Civil Engineering Infrastructures Journal xx,xx
DOI: 10.22059/CEIJ.2024.364871.1956

Prediction of Compressive Strength of Geopolymer Fiber Reinforced Concrete Using Machine Learning

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Received: 11/09/2023
Revised: 02/01/2024
Accepted: 16/03/2024

Abstract: Geopolymers represent a cutting-edge class of inorganic materials that provide a sustainable substitute for conventional cement and concrete. Through meticulous combinations and ratios of elements like fly ash (FA), silica fume, ground granulated blast slag (GGBS), alkaline solutions, aggregates, superplasticizers, and fibers, geopolymer concrete mixes are generated as part of the experimental program. The investigation concentrates on predicting the 28-day compressive strength, a pivotal parameter in assessing concrete performance. The dataset comprises 96 data points, and two advanced techniques, namely Support Vector Regression (SVR) and Artificial Neural Networks (ANN), are harnessed for this research. The ANN demonstrates an R^2 value of 0.992 on the training dataset, indicating its capacity to elucidate around 99.2% of the variability. On the other hand, SVR boasts an R^2 value of 0.995, signifying an ability to account for about 99.5% of the variance. When applied to the testing data, the ANN achieves an R^2 of 0.96, while SVR attains an R^2 of 0.99. This study suggests that SVR exhibits slightly superior performance in elucidating variance within the testing dataset.

Keywords: ANN, Fly ash, GGBS, Soft computing.

Introduction

Reinforced concrete (RC) is a global construction material used worldwide, supported by a substantial global cement production, estimated to be approximately 4.6 gigatons (Gt) in 2015. Despite its widespread use and durability, RC structures can face challenges over time due to various factors, such as environmental exposure, chemical attack, or structural damage caused by external events (Jindal et al; 2023). Interventions are often necessary to maintain the load-carrying capacity and extend the service life of existing RC structures. Over the last few decades, externally bonded composite materials have emerged as an effective solution for rehabilitating and enhancing RC structures. Among these materials, fiber-reinforced cementitious matrix (FRCM) composites have gained significant attention as an alternative to traditional fiber-reinforced polymer (FRP) composites (D'Antino et al. 2014; Tayeh et al. 2021; Wong 2022). Both FRCMs and FRPs consist of continuous high-strength fibers embedded within a matrix, but they differ in the composition of the matrix material (Wang et al. 2009).

Furthermore, FRCMs exhibit excellent compatibility with concrete, which promotes a strong bond between the composite material and the existing structure (Carloni et al. 2015). Alkali-activated materials are a diverse group of inorganic materials that include a novel category known as geopolymers (Qaidi et al. 2022). These materials not only provide alternatives to traditional cement-based products but also mitigate environmental impacts by reusing industrial byproducts and reducing carbon emissions (Kumar et al. 2023).

Polypropylene fibers (Althoey et al. 2023; Tayeh et al. 2022) are commonly utilized to control cracking in concrete, but they may not be ideal for geopolymer composites due to this weak interaction. Steel fibers are a popular choice for reinforcing cementitious composites. Steel fibers' tensile strength and ultimate elongations can vary significantly, ranging from 310-2850 MPa and 0.5-3.5%, respectively (Al-Majidi et al. 2017; Sukontasukkul et al. 2018; Wang et al. 2018). The corrugated surface enhances the interaction between the steel fibers and the binder, improving the composite material's performance and strength (Wang et al. 2018; Yin et al. 2015). One significant application of recycled synthetic fibers lies in the construction industry, offering an effective solution for disposing of commonly consumed plastics like polyethylene terephthalate (PET) and polypropylene (PP) on a global scale (Siddique et al. 2008). Among the synthetic fibers used in construction PP, polyvinyl alcohol (PVA), polyethylene (PE), and PET are the most prevalent ones(Farooq et al. 2019; Mastali et al. 2018; Ranjbar et al. 2016; Sukontasukkul et al. 2018). PP, derived from the monomeric C_3H_6, is a cost-effective option with inert characteristics in high pH cementitious environments(Farooq et al. 2019). It helps control plastic shrinkage cracking in concrete and allows for easy dispersion (Larena and Pinto 1993). It does have drawbacks such as poor thermal resistance, low modulus of elasticity, and difficulty in forming a strong bond with cementitious matrices due to its inherent hydrophobic nature(Banthia and Gupta 2006; Mu et al. 2002; Yin et al. 2015). On the other hand, PET fibers, produced by recycling PET bottles, exhibit mechanical properties comparable to PP and nylon fibers while being more cost-effective and environmentally friendly to produce (Ochi et al. 2007).

Soft computing (SC) is an effective approach for addressing complex problems, particularly when mathematical models struggle to express relationships among parameters. SC offers a notable advantage in solving nonlinear and linear problems by accommodating intricate relationships that may be challenging to model mathematically (Ghanbari et al. 2017). A key strength of SC lies in its ability to incorporate human-based knowledge, recognition, understanding, and learning into computational processes (Vadel et al. 2019). In recent years, researchers have increasingly harnessed artificial intelligence (AI) methods and machine learning (ML) techniques as integral components of SC in predicting various properties of concrete. AI and ML, as sub-branches of SC, bring advanced computational capabilities to the forefront (Shariati et al. 2022).

However, accurately predicting the compressive strength of geopolymer concrete (GPC) poses challenges due to the significant influence of physical and chemical variables. Fortunately, AI and ML have emerged as promising solutions to enhance accuracy and efficiency in predicting concrete strength (Naghibzadeh et al. 2022). While traditional regression methods lacked accuracy, ML methodologies have significantly improved predictions, the advanced techniques such as genetic engineering programming (GEP), SVR, ANN, and ensemble approaches (Sahu et al. 2023). SVR constructs hyperplanes that best separate data points based on their features, enabling it to make precise predictions (Li et al. 2022; Shariati et al. 2022). Its ability to handle high-dimensional data and capture nonlinear relationships has made SVR a popular choice in concrete strength estimation. Inspired by the human brain's functioning, ANN is a deep learning technique capable of learning and generalizing from large datasets (Kaveh and Khavaninzadeh 2023). As ANN layers process and transform input data, the model comprehensively understands the relationships between variables, leading to highly accurate predictions. Ensemble approaches combine multiple models to improve predictive accuracy by leveraging the strengths of individual algorithms (Huang et al. 2023).

The primary aim of the current research is to create models that can predict experimental data by utilizing two specific techniques: SVR and ANN. The focus of this study is centered around geopolymer concrete, a unique type of concrete made from components such as FA, silica fume, GGBS, as well as polyvinyl alcohol fiber (PVA) and steel fiber. To evaluate the effectiveness of the prediction models (SVR and ANN), the parameter chosen for analysis is the compressive strength of the geopolymer concrete after a curing period of 28 days. This 28-day compressive strength is a critical indicator of the concrete's performance and durability. By using the SVR and ANN models, the study aims to establish accurate predictions of this compressive strength based on the specific combinations of materials used in the geopolymer concrete.

Materials and Data Demonstrations

The experiment involves the development of a novel type of concrete called geopolymer hybrid fiber-reinforced concrete. This concrete is designed to have enhanced strength and durability by combining various materials and fibers. The main components used in this experiment are FA, Silica fume, GGBS, alkaline solutions, fine and coarse aggregates, superplasticizers, and a hybrid combination of steel fiber and polyvinyl alcohol (PVA) fiber. Concrete relies on binding agents to ensure that its components are properly linked together. In addition to binding materials, concrete also contains fine and coarse aggregates like sand and gravel. The experimental program involves creating different concrete mixes by varying the proportions of these materials. The specific combinations and ratios of FA, Silica fume, GGBS, alkaline solutions, aggregates, superplasticizers, and hybrid fibers are detailed in Table 1 of the experiment. This mix design is a roadmap for producing batches of geopolymer hybrid fiber-reinforced concrete with consistent and controlled properties.

Table 1. Mix design of the experimental program

Mix Designations	P0S1	P0S2	P0S3	P1S4	P1S0	P2S0	P3S0	P4S0
FA	585	585	585	585	585	585	585	585
Silica fume	32.5	32.5	32.5	32.5	32.5	32.5	32.5	32.5
GGBS	32.5	32.5	32.5	32.5	32.5	32.5	32.5	32.5
Na_2SiO_3	156	156	156	156	156	156	156	156
NaOH	104	104	104	104	104	104	104	104
Fine Aggregate	850	850	850	850	850	850	850	850
Coarse Aggregate	800	800	800	800	800	800	800	800
Super Plasticizer	10	10	10	10	10	10	10	10
Polyvinyl Alcohol Fiber	0	0	0	0	0.10%	0.20%	0.30%	0.40%
Steel Fiber	0.10%	0.20%	0.30%	0.40%	0	0	0	0

*P1S0 = Polyvinyl alcohol fiber 0.1% and Steel fiber 0%.

ML approaches necessitate a diverse set of input variables (Wang et al. 2018). These input variables and the corresponding outputs are derived from an experimental program. This specific study focuses primarily on predicting the 28-day compressive strength, a critical parameter for evaluating concrete performance. The models employed for this purpose involve a selection of input variables, and their correlation with the 28-day compressive strength is investigated. The chosen input variables encompass a variety of factors that contribute to the properties of the concrete mixture. These variables include cement, water, sand, coarse aggregate, superplasticizer, silica fume, FA, alkali/binder ratio, steel fiber, and PVA fiber. Each of these variables plays a distinct role in shaping the characteristics of the final concrete product.

The dataset used in this study comprises 96 data points, each representing a specific combination of input variables and the corresponding 28-day compressive strength. These data points serve as the basis for training and testing the ML models.

Table 2 presents a comprehensive summary of the statistical analysis conducted on the input variables. The statistics presented in the table include the mean, standard deviation, minimum value, and maximum value for each input variable. These statistics collectively offer a thorough understanding of the variability and central tendencies within the input dataset.

Table 2. Statical description of input variables

	Total	Mean	SD	Min.	25%	50%	75%	Max.
FA	96	552.5	26.67	520	520	552.50	585	585
GGBS	96	48.75	13.34	32.5	32.5	48.75	65	65
Silica fume	96	48.75	13.34	32.50	32.50	48.75	65	65
NaOH	96	110.6	14.61	91	100.50	110.50	120.3	130
Na_2SiO_3	96	165.75	21.92	136.50	151.13	165.75	180.4	195
Coarse aggregate	96	850	0	850	850	850	850	850
Fine aggregate	96	800	0	800	800	800	800	800
alk/b	96	0.425	0.056	0.35	0.3875	0.425	0.46	0.50
Superplasticizer	96	10	0	10	10	10	10	10
Polyvinyl alcohol fiber	96	0.125	0.14	0	0	0.05	0.2	0.40
Steel fiber	96	0.125	0.14	0	0	0.05	0.2	0.40
Compressive Strength	96	38.81	8.56	21.56	32.26	38.46	44.25	58.8

Methodology

In this study, ML models were employed to estimate the compressive strength of a material, and these models were implemented using Python code through the Anaconda software platform. Anaconda Navigator is a hub for accessing Python and other programming languages crucial for data science and machine learning applications. It emphasizes activities like package development and maintenance to support these tasks effectively. The study employed three distinct techniques, namely ANN and SVR, to predict the compressive strength of a material. These techniques are widely used in ML for regression tasks, where the goal is to predict a continuous numerical output. To assess the accuracy of the predictions generated by these models, the R^2 was utilized. The R^2 value is a metric that ranges from 0 to 1, with higher values indicating better alignment between the predicted outcomes and the actual measured values. Furthermore, the study conducted rigorous evaluations to gauge the models' performance. This involved statistical checks and error assessments, including Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE). These metrics offer insights into how well the models' predictions align with the actual data by measuring the average magnitude of errors. A lower MAE and RMSE indicate better predictive accuracy and a smaller deviation between predicted and actual values.

The data set is generated from the experimental programs. The process involved organizing a dataset into two subsets: a training set and a test set. In the 70-30 data split, a dataset is partitioned into two subsets: 70% is allocated for training a model, and the remaining 30% is reserved for testing the model's performance. Each example in these sets was broken down into individual instances of input features, also known as independent variables, which were associated with a specific target or dependent variable to be predicted. The input features utilized in this analysis were chosen to represent quantifiable aspects that experiments could measure. These features were carefully defined and structured to provide an advantageous learning environment for the various models being evaluated (Fig. 1). This structured setup ensured that the models could learn effectively from the data. The ANN underwent a process of manual fine-tuning to achieve a reasonable level of accuracy in predicting the target variable. This fine-tuning process involved adjusting the model's internal parameters and architecture to minimize prediction errors and enhance performance. Subsequently, the hyperparameters of the ANN were determined based on the outcomes of this initial manual fine-tuning (Pratap et al. 2023). Hyperparameters are settings external to the model but influence its learning process. SVR aims to find the optimal function that best captures the underlying patterns in the data while maintaining a certain margin of error. The fundamental idea is to identify a hyperplane that effectively fits as many data points as possible within a specific epsilon (ε) tube, where the goal is to minimize the deviation of data points from the predicted values while allowing for a controlled tolerance. SVR employs a mathematical approach to determine the optimal hyperplane by solving a constrained optimization problem. One of the strengths of SVR is its ability to handle non-linear relationships between variables by utilizing kernel functions. These functions transform the original feature space into a higher-dimensional space, enabling the algorithm to capture complex patterns that might not be apparent in the original data.

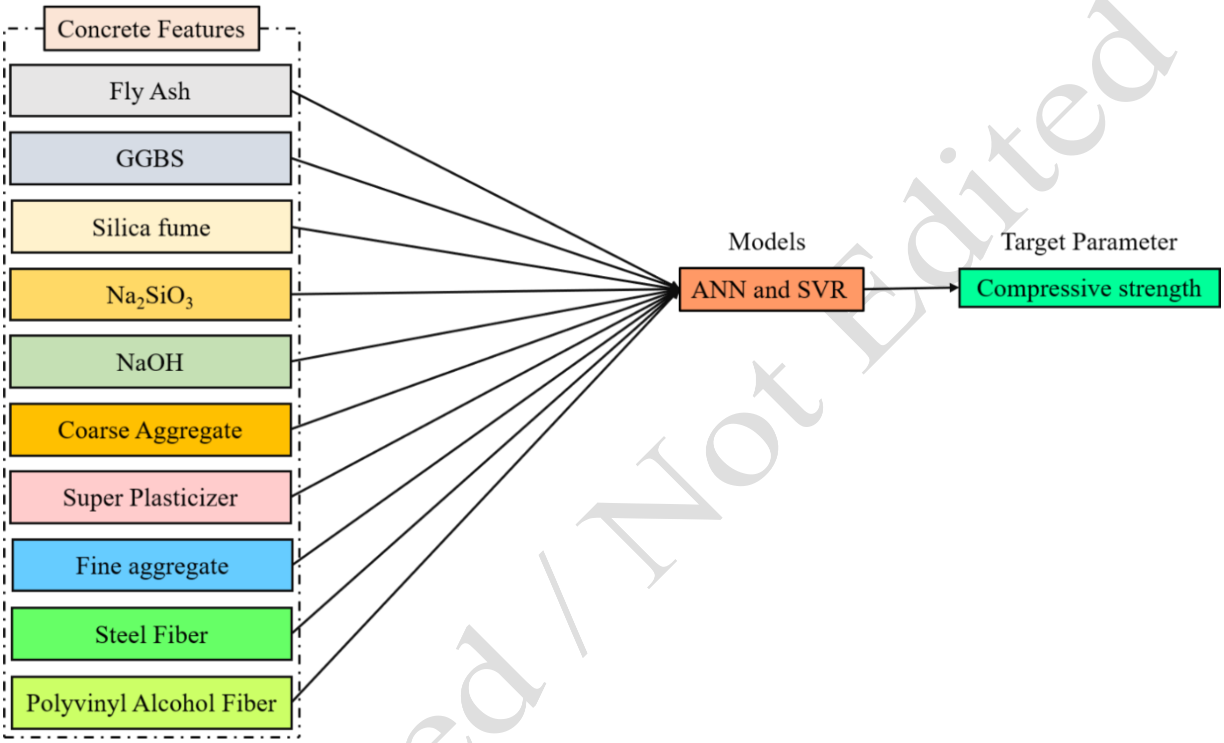
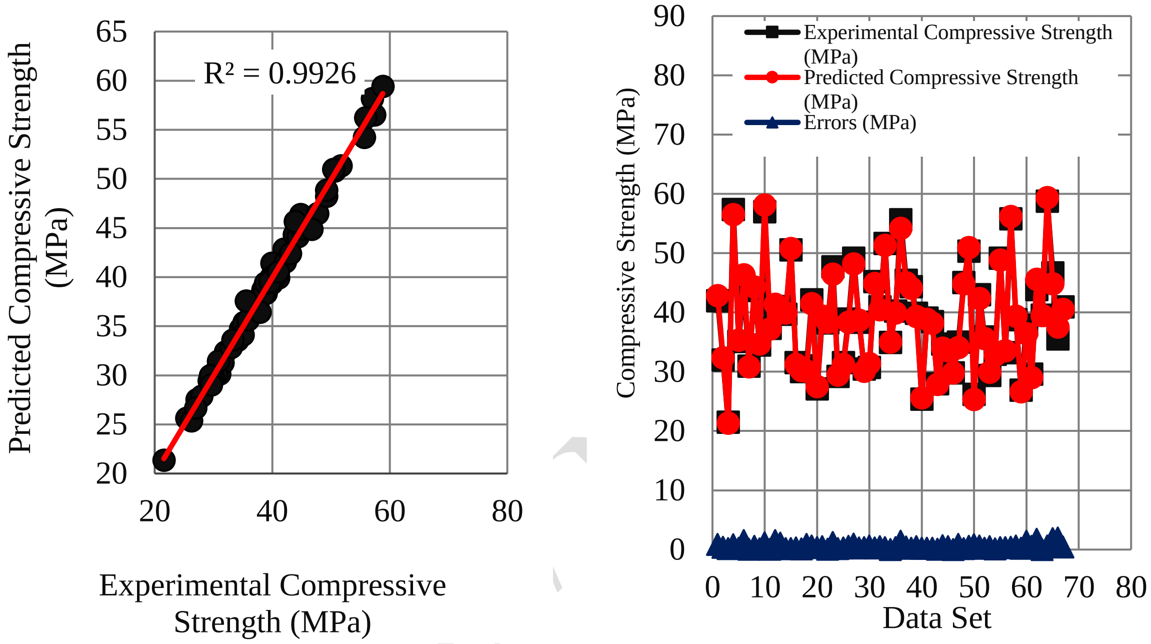


Fig.1. An input and output roadmap for the ANN and SVR algorithms

Results and discussions

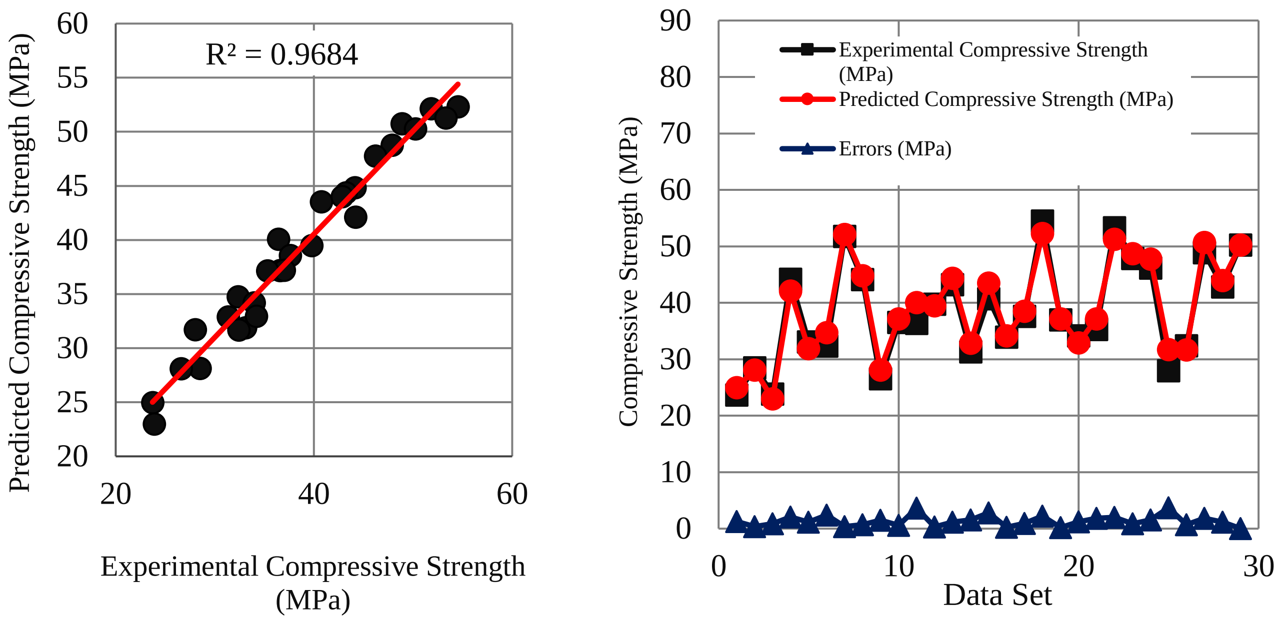
The study evaluates the predictive accuracy of the ANN model by comparing its predicted outcomes to the actual measured compressive strengths. The analysis involves two main aspects: the statistical comparison pattern and the model's performance metrics. In terms of statistical analysis, the study assesses the pattern of outcomes obtained from the actual testing of geopolymer concrete samples and the predictions made by the ANN and SVR models.

The R^2 value serves as an indicator of how well the model's predictions match the actual data. In this case, the R^2 value of 0.9924 for training and 0.9672 for testing signifies an excellent performance of the ANN model in accurately calculating the compressive strength outcomes. Figures 2(a) and 3(a) visually represent these high R^2 values, highlighting the closeness of the model's predictions to the real data points. On the other hand, Figures 2(b) and 3(b) provide a graphical depiction of the distribution of the investigated outcomes compared to the estimated outcomes by the ANN model. These figures allow for a direct comparison, revealing the model's efficacy in capturing the trend of the actual outcomes. The study also addresses the errors associated with the ANN model's predictions. This study analyzes the spread of errors in terms of the largest, lowest, and average error values. For the training phase, the largest error is 2.003 MPa, the lowest error is 0.0314 MPa, and the average error is 0.5646 MPa. Similarly, for the testing phase, the largest error is 3.69 MPa, the lowest error is 0.028 MPa, and the average error is 1.356 MPa.



(a) (b)

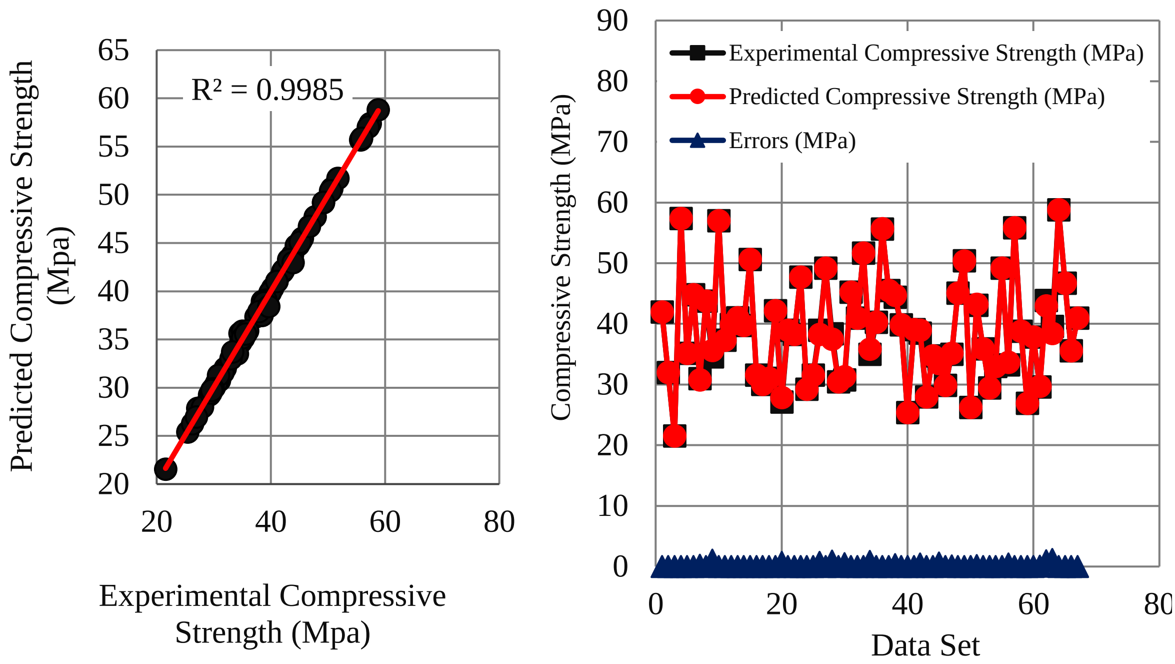
Fig. 2. (a) Relation between experimental and predicted values for training model of ANN (b) Distribution of experimental, predicted and error values for training model of ANN



(a) (b)

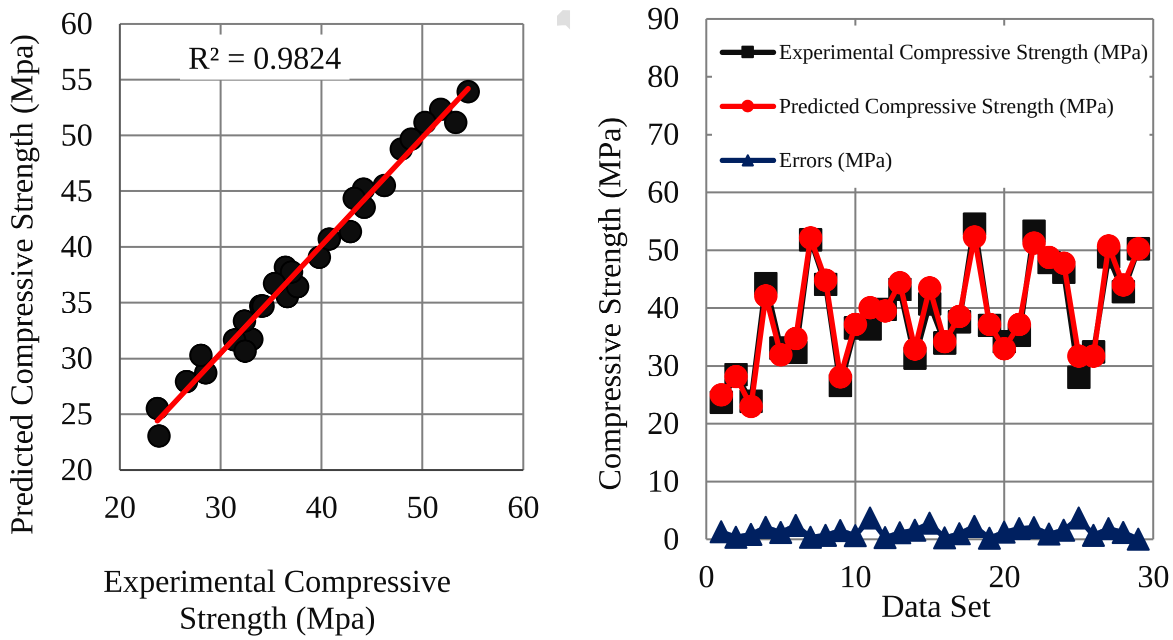
Fig. 3. (a) Relation between experimental and predicted values for a testing model of ANN (b) Distribution of experimental, predicted and error values for a testing model of ANN

The SVR model demonstrates exceptional performance in accurately predicting compressive strength outcomes, as evidenced by high R^2 values of 0.9985 (Fig. 4a) for training and 0.9908 (Fig. 5a) for testing. These values highlight the strong alignment between the model's predictions and actual data points. This closeness between predicted and real values is visually represented in the figures. Conversely, Figures 4(b) and 5(b) visually illustrate how the SVR model's estimated outcomes compare to the investigated outcomes. This direct comparison underscores the model's ability to capture the underlying trends in the actual data (Li et al. 2022). The study also delves into the errors associated with the SVR model's predictions, examining their distribution (Sahu et al. 2023). The analysis of error distribution entails the consideration of the largest, smallest, and average error values. During the training phase, the most significant error observed is 1.164 MPa, while the smallest error is 0.00053 MPa, and the average error is 0.1389 MPa. Similarly, in the testing phase, the largest error amounts to 2.287 MPa, the smallest error is 0.152 MPa, and the average error is 1.0366 MPa.



(a) (b)

Fig. 4. (a) Relation between experimental and predicted values for training model of SVR (b) Distribution of experimental, predicted and error values for training model of SVR



(a) (b)

Fig.5. (a) Relation between experimental and predicted values for the testing model of SVR (b) Distribution of experimental, predicted and error values for a testing model of SVR

The table 3 present the performance metrics of two different machine learning algorithms, ANN and SVR, on a dataset. These metrics are commonly used to evaluate the quality of predictive models. This column simply lists the two machine learning algorithms being compared, which are ANN and SVR. These are different techniques used for regression tasks, where the goal is to predict a continuous numerical output. The ANN has an R^2 of 0.992 on the training set, indicating it explains about 99.2% of the variance, and SVR has an R^2 of 0.995, indicating it explains about 99.5% of the variance. Both values are very high, suggesting strong performance on the training data. ANN has an RMSE of 0.73, while SVR has an RMSE of 0.32. Lower RMSE values indicate better model accuracy, so SVR is performing better on the training data in this regard. ANN has an MAE of 0.56, and SVR has an MAE of 0.13. Again, lower MAE values indicate better accuracy, and SVR has a lower MAE, suggesting better performance on the training data. ANN has an R^2 of 0.96 on the testing data, while SVR has an R^2 of 0.99, indicating that SVR performs slightly better in terms of explaining variance in the testing data. ANN has an RMSE of 1.65, and SVR has an RMSE of 0.81. Again, lower RMSE values are better, so SVR outperforms ANN on the testing data. ANN has a MAE of 1.35, while SVR has a MAE of 0.53. Like RMSE, lower MAE values indicate better accuracy, and SVR is more accurate on the testing data.

Table 3: Training and testing results data

Algorithms	Training			Testing		
	R^2	RMSE	MAE	R^2	RMSE	MAE
ANN	0.992	0.73	0.56	0.96	1.65	1.35
SVR	0.995	0.32	0.13	0.99	0.81	0.53

Conclusions

This research successfully demonstrates the development of geopolymer concrete through a combination of fibers, FA, and GGBS as precursor materials. Elaborate prediction studies are conducted involving partial replacement of FA with GGBS and silica fume. The conclusions drawn from the results and interpretations can be summarized as follows:

- The performance of the prediction models is assessed using the coefficient of determination (R^2). The ANN achieves an R^2 of 0.992 on the training set, explaining approximately 99.2% of the variance, while the SVR obtains an R^2 of 0.995, explaining about 99.5% of the variance. On the testing data, the ANN's R^2 is 0.96, whereas the

SVR's R^2 is 0.99. This indicates that SVR slightly outperforms ANN in terms of explaining variance in the testing data.

- The analysis of error distribution involves assessing the largest, smallest, and average error values. During the training phase, the most significant error observed is 1.164 MPa, while the smallest error is 0.00053 MPa, and the average error is 0.1389 MPa. Similarly, in the testing phase, the largest error amounts to 2.287 MPa, the smallest error is 0.152 MPa, and the average error is 1.0366 MPa.
- Overall, both models demonstrate strong performance on the training data, with SVR having a slight advantage in terms of RMSE and MAE. However, when applied to unseen testing data, SVR maintains its superior performance in terms of RMSE, MAE, and R-squared, suggesting that SVR is the more suitable model for this specific dataset. The importance of evaluating a model's performance on both training and testing data is highlighted by the results presented in this table.

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