

Mechanical Strength Prediction of Nano-Silica Concrete Composites Using Machine Learning Techniques

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Abstract

Nano-silica, or nanosilica, refers to silicon dioxide nanoparticles, which are a kind of silica (SiO_2) with diameters that often fall below 100 nanometers. This nanomaterial has attracted considerable attention because of its distinctive characteristics and diverse array of uses, notably in augmenting the performance of materials such as concrete. The integration of nanoparticles with cementitious matrix in nano-silica concrete offers a viable approach to improving the mechanical characteristics and longevity of concrete constructions. The use of machine learning (ML) techniques to forecast the strength properties of nano-silica concrete is investigated in this work. Machine learning (ML) methods provide a data-driven method for properly forecasting the compressive strength, flexural strength, and other pertinent mechanical parameters by making use of the inherent complexity of nanomaterial interactions inside the concrete matrix. Compiling a large dataset with different mix designs, nano-silica concentrations, curing settings, and testing parameters is the research's main task. After the dataset's significant features are extracted using feature engineering approaches, the model is subjected to validation, testing, and training phases. Regression models, support vector machines, artificial neural networks, and other machine learning techniques are tested to see which method works best for strength prediction. The impact of various hyperparameters and feature selection techniques on the models' prediction performance is also examined in this study. The findings show that machine learning (ML) based models show promise in precisely forecasting the strength characteristics of nano-silica concrete. This provides important information for mix design optimisation and improving the overall performance of concrete structures in construction applications.

Keywords: Concrete composites; mechanical properties; nano-silica; artificial neural network; machine learning techniques

INTRODUCTION

Nano-silica is mostly comprised of silicon dioxide (SiO_2), which is the same chemical component included in regular sand, quartz, and conventional silica used in diverse industrial procedures. Nevertheless, the minute size at the nano-scale confers unique characteristics that set it apart from its larger cousin. Silicon (Si) is the primary atom found in the silica molecule. Each silicon atom forms

covalent bonds with four oxygen atoms, resulting in a repeating structure of SiO_4 tetrahedra. The SiO_4 tetrahedra in nano-silica exhibit a high degree of organisation, but at a much-reduced size. Nano-silica displays distinct characteristics as a result of its diminutive dimensions and expansive surface area: The nanoscale dimensions of silica result in a substantially increased surface area compared to larger bulk forms, hence promoting greater reactivity and contact with other substances [1,2].

Nano-silica is often characterised by an amorphous structure, meaning it does not possess a

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well-defined crystalline order over long distance. This lack of crystallinity is responsible for its heightened reactivity. Nano-silica has enhanced reactivity due to its enlarged surface area and amorphous form, rendering it highly responsive in chemical reactions and effective as a reinforcing agent in composites. Nano-silica particles possess such minuscule dimensions that they do not disperse visible light, rendering them transparent in many applications such as coatings. Applications Specifically in the context of concrete, nano-silica is often used to improve the characteristics of the material [3,4]. It functions as a pozzolanic substance, chemically interacting with calcium hydroxide ($\text{Ca}(\text{OH})_2$) generated during the process of cement hydration. This reaction results in the formation of extra calcium silicate hydrate (C-S-H), which is the main component responsible for providing strength to concrete. The little particles fill the tiny empty spaces in the concrete structure, resulting in a more compact material with decreased permeability and enhanced longevity. Nano-silica improves the durability of concrete by enhancing its resistance to environmental damage, such as freeze-thaw cycles and chemical assault, by the refinement of pore structure and reduction of porosity [5,6].

Nano-silica is used in coatings due to its capacity to enhance scratch resistance, durability, and adhesion. Polymer composites are incorporated into polymers to enhance mechanical qualities, such as tensile strength and thermal stability. In the field of healthcare, nano-silica is being investigated for its biocompatibility, making it a promising candidate for drug delivery systems and as a diagnostic tool in medical applications. Nano-silica may be produced using a variety of methods: The Sol-Gel Process refers to the transformation of a liquid system, known as a "sol" (mostly consisting of colloidal particles), into a solid phase called a "gel". Flame Synthesis: The process of oxidising silicon tetrachloride (SiCl_4) in a flame result in the formation of nano-silica particles. Precipitation refers to the process of creating nano-silica particles by forming them from a solution that contains an excess amount of silica precursor. This is often followed by intentionally causing the particles to come together in a controlled manner [7,8].

Although nano-silica has several advantageous uses, it is crucial to take into account its potential effects on the environment and human health. The act of breathing in nano-silica particles might present potential dangers to the respiratory system, so it is crucial to follow certain procedures and use protective gear. The long-term environmental consequences of nano-silica are now being studied, highlighting the need for appropriate manufacture and disposal methods. Nano-silica, which is mostly made up of silicon dioxide, has distinct characteristics as a result of its very small size at the nanoscale and its large surface area. Due to its chemical reactivity and capacity to improve material characteristics, it is very beneficial in concrete technology, coatings, composites, and several other applications. Nevertheless, it is essential to effectively control the environmental and health consequences by using secure handling methods and practising responsible use [9,10].

Nano silica in concrete compositions improves mechanical qualities such as compressive strength, flexural strength, and abrasion resistance [11,12]. Nanoscale particles fill the holes and gaps in the concrete matrix, making the structures denser and more compact. This enhanced microstructure increases concrete's resilience and endurance, making it less prone to cracking, erosion, and deterioration over time [13,14]. The pozzolanic process of Nano-silica reduces the porosity and permeability of concrete, thereby preventing the intrusion of water, chloride ions, and other hazardous elements. As a result, concrete structures are more resistant to moisture penetration, chemical attacks, and embedded reinforcement corrosion [2,15]. Despite its tiny particle size, nanosilica improves dispersion and uniform distribution in concrete mixes. This enhances the workability and cohesiveness of new concrete, allowing for easier placing and compaction. Nano silica-modified concrete has improved rheological qualities, allowing construction professionals to produce smoother finishes and sharper detailing even in complex formwork designs [16,17]. Nano silica's capacity to modify the microstructure of concrete reduces the danger of thermal cracking caused by temperature differentials during hydration and curing [18,19]. Nano silica-modified concrete has better thermal stability and resilience to temperature-induced stresses because it has fewer capillary holes and faster hydration kinetics. This is especially useful in locations prone to adverse weather conditions. The use of nano

silica in concrete is consistent with sustainable building methods since it optimises material utilisation and reduces the total environmental impact of construction projects (20,21). The improved performance and durability of nano silica-modified concrete help to extend its service life, decreasing the need for frequent repairs, maintenance, and material replacement. Furthermore, the pozzolanic characteristic of nano silica allows for the partial substitution of cement, lowering greenhouse gas emissions connected with cement manufacturing. Nano silica is a game-changing development in concrete technology, providing a comprehensive approach to improving the performance, sustainability, and lifespan of concrete buildings. Its numerous benefits include increased strength, durability, workability, and environmental sustainability, making it an important addition to current building procedures [4,10,22].

Machine learning techniques have revolutionised several sectors in recent years, and construction is no different [23–25]. One especially intriguing use is estimating the mechanical characteristics of nano-silica concrete. Because of its distinct features, correctly evaluating nano silica's strength and other mechanical qualities is difficult. However, with breakthroughs in machine learning algorithms and data analytics, researchers and engineers can now construct strong models capable of accurately predicting these traits [26,27]. Machine learning is used to forecast the strength and mechanical qualities of nano silica concrete by using massive quantities of data, such as material compositions, mixing ratios, curing settings, and test results from experimental research. Machine learning algorithms may find complicated patterns and correlations in data that traditional analytical approaches may miss [28,29].

The adoption of machine learning techniques represents a paradigm change in our approach to concrete research and design. Rather of relying simply on empirical formulae or theoretical models, machine learning enables us to use data-driven insights to optimise concrete formulations, forecast material behaviour, and ultimately increase the performance and durability of nano-silica concrete structures [30,31]. These algorithms are trained on past data to understand the underlying correlations between input parameters and output variables, allowing them to make precise predictions for new data instances. Researchers and engineers may speed up material characterisation, save experimental costs, and accelerate the creation of novel concrete formulations by using machine learning approaches into the strength prediction of mechanical characteristics of nano silica concrete. Furthermore, these predictive models offer useful insights for optimising mix designs, improving quality control procedures, and assuring the long-term durability and sustainability of concrete buildings [32–34]. Overall, to forecast the mechanical characteristics of nano silica concrete is a huge step forward in materials science and construction engineering, providing new prospects for concrete innovation and optimisation [35,36].

Concrete design and construction rely heavily on compressive strength (CS) as a quality control metric. CS is widely used because to its ease of testing and strong association with other important metrics like as tensile strength and durability. Structural engineers use (CS) extensively in their design process [37]. Designing and producing concrete requires trial and error owing to its complexity and variability. Concrete's physical and chemical qualities vary greatly according to its many constituents, including as cement, water, SCMs, aggregates, and admixtures. Environmental variables like temperature and humidity may significantly affect the characteristics of concrete, making the problem more difficult. A strong predictive model can optimise mixes to fulfil design criteria and increase efficiency [38]. In comparison to prior methodologies, machine learning in concrete analysis allows for faster and more accurate processing of vast amounts of data. Engineers can save time and money by improving mix design and eliminating experimental testing. ML can reveal subtle linkages and correlations that traditional statistical methods may miss. Using machine learning to replicate the complex structure of concrete might be an effective way. To forecast the CS of concrete, a variety of machine learning models such as ANNs, SVMs, DTs, and RFs were utilised. A dataset of 625 experimental tests was analysed using machine learning algorithms (DT, RF, SVM, KNN, and ANN) [39]. Figure. 1 shows the model of multi-layer perceptions.

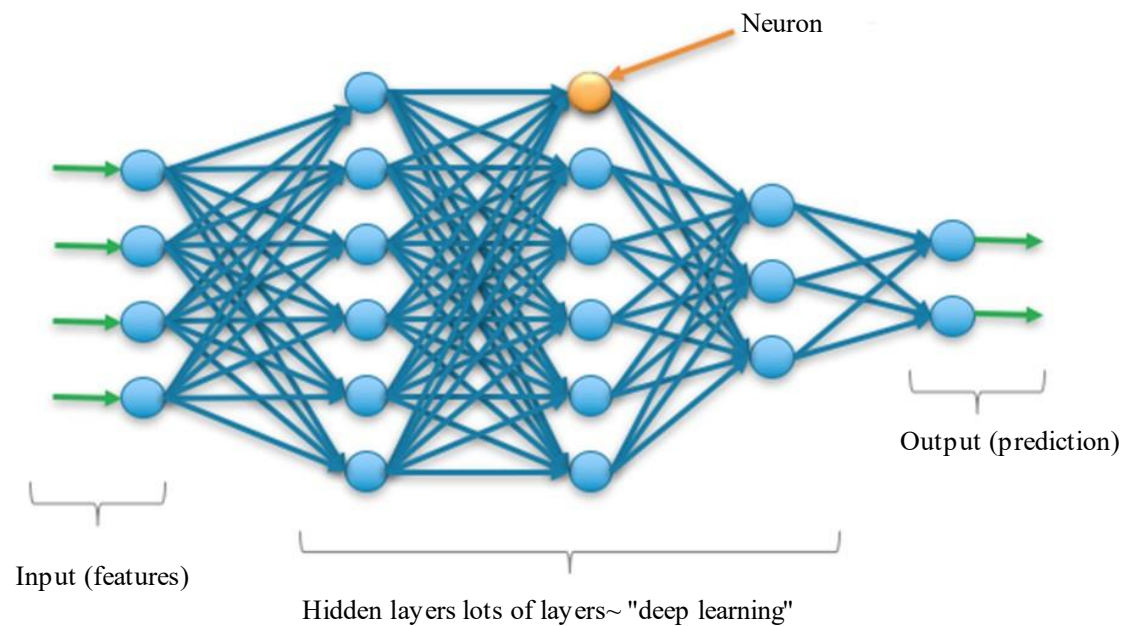


Figure 1. Multilayer perceptron (MLP) model.

Adding NS to the cementitious matrix hastens hydration and increases plasticizer demand, affecting the fresh and hardened characteristics and complicating the system. Because of the multiple factors that impact NS-modified concrete's mechanical properties, a comprehensive tool is required to investigate and estimate the output parameters [40,41].

RESEARCH SIGNIFICANCE

This work aims to use NS-modified concrete in order to increase the accuracy of CS, which would lead to more efficient design and cost reductions. When compared to traditional testing processes, these technologies provide speedy and accurate predictions while saving labour, time, and money. This approach eliminates the need for physical testing and instead use machine learning to enhance CS estimate in NS-modified concrete, resulting in more efficient and cost-effective building methods. Incorporating NS into concrete increases strength and durability, enabling sustainable construction techniques. The research seeks to improve durability and sustainability, offering a cost-effective and ecologically responsible option for the building industry.

METHODOLOGY

Concrete science procedures generally involve six phases of machine learning. The steps are: issue formulation, data gathering, pre-processing, model building, assessment, and deployment. ML models can help identify novel concrete compositions with desirable qualities. The mixes are validated using empirical or computer investigations [42]

Data Collection

This study analysed 1143 data points from 39 peer-reviewed research publications on the CS of concrete with NS. Datasets from each publication are included, along with the size and specific surface area (SSA) of the NS used in experiments. These factors influence CS significantly. The table describes the form of the specimens used in the investigations. This information is crucial for understanding the experimental setting and comparing findings across different studies. The database contains test results for cylindrical and cubic samples in various sizes. Before training and evaluating the model, the CS of cube samples of different sizes (100 mm, 150 mm) are translated to 150 mm cubes, and $\phi 100 \times 200$ mm and $\phi 150 \times 300$ mm cylinders are transformed to $\phi 150 \times 300$ mm. The $\phi 150 \times 300$ mm cylinders are converted to 150 mm cubes. All concrete samples' compressive strength (CS) was calculated as $150 \times 150 \times 150$ mm³. Figure 2 explains the flow of machine learning process.

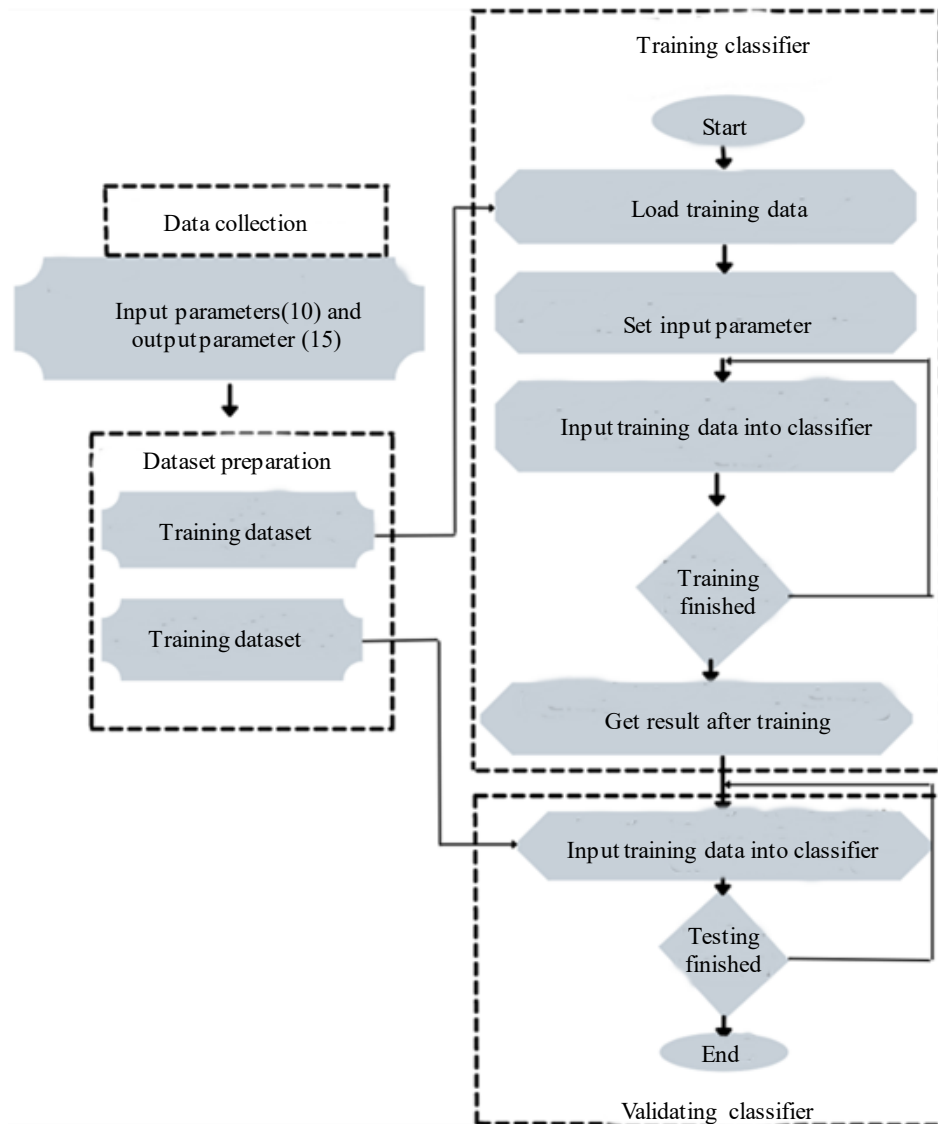


Figure 2. Flow of machine learning process.

A link was found between NS size and SSA, consistent with previous studies. To guarantee uniformity, studies with just the NS size were transformed to SSA values based on the correlation and utilised as parameters in the research. In pozzolanic materials, the SSA, not particle size, regulates the quantity and rate of reactant. Including the SSA grain size as a variable in models, rather than the NS grain size, was expected to improve predictive power.

The last diagram shows that many concrete samples have a compressive strength (CS) ranging from 20 to 80 MPa. Cement has an essentially typical distribution. NS has a left-skewed distribution, with most samples falling between 0 and 20 kg/m³. The data for W/B clusters around 0.4. To assess correlation, Pearson correlation coefficients are provided in the picture. The figure shows the expected negative connection between W/B and CS.

Despite a consistent W/B ratio, CS levels might vary significantly. The picture illustrates how the factors interact and impact the CS values. To establish which parameters, have the most and least impact on production, correlations between them must be determined. Using Pearson correlation, researchers may determine the factors that have the greatest influence on the intended output by analysing the size and direction of correlations between variables. This approach helps create reliable models. Table 1,

shows the mix design and statistical features of the output and input parameters. Python was used to code and optimise the models.

Table 1. Mix design.

Variables	Maximum	Minimum	Median	Mean	StD*
Cement (kg/m ³)	690	80	394	374.2	113.7
Water (kg/m ³)	246.7	104	180	174.9	24.1
FA (kg/m ³)	427.5	0	0	41.1	71
NS (kg/m ³)	60	0	5	6.9	8
GGBS (kg/m ³)	320	0	0	14.7	55.2
SF (kg/m ³)	80	0	0	3.2	10.5
C-Agg (kg/m ³)	1307	654	1058	1035.7	167
F-Agg (kg/m ³)	1063	472	725	757.8	137.2
W/B	0.73	0.2	0.41	0.42	0.1
Age (day)	365	1	28	33.4	43.8
SP (kg/m ³)	24.5	0	2.93	3.8	3.8
SSA of NS (m ² /g)	560	41	162	192	112.1
CS (MPa)	128.82	4.48	49	50.22	20.4

MACHINE LEARNING MODELS

AI and machine learning (ML) are gaining popularity across sectors due to their ability to improve efficiency and precision in operations. AI and machine learning (ML) may significantly enhance the outcomes and profitability of concrete-related operations. ML algorithms may build prediction models from empirical data without knowing the physical causes. These characteristics make them ideal for forecasting material qualities like concrete's CS, which are impacted by several inputs.

Artificial Neural Network (ANN)

ANNs are machine learning algorithms that mimic human brain structure and function. ANNs have shown promising results in regression and classification issues across several areas, is a typical method for learning. ANNs improve their neural connection weights to recognise patterns in the data. To train ANNs, input-output pairs are sent into the network and weights are adjusted until the desired output is achieved for each input.

After training, ANNs may accurately predict output for new input data. ANNs provide several benefits over traditional machine learning techniques. They can learn and maintain complicated patterns and relationships in enormous volumes of high-dimensional data. They can manage noisy and missing data.

Linear Regression (LR)

Linear regression (LR) is a fundamental statistical approach that is commonly used in predictive modelling, including predicting compressive strength in concrete. In the context of concrete, compressive strength is an important mechanical attribute that has a direct impact on structural integrity and performance. Linear regression provides an easy way to simulate the link between many factors impacting compressive strength and the actual strength values acquired from laboratory testing. This linear equation is often represented by a line or hyperplane, and its parameters are calculated using an optimisation approach to minimise the sum of squared errors between expected and ground actual values.

Decision Trees (DT)

Decision trees are supervised machine learning techniques that use a tree-like structure to anticipate desired output. Leaf nodes represent class labels and branches indicate related information. DT approach offers benefits such as ease of learning, interpretation, and visualisation. This strategy works

for both classification and regression issue and integrates decision-making techniques into the DT framework. DTs partition data into smaller sections according on input factors. The technique selects the best variable and splitting point to minimise error metrics like MSE. However, DTs are not without restrictions. Overfitting can occur when trees are too complicated or big. When applied to new data, this may result in poor generalisation performance.

Random Forest (RF)

RF is an ensemble approach that combines many DTs to create a more robust and accurate model, addressing overfitting issues. RF uses several DTs. This method reduces overfitting, increasing the model's ability to generalise. RF provides several advantages and benefits. Firstly, it demonstrates good accuracy, especially for huge databases. Furthermore, RF is quite easy and quick to deploy. Research has shown that RF is more accurate than other ML-based techniques. The number of trees significantly affects the accuracy of an RF model, as explained above.

Stochastic Gradient Descent (SGD)

SGD is a popular optimisation approach for training different models. The SGD Regressor excels at processing huge datasets in short batches, making it ideal for such circumstances. It provides flexibility by allowing users to pick suitable loss functions and penalties based on the regression problem.

Support Vector Machines (SVM)

SVM strategy improves model accuracy by focusing on errors over a preset threshold (ϵ). Vapnik developed this method, which is based on statistical learning theory. SVM is a valuable technique in machine learning since it uses hyperplanes to categorise information.

K-Nearest Neighbours (KNN)

Fix and Hodges created the KNN method in 1951, KNN predictions is strongly dependent on the distance and similarity functions used. In KNN regression, continuous variables are often represented by the Minkowski distance function (Eq. 7). Experimentation revealed that three neighbours provide the maximum accuracy ($R^2 = 0.84$) for the test set. We used an iterative algorithm to find the optimal model and number of neighbours. We created and trained KNN regression models for each neighbour count, and then calculated the R^2 score.

RESULTS AND DISCUSSIONS

Evaluate Accuracy

Prediction models may be evaluated using numerous approaches. This study assesses models using popular performance measures, including R^2 for both train and test sets, RMSE, MSE, and MAE. Metrics assess the accuracy of prediction models by comparing actual and anticipated values. The performance metrics for each model. Eq. 1 – 6 are used to calculate the errors between actual value and predicted values (Table.2)

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \bar{y}_i)^2 \quad (1)$$

Where $\bar{y}_i$ are the predicted value and y is true the value

$$R^2 = \frac{(n \sum x_i y_i - \sum x_i \sum y_i)^2}{(n \sum x_i^2 - (\sum x_i)^2)(n \sum y_i^2 - (\sum y_i)^2)} \quad (2)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |x_i - y_i| \quad (3)$$

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

$$RAE = \frac{\sum_{i=1}^n |x_i - y_i|}{\sum_{i=1}^n |x_i - (1/n) \sum_{i=1}^n x_i|} \quad (5)$$

$$RRSE = \sqrt{\frac{\sum_{i=1}^n (x_i - y_i)^2}{\sum_{i=1}^n (x_i - (1/n) \sum_{i=1}^n x_i)^2}} \quad (6)$$

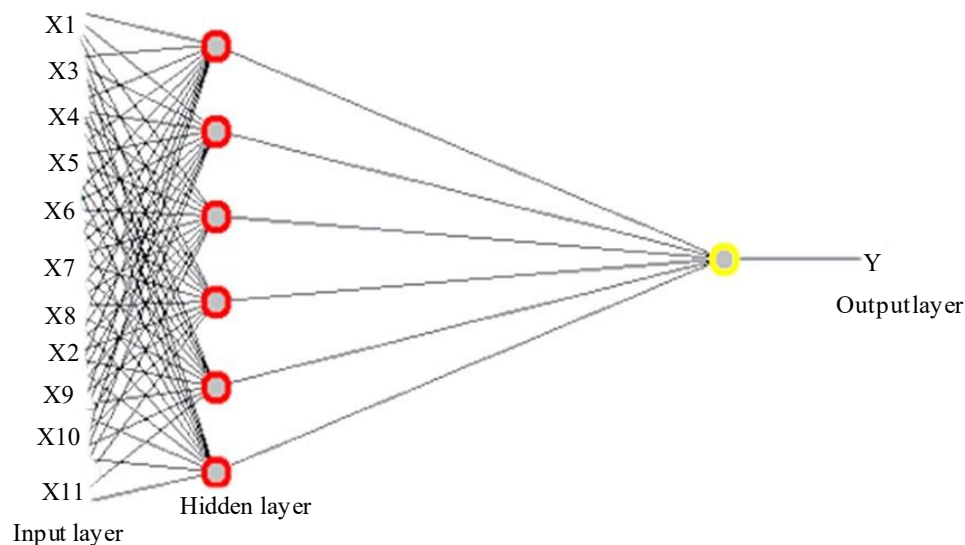
Table 2. Performance of various models.

Algorithm	MAE	MSE	Error (RMSE)	Accuracy (R2)	
				Train	Test
LR	9.83	181.1	13.5	0.61	0.52
DT	12.3	255	16	0.44	0.37
SVM	10.4	216	14.7	0.56	0.52
SGD	9.7	163.3	12.8	0.6	0.54
KNN	6.25	74.3	8.6	0.89	0.81
RF	3.5	26.05	5.1	0.99	0.93
ANN	3.94	31.87	5.6	0.97	0.92

The RF model outperformed the other techniques in terms of RMSE, R2, and accuracy, although they are similar. The RF and ANN models perform similarly and are equally suitable for calculating the CS of concrete. The nonlinear relationship between input parameters and CS may explain why LR models perform worse than others. All models with an R2 value over 0.85 are highly reliable in predicting the CS of NS-containing concrete. The dataset is complicated due to variances in laboratory settings, equipment, and NS dispersion strategies, as well as data from several areas with different climates and aggregate resources. An R2 value above 0.85 indicates a credible outcome. Figure 3 depicts the neural network prediction model.

Analyse The Relevance of Features

Each variable's importance score is determined using the permutation feature importance approach. This method neutralises the influence of each feature and assesses the model's reliance on it. This approach measures the impact of shuffled feature values on model performance, providing a more reliable assessment of feature relevance. Examining the influence of several elements on concrete's CS highlights their importance in model evaluation. The W/B is the most important element among the others. Following W/B, age and SP have significant roles. As W/B drops, increasing SP dose may have an influence on CS.

**Figure 3.** Neural network prediction model.

CONCLUSIONS

Estimating the compressive strength (CS) of concrete is challenging owing to factors such as ingredient type, dose, homogeneity, curing conditions, compaction, curing duration, ambient variables, and equipment employed. Adding NS to concrete mixtures complicates the situation, we may derive the following conclusions:

1. RF and ANN models exhibited the maximum accuracy in predicting the CS of concrete with NS, with R2 values of 0.93 and 0.92, respectively. Both models can predict CS with up to a 10% inaccuracy. These ratings are considered robust, given the complexity of the problem and the unpredictability of input factors.
2. As predicted, the LR model had the lowest dependability.
3. This study's dataset has a considerable impact on identifying the most crucial element determining the CS, as compared to other models in the literature.
4. The RF model's PDP suggests that an NS dose of 10 kg/m³ is best for obtaining desired characteristics.

This study's ML models were trained on a dataset from the literature; hence their capabilities are restricted. A larger data collection is necessary for more trustworthy models.

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