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Use of Artificial Neural Networks for Prediction of Properties of Self-Sensing Concrete

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Abstract **–** Nanomaterials such as carbon nanotubes and carbon nanofibers are used as reinforcement for concrete, enhancing its compressive and flexural strength, and durability, and providing additional properties such as electrical conductivity. Hence, CNT/CNF reinforced concrete composite material is multifunctional material which may be used in structural capacity as well as structural health monitoring purposes. Although this material can be superior to traditional concrete, extensive and costly procedures of fabrication are hindering its practical potential. Concrete mix design methods are commonly used during the design of such composites, however, since these methods cannot give direct connection between the recipe and the end-product, every composite must be put through testing and iteratively adjusted until the appearance of wanted results.
This paper proposes application of artificial neural networks for predicting properties of CNT/CNF concrete composite materials. Artificial neural networks in mix design have been developed for various types of concrete, commonly to predict only compressive strength as the primary property of concrete. However, self-sensing concrete is used primarily for its piezoresistivity and enhanced strength is only the consequence of the existence of nanofillers. Hence, the paper investigates prediction of compressive and flexural strength as well as electrical resistivity of 468 concrete mixtures by developing 3 different datasets comprehended by 6 ANN models. The models show some interesting results and point toward the necessity of further investigations on this topic and possible improvements.

Keywords**:** Carbon nanotubes, Carbon nanofibers, Self-sensing concrete, Concrete mix design, Artificial neural networks.

1. Introduction

Carbon nanotubes (CNTs) and carbon nanofibers (CNFs) are a familiar topic within the field of structural health monitoring. These materials can be used as nanofillers in concrete, where their role is twofold. Firstly, when the percolation threshold is crossed, it is considered that electrically conductive network is formed in the insulating concrete matrix. Secondly, mechanical properties such as compressive and flexural strength are enhanced by the presence of nanofillers which have superior characteristics compared to the concrete matrix. So, these composite materials are used primarily as sensors for monitoring cracking and other structural damage while functioning as structural elements able to withstand extraordinary loading. One of the problems arising with practical implementation of CNT or CNF reinforced concrete is slow and relatively expensive fabrication. Namely, these materials are applied only after a process of adjusting the mixture recipe in terms of ingredients and weight fraction of nanofillers. Due to the possibility of various mishaps during fabrication, extensive testing procedure is necessary to establish mechanical properties of these composite materials, which leads to additional waste of time and funds.

This paper proposes useful and more sustainable design method for CNT/CNF reinforced concrete that can be achieved through application of machine learning, more specifically, artificial neural networks. Machine learning methods are now present in the scientific community across all fields and areas of research. Among machine learning methods, artificial neural networks are the most prominent within the field of concrete mix design. Artificial neural networks (ANNs) are distinguished by the ability of solving complex problems that cannot always be mathematically described and by their flexibility, adaptability, and user-friendliness. ANNs may be applied for a variety of specific tasks and have shown themselves useful in mix design of various types of concrete. Most of the ANN models serve to predict the compressive strength as primary property of concrete, and other properties such as flexural strength [1-19], electrical properties [3,7,20-30], slump [31], elastic modulus [32], Poisson's ratio [33], etc. are investigated seldomly. Because of the specific nature of CNT/CNF concrete composite materials, the idea of the author is to investigate compressive strength, flexural strength, and electrical resistivity using ANN models. Using the traditional four-ingredient concrete reinforced with nanomaterials as a starting point, different models and new practice in concrete mix design may be developed, as well as further implementation of self-sensing concrete in regular civil engineering practice.

2. Development of ANN Models

Development of ANN models consisted of forming datasets, data analysis and processing, and building of ANN models. Data is collected from experimental investigations published in open access journals throughout the last decade. Artificial neural network models were developed using Matlab Neural Fitting tool.

2.1. Self-sensing Concrete

Research work consists of collecting data from available literature on compressive strength, flexural strength, and electrical properties of CNT/CNF reinforced concrete composite material. The data consists of results of laboratory testing, obtained from investigations chosen based on concrete ingredients. After the data is collected, it is checked, and inconclusive or somewhat strange results (outliers) are rejected while applicable results remained. Finally, three datasets are formed to show compressive strength, flexural strength, and electrical resistivity individually. It should be noted that tested electrical properties included electrical conductivity, resistivity, and/or resistance. All values were analytically transformed to electrical resistivity to form a comprehensive dataset. Total of 468 mixtures were collected from 35 investigations [1-30,34-38]. Observed mixtures represent traditional four-ingredient concrete with addition of CNTs or CNFs and supporting materials for improved dispersion. Due to the presence of CNTs and CNFs, additional materials are used to avoid phenomena such as high-air content (foaming), segregation, and low dispersion quality. OPC with strength class of 42.5 MPa and 52.5 MPa is favourable for its purity, leading to minimal side effects. Water was distilled, sonicated, or tap, fine aggregate was natural or manufactured siliceous sand, and coarse aggregate was gravel or crushed limestone. Only additional material which was considered as a part of the mixture within datasets is superplasticizer since its weight goes as high as 2% of the cement weight, and it affects the amount of water which further affects electrical sensitivity of hardened concrete composite material. Materials and their weights are presented in Table 1. Nanomaterials are of high purity, commonly purchased in the form of powder. Materials used as support for the dispersion of nanomaterials are surfactants, as follows: polyethylene glycol aromatic imidazole (TNWDIS) [1,11,12], sodium dodecyl benzene sulfonate (NaDDBS, SDB) [8,25,26,34], lignosulfonic acid sodium salt (SLS) [20-24], sodium lauryl with defoamer (SLDS), Triton X-100 (TX), gum arabic (GA), and cetyltrimethylammonium ammonium bromide (CTB) in [34], polycarboxylate based surfactant (SFC) [3-6,14,15], Adva Cast 575 [10,16], polyvinylpyrrolidone (PVP) [11], sodium dodecyl sulfate (SDS) [18,30], Dolapix PC67 [12]. Some dispersions are achieved without the help of surfactants [2,17,27,28,36,37]. These surfactant materials were not included as part of input data because of the negligible amounts they were used in, different procedures of dispersion not comprehended by the dataset, and the fact that they influence dispersion quality rather than final properties of concrete. Except for the weights of ingredients, common input neurons for all three datasets also included cement class and functionalization of nanomaterials with 0/1 designations. Cement class was represented by 1 for 42.5 MPa and 0 for 52.5 MPa. Functionalization was comprehended only by its existence (yes=1; no=0), without going further into the exact nature of the process.

Table 1. Summary of materials

Material	Minimum material/cement ratio	Maximum material/cement ratio	Minimum weight [kg/m^3]	Maximum weight [kg/m^3]
Cement	-	-	317.61	1875
Water	0.2	0.79	121.6	789.48
Fine aggregate	0	6	0	1994.4
Coarse aggregate	0	2.21	0	1015
Superplasticizer	0	0.02	0	27.27

CNTs	0	0.02	-	-
CNFs	0	0.025	-	-

Mortar and concrete mixtures were obtained through several different processes. Composite material fabrication in all experimental investigations followed the algorithm of mixing the dispersion, achieving satisfactory dispersion, mixing in the dispersion with dry concrete ingredients and water, moulding, and curing until testing. Although dispersion processes widely differentiate, quality of dispersions was verified by SEM analysis. Mixing of dispersion and concrete was done manually or automatically using mechanical agitator and/or rotary mixer. Geometry of moulding varies for different mixtures and specimens, depending on the nature of testing. Demoulding age was addressed within the dataset, where the 24 h duration was denominated as 0 and 48 h as 1. Curing duration varied depending on the testing date and was provided accordingly. Age of specimens was included in the input. Curing durations of 3, 7, 14, 20, 21, 28, 90, and 120 days are noted as a significant factor on the final strength and conductivity of specimens. Some investigations dealing with electrical testing addressed the issue of polarization effect. Polarization effect was addressed after the curing process by testing the variation of current intensity [20-24]; by drying the specimens at temperatures of 60°C and/or 95°C for 3 days [6]; and by fixing the current intensity with an AC/DC current source [27]. Flexural strength was tested on parallelepiped specimens with different sets of dimensions (Table 2) which have been exposed to three-point or four-point standard bending tests. Testing of compressive strength was carried out by standard compression press on parallelepiped and cylindrical specimens. Experimental investigations which examined electrical properties of CNT/CNF reinforced concrete composite material followed testing procedures of two-probe and four-probe method. Results of electrical tests included electrical resistance, resistivity, or conductivity. Hence, all results were analytically transformed into a comprehensive set giving only values of electrical resistivity.

2.2. ANN models

Datasets for ANN models were made based on information about mixtures, specimen preparation, testing procedures and results of testing. Three independent datasets were made for each property which represents an output signal. All datasets have 11 common input neurons representing the weights of cement (CEM), water (WAT), fine aggregate (FA), coarse aggregate (CA), and superplasticizer (SPL) per cubic meter of concrete, weight fraction of nanomaterials relative to the weight of cement (CNT, CNF), cement class (CLASS), functionalization (FUNC), demoulding age (D-AGE), age of specimen at the time of testing (AGE). Neurons which differentiate between datasets represent relevant specimen geometry and output, as it is shown in Table 2.

Table 2. Additional neurons per each dataset

Data set	Input	Input	Input	Input	Input	Input	Input	Output	Total # of tuples	Min. output value	Max. output value
1	C-S_A	C-S_B	C-S_C	C-S_D	C-S_E	C-S_F	C-S_G	COM-S	346	4.4 MPa	152 MPa
	4x4x8 cm	4x4x4 cm	5x5x5 cm	7x7x7 cm	20x10 cm	15x15 cm	7.5x15 cm				
2	C-S_A	C-S_B	C-S_C	C-S_D	C-S_E			FLEX-S	219	0.5851 MPa	16.7 MPa
	4x4x16 cm	2.5x4x8 cm	2x2x8 cm	10x50x50 cm	15x15x15 cm						
3	C-S_A	LENGTH						RESIST	173	10 Ω·cm	84100 Ω·cm
	min/max	min/max									

All values of input and output except of CLASS, FUNC, and D-AGE are normalized by min/max normalization with [0,1] value interval. Datasets are divided into training, testing and validation subsets. Division ratios between subsets for training/testing/validation are given in Table 3, while tuples are randomly divided with minimal repetition. All ANN models are based on similar architecture. Considering the size of datasets, Levenberg-Marquadt (LM) algorithm is commonly used for moderately sized network with up to a few hundred weights. Activation function is sigmoid because of the smooth gradient and functioning within [0,1] interval. Initial weights and biases are automatically assumed by the fitting tool and iteratively adjusted as the learning proceeds with the backpropagation. Model parameters are automatically prescribed by the Matlab neural fitting tool. In this case, the prescribed network is "*shallow*" meaning that there is only one hidden layer, while the number of hidden neurons is adjusted. Number of neurons in the hidden layer is a parameter which is set according to the number of input neurons and overall size of the network. Eq. (1) and Eq. (2) define the number of neurons of the hidden layer according to [39] and were adopted for the ANN models.

$$N_h = N_i \tag{1}$$
$$N_h = N_i \cdot 2 + 1 \tag{2}$$

To resume, there are 2 models for every dataset giving a total of 6 models. Each model is feed-forward backpropagation shallow neural network with sigmoid activation function, differentiating in subset ratios and number of neurons in the hidden layer. Table 3 is showing parameters describing all models.

Table 3. Summary of parameters describing all ANN models.

Model	Input nodes	Hidden layer	Hidden nodes	Testing [%]	Training [%]	Validation [%]	Max. epoch	Algorithm	Activation function
COM-S1	18	1	18	80 (276)	10 (35)	10 (35)	1000	trainlm	sigmoid
COM-S2	18	1	37	80 (276)	10 (35)	10 (35)	1000	trainlm	sigmoid
FLEX-S1	16	1	16	80 (175)	10 (22)	10 (22)	1000	trainlm	sigmoid
FLEX-S2	16	1	33	80 (175)	10 (22)	10 (22)	1000	trainlm	sigmoid
RESIST1	13	1	13	85 (147)	10 (17)	5 (9)	1000	trainlm	sigmoid
RESIST2	13	1	27	85 (147)	10 (17)	5 (9)	1000	trainlm	sigmoid

3. Results and discussion

Flowchart describing the process of developing an ANN model is shown in Figure 1. After generating the models, mean squared error (MSE) and coefficient of regression (R) are investigated and compared.

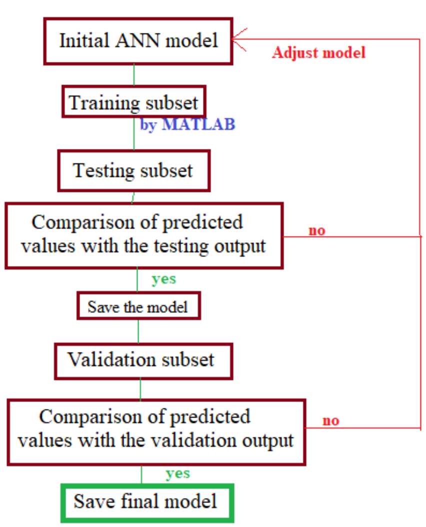

Figure 1. Flowchart for model development

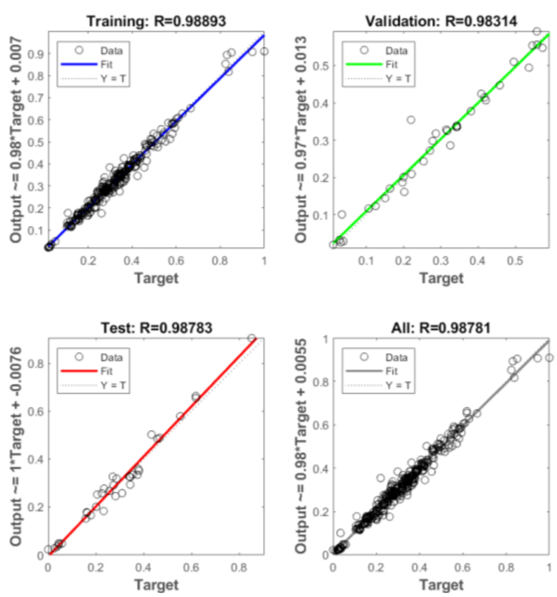

Figure 2. Regression plot for model COM-S1

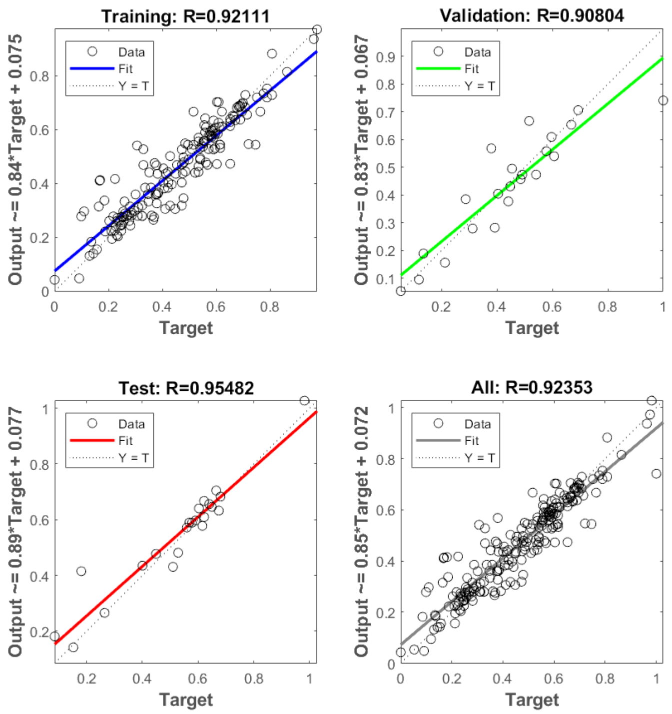

Figure 3. Regression plot for model FLEX-S2

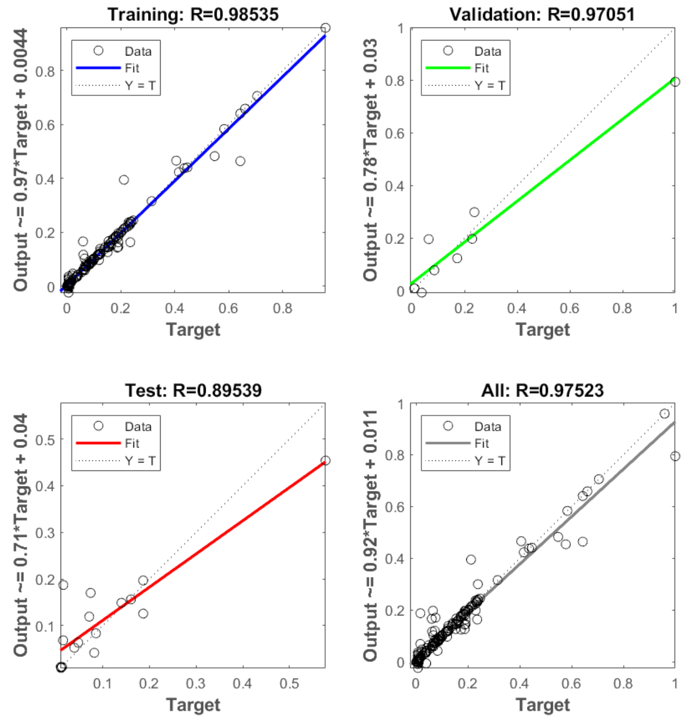

Figure 4. Regression plot for model RESIST2

Table 4 shows results of training the models. Regression coefficients are showing that all models are more or less successful with matching generated and target output value. However, there are some differences appearing regarding the mean square error factor and especially number of iterations needed for the generalization of the network.

Table 4. Results of training for all ANN models

Model	R	MSE	Epoch
COM-S1	0.9878	0.000935	52
COM-S2	0.9713	0.00297	17
FLEX-S1	0.9125	0.00915	12
FLEX-S2	0.9235	0.00781	24
RESIST1	0.9123	0.00113	20
RESIST2	0.9752	0.00766	60

Small number of training iterations may be prescribed to the small sample sizes of all three dataset, and hence subsets. Even so, model COM-S1 and RESIST2 have converged at a fairly high epoch number comparing to other models. Since the number of hidden neurons differentiate between these two models, the occurrence may be prescribed to higher quality of data in case of COM-S1. Model COM-S1 has the biggest sample size (346 tuples), and number of hidden neurons is equal to the number of input neurons, so, relatively longer generalization period may be caused by the presence of outliers in the sample.

Model RESIST2 has the smallest sample size with 173 tuples. Number of hidden neurons for this model is 27 which is relatively high giving that there are 13 input neurons and smaller sample, which may be causing more iterations during the training process. Best validation performance occurs just at epoch 54, however the performance plot shows smooth MSE curve per epoch. Models FLEX-S1 and FLEX-S2, with flexural strength as the output, have shown the weakest performance overall. Regression coefficient is the lowest in both models, mean square error is highest, and the number of iterations is not very conceivable in terms of accomplishing usable generalization. This may point at various problems including sample size, subset division, number of hidden neurons, and data quality. Supposedly, results would differ in case of varying subset division in combination with variations of the number of hidden neurons and changing the activation function to hyperbolic tangent function.

4. Conclusion

This paper describes the development of 6 ANN models based on 35 experimental investigations of CNT or CNF reinforced concrete. Investigation considered only experimental results that are usable for it, excluding non-standardized testing, outlying or unacceptable results, etc. For purposes of building ANN models, three different datasets were formed, first giving compressive strength, second giving flexural strength, and third giving electrical resistivity of the concrete composite material as output signals. All models have similar architectures with only one hidden layer. Each dataset was used for training 2 models differing in the number of hidden neurons. ANN models were developed, trained, tested, and validated using Matlab neural fitting tool. Results showed that models overall have relatively good behaviour, however, small number of iterations may imply false positive results. In order to get clearer picture of the condition of the network, more variations and additional investigations of each dataset should be made.

This investigation was made as the initial stage of testing the application of ANNs for CNT or CNF reinforced concrete composite materials. Experimental results used here present the baseline for development of numerical simulations for material behaviour of these composites. Future work includes developing numerical models using ANSYS and using the results of finite element model analysis for building new datasets which will accommodate comprehensive ANN models with three outputs, namely, compressive strength, flexural strength, and electrical property. Hopefully, this work will show that fabrication of nano-reinforced self-sensing materials can be more feasible and usable for practical purposes and inexperienced users. Through application of ANN, real-time monitoring of RC structures could become more cost-efficient, reach further practices, and not represent a luxury intended only for a privileged few.

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