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Machine learning-based estimation of concrete compressive strength: a multi-model and multi-dataset study

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Abstract

Concrete is a commonly used construction material due to its favorable engineering properties, such as high compressive strength, good durability, and resistance to corrosion. Accurate predictions of the compressive strength of this material significantly reduce the time and effort required by laboratory tests. The current paper aims to compare the performance of prominent machine learning-based approaches used for predicting the compressive strength of concrete. In addition, 11 historical datasets, collected from the literature, are used. The diversity of the input features, the data dimensionality, and the number of instances can be helpful to evaluate the generalization capability of the employed machine learning models. Repetitive data sampling processes, consisting of 20 independent runs, are carried out to obtain the machine learning models' performances. Through experiments, it can be shown that the gradient boosting machines

attain the best performance. Notably, the extreme gradient boosting machine has achieved the best outcome in five historical datasets.

Keywords: Concrete Compressive Strength; Gradient-Boosting Machine; Machine Learning; Regression Models; Comparative Study.

1. Introduction

Concrete has been commonly used in construction due to its favorable engineering properties such as high compressive strength, good durability, resistance to corrosion, etc. (Chung et al. 2021). Basically, a concrete mix consists of four primary constituents: fine aggregate, coarse aggregate, cement, and water. These constituents can be easily accessed in the local market. These advantages allow concrete to be widely used in various forms of construction projects around the globe. Moreover, in recent years, many studies have found that supplementary materials like fly ash (PFA) (Gomaa et al. 2021), blast furnace slag (GGBS) (Kandiri et al. 2020), silica fume (Kang et al. 2021), and many other industrial/agricultural waste or by-products can be blended into concrete to meliorate its mechanical properties. Han et al. (2020) points out that the inclusion of those supplementary materials into concrete offers significant environmental benefits and also enhances the longevity and resiliency of concrete structures.

Among various concrete properties, the compressive strength (CS) is apparently the most critical since this index directly governs the structural safety and must be specified to determine the performance of concrete structures throughout their lifecycles (Zhao et al. 2022). When designing concrete mixes, one significant challenge is to select appropriate materials to achieve a targeted compressive strength. Therefore, it is of immense advantage to possess reliable predictive models that can yield accurate estimation of the CS based on the amount or proportion of the concrete components. These models can help to come up with meaningful predictions that can help to reduce the time and cost required for making and testing samples.

Historical data plays a crucial role in constructing robust prediction models. Recent studies with extensive data collection and model performance comparison have demonstrated the advantages of advanced ML models over conventional statistical regression analysis-based models (Ben Chaabene et al. 2020). Accordingly, various ML-based models have been proposed in the literature. Artificial Neural Network (ANN) and Genetic Programming (GP) was used in (Chopra et al. 2016) to predict the CS at 28, 56, and 91 days. One advantage of the GP is its capability of constructing predictive formulas used for the CS prediction. However, using the collected dataset, the authors find that ANN is preferable to the GP with respect to predictive accuracy.

ANN was also utilized in (Hocine 2018) to estimate the CS of limestone filler concrete and high-performance concrete (HPC), respectively. Although ANN-based models are capable nonlinear regressors, their performance substantially depends on the training algorithms. Current training methods of ANNs rely on stochastic gradient descent-based algorithms that are susceptible to being trapped in sub-optimal solutions. Gene expression programming was used in (Shahmansouri et al. 2020) to estimate ground granulated blast-furnace slag blended concrete. Using a dataset consisting of 351 specimens, the authors successfully constructed predictive formulas with high degrees of data fitting.

Zhang and Aslani (2021) proposed a data-driven approach based on a back-propagation neural network incorporating ultrasonic pulse velocity for estimating the CS of lightweight aggregate concretes. Nguyen et al. (2021) develops predictive models based on support vector machine regressor (SVM), ANN, gradient boosting machine (GBM), and extreme gradient boosting

(XGBoost) for estimating the CS of HPC. The authors find that GBR and XGBoost perform better than SVM and ANN. Nevertheless, this paper has not explored the capability of XGBoost in predicting the CS of other widely-used concretes (e.g., self-compacting concrete and class F fly ash-blended concrete). An intelligent approach that hybridizes a genetic algorithm and a backpropagation neural network is proposed in (Zhang et al. 2021) for predicting the CS of rubberized concrete.

GBM was also used in (Rathakrishnan et al. 2022) to model the CS of concrete mixes blended with ground granulated blast-furnace slag. Ensemble learning models based on Adaptive boosting machine, GBM, XGBoost, and random forest were proposed in (Li and Song 2022). The mixtures include admixtures such as fly ash and silica fume. The authors observed good performance of GBM that achieved a coefficient of determination (R^2) up to 0.96. Naser et al. (2022) applied Multivariate Adaptive Regression Splines (MARS) for estimating the CS of green concrete; MARS obtained the most desired performance (with $R^2 = 0.89$) which is better than that of SVM and random forest. A study in (Hoang 2022) reported superior performances of neural computing models and XGBoost over other data-driven approaches for predicting the CS of self-consolidating concrete; however, the predictive capabilities of MARS and piecewise linear regression models have not been investigated.

In general, recent reviews and comparative works (Ben Chaabene et al. 2020; Khambra and Shukla 2021; Mirrashid and Naderpour 2020) point out an increasing trend of using advanced data-driven tools in estimating this crucial mechanical property of concrete. However, the inclusion of various mineral additions, supplementary materials, and admixtures increases the complexity of the concrete. Thus, it is beneficial for the research community and practitioners to obtain information regarding the predictive capability of prominent ML models in estimating the CS of samples stored in various historical databases.

The current paper aims to compare the capabilities of prominent ML models, including XGBoost, GBM, SVM, MARS, GP, ANN, and sequential piecewise linear regression (SPLR). The selections of the first six models are based on reviewing recent works on ML-based CS prediction (Naser et al. 2022; Nguyen et al. 2021; Tanyildizi and Çevik 2010; Ullah et al. 2022; Zhang and Aslani 2021). In addition, the SPLR model has been shown to be a capable nonlinear regressor (Hoang 2019); however, its performance in modeling the CS has not yet been investigated. Furthermore, 11 historical datasets, gathered from previous experimental works, are employed to train and test the ML models. Repeated data sampling processes, consisting of 20 runs, are performed to obtain statistical criteria that express the performance of the models.

The current study aims to report the prediction results of the employed ML models in estimating the CS of concretes in multiple datasets. The outcomes of this paper may serve as initial guidance for researchers in selecting appropriate ML models for the task of interest. Since data samples are crucial for constructing reliable ML models, the scope of the paper is limited to the datasets that are openly accessed via data repositories or reported in reliable sources such as academic journal articles. Accordingly, the current work contributes to the body of knowledge in the following aspects:

(i) This study investigates the performances of a wide range of ML models, including the powerful methods of gradient boosting machines, for predicting the CS of concretes.

(ii) Although XGBoost has shown outstanding performances in modeling the mechanical properties of HPC, its capability in estimating the CS of other concretes (e.g., self-compacting concrete, class F fly ash-blended concrete, rubberized concrete) has not been fully explored.

(iii) Datasets representing diverse types of concrete are gathered from previous works to construct and test the ML approaches.

(iv) Through experiments, it can be shown that the gradient boosting machines cannot attain the best performance in all datasets. Nevertheless, SVM, MARS, and GP may outperform the gradient-boosting-based models in predicting the CS of certain types of concrete.

2. The employed machine learning models

2.1 Extreme gradient boosting machine (XGBoost)

XGBoost (Chen and Guestrin 2016) is an improved version of the standard the gradient boosting algorithm (Friedman 2002). This method is essentially an ensemble of boosted regression trees. The training process of the ML method is fast since it can be executed in parallel (Zhang et al. 2019). Let $D = \{(\mathrm{x_i}, \mathrm{y_i})\}$ be a collected dataset including *n* samples and *d* predictor variables. The XGBoost employs *Z* additive functions for estimating the target variable of the CS as follows:

$$\hat{y} = \phi(\mathrm{x_i}) = \sum_{z=0}^{Z-1} f_z(\mathrm{x_i}) \tag{1}$$

where $f_z \in F$ is the space of tree-based regressors. $\hat{y}$ represents the estimated CS value.

The objective function used in the model training phase is given by:

$$L^t = \sum_{i=0}^{n-1} l(\mathrm{y_i}, \hat{y}_i^{\,t}) + \Omega(\mathrm{f_t}) = \sum_{i=0}^{n-1} l(\mathrm{y_i}, \hat{y}_i^{\,t-1} + \mathrm{f_t}(\mathrm{x_i})) + \Omega(\mathrm{f_t}) \tag{2}$$

where *l* is a loss function which calculates the deviation between the predicted (y_i) and the actual variable ($\hat{y}_i$) of the concrete CS at an iteration *t*. $\Omega(\mathrm{f})$ denotes a function that regularizes the model complexity.

The regularization function $\Omega(\mathrm{f})$ is stated as follows:

$$\Omega(\mathrm{f}) = \gamma T + \frac{1}{2}\lambda \sum_{j=0}^{T-1} w_j^2 \tag{3}$$

where γ is the minimum reduction coefficient and λ denotes the regularization parameter. *T* represents the number of leaves in a classification tree and *w* is the weights associated with the leaves.

2.2 Gradient boosting machine (GBM)

GBM iteratively aggregates an ensemble of regressors to attain a powerful learner with enhanced fitting accuracy. This ML method can be viewed as a numerical optimization approach that establishes an additive model that reduces the value of a loss function (Friedman 2001). For regression problems, the commonly used loss function is the mean squared error (Touzani et al. 2018). Hence, the GBM model iteratively incorporates a new regression tree into an ensemble iteratively; the goal is to minimize the loss function. Via the process of fitting regressors to the prediction errors, the performance of an ensemble is enhanced in regions where it did not well fit the data. The GBM model operates by fitting a decision tree f^k at k^{th} iteration using the residual of the previous iteration $r_{k\text{-}1}$. Accordingly, the updated model $f(x)$ is computed as follows:

$$f(x) = f(x) + \alpha f^k(x) \tag{4}$$

Subsequently, the residual r_k is updated as follows:

$$r_k = r_{k-1} - \alpha f^k(x) \tag{5}$$

2.3 Support vector machine (SVM)

SVM (Drucker et al. 1996) utilizes a margin of tolerance (ε) for fitting a nonlinear function that describes the functional relationship between the mechanical parameter of concrete and the concrete mix's constituents. This ML model minimizes the training error and searches for a hyperplane that has a maximal margin. Additionally, the kernel function is used to cope with nonlinearity. In detail, the kernel function has the role of mapping the input data from the original space to a high-dimensional space. In this new space, a linear regression model is trained to fit the collected dataset.

The training phase of a SVM model constructs a model $f(x)$ that minimizes the structural risk in the feature space; $f(x)$ can be expressed as follows:

$$f(x) = w^T \varphi(x) + b \tag{6}$$

where $\varphi(x)$ denotes the aforementioned nonlinear mapping; w and b are the parameters of a SVM model.

The w and b are used to specify a SVM model. The training phase of a SVM model is equivalent to the following constrained optimization problems:

$$\text{Min. } \frac{1}{2}\| w \|^2 + C\sum_{i=1}^{N}(\xi_i + \xi_i^*) \tag{7}$$

$$\text{subjected to } \begin{cases} y_i - (\langle w, \varphi(x_i)\rangle + b) \le \varepsilon + \xi_i \\ (\langle w, \varphi(x_i)\rangle + b) - y_i \le \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \ge 0 \end{cases}$$

where C denotes the complexity coefficient; ξ_i and ξ_i^* are the slack variables (Drucker et al. 1996); $i = 1, 2, \ldots, N$ and N is the number of records in the training set.

2.4 Multivariate adaptive regression splines (MARS)

MARS, proposed in (Friedman 1991), constructs a nonlinear mapping relationship by dividing the learning space into regions of independent variables. In addition, this ML model employs piecewise linear functions and an adaptive training approach for model construction. A MARS model can be understood as a set of basis functions that describe the relationship between predictor variables and the CS. A basis function can be expressed as follows:

$$b_m(x) = \max(0, C - x) \text{ or } b_m(x) = \max(0, x - C) \tag{8}$$

where b_m is a basis function; x is an influencing factor of the CS of concrete; C is a tuning parameter that governs the process of separating x into regions.

Using the concept of the basis function, the general model can be expressed as follows:

$$f(x) = \alpha_0 + \sum_{m=1}^{M}\alpha_m b_m(x) \tag{9}$$

where $\alpha_0, \alpha_1, \ldots, \alpha_M$ denote the parameters of MARS; $f(x)$ yields the predicted outcomes of the CS. M represents the number of the model's parameters.

2.5 Genetic programming (GP)

GP (Koza 1994) is a ML approach inspired by real-world biological systems. This ML method is capable of generating mathematical equations (also called programs) to describe the behaviors of nonlinear systems. Thus, this method can be used to construct predictive equations used for estimating the CS. This ML method does not require any assumptions about the prior form of the mapping relationships. The structures of the predictive models, expressed in the form of equations, as well as their parameters, are learned by GP. The basic operations of a GP model are described as follows (Koza 1994; Searson 2015): (1) the generation of a set of random programs (2) the assessment of programs with a specified fitness function; (3) the generation of new programs based on the processes of reproduction, mutation, and crossover; (4) the processes of self-adaptation and fitness-based evaluation; and (5) the selection of the best program via fitness comparison.

2.6 Artificial neural network (ANN)

ANN is essentially an interconnected network of individual neurons (Haykin 2008). This ML method is capable of simulating the processes of learning and generalization in the human brain. There is a nonlinear activation function in each neuron; this function is used to process the input signals. To construct an ANN-based CS prediction model, a historical dataset is first collected. Subsequently, the back-propagation framework (Rumelhart et al. 1986) coupled with an optimizer is employed to fit the parameters of an ANN. An ANN is typically specified by its weight matrices: the matrix W_1 that connects the input layer to the hidden layer and the matrix W_2 that represents the link between the hidden layer and the output layer. In addition, there are vectors of bias associated with each layer.

The ANN model used for estimating the CS can be stated as follows:

$$f(x) = b_2 + W_2 \times \sigma(b_1 + W_1 \times x) \tag{10}$$

where x is the matrix of input variables; σ denotes the activation function. b_1 and b_2 are vectors of bias.

In the case of nonlinear function approximation, the Mean Square Error (MSE) loss function is often employed. Additionally, the sigmoid activation function can be used (Bishop 2011). The adaptive moment estimation (Adam) (Kingma and Ba 2015) is the state-of-the-art optimizer employed for training the ANN model. The Adam is an effective optimizer that relies on information about the first-order gradient of an objective function. To train an ANN-based model, the objective function is MSE. This algorithm harnesses the information obtained from the average of the second moments of the gradients to enhance the performance of the optimization process.

2.7 Sequential piecewise linear regression (SPLR)

A piecewise linear regression model (PLRM) is a ML approach that uses individual linear models to fit a portion of the training data. The transition location between separated domains of input features is often called a breakpoint or a knot (Breiman 1993; Ryan and Porth 2007). The appropriate value of a knot is estimated from the training dataset. SPLR, described in (Hoang 2019), employs a sequential algorithm to compute the knots of a PLRM. The training process of the SPLR relies on a set of hinge functions (Breiman 1993). This function basically separates the training data into separate domains in which individual linear models can be used to fit the dataset locally.

A SPLR model having one predictor variable X and one break point b is given by:

$$\begin{aligned} Y = {} & \beta_o + \beta_{11} \max(0, sign(X - b)) + \beta_{12} \max(0, sign(b - X)) + \beta_{21} \max(0, X - b) \\ & + \beta_{22} \max(0, b - X) \end{aligned} \tag{11}$$

where β_0, β_{11}, and β_{12} denote the bias parameters; β_{21} and β_{22} represent the slope parameters of the two linear models separated by a knot.

A general SPLR model used for estimating the CS values is expressed as follows:

$$Y = \sum_{d=1}^{D} \sum_{v=1}^{V_d} LF_{d,v}(X_d) \quad (12)$$

where d is the index of the independent variables (e.g. the components of a concrete mix); D is number of predictor variables; v denotes the index of the hinge function of the d^{th} independent variable; V_d represents the number of hinge functions of the d^{th} independent variable.

3. The collected datasets

To assess the capability of the employed ML models, this study has selected 11 historical datasets compiled by the previous works. In these datasets, the number of features ranges from 4 to 10. The number of data samples is from 70 to 1030. The selected datasets include normal concrete (Al-Jamimi et al. 2022), high-strength concrete (Al-Shamiri et al. 2019), self-compacting concrete (Kovačević et al. 2022), lightweight concrete (Tanyildizi and Çevik 2010; Ullah et al. 2022), and high-performance concrete (Videla and Gaedicke 2004; Yeh 1998). In addition, concrete with the alternative binder of ground granulated blast-furnace slag (GGBS) (Shahmansouri et al. 2020) and the alternative aggregate of rubber (Gesoğlu et al. 2009) are also considered. The diversity of the features and the number of data instances can be helpful to reveal the overall predictive capability of the ML approaches.

Table 1. The employed datasets

Dataset	Number of input features	Number of samples	Description	Reference
1	7	108	Plain and blended cement concretes	(Al-Jamimi et al. 2022)
2	5	324	High-strength concrete	(Al-Shamiri et al. 2019)
3	8	70	Rubberized concretes	(Gesoğlu et al. 2009)
4	7	262	Self-Compacting Concrete with Class F Fly Ash	(Kovačević et al. 2022)
5	8	144	Concrete containing fly ash and silica fume	(Pala et al. 2007)
6	5	117	Concrete containing ground granulated blast-furnace slag (GGBS)	(Shahmansouri et al. 2020)
7	6	96	Lightweight concrete containing silica fume	(Tanyildizi and Çevik 2010)

8	4	191	Lightweight foamed concrete	(Ullah et al. 2022)
9	10	195	Portland Blast-Furnace Slag Cement High-Performance Concrete	(Videla and Gaedicke 2004)
10	8	1030	High performance concrete	(Yeh 1998)
11	10	323	Concrete with manufactured sand	(Zhao et al. 2017)

The compiled datasets are summarized in **Table 1,** which provides information regarding the number of features, number of samples, descriptions, and sources of the data. **Table 2** provides an overview of the variables in each dataset. Furthermore, the frequency of the predictor variables is provided in **Fig. 1**. It is noted that to standardize the range of the variables, this study relied on the Z-score normalization approach. The Z-score normalization equation is given by:

$$X_Z = \frac{X_O - \mu_X}{\sigma_X} \tag{13}$$

where X_Z and X_O are the standardized and original variables (e.g., components of a concrete mixture), respectively. μ_X and σ_X represent the mean and standard deviation of the independent and response variables, respectively.

Table 2. The predictor variables

Input variables	Note	Dataset										
		1	2	3	4	5	6	7	8	9	10	11
Water content	X_1	x	x	x	x	x	o	o	o	x	x	x
Cement content	X_2	x	x	x	x	x	o	x	x	x	x	o
Water to cement ratio	X_3	o	o	o	o	o	o	x	x	o	o	x
Water to binder ratio	X_4	o	o	o	o	o	o	o	o	o	o	x
Silica fume content	X_5	x	o	x	o	x	x	x	o	x	o	o
Fly ash content	X_6	x	o	o	x	x	o	o	o	o	x	o
Coarse aggregate content	X_7	x	x	x	x	x	o	o	o	x	x	o
Fine Aggregate content	X_8	x	x	x	x	x	o	o	x	x	x	o
Superplasticizer content	X_9	o	x	x	x	o	o	x	o	x	x	o
Crump rubber content	X_{10}	o	o	x	o	o	o	o	o	o	o	o
Tire chips content	X_{11}	o	o	x	o	o	o	o	o	o	o	o
High-rate water reducing agent content	X_{12}	o	o	o	o	x	o	o	o	x	o	o
NAOH concentration	X_{13}	o	o	o	o	o	x	o	o	o	o	o

Natural zeolite content	X_{14}	o	o	o	o	o	x	o	o	o	o	o
Ground granulated blast-furnace slag content	X_{15}	o	o	o	o	o	x	o	o	o	o	o
Temperature	X_{16}	o	o	o	o	o	o	x	o	o	o	o
Pumice aggregate	X_{17}	o	o	o	o	o	o	x	o	o	o	o
Foam	X_{18}	o	o	o	o	o	o	o	x	o	o	o
Entrapped air content	X_{19}	o	o	o	o	o	o	o	o	x	o	o
Blast Furnace Slag	X_{20}	o	o	o	o	o	o	o	o	o	x	o
Compressive strength of cement	X_{21}	o	o	o	o	o	o	o	o	o	o	x
Tensile strength of cement	X_{22}	o	o	o	o	o	o	o	o	o	o	x
D_{max} of crushed stone	X_{23}	o	o	o	o	o	o	o	o	o	o	x
Stone powder content in sand	X_{24}	o	o	o	o	o	o	o	o	o	o	x
Fineness modulus of sand	X_{25}	o	o	o	o	o	o	o	o	o	o	x
Sand ratio	X_{26}	o	o	o	o	o	o	o	o	o	o	x
Slump	X_{27}	o	o	o	o	o	o	o	o	x	o	o
Concrete age	X_{28}	x	o	o	x	x	x	o	o	x	x	x

Note: The symbols ‘o’ and ‘x’ denote an inclusion and exclusion of a variable, respectively.

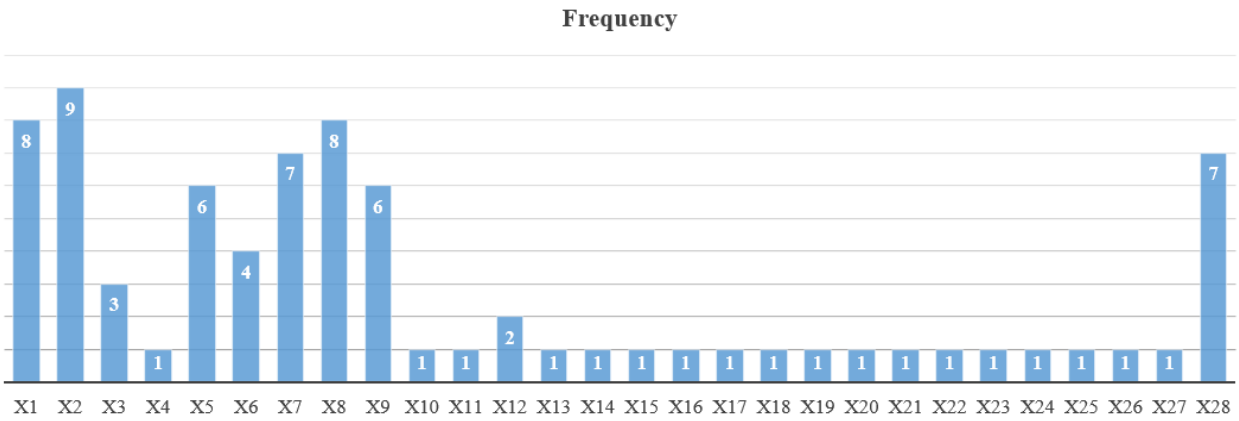


Fig. 1 The frequency of the predictor variables

4. Experimental results and discussion

The performance of the ML models with respect to the datasets of concrete strength samples is reported in this section of the article. For each dataset, 90% of the samples are used for training the prediction models; 10% of the dataset is used for testing the models’ predictive capability. To evaluate the ML models, the root mean square error (RMSE), mean absolute percentage error (MAPE), and coefficient of determination (R^2) are computed. The equations used to calculate those indices are presented in the following manner:

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - t_i)^2} \tag{14}$$

$$MAPE = \frac{100}{N} \times \sum_{i=1}^{N} \frac{|y_i - t_i|}{y_i} \tag{15}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(t_i - y_i)^2}{\sum_{i=1}^{N}(t_i - \bar{t})^2} \quad (16)$$

where t_i and y_i are the experimental and estimated CS of the i^{th} sample, respectively. N denotes the number of samples. $\bar{t}$ is the mean of the actual CS.

The RMSE measures the deviations between the experimental and estimated CS values. It is actually the square root of the second sample moment of the deviations between estimated and actual values. This index aims to aggregate the magnitudes of the residuals in predictions for various data points into a single measurement, indicating the prediction error of a CS prediction model. The RSME is always non-negative and a RMSE of 0 implies a perfect fit to the collected data. Generally, the lower the RMSE is, the better the ML model is. However, since the RMSE is scale-dependent, it is only valid to compare models fitting one dataset. The MAPE expresses the relative error of the model prediction. Similar to the RMSE, a small value of the MAPE indicates a good ML model. In addition, the R^2 represents the proportion of the variation in the CS of concrete that can be captured by the ML models (Mendenhall and Sincich 2011). A R^2 = 1 demonstrates a perfect regression model. Generally, the higher the $R^2$is, the better the ML model is.

In this study, the XGBoost model is constructed with the built-in functions provided by the Python library of (XGBoost 2021). The GBM, SVM, and ANN models are built with the Scikit-Learn library (Pedregosa et al. 2011). The MARS and GP are developed using the MATLAB toolboxes provided in (Jekabsons 2016) and (Searson 2015), respectively. The SPLR model is constructed in MATLAB by the author. It is noted that the five-fold cross validation processes (Wong and Yeh 2020) were employed to set the free parameters of the ML models.

Table 3. Prediction performance of the models in terms of RMSE

Data	Models						
	XGBoost	GBM	SVM	MARS	GP	ANN	SPLR
1	1.57	1.78	1.33	1.58	**1.24**	1.97	2.45
2	**0.31**	0.47	0.92	0.93	1.55	1.62	2.02
3	2.61	2.34	**1.2**	1.36	1.92	1.96	2.27
4	5.74	**5.21**	7.11	7.52	8.09	8.15	6.35
5	**2.78**	2.91	6.02	3.07	3.9	6.01	5.6
6	2.85	2.72	**2.24**	3.08	3.09	3.67	3.45
7	2.33	2.24	2.43	**2.15**	2.24	2.85	2.5
8	3.54	**3.14**	4.51	5.28	5.77	4.52	5.04
9	**3.6**	**3.6**	12.02	4.12	4.27	6.72	4.23
10	**4.14**	4.19	5.26	6.21	6.48	5.93	6.33
11	**2.58**	2.63	4.74	2.99	5.44	5.47	4.96

Note: Bold texts indicate the best outcomes.

Table 4. Computational time (s)

Data	Concrete strength prediction models

	XGBoost	GBM	SVM	MARS	GP	ANN	SPLR
1	0.03	0.03	0.01	0.12	96.38	0.04	0.05
2	0.03	0.08	0.14	11.33	222.92	0.08	0.05
3	0.03	0.04	0.01	0.10	1.70	0.05	0.06
4	0.04	0.13	0.04	21.15	227.53	0.14	0.70
5	0.03	0.04	0.01	3.80	101.20	0.04	0.03
6	0.03	0.02	0.02	1.50	103.18	0.21	0.06
7	0.03	0.01	0.01	0.06	101.44	0.07	0.08
8	0.04	0.02	0.01	0.13	103.64	0.11	0.03
9	0.03	0.03	0.01	0.66	100.40	0.15	0.75
10	0.06	0.20	0.15	7.30	968.45	0.40	0.29
11	0.03	0.10	0.02	10.87	19.00	0.17	0.14

The performances of the employed ML models in each dataset are presented in **Table 3** and **Table 4**. In **Table 3**, the model accuracy is presented in terms of the average RMSE obtained from the testing phase. The bold figures indicate the best outcomes. As can be observed from the experimental results, the XGBoost model has achieved the best performances in 5 out of 11 datasets. The GBM model is the second best model with 5 times being the 1st rank. The SVM model has been ranked as the best model twice. Meanwhile, each of the MARS and GP models attains the best outcome in one dataset. The model ranking is further demonstrated by **Fig. 2**. **Table 3** reports the average computation time of each model with respect to different datasets. It can be seen that the XGBoost's training phases are fast, with the average training time ranging from 0.03 to 0.06s. On the contrary, the GP requires much longer computational cost for model training; its training time can go up to 968s in the dataset 10. It is understandable because the training phase of the XGBoost model can be carried out in parallel. Meanwhile, the evolutionary operations performed by the GP's populations require much higher computational cost to accomplish.

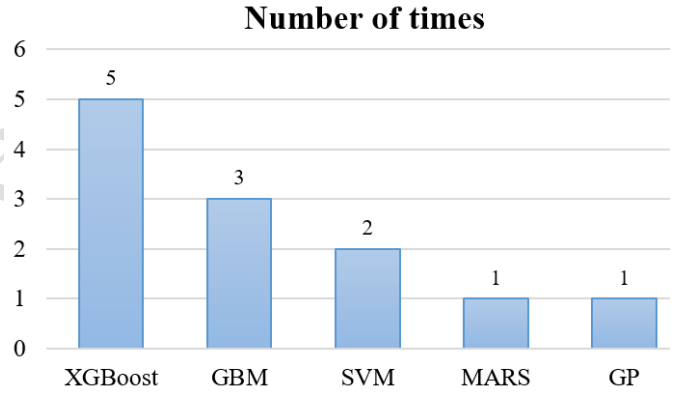


Fig. 2 The number of times that the model achieves the 1st rank

Table 5. Performances of the best models (from dataset 1 to dataset 6)

Dataset	The best model	Performance indices	Mean	Std.
1	GP	RSME	1.24	0.36
		MAPE (%)	3.25	1.02
		R^2	0.97	0.03

2	XGBoost	RSME	1.55	0.16
		MAPE (%)	2.48	0.35
		R^2	0.97	0.01
3	SVM	RSME	1.20	0.34
		MAPE (%)	2.93	1.47
		R^2	1.00	0.00
4	GBM	RSME	5.21	0.88
		MAPE (%)	12.34	2.45
		R^2	0.91	0.03
5	XGBoost	RSME	2.78	0.62
		MAPE (%)	5.13	1.33
		R^2	0.98	0.01
6	SVM	RSME	2.24	0.67
		MAPE (%)	2.72	0.78
		R^2	0.93	0.05

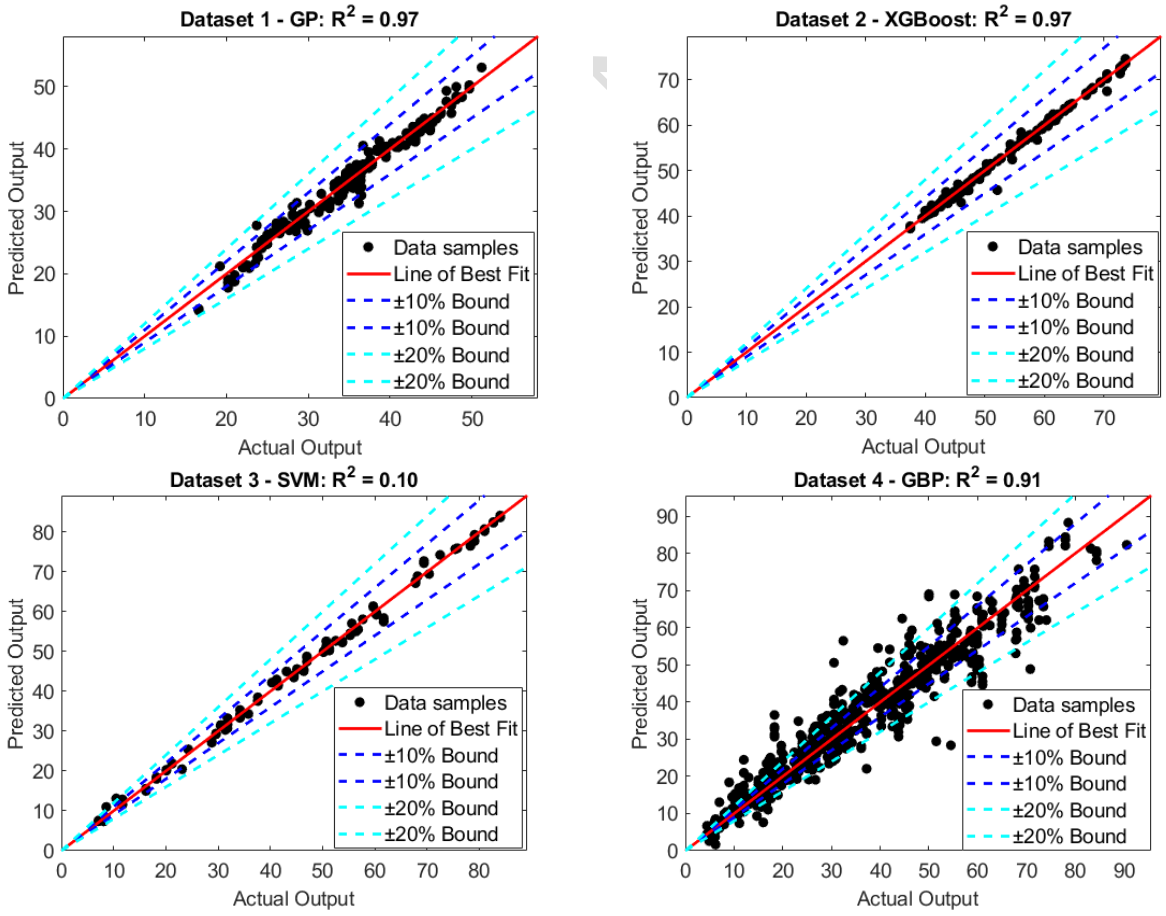
Table 6. Performances of the best models (from dataset 7 to dataset 11)

Dataset	The best model	Performance indices	Mean	Std.
7	MARS	RSME	2.15	0.39
		MAPE (%)	8.28	2.85
		R^2	0.95	0.03
8	GBM	RSME	3.14	0.95
		MAPE (%)	19.20	10.30
		R^2	0.94	0.05
9	XGBoost	RSME	3.60	0.63
		MAPE (%)	4.90	1.03
		R^2	0.97	0.01
9	GBM	RSME	3.60	0.69
		MAPE (%)	4.87	1.12
		R^2	0.97	0.01
10	XGBoost	RSME	4.14	0.44
		MAPE (%)	9.97	1.14
		R^2	0.94	0.02
11	XGBoost	RSME	2.58	0.85
		MAPE (%)	5.10	5.00
		R^2	0.97	0.02

In addition, the detailed performance of the best model associated with each dataset is presented in **Table 5** and **Table 6**. As can be seen from the experimental results, the ML models are able to fit the datasets to a high degree. These results clearly demonstrate the capability of the ML models in CS prediction of various types of concrete. In general, the MAPE of the CS

estimations can be as low as 2.48% in the case of the XGBoost used for predicting the high-strength concrete samples provided in the dataset 2 (Al-Shamiri et al. 2019). The R^2 values in all datasets are higher than 0.90 which indicates a sufficient degree of variance explanation. Additionally, in 8 out of 11 datasets, the R^2 is greater than or equal to 0.95. The SVM model used for predicting the CS of rubberized concrete achieves the R^2 of roughly 1 which indicates a nearly perfect fit. The scatter plots providing the overview of the data fitting results are presented in **Fig. 3**. Herein, the red straight line represents a perfect fit. The nearer the data points (denoted as black circles) to the red line, the better they are fitted by the ML models. The lines of ±10% and ±20% bounds are also added to inspect the magnitude of the models' residuals.

Most of the prediction errors lie within the ±20% bound. The dataset 4 (self-compacting concrete blended with class F fly ash), the dataset 8 (lightweight foamed concrete), and the dataset 10 (high-performance concrete) have high proportions of data beyond the ±20% bound. One possible reason for this phenomenon is that the complexity of the mapping functions between the CS and its influencing factors hidden in those data is high. Notably, the number of influencing factors used by the dataset 8 is 4 which is quiet limited. It is possible that the CS values of the lightweight foamed concrete samples are affected by other explanatory factors that are not yet covered by the current work. Datasets 1, 2, 3, 5, 6, and 9 have the major proportion of the samples lying within the ±10% bound; this fact indicates a strong correlation between the estimated and the observed CS values.



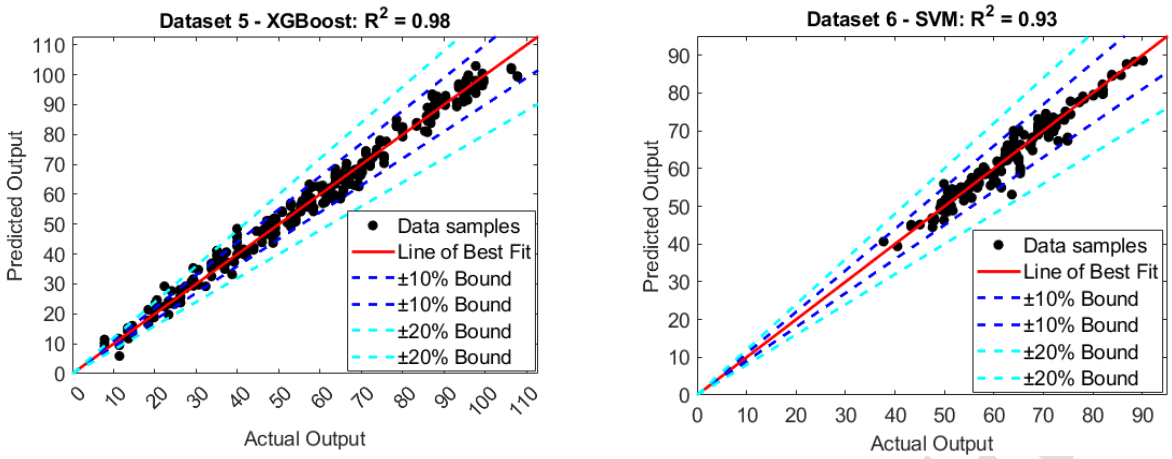
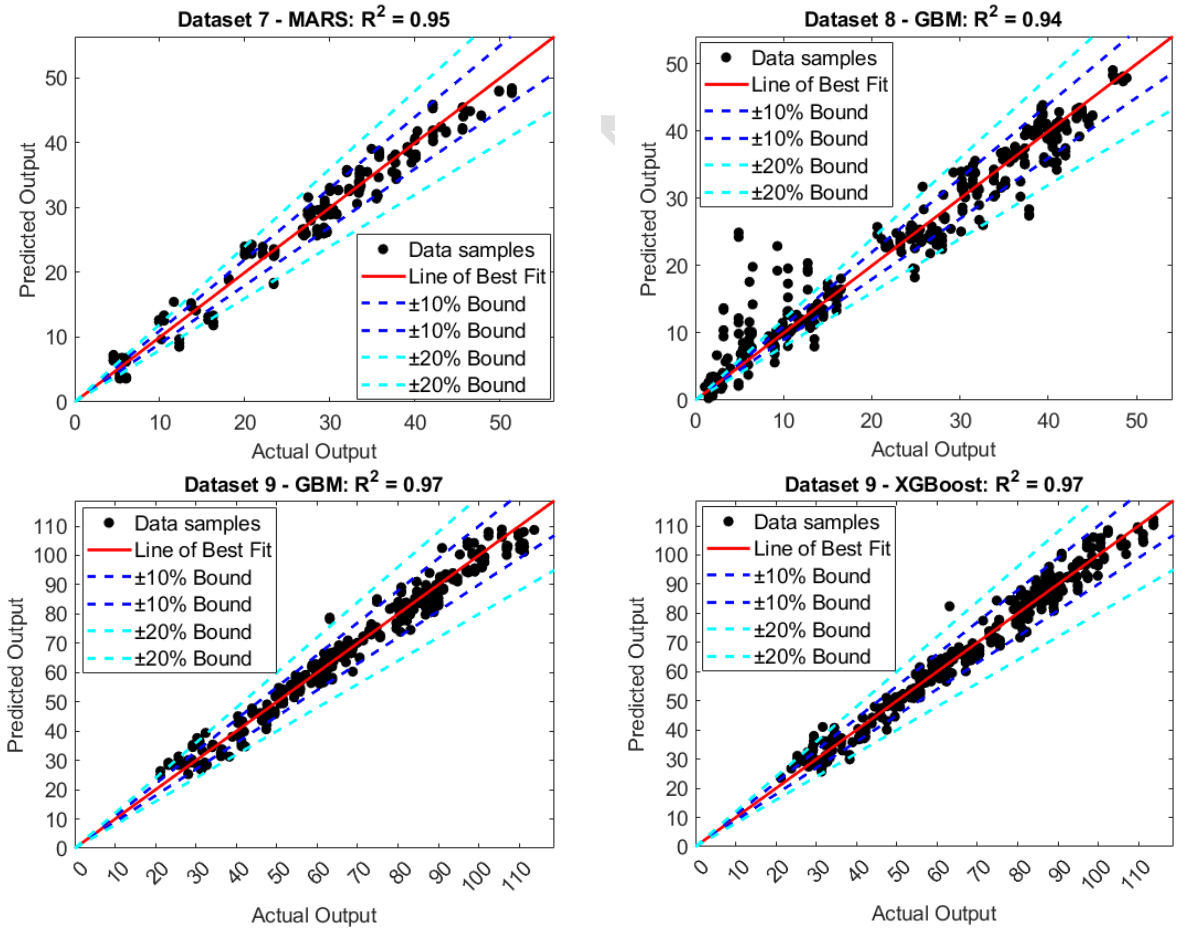


Fig. 3 Line of best fit plots



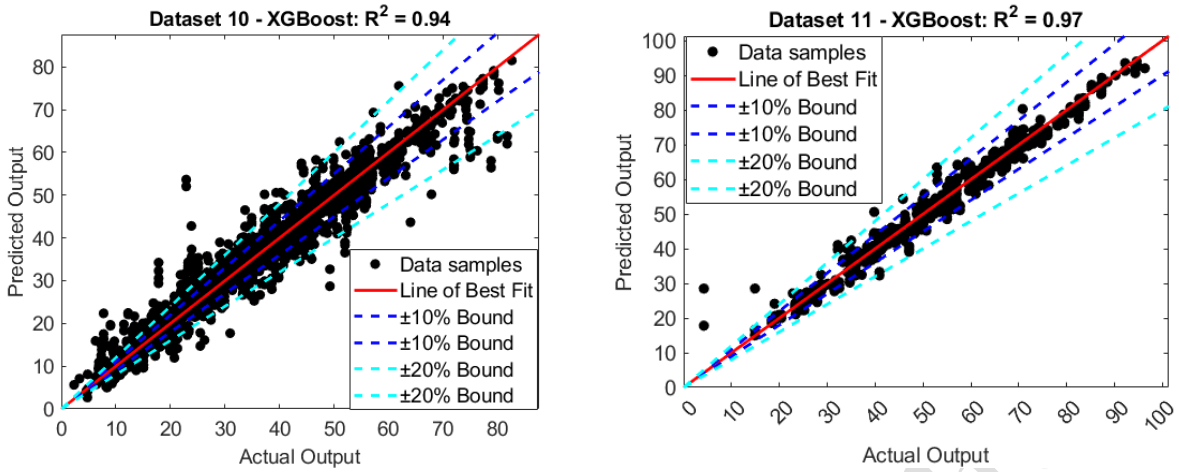


Fig. 3 Line of best fit plots (cont)

Table 7. Summary of the models' rank

Models	Dataset										
	1	2	3	4	5	6	7	8	9	10	11
XGBoost	3	1	7	2	1	3	4	2	1	1	1
GBM	5	2	6	1	2	2	2	1	1	2	2
SVM	2	3	1	4	7	1	5	3	7	3	4
MARS	4	4	2	5	3	4	1	6	3	5	3
GP	1	5	3	6	4	5	3	7	5	7	6
ANN	6	6	4	7	6	7	7	4	6	4	7
SPLR	7	7	5	3	5	6	6	5	4	6	5

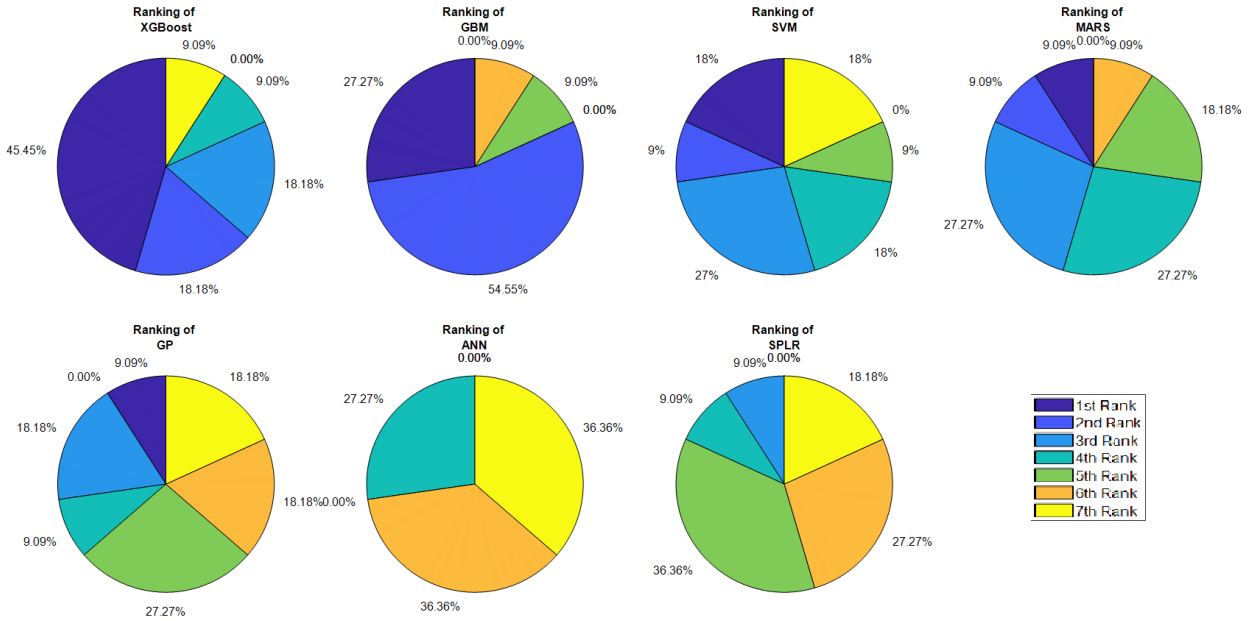


Fig. 4 Percentages of the model rankings

Table 7 and **Fig. 4** summarize the ranks of the ML models with respect to different datasets. Apparently, the XGBoost is the best model with five 1st ranks, two 2nd ranks, and two 3rd ranks. The GBM model is the second best one with three 1st ranks and six 2nd ranks. The SVM model succeeds the GBM model with two 1st ranks, one 2nd ranks, and three 3rd ranks. Each of the GP and MARS models achieves one 1st rank. However, MARS achieves the 2nd rank in one dataset. In addition, the highest rank of SPLR is 3rd; the rank of the ANN model never goes higher than 4th. Comparing the performances of these two models in other datasets, it can be concluded that the result of SPRL is slightly better than that of ANN. Thus, the outcomes of this study are in line with the previous works of (Nguyen et al. 2021) and (Kang et al. 2021) which points out the advantage of the XGBoost and GBM models. However, the SVM, MARS, and GP models can also be the models of choice in the tasks of predicting the CS of the rubberized concrete, concrete containing ground granulated blast-furnace slag (GGBS), and lightweight concrete containing silica fume. More detailed regarding the performances of the ML models are reported in Appendix 1 (boxplots of the model performance) and Appendix 2 (detailed model ranking).

5. Concluding remarks

CS is considered the most important mechanical property of concrete. This index serves as a crucial indicator of the concrete quality. Reliable prediction of the CS can significantly assist construction material engineers and researchers in the task of concrete mixture design. This study carried out a large-scale comparative study which investigates the performance of the prominent ML models used in estimating the CS of 11 historical datasets. The number of explanatory variables in these datasets ranges from 4 to 10. The number of samples ranges from 70 to 1030. XGBoost, GBM, SVM, MARS, GP, ANN, and SPLR are employed and their performances are benchmarked with the indices of RMSE, MAPE, and R^2. Repetitive data sampling processes, consisting of 20 independent runs, are used for reliably assessing the model predictive capability.

Experimental results point out that the XGBoost model has achieved the most desired outcomes with 5 times of 1st rank. Its performance is followed by the GBM, SVM, MARS, and

GP. The highest rank that the SPRL achieves is 3rd; its performance is slightly better than that of ANN. In general, XGBoost and GBM are the models of choice when dealing with the task of CS estimation. However, SVM, MARS, and GP should also be attempted for estimating the CS of the rubberized concrete, concrete containing ground granulated blast-furnace slag (GGBS), and lightweight concrete containing silica fume.

The prediction of the CS of diverse concrete types is a highly active research topic. Therefore, there are various datasets of concrete strength that are documented in the literature. In addition, researchers continuously compile, analyze, and report the testing records of the CS of concrete. Hence, due to the limited time frame of the current study, the selected datasets in the current work cannot be comprehensive and cover all relevant datasets. In addition to the selected ML models, many other advanced methods (e.g., sophisticated ensembles of decision trees, light gradient boosting machines, neural networks trained by novel metaheuristic algorithms, etc.) also have potential for the task of interest.

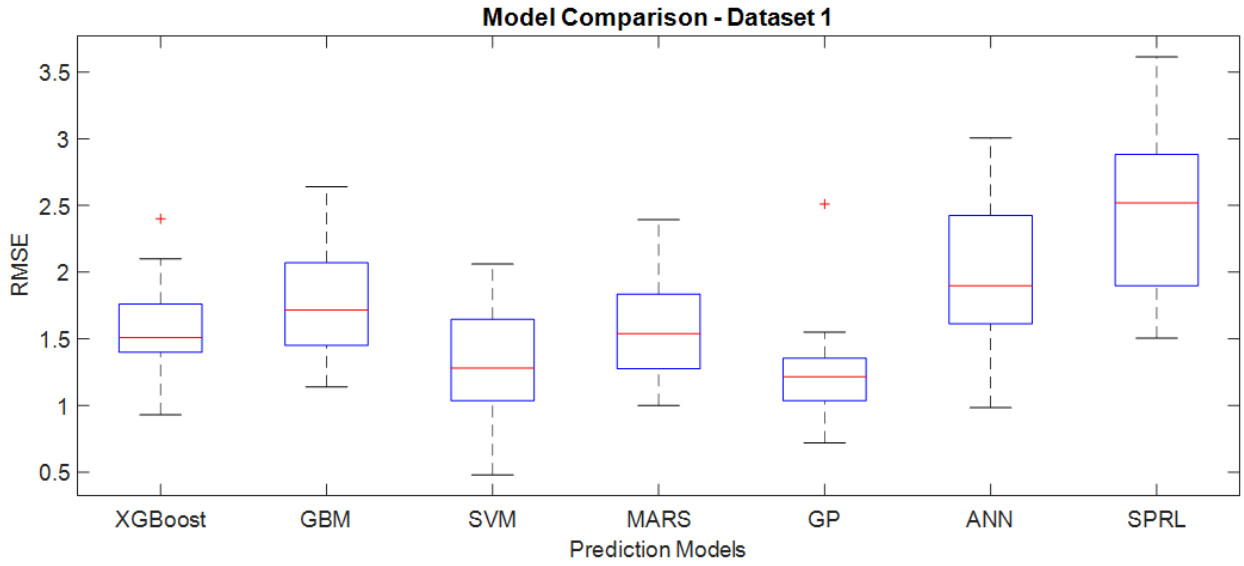
Accordingly, the current work can be extended in multiple ways: (i) the investigation of other advanced ML methods such as deep learning regression (Zeng et al. 2022), hybrid ensemble learning (Cao et al. 2022), metaheuristic-trained ANN (Zhang et al. 2021), and ensemble deep neural networks (Barkhordari and Massone 2022), (ii) the collection of more experimental datasets used for model validation, and (iii) the applications of advanced feature selection for enhancing the model performance.

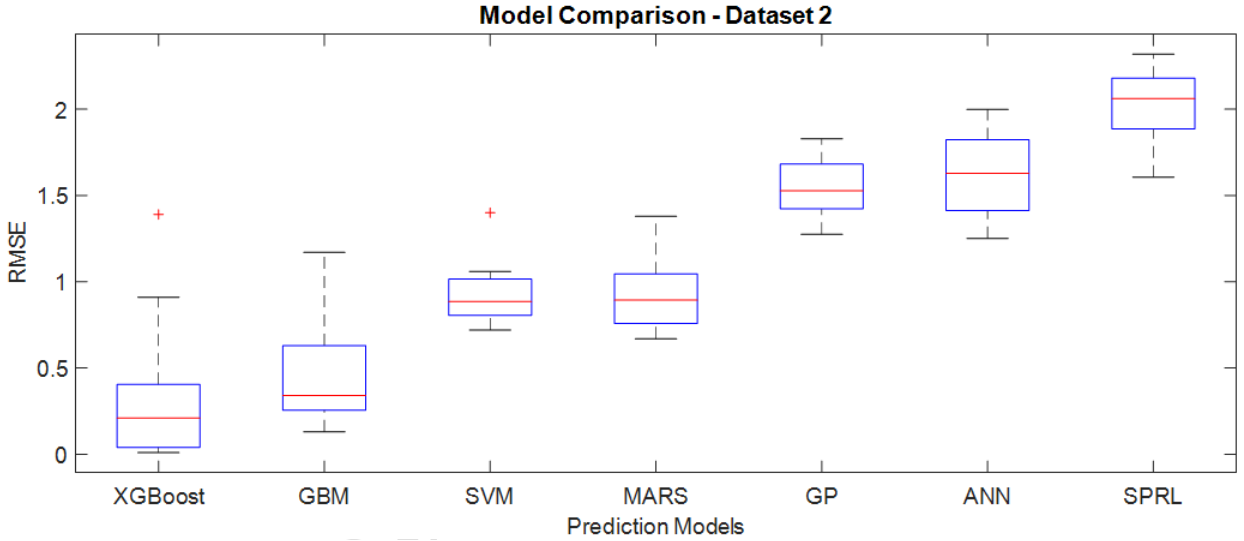
Supplementary material

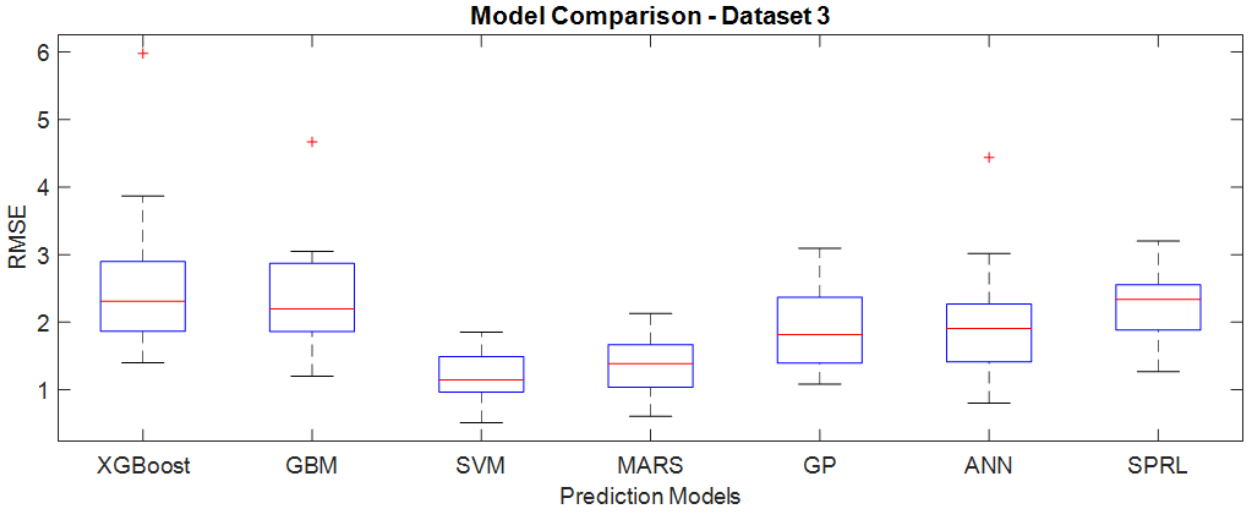
The datasets used to support the findings of this study are deposited in Github repository as follows: https://github.com/NHDDTUEDU/CS_ML.

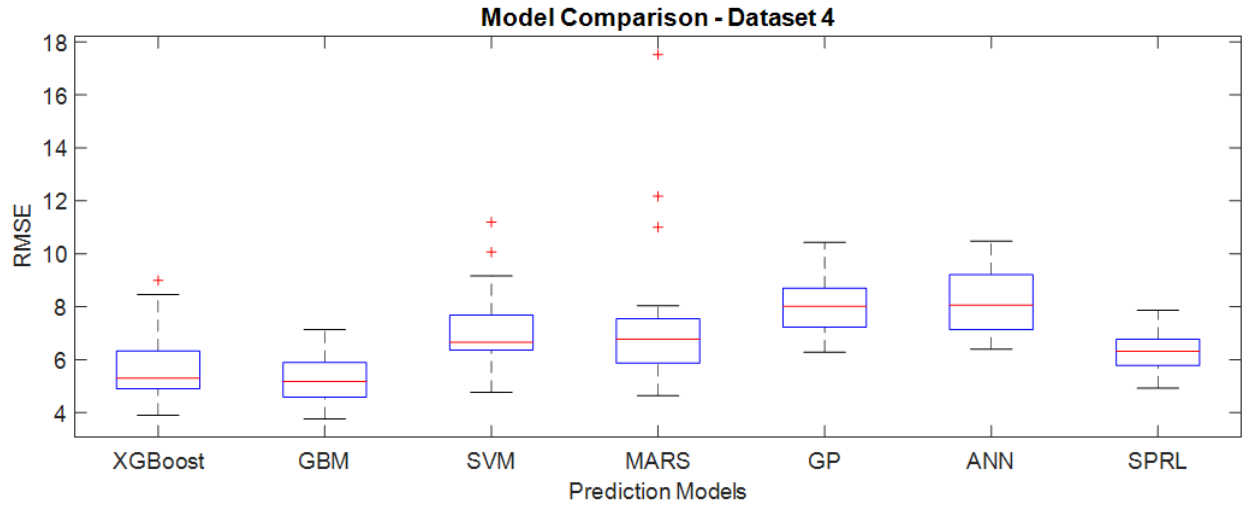
Appendix 1

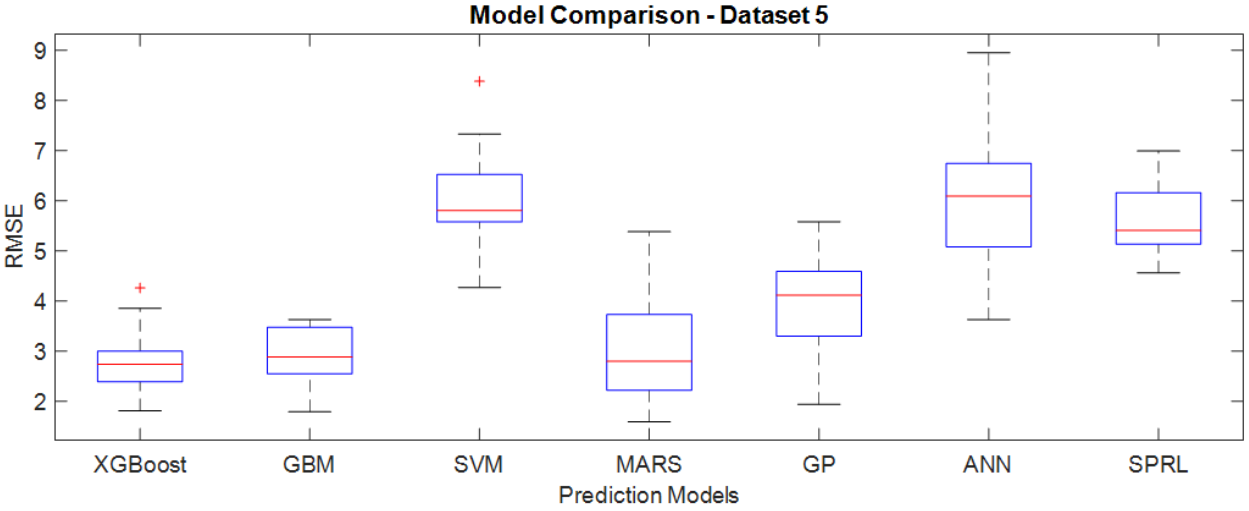
Boxplots of the model performance

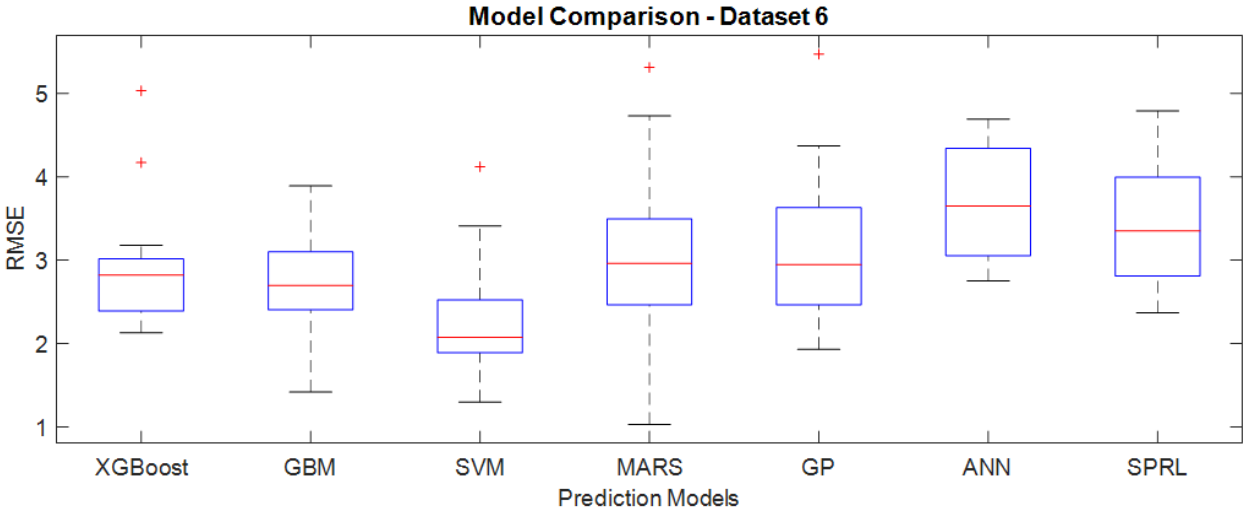

Model Comparison - Dataset 1
RMSE
3.5
3
2.5
2
1.5
1
0.5
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models

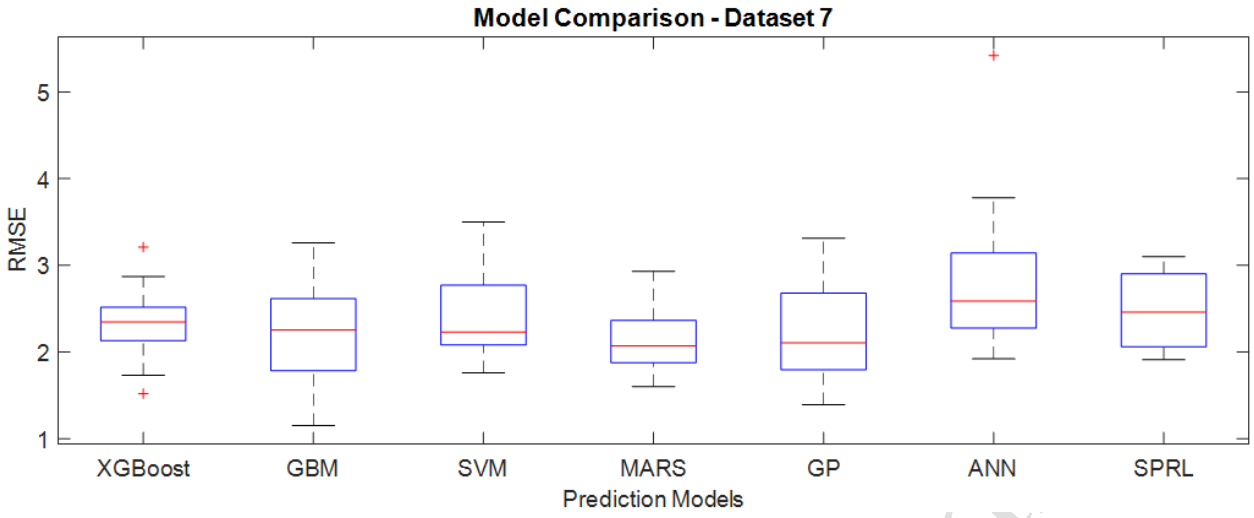

Model Comparison - Dataset 2
RMSE
2
1.5
1
0.5
0
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models

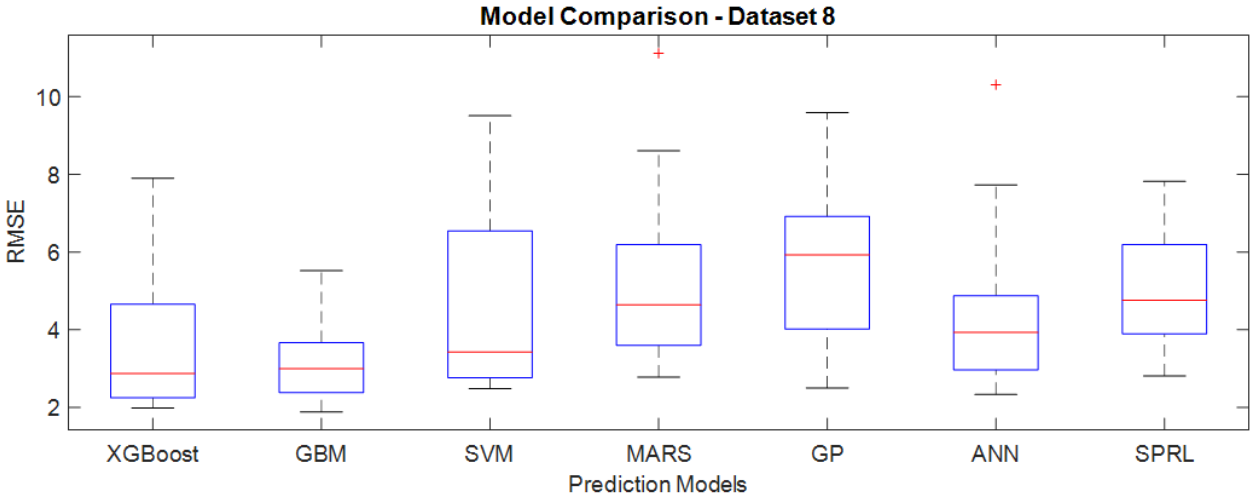

Model Comparison - Dataset 3
RMSE
6
5
4
3
2
1
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models

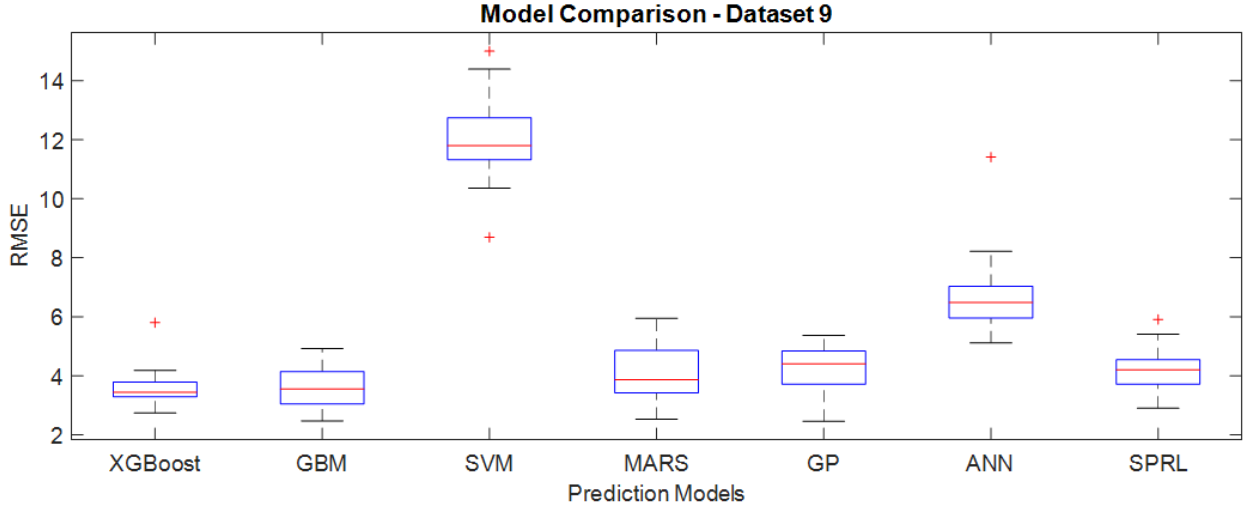

Model Comparison - Dataset 4
RMSE
18
16
14
12
10
8
6
4
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models

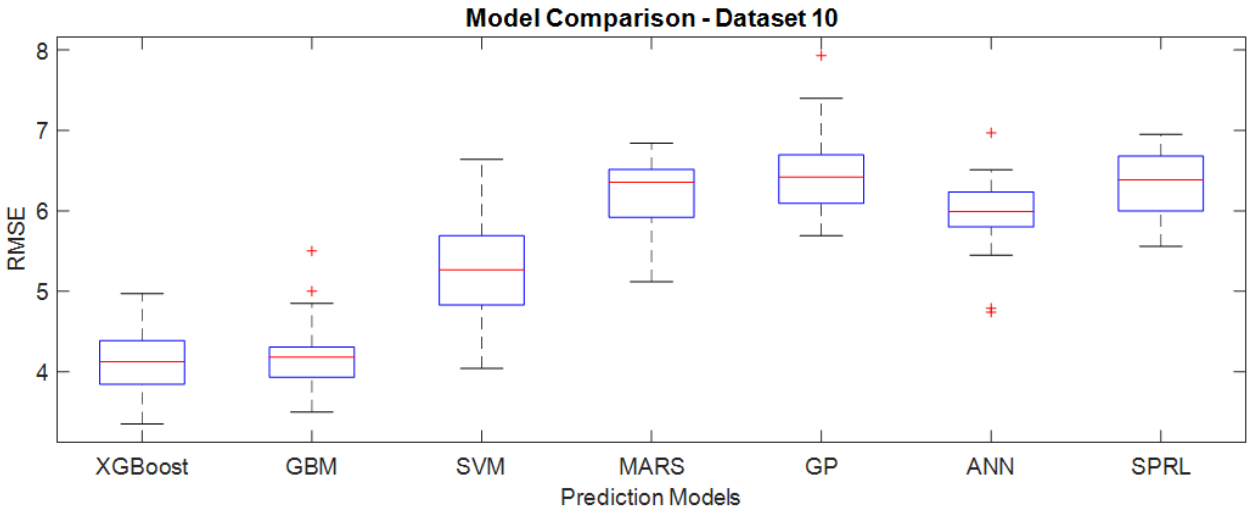

Model Comparison - Dataset 5
RMSE
9
8
7
6
5
4
3
2
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models

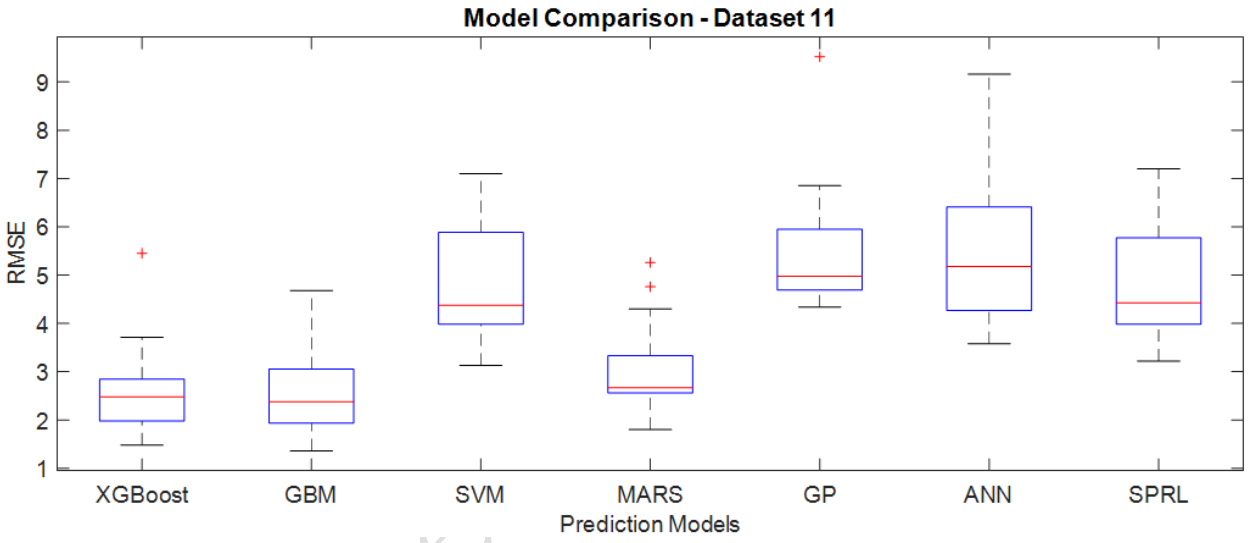

Model Comparison - Dataset 6
RMSE
5
4
3
2
1
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models


Model Comparison - Dataset 7
RMSE
1
2
3
4
5
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models


Model Comparison - Dataset 8
RMSE
2
4
6
8
10
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models


Model Comparison - Dataset 9
RMSE
2
4
6
8
10
12
14
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models


Model Comparison - Dataset 10
RMSE
8
7
6
5
4
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models


Model Comparison - Dataset 11
RMSE
9
8
7
6
5
4
3
2
1
XGBoost
GBM
SVM
MARS
GP
ANN
SPRL
Prediction Models

Appendix 2

Models' ranking

Table A2. Ranking of the models

Dataset	Models	RMSE	Ranking
1	GP	1.24	1
	SVM	1.33	2
	XGBoost	1.57	3
	MARS	1.58	4
	GBM	1.78	5
	ANN	1.97	6
	SPRL	2.45	7
2	XGBoost	0.31	1
	GBM	0.47	2
	SVM	0.92	3
	MARS	0.93	4
	GP	1.55	5
	ANN	1.62	6
	SPRL	2.02	7
3	SVM	1.20	1
	MARS	1.36	2
	GP	1.92	3
	ANN	1.96	4
	SPRL	2.27	5
	GBM	2.34	6
	XGBoost	2.61	7
4	GBM	5.21	1
	XGBoost	5.74	2
	SPRL	6.35	3
	SVM	7.11	4
	MARS	7.52	5
	GP	8.09	6
	ANN	8.15	7
5	XGBoost	2.78	1
	GBM	2.91	2
	MARS	3.07	3
	GP	3.9	4
	SPRL	5.6	5
	ANN	6.01	6
	SVM	6.02	7

Table A2. (cont)

Dataset	Models	RMSE	Ranking
6	SVM	2.24	1
	GBM	2.72	2
	XGBoost	2.85	3
	MARS	3.08	4
	GP	3.09	5
	SPRL	3.45	6
	ANN	3.67	7
7	MARS	2.15	1
	GBM	2.24	2
	GP	2.24	3
	XGBoost	2.33	4
	SVM	2.43	5
	SPRL	2.50	6
	ANN	2.85	7
8	GBM	3.14	1
	XGBoost	3.54	2
	SVM	4.51	3
	ANN	4.52	4
	SPRL	5.04	5
	MARS	5.28	6
	GP	5.77	7
9	XGBoost	3.60	1
	GBM	3.60	2
	MARS	4.12	3
	SPRL	4.23	4
	GP	4.27	5
	ANN	6.72	6
	SVM	12.02	7
10	XGBoost	4.14	1
	GBM	4.19	2
	SVM	5.26	3
	ANN	5.93	4
	MARS	6.21	5
	SPRL	6.33	6
	GP	6.48	7

Table A2. (cont)

Dataset	Models	RMSE	Ranking
11	XGBoost	2.58	1
	GBM	2.63	2
	MARS	3.94	3
	SVM	4.74	4
	SPRL	4.96	5
	GP	5.44	6
	ANN	5.47	7

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