MACHINE LEARNING-BASED PREDICTIVE MODELLING OF LAMINATED COMPOSITES

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ABSTRACT

Laminated composite plates and shells are widely used in aerospace, marine, and automotive industries. Their structural response can be tuned by modifying the stacking sequence, but accurate modelling requires computationally expensive finite element (FE) analysis. This study develops machine learning-based predictive models as surrogates for FE analysis to predict the first natural frequency of laminated composites. Two problems are considered, a 2-variable low-dimensional (LD) problem and a 16-variable high-dimensional (HD) problem. Six machine learning models were trained and evaluated. For the LD problem, support vector regression (SVR) performed best (R^2 = 0.9972, MSE = 0.0097). For the HD problem, Gaussian process regression (GPR) outperformed others (R^2 = 1.000, MSE $\ll$ 0.0001), effectively handling complex nonlinearities. The results highlight SVR's suitability for simpler cases and GPR's superior predictive accuracy for high-dimensional design spaces.

KEYWORDS

Laminated composite, Machine learning, Prediction, AdaBoost, MLP, Random Forest, Gaussian process, SVM

1 INTRODUCTION

Composite material is made of two or more constituent materials with significantly different chemical or physical properties which, when combined, produce a material with characteristics different from the individual components. The material after formation has a property far better than the individual ones. The composite material becomes lighter, more robust and less expensive than the traditional material. Different professionals have employed composite materials to limit their ingenuity and creativity. Further, composite has played an important role in moving towards industrial use and brought a revolution in material usage [Gilbert 2017, Karger-Kocsis 1995]. It is being used by different industries, like transport, construction, energy, sports, health etc. For example, automotive industry [Hallal 2013] has utilized the composites to reduce vehicle mass and improve driving performance all around. Composites have helped the designers build luxurious and high-end cars [O'Rourke 1990]. In aerospace, it has helped save fuel costs by adding a lightweight material with strength. Now, it has been part of half of the mass of a commercial carrier. The advanced composite fuselage used in aircraft improves performance, safety and reliability. It has even helped in making powerful rockets for future space tourist flights. Even in construction, the researchers have prized out the composites having better corrosion resistance, structural strength, insulation capacity, design flexibility and fatigue resistance [Banakar 2012] which have helped in making different sky-touching monuments and heavy load bearing bridges with unique designs. It has also contributed to green energy spaces by proving more substantial and longer rotor blades for wind turbine to produce wind energy. Adding to the part of medical use [Oka 2011], composites have helped patients in rehabilitation and prolonged their abilities. Different medical manufacturers prefer composites to manufacture various medical equipment. Overall, composites have reached every corner from home furnishing to space equipment and have given clean and sustainable materials. It has also added sustainability to grow more in different industries in perspective of material use and has called out to have a good scope of lightweight material with high strength [Prashanth 2017], durability, design flexibility [Ma 2021], excellent chemical and corrosion-resistant properties for different uses [Mangino 2007, Qin 2006].

Various researchers have adopted machine learning (ML) algorithms to optimize and predict the behaviour of complex engineering problems [Nag 2024] [Mpia 2024]. Simulating and analyzing are more common than prototyping due to significant savings in cost and time [Chen 2019]. Similarly, prediction of responses using ML algorithms is economical rather than simulating using physics-based models. It reduces overall computation cost and time. The era is transforming from design-based concepts to data-driven approaches based on ML techniques. Many researchers have applied regression and classification techniques to make accurate predictions. Kaveh et al. [Kaveh 2021] considered four ML algorithms, i.e. random forest, deep learning, decision tree and multiple linear regression to establish a relationship between fiber angle and buckling capacity of cylinders under bending-induced load. It was observed that deep learning ML model had the smallest error with substantial reduction in overall computation cost and time. Tiryaki et al. [Tiryaki 2014] utilized multiple linear regression and artificial neural network (ANN) to predict heat-treated wood's compressive strength. The results showed that ANN would provide closer results with minor errors than multiple linear regression.

Yang et al. [Yang 2018] proposed application of a deep learning model to predict stiffness of high contrast elastic composites. Gu et al. [Gu 2018] employed linear regression and convolution neural network to a composite system to predict its various mechanical properties, including toughness and strength. Marani et al. [Marani 2020] validated the application of different regression techniques, i.e. random forest, gradient boosting and extreme gradient boosting to predict compressive strength of PCM-integrated cementitious composites. Zhang et al. [Zhang 2021] employed the Gaussian process regression model to predict delamination factors during drilling of carbon fiber-reinforced plastic composite. Kordijazi et al. [Kordijazi 2020] proposed the application of three ML algorithms, e.g. linear regression, ANN and multivariate polynomial regression to envisage the wetting properties of iron-based composites. Le et al. [Le 2021] also used the Gaussian process regression for prediction of tensile strength of polymer carbon nanotube composites.

Most of the research works cited above on ML modelling of composite systems have a narrow purview, either in terms of data used or number of design variables or complexity and spread of the design space. Typically, most of the works are limited to 30 data points, 3-5 design variables and a very narrow range of design variables. As such, these problems pose very limited challenges to ML algorithms. Considering a laminate stacking sequence design problem, Kalita et al. [Kalita 2021] carried out a comprehensive study on the effect of different basis functions of radial basis function ML models on their accuracy and prediction quality.

In this paper, a similar laminate stacking sequence design problem is considered. The frequency characteristics of the laminated composites can be expressed as functions of the stacking sequence. However, the range of ply angles for each stacked layer is ±90°, which imposes a significant challenge to ML algorithms in terms of vastness of the design space. In this paper, six different ML predictive algorithms, i.e. Linear regression, random forest (RF), adaptive boosting (AdaBoost), support vector machine (SVM), multilayer perceptron and Gaussian process regression are applied to model the laminate design problem and identify the best performing predictive model with respect to some popular statistical metrics, while addressing two different problems with different dimensions.

2 METHODOLOGY

2.1 Machine learning algorithms

To develop predictive models for laminated composite structures, six widely used supervised learning algorithms were selected: linear regression (LR), random forest regression (RFR), adaptive boosting (AdaBoost), support vector regression (SVR), multilayer perceptron (MLP), and Gaussian process regression (GPR). Each of these algorithms has distinct advantages and suitability depending on the complexity of the problem. Their key principles and selection rationale are discussed below.

2.1.1 Linear regression

Linear regression is one of the simplest supervised machine learning models, which assumes a linear relationship between input variables (design parameters) and the output (natural frequency). The model fits a straight-line equation:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_n X_n + \varepsilon \tag{1}$$

where β_0 is the Y-intercept and β_1 is the slope of the line, ε is the random error term, n number of independent variables.

LR was included as a baseline model to evaluate how well linear approximations capture the composite response.

2.1.2 Random Forest

Random forest is an ensemble-based method that constructs multiple decision trees using different subsets of training data. Predictions from each tree are aggregated to improve accuracy and reduce overfitting. The key advantage of RFR is its ability to model complex nonlinear relationships while maintaining robustness against noise and overfitting.

$$\hat{Y} = \frac{1}{T}\sum_{t=1}^{T} f_t(X) \tag{2}$$

where $f_t(X)$ represents individual decision trees. RFR was chosen for its strong performance in moderate-dimensional problems where relationships between design variables and response functions are highly nonlinear.

2.1.3 Adaptive boosting

AdaBoost is an iterative ensemble learning technique that combines multiple weak learners (typically decision stumps) into a strong predictive model. It assigns higher weights to misclassified samples in each iteration, forcing subsequent weak learners to focus on difficult-to-predict instances. The final prediction is obtained as a weighted sum of all weak models:

$$F(X) = \sum_{m=1}^{M} \alpha_m h_m(X) \tag{3}$$

where $h_m(X)$ represents weak learners, and α_m are their assigned weights. AdaBoost was selected for its ability to improve model accuracy in cases where individual models struggle to generalize well.

2.1.4 Support vector machine

SVR is a kernel-based learning algorithm that maps input features into a higher-dimensional space to find an optimal regression hyperplane. Unlike linear regression, SVR aims to minimize errors within a margin of tolerance (ϵ-insensitive loss function), ensuring robustness against outliers:

$$\min_{w,b} \frac{1}{2} \parallel w \parallel^2 \quad \text{subject to } |Y - (wX + b)| \le \epsilon \tag{4}$$

where w and b define the hyperplane. SVR was chosen because it excels in capturing nonlinear dependencies in low-dimensional problems, as demonstrated by its superior performance in the 2-variable LD case.

2.1.5 Multilayer perceptron

MLP is a type of artificial neural network (ANN) that consists of multiple layers: an input layer, hidden layers, and an output layer. Each neuron applies an activation function (e.g., ReLU, sigmoid) to process weighted sums of inputs:

$$h(x) = f(WX + b) \tag{5}$$

where W represents connection weights and b represents biases. MLP was included due to its strong capability in approximating complex functions, especially in cases where interactions between design variables are highly nonlinear.

2.1.6 Gaussian process regression

GPR is a nonparametric Bayesian approach that models the relationship between input and output variables using a probabilistic framework. It assumes that any finite set of observed data points follows a joint Gaussian distribution:

$$Y(X) \sim \mathcal{GP}\big(\mu(X), K(X, X')\big) \tag{6}$$

where $\mu(X)$ is the mean function and $K(X, X')$ is the kernel function modelling data correlations. GPR was chosen for high-dimensional problems because it provides uncertainty quantification and handles sparse data efficiently. Its superior performance in the 16-variable HD problem confirmed its ability to generalize well in complex design spaces.

2.2 Model evaluation method

The accuracy of any machine learning model is one of the essential parts to be calculated. To evaluate the model's performance, different performance metrics, MSE, MAE and R^2 or Coefficient of determination metrics, are used in regression analysis.

2.2.1 R-square

Coefficient of determination is the most used accuracy metric in regression tasks. It is a measure of the amount of variance in the data explained by the developed model. R^2 is determined by.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(x_i - \hat{x})^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2} \tag{7}$$

where x_i = actual value of x, $\bar{x}$ = Mean value of x, $\hat{x}$ = Predicted value of x.

2.2.2 Mean absolute error

Mean absolute error (MAE) are metrics which is being used for getting the accuracies of model. It measures the level of accuracy being reached over there using the model. It says about how much deviation is there from the actual. The average of mean absolute difference between the actual and predicted value in dataset is further calculated as

$$MAE = \frac{1}{N}\sum_{i=1}^{N}|x_i - \hat{x}| \tag{8}$$

2.2.3 Mean square error

Means square error measures the degree to which overall sample deviates from the actual value to the predicted one.

$$MAE = \frac{1}{N}\sum_{i=1}^{N}(x_i - \hat{x})^2 \tag{9}$$

2.2.4 Median error

The median error is computed as

$$\mathrm{Med.\,Error}\ (x, \hat{x}) = \mathrm{median}\ (|x_1 - \hat{x}_1|, \ldots, |x_n - \hat{x}_n|) \tag{10}$$

2.2.5 Median absolute error

Median absolute error is used to compare the true observed response with predicted response in regression. It is calculated as

$$\mathrm{Med.\,Error}\ (x\,, \hat{x}) = \mathrm{median}\ (|x_1 - \hat{x}_1|, \ldots, |x_n - \hat{x}_n|) \tag{11}$$

2.3 Objectives and problem description

The prime objective of this paper is to assess the utility of six popular ML regression algorithms in developing accurate prediction models for laminate composite systems. For this task linear regression (LR), random forest regression (RFR), Ada Boost regression (ABR), support vector regression (SVR), multi-layer perceptron regression (MLP), gaussian process regression (GP) are selected. The developed models are assessed using a variety of metrics like mean square error (MSE), R- square(R^2), mean absolute error (MAE), etc. on training as well as independent test data.

Two test problems of varying dimensionality are considered in this work. The first problem is a 2-variable low dimensional (LD) problem. Here, the objective is to accurately predict the first natural frequency using the ply-angles as the design variables. The range of the ply angles is ±90°. Similarly, for the second problem, a 16-variable high dimensional (HD) problem is selected. Here too the ply angles of the 16 layers are the variables which can vary between ±90°.

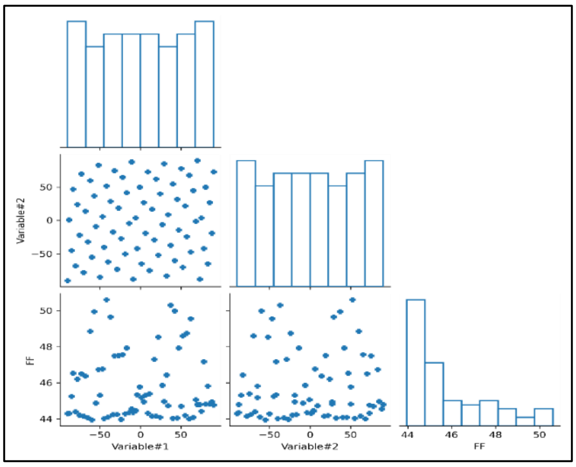

Figure 1. Pair plot diagram for the design and response variable for low dimensional problem

3 RESULT AND DISCUSSION

3.1 Low-dimensional problem

In this LD problem, a square symmetric simply supported composite of 4-ply material graphite-epoxy composite laminate is considered where the ply angles are considered as a design variable. The data analyzed using various ML models are utilized from Kalita et al. [20]. For the LD problem, the thickness to side ratio of the composite plate is being taken as 0.0005. The first natural frequency is obtained using FEM analysis [20]. The training dataset is design using a Hammersley design and contains 72 data points. A random sampled independent test dataset of 20 datapoints is also used.

3.1.1 Data visualization

The training data is visualized using pair plot diagram as shown in Figure 1 which gives the correlation between the different design variables and a response providing the relationship between the different variables of data. It is seen that due to the use of Hammersley design the data points are uniformly distributed in the search space. The effect of both the variables is seen to be similar on the first natural frequency.

In Figure 2 the data is described by Pearson correlation heatmap which shows the correlation between the input and output parameters. The responses show no correlation between the two independent variables which exhibit the lack of multicollinearity, an important assumption for statistical regression models. The first natural frequency also has a very low correlation with the input variables. This indicates that the dependent variable has very small linear relation with the independent variables and thus algorithms that rely on mapping only linear relations will have low predictive power.

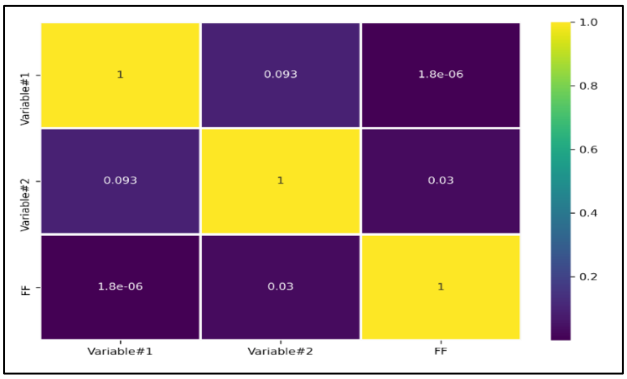

Figure 2. Correlation heatmap between frequency and variables for LD problems

Random Forest has performed well in testing data for the low dimensional problem. Compared to all the models over here, the support vector regression has performed well with R^2 0.99, i.e., relatively closer to 1 in the training data. All other models show the negative result in the R^2 case, which directly means that the model is performing worse than the mean value line. MSE is quite similar to MAE, but the square of the difference between the model prediction and the training dataset is being calculated instead of using the absolute value. MLP has shown a higher value for MSE, i.e., 157.22, and MAE for the same is 10.13 in the case of the training dataset.

Metric	R^2	MSE	MAE	MSLE	MedAE
LR	0.0009	3.4416	1.5338	0.0015	1.4225
RFR	0.9487	0.1768	0.3153	0.0001	0.2103
ABR	0.8541	0.5024	0.5767	0.0002	0.5801
SVR	0.9972	0.0097	0.0976	0	0.0999
MLP	-44.6443	157.2276	10.1354	0.1251	8.7607
GPR	1	<<0.0001	<<0.0001	<<0.0001	<<0.0001

Table 1. Performance metrics for the training data of LD problem

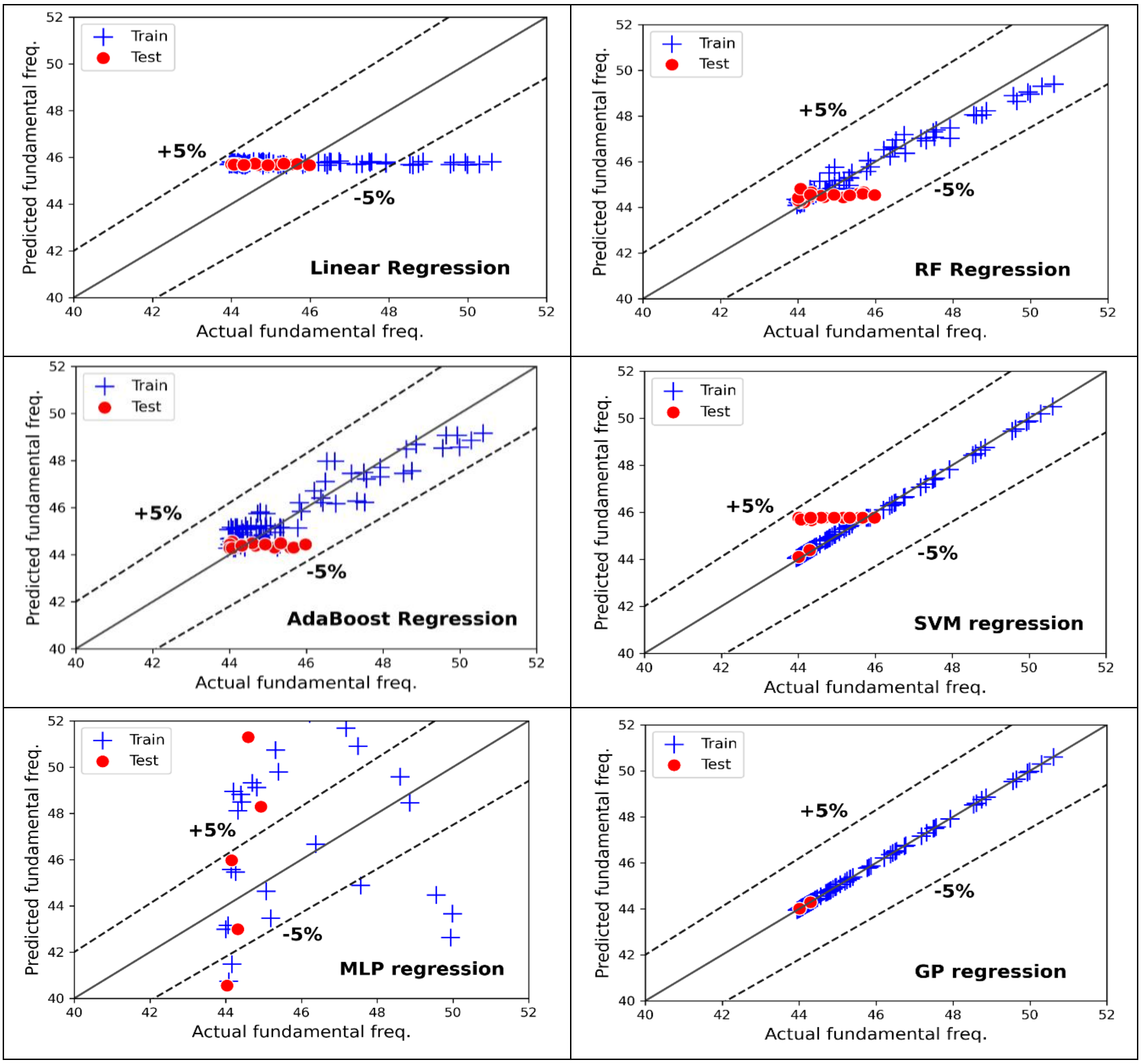

Figure 3. Comparisons of ML regression model for low dimensional problems

Similarly, the gaussian process regression has shown a huge value of MSE, i.e., 1799. It shows the presence of lots of outliers, hindering the model's prediction accuracy. The MSE value is considered a good value as it is closer to 0. Compared to all in Random Forest MSE value is 0.17 and SVR is 0.009, much closer to 0 in training and testing; RFR has performed well and has an MSE value of 0.39.

Metric	R^2	MSE	MAE	MSLE	MedAE
LR	-2.5456	1.5529	1.0837	0.0007	1.349
RFR	0.1082	0.3906	0.4965	0.0002	0.3244
ABR	-0.2524	0.5485	0.5791	0.0003	0.4822
SVR	-2.1635	1.3855	0.9759	0.0007	1.1453
MLP	-187.2959	82.4693	8.3881	0.0428	9.0981
GPR	-4107.0268	1799.2209	40.2359	13.148	44.329

Table 2. Performance metrics for testing data of LD problem

3.2 High-dimensional problem

For the HD problem, a simply supported 32-ply square symmetric composite laminate is considered. The16-ply angles are considered as the design variables. The ratio between thickness to the side is 0.04. The training data for the HD problem is designed as per Hammersley design containing 712 datapoints and the testing data is made of 50 randomly sampled datapoints.

Multivariate analysis is done to visualize the data. Fig 4 shows the heatmap (correlation matrix) graph. It is observed that there is no correlation found among the design variables. Thus, there is no multicollinearity in the data. However, the output response i.e., the first natural frequency too does not show any linear dependencies on the 16 design variables.

Similarly, the data is being analyzed for the high dimensional problem and the different performance metrics were taken into consideration to analyze the performance of other models being executed. The coefficient of determination, i.e., R^2 values, is examined and found that random forest, support vector and GPR have performed well, and residuals are closer to the fit line. The performance was too weak for all the models to determine the lack of proper determination between the dependent and independent variables in testing data.

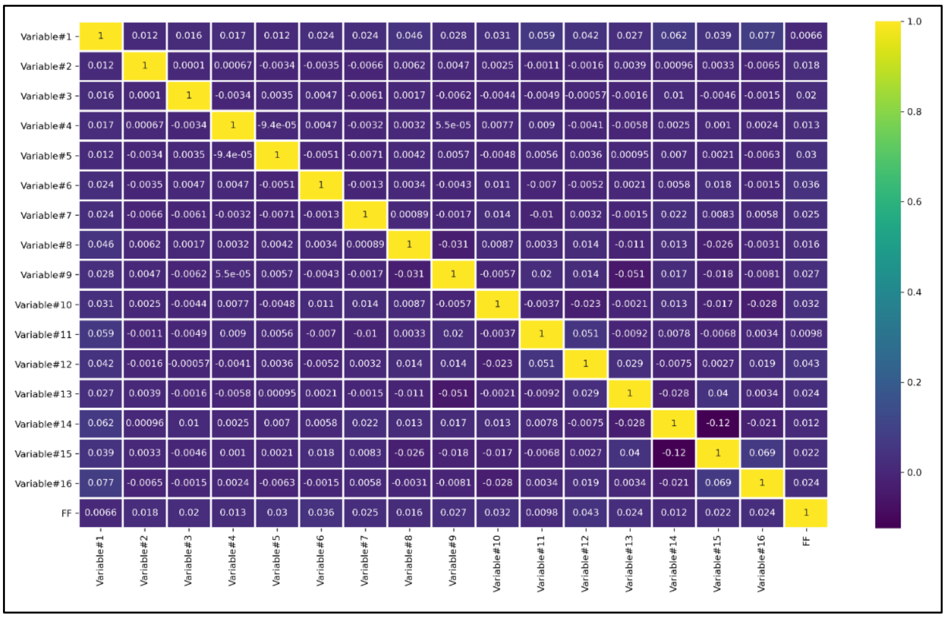

Figure 4. Correlation heatmap between frequency and variables for High Dimensional problems

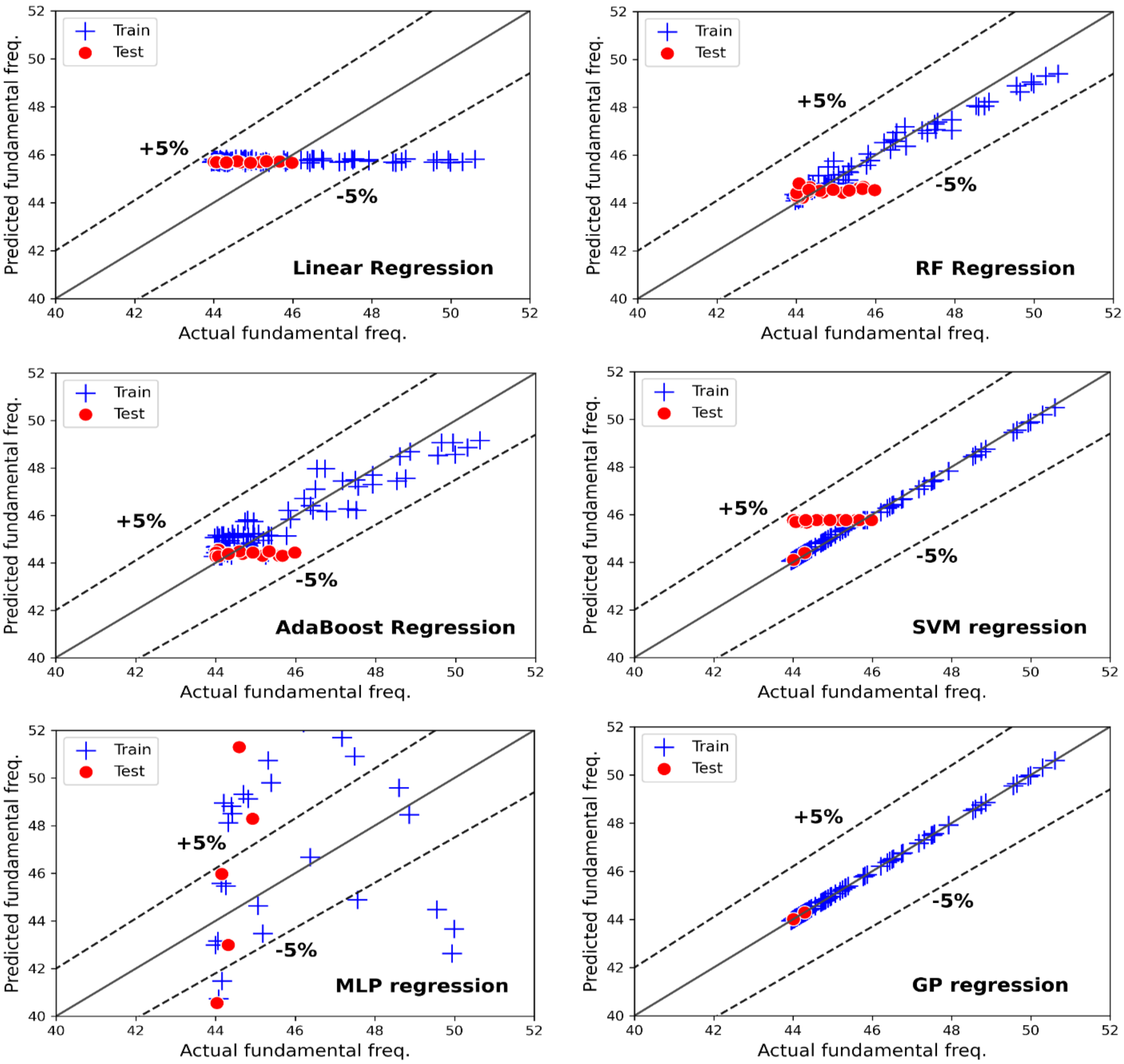

Figure 5. Comparisons of ML regression model for High dimensional problem

Metric	R^2	MSE	MAE	MSLE	MedAE
LR	0.0095	2.1465	1.1868	0.0009	0.9928
RFR	0.8955	0.2264	0.374	0.0001	0.2992
ABR	0.2026	1.7279	1.0789	0.0007	0.9292
SVR	0.9955	0.0097	0.098	0	0.1
MLP	0.839	0.3488	0.4559	0.0001	0.3692
GPR	1	<<0.0001	<<0.0001	<<0.0001	<<0.0001

Table 3. Performance metrics for the training data of HD problem

Metric	R^2	MSE	MAE	MSLE	MedAE
LR	-1.8727	17.927	3.7442	0.0081	4.5364
RFR	-0.5119	9.4352	2.6458	0.0043	2.6073
ABR	-1.1341	13.3179	3.0807	0.006	2.8376
SVR	-2.3469	20.8862	4.0056	0.0093	5.2132
MLP	-32.1258	206.7222	10.4069	0.351	7.1385
GPR	-321.7474	2014.1092	44.3595	14.3983	43.8912

Table 4. Performance metrics for testing data of HD problem

4 CONCLUSIONS

This study investigates the predictive modeling of laminated composites using machine learning techniques. Based on the analysis, the following key findings are highlighted—

1. For low-dimensional (LD) problems, support vector regression (SVR) demonstrated the best performance, achieving an R^2 value of 0.9972 and MSE of 0.0097, making it a strong candidate for simpler cases.
2. For high-dimensional (HD) problems, Gaussian process regression (GPR) outperformed all other models, achieving $R^2 = 1.000$ and an extremely low MSE $\ll 0.0001$, demonstrating its capability to handle complex nonlinear relationships.
3. Random forest regression (RFR) and AdaBoost showed competitive performance, particularly in moderate-dimensional cases, but struggled with scalability in very high-dimensional spaces.
4. The lack of multicollinearity in design variables was confirmed using correlation heatmaps, ensuring that machine learning models were not biased due to redundant inputs.
5. The results provide a valuable reference for optimizing composite structures, particularly in aerospace, automotive, and marine applications where computational efficiency is critical.

Future work will explore hybrid machine learning models and deep learning approaches to further enhance predictive accuracy and generalization for complex laminated composite systems.

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