Modeling of thermal conductivity of concrete by using artificial neural networks approaches

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Abstract:

The energy consumption of buildings presents a significant concern, which has led to a demand for building materials with better thermal performance. For this reason, determining the thermal properties of materials is essential information in the search for more energy-efficient materials. However, many time-consuming characterization experiments associated with high costs are required to ensure high accuracy and precision. Thermal conductivity (TC) is among the most relevant properties, which allows for measuring the material's heat transfer resistance. Due to the impracticality of predicting this thermal property in experimental tests, this study seeks to develop a methodology based on artificial neural networks (ANN) to predict the thermal conductivity of different types of concrete through its chemical composition. This work is broken down into two parts. The first one contains a feedforward backpropagation neural network (Multilayer Perceptron, MLP) to predict TC based on 200 experimental data sets of various types of concrete. Then, a Generative Adversarial Network (GAN) is used to expand the size of the training dataset to improve the performance of the first neural network. Currently, the model is implemented in Python, and different ANN structures varying the number of layers and neurons have been tested to find the best accuracy. The MLP model was developed using two hidden layers containing 200-100 neurons. It performed reasonably well on the training and validation dataset with an RMSE of 0.176, 0.183 W/m-K, and R^2 of 0.98 and 0.96, indicating a remarkable consistency between the predicted and the tested results. Furthermore, early GAN results show that it can generate data with reasonable accuracy with R^2 of 0.7. In the near future, we intend to increase the dataset and improve the model. Furthermore, the outcomes from this model can be helpful for the development of materials required for more energy-efficient buildings, providing quantitative information and helping the decision-makers in the construction sector.

Keywords: Artificial neural networks, MLP, GAN, Building materials, Concrete, Thermal conductivity.

1. Introduction

Due to the constant concern about the energy consumption of buildings, there is a growing demand for building materials to improve thermal performance. Utilizing thermal efficiency materials in the construction sector is necessary as they preserve indoor thermal comfort, despite fluctuations in the outdoor environment conditions [1]. Many building materials, such as concrete, masonry, and specific stones, can also be used as thermal energy storage materials. As energy efficiency relies on the material's thermal properties, an accurate prediction of their properties is vital for optimizing their performance in a building.

Concrete is one of the most used materials in construction and as a thermal energy storage material (TES) due to its unique features, such as high compressive strength, heat capacity, and low cost. However, as its chemical composition can vary significantly, its properties can undergo significant variations. For this reason, and in order to be effective as a TES material, it is crucial to have an ideal composition to ensure that its thermal properties meet the required design specifications [2].

Due to the search for more energy-efficient materials, many studies focus on analyzing the thermal properties of construction materials, such as thermal conductivity. This property is essential when evaluating

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the ability to transfer and store heat, which is directly related to finding and developing more energy-efficient materials. Therefore, a predictive model that can accurately estimate the thermal behavior of these materials would be beneficial in optimizing their use. In addition, several areas of engineering have used machine learning to perform data processing and analysis tasks due to its high efficiency.

Machine learning (ML) models can be used to develop such predictive models by learning from large datasets and finding patterns that can be used to make predictions. By incorporating ML, the predictive models can adapt to varying conditions and continuously improve their accuracy, making them a valuable tool in optimizing the performance of building materials [3]. Among the machine learning-based models, the Artificial Neural Network (ANN) is one of the most employed ones to solve complex problems and has various applications in several fields [4], [5]. The importance of ANNs lies in their ability to learn and make decisions based on data, which makes them highly valuable in different areas. ANN is composed of a set of networks of interconnected nodes, which work together to learn complex relationships between a group of inputs and outputs, making them well-suited for predicting some values based on a variety of parameters. In this way, ANNs can be used to solve problems that conventional or other computational methods have difficulties [6].

ANNs provide an alternative method for predicting concrete properties that is faster, cheaper, and more accurate than traditional methods. Although it has been applied to properties prediction, a few papers are progressing on models to determine the thermal properties. Additionally, the papers do not have a generalist model, which only focuses on specific types of concrete. This work intends to fill this gap, and the novelty is the development of a methodology using an ANN model to predict the thermal properties of concrete containing different types of materials such as slag, lightweight and recycled aggregates, fibers, and others. For this methodology, a Neural Network model for predicting thermal conductivity will be developed based on the constituents' composition and the concrete's density. The objective of the developed model is to extend it to other building materials, which can improve the performance and efficiency of these materials, making them more effective and cost-efficient.

2. Background

Concrete is a composite material made of cement, water, and fine and coarse aggregates, which let the designers select the components and create mixtures with distinct physical and chemical characteristics [7]. Adjusting these materials and their quantities allows the properties of both fresh and hardened states to be tailored to achieve the design specifications. For this reason, some works have developed an ANN to predict the properties of concrete. Over the years, ANN has been applied to predict different properties of concrete due to its ability to model complex non-linear relationships. After training the neural network, it can predict concrete properties such as compressive strength, slump, and workability with high accuracy. Many works have been published using different structures of a neural network, such as a backpropagation neural network (BPNN) [8], multilayer perceptron (MLP) [9], and radial basis function neural network (RBNN) [10].

Regarding the property predictions, the mechanical properties are the most evaluated, with compressive strength being the most investigated in different machine learning models. For example, Kandiri et al. estimated the compressive strength using a hybrid model of ANN and salp swarm algorithm [11], Abellán-García trained an MLP model to forecast the compressive strength for a given ultra-high-performance concrete (UHPC) mixture design [12]. Besides that, another work also developed an ANN with a feedforward backpropagation algorithm to predict the slump flow and compressive strength of UHPC while incorporating silica fume, limestone powder, recycled glass powder, and FCC [13].

Although many studies are developing new models to predict the properties of concrete, only a few papers investigated thermal conductivity or other thermal properties. Fidan et al. [14] trained different structures of an ANN model to predict thermal conductivity through five parameters – density, compressive strength, tensile strength, porosity, and ultrasonic pulse velocity. The best solution performance was achieved with a neural network with three layers and the following neurons sequence of 5, 25, and 1 in each layer. Sargam et al. [9] evaluated nine machine learning models, and MLP showed the highest prediction accuracy using the maxout activation function and three hidden layers, each containing 100 neurons. Kurpińska et al. [15] also investigated the influence of varying the number of neurons in the hidden layer to forecast the thermal conductivity of lightweight concrete. The model presented a sigmoid function and a structure with four layers: an input layer with two neurons, the first hidden layer varying from 2 to 12, the second hidden layer ranging from 2 to 17, and the output with one neuron. Kursuncu et al. [16] used ANN and ANOVA to investigate the effect of partial replacement of waste marble powder and rice husk ash instead of fine aggregate and cement into foam concrete. The results indicated ANN as the most adequate to estimate the thermal conductivity. Gence et al. [17] compared two neural networks RBNN and MLP to predict the thermal conductivity of concrete with vermiculite and concluded that RBNN had greater accuracy.

Different types of ANNs have been successfully applied to predict the thermal conductivity of concrete. ANN with a backpropagation algorithm is the most popular method for prediction. In order to show the effectiveness of ANN, some comparative studies have been conducted, as listed in Table 1.

Table 1. Comparative studies of different ANN-based methods to predict thermal conductivity.

Reference	ML method	Concrete	Number of inputs	Number of hidden layers	Neurons of hidden layers	Number of outputs	Number of datasets	Activation function	Evaluation criteria
Sargam et al. [18]	MLP	Concrete containing modern constituent materials	3,5,6,8,9,10,13	3	100 100 100	1	213	Maxout	MAE
Fidan et al. [14]	ANN	Concrete	5	1	5,10,15, 20,25	1	132	Tansig	MAE, MAPE, RMSE, R^2
Kurpińska et al. [15]	Backpropagation NN	Lightweight concrete	2	2	2-12 2-17	1	15	Sigmoid	MSE
Kursuncu et al. [16]	ANN	Foam concrete	-	-	-	1	18	Sigmoid	R
Gencel et al. [17]	Radial basis NN / MLP	Concrete with vermiculite	5	1	3	1	20	Non-linear	RMSE, MSE, R
Lee et al. [19]	Backpropagation NN	Concrete	11	2	20 20	1	152	Sigmoid / linear	MSE, R
Ozel and Topsakal [20]	Backpropagation NN	Construction materials	2	1	1	1	110	-	RMSE, R^2

Besides the literature review, a generic bibliometric analysis was performed to identify the most relevant and influential literature in the research domain of the employment of machine learning to predict the properties of concrete, which can facilitate the identification of critical research gaps and areas for future investigation. To proceed with this analysis, VOSviewer was used. It visually represents the research and enables researchers to find insights into the research domain [21]. Consequently, it can lead to more effective development of prediction models of thermal properties.

In order to evaluate the development of the research regarding property predictions using machine learning, a bibliometric study in the Web of Science database was performed. The following query, "concrete" AND "properties" OR "thermal conductivity" AND "machine learning" OR "artificial neural network" OR "ANN", and search criteria that were used in this bibliometric study summarized a total of 1508 documents that were published between 2000 and 2023. Then, the overall results were inserted in VOSviewer to analyze the keywords present in each paper's title or abstract, which generated the overlay cluster representing the development of the research over the years (Figure 1).

Figure 1 depicts the trend of integrating machine learning techniques with optimization for property prediction over the years, proving that machine learning models are a very actual research line with great expectations of development in this area. Although the ANNs are dated between 2018 and 2019, they are still being explored due to their effectiveness. Although many works employ ANN to predict mechanical properties, it is possible to observe the investigation of some chemical properties.

Therefore, after the literature and the bibliographic review, we noticed a gap in prediction models regarding thermal properties using machine learning models. This study aims to fill this gap and develop a method to predict the thermal conductivity of concrete. Additionally, we intend to build a model for data augmentation that has been used in many fields.

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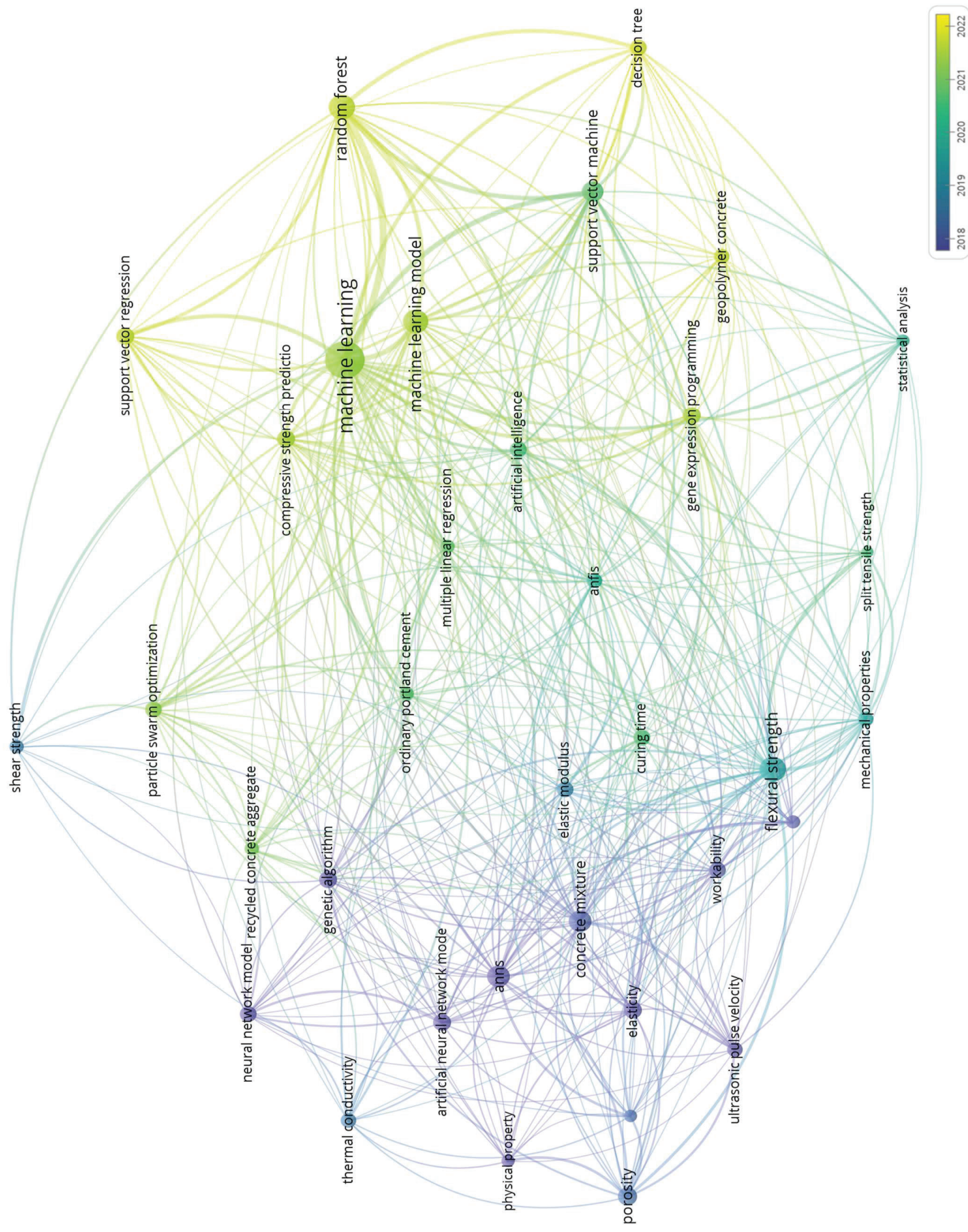

Figure 1. Cluster based on keywords (Overlay visualization).

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3. Methodology

The following methodology outlines the development of an ANN model for predicting the thermal conductivity of concrete based on its features, which enables the evaluation of the model potential to foresee this property and shows the efficiency in the prediction speed when compared to the time-consuming experiments, which will provide a reliable model to predict the concrete's thermal conductivity. This methodology is broken down into three steps (Figure 2).

The first one corresponds to the literature review and data collection of a diverse variety of concrete. Collecting the database is the primordial step in building the predictive model, as the ANN will learn from this data. If it presents an inadequate representation of the problem, the model cannot predict the property effectively, thus reducing the model's reliability. Furthermore, for the model to be representative, there must be a sufficiently large amount of data to ensure diversity. In this step, it is necessary to define the dependent and independent variables, that is, to recognize which properties affect the output response of the model. First, the model's inputs and outputs are defined according to the available data and the dependent variables. Then, the available data sets from the literature are organized in a CSV file to develop the ANN model. The second one is related to the general process of building the ANN model to predict thermal conductivity, i.e., the selection of an appropriate neural network architecture for the prediction task, defining the learning rate of the neural network, the number of hidden layers and neurons in each layer, and the metrics to find the best model for the dataset. The last step is analyzing a case study, where the dataset based on previously published works is plugged into the model to evaluate its accuracy. Besides that, a Generative Adversarial Network (GAN) is also developed for data augmentation to improve the model and guarantee a good prediction. Then, both neural networks are implemented to strengthen the final model. Figure 3 summarizes the key steps and the necessary data.

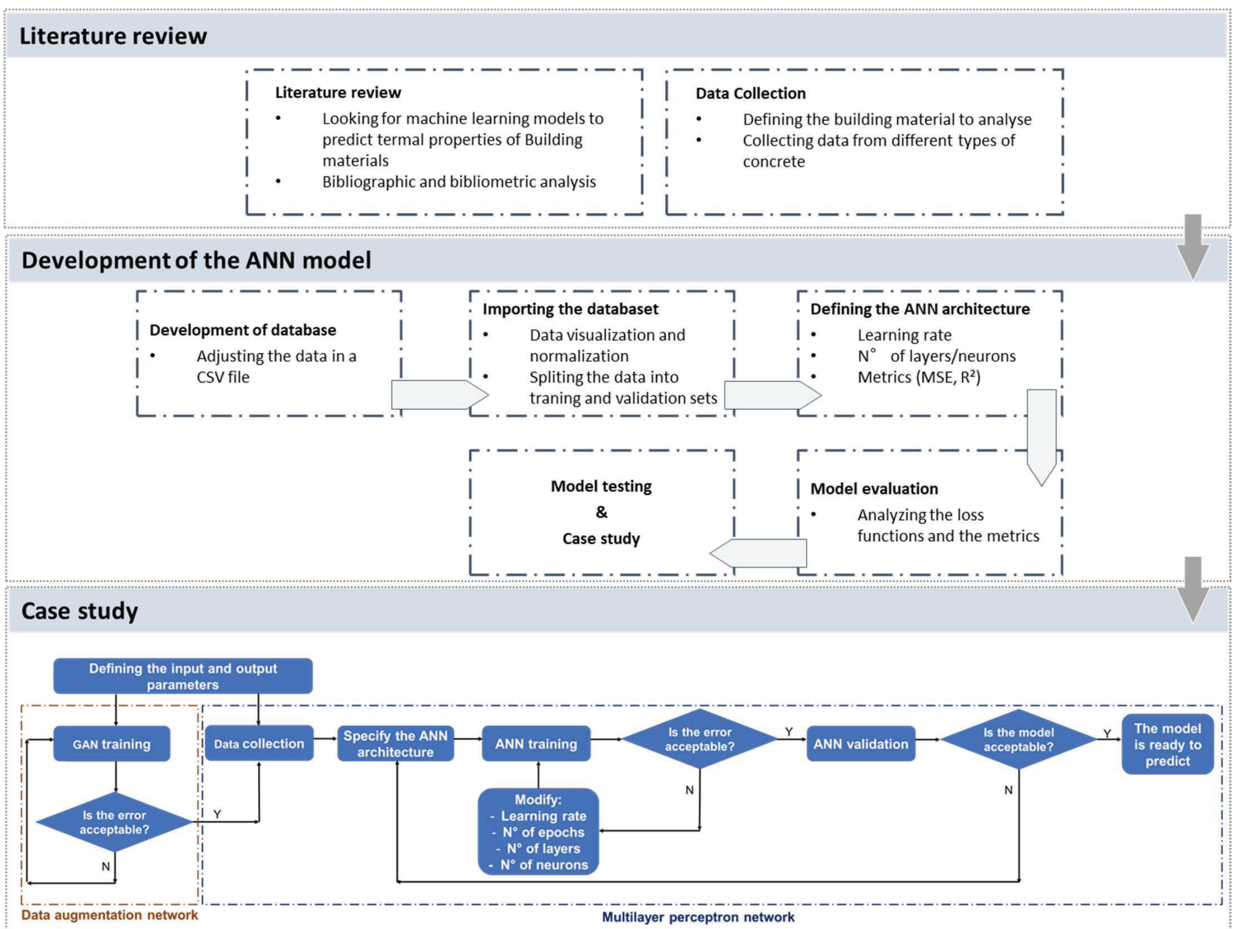

Figure 2. Methodology framework

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4. Case study

This case study demonstrates the potential for ANNs to improve the accuracy and efficiency of material property predictions, with important implications for energy-efficient building construction. The case study explores the use of ANNs to predict the thermal conductivity of different types of concrete.

4.1. Database

The database for developing the neural network model was obtained from the literature. This work conducted a comprehensive literature review to create a dataset of 200 points from various relevant articles published in the literature. Furthermore, in order to build an ANN model, data related to the composition and density of each type of concrete were collected and organized to plug into the model. Table 2 presents a sample of the training dataset obtained from the literature.

Table 2. Sample of the training dataset

Density	w/c	Water	Cement	Ceramic powder	Fine agg.	Coarse agg.	Nat. agg.	Fly ash	Silica Fume	Slag	Fiber	Adm.	Splast.	Foam Vol.	TC
1530	0,5	510	1020	0	0	0	0	0	0	0	0	0	0	0	0,6
1530	0,5	510	1020	0	0	0	0	0	0	0	0	0	0	0	0,7
1740	0,33	432	1308	0	0	0	0	0	0	0	0	0	0	0	0,9
1740	0,33	432	1308	0	0	0	0	0	0	0	0	0	0	0	1
2340	0,44	170	387	0	736	1115	0	0	0	0	0	0	0	0	1,1
2340	0,44	170	387	0	736	1115	0	0	0	0	0	0	0	0	1,3
2240	0,49	190	385	0	701	1096	0	0	0	0	0	0	0	0	1,3
2240	0,49	190	385	0	701	1096	0	0	0	0	0	0	0	0	1,4
2260	0,62	183	294	0	701	1236	0	0	0	0	0	0	0	0	1,6
2414	0,62	183	294	0	701	1236	0	0	0	0	0	0	0	0	1,7
1475	0,5	175	350	0	700	250	0	0	0	0	0	0	0	0	1,1
2042	0,5	292	583	0	1167	0	0	0	0	0	0	0	0	0	1,2
1475	0,5	175	350	0	700	250	0	0	0	0	0	0	0	0	1,3
3075	0,5	175	350	0	700	1850	0	0	0	0	0	0	0	0	1,7
1475	0,5	175	350	0	700	250	0	0	0	0	0	0	0	0	1,8
2358	0,48	145	242	0	707	1204	0	60	0	0	0	0	0	0	1,1
2358	0,48	145	242	0	707	1204	0	60	0	0	0	0	0	0	1,1
2358	0,48	145	242	0	707	1204	0	60	0	0	0	0	0	0	1,2
2358	0,48	145	242	0	707	1204	0	60	0	0	0	0	0	0	1,2
2358	0,48	145	242	0	707	1204	0	60	0	0	0	0	0	0	1,3
2349	0,37	161	439	0	621	1128	0	0	0	0	0	0	0	0	1
2349	0,37	161	439	0	621	1128	0	0	0	0	0	0	0	0	1,4

4.2. Artificial Neural Network Model

A neural network is a structure of layers of interconnected artificial neurons, which receive an initial input, process the information, and produce an output. Figure 3 represents a graphical representation of this mechanism. Each input (X_i) is multiplied by the weight (W_i) and summed with each other and added the bias value (b). Then, the result is transferred to the activation function, which adjusts the final output. The essential elements of a neural network are the inputs, outputs, artificial neurons, weights, activation functions, and hidden layers. According to the problem to be solved, these elements are varied until the model obtains outputs closer to the actual values. For example, and the activation functions, there are several possibilities, which are tangent sigmoid (tansig), linear (purelin), tri-angular basis (tribas), radial basis (radbas), and logarithmic sigmoid (logbas) [14]. During training, the complex relationships between the input data and the target values are trained to find specific patterns, and the weights are updated according to the learning technique until the predicted values reach a tolerance limit.

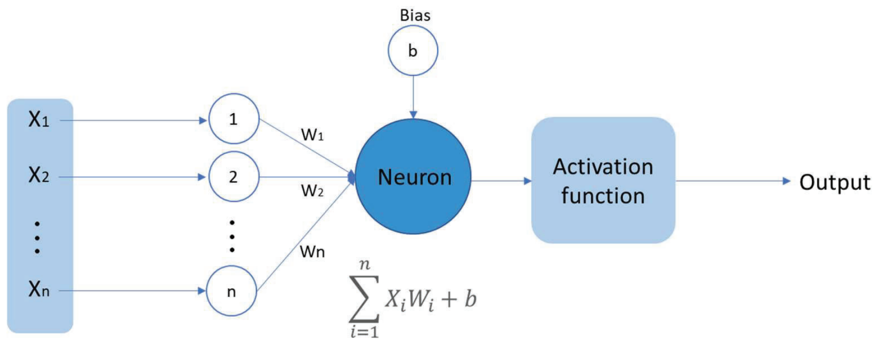

Figure 3. Graphical representation of a neuron

The developed artificial neural network model was built to predict the thermal conductivity of concrete based on chemical properties. To train the ANN with thermal conductivity as the output, this research utilized experimental data reported by previous researchers with thirteen parameters: the water-cement ratio, the unit water weight, the unit cement weight, the unit of ceramic powder, the unit fine aggregate weight, the unit coarse aggregate weight, the unit natural aggregate weight, the unit fly ash weight, the unit silica fume weight, the unit slag weight, the unit fiber weight, the unit superplasticizer weight, and density.

The ANN implemented was a Multilayer perceptron (MLP). It is a feedforward network that consists of an input layer, one or more hidden layers, and an output layer, as shown in Figure 4. Various combinations of network architecture were examined to evaluate the optimum model. The MLP model was built with an input layer with 13 neurons, some hidden layers varying the neurons in each layer, and 1 output layer with 1 neuron. In order to determine the best performance values, different activation functions, neuron numbers, and hidden layers were designed to perform the property prediction. This study tested different activation functions and used the backpropagation algorithm as the learning algorithm because it had been extensively used in previous studies.

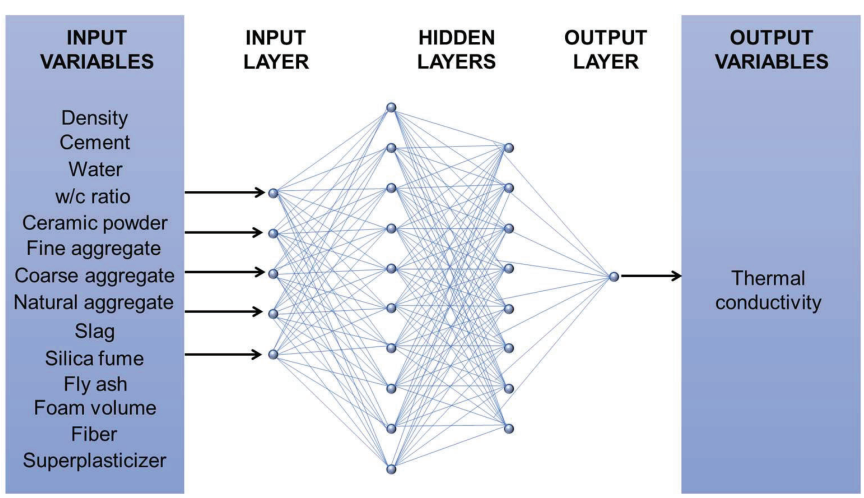

Figure 4. Example of the MLP model

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4.3. Generative Adversarial Network

A Generative Adversarial Network (GAN) aims to generate new data based on a real database. The GAN captures the distribution patterns of the real data and creates new examples from this distribution. Its framework comprises two distinct deep neural networks: the generator and the discriminator network, which work together to train the GAN to produce realistic data that are difficult to differentiate between the generated and the data (Figure 5). First, the generator initiates the process, which takes a random noise as an input, creating samples similar to the original dataset. Following this, the discriminator tries to distinguish the data and inform which ones are real or fake. During the training, the generator loss and the discriminator loss are evaluated, allowing the generator to get better and better at producing new artificial data and the discriminator to find if they are real.

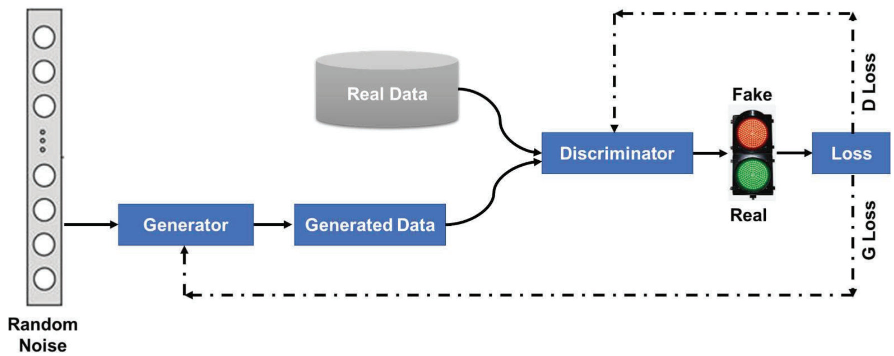

Figure 5. Flowchart of a Generative Adversarial Network (GAN)

5. Results

The first part of this study implemented an MLP model using Fastai, the most updated library to develop neural networks in deep learning. As previously mentioned, the model was developed to predict the thermal conductivity of concrete by utilizing the different compositions and densities as the input parameters.

Firstly, the dataset was plugged into the model and divided into two categories: training (80%), validating, and testing (20%), also used to train the GAN. Then, some features of the model were specified, such as the hyperparameters, metrics, activation, optimization, and loss functions. Table 3 summarizes the main features of this model.

For this study, some hyperparameters were varied during training to achieve the lowest value of the loss function and the highest values of the metrics selected. It used a combination of metrics to compare the model's overall performance. The chosen metrics were the Root Mean Squared Error (RMSE) and the coefficient of determination (R^2); both are frequently adopted to evaluate the prediction quality regarding the variations in the dataset. The learning rate and the number of epochs were kept fixed.

Table 3. Main features of the MLP model

Hyperparameters
Hidden layers = [1, 2, 3, 4]
Batch size = 32
Learning rate = 0.001
Epochs = 40
Metrics
RMSE

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R^2
Activation function
ReLU
Optimization function
Stochastic Gradient Descent (SGD)
Loss function
MSE

The numbers of the hidden layers and the neurons have been tested to determine the optimal structure of the ANN model. In order to select the best architecture, it was evaluated the loss function and the metrics. Table 4 displays some of the neural network architecture tested in this work. It can be observed that the best model presents a structure of 2 hidden layers with 200 and 100 neurons, achieving an RMSE of 0.111 W/m.K and R^2 of 0.984 for the training dataset. Regarding the test dataset, the metrics values were 0.183 and 0.96, respectively.

Table 4. Performance indices and metrics of the MLP model

Layers	ANN Architecture	Train Loss	Valid Loss	RMSE	R^2
4	200 – 100	0.083	0.012	0.111	0.984
5	200 – 100 – 50	0.107	0.024	0.155	0.968
5	200 – 100 – 40	0.099	0.037	0.192	0.950
5	200 – 100 – 30	0.087	0.028	0.167	0.960
5	200 – 100 – 20	0.012	0.037	0.191	0.949
6	200 – 100 – 50 – 25	0.102	0.064	0.253	0.918

To the best model evaluated, the loss function versus the number of epochs was analyzed, as seen in Figure 6. Although the number of epochs during the training was set as 40, we can observe the decreasing rate of the loss function over the epochs numbers, and after the setpoint, the loss function tends to be the smallest value in both datasets.

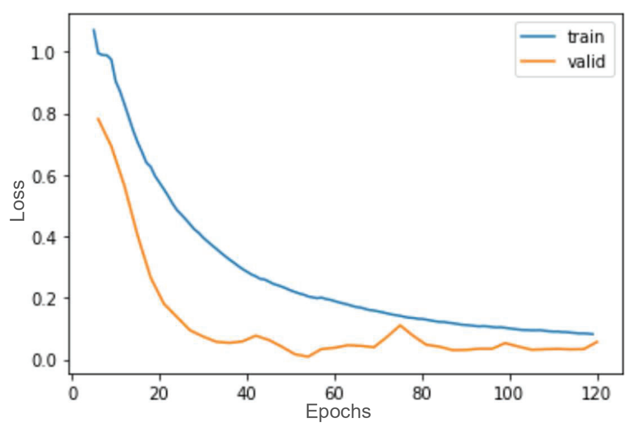

Figure 6. Loss function during the training

Comparing our results with previous works, although the model developed presents an accuracy as high as the other papers, this work brings a greater variety of the constituents of concrete. Fidan et al. [14], using a dataset with 132 entries, developed an ANN with an R^2 performance of 0.996. Sargam et al. [18], the only one to implement a neural network with a larger dataset, presented RMSE and R^2 of 0.117 and 0.964 for the training set and 0.215 and 0.894 for the validation set.

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The second part of the study considered the implementation of a GAN for data augmentation. As can be observed in Table 4, increasing the number of layers did not improve the model's learning capacity or performance. If we increase the hidden layers of the model with a small dataset, the model can overfit. For this reason, the metrics and the loss function exhibited higher values. In order to solve this issue, we intend to develop GAN to increase the dataset, creating new synthetic data based on the real data used to develop the MLP model. It will avoid the overfitting process and make the model more robust with extensive dataset training.

This part of the study is broken down into two steps. The first step of GAN training is the generation of a synthetic dataset, and the second is the integration of the MLP and GAN to train the model on both real and artificial datasets. The implementation of GAN used a specific library to create tabular data (Tabgan). The first result showed a promisor result with R^2 of 0.710. The next step of this work will include this new data and verify the performance of the MLP model and if the neural network structure will change.

6. Conclusion

Determining the thermal conductivity of concrete is vital to analyze the thermal behavior of the concrete. Nonetheless, the conductivity value depends on various variables, including composition, porosity, temperature, etc. Thus, a dataset containing the thermal conductivity values of concrete and other parameters related to its composition was developed from published works. This paper proposed a prediction methodology integrating a Multilayer Perceptron (MLP) and Generative Adversarial Network (GAN) models. The first part of the study showed that MLP predictions agree with the thermal conductivity values found in the literature, presenting RMSE and R^2 values of 0.183 and 0.96 for the validation dataset. Therefore, it can be used to predict thermal conductivity with high accuracy. Besides that, the first step of GAN indicated that it could generate reliable synthetic data to be included in the original dataset.

This work is part of a broader effort to develop a methodology for predicting the thermal properties of building materials using ANN. As the contribution of this study, the authors intend to demonstrate the feasibility of the proposed method to predict the thermal conductivity of different types of concrete and show that a GAN model can be used for data augmentation based on a small dataset and present a reliable model. Then, the ultimate goal of this research is to extend the model developed for concrete to other materials, thereby advancing the field of energy efficiency and enabling the development of new energy storage solutions that can meet the growing demands of the future. Additionally, integrating artificial intelligence techniques enhances the intelligence and feasibility of TES systems. By developing models that can predict thermal properties, researchers can improve the performance and efficiency of these materials, making them more effective and cost-efficient. Besides that, the ability to predict the thermal properties of building materials will also facilitate the development of new energy storage solutions that can meet energy demands, ensuring a more sustainable and energy-efficient future for the next generations.

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