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RESEARCH PAPER

Gradient Boosting Hybridized with Exponential Natural Evolution Strategies for Estimating the Strength of Geopolymer Self-Compacting Concrete

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Abstract

The current global demand to minimize carbon dioxide (CO_2) emissions from Portland cement manufacturing processes has led to the use of environmentally friendly additives in cement products. The so-called green cementitious composites have become increasingly essential in the design of cementitious composite mixtures, providing the environmental compatibility of concrete as a building material. Engineers face a difficult problem in predicting the mechanical properties of green composites due to their changing nature under various circumstances. Machine learning models then emerge as surrogate models to perform this difficult task. The very design of such models has become a challenge for machine learning. This study presents a gradient boosting algorithm hybridized with Natural Exponential Evolution Strategies inspired by nature to predict the mechanical properties of geopolymeric self-compacting concrete. The hybrid model is used to evolve the parameters, automating the selection of the best set of internal parameters to estimate the strength properties of geopolymer self-compacting concrete. Results show the predictive ability superiority of machine learning models and optimization algorithms hybridization compared to manually tuned models. In addition, this approach can minimize laboratory work, potentially optimize experimental design, and reduce sample production time and associated activity burden.

Keywords: Geopolymer self-compacting concrete; gradient boosting; evolution strategies; carbon dioxide; portland cement

1. Introduction

The use of ecologically friendly admixtures in the manufacture of so-called green cementitious composites has lately become increasingly essential in cementitious composite mixture design. This is primarily due to a recent global trend of minimizing the emission of carbon dioxide (CO2) from Portland cement manufacturing processes [42]. Fly ash, silica fume, and ground granulated blast furnace slag (GGBFS) are some of the environmentally friendly admixtures used in concrete [16]. In addition, the fact that these minerals are leftovers from numerous industrial operations is another rationale for their utilization [18].

Various industrial activities are considered to be environmentally detrimental; nonetheless, evidence indicates that the building industry is the most significant contributor to global greenhouse gas (GHG) emissions [60]. Portland Cement (PC) has a substantial influence on GHG emissions as it is an essential component of concrete [9]. Despite the benefits of PC, its production contributes to

about 7% of total man-made CO2 emissions into the environment [23]. Around half of the emitted CO2 by the cement factory comes from the calcination reaction process that involves CO2 extraction from CaCO3 to form CaO; the other half is due to energy consumption throughout the cement production process [7]. PC is produced at a rate of almost 4000 million tons per year, making it the most used binder in construction [48]. According to estimates, global PC usage will exceed 6000 million tons per year by 2060 [53]. GGBFS is produced as a fine waste powder by the metallurgy sector after blast furnace grinding. Recently, there has been an increase in research into the behavior of GGBFS concrete properties [33, 41]. Laboratory tests are required in the traditional methods for determining the compressive strength of a concrete mixture; however, these examinations are both expensive and laborious. For instance, testing one series of composites in the European Union costs at least 100 euros. Moreover, due to these tests' destructiveness, they are not recommended on existing structures without demolishing a portion of the structure to get the required core sample for the tests. Another drawback of destructive testing is that it is normally done after 28 days and occasionally even after 90 days. As a result, the traditional process is ineffective, and the environmental concern of such green composites gets higher. The need for more research into innovative alternative binders that use less energy to manufacture and emit less pollution has been highlighted [62]. The usage of geopolymers [31] has been suggested as a way to mitigate the aforementioned owing to the environmental friendliness of geopolymers-based concretes as construction materials. It is made by using alkali activators like sodium hydroxide and sodium silicate to activate the cementitious property of solid aluminosilicate materials like fly ash, metakaolin, or GGBFS at a low curing temperature in an alkaline medium [14]. As a green material, geopolymer has an 80 percent smaller carbon footprint than PC [15]. It has been utilized to make structural elements used in buildings, such as beams, piles, and columns [25, 24]. Some of the factors that affect the CS of GPC include the silicate: hydroxide ratio, alkali activator: solid materials ratio, the type of alkali activator, and the number of solid materials used [32].

Engineers face a difficult problem in predicting the CS of GPC because of its changing nature due to a variety of circumstances [44]. As a result, a numerical model capable of accurately predicting the strength performance of this type of concrete, such as a soft computing model, is required to address this issue [2, 68, 70]. More complex data analysis must be used in such a scenario as well [5, 30]. In civil engineering, the use of machine learning to solve a variety of problems has been reported [72, 69]. Such applications include the prediction of CS and tensile strength [8, 50], the prediction of the adhesion between layers of cementitious composites [13, 12, 59], prediction of concrete strength [71, 57], prediction of the parameters of soil strength and soil safety factor [29, 46], among others.

Data intelligence models are alternatives to produce accurate models for green cementitious properties, avoiding expensive laboratory experiments and the work of specialized labor. Recently, some efforts can be highlighted in the literature to predict and model mechanical properties through machine learning and deep learning models. [43] implemented decision trees and support vector machines to predict the compressive strength of silica fume concrete. Other machine learning models such as support vector machines, [27, 26, 28] and neural networks [56, 58, 61], random forests [38, 10, 21], and gaussian processes [52, 37] have been used as successful data-driven tools for green concrete modeling.

Nature-inspired approaches have also been employed to deal with the nonlinear characteristics of green concrete mechanical properties. [55] and [54] developed a multi expression programming (MEP) approach to develop predictive models for modeling the mechanical properties of sugarcane bagasse ash green concrete. [45] used an evolutionary learning strategy for modeling the compressive strength of sustainable concrete mixtures. [6] modeled the properties of concrete mixtures containing natural zeolite using a metaheuristic-based machine learning method.

Deep learning has also gained increasing attention of researchers due to its modeling capabil-

ities. [35] employed deep learning neural networks to model the reinforcement mechanisms in the microstructure of graphene oxide-silica (GOS) reinforced portland cement composites. [36] implemented a convolutional neural network to predict the mechanical properties of eco-efficiency concrete containing diatomite and iron ore tailings. Despite the excellent results reported, deep learning models have some disadvantages. These models generally require large datasets and a lot of computational resources for training, resulting in complex models with low interpretability [3].

The gradient boosting model has also been successfully applied to problems of predicting the mechanical properties of sustainable concretes [66, 34, 51, 21, 63]. The gradient boosting model is constructed using the ensemble strategy, combining several simple models resulting in an accurate final model. These features allow handling complex data with non-linear behavior and accommodating noise in the data [39]. Unlike deep learning models, gradient boosting does not present a great complexity in the resulting training that is not computationally expensive [1]. In the same way, the number of parameters to be determined in the gradient boosting model is moderate. In this context, using metaheuristics is attractive to decide on the best parameters that allow exploring the model's predictive capacity [17, 64].

The current study presents a machine learning model approach implementing the gradient boosting model assisted by an evolutionary algorithm resulting in a hybrid model. The hybrid model is used to evolve the parameters, automating the selection of the best set of internal parameters for estimating the strength properties of geopolymer self-compacting concrete. This research aims to understand the role of the gradient boosting algorithm in predicting the mechanical properties of self-compacting concrete. In addition, this paper assesses the performance of the exponential natural evolution strategy optimization algorithm for searching the internal parameters and the accuracy of the machine learning algorithm results. The results show that the proposed strategy results in a model with greater predictability that can be used as a tool to assist in the performance of tests as well as in the prediction of the strength of hardened self-compacting concrete.

2. Material and Methods

This section explains the background for developing the model presented in this paper. First, the dataset is presented, and its statistical properties are described. The correlation between input data and outcomes is also shown. Then, the mathematical formulation of the machine learning model is elaborated in detail, emphasizing the parameters that influence its performance. Additionally, the Exponential Natural Evolution Strategies optimization algorithm is presented with the necessary information to show the hybridization procedure. Then, the computational framework is shown in detail, and the problem of searching for internal parameters of the machine learning model is presented as an optimization problem. Finally, the section describes the cross-validation strategy combined with the suitable metrics used to evaluate the model's performance.

2.1 Self-compacting Concrete Dataset

The experimental work was conducted by [8] using raw materials and fresh mix properties as predictors and strength properties as the response. The tests were performed on low calcium fly ash (ASTM class F), ground granulated blast furnace slag (GGBS) and silica fumes as Pozzolanic materials. The workability of the mixtures was assessed through 5 variables: slump flow, T50 cm, V-funnel, L-box, and J-ring tests. The hardened properties measured were compressive strength, split-tensile strength, and flexural strength.

Nine input variables were used to characterize the samples: fly ash, GGBS, silica fume, slump flow, T50 cm flow, L-box, V-funnel, J-ring and curing age. In addition, three output variables associated with hardened properties were modeled: compressive strength, split-tensile strength and flexural strength. Table 1 shows the basic statistics for input and output variables.

Table 1: *Dataset basic statistics. CS: Compressive strength, TS; Split-tensile strength and FS: Flexural strength.*

Input data	min	mean	std	max
Fly ash (kg/m^3)	270.00	385.71	55.70	450.00
GGBS (kg/m^3)	0.00	38.57	51.86	135.00
Silica fume (kg/m^3)	0.00	19.28	25.93	67.50
Slump flow (mm)	650.00	670.00	13.41	690.00
T50 cm (s)	3.00	4.02	0.57	4.70
L-box	0.88	0.92	0.03	0.96
V-funnel (s)	9.30	11.11	1.52	14.00
J-ring (mm)	3.00	4.34	0.83	5.40
Age (days)	7.00	16.33	8.94	28.00
Outputs	**min**	**mean**	**std**	**max**
CS (kN/m^2)	24.67	32.82	3.45	38.55
TS (kN/m^2)	1.04	3.31	1.05	4.62
FS (kN/m^2)	1.03	3.49	1.13	4.82

Figure 1 shows the correlation coefficients for the dataset. As observed in the figure, the specimens' age does not correlate with the other input variables. Such behavior comes from the constitution of the specimens and is not related to the curing time. Likewise, the curing time has no interference with the composition of the specimens. On the other hand, age strongly correlates with different resistances, as observed by the positive correlation values with the output variables: 0.85 for Compressive strength, 0.86 for Split-tense strength, and 0.79 for Flexural strength.

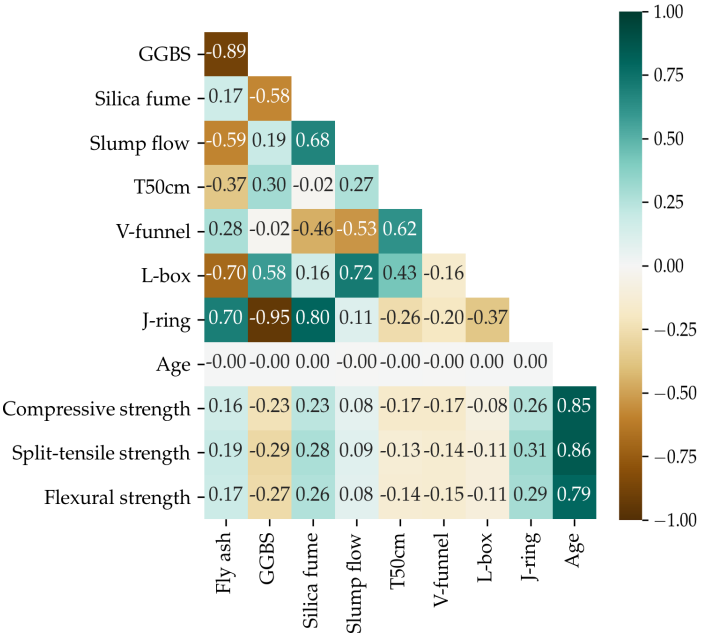

Figure 1: *Correlation coefficients among input and output variables.*

2.2 Gradient Boosting

Extreme Gradient Boosting (XGB) is one implementation of Gradient Boosting based on decision trees where errors are minimized by gradient descent. It has good performance and is considerably fast when compared to other implementations of gradient boosting, being utilized for supervised learning [47]. The XGB works as follows [11]: Considering a dataset that has m characteristics and an n number of samples $(x_1, y_1), ..., (x_n, y_n)$ where $x_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$, $i = 0, ...n$. Let $\hat{y}_i$ be the estimated output of an ensemble tree method obtained from the equations:

$$\hat{y}_i = \phi_M(x_i) = \sum_{k=1}^{M} f_k(x_i), \qquad f_k \in \mathbb{F} \tag{1}$$

where M represents the number of trees in the model, f_k represents the kth decision tree. The decision tree f_k has its depth less than or equal to m_{depth}.

In the additive boosting method the approximation is increasingly constructed as

$$\phi_M(x) = \phi_{M-1}(x_i) + \eta f_n(x_) \tag{2}$$

where η is the rate of learning and $f_n(x_i)$ a decision tree adjusted for minimizing the loss function L_n

$$L(\phi) = \sum_i l(y_i, \phi_{M-1}(x_i)) + \frac{1}{2}\lambda\|w\|^2 \tag{3}$$

where $l = |\hat{y}_i - y_i|$ is the loss function, $\hat{y}_i$ the predicted output and y_i the actual output, T is the number of leaves of the tree and w is the weight of each leaf, and λ is the L_2 regularization term on weights.

2.3 Exponential Natural Evolution Strategies

Natural Evolution Strategies (NES) is a family of evolution strategies that iteratively update a distribution using information from a gradient estimated based on data from the parameters of the distribution itself [67]. The general procedure is as follows: the parameterized search distribution produces a population of solutions. Then the fitness function is evaluated on each of these candidate solutions. The distribution parameters also include the evolution strategy parameters (in the case of a Gaussian distribution, these parameters are the mean and the covariance matrix). This strategy allows the algorithm to learn the landscape structure adaptively.

From the population of candidate solutions, the NES estimates a gradient in the parameters of the candidate solutions to generate new solutions with the highest expected fitness. Unlike the usual gradient method, the NES performs a second-order method that renormalizes the update. This step is crucial as it avoids oscillations, premature convergence, and undesired effects resulting from a specific parameterization. This process is repeated until a stopping criterion is met.

The Exponential Natural Evolution Strategies (xNES) is an improvement of the Natural Evolution Strategy methodology where the natural gradient is pursued to update the parameters in search of higher expected fitness [19]. Let d be the dimension of the problem, f the fitness function, μ the mean, A the covariance matrix, n the population size, z_i the sample in local coordinates, x_i is the candidate solution coordinates, $N(0, I)$ a normal distribution, G the gradient in the natural coordinate system,η_B the covariance learning rate, η_μ the mean learning rate, η_σ the scale learning rate, and u_i the utility function used for fitness shaping. The pseudo-code of xNES is presented in Algorithm 1.

The variables described previously are given below:

$$n = 4 + [3\log(d)] \tag{4}$$

$$\eta_\mu = 1 \tag{5}$$

$$\eta_\sigma = \eta_B = \frac{3}{5} \cdot \frac{3 + \log(d)}{d\sqrt{d}} \tag{6}$$

$$u_i = \frac{\max(0, \log(\frac{n}{2} + 1) - \log(i))}{\sum_{j=1}^{n} \max(0, \log(\frac{n}{2} + 1) - \log(j))} - \frac{1}{n} \tag{7}$$

The stopping criteria are commonly the number of fitness function evaluations or a user-defined number of generations.

Data: $d \in \mathbb{N}, f : \mathbb{R}^d \to \mathbb{R}, \mu \in \mathbb{N}^d, A \in \mathbb{N}^{dxd}$
$\sigma \leftarrow \sqrt[d]{|det(A)|}$
$B \leftarrow A/\sigma$
while *stopping condition not met* **do**
  for $i \in \{1, ..., n\}$ **do**
    $z_i \leftarrow N(0, I)$
    $x_i \leftarrow \mu + \sigma B \cdot z_i$
  end
  $sort\{(z_i, x_i)\}$ with respect to $f(x_i)$
  $G_\delta \leftarrow \sum_{i=1}^{n} u_i \cdot z_i$
  $G_M \leftarrow \sum_{i=1}^{n} u_i \cdot (z_i z_i^T - I)$
  $G_\sigma \leftarrow tr(G_M)/d$
  $G_B \leftarrow G_M - G_\sigma \cdot I$
  $\mu \leftarrow \mu + \eta_\mu \cdot \sigma B \cdot G_\delta$
  $\sigma \leftarrow \sigma \cdot exp(\eta_\sigma/2 \cdot G_\sigma)$
  $B \leftarrow B \cdot exp(\eta_B/2 \cdot G_B)$
end

Algorithm 1: The xNES Algorithm.

2.4 Hybrid Computational Approach

Figure 2 shows the framework responsible for producing an optimized parameters machine learning model. A hybrid approach was used where an optimization algorithm, in this case, xNes, acts to enhance machine learning model results. The algorithm seeks to minimize the target metric at each iteration. RMSE was chosen as the target metric. Each individual in the population embodies a set of different machine learning model internal parameters values. The initial population is randomly generated, and new parameter sets are tried at each iteration according to the optimization algorithm strategy. In this work, we used a population of 25 individuals throughout algorithm execution.

The Gradient Boosting model depends on the adjustment of four parameters, Learning rate, number of weak estimators, Maximum depth, and Regularization parameter. Then, each candidate solution results in a 4 variable set. Table 2 describes the parameters optimized by xNES and their respective search domain.

A new machine learning model is trained and tested whenever the optimization algorithm generates a new parameter set. The training process uses a k-fold cross-validation strategy with k=7. In the testing process, the RMSE of that candidate solution is calculated and used as the fitness function in the optimization algorithm. The xNES steps shown in Algorithm 1 are followed until the stopping criterion is reached, herein, 40 iterations. At each iteration of the algorithm, to generate a new population, the previous population is ranked, the gradient in the natural coordinate system is calculated, and strategy parameters update.

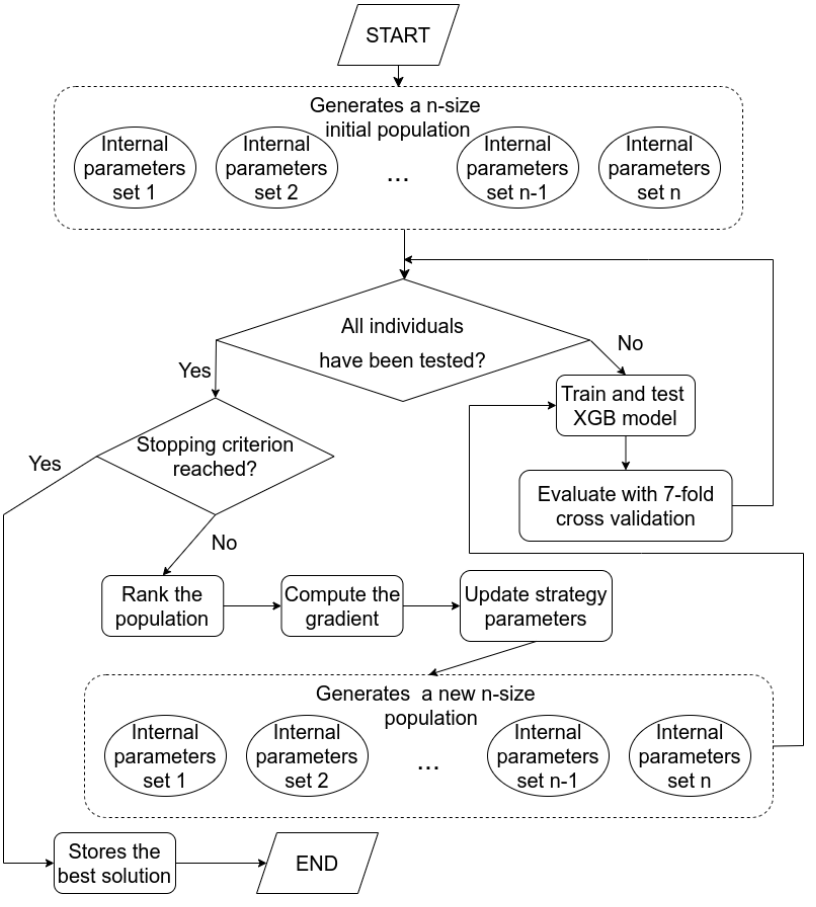

Figure 2: *Flowchart of Exponential Natural Evolution Strategies and Gradient Boosting hybrid approach.*

After the stopping criterion is met, the evolutionary cycle ends and the best solution found contains a model with optimized internal parameters. This procedure is performed repeatedly independently to obtain the hybrid algorithm's overall performance and stability metrics.

Table 2: *Encoding of candidate solutions. The column IP indicates the Internal Parameter in the xNES encoding.*

Estimator	Encoding	Description	Settings/Range
XGB	x_1	Learning rate, η	$[10^{-6}, 1]$
	x_2	No. weak estimators, M	[10, 500]
	x_3	Maximum depth, m_{depth}	[1, 20]
	x_4	Regularization parameter, λ	[0, 100]

3. Results and Discussion

The computational framework presented in Figure 2 was implemented on python programming language based on implementations adapted from pandas [40], NumPy [22], and scikit-learn framework [49], running on a computer environment described as follows: Intel(R) Core(TM) i7-9700F

(8 cores of 3 GHz, and cache memory of 6MB), 32 GB RAM, and operating system Linux Ubuntu 18.

The computational framework was executed 30 times independently, with different random seeds to gather statistical information on the models' performance. The XGB model training depends on random numbers. As a consequence, different random seeds may lead to different performances. Besides, the dataset was shuffled before the 7-fold split on each independent run. This procedure was adopted to add robustness to the results obtained by the hybrid model. The metrics shown in Table 3 were used for models' assessment.

Table 3: *Performance metrics: y_i is the observed value, $\hat{y}_i$ is the correspondent predicted value, $\hat{y}_i$ is the mean of the measured values, and N is the total number of samples in the dataset.*

Name	Expression
R^2	$\sum_{i=1}^{N}(\hat{y}_i - \hat{y}_i)^2 / \sum_{i=1}^{N}(y_i - \bar{y})$
MAE	$\frac{1}{N}\sum_{i=1}^{N}\lvert y_i - \hat{y}\rvert$
RMSE	$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y})^2}$
MAPE	$\frac{100}{N}\sum_{i=1}^{N}\left\lvert\frac{y_i - \hat{y}}{y_i}\right\rvert$

Table 4 shows the results obtained after 30 independent runs of the computational framework outlined in Figure 2. The first column of Table 4 indicates the output variable where CS indicates compressive strength, FS represents the flexural strength, and TS the split-tensile strength. The second column shows the machine learning and soft computing models used for comparison. The acronym XGB represents the hybrid gradient boosting model, while the ANN model is a neural network and the GEP a gene expression model both developed by [8]. Results in parentheses indicate the value of the standard deviation calculated in the 30 independent runs. The statistical metrics obtained for ANN and GEP were calculated under the same dataset. The performance reported by [8] is then used as the benchmark for the approach developed in this study. The third, fourth, fifth and sixth columns show the results for the metrics for Coefficient of Determination (R^2), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE) and Mean Absolute Percentage Error (MAPE), respectively. Metrics that were not available or could not be calculated were left blank. GEP model was implemented in this study, which allowed the calculation of all performance metrics for comparisons.

The results in Table 4 show that the proposal presented in this paper presented better results for all metrics than those reported by [8]. In addition, the model presented consistent results throughout the independent runs, as can be verified by the low value of the standard deviations compared to the averages obtained by the hybrid model. A considerable improvement was obtained in the modeling of CS and FS, as can be seen by the coefficient R^2.

Considering RMSE and MAE metrics, we can also observe that the values reached by the hybrid model were half for the RMSE and MAE metrics for all output variables, CS, FS and TS. On the other hand, the mean percentage error for FS and TS was slightly better than ANN and GEP. As observed in the table, using mean percentage error as a reference, there was a reduction of 12% for FS and 8% for TS. In contrast, the MAPE for the CS had a considerable improvement reaching an average value of 3.36%, much lower than the 11.1% calculated for the reference paper.

Table 4: *Results obtained averaged 30 independent runs of the computational framework. Values in parentheses indicate the standard deviation. Results for ANN and GEP reported by [8].*

	Estimator	R^2	RMSE	MAE	MAPE
CS	XGB	0.800 (0.041)	1.500 (0.150)	1.093 (0.121)	3.360 (0.363)
	ANN	0.455 (—)			
	GEP	0.455 (—)	3.33 (—)	2.02 (—)	11.10 (—)
FS	XGB	0.920 (0.041)	0.305 (0.076)	0.217 (0.050)	8.621 (2.412)
	ANN	0.568 (—)			
	GEP	0.567 (—)	0.810 (—)	0.690 (—)	9.822 (—)
TS	XGB	0.936 (0.030)	0.253 (0.060)	0.182 (0.047)	7.921 (2.132)
	ANN	0.730 (—)			
	GEP	0.729 (—)	0.550 (—)	0.420 (—)	8.605 (—)

Taylor diagrams [65] provide a way to graphically summarize how closely a model (or a set of models) matches observations. The similarity between the two standards is quantified in their correlation, their centered mean square difference, and the amplitude of the variations (represented by their standard deviations). These diagrams help assess various aspects of models or assess the relative predicting ability of different models.

Figure 3 shows the Taylor diagrams for compressive strength, flexural strength and split-tensile strength. Each dot represents an independent run. A total of 30 runs were performed. The Taylor diagrams show that the results were consistent across all runs. The simulations result in red dots in dense clusters in all three analyzed cases. For the Compressive strength, the values of correlation coefficients were greater than 0.80. For flexural strength and split tensile strength, the coefficients were greater than 0.90, indicating an excellent fit to the experimental data.

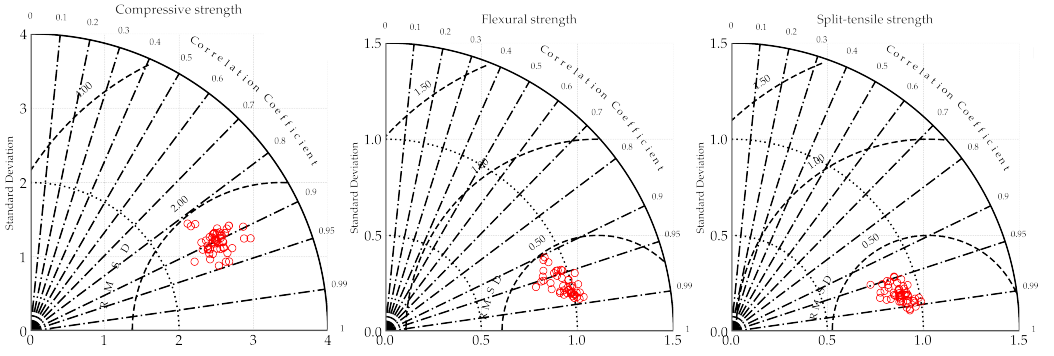

Figure 3: *Taylor diagrams for compressive strength, flexural strength and split-tensile strength. Each dot represents an independent run. A total of 30 runs were performed.*

The accurate results are due to the predictive capacity of the gradient boosting model combined with the search for the best parameters performed by the xNES algorithm. This process leads to robust and reliable results as it was implemented in a 7-fold cross-validation strategy with shuffling, which minimizes the empirical structural risk of the model outcomes [4], ensuring the reliability of the predictive capacity of the hybrid model.

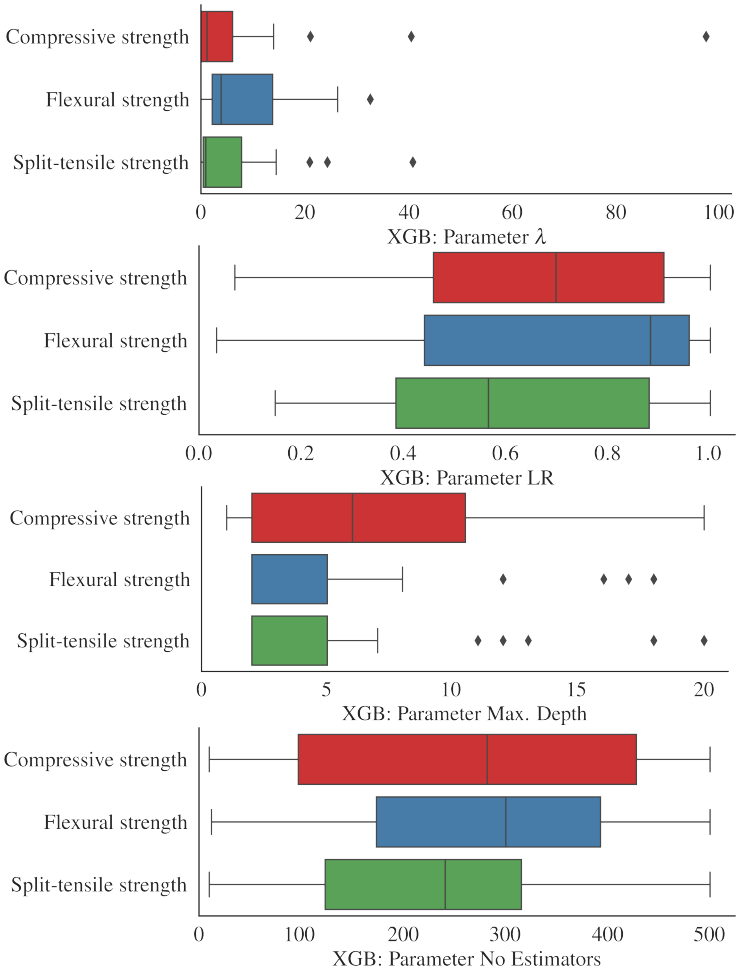

Figure 4: *Distribution of internal parameters.*

Figure 4 shows the distribution of internal parameters over 30 independent runs. The parameters found for the best individual in the population were chosen to build the machine learning model in each independent run. The boxplots depicted in figure 4 show the variation of the internal parameters. This distribution can suggest or indicate possible values for the choice of parameters in similar problems that were not addressed in this study. The boxplots representation was chosen because it allows a good idea of the distribution by parameters by presenting relevant information such as the median, the interquartile range, and possible outliers.

The learning rate showed a similar interquartile range for the three outcomes, but the median value was higher for flexural strength, with learning rates closer to 1. The learning rate indicates how quickly the model learns. Each tree added modifies the overall model, and the learning rate controls the magnitude of the changes, as can be verified in Eq (2). The lower the learning rate, the slower the model learns. The advantage of the slower learning rate is that the model becomes more robust and efficient, leading to better performance.

The tree depth was greater for the compressive strength. A greater depth value indicates that more complex models were used to compose the additive boosting model. The median depths in the final models were smaller than 5, presenting outliers for flexural and split-tensile strength. The median

values for the penalization in the loss function are smaller than 20 for all outputs. The interquartile interval for the number of estimators M lies between 100 and 400 estimators for all outcomes, with median values around 300 for compressive and flexural strength and M = 250 estimators for tensile strength.

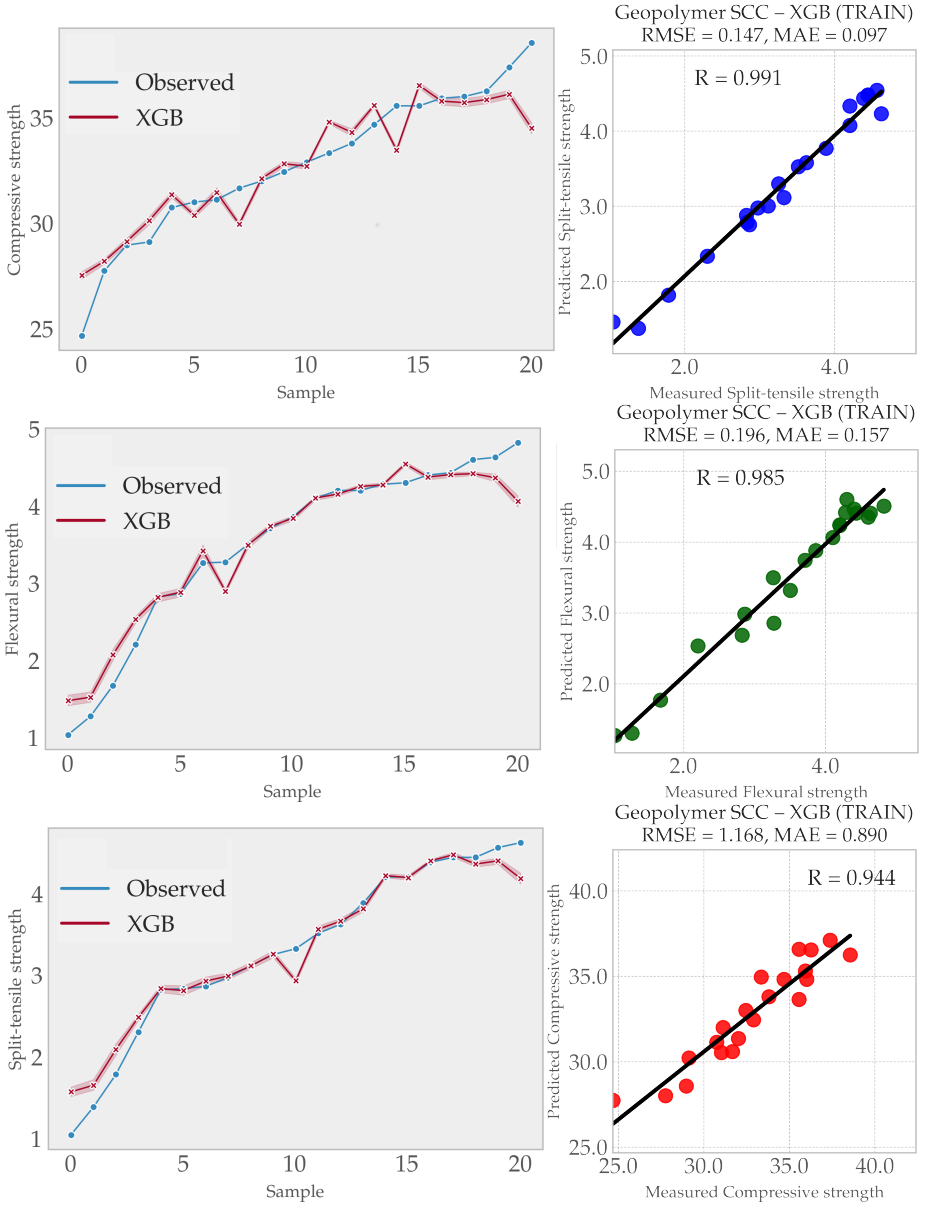

Figure 5: *Left: Comparison of observed and predicted values averaged (over 30 runs). Top: Compressive strength, middle: Flexural strength and bottom: Split-test strength. Right: Scatter plots for the best model in 30 runs according to RMSE for Compressive strength, Flexural strength and Split-test strength.*

Figure 5 shows the comparison between the observed values and the average in 30 runs of the predicted values (left) and the scatter plot of the best model in 30 runs according to the RMSE (right).

The red curve of the mean values predicted by the XGB model also presents a shaded area representing the 95% confidence interval of the predictions. We can see that the confidence interval inside the curve is small, as seen from the small standard deviation values in the Table. The scatterplot plots show the best performance of the models over 30 runs with the associated metrics that were calculated. In addition, an excellent fit of the predicted and real strength values is observed for compressive, split-tensile and flexural strength.

The relationship between the composition of the mixture and the mechanical properties of self-compacting hardened GGBS concrete is different from conventional concretes. These characteristics increase challenges to modeling such properties with machine learning models. GGBS concrete allows the reduction of cement, replacing it with blast furnace slag, reducing cost and environmental impact. The replacement can attain approximately 35% cement by the blast furnace slag. GGBS concrete is a mixture that presents mechanical properties superior to conventional concrete and with the advantage of fewer voids. The drawbacks of modeling the relationship between the characteristics of fresh concrete and its the mechanical properties reported in the literature are easy to perceive when observing the results reported by [8] in Table 4. On the other hand, the hybrid model proposed in this study achieved better results due to the synergy between the machine learning model and the nature-inspired optimization algorithm. The relevance of this research is due to the combination of a robust machine learning model and an efficient and easy-to-implement search algorithm. The gradient boosting model efficiently exploited its parameters by the nature-inspired xNES algorithm, resulting in outstanding performance even with a limited dataset.

The contribution of this study is the proposal of a hybrid approach for a machine learning-based tool for predicting the mechanical properties of self-compacting concrete. The computational framework is flexible and allows automatic search of the machine learning model. The limitation of this study lies in the small dataset, which does not allow a comprehensive and robust assessment of the model's performance. Testing the model on larger sets is recommended, but obtaining more data is costly and time-consuming. In addition, the model presents deficiencies in interpretability, which is interesting for the understanding of structural designers and engineers at the construction site. An improvement to the proposed approach is the automatic selection of input variables [20] aiming to produce models with similar accuracy levels but with few variables, reducing the model complexity.

4. Conclusion

This study focused on developing a gradient boosting algorithm hybridized with nature-inspired Exponential Natural Evolution Strategies to predict the mechanical properties of geopolymer self-compacting concrete. The algorithm developed in this paper was compared with other strategies such as neural network approach and gene expression programming to better understand the performance of the proposed approach.

i. The hybrid algorithms showed better performance with minor errors between observed and predicted values.
ii. The level of accuracy of the hybrid technique was compared with other soft-computing models and led to a more robust and more accurate model indicated for compressive strength, split-tensile strength, and flexural strength, observed by the averaged correlation coefficients (R^2) value equal to 0.80, 0.92, and 0.936, respectively.
iii. The smallest error values, MAE (1.093 MPa for CS, 0.217 MPa for FS, and 0.182 MPa for FS), also confirm the high accuracy of the hybrid model, while other algorithms present higher values for these errors.
iv. The application of several statistical metrics also confirms that the proposed model improves the model's precision, minimizing the error difference between the desired and predicted results.

The machine learning approach combined with an evolutionary search on internal parameters

provides an accurate alternative to model the relationship between the constituents of concrete mixtures and the mechanical properties. Combining a robust machine learning model com with an efficient model optimization algorithm attained better results than those previously reported in the literature. However, the size of the dataset did not allow a comprehensive evaluation of performance. In addition, one of the limitations of the model is its low interpretability. This aspect is relevant because it predicts the strength properties of concrete since it is a time-consuming task to have a result of concrete strength. This approach can minimize laboratory work, potentially optimize experimental planning, and reduce specimen production time and the burden of associated activities.

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