were a superplasticizer, a viscosity modifying agent, nano-clay, C-S-H seeds and an accelerator with a water-reducing effect. A rotary rheometer was used to measure the viscosity and the dynamic yield stress of both mortar and cement-paste mixtures. Additional tests were conducted such as the small Abrams cone and the ASTM C1437 flow test. Several predictive algorithms were developed and compared, in which artificial neural networks were used. Furthermore, to enhance the performance of the neural network, a genetic algorithm was used to optimize the network parameters. To evaluate the performance of the models, the normalized root mean square error (NRMSE), and coefficient of determination (R^2) were calculated. This approach is a single-objective prediction which yields promising capability to predict the wet properties of both mortar and cement pastes, which can be later expanded into a multi-objective approach.

Keywords: Artificial neural networks, genetic algorithms, wet properties, mix design, 3D printing.

1 Introduction

In recent years, artificial intelligence (AI) has been increasingly utilized to solve complex problems across many engineering sectors. Civil engineering is among them, where AI has been applied for the prediction of concrete properties, such as compression strength, drying shrinkage, filling capacity, concrete durability, segregation and slump [1-6]. The majority of the studies in this field use artificial neural network algorithms (ANN), tree-based models, and fuzzy logic. The combination of AI methods with optimization techniques is also promising. ANN has been implemented along with the whale algorithm or the multi-objective grey wolves technique, whereas the adaptive network based fuzzy inference system has been used with genetic algorithms [2-4]. These studies confirm that AI techniques are a promising avenue to predict the properties of concrete materials.

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In this study, the main objective is to develop ANN models that can predict the wet properties of mortar and cement-paste mixes. Two different methods were compared: the leave-one-out cross validation method and the genetic algorithm (GA) optimization technique which divides the available dataset into training and testing data with proportions of 70% and 30%, respectively. The GA technique was applied to investigate an increase in the prediction performance of the ANN model in searching the optimal parameters. Sixteen formulations were available from a previous study of Charrier and Ouellet-Plamondon [7] where six early age property measurements were conducted, such as rheological and slump tests. The objective of the present study is the prediction of those six properties, namely the yield stress, viscosity, and mini-slump test for cement-paste mixes and slump, flow and deformation tests for mortar mixes for 3D printing applications. The coefficient of determination (R^2) and the normalized root mean squared error (NRMSE) were employed to evaluate the effectiveness of the proposed models and to compare the two different methods.

2 Materials and testing methods

2.1 Materials and mix design

Binder and admixtures. The cement that was used in this study is the GUb-8SF which is a binary cement with silica fume and a specific gravity of 2.8. A local sand was selected with specific gravity of 1.65 and the water used was tap water. The selected admixtures were five in total; a superplasticizer (SP), an accelerator (A), the C-S-H seeds (X), nanoclay (C), and a viscosity modifying agent (VMA). The SP, A, X were added to control the workability of each mixture. The A and X are strength-enhancing admixtures which are also known to improve cement hydration. Finally, the VMA and C were used to increase the stability of the mix. The solid content of the admixtures was determined according to ASTM C494 [8]. Further details can be found in the published study

Mix design. For the mortar mixes, the sand/cement ratio was selected to be 1.8. Based on literature this ratio results in a mortar mixture with acceptable pumpability-extrudability. The water/cement ratio was a fixed proportion of 0.345 for all of the mixes, both for cement-paste and mortar mixes. In this ratio, the water content of each admixture was included. The water content of each admixture was determined by measuring the residue of each admixture with oven drying, according to ASTM C494 [8]. Furthermore, the dosage for each admixture was determined based on the literature review [7] and experimental tests with different dosages that were conducted in a preliminary study. The quantities of SP, C, A, X and VMA used were 0.26%, 0.50%, 0.70%, 0.30% and 0.004% of the cement weight, respectively. A two-level full-factorial design was implemented for the experimental design, where the admixtures except for SP were either present in the aforementioned amounts or absent. It is always preferable to do a factorial design. The only exception is if the admixtures do not interact with each other with absolute certainty. Factorial design can also reduce the number of runs necessary, resulting in prompt convergence. The SP was included in all mixes to reduce the water content. Hence, the total amount of the mixes was $2^4=16$. Finally, all the admixtures were added to the water just before the addition of the binder, apart from the C admixture which was dry mixed with the binder. The mixing procedures for the cement paste were made according to ASTM C1738 [9]. The 16 mixes and the six testing methods are explained in [7, 10].

3 Artificial intelligence

In 3D concrete printing a common challenge is the development of a suitable mixture. Some of the most important properties of the mixture are the flowability, extrudability, and buildability [11-13]. However, in general those properties tend to be contradictory to each other. In order to address this problem, artificial intelligence can be utilized to develop the best possible mixture. Compared to linear and quadratic models, machine learning provides better predictive performance of the concrete mixture properties, such as compressive strength and slump [3]. At an early stage of the study, the two most prevalent algorithms were compared, the random forest (RF) and the artificial neural network algorithms (ANN). The preliminary results showed better accuracy of the ANN. Thus, only the results of the latter are discussed herein in detail.

3.1 Algorithms

Neural Network. The ANN can be described as an interconnected system of nodes inspired by the biological neural networks of the human brain. The ANN consists of three basic components, namely the input, hidden, and output layers. This model is trained in order to predict the output from a provided input. Compared with traditional computational models, the advantages of ANN are that it does not require predefined constraints and it is powerful in large data problems. Furthermore, ANNs can observe a pattern during training or identify complex nonlinear relationships in the data itself. ANNs have been used in concrete mixture design where the input and output layer nodes are decision variables and objectives, respectively. Training the network with a dataset changes the weights between the nodes and increases the predictive performance [3].

Evaluation. In order to evaluate the performance of the models, the normalized root mean square error (NRMSE), and coefficient of determination (R^2) are calculated. The NRMSE is the normalized mean squared difference between targets and outputs, and R^2 describes the correlation between outputs and targets. In brief, lower NRMSE and higher R^2 (with a range between 0 and 1) show better accuracy of the model.

3.2 Methodology

Cross-validation: Leave-one-out. Following the approach of [10], the first algorithm that was developed in MATLAB was a neural network with the leave-one-out cross-validation method. As the author mentions, this method was chosen in order to avoid overfitting of the model. The available dataset was 16 different mixes; therefore, the training of each network was made from the 15 out of the 16 samples in total and the remained sample was used for testing. As a result, the developed algorithm produced 16 different networks which were compared by calculating the NRMSE and R^2. Linear, quadratic and cubic regressions were performed to achieve better results. Furthermore, each network is consisted of three layers, namely the input, output and one hidden layer with ten neurons. The input neurons were the types of admixtures that were used, whereas the output is one property of the material, such as the yield stress, viscosity or mini-slump. The selected training function of the network updates the bias and weight values according to Levenberg-Marquardt optimization. This minimizes a combination of squared errors and weights and then determines the correct combination to produce a network that generalizes well. The process is called Bayesian regularization backpropagation [14].

Optimization algorithm and 70/30 rule. A testing plan is used to ensure that the evaluation provides realistic estimates of model performance on unseen data. Generally, one of the main steps is to split the data into training and testing sets. The proportions of split may vary depending on the project, although 70/30 is the most common, where 70% is for training and 30% for testing. In the first few attempts to apply this methodology to this network, the number of the hidden layers and neurons along with the training method, remained the same as the ones of the leave-one-out-cross validation method. The genetic algorithm was later selected in order to optimize the parameters of the network depending on the property to be predicted. The genetic algorithm (GA) is one of the oldest and most widely used evolution algorithms (EA). GA is inspired by the natural evolution of species, where the population adapts and evolves based on the environmental conditions. It consists of a population of individuals in which each one represents a potential solution to the problem. Similarly, to other EAs, a GA develops a random population of candidate solutions and iteratively forms subsequent populations of solutions by the selection, crossover, and mutation of a portion of the best solutions. The number of the total population can be gradually increased in each iteration [3]. The parameters that were tested to improve the predictive performance of the neural networks were the number of hidden layers, the number of neurons of each hidden layer, the number of neurons of the output layer and the training method. Since the number of the neurons in the output layer was a parameter, single and multi-objective predictions were performed. The goal of the genetic algorithm was to simultaneously maximize the R^2 and minimize the NRMSE. The second selected training function is a network training function that updates bias and weight values according to Levenberg-Marquardt optimization. Typically, it is the fastest backpropagation algorithm, despite requiring more virtual memory than other algorithms [14].

4 Results and discussion

The first approach was to use linear regression and to compare the 16 different combinations of the training and testing sets. The linear regressions of the networks for predicting the properties of the cement paste are shown in Fig. 1. The black dots represent the training data, whereas the red dot is the testing sample. The best performance for the yield stress was achieved in the 14th network, with R^2=0.999 and NRMSE=0.013. The testing sample was the 3rd mix and the rest were used for training the network.

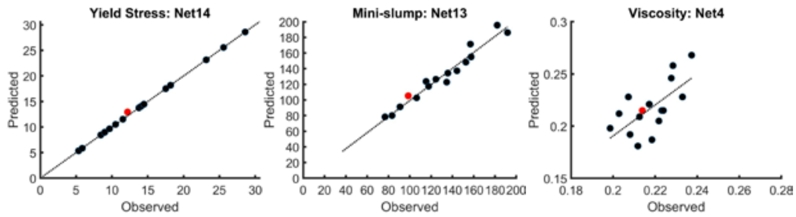

Fig. 1. The linear regression that was performed for the 14th network of yield stress (Fig. 1a), 13th network of mini-slump (Fig. 1b) and 4th network of viscosity (Fig. 1c) of the cement paste.

Moreover, the best network for predicting the mini-slump was the 13th network, with R^2=0.958 and NRMSE=0.054. The testing sample was the 4th mix and the rest were used for training the network. However, concerning the network for the viscosity, the predictive performance was below an accepted value, as the R^2 and NRMSE were 0.44 and 0.084 respectively.

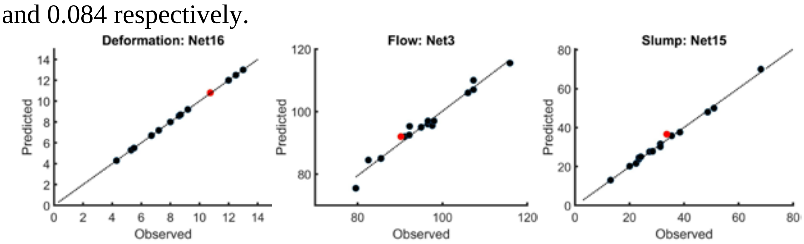

Fig. 2. The linear regression that was performed for the 16th network of deformation (Fig. 2a), the 3rd network of flow (Fig. 2b) and 15th network of slump (Fig. 2c) of the mortar.

Predicting the properties of the mortar mixes was also feasible. The predictive performance of the networks was even better than those of the cement paste. Particularly, in the 16th network with the deformation as the only objective, the R^2 was greater than 0.999 and the NRMSE was 0.002. Concerning the flow, the best network was the 3rd with R^2 and NRMSE being 0.97 and 0.0018 respectively. As for the slump, which is the third and final property measured for the mortar mixes, the 15th was the best network in which the R^2 was 0.994 and the NRMSE was 0.033.

The linear regressions of all the properties had strong correlation except for the viscosity of the cement paste. With the aim to develop a better network for the viscosity, a second approach was attempted by comparing linear, quadratic and cubic regressions. This approach was not only used for the viscosity, but also for all of the six properties to observe if there will be any further improvement in performance. The best performance among the cement paste properties was achieved by the 14th network for predicting the yield stress, with R^2=0.999 and NRMSE=0.013 with quadratic regression. However, the performance was the same as the linear regression. The testing sample was the 3rd and the rest was used for training the network.

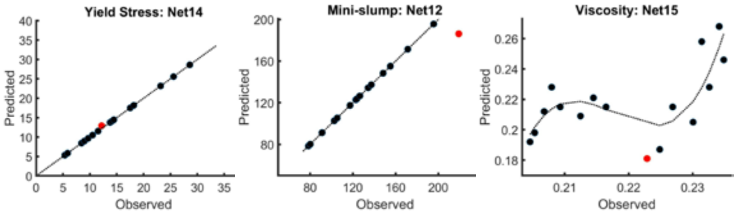

Fig. 3. The quadratic regression that was performed for the 14th network of yield stress (Fig. 3a) and the cubic regression for the 12th network of mini-slump (Fig. 3b) and the 15th network of viscosity (Fig. 3c).

Moreover, the best network for predicting the mini-slump was the 12th network, with R^2=0.994 and NRMSE=0.063 with cubic regression. The testing sample was the 5th and the rest was used for training the network. In this non-linear network, there was a minor improvement in the performance compared with the linear regression. Furthermore, the best network for predicting the viscosity of the cement paste was the 15th network, with R^2=0.687 and NRMSE=0.094 with cubic regression. The regression showed almost a strong correlation, $R^2 \sim 0.7$. Thus, it was considered acceptable. The testing sample was the 2nd and the rest was used for training the network.

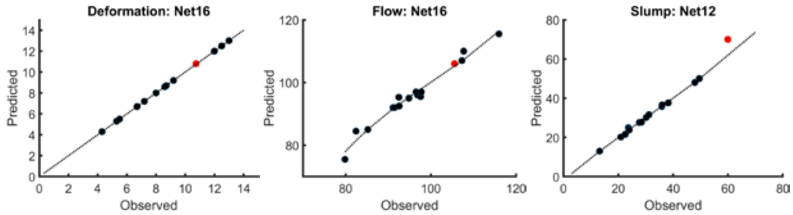

Fig. 4. The quadratic regression that was performed for the 16th network of deformation (Fig. 4a) and the cubic regression for the 16th network of flow (Fig. 4b) and 12th network of slump (Fig. 4c).

The best performance among the mortar properties was achieved by the 16th network for predicting the deformation, where the R^2 was greater than 0.999 and the NRMSE was 0.002 with quadratic regression. However, the performance was also the same as the linear regression. The testing sample was the 1st and the rest was used for training the network. Concerning the network for the flow, the 16th was the best network where the R^2 and NRMSE were 0.976 and 0.0017 respectively with cubic regression.

The performance was slightly improved, and the testing sample was the 1st. As for the slump, the best network was the 12th with R^2 equal to 0.997 and NRMSE 0.079 with cubic regression. The testing sample was the 5th, with a modest improvement over the linear regression. In brief, the leave-one-out cross-validation method was applied successfully for both the mortar and cement paste properties, and the results of the evaluation methods were acceptable. However, despite the good results for the R^2 and the NRMSE, the figures above, such as Fig. 3b of the mini-slump or Fig. 3c of the viscosity, also reveal a noticeable error between the prediction and observed values of the testing sample. This implies that the predictive performance is not realistic and that most of the networks are overfitted. This fact can be explained by the big imbalance between the training (94%) and testing (6%) data.

In order to face the above-mentioned problem, new networks were created with a better split of the available dataset. Based on the literature, the most common proportions of the two sets, training and testing, is 70 and 30 percentage respectively. However, a better balance of training and testing data alone does not guarantee an improvement in the model. For this, it is essential to use a suitable algorithm to discover the optimal parameters of the network. To overcome this problem, the genetic algorithm was used. The maximum generations of the algorithm were selected to be 50, the number of candidate solutions of the first generation was 80 and at every new generation the number was increased by 40. Depending on the cement parameter being modeled, different parameters were considered to be the best for each individual network. However, there were a few common parameters that were used in all networks. Specifically, the best training method was the Levenberg-Marquardt, the performance method was the mean squared error, and the networks with only one hidden layer performed better. The data was divided into two parts, the training and testing. However, the division was conducted prior to entering the data to MATLAB network function. Hence, only the training data was input to the network and the 'dividetrain' function was selected to assign all data of the training set only. Testing of the network was performed with linear regression, and the results were used as input for the genetic algorithm. Finally, in order to reduce the amount of time required for the overall algorithm, the number of the maximum epochs of each network was selected to be 400.

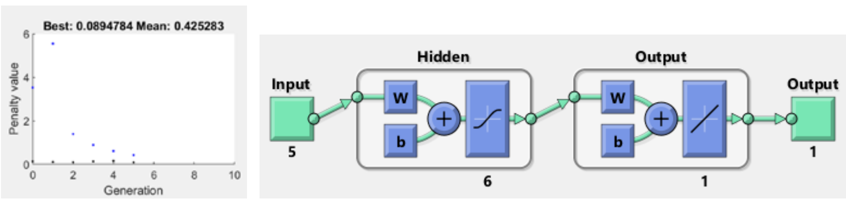

Fig. 5. Examples of the genetic algorithm and of a network in Fig. 5a and Fig. 5b respectively. In Fig. 5a, the results of the initial and first four generations are depicted. In Fig. 5b, the general form of a network with three layers is shown; the input, output and one hidden layer with 6 neurons.

The number of output neurons, or objectives, was also a parameter. Several attempts were made to create multiple output networks; for instance, training two networks in total, one for the cement paste's properties and another one for the mortars where each one had three objectives, or only one network with six objectives. However, the best predictive performance was achieved when each network had only one objective, hence the final number of the networks that were developed were six in total. As a result, each property of the mortar and cement-paste mixes has a separate optimized network. In the following discussion, each network is explained separately along with figures of the linear regression. In each figure, the black dots depict the training data set, 11 mixes, whereas the red dots, remaining 5 mixes, are the testing dataset. Finally, the training and testing data were randomly selected every time at each iteration of the genetic algorithm. However, based on the final results, the best mixes for training all networks were the 2nd, 3rd, 5th, 7-11th, 13-15th mixes and the rest were used for testing the network.

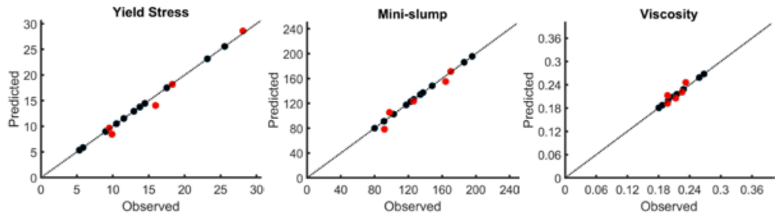

Fig. 6. The linear regression that was performed for the network with the yield stress (Fig. 6a), the mini-slump (Fig. 6b), and viscosity (Fig. 6c) of the cement paste as the only objective.

For the best network with the yield stress as the only objective, the R^2 was 0.9924 and the NRMSE was 0.0629. In order to achieve those results, the number of the neurons on the hidden layer was six in total. Concerning the network for the mini-slump, the R^2 and NRMSE was 0.9833 and 0.00263, respectively. In this network, the best performance was achieved with the number of the neurons on the hidden layer to be ten in total. As for the viscosity, the improvement was evident as the R^2 was 0.9426 and the NRMSE was 0.023. The network performed better with eleven neurons in total on the hidden layer.

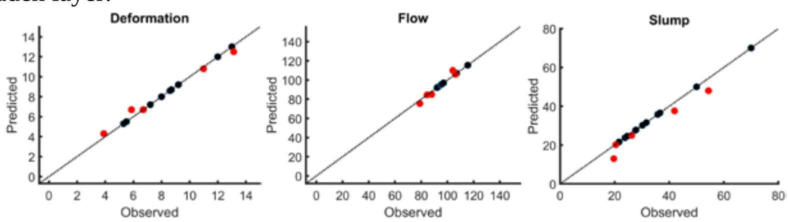

Fig. 7. The linear regression that was performed for the network with the deformation (Fig. 7a), flow (Fig. 7b) and the slump (Fig. 7c) of the mortar.

Furthermore, for the best network with the deformation as the only objective, the R^2 was 0.9921 and the NRMSE was 0.0263. In order to achieve those results, the number of the neurons on the hidden layer was seven in total. For the network for the flow, the R^2 and NRMSE were 0.9722 and 0.00176, respectively. In this network, the best performance was achieved with the number of the neurons on the hidden layer to be seven in total. As for the slump, which is the third and final property measured for the mortar mixes, the R^2 was 0.9715 and the NRMSE was 0.0685. The network performed better with four neurons in total on the hidden layer. The summary of the results is presented in Table 1.

Table 1. Summarizing all the results of leave one out cross validation method (1st) and 70/30 method with genetic algorithm (2nd)

Mixture	Test/Property	R^2			NRMSE		
		1st Method		2nd Method	1st Method		2nd Method
		Linear	Quadradic, cubic	Linear	Linear	Quadradic, cubic	Linear
Cement paste	Yield Stress	0.999	0.999	0.9924	0.013	0.013	0.0629
	Mini Slump	0.958	0.994	0.9833	0.054	0.063	0.0263
	Viscosity	0.44	0.687	0.9426	0.084	0.094	0.023
Mortar	Deformation	>0.999	>0.999	0.9921	0.002	0.002	0.0263
	Slump	0.994	0.997	0.9715	0.033	0.079	0.0685
	Flow	0.97	0.976	0.9722	0.018	0.017	0.0176

5 Conclusion and future work

Based on the evaluation methods that were applied, the leave-one-out cross validation method with quadratic and cubic regression perform slightly better for most properties. On the other hand, the 70/30 method with GA can predict the viscosity of the cement paste better than the cross-validation method. The viscosity was the most difficult property to be predicted without changing the controllable factors of the network, such as the number of the neurons in the hidden layer. Finding the right values of those factors would be hard to be achieved without the GA method. However, the proportion of the training data of the dataset was different, specifically 96% and 70% respectively on the two methods. As a general conclusion, predicting properties for new mixes is possible by employing these two methods, although, the second method is the suggested one. Despite the fact that the available dataset was small, it was adequate for training and validating the developed networks. However, the testing of those networks will be made with new unseen data. Hence, as a next step, the prediction accuracy of the developed networks will be validated by forming new mixtures and testing them in the lab. More data will be added with the aim to have a large and diverse data set. Additionally, new attributes and objectives will be added by employing new tests on cement pastes and mortars, such as calorimetry and compression tests. Finally, multi-objective optimization algorithms will be developed with the aim to design optimum mortar mixes suitable for 3D printing applications, by achieving the desired properties, reducing the overall cost and forming more eco-friendly mixes.

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