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Interpretable Machine Learning and PSO-Based Optimization for Predicting the Mechanical Performance of Steel Fiber-Reinforced Recycled Aggregate Concrete: A Dual Focus on Compressive and Splitting Tensile Strengths

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ABSTRACT

The study selected Multilayer Perceptron (MLP), Gaussian Process Regression (GPR), and Extreme Gradient Boosting (XGBoost) as the ML algorithms to develop models that estimate the compressive strength (fcu) and splitting tensile strength (fsp) of steel fiber-reinforced recycled aggregate concrete (SFR-RAC). The study had 465 compressive strength and 339 splitting tensile strength samples from concrete mixes with contrasting proportions. The training and evaluation of models used an 80/20 split, and their hyperparameters were improved through Particle Swarm Optimization (PSO). Assessing how well the models work was done with four statistical measurements: coefficient of determination R^2, mean absolute error (MAE), root mean squared error (RMSE), and mean absolute percentage error (MAPE). XGBoost could predict outcomes more effectively than any model, and RF or MLP were close behind. To find out how the inputs affect the model results, feature importance analysis and SHapley Additive exPlanations (SHAP) were carried out. It was shown that the water content, the amount of cement, and the proportion of fibers in the concrete all affect its strength. These proposed models explain in detail how SFR-RAC mixtures work, which helps create environmentally friendly concretes with outstanding strength. Later research could use more data and predictor variables to see if these models apply well.

INTRODUCTION

In recent years, there has been an increased demand for the construction industry to use sustainable practices to help the environment and use resources wisely. Another method worth considering is recycled aggregate concrete (RAC), which replaces part or all the natural aggregate with demolished concrete. By using this method, we cut down on landfill waste and conserve nature, in support of global goals for sustainability (Zhang *et al.,* 2020). Even though RAC helps the environment, it usually performs less well mechanically than NAC, chiefly because recycled aggregates are not as uniform and may still contain some contaminants.

A significant drop in compressive strength, as well as decreases in splitting tensile strength and elastic modulus, is reported in studies about Recycled Asphalt Concrete (RAC) (Kou *et al.*, 2007; Yang, 2014). Extensive steel fiber addition created steel fiber-reinforced recycled aggregate concrete (SFR-RAC) to make RAC perform better mechanically. Using steel fibers leads to better crack resistance, strength, and the ability to withstand pressure, reducing any harmful effects from recycled aggregates (Zhang *et al.*, 2023; Chen *et al.*, 2022).

Liu *et al.* (2023a) and Li and Ma (2017) show that including steel fibers results in better performance against compression, tension, fatigue, and impact, suggesting SFR-RAC is a good choice for structures that need improved durability and flexibility. However, it is not easy to predict the strength of SFR-RAC because of the nonlinear connections among fiber, aggregate, water, and binder. People typically test SFR-RAC in a lab and look at empirical data to describe their mechanics (Gao *et al.*, 2017; Carneiro *et al.*, 2014).

They may give us helpful information, but the process is costly, requires a lot of time, and has restrictions because of differences in materials and mixing. Also, empirical models cannot capture all the complex relationships in material behavior, making them less suitable for use with various mixes and conditions (Ge *et al.*, 2021).

ML has played a significant role in modeling and anticipating complicated engineering processes, allowing for dealing with extensive data sets, uncovering patterns, and going beyond traditional models' limitations. Artificial neural networks (ANN), support vector machines (SVM), Gaussian process regression (GPR) and ensemble approaches such as extreme gradient boosting (XGBoost) have proven helpful in predicting the strength and other properties of concrete and construction materials (Mawlood *et al.*, 2021; Gong *et al.*, 2023; Uddin & Lu, 2024).

They are experts at recognizing how certain features interact, allowing them to forecast results more accurately than traditional regression. Practical search algorithms such as Particle Swarm Optimization (PSO) are often used to help optimize the hyperparameters of ML models and boost their performance and stability (Chen *et al.*, 2021; Cao *et al.*, 2022).

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Adding techniques such as SHapley Additive ExPanations (SHAP) and Partial Dependence Plots (PDP) to models has helped civil engineering research better explain why a model behaves the way it does and how different components affect its results (Zeng *et al.*, 2022; Pallapothu *et al.*, 2023). The purpose of this study is to improve how SFR-RAC mechanical properties are modeled using Multilayer Perceptron (MLP), Gaussian Process Regression (GPR), and Extreme Gradient Boosting (XGBoost). The aim of using Particle Swarm Optimization is to optimize the hyperparameters of each model, which increases their accuracy and ability to generalize.

In addition, interpretable machine learning approaches are applied to this study, which explains the impact of different mix design factors on concrete performance and aids in making better mixture designs. Using machine learning, optimization, and explanatory evaluations supports the growth of sustainable high-performance concrete materials and leads to more utilization of SFR-RAC for purposes such as building structures. Results are expected to help experts in concrete engineering focus on protecting the environment and ensuring good mechanical performance.

MATERIALS AND METHODS

The study constructed a dataset containing 465 samples for fcu (compression strength) and 339 for fsp (splitting tensile strength), with main input features such as cement level, water-binder ratio, the proportions of fine and coarse aggregates, quantity of recycled aggregate, steel fiber ratio, and fiber sizes. Data was edited to fix any missing values, mainly in the fsp data column, by replacing them with the average value and removing incomplete rows. A StandardScaler was run to ensure that the features had the same scale, which assists in the model doing well and being measured fairly. The data was split up so part of it was used to train and the other part was used to test three machine learning models—Multilayer Perceptron (MLP), Gaussian Process Regression (GPR), and eXtreme Gradient Boosting (XGBoost)—in predicting both variables. The cross-validation method was used via Particle Swarm Optimization to ensure that overfitting would not affect the results. After making the prediction, Particle Swarm Optimization (PSO) was used to find the best mix that balances the strength and cost of the concrete. Then, SHapley Additive exPlanations (SHAP) were used to determine individual input variables' role in the model's output, making the predictions more transparent and reliable.

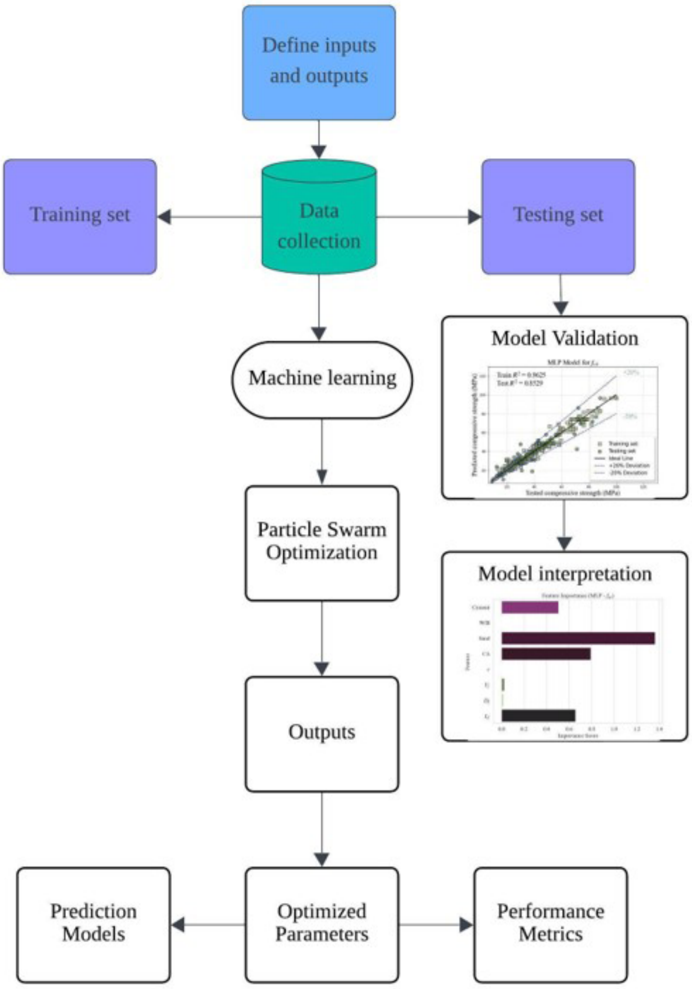


Figure 1: Model proposal

Fundamental ML Models

Multilayer Perceptron

Multilayer Perceptron (MLP) implements supervised machine learning that uses artificial neural networks. It approximates complicated nonlinear functions by allowing input data to go through different layers of connected neurons. Each neuron takes a weighted total of all its inputs and then uses an activation function (like ReLU or sigmoid) to improve the neural network. MLP is trained by employing backpropagation, which lowers the prediction error by adjusting the weights with gradient descent. It is beneficial for studying complex patterns in data of many dimensions, including concrete mix design data.

Equation if Statement

$y=\sigma(\sum^{n}_{(i=1)} w_i x_i+b)$

Where y is the output of the neuron; σ is the activation function (e.g., ReLU, sigmoid); xi is the i-th input feature; wi is the weight associated with the i-th input feature; n is the total number of input features; b is the bias term.

Gaussian Processes are used in Regression (GPR). In Gaussian Process Regression (GPR), the output values are assumed to be distributed like a multivariate normal distribution. Instead of deciding on a set of fixed weights as neural networks do, GPR provides a probability distribution for functions and bases its predictions on the mean and variation of this distribution. That's why it supplies an estimate of how uncertain the forecast is and the predicted value. GPR is best for simple data and scenarios requiring measuring your accuracy with each prediction.

Gaussian Process Regression (GPR)

Gaussian Process Regression (GPR) is a model that does not depend on parameters and views the outputs as being taken from a multivariate normal distribution of values. Neural networks use a fixed number of weights, but by contrast, GPR defines a distribution and uses its principal value and scatter to make predictions. This makes it able to estimate how sure it is about its predictions. GPR excels at solving minor problems and in cases where showing the exactness of a prediction matters.

The following equation provides a mathematical explanation of the prediction process:

$\hat{y}(x_*)=K(x_*, X)\,[K(X,X)+\sigma^2_n I]^{(-1)}\, y$

Where y (x*) is the predicted value at the test input x*; K(x*, X) is the covariance vector between the test input x* and the training inputs X; K(X,X) is the covariance matrix between training inputs; σ^2_n is the variance of the Gaussian noise; I is the identity matrix; y is the vector of observed target values in the training data.

eXtreme Gradient Boosting (XGBoost)

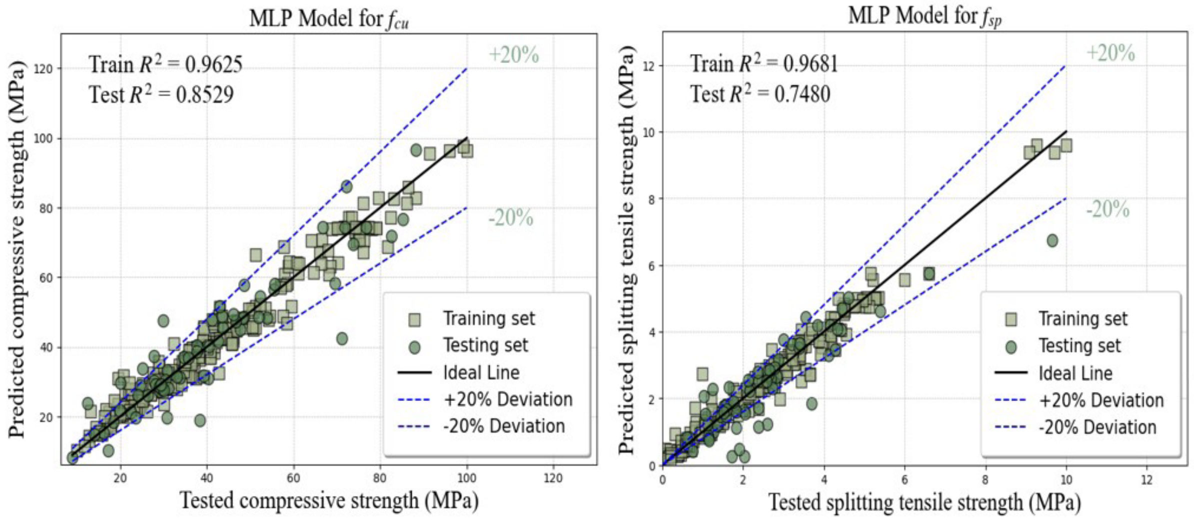
XGBoost stands for Extreme Gradient Boosting and is based on using decision trees and gradient boosting together. It creates a series of trees, with each new tree fixing the problems seen in the previous trees. The algorithm strives to improve prediction accuracy and keep complexity low by working on a regularized objective function, which makes it efficient and superior in results. Many people agree that XGBoost delivers excellent outcomes and does so quickly when handling concrete strength prediction.

This prediction process can be mathematically expressed as follows:

$$Obj = \sum_{i=1}^{n} \square\, l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \square\, \Omega(f_k)$$

Where

Obj is the overall objective function to minimize; $l(y_i, \hat{y}_i)$ is the loss function between actual target y_i and predicted value $\hat{y}_i$; n is the number of training samples; $\Omega(f_k)$ is the regularization term for the k-th tree fk; K is the number of trees in the model.



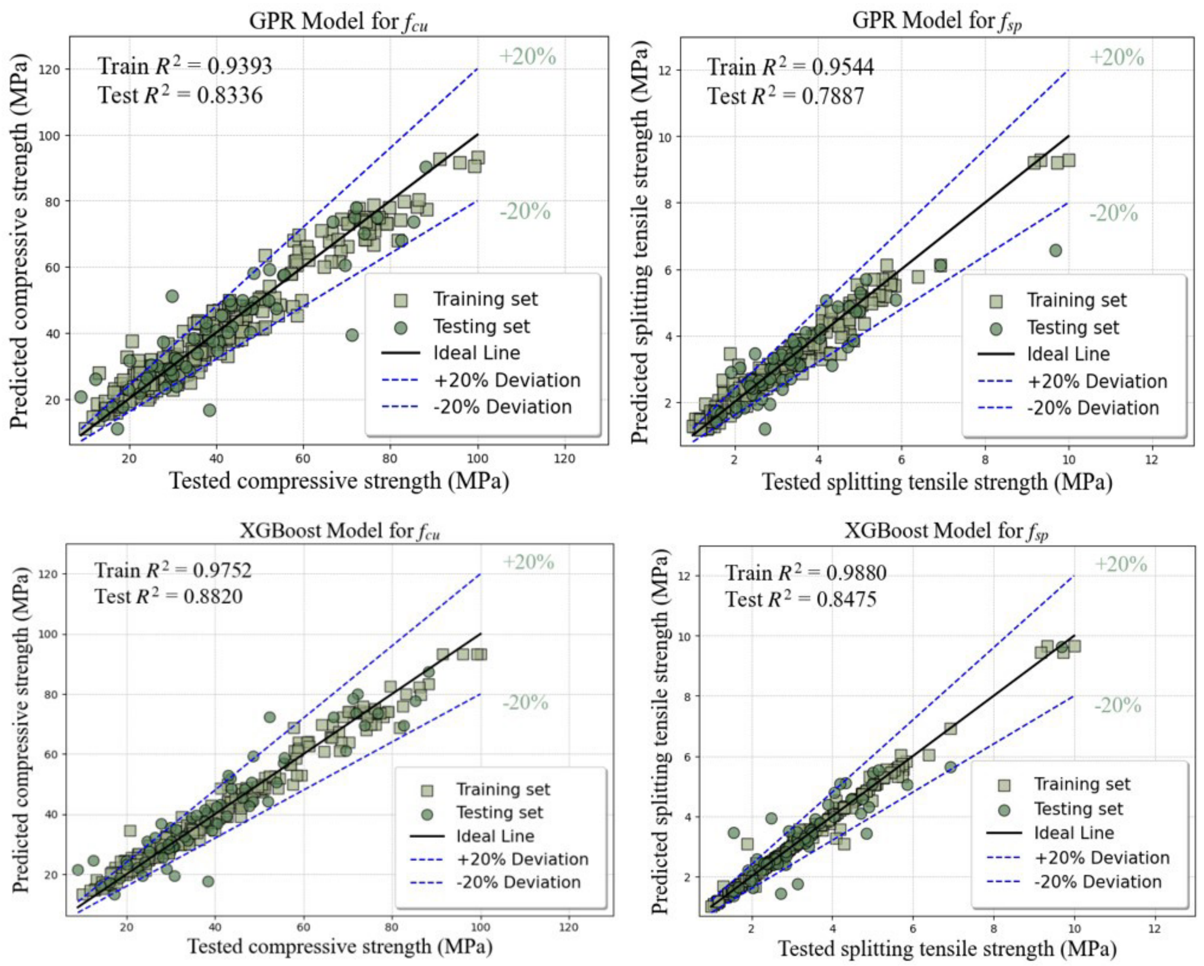


Figure 2: Prediction results of each ML models

Model Development

Regression Evaluation Criteria

Evaluating how well machine learning models forecast is done by measuring Root Mean Square Error (RMSE), Mean Absolute Percentage Error (MAPE), Nash-Sutcliffe Efficiency (NSE), Relative Percentage Difference (RPD) and Akaike Information Criterion (AIC). Here is the process for calculating these forms of evaluation metrics:

$R^2=1-(\sum^n_{(i=1)} (y_i-\hat{y}_i)^2)/(\sum^n_{(i=1)} (y_i-\_y)^2)$

$RMSE=\sqrt{(1/n \sum^n_{(i=1)} (y_i-\hat{y}_i)^2)}$

$MAE=1/n \sum^n_{(i=1)} |y_i-\hat{y}_i|$

$MAPE=(100\backslash\%)/n \sum^n_{(i=1)} |(y_i-\hat{y}_i)^2)/y_i|$

Table 1: Statistical metrics of different ML models on the test set

Item	type	Training				Testing			
		R^2	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE
fcu	GPR	0.939	3.831	2.997	6.333%	0.834	6.033	4.050	8.719%
	MLP	0.962	3.011	2.155	4.424%	0.853	5.673	3.787	7.770%
	XGBoost	0.975	2.446	1.752	3.596%	0.882	5.080	3.739	8.098%
fsp	GPR	0.954	0.455	0.321	8.727%	0.789	0.905	0.594	13.345%
	MLP	0.968	0.381	0.260	6.792%	0.748	0.989	0.672	16.566%
	XGBoost	0.988	0.235	0.089	11.396%	0.850	0.763	0.466	11.396%

Particle Swarm Optimization (PSO)

In Particle Swarm Optimization (PSO), the intelligent groupings of birds or fish inspire the search for solutions. In 1995, Kennedy and Eberhart introduced the algorithm, which efficiently solves optimization problems with many variables [80]. In the research, the authors applied PSO to find the best values for their machine learning models' hyperparameters, which helped improve the prediction of Steel Fiber-Reinforced Recycled Aggregate Concrete (SFR-RAC). In the swarm, every particle stands for a possible solution, which is identified by its position and velocity. When optimizing, particles update their spots by aiming for their very best positions (pbest) and the best position among all particles (gbest). The system is updated using these equations for speed (velocity) and position.

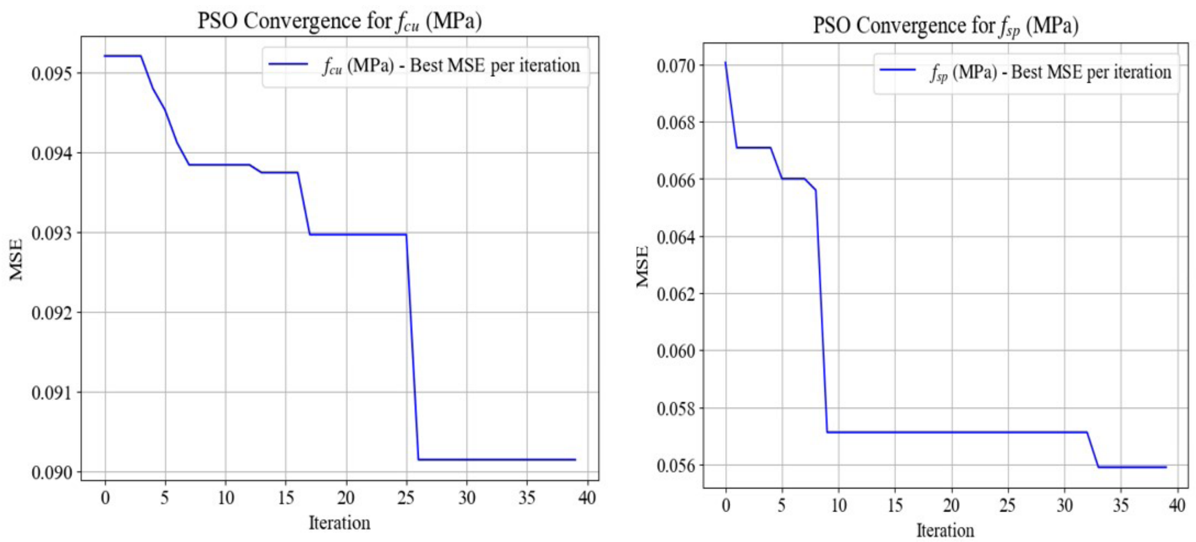


Figure 3: Convergence of PSO Optimization for fsp and fcu (MPa)

$v_i^{(t+1)} = w \cdot v_i^t + c_1 \cdot r_1 \cdot (pbest_i - x_i^t) + c_2 \cdot r_2 \cdot (gbest - x_i^t)$

Where $v_i^{(t+1)}$ the updated velocity of the particle i; w is inertia weight (balances exploration and exploitation); c_1 is a cognitive coefficient (self-confidence); c_2 is social coefficient (swarm confidence); r_1, r_2 are random numbers in [0,1]; $pbest_i$: personal best position of particle i; gbest the global best position found by the swarm; x_i^t is the current position of a particle i.

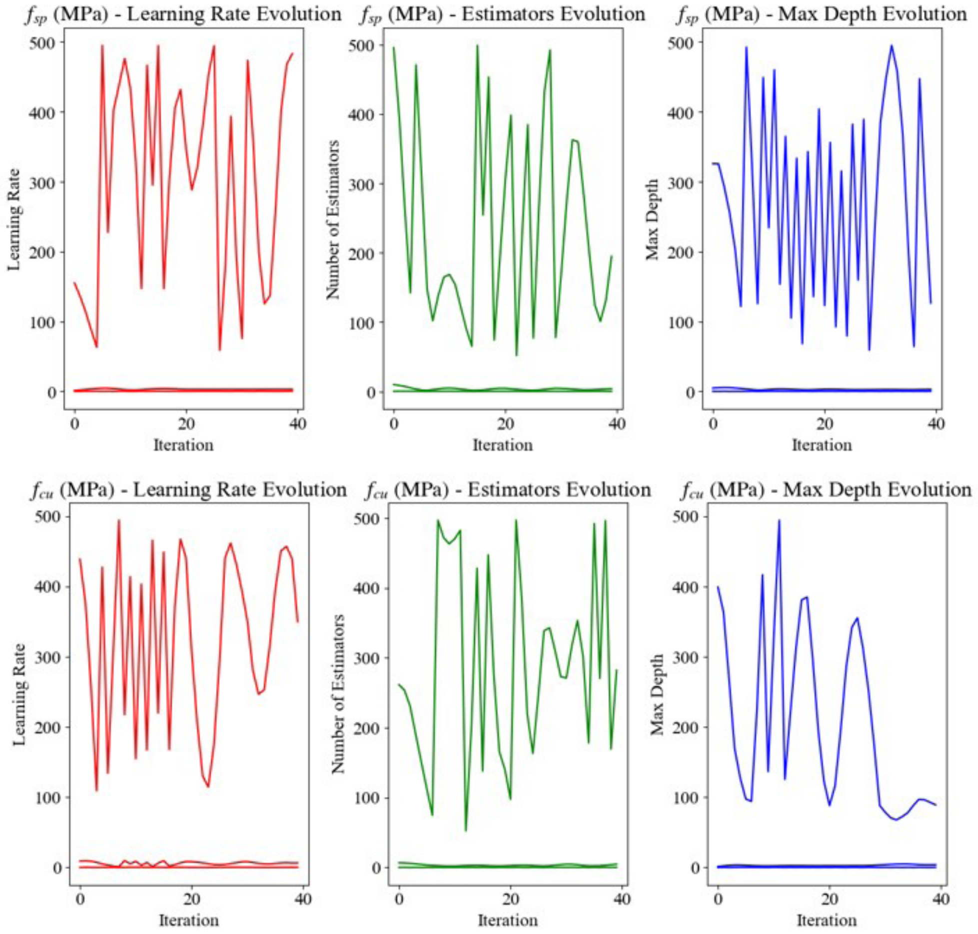


Figure 4: Hyperparameter Evolution for fcu and fsp Models

Table 2: Impact of Particle Swarm Optimization on Metrics

ML algorithms		**Compressive strength (fcu)**			**Splitting tensile strength (fsp)**		
		R^2	**RMSE**	**MAPE**	**R^2**	**RMSE**	**MAPE**
GPR	Before	0.834	6.033	8.719%	0.789	0.905	13.345%
	After	0.905	4.553	7.284%	0.936	0.497	9.115%
MLP	Before	0.853	5.673	7.770%	0.748	0.989	16.566%
	After	0.911	4.420	7.061%	0.878	0.689	12.415%
XGBoost	Before	0.882	5.080	8.098%	0.850	0.763	11.396%
	After	0.904	4.594	7.165%	0.923	0.546	8.709%

RESULTS AND DISCUSSION

Model Development

Figure 2 helps compare the predictive success of Gaussian Process Regression (GPR), Multilayer Perceptron (MLP) and Extreme Gradient Boosting (XGBoost), for estimating compressive strength (fcu) and splitting tensile strength (fspBlue dots stand for the training data, and red dots are used for the testing data; on the x-axis are the actual values, and the y-axis gives the predicted ones. Table 3 provides the models’ performance by reporting R^2, RMSE, MAE, and MAPE. The blue dashed lines in Figure 4 show where the ±20% margin of error is located.
XGBoost shows the best performance for fcu prediction, getting an R^2 of 0.975 and a RMSE of 2.446 in training, plus an R^2. Because both training and testing MAPEs were under 10%, the model can generalize well, and most predicted results are near the ±20% mark. Scatter plots confirm that the line drawn through the predictions is close to the ideal line.

MLP also gives good results for fcu, having a training R^2 of 0.962 and a test R^2 of 0.853 and matching RMSE values of 3.011 and 5.673. When the MAPE values for training are 4.424% and for testing 7.770%, MLP offers stable and functional predictions within the ±20% range.

The GPR model may not be exactly as accurate as XGBoost or MLP for fcu measurements, but it still does well with a training R^2 of 0.939 and a testing R^2 of 0.834 and with MAPE values of 6.333% and 8.719%. GPR’s scatter plot indicates that points are more clustered around the ideal line than what was seen with KNN at the start of the exercise, showing it is exceptionally reliable when outcomes don’t differ much from what’s expected.

XGBoost comes out on top here as well, having a training R^2 of 0.988 and RMSE of small value 0.235. It still performs well, with an R^2 of 0.850, an RMSE of 0.763 and the same MAPE of 11.396% in testing as in training, proving reliable generalization. The forecasts are generally close to 20% under or over the real values, as is shown in the graph.

MLP does well in explaining fsp, getting training and testing R^2 of 0.968 and 0.748. The testing MAPE rises dramatically to 16.566%, indicating that some predictions in testing go out of the ±20% band.

Most of the results are along or near the ideal result for both XGBoost and MLP which means about 80% of the data points are within the ±20% error zone for fcu and fsp. GPR continues to produce strong results, though its performance falls behind the other two in tests of forward selection path accuracy. XGBoost and MLP have proven to accurately describe the behavior of steel fiber-reinforced concrete, while GPR remains a trustworthy but slightly less precise alternative.

Effect of Particle Swarm Optimization (PSO)

Particle Swarm Optimization (PSO) was used to find the best GPR, MLP and XGBoost hyperparameters for estimating the fcu and fsp values. The model was repeatedly updated to minimize errors by measuring the performance metrics from testing samples (figure 4).

As shown in Table 2, each algorithm saw significant gains in performance because of using PSO. As for compressive strength (fcu), the R^2The GPR model’s value increased to 0.905, and the RMSE fell to 4.553, so the MAPE improved as well, from 8.719% to 7.284%. The changes mean that the model gives more accurate predictions and is tighter in grouping values within ±20%.

PSO helped the MLP achieve good improvements as well. R^2The RMSE went up from 0.853 to 0.911, the RMSE fell from 5.673 to 4.420, and the MAPE was cut from 7.770% to 7.061%. These improvements improve the ability to make predictions on unseen data and lower the risk of overfitting, mostly for compressive strength.

Even when the XGBoost model had already done well, optimization through PSO improved its results. The correlation increased to 0.904, error was reduced to 4.594 and the percentage error was improved to 7.165%. The outcomes validate that the model can work correctly with fine-tuned parameters.

PSO also achieved remarkable results when predicting splitting tensile strength (fsp). For GPR,R^2 grew from 0.789 to 0.936, RMSE lowered from 0.905 to 0.497, and MAPE went from 13.345% to 9.115%. After performing optimization, GPR is more reliable in revealing the nonlinear behavior of tensile strength.

There were significant improvements in fsp prediction using the MLP model. R^2 went up from 0.748 to 0.878, RMSE was reduced from 0.989 to 0.689, and MAPE decreased from 16.566% to 12.415%, which shows a more stable and improved prediction after improving the model.

Once optimized, the XGBoost model showed it was still strong, resulting in R² rising from 0.850 to 0.923, RMSE decreasing from 0.763 to 0.546 and MAPE falling from 11.396% to 8.709%. Because of these values, PSO was able to adjust the model better, resulting in more accurate predictions of splitting tensile strength.

Overall, the table shows that Particle Swarm Optimization helped considerably lift model performance. For the target variables used (fcu and fsp), PSO regularly increased the R² value, making the predictions more accurate, generalizable, and reliable. Table 5 shows the optimal values for each model's hyperparameters, which confirms that the optimization process works well.

Interpretation of Modeling Results

Shapley Additive Explanation (SHAP)

According to the plots of the features importance (figures 5 and 6) that can be obtained through the MLP model due to the estimation of the compressive strength (fcu) as well as splitting tensile strength (fsp) of the reinforced concrete and steel fiber aggregate, the following conclusion can be made:

In compressive strength (fcu), the most important predictor is the Cement and Sand, followed by Cement in order of importance. Close behind sand is a significant showing that the two elements were the major contributors to the prospect of the compressive strength determination by the model. Moderate relations are also given to Coarse Aggregate (CA), but the rest of the properties, such as the Water-to-Binder ratio (W/B), Density (r), Fiber Volume Fraction (Vf), Fiber Diameter (Df), and Fiber Length (Lf) are evaluated as relatively unimportant. That implies that the mechanical spine behind the compressive strength resides mainly in the core matrix components, such as cement and sand, and not the fiber and density parameters.

When comparing it, in case of splitting tensile strength (fsp), the importance chart is led by Sand, followed by CA, Lf and Cement. This tendency means that cement remains essential, but fiber length and coarse aggregates are more effective factors to resist the action of tensile stress. Noteworthy, Lf is much more critical when it comes to fsp than when in the case of fcuThis indicates the increased crack-bridging and tensile behavior exhibited by the fibers. Though Vf and Df do not have much effect in either of the cases, a little increased contribution in fsp concurs with the common intention of the fibers to improve tensile performance. The inertial contributions W/B and r continue to be very insignificant contributors to fsp unlike in the conventional cases.

Generally, the information in these plots points out that compressive strength is more predictable using binder-rich materials such as cement and sand, whereas tensile strength is more widely predictable with sand, CA and fiber length being decisive. These differences determine the formation of concrete mix design relying on compressive or tensile performance preference.

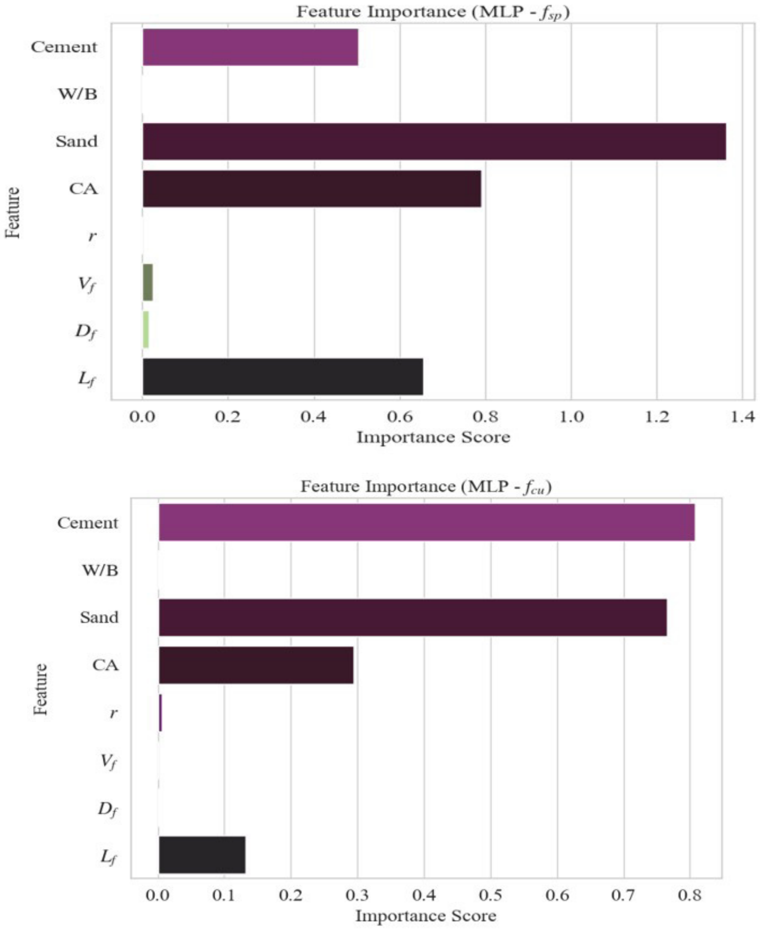


Figure 5: Feature Importance – MLP Model (fcu)

MLP Learning Curve (RMSE)

Figure 7 is the result of the learning curve of the MLP (Multilayer Perceptron) regressor, and the measure used was RMSE, which was plotted against the training example. The red curve gives training error, whereas the green curve gives cross-validation error, and the shaded area shows the standard deviation across the folds. When the sample size is small, the model will have a low training error and a large, fluctuating cross-validation error because of overfitting and poor generalization. As we have more and more training examples, we can see the training error increasing slowly, whereas the cross-validation error keeps decreasing until it becomes steady. It is also important to note that, after about 200 training samples, the two curves NP and FC merge, and the RMSE values become close to each other and relatively low. This unity indicates that the model is doing a good generalization with sufficient data, and there is no occurrence of underfitting or overfitting at this point. The fact that the error between training and validation errors is converging, along with the decreasing variance, implies that the model takes advantage of more data and is learning meaningful patterns that are important to the task of making the prediction.

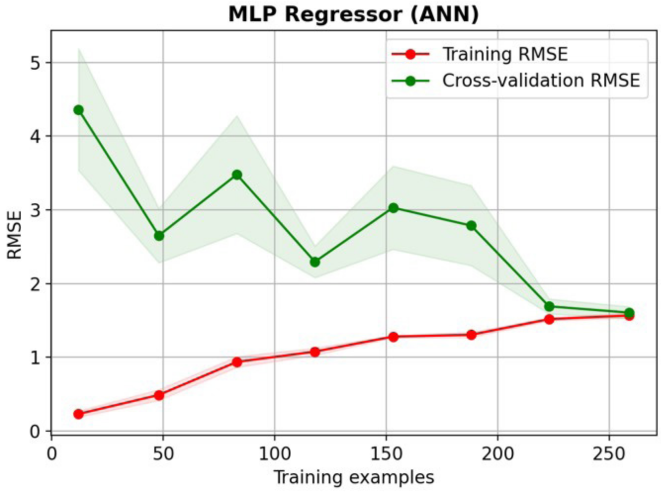


Figure 6: Feature Importance – MLP Model (fsp)

CONCLUSION

The present study has put forward a complete approach toward forecasting and optimization of mechanical behaviors of the steel fiber reinforced recycled aggregate concrete, with the two-fold objectives being the compressive strength (fcu) and splitting tensile strength (fsp). The following stages offered the following: machine learning (MLP, GPR, XGBoost) models adequately predicted the target characteristics regarding various material features. They showed that the models possessed strong predictive ability, and the machine learning methods can effectively model complex, non-linear relationships in concrete behavior. The second phase involved particle swarm optimization (PSO) to select the best proportions of the mix to ensure maximum mechanical performance. This optimization step allowed finding optimal combinations of essential variables in terms of inputs through providing a realistic course of action toward improving concrete properties, which also considers the variability and trade-offs of interest in mixing design. Lastly, the contribution of each feature to the model outputs was interpreted using SHAP (SHapley Additive exPlanations). The interpretability analysis showed that cement and sand have the most significant variables in predicting compressive strength, whereas splitting tensile strength is more responsive to fiber variables, including (Vf) and Lf. The insights confirm the predictive models and offer much-needed advice on mix design optimization (to achieve more performance from the design). The combination of machine learning, optimization, and explainable AI would provide a high-potential and interpretable cost function to spearhead the development of sustainable and high-performance concrete designs considering recycled aggregates and steel fibers.

CRediT Authorship Contribution Statement

Hamza Naciri: Participated in the draft of the first manuscript, development of software, development of a methodology, exploration, and formal analysis of data. Ouahib Alaoui: Contributed to the review and editing of the manuscript, contributed to guidance and methodological contribution and verified the results. Hamza Zaouri: Has taken part in the editing and manuscript preparation and verification of findings.

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