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Predicting the flexural strength of 3D-printed geopolymer reinforced concrete using machine learning techniques

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ABSTRACT

Both geopolymer concrete and 3D printing are innovative trends in construction materials science. This study investigates the prediction of 3D printed geopolymer reinforced concrete due to lack of information and studies on the prediction of 3D printed geopolymer reinforced concrete. This study investigated for the first time the flexural strength of 3D printed reinforced concrete through compressive strength with concrete mix design. Rigid, Lasso, elastic net, random forest, gradient boosting, decision tree, support vector machine regression and k-nearest neighbor are examined in this study. Considering to this study, compressive strength and flexural strength have more than 0.97 relationship. Moreover, the best result was for gradient boosting, random forest and k-nearest neighbor with 0.85 and 0.89.

KEYWORDS

3D printing concrete • 3D printing reinforced concrete • auxetic • geopolymer • prediction

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Introduction

Geopolymer concrete is a type of green concrete that reduces the negative effects of using concrete and cement, which is why many researchers use geopolymer concrete [1]. Cement production and use releases large amounts of carbon dioxide into the atmosphere, while geopolymer concrete can reduce this amount by eliminating cement [2].

The geopolymer concrete has high potential strength such as high compressive strength, low alkaline expansion, low shrinkage and etc. [3,4]. Amin et al. [5] studied the geopolymer concrete with fly ash, metakaolin, and slag. They found that compressive strength is more than 60 MPa, tensile strength is more than 6.2 MPa and flexural strength is more than 9.2 MPa. Silica fume and micro silica, with a high percentage of silicon, can improve mechanical properties such as compressive strength of geopolymer concrete [6]. Wu et al. [7] analyzed geopolymer concrete with silica fume and sodium silicate as activator. They found that compressive strength can achieve more than 43.63 MPa. Adding microsilica and silica fume as powder form to geopolymer concrete can create aluminosilicate (N-A-S-H) geopolymer gel. In addition, sodium silicate solution as an activator is a good option for addition to geopolymer concrete [8]. Gel products are calcium silicate gel (C-S-H) converted to calcium aluminosilicate gel (C-A-S-H) [9].

De Oliveira et al. [10] have proven the high durability of geopolymers. Mintsaev et al. [11] studied features of the synthesis of construction geopolymer composites. A. Jan et al. [12] found that when 0.25 % polypropylene fibers (PPF) were added to geopolymer concrete, the compressive strength improved by more than 3.73 %. Some studies show that different types of fiber such as steel, basalt and etc. can improve the mechanical properties of concrete such as compressive, tensile and flexural strengths [13–15]. According to Levkina and Titova [16], the use of innovative products, such as geopolymers, can become an impetus for the development of small businesses in the regions.

Despite the above studies, there is a lack of information and research on the prediction of 3D printed geopolymer reinforced concrete. This study first investigated the flexural strength of 3D printed geopolymer reinforced concrete through compressive strength with concrete mix design. This study considers the stiff methods, lasso, elastic net, random forest, gradient boosting, decision tree, support vector regression and K-nearest neighbors. It is necessary to identify the relationship between compressive strength and flexural strength. The aim of the study is to predict the flexural strength of 3D-printed reinforced concrete using machine learning methods. The tasks were:

1. Establishing the relationship between the compressive and flexural strengths of concrete and identifying the best predictive models.
2. Identifying the influence of various factors on the mechanical properties of 3D-printed reinforced concrete.
3. Determining the potential for the innovative results obtained.

Materials and Methods

Materials

This study was conducted on geopolymer concrete containing microsilica and sodium silicate. In this research, in order to investigate the effect of microsilica geopolymer concrete and different aggregates, fine and coarse aggregates were mixed in different proportions (Fig. 1). Sodium silicate was sprayed on the concrete as an activator during the curing period due to the creation of an alkaline environment due to the creation of a geopolymer activator. Table 1 shows the mixture design of current study concrete.

Methodology

The compressive strength is based on the ASTM C109 [17] for cube (5 × 5 × 5 cm^3), and flexural strength as three-point bending strength as prism (16 × 4 × 4 cm^3) [18].

Table 1. Current study mixture design

Sample	Micro silica, kg/m³	Water, kg/m³	Fine aggregate, kg/m³	Coarse aggregate, kg/m³	Marble powder, kg/m³	Glass powder, kg/m³	Super-plasticizer, kg/m³
CF100	600	370	1180	0	150	200	55.5
CF80	600	370	944	236	150	200	55.5
CF60	600	370	708	472	150	200	55.5
CF40	600	370	472	708	150	200	55.5
CF20	600	370	236	944	150	200	55.5
CF0	600	370	0	1180	150	200	55.5

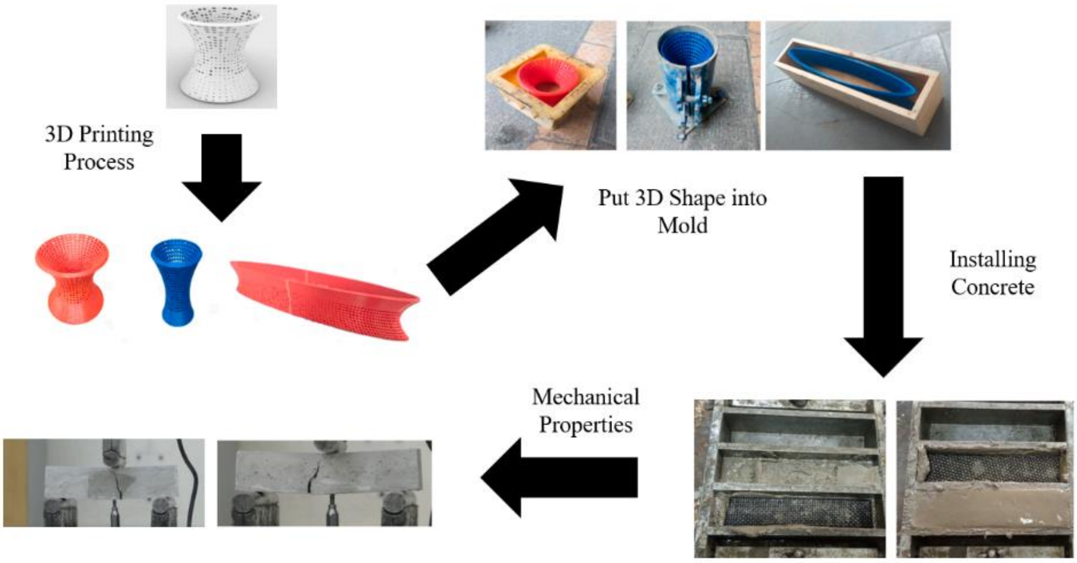

Fig. 1. Scheme of 3D printed reinforced concrete based on [18,19]

Regressions

In this study, Rigid, Lasso, elastic net, dissection tree, random forest, GBoost, SVR and KNN used (Table 2).

Table 2. Current study mixture design

Regression	Alpha	max_depth	min_samples_leaf	min_samples_split	_estimators	learning_rate	C	gamma	kernel
Ridge	0.615	–	–	–	–	–	–	–	–
Lasso	0.885	–	–	–	–	–	–	–	–
Random forest	–	20	1	4	50	–	–	–	–
Gradient boosting	–	9	–	4	50	0.124	–	–	–
SVR	–	–	–	–	–	–	92.76	10.0	rbf

In this term, ridge regression illustrated in Eq. (1) decreases errors and obtains more accuracy [20,21]:

$$v = \delta_0 + \delta_1 w_1 + \delta_2 w_2 + \delta_3 w_3 + \delta_4 w_4 + \varepsilon + \lambda \sum (\delta_1^2 + \delta_2^2 + \delta_3^2 + \delta_4^2), \quad (1)$$

where v is the dependent variable, w is the independent variable, δ_0 is the y-intercept and δ_1 is the regression coefficient representing the change in v concerning the change in w, also called the slope, and λ is the ridge regression penalty ratio, ε is the error term, $\sum(\delta_i^2)$ represents the sum of the squares of the coefficients.

Lasso regression means least absolute shrinkage and selection operator (LASSO). Lasso regression is a usual regression for solving multicollinearity issues, while unlike ridge regression, results in some coefficient predictions are equal to zero. Equation (2) shows the Lasso regression equation [21,22]:

$$v = \delta_0 + \delta_1 w_1 + \delta_2 w_2 + \delta_3 w_3 + \delta_4 w_4 + \varepsilon + \lambda \sum |\delta_1| + |\delta_2| + |\delta_3| + |\delta_4|, \quad (2)$$

Support vector machine (SVM) is a classification method for machine learning. In fact, support vector regression is solving problem by SVM as a regression. SVR can solve nonlinear and problems with high-dimensional [23–25].

Elastic net is a linear regression that combines two types of penalty functions to refine the best predictions. The best prediction is analyzed by the Scikit-learn package with a parameter in the range [0,1]. This algorithm is much closed for lasso prediction as the minimum contraction and selection operator. This algorithm reduces the complexity of the algorithm [26,27].

Decision tree is used for classification and prediction as a regression algorithm. In this algorithm, direct nodes are considered as root nodes and internal nodes are called leaf nodes. Usually, nodes in direct tree algorithm predict data category or direct data [28–30].

K-nearest neighbor is a supervised machine learning algorithm that solves problems with a small amount of data, usually for classification, but other studies also use it as regression. KNN solves the problem by finding the distance between the query and all the examples in the data by selecting a certain number of examples (k) close to the query, then averaging the labels in the case of a regression problem. The k-nearest neighbor algorithm is as follows [31]:

$$\bar{y} = \frac{1}{k} \sum_{j=1}^{k} y_i, \quad (3)$$

where y_i are actual values of the output characteristic and x_i are training examples attributes, x is test point, k is the number of nearest instances.

Random forest is an effective method that gives consistent answers. The reliability of the random forest method is related to the nature. Random forest is an advanced method related to decision trees with high efficiency [32,33]. All types of regression are applied to find the best prediction result to find the optimal and best result.

Validation

To find the verified prediction, the correlation coefficient (R^2) as expressed in Eq. (3), mean absolute errors (MAE), and root mean squared errors (RMSE) have been established [34]:

$$R^2 = 1 - \frac{\sum (y - \hat{y})^2}{\sum^n (y - \bar{y})^2}. \quad (4)$$

RMSE calculates the average deviation of each actual data point and the predicted results [35]:

$$RSME = \sqrt{\frac{1}{n} \sum^n (y - \hat{y})^2}. \quad (5)$$

Data collection

To data collection in this study, concrete mixture designs and concrete mechanical properties have been selected as the main parameter, in fact, compressive strength known as main character and the flexural strength known as the predictive character. This study used 3D printing study to collect data to find the concrete mixture and mechanical properties [18,19,36–39]. Due to lack of information about 3D printed reinforced concrete, Gaussian Noise has been selected to increase data more than 2000 with regard pervious data study.

Results

Hyperparameter and data

This heat map visually shows the distribution and intensity of different properties or components in a concrete mixture. A colour spectrum is used to highlight differences, with warm colours (such as red) representing higher values and cool colours (such as blue) representing lower values. This helps to quickly identify patterns, correlations, or anomalies in the data.

Figure 2 heat map visually displays the relationships between the various components of concrete and its mechanical properties. Correlation values close to 1 indicate a strong and direct relationship between the variables, while values close to (-1) indicate a strong and inverse relationship. For example, the strong negative correlation between water and compressive strength (-0.94) indicates that increasing the amount of water significantly reduces the compressive strength of concrete. On the other hand,

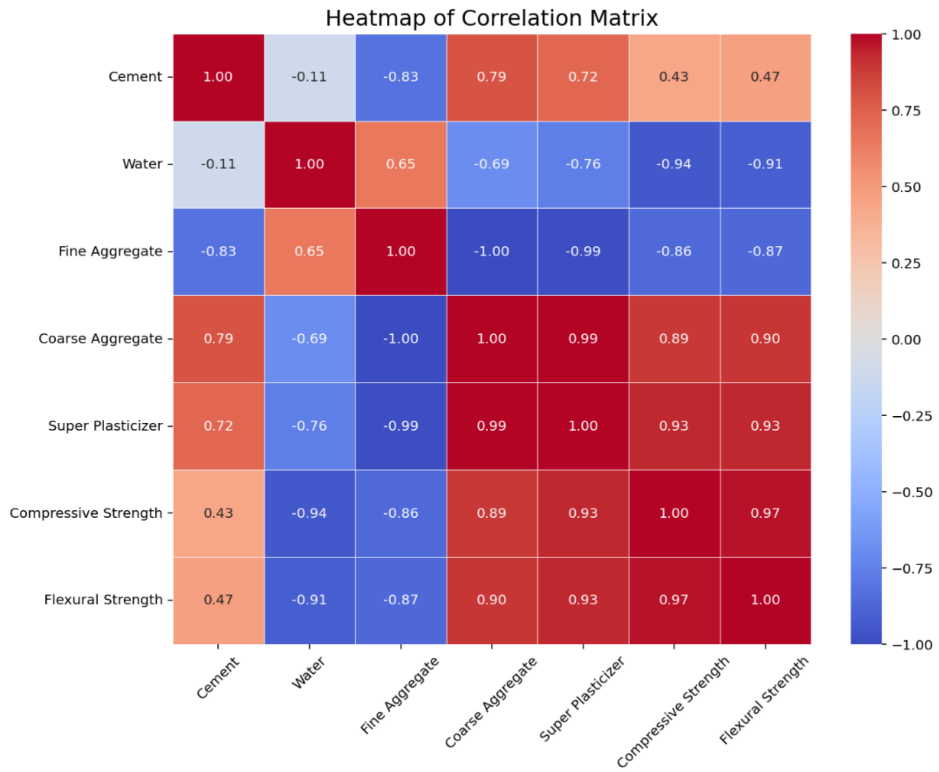

Fig. 2. Heatmap of concrete

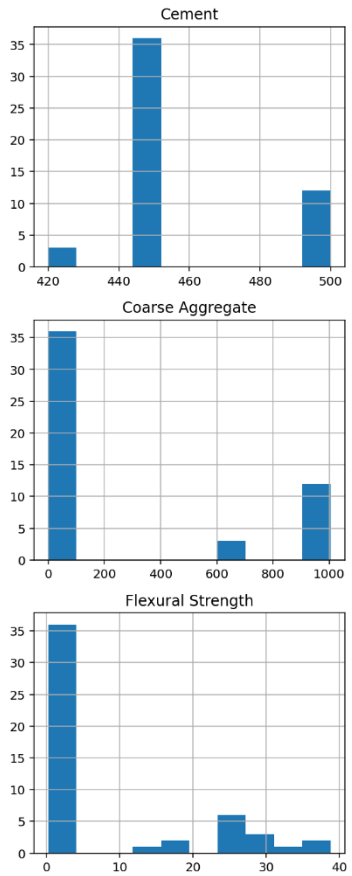

Fig. 3. Data distribution of current study

the positive correlation between coarse aggregate and compressive strength (0.89) indicates a positive effect of this material on increasing strength. Moreover, flexural strength and compressive strength have more than 0.97 positive effect. According to heat map water and fine aggregates have negative effect on the compressive and flexural strength, which means increasing fine aggregates and water can decrease the compressive and flexural strengths.

Figure 3 shows the distribution of the data collected in this study. This graph visually shows the dispersion and concentration of data related to concrete mix design and its mechanical properties. By examining this graph, it is possible to identify patterns in the data and use it for further analysis.

In the second part, Fig. 3 shows how the data is distributed across different ranges. This distribution helps researchers better understand the relationship between different variables, such as the compressive and flexural strengths of concrete. It can also reveal outliers or unusual data that may affect the results.

Finally, Fig. 3 serves as an auxiliary tool to verify the quality of the data used in machine learning models. By viewing this graph, researchers can ensure that the data has been collected in a balanced and representative manner, which increases the accuracy of the predictions made by the models.

Figure 4 in this study shows the scatter plot between flexural strength, compressive strength and other related data. These plots are plotted in pairs to clearly show the linear or nonlinear relationships between different variables. In the second part, Fig. 4 shows how other factors such as cement content, water and aggregates affect the strength of concrete. For example, increasing the water content reduces the compressive and flexural strengths, while cement and coarse aggregates have a positive effect on the strength of concrete. These relationships help researchers to understand the factors affecting the mechanical properties of concrete and design prediction models more accurately.

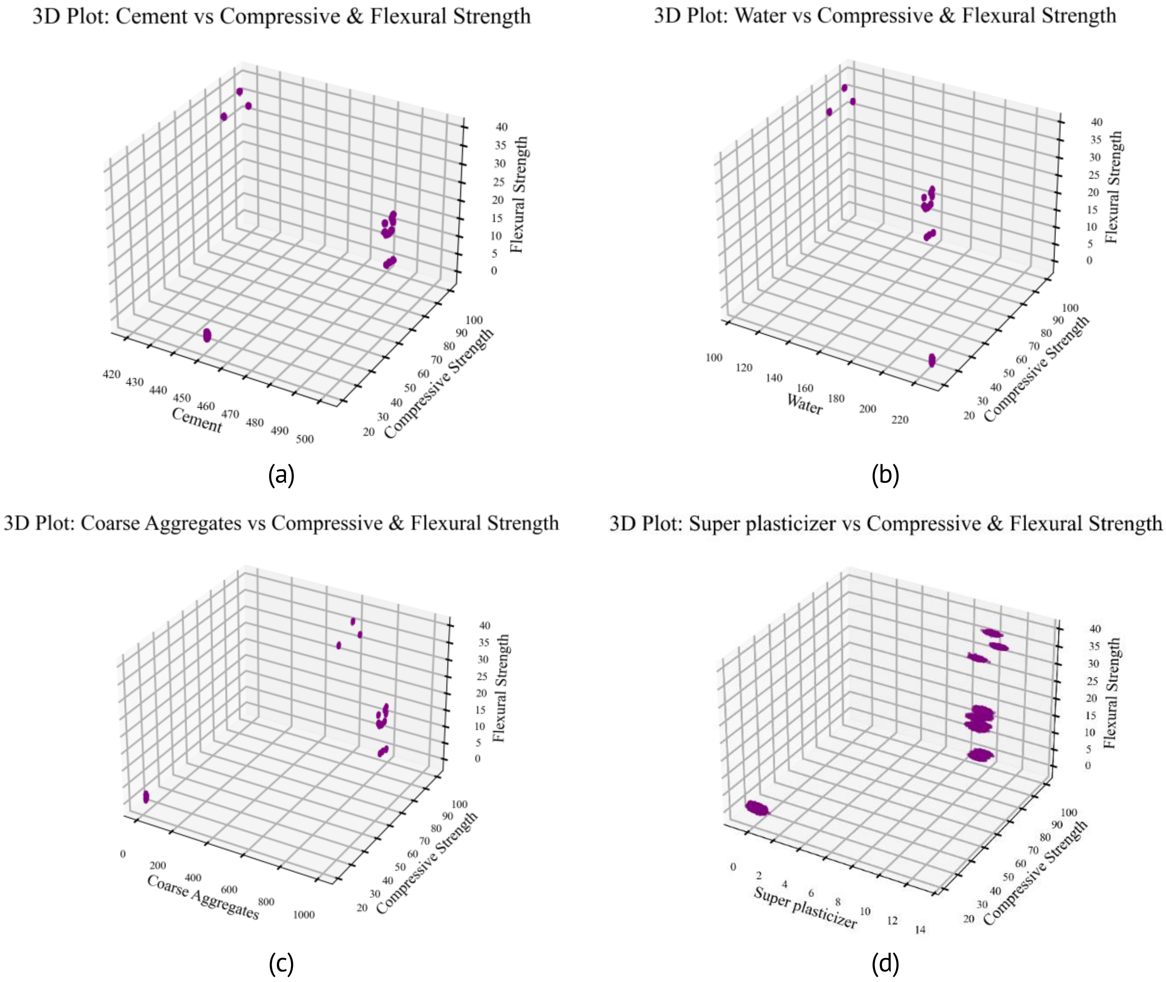

Fig. 4. The scatter plot between flexural strength, compressive strength and other data: (a) cement, (b) water, (c) coarse aggregates, (d) super plasticizer

Finally, Fig. 4 is used as an aid to validate data and machine learning models. By comparing the dispersion of the actual and predicted data, we can evaluate the accuracy of different models. These graphs also show that some models, such as Gradient Boosting and Random Forest, were able to identify patterns in the data well and provide more accurate predictions.

Figure 5(a) shows a multi-bar diagram of the gradient reinforcement model that ranks the factors affecting a system (i.e., concrete strength). In this diagram, cement is identified as the most important factor (around 0.35) as the key factor, while fine aggregate and water are in the next ranks. Other products such as superplasticizer and coarse aggregate have negligible or close to zero effects. These results indicate that the model considers cement as the most important variable in its prediction.

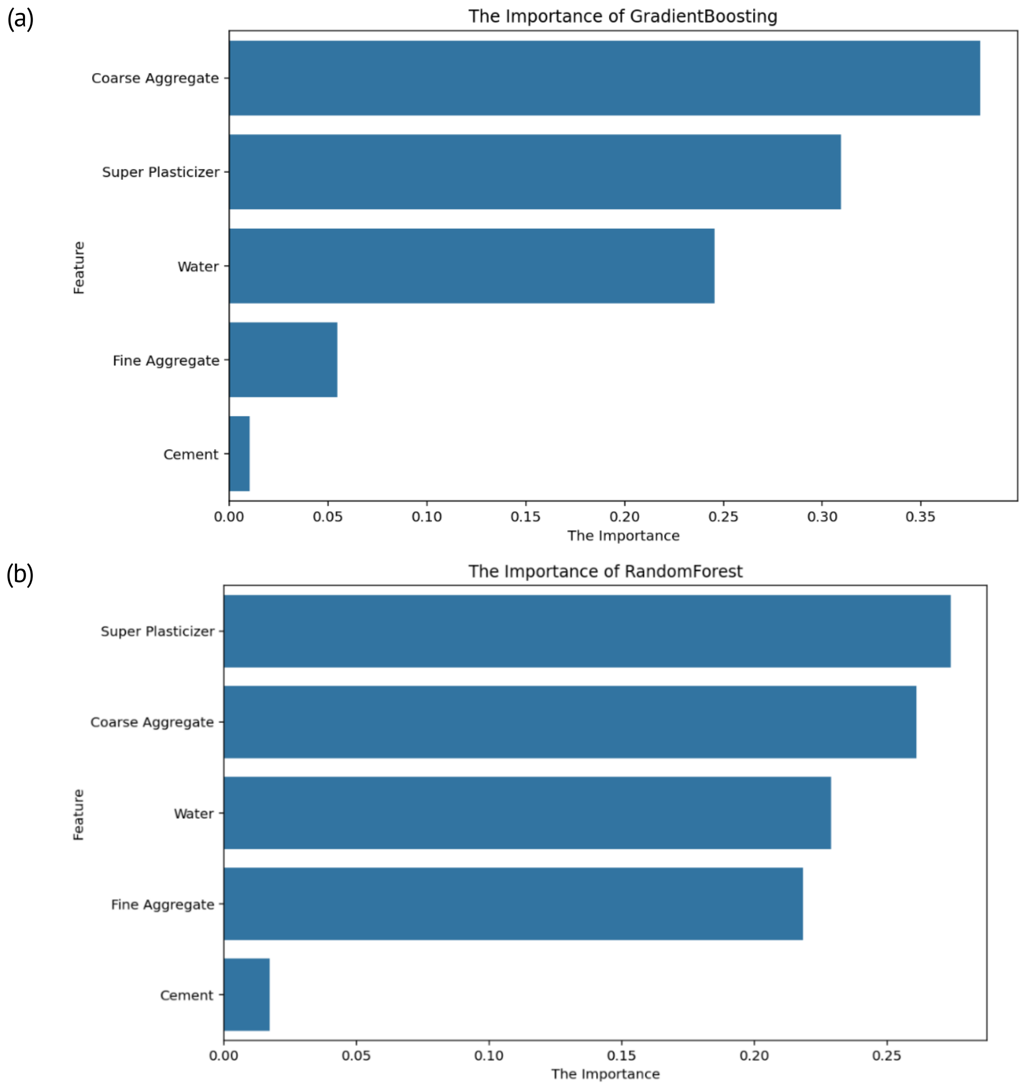

Fig. 5. The importance and features: (a) GBoost; (b) random forest

Figure 5(b) shows the importance of variables in the random forest model, indicating the influence of each factor on the model predictions. In this plot, cement is identified as the most influential variable with an importance of about 0.25. This is followed by fine aggregate and water with an importance of about 0.15 and 0.10, respectively. Other variables such as super plasticizer, coarse aggregate and unspecified Feature are less important, with some of them having a negligible impact on the model. These results indicate that cement plays a key role in the predictions of this model.

Regressions

All regression results are shown in Fig. 6. Considering to regression results the most data are divided by to clusters, however in KNN and random forest regressions three clusters are existed. In the first cluster, data are complex and close together, while data in the middle of data set are scatters.

Table 3 compares the performance of eight different regression models based on two metrics: r^2 (coefficient of determination) and RMSE (root mean square error). The models

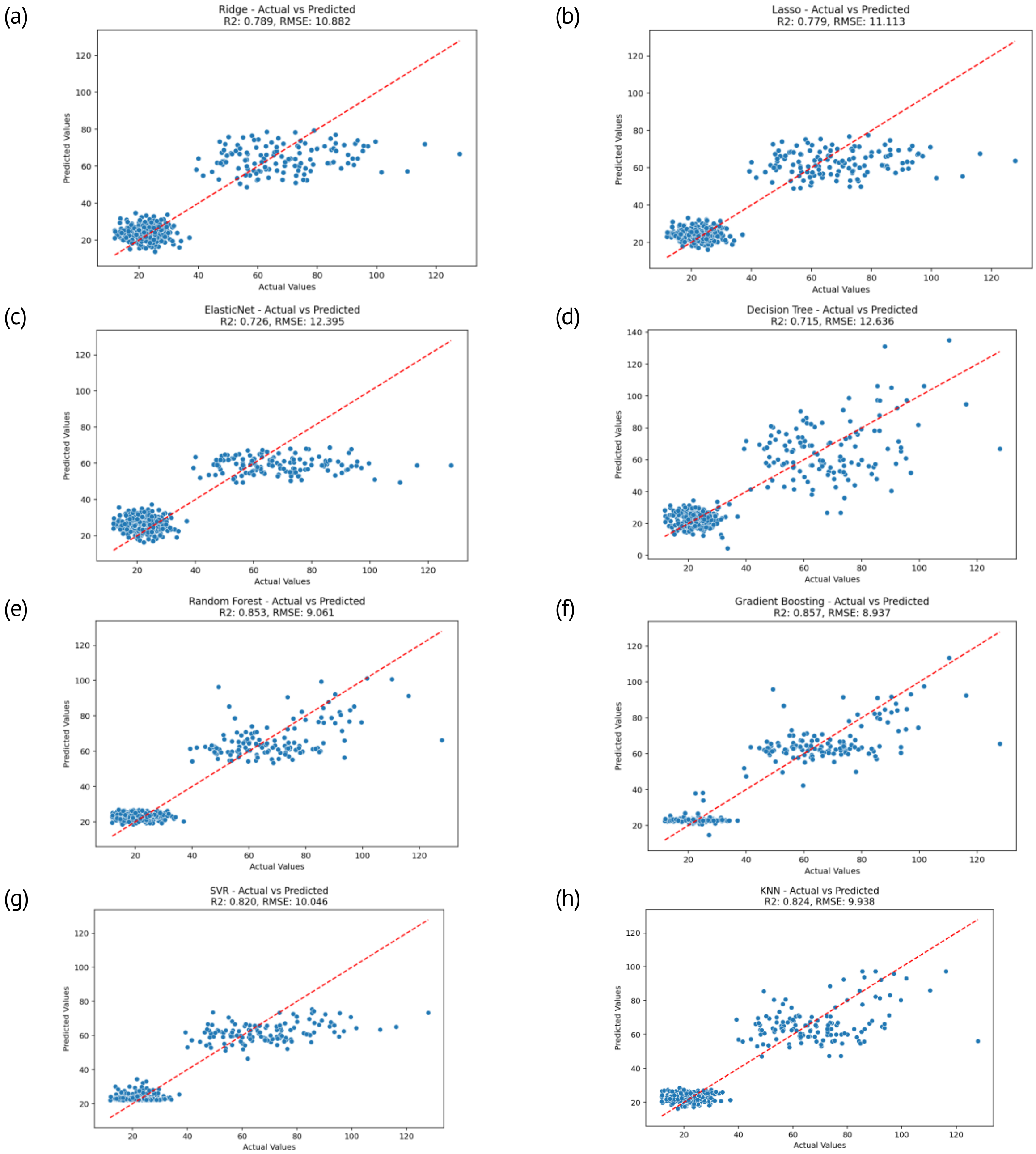

Fig. 6. Regression results: (a) Rigid; (b) Lasso; (c) elastic net; (d) dissection tree; (e) random forest;(f) GBoost; (g) SVR; (h) KNN

Table 3. Regression results of current studies

Regression	***R***^{2}	**RSME**
Rigid	0.78	10.88
Lasso	0.77	11.11
Elastic net	0.12	12.39
Decision tree	0.71	12.63
Random forest	0.85	9.06
GBoost	0.85	8.93
SVR	0.81	10.04
KNN	0.89	9.93

studied include ridge regression (Rigid), lasso (Lasso), elastic net (elastic net), decision tree (decision tree), random forest (random forest), gradient boosting (GBoost), support vector regression (SVR), and k-nearest neighbour (KNN). Among these models, GBoost and random forest performed best with R^2 of 0.85 and RMSE of 8.93 and 9.06, respectively. these results indicate that these two models are able to explain the variance of the data and have low prediction error.

In contrast, the elastic net model has the weakest performance with a very low r^2 (0.12) and a high RMSE (12.39), which is probably due to the model not matching the data structure or its parameters being incorrectly set. The rigid, lasso and SVR models have average performance with r^2 values between 0.77, 0.81, and RMSE between 10.04 and 11.11. Although these models are acceptable, they have lower accuracy than GBOOST and random forest. Also, the KNN model has a relatively high RMSE (9.93) despite a high r^2 (0.89), which may be overfitting in some data.

Finally, it can be concluded that GBOOST is recommended as the best model, as it has the highest r^2 and lowest RMSE, which provides a good balance between accuracy and generalizability. However, the final model choice also depends on the specific project needs and computational costs. For example, if the interpretability of the model is important, random forest is a better option, while KNN may be more suitable for low-dimensional data. Also, tuning the hyperparameters of weaker models such as elastic net can help improve their performance.

The Taylor plot clearly shows that the GBoost and Random Forest models have higher accuracy in predicting flexural strength compared to other models. The best results of regression were for KNN, Random Forest and GBoost. Other studies are investigated on this type of regressions. For example, Zhu et al. [40] studies basalt fiber reinforced concrete with PSO-KNN method, they found that this method have more than 0.96 and 0.98 accuracy with R^2. Elastic Net was a powerful regression, however in this

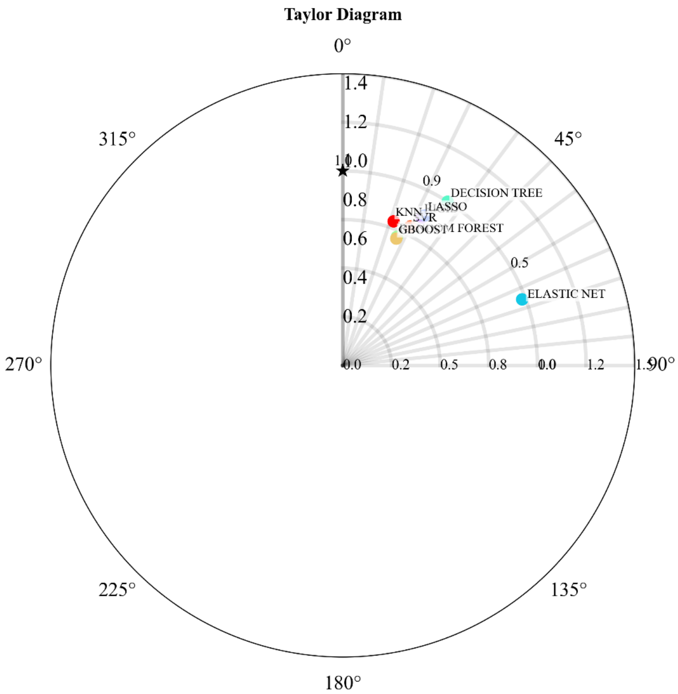

Fig. 7. Taylor diagram

study result of this regression was 0.12, while other studies show that when concrete predicted with Elastic Net regression, result is more than 0.98 [27]. These two models are located near the centre of the plot and have high correlation, indicating a good match between the actual data and the data predicted by these algorithms. In contrast, models such as Elastic Net, which are further away from the reference point, show poorer prediction performance. The use of the Taylor plot in this study is an effective visual tool for making the final decision in choosing the most appropriate machine learning algorithm (Fig. 7).

The obtained results are in good agreement with the results of independent authors, for example [41]. The obtained results are applicable in the design of 3D printed reinforced concrete.

Conclusions

This study investigated the prediction of flexural strength of 3D printed reinforced concrete using machine learning techniques.

1. The results showed that there is a strong relationship between the compressive and flexural strengths of concrete with a correlation coefficient of more than 0.97, which allows for more accurate prediction of flexural strength. Also, the gradient strengthening, random forest, and KNN models were identified as the best predictive models with R^2 values of 0.85, 0.85, and 0.89, respectively.
2. Among the key findings of this study was the significant effect of cement as the most important factor on concrete strength and the negative effect of water and fines on mechanical properties. These results not only help to better understand the behavior of 3D printed reinforced concrete but also provide valuable guidance for optimizing concrete mixing designs in the future. Also, the use of machine learning methods in this field is a new step towards increasing accuracy and reducing laboratory costs.
3. Finally, as one of the first comprehensive studies on the prediction of flexural strength of 3D printed reinforced concrete, this research paves the way for future research in this field. Despite the promising results, there is a need to develop more accurate models with more extensive data and to investigate the influence of other parameters such as fiber type and printing geometries.

CRediT authorship contribution statement

Mohammad Hematibahar : writing – review & editing, writing – original draft; **Makhmud Kharun** : writing – original draft, conceptualization; **Roman S. Fediuk** : writing – original draft, investigation; **Nikolai I. Vatin** : writing – original draft, supervision; **Maxim G. Porvadov** : writing – original draft, data curation; **Linar S. Sabitov** : writing – review & editing, writing – original draft.

Conflict of interest

The authors declare that they have no conflict of interest.

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