

Predictive Modeling of Compressive Strength for Additively Manufactured PEEK Spinal Fusion Cages Using Machine Learning Techniques

Narain Kumar Sivakumar¹, Sabarinathan Palaniyappan^{2,*}, Mahdi Bodaghi³, P Mohammed Azeem⁴,

G S Nandhakumar¹, Santhosh Basavarajappa⁵, Saravanan Pandiaraj⁶, Mohamed Ibrahim Hashem⁵

¹ Centre for Additive Manufacturing, Chennai Institute of Technology, Chennai, Tamilnadu 600069, India

² Centre for Molecular Medicine and Diagnostics, Saveetha Dental College, Saveetha Institute of Medical and Technical Sciences, Saveetha University, Chennai, Tamilnadu, India.

³ Department of Engineering, School of Science and Technology, Nottingham Trent University, Nottingham, NG11 8NS, UK.

⁴ Department of Computer Science, Chennai Institute of Technology, Chennai, Tamilnadu 600069, India.

⁵ Department of Dental Health, College of Applied Medical Sciences, King Saud University, P.O. Box 10219, Riyadh 11433, Saudi Arabia.

⁶ Department of Self-Development Skills, King Saud University, Riyadh, 11362, Saudi Arabia.

Corresponding author: Sabarinathan14010@mech.ssn.edu.in

Abstract

The current study delves into the utilization of Machine Learning (ML) algorithms to evaluate the mechanical properties of additively manufactured PEEK spinal fusion cages. In this research, a range of ML models, including Linear Regression (LiR), Lasso Regression (LaR), Decision tree (DT), and K-Nearest Neighbor (KNN) are harnessed to enhance compressive strength prediction. Ensemble learning techniques such as bagging, boosting, and stacking are applied to identify the most accurate ML model in terms of achieving heightened accuracy and minimized errors. To facilitate this, spinal fusion cages are 3D printed using the Fused Filament Fabrication (FFF) technique and subsequently tested using a Universal Testing Machine (UTM). The development of ML models involves the exploration of independent material-extrusion factors, encompassing layer height (0.1 mm, 0.2 mm, 0.3 mm), printing temperature (370°C, 390°C, 410°C), printing speed (10 mm/sec, 30 mm/sec, 50 mm/sec), infill density (40%, 70%, 100%), build orientation (0°, 45°, 90°), and line width (0.1 mm, 0.2 mm, 0.3 mm). The robustness and effectiveness of the developed ML models in predicting compressive strength properties are optimized through comprehensive error metric analysis. The results indicate that the LiR model, particularly when implemented under the boosting ensemble technique, demonstrates the highest accuracy with a Mean Absolute Error (MAE) of 0.657, Root Mean Square Error (RMSE) of 0.758, and Median Absolute Error (MedAE) of 0.634. This underscores the potential of LiR for precise compressive strength prediction in 3D-printed PEEK spinal fusion cages for spinal and maxillomandibular reconstruction.

Keywords:

Additive manufacturing; Spinal fusion cage; Compressive strength; Machine learning; Medical and dental devices.

1. Introduction

Spinal fusion cages, also called intervertebral or spinal implants, stabilize vertebrae and promote fusion in spinal surgery [1]. They are specifically designed for conditions like degenerative disc disease, spondylolisthesis, or spinal fractures [2], the procedure replaces damaged discs with these cages [3]. Their hollow cylindrical or rectangular structure allows for bone graft placement [4]. The main objectives include restoring disc height, maintaining alignment, providing stability, and aiding fusion between adjacent vertebrae [5]. During the surgical procedure, the surgeon first removes the affected disc, prepares the neighboring vertebrae, and the cage is immediately inserted for ensuring stability and height restoration. To promote fusion, bone graft material is packed around the cage, sourced from the same patient (autograft), a donor (allograft), or an artificial bone graft material [6]. The cage serves as a supportive framework over time, facilitating fusion between the vertebrae [7].

Spinal fusion cages conventionally undergo subtractive manufacturing like CNC machining, involving various processes such as fixturing, milling, drilling, turning, polishing, and etching [8]. These processes introduce stresses and voids, diminishing the cage's lifespan and negatively impacting patient outcomes [9]. In contrast, additively manufactured spinal fusion cages require no post-manufacturing processes, and evidence indicates their superior performance compared to conventionally manufactured cages [10].

The Additive Manufacturing (AM) technique involves layer-wise material deposition for component development [11]. Moreover, its rising demand, driven by its capability for intricate design profiles, is evident across sectors like aerospace, marine, biomedical, automobile, and architecture [12, 13]. The AM technique is categorized into seven classes by ASTM F2792 standards [14]. This study specifically employs the Fused Filament Fabrication (FFF) AM technique for fabricating spinal fusion cages.

Titanium and PEEK (Polyether-ether-ketone) are considered the two primary materials used to manufacture spinal fusion cages [15]. Titanium is known for its high strength, and stiffness, making it suitable for load-bearing applications [16]. A few studies dealing with the development of titanium spinal fusion cages are discussed as follows. Wu et al. developed a Ti_6Al_4V fusion cage by SLM technique and performed surface modification and heat treatment to enhance the stiffness, fatigue strength, and osteogenic differentiation characteristics. They reported that the sandblasting and chemical etching increased cell proliferation and osteoblast mineralization. In addition, the fatigue life of the cage improved with reduced residual stress [17].

On the other hand, PEEK is a high-performance thermoplastic that is valued for its inertness and biocompatibility in the body, making it compatible with the body's tissues [18]. PEEK implants have a modulus similar to bone and are less stiff than titanium, allowing for optimal load sharing [19]. This helps in reducing stress shielding and subsidence rates. Additionally, PEEK does not cause any artifacts

during medical imaging, ensuring complete radiolucency during CT, MRI, and X-ray scans [20]. These significant qualities of PEEK make them suitable for developing biocompatible spinal fusion cages. In recent years, the PEEK spinal fusion cages have been fabricated by AM techniques like FFF and SLS. Among the two techniques, the FFF technique is widely employed for fabricating PEEK spinal fusion cages in contrast to the SLS technique due to reduced wastage of material [21].

Only a few studies have been conducted on the production of PEEK spinal fusion cages, with some notable examples outlined below. Basgul et al. studied the impact of printing speed on the mechanical characteristics of the 3D-printed PEEK spinal fusion cages. They stated that the porosity of the 3D printed cage increased with a maximum printing speed of 3000 mm/min. In addition, they added that printing speeds less than 1500 mm/min enhanced mechanical strength [22]. Saini et al. investigated the effect of bed, nozzle, and chamber temperature on the mechanical and thermal characteristics of the 3D PEEK spinal fusion cages. They reported that, as the levels of thermal parameters of the FFF technique increase, the mechanical properties and crystallinity are enhanced due to the increased degree of layer fusion [23]. Basgul et al. fabricated PEEK lumbar spinal cages and evaluated the effect of nozzle diameter, cage counts in a single take, and printing speed on the mechanical characteristics of additively manufactured PEEK lumbar spinal fusion cages. They found that the mechanical characteristics of the additively manufactured PEEK spinal fusion cages increase with an increase in the cooling time [24]. During the fabrication of PEEK spinal fusion cages by the FFF AM technique, the material-extrusion factors employed during the course of fabrication have a significant role towards bonding and surface morphology of deposited material layers [25]. The superior mechanical and energy absorption characteristics of PEEK spinal fusion cages solely depend on the material-extrusion factors. In order to achieve enhanced mechanical characteristics, the material-extrusion factors need to be optimized and investigated effectively. In general, the material-extrusion factors are optimized by various conventional optimization techniques like Taguchi, Response Surface Methodology (RSM), Grey Wolf Optimization (GWO), etc. Some of the studies dealing with the optimization of material-extrusion factors using conventional techniques are discussed here.

Popović et al. carried out optimization for printing factors like printing speed and printing temperature concerning the roughness and tensile strength of PLA components. They reported that a printing temperature of 190°C and 40 mm/min developed a considerable tensile strength and roughness [26]. Kumar et al. explored the significance of various factors like layer height, fan speed, infill pattern, printing speed, bottom/top pattern, bed temperature, top/bottom layer counts, printing temperature, infill density, shell counts, and flow rate on tensile strength and Young's modulus using Grey-Taguchi optimization technique. They observed that the layer height had a significant impact on the tensile strength and Young's modulus of the PLA components [27]. Pulipaka et al. investigated the impact of print speed, nozzle temperature, layer height, platform temperature, and infill percentage on the compressive strength and tribology characteristics of PEEK components using the Taguchi optimization

technique. They concluded that factors like nozzle temperature and layer height had a significant influence on the surface roughness and Young's modulus of the developed PEEK component [28].

To optimize the AM process effectively, the Machine Learning (ML) approach has been considered in recent years [29]. The ML approach is significant in optimizing the AM process for several reasons like complex relationships, utilizing data-driven insights, handling nonlinearities, etc [30]. Mohammed et al. predicted the friction coefficient using machine learning algorithms on the silicon wafer coated with graphite and talc, and a liquid filler such as Perfluoropolyether (PFPE). The results show that the ANN algorithm observes the best R2 metrics compared to all other selected ML models [31]. Similarly, Prajapati et al. optimized the mixed lubrication parameters using the machine learning technique. Multi-layer perceptron (MLP) model with hyperparameter tuning and fivefold cross-validation exploits better accuracy compared to the random forest regression model [32].

A few studies have focused on optimizing material-extrusion factors through an ML approach, and some notable ones include the following. Ranjan et al. deployed ML models for determining the effect of parameters like spray layer counts, infill density, and infill pattern on the flexural strength of the developed composite. They found that the Random Forest model developed higher prediction accuracy and fewer errors concerning the flexural strength of developed composites [33]. Agarwal et al. employed various machine learning algorithms like Random Forest, Support Vector Regression, K-Nearest Neighbor (KNN), and Decision Tree (DT) for predicting the compressive strength of PLA bone screws. The ML models were constructed using wall thickness, layer height, infill pattern, and infill percentage. The Random Forest model reported a higher degree of prediction accuracy in terms of compressive strength [34].

The current study focuses on 3D printing PEEK spinal fusion cages and optimizing material-extrusion factors with ML models, including Linear Regression (LiR), Lasso Regression (LaR), Decision tree (DT), and K-Nearest Neighbor (KNN). Ensemble learning techniques like Bagging, Boosting, and Stacking enhance the ML model's performance. Hyperparameter tuning is employed for each model to improve the prediction accuracy. The best model, identified through a higher coefficient of fit and fewer errors, optimizes material-extrusion factors for attaining higher compressive strength. The data visualization plots, such as the Box-whisker plot, Pair plot, and Partial Dependency plot help in interpreting the impact of the input factors concerning the output response. The influential factors and their percentage contributions are evaluated using the best ML model. The train and test data are analyzed with scatter and residual plots. The error metrics like Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Median Absolute Error (MedAE) are calculated for all ML models and ensemble techniques. This ML approach effectively optimizes PEEK spinal fusion cages, enhancing compressive strength and energy absorption for implantation conditions.

2. Experimental procedure

2.1. Materials

The FFF technology is capable of handling both low-temperature and high-temperature polymers. For the current research, the FFF 3D printer (Make: Creatbot, India) is employed for the fabrication of PEEK spinal fusion cages. The commercially available medical grade PEEK filament was procured from kexcelled3d, China as depicted in Figure 1. Figure 1 shows the FFF-based PEEK printer and its print bed employed during the fabrication of PEEK spinal fusion cages.

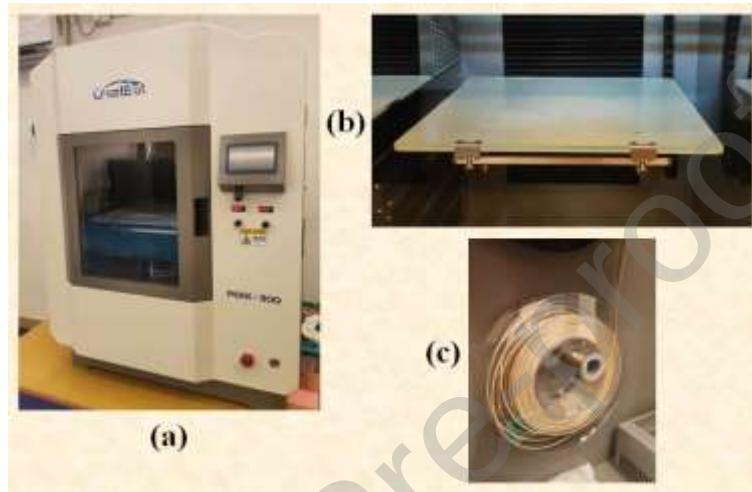


Figure 1. (a) PEEK 3D printer, (b) Print bed, and (c) PEEK 3D printing filament.

2.2. Design and fabrication of PEEK spinal fusion cages

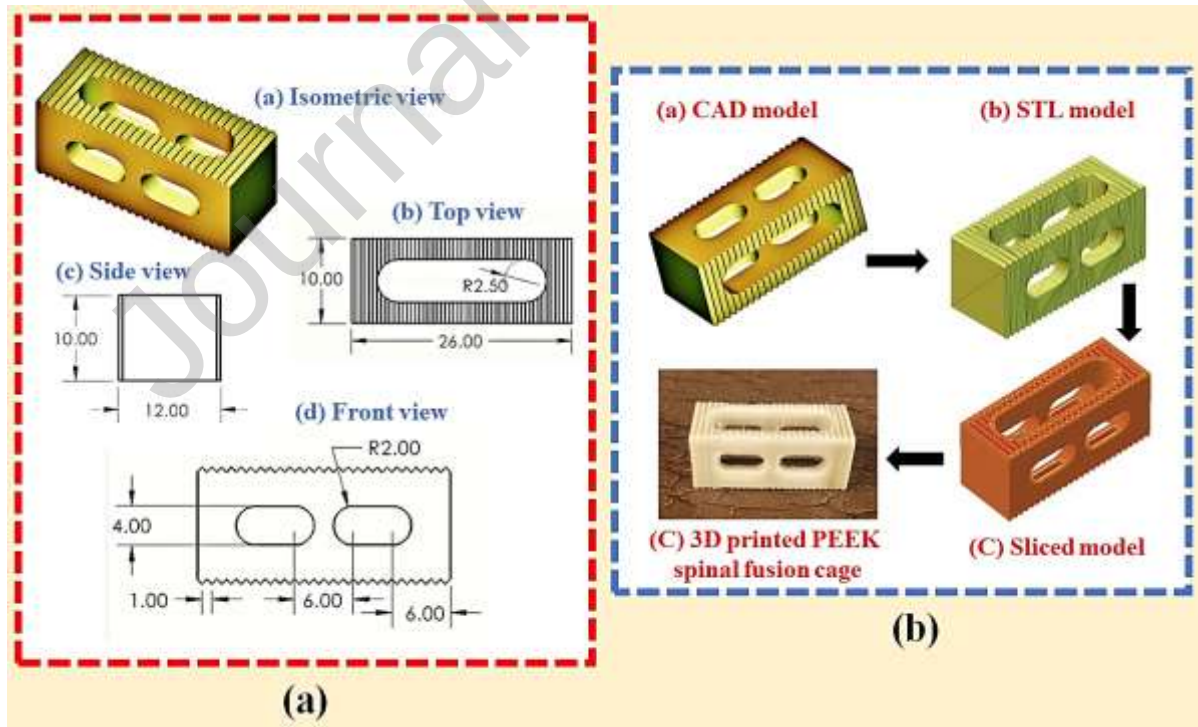


Figure 2. (a) Spinal fusion cage design and (b) CAD to 3D model.

The fabrication of spinal fusion cage by the FFF technique contains three vital steps. The first step involves the design modeling of the PEEK spinal fusion cage using CAD software (Ntopology, Make:

New York, USA) with dimensions as illustrated in Figure 2 (a). And then, the second step involves saving the developed design in CAD format which is then converted into stereolithography (.stl) files. The third step includes the slicing of the stereolithography files into G-codes using suitable slicers. The G-codes refer to the set of procedures given to the 3D printer which will be carried out during the printing process. The developed G-code is then saved in the storage device. This storage device is given as input for the FFF-based 3D printer for fabricating the PEEK spinal fusion cages. Figure 2 (b) also depicts the various steps involved in the conversion of the CAD model into a 3D model. During the fabrication process, certain material-extrusion factors are kept to be constant. The constant material-extrusion factors employed during the 3D printing process are as follows: a chamber temperature of 90°C, a bed temperature of 130°C, an infill flow rate of 100 %, a wall thickness of 0.1 mm, and a raft-type bed adhesion.

2.3. Selection of input material-extrusion factors

To minimize the need for numerous experiments while maintaining the influence of each material-extrusion factor, the Design of Experiments (DOE) technique is utilized. An L_{27} orthogonal array is created by manipulating the levels of different material-extrusion factors like layer height (0.1 mm, 0.2 mm, 0.3 mm), printing speed (10 mm/sec, 30 mm/sec, 50 mm/sec), printing temperature (370°C, 390°C, 410°C), infill density (40 %, 70 %, 100 %), build orientation (0°, 45°, 90°), line width (0.1 mm, 0.2 mm, 0.3 mm). For every individual experimental trial, six test samples are fabricated and mechanically evaluated. As a result, a group of 162 samples are 3D printed for 27 trials. These 162 samples help in optimizing the material-extrusion factors concerning the compressive strength of the fabricated cages. Table 1 proclaims the L_{27} orthogonal array and compressive strengths of corresponding PEEK spinal fusion cages.

Table 1. L_{27} orthogonal array for training and testing ML models.

Sl. No	Layer Height (mm)	Printing Speed (mm/sec)	Printing Temperature (°C)	Infill Density (%)	Build Orientation (°)	Line Width (mm)	Compressive Strength (MPa)
1	0.1	10	370	40	0	0.1	71.22
2	0.1	10	370	40	45	0.2	62.96
3	0.1	10	370	40	90	0.3	76.91
4	0.1	30	390	70	0	0.1	86.92
5	0.1	30	390	70	45	0.2	74.24
6	0.1	30	390	70	90	0.3	83.55
7	0.1	50	410	100	0	0.1	91.04
8	0.1	50	410	100	45	0.2	82.74
9	0.1	50	410	100	90	0.3	85.13
10	0.2	10	390	100	0	0.2	75.73
11	0.2	10	390	100	45	0.3	66.83
12	0.2	10	390	100	90	0.1	77.31
13	0.2	30	410	40	0	0.2	84.04
14	0.2	30	410	40	45	0.3	72.10
15	0.2	30	410	40	90	0.1	79.06
16	0.2	50	370	70	0	0.2	68.84
17	0.2	50	370	70	45	0.3	62.70

18	0.2	50	370	70	90	0.1	75.00
19	0.3	10	410	70	0	0.3	72.92
20	0.3	10	410	70	45	0.1	64.50
21	0.3	10	410	70	90	0.2	76.11
22	0.3	30	370	100	0	0.3	67.38
23	0.3	30	370	100	45	0.1	69.86
24	0.3	30	370	100	90	0.2	70.09
25	0.3	50	390	40	0	0.3	65.41
26	0.3	50	390	40	45	0.1	64.49
27	0.3	50	390	40	90	0.2	69.14

2.4. Mechanical testing of fabricated PEEK spinal fusion cages

The manufactured PEEK spinal fusion cages are mechanically evaluated using a Universal Testing Machine (UTM, Make: Bluestar, India). This UTM boasts a maximum loading capacity of 50 kN. To perform the compression test, the ASTM F 2077 standards are followed, employing a loading rate of 1 mm/min. During the compression testing process, the PEEK spinal fusion cages are positioned between the loading plates, and compressive loads are applied to each cage. As six cages are fabricated for each unique test condition, the mean compressive strengths of these six tested cages are employed as input data for various ML models.

2.5. Machine Learning models

This study proposes the utilization of ML models such as LiR, LaR, DT, and KNN for making predictions concerning the compressive strength of the 3D-printed PEEK spinal fusion cages. A detailed explanation regarding the employed machine learning models can be found in the upcoming sections.

Figure 3 depicts the schematic flow of the current study.

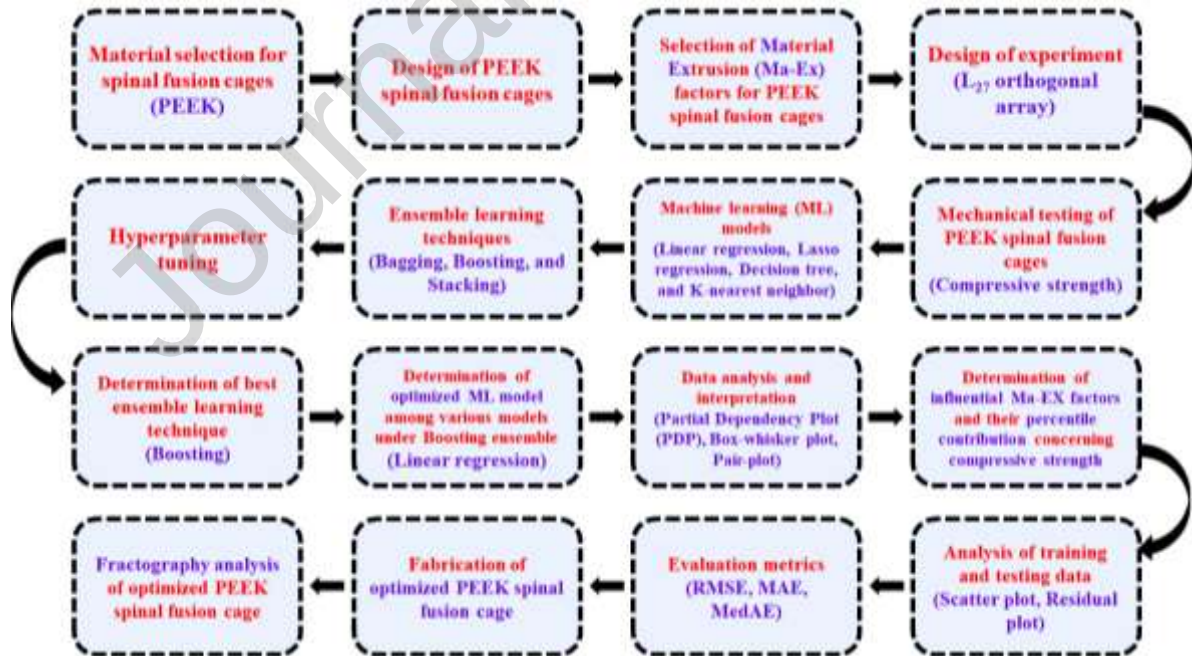


Figure 3. Schematic flow of the current study.

2.5.1 Linear Regression

Linear Regression (LiR) is one of the fundamental supervised machine learning algorithms that is primarily used for finding the relationship between variables and making predictions. It is a regression model that predicts the target value based on independent variables. The LiR algorithm works by finding the coefficients of the line that best fits the data points. The line is determined by computing the slope and intercept values that reduce the sum of squared distances between the line and the data points to the minimum. Once fitted, the line can be employed to forecast the dependent variable's value for any given independent variable value. In regression analysis, the dependent variable is commonly known as the outcome variable, criterion variable, or regressand. Conversely, the independent variable is often referred to as exogenous variable, predictor variable, or regressor.

2.5.2 Lasso Regression

Lasso Regression (LaR) is indeed recognized as a penalized regression method. It excels in enhancing prediction accuracy compared to various other regression models. It is particularly valuable for improving model interpretability. Moreover, the primary objective of LaR is to identify the optimal model for predicting the response variable by carefully choosing a subset of the available predictor variables. LaR varies from other regularization approaches such as ridge regression by imposing a penalty on the size of the regression coefficients and feature selection by reducing the coefficients toward zero. The size of the penalty is controlled by a tuning parameter, which determines the degree of regularization. The LaR model consists of a parameter called “Alpha” which helps in tuning the LaR using a Lasso CV. This is highly recommended when working with high-dimensional data, where the number of predictor variables exceeds the number of observations.

2.5.3 Decision Tree

Decision tree (DT) is a supervised machine-learning model that can be used for both classifications as well as regression analysis. A DT is a graphical representation of decision rules and their outcomes in the form of a tree. The nodes of the tree correspond to a choice or event, while the edges represent the conditions or decision rules. Data is split based on a specific parameter, and the model is trained using a set of distinct values. One of the significant advantages of DT is that it can handle both numerical and categorical data. Within a DT model, decision nodes and leaves serve distinct roles. Decision nodes and leaves are used to represent predicted class labels and feature values, respectively. Internal nodes within the tree correspond to dataset features and act as decision points. The branches of the tree signify the decision rules, and the ultimate outcomes of the model are conveyed through the leaf nodes.

2.5.4 K-Nearest Neighbor

K-Nearest Neighbor (KNN) regression is very effective while handling non-linear relationships between features and target variables. During the course of training, the KNN model stores the feature vectors and corresponding target values while predicting the regression that utilizes a distance metric parameter such as Euclidean distance or Manhattan distance to identify the k closest neighbors to predict a new data point in the feature space. A decrease in the value of K results in a regression line that is more flexible and less smooth, whereas an increase in the value of K yields a smoother regression line.

at the potential expense of increased bias. After identifying the KNNs, the model proceeds to compute the average of the target values associated with these neighboring data points. This calculated average value is then employed as the predicted value for the new data point being evaluated by the algorithm.

2.6 Ensemble learning techniques

Ensemble learning is a strategy that merges multiple individual models to enhance generalization performance. It is widely employed to boost the accuracy and dependability of machine learning models by amalgamating predictions from sub-models. This approach contributes to improved model generalization, reduced model variance, and more effective model exploration. There are several ensemble techniques available, each distinguished by how it combines the predictions of sub-models. Some of the well-known ensemble models are as follows: Bagging, Boosting, and Stacking.

2.6.1 Bagging

Bagging is an ensemble learning technique that focuses on enhancing the performance of base regression models by generating multiple models on various subsets of the training data and combining their predictions. The objective of the bagging technique is to reduce variance and prevent overfitting, which ultimately leads to better generalization and accuracy of the model on new data. In the case of bagging, the input data for training a model is drawn by the replacement technique. After that, the predictions of all models are aggregated using methods such as voting or averaging to generate the final prediction.

2.6.2 Boosting

Boosting is a prominent ensemble learning technique that comprises multiple weak learners for developing a single strong model. The objective of boosting is to increase the accuracy of the weak models by altering the weights of the training data to focus on the misclassified data points. This is accomplished by training weak models on modified versions of the training data iteratively, where the weights of the misclassified data points are increased. Boosting technique generally concentrates on developing a model with a higher degree of fit. The boosting technique develops accurate models by combining the predictions of all the weak models with higher weights. The boosting technique seems to be effective in terms of reducing bias and variance and improving the overall accuracy of the model. AdaBoost or Adaptive Boosting has become the most widely employed boosting model since it combines numerous weak learners to develop a strong learner. AdaBoost assigns weights to the selective sample in the training set and the weights of the misclassified samples are increased after each iteration.

2.6.3 Stacking

Since each model is known for its corresponding strengths and weaknesses, the stacking technique helps in reducing the errors and increasing the model's prediction efficiency by combining the predictions of the multiple base models with a meta-model. The stacking process typically involves three steps which are as follows. The first step involves splitting the training data into several subsets and training multiple base models on each subset. The consecutive step involves the predictions of the respective base models

and then employed as an input for the meta-model. In the third step, the meta-model is then trained to predict the outcome based on the predictions of the respective base models. Finally, the meta-model is capable of combining the predictions of each base model by assigning weights to them which in turn results in a more accurate final prediction.

2.6.4 Hyperparameter tuning

Parameter tuning is the process of selecting the optimized set of parameters to enhance a machine-learning model in terms of accuracy and efficiency. A poorly tuned model will lead to decreased model accuracy, longer training duration, and wastage of computational resources. There are several methods for performing parameter tuning like: Grid search, Random search, etc. Grid search is a fundamental approach for hyperparameter tuning in machine learning. This method involves creating a model for every possible combination of hyperparameter values, evaluating the performance of each model, and then selecting the set of parameters that produces the best result.

2.7 Data interpretation plots

For the current study, the data interpretation plots like Partial Dependency Plot (PDP), Box whisker plots, Pair plots, Residual plots, and Scatter plots have been considered and their significances are discussed in the upcoming sections.

2.7.1 Partial Dependency Plot (PDP)

In general, the Partial Dependency Plot (PDP) provides a comprehensive view of the relationships between input features and target response in ML models. PDP plots are used to analyze how changes in a specific feature or feature impact the model's output. Moreover, PDP assists in assessing the consistency of predictions and identifying which components within the model exert the most significant influence on the target variable.

2.7.2 Box whisker plots

The Box whisker plots provide an informative visualization of the distribution and statistical properties of a dataset or model predictions. They additionally make it possible to see variations in data such as differences in central tendency, skewness, identifying patterns, trends, or discrepancies in the data. Box whisker plots are useful for discerning the extremes of specific features and understanding how different elements influence the outcome.

2.7.3 Pair plots

The Pair plots provide a visual perspective on the relationship between two continuous variables in a data set. Each data point is represented as a dot on the two-dimensional plane or a cartesian system. In the present study, the material-extrusion factors are plotted on the X-axis, while the output parameter such as compressive strength is plotted on the Y-axis.

2.7.4 Residual plots

A Residual plot is a graphical representation that illustrates the differences between the observed values and the predicted values. The primary purpose of residual plots in ML is to serve as a visual tool for

comprehending the performance and quality of the predictive model. Residual plots are mainly useful for identifying outliers, influential data points, and missing patterns in the model.

2.7.5 Scatter plots

A scatter plot is a visual representation of data points in a two-dimensional coordinate system. In the current study, the scatter plot enables the correlation between the actual points and the predicted points. A smaller gap between predicted and actual data points signifies the model's ability to make precise predictions, while a wider gap suggests that the model's predictions are likely to have a higher degree of error.

2.8 Error metrics

The error metrics are used to examine the quality and accuracy of the ML models. These error metrics provide quantitative measures that help in determining the efficiency of the model and facilitate comparisons between different models. Various error metrics like RMSE, MAE, and MedAE are considered for the current study and they are discussed in the following sections.

2.8.1 Root Mean Square Error

RMSE is a statistical measure commonly used to assess the accuracy of the model's predictions. To calculate RMSE, the average of the squared differences between the predicted values and the actual values is taken and squared. The lower the RMSE value, the better the fit between predicted and actual values. The mathematical formula for RMSE is depicted in Equation (1).

$$RMSE = \sqrt{\sum_{i=1}^n \frac{(yp_i - ym_i)^2}{n}} \quad (1)$$

2.8.2 Mean Absolute Error

MAE is a widely employed metric in predictive modeling for evaluating the accuracy of models. It computes the average absolute difference between the predicted values and the actual values within a dataset. MAE is not highly sensitive to outliers as it treats all errors equally. MAE is an easy and direct interpretable metric that is particularly suitable for tasks focused on minimizing the average error of a particular model. It is commonly utilized with other evaluation metrics like RMSE or MSE to provide a more comprehensive assessment of the model's performance. The mathematical formula for MAE is depicted in Equation (2)

$$MAE = \frac{1}{n} \sum_{i=1}^n |yp_i - ym_i| \quad (2)$$

2.8.3 Median Absolute Error

MedAE is an error metric in machine learning that measures the accuracy of the predictive model that is less sensitive to outliers. It is determined by calculating the median of the absolute differences between the predicted and actual values within the dataset. The MedAE is particularly valuable when working with data that exhibits skewed distributions or contains extreme values. The mathematical formula for MedAE is depicted in Equation (3)

$$MedAE = (|A_i - \text{median}(A_i)|) \quad (3)$$

3 Results and discussion

3.1 Determination of the best ML model

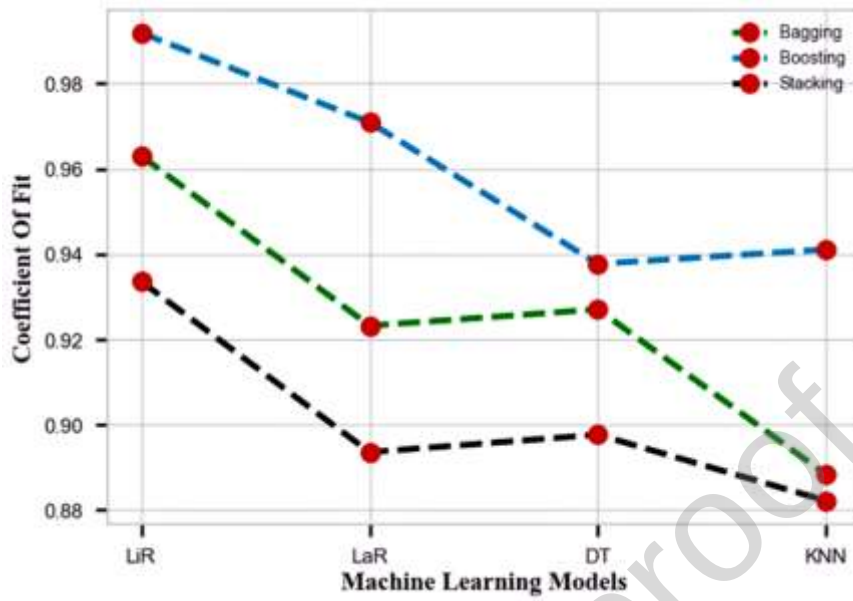


Figure 4. Coefficient of fit for various ML models under different ensemble techniques.

With the assistance of the Coefficient of fit (R^2) value, the best ML model is determined among various ML models like LiR, LaR, DT, and KNN. The term “Coefficient of fit” determines the fitness of the developed ML model concerning the dataset. The R^2 value varies within a liable range of 0 to 1. As the R^2 value increases from 0 to 1, the fitness of the ML model increases. From Figure 4, it is evident that the boosting ensemble technique has attained a higher R^2 value. Among the various ML models in boosting ensemble technique, the LiR model attained a R^2 value of 0.992. Moreover, the LiR model developed a higher coefficient of fit in the instance of all ensemble learning techniques. Finally, the LiR model from the boosting ensemble technique is considered for data analysis and interpretations which are discussed in the upcoming sections.

3.2 Data analysis and interpretation

The LiR model from the boosting ensemble learning technique is the most optimized ML model for the current study. The results obtained from the LiR model are interpreted with the assistance of PDP, Box whisker plot, and Pair plot.

The PDP helps in identifying the influence of input material-extrusion factors on the output response (compressive strength) in terms of partial dependency. Figure 5 depicts the PDP of input material-extrusion factors like layer height, printing speed, printing temperature, infill density, line width and build orientation on the compressive strength of 3D-printed PEEK spinal fusion cages. The Box whisker plots help in the determination of median compressive strength as shown in Figure 6. The pair plot demonstrates a correlation between the input factors and output response with concern to a particular input factor and it is depicted in Figure 7.

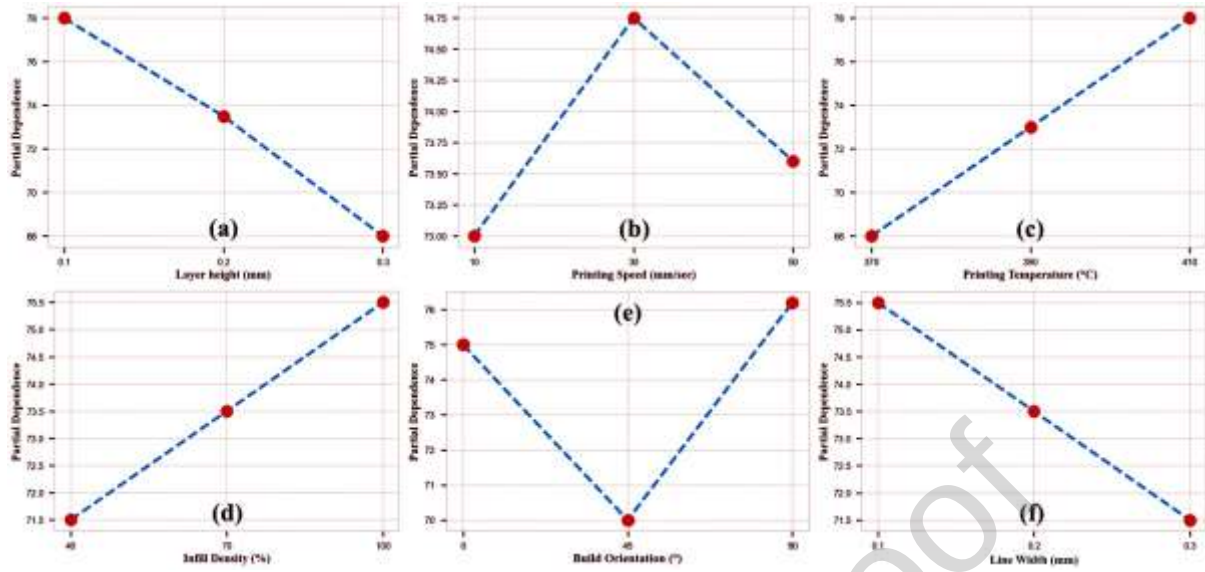


Figure 5. Partial Dependency Plot (PDP) of input material-extrusion factors.

The PDP of compressive strength concerning layer height is presented in Figure 5 (a). It is clear that a higher partial dependence value of 78 is developed by spinal cages fabricated at a layer thickness of 0.1 mm. At a lower layer thickness of 0.1 mm, the PEEK material gets deposited with a significantly lower thickness which in addition results in the deposition of higher layers. Moreover, the lower layer thickness contributes to lower structural deviations in the contour of the developed spinal cage which effectively reduces lateral stress concentrators. In the case of gradually increasing layer thickness of 0.2 mm and 0.3 mm, the respective partial dependence values of 73.5 and 68 are observed. From these results, it can be inferred that compressive strength has a direct correlation with layer count. As the layer count increases (layer thickness decreases), the load-bearing capacity of the respective cage increases which contributes to higher compressive strengths and the vice-versa takes place in the instance of lower layer counts. From Figure 6 (a), it can be inferred that 0.1 mm layer height resulted in a higher median compressive strength of 82.9 MPa with a negative skewness. On the other hand, 0.2 mm and 0.3 mm layer heights developed respective median compressive strengths of 75 MPa and 69.25 MPa. A similar remark was made by El Magri et al., in the instance of PEEK components. They reported a maximum ultimate tensile strength at a lower layer height of 0.1 mm [35].

The PDP of compressive strength concerning printing speed is depicted in Figure 5 (b). It is clear that a higher partial dependence value of 74.75 is developed by spinal cages fabricated at a printing rate of 30 mm/sec. When the printing speed is set at 30 mm/sec, the PEEK material is deposited with precision, particularly at the spinal cage's contours. Moreover, this speed fosters improved bonding between consecutively deposited PEEK layers, leading to a substantial enhancement in compressive strength. Conversely, at a lower printing speed of 10 mm/sec, there is a risk of PEEK material over-melting because it remains exposed to the nozzle's elevated temperature for a longer duration. This prolonged exposure can have an adverse effect on compressive strength. On the contrary, in the instance of a higher printing rate of 50 mm/sec, the under-melting of PEEK material takes place which develops

lower inter-layer bonding and contributes to lower compressive strengths. The partial dependence values of 73 and 73.60 were observed at 10 mm/sec and 50 mm/sec. From Figure 6 (b), it is evident that the 30 mm/sec printing rate developed the highest median compressive strength of 74.4 MPa. The median compressive strengths of 72.86 MPa and 69.1 MPa were observed at 10 mm/sec and 50 mm/sec printing speeds.

The PDP of compressive strength concerning printing temperature is depicted in Figure 5 (c). It is clear that a partial dependence value of 78 is developed by spinal cages fabricated at a printing temperature of 410°C. At a printing temperature of 410°C, the proper fusion of PEEK material takes place effectively leading to no in-line gaps between deposited PEEK layers. The effective fusion of PEEK layers contributes to higher compressive strengths. On the other hand, at lower printing temperatures of 370°C and 390°C, the deposited PEEK layers don't fuse effectively leading to a higher degree of in-line gaps between the deposited PEEK layers. The in-line gaps lead to a decrease in the compressive strength of respective fusion cages. From Figure 6 (c), the respective median compressive strengths of 69.85 MPa, 74.3 MPa, and 79 MPa are developed at printing temperatures of 370°C, 390°C, and 410°C. Saini et al. also made a similar observation in the context of PEEK spinal fusion cages. They also reported a similar phenomenon where the maximum compressive strength is observed at 410°C [23].

The PDP of compressive strength concerning infill rate is depicted in Figure 5 (d). It is clear that a partial dependence value of 75.5 is developed by spinal cages fabricated at an infill rate of 100 %. At an infill rate of 100 %, the inter-line spacing between the consecutive infill lines is significantly lower which in turn develops higher relative density and significantly results in higher compressive strength. In the instance of lower infill rates like 40 % and 70 %, the lower partial dependence values of 71.5 and 73.5 are observed. At lower infill rates, the relative density of the respective spinal cage reduces significantly due to higher inter-line spacing. Figure 6 (d) depicts the respective median compressive strengths of 71.24 MPa, 74.32 MPa, and 75.72 MPa achieved at corresponding infill densities of 40%, 70%, and 100%. A similar observation was made by Srinivasan et al., for PETG parts. They reported that the ultimate tensile strength of PETG parts increases with an increase in infill density from 20 % to 100 % [36].

The PDP of compressive strength concerning build orientation is depicted in Figure 5 (e). It is clear that a partial dependence value of 76.2 is developed by spinal cages fabricated at a build orientation of 90°. At 90° build orientation, the spinal cage is printed in the vertical direction with successive deposition of PEEK material. In the instance of spinal cages developed along 90° orientation, the layer counts are higher than the 0° and 45° orientated spinal cages at a constant layer thickness which accounts for higher compressive strength. The spinal cages fabricated in the 0° horizontal orientation developed a partial dependence value of 75. At 0° horizontal orientation, the PEEK material is deposited in the horizontal orientation with lower layer counts within the spinal cage profile. The horizontally oriented PEEK layers get delaminated at the instance of compression test which drastically reduces load bearing capacity. The spinal cages developed in the 45° orientation comprise higher layer counts than the 0°

oriented spinal cages in an inclined orientation. The 45° oriented layers begin to slide at the initial stage of compressive loading resulting in the lowest partial dependence value of 70 among various build orientations due to inclined orientation. From Figure 6 (e), the respective median compressive strengths of 72.95 MPa, 66.8 MPa, and 76.9 MPa are observed at corresponding build orientations of 0°, 45°, and 90°. A parallel remark was made by Mathiazhagan et al., in the case of hydroxyapatite particles reinforced composite tubes [37].

The PDP of compressive strength concerning line width is depicted in Figure 5 (f). It is clear that a partial dependence value of 75.5 is developed by spinal cages fabricated at a line width of 0.1 mm. At a lower line width of 0.1 mm, the number of consecutive printing lines within a given deposited layer is higher and finer leading to lower porosity between the consecutive printing lines. As the porosity decreases, the rate of crack propagation decreases which results in higher compressive strengths. At higher line widths of 0.2 mm and 0.3 mm, the porosity between the internal printing lines increases leading to lower partial dependence values of 73.5 and 71.5. From Figure 6 (f), the median compressive strengths of 75.1 MPa, 74.2 MPa, and 72.05 MPa were observed at line widths of 0.1 mm, 0.2 mm, and 0.3 mm respectively. Therefore, the optimized level of input material-extrusion factors for attaining higher compressive strength will be a layer height of 0.1 mm, a printing speed of 30 mm/sec, a printing temperature of 410°C, an infill density of 100 %, a build orientation of 90° and a line width of 0.1 mm.

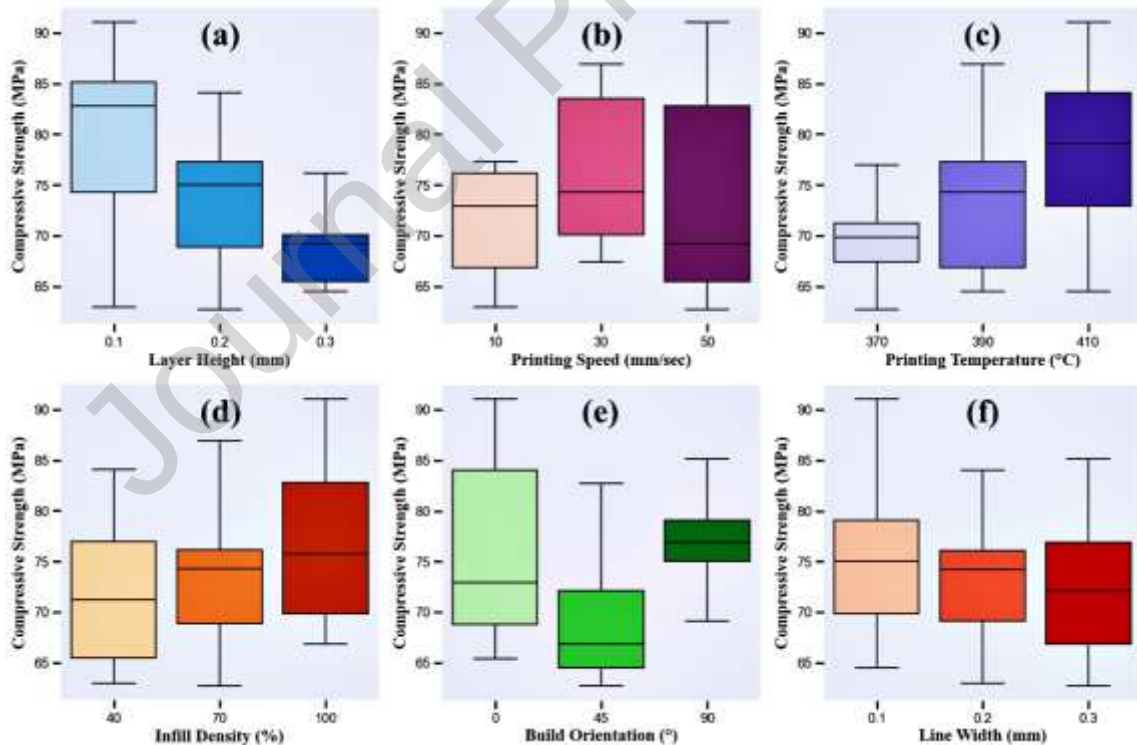


Figure 6. Box-whisker plot of material-extrusion factors on the compressive strength of 3D printed PEEK spinal fusion cages.

With the help of LiR model, the sequence of input material-extrusion factors is arranged in chronological order depending on their impact on developed compressive strength, and their respective

percentile contributions are determined. The sequence of material-extrusion factors depending on their impact on the compressive strength is layer height > printing temperature > build orientation > printing speed > infill density > line width. Among the various input material-extrusion factors, the layer height developed a major influence of 25.917 %. The printing temperature followed layer height by 22.894 %. The build orientation and printing speed followed layer height by 20.951 % and 11.879 %. Finally, the material-extrusion factors like infill density and line width hold the least contribution of 11.232 % and 7.127 %.

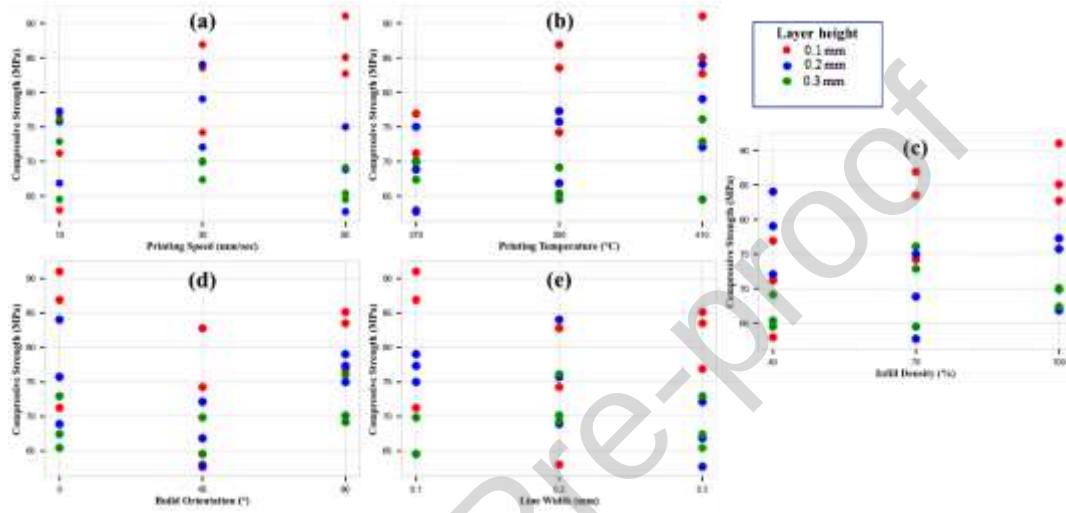


Figure 7. Pair-plot of (a) Printing speed, (b) Printing temperature, (c) Infill density, (d) Build orientation, and (e) Line width on the compressive strength of 3D printed PEEK spinal fusion cages.

Figure 7 depicts the pair-plot representation of independent material-extrusion factors like printing speed, printing temperature, build orientation, infill density, and line width on the output response of the 3D printed PEEK spinal fusion cages (compressive strength) with respect to layer height at different levels like 0.1 mm, 0.2 mm, and 0.3 mm. The pair-plot develops a pairwise relationship between the material-extrusion factors and compressive strength. From Figure 7, the input material-extrusion factors like printing temperature and infill density developed a positive correlation with the compressive strength of 3D-printed PEEK spinal fusion cages. Whereas input material-extrusion factors like line width developed a negative correlation with the compressive strength of 3D-printed PEEK spinal fusion cages. Finally, the layer height factor developed a significant influence on the compressive strength in comparison to other material-extrusion factors.

3.3 Analysis of training and testing data

The accuracy of training and testing data is analyzed using scatter plots which are depicted in Figure 8 and 9. The scatter plots visually depict the relationship between the actual train data and the corresponding predicted values generated by each model. By examining the distance between every individual actual and predicted train point in the scatter plots, the performance of the ML model in predicting the accuracy of the model is evaluated. From Figure 8, it is evident that the LiR model has

higher accuracy in terms of predicting the target variable by resulting in a higher degree of overlapping between the actual and predicted values of the train data when compared to other ML models.

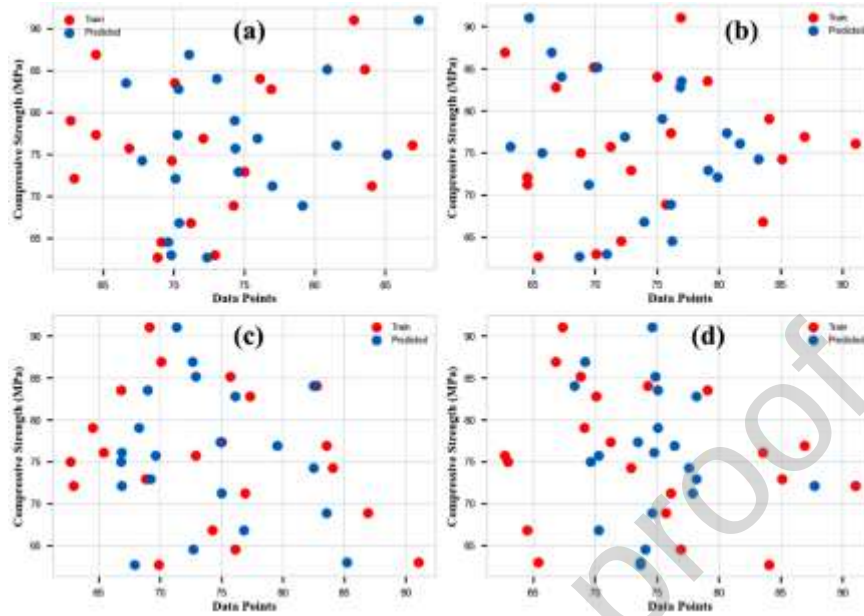


Figure 8. Actual and predicted values of train data for various ML models (a) LiR, (b) LaR, (c) DT, (d) KNN.

Figure 9 depicts the accuracy of the ML models in the instance of test datasets. From Figure 9, the actual test data and the respective predicted data plotted in the scatter plot seem to overlap. The overlapping of the actual and predicted test data refers to the increased accuracy of the respective ML model. Among the various ML models in Figure 9, the LiR model developed the highest accuracy in terms of predicting the compressive strength of 3D printed PEEK spinal fusion cages due to the increased overlapping of datasets.

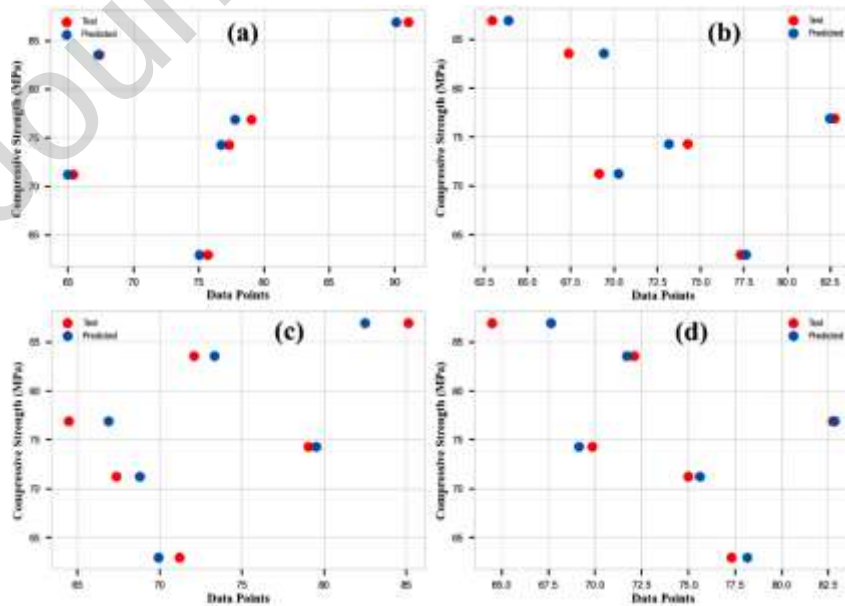


Figure 9. Actual and predicted values of test data for various ML models (a) LiR, (b) LaR, (c) DT, (d) KNN.

Figure 10 demonstrates the residual plots of various ML models which help in determining the performance of the train and test dataset of the 3D-printed PEEK spinal fusion cages. The residual plot depicts the graphical representation between the respective residuals and predicted values. It helps in representing the relation between two correlated variables within the same range. The respective residuals are represented along the y-axis whereas the predicted values are represented along the x-axis. From Figure 10, it is clear that the LiR model has attained the test data points within a lower range starting from - 2.5 to 2.5. On the contrary, the other ML models have a wider range of test data points ranging from - 5 to 5. Therefore, it can be concluded that the LiR model is the most prominent ML model for predicting the compressive strength of the 3D-printed PEEK spinal fusion cages.

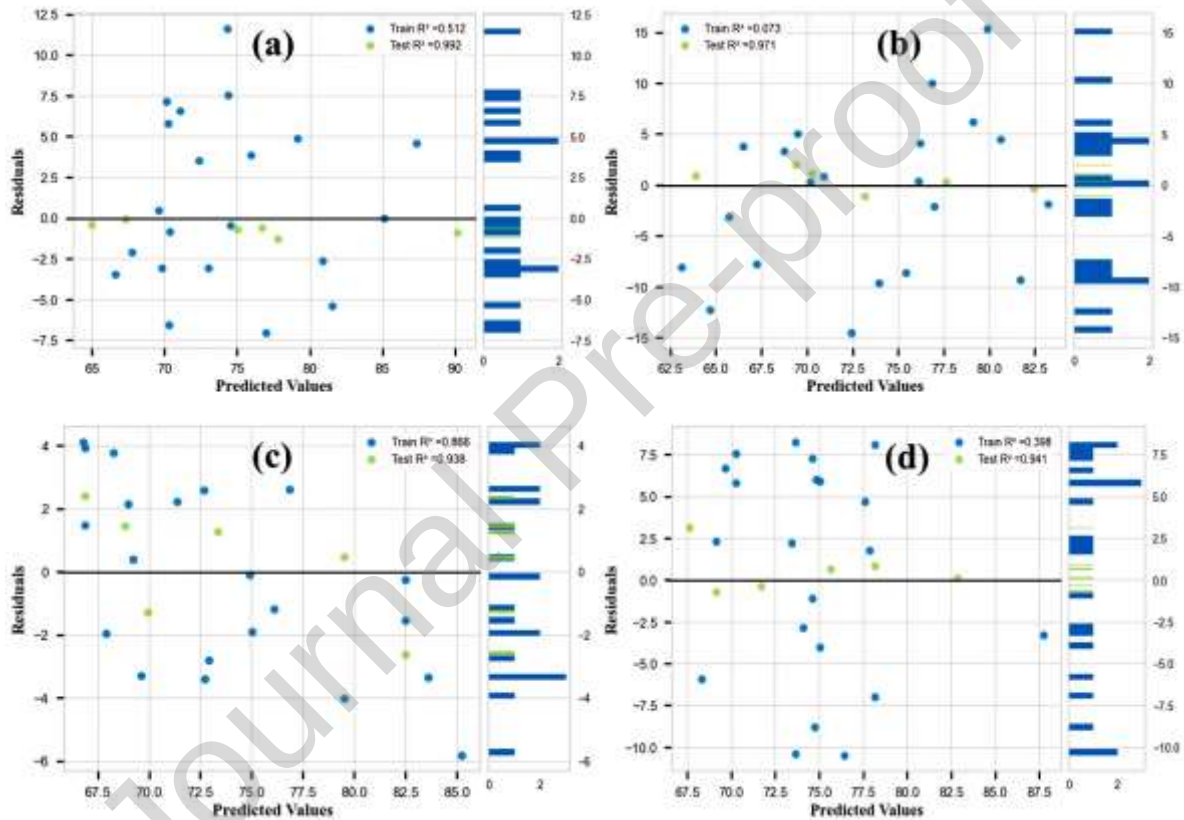


Figure 10. Residual plot of various ML models (a) LiR, (b) LaR, (c) DT, (d) KNN.

3.4 Evaluation metrics

Table 2. Error metrics of various ML models for the test dataset

Error metrics	Root Mean Square Error (RMSE)	Mean Absolute Error (MAE)	Median Absolute Error (MedAE)
LiR	0.758	0.657	0.634
LaR	1.121	0.958	1.001
DT	1.739	1.578	1.358
KNN	1.396	0.971	0.669

The adequacy of train and test data points is evaluated with the assistance of error metrics. For the current study, the error metrics like RMSE, MAE, and MedAE are considered. These error metrics are

well enough to determine the adequacy of the predictive model. Figure 11 presents the error metrics of various ML models under boosting ensemble learning techniques for test data points.

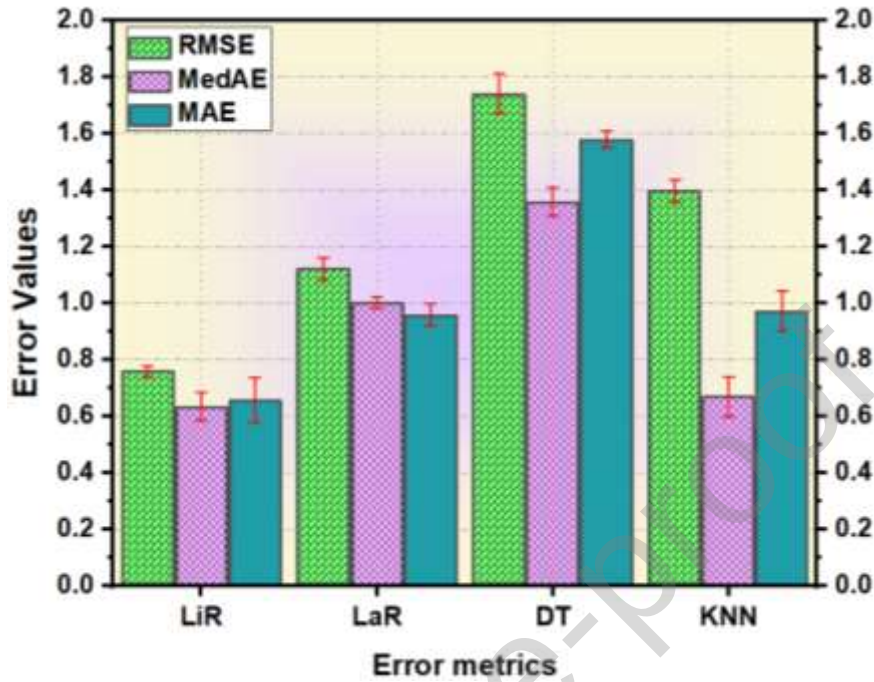


Figure 11. Error metrics of various ML models (a) LiR, (b) LaR, (c) DT, (d) KNN for the test dataset.

From Figure 11, the LiR model attained the least level of error metrics like RMSE of 0.758, MAE of 0.657, and MedAE of 0.634. Table 2 lists error metrics of the various ML models under boosting ensemble learning technique for test data points. From Table 2, the LiR model under the boosting ensemble technique seems to be the most accurate ML model in predicting the compressive strength of the 3D-printed PEEK spinal fusion cages.

3.5 Characterization of printed sample with effect of process parameters

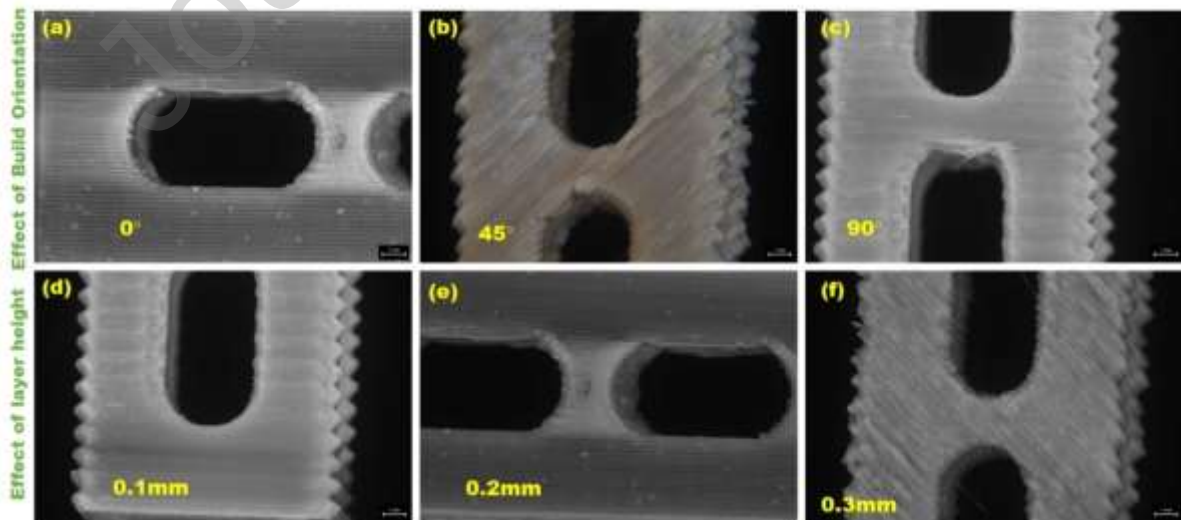


Figure 12. Stereomicroscopy images of 3D printed PEEK samples (a) 0°, (b) 45°, (c) 90° printing orientation, (d) 0.1mm, (e) 0.2mm and (f) 0.3mm layer height.

The print resolution of the developed biomedical implants depends on the material-extrusion factors. Figure 12 (a-c) shows the build orientation of the 3D-printed spinal fusion cage. It is evident that 0° and 90° build orientation has better layer adhesion when compared with the 45° build orientation. In the case of 45° build orientation, there is a greater number of layer shrinkage and uneven deposition of the printed layers, this may end up in failure initiation point under compressive loading. In the case of 90° printed samples exploits the greater number of printed layers when compared with other 45° and 0° printed samples. This may withstand more loads when compared with minimal-layer printed samples. Figure 12 (d-f) shows the impact of layer height on the 3D-printed spinal fusion cage. The result clearly shows that, at 0.3 mm layer height the surface qualities are poor and the interlayer adhesion between the successive layers. In the case of 0.1 mm of layer height, the layer adhesion and print surface quality were good. The interfacial adhesion was better based on the cohesive force between the print layers. This results in experiencing better load transferring capacity on the prepared fusion cage with fewer voids, defects, and good surface quality [38].

3.6 Performance study of the optimized 3D printed PEEK spinal fusion cage

The optimized PEEK spinal fusion cages are fabricated at the optimized level of input material-extrusion factors like a layer height of 0.1 mm, a printing speed of 30 mm/sec, a printing temperature of 410°C , an infill density of 100 %, a build orientation of 90° , a line width of 0.1 mm. Figure 13 represents the stress-strain curve obtained for the optimized PEEK spinal fusion cage. The optimized PEEK spinal fusion cage reports a higher compressive strength of 92.154 MPa.

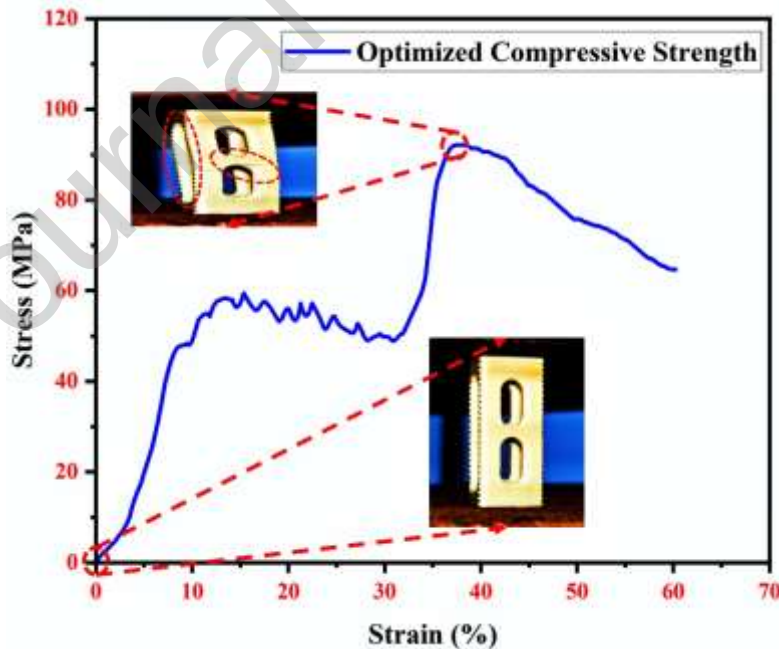


Figure 13. Stress-Strain curve of the optimized PEEK spinal fusion cage.

From Figure 12, it can be inferred that the optimized PEEK spinal fusion cage undergoes a progressive mode of crushing, lateral buckling, and interlayer delamination. Initially, the optimized cage undergoes step-by-step crushing within the strain range of 10 % to 30 %. In addition, the fluctuation in the

respective strain range denotes the progressive crushing failure mode. Then, the optimized cage develops lateral buckling failure within the strain range of 30 % to 37 %. Finally, when the optimized cage is strained to 40 %, the ultimate compressive strength of 92.154 MPa is attained and then consequently the cage is subjected to interlayer delamination.

4 Conclusion

In recent years, 3D printing has become one of the inevitable technologies in biomedical device development and they are facing many upgradations trend in technological adaptation. In this study, various machine learning algorithms were adapted to improve the printing process parameters of the PEEK spinal fusion cage with respect to the compressive strength properties. These machine learning algorithms are beneficial in optimizing the mechanical properties, print quality, and effective printing parameters concerning the particular type of implants. The following conclusions can be drawn from the present study:

1. The optimized level of input material-extrusion factors for attaining higher compressive strength are a layer height of 0.1 mm, a printing speed of 30 mm/sec, a printing temperature of 410°C, an infill density of 100 %, a build orientation of 90°, a line width of 0.1 mm.
2. The LiR model under the boosting ensemble technique seems to be the most accurate ML model in predicting the compressive strength of the 3D-printed PEEK spinal fusion cages.
3. The least error from the testing data is observed on the LiR model with a RMSE of 0.758, MAE of 0.657, and MedAE of 0.634.
4. The optimized PEEK spinal fusion cage undergoes a progressive mode of crushing, lateral buckling, and interlayer delamination.
5. The summarized data are expected to be the key results for the development of ML-based systems and can adopt more input parameters to customize implants fabricated by 3D printing technologies.

Acknowledgement

The authors extend their appreciation to the Researchers Supporting Project (no. RSPD2024R680), King Saud University, Riyadh, Saudi Arabia, for funding this study.

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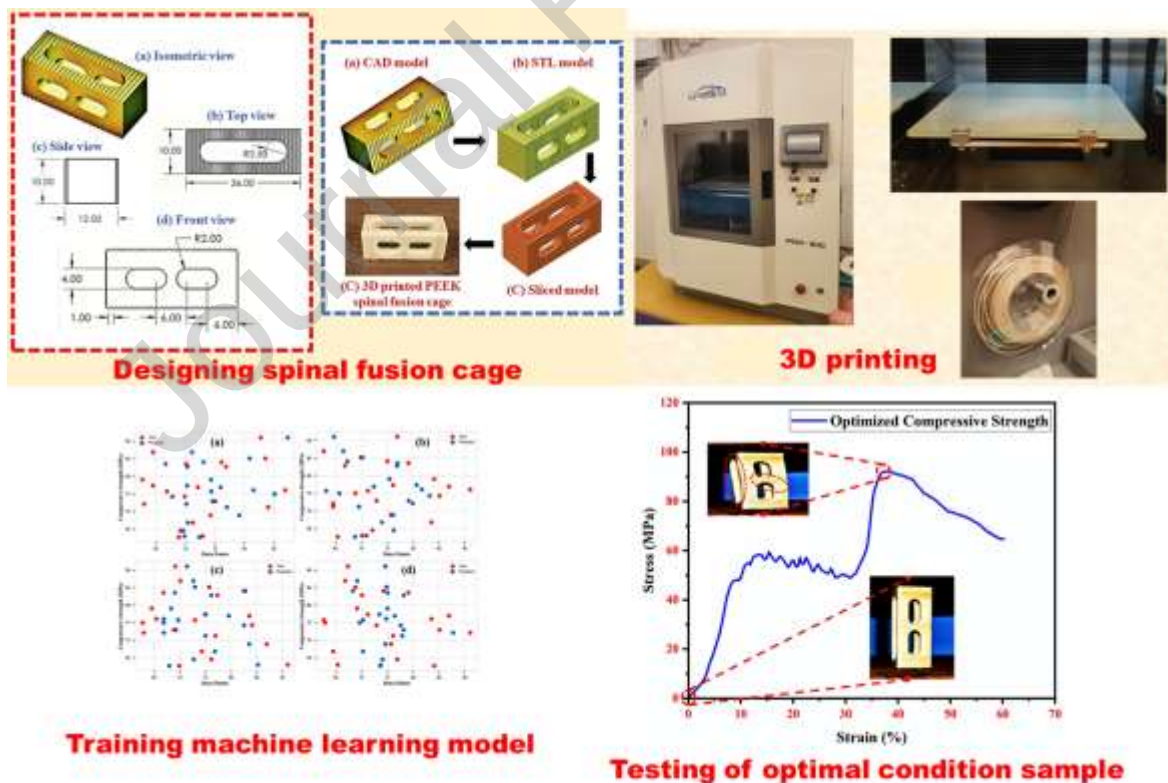
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Graphical abstract



Credit author statement

Narain Kumar Sivakumar: Writing- Review & Project administration

Sabarinathan Palaniyappan: Conceptualization, Investigation, Resources. Writing- Review & Editing,

Mahdi Bodaghi: Writing- Review & Editing,

P Mohammed Azeem: Data acquisition and Validation

G S Nandhakumar: Data acquisition and Validation

Santhosh Basavarajappa: Resources, Data acquisition and Validation

Saravanan Pandiaraj: Resources, Data acquisition and Validation

Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Highlights

- 3D-printed PEEK spinal fusion cage is fabricated by 3D printing technology.
- Machine learning (ML) algorithms to evaluate the mechanical properties of additively manufactured PEEK spinal fusion cages.
- Optimized PEEK spinal fusion cage reports a highest compressive strength of 92.154 MPa.
- Linear Regression model implemented under the boosting ensemble technique, demonstrates the highest accuracy on the compressive properties.