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Artificial Intelligence for Mechanical Property Prediction of Multi-Material Gyroid Structures

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Abstract

Mechanical property predictions in multi-material lattice structures are very important in order to optimize lightweight designs in the field of engineering and biomedical applications. In this work, the behaviour of gyroid structures made of thermoplastic polyurethane (TPU) and polylactic acid (PLA) was predicted using machine learning (ML) algorithms. This study incorporates two key design parameters (PLA percentage and relative density) of gyroid structures. Since TPU content is complementary to PLA, it was not used as an independent variable. Three mechanical properties were assessed as target outputs: elastic modulus (EM), energy absorption (EA), and peak stress (PS). A systematic comparison of five ML algorithms (artificial neural networks, support vector regression, random forest, decision tree, and CatBoost) was carried out using the mean absolute error (MAE), root mean squared error (RMSE), and mean arctangent absolute percentage error (MAAPE) for each property. The results indicated that CatBoost maintained consistently well-balanced predictive performance. Meanwhile, random forest exhibited the highest robustness and scale-independent performance across all mechanical properties.

Keywords
Machine Learning, Multi-Material Structures, Gyroid Structures, Mechanical Property Prediction and Metamaterials

1. Introduction

Additive manufacturing (AM), which is also known as 3D printing, has revolutionized structural design. It has made it possible to create complicated lattice materials with specialized applications such as lightweight parts, protection equipment, as well as medical implants. Among different mechanical metamaterials, triply periodic minimal surface (TPMS) lattices, particularly gyroid structures, stand out because of their smooth curvature, continuous load paths, and manufacturability without support structures when fabricated by fused deposition modelling (FDM) (Teawdeswan and Dong 2024). Inherent design flexibility of gyroids enables control of mechanical performance, including stiffness and energy absorption capacity, by changing design parameters (Teawdeswan and Dong 2024). Multi-material additive manufacturing (MMAM) is a new technology that has opened up the design space of these lattices by allowing one to incorporate contrasting mechanical behaviour materials. Combining polylactic acid (PLA), a stiff and brittle polymer, with thermoplastic polyurethane (TPU), a soft and ductile polymer, allows a single structure to simultaneously exhibit strength, elasticity, and energy absorption capabilities. Teawdeswan and Dong (2024) demonstrated that the mechanical response of PLA–TPU gyroid lattices can be precisely tuned by adjusting both relative density and the fraction of stiff and flexible phases. However, the highly nonlinear and coupled effects between these parameters make analytical prediction difficult and conventional finite element (FE) approaches computationally demanding.

Machine learning (ML) provides an effective approach by capturing complex, multidimensional relationships between design parameters and mechanical responses with high predictive accuracy and low computational cost (Zhang et al.

2021). Studies have shown the use of ML algorithms for lattice structures' mechanical property predictions. Zhang et al. (2021) achieved high prediction accuracy for titanium TPMS structures using an Adaboost regression model. Li et al. (2025) demonstrated that a back propagation neural network could effectively correlate multiple TPMS parameters with yield strength and optimize the performance of gyroid–diamond lattices. However, most studies have focused on single-material structures. Therefore, there is a research gap in data-driven modelling of multi-material structures. Mechanical behaviour of dual-phase structures, in which load transfer is through interfaces between dissimilar materials, is under-investigated from the predictive perspective. To overcome this issue, it is necessary to establish a systematic approach that links structural and compositional design variables to mechanical properties in a forward sense, so that the correct and efficient estimation of performances can be made before fabrication.

In this work, ML algorithms are used to predict elastic modulus (EM), energy absorption (EA), and peak stress (PS) of PLA-TPU based gyroids. Prediction performance of different regression algorithms (artificial neural networks, support vector regression, random forest, decision tree, and CatBoost) was carried out based on the mean absolute error (MAE), root mean squared error (RMSE), and mean arctangent absolute percentage error (MAAPE) of each property to identify the most robust algorithm for this forward prediction task.

1.1 Objectives

The objective of this research is to implement and evaluate ML algorithms for forward prediction of mechanical properties — specifically elastic modulus (EM), energy absorption (EA), and peak stress (PS) — in multi-material gyroids composed of PLA and TPU. The specific objectives are to:

1. To implement Artificial Neural Networks (ANN), Support Vector Regression (SVR), Random Forest (RF), Decision Tree (DT), and CatBoost for the forward prediction of mechanical properties.
2. To evaluate model performance using standard statistical metrics such as MAE, RMSE, and MAAPE.

2. Literature Review

Traditionally, finite element analysis (FEA) and experimentation are utilized to derive mechanical properties of additively manufactured lattice structures. Though these methods are accurate, they are computationally intensive and limited in scalability. Recently, advancements in supervised and deep learning have enabled the construction of data-driven models capable of mapping complex relationships between structure, composition, and mechanical properties. These have sped up the complex design process of mechanical metamaterials.

Numerous studies have successfully applied machine learning algorithms to predict mechanical properties of different lattice structures. Ma et al. (2022) implemented support vector regression (SVR) to predict the elastic modulus and yield strength of a 3D printed unit cell. Their model used voxel-based entropy features along with porosity and base material stiffness, achieving results comparable to FEA but in a fraction of the time. Similarly, Bai et al. (2024) applied artificial neural networks (ANNs) to predict Young's modulus and yield strength of lattice structures. On the basis of the Gibson–Ashby model, they separated the data into bending- and stretching-dominated groups. They achieved impressive accuracy, showing that physically informed classification improves learning efficiency.

Prada Parra et al. (2024) employed a range of supervised learning algorithms to predict the elasticity and strength of additively manufactured fibre-reinforced polymer composites. According to their analysis, fibre content is the most influential parameter for their prediction. In their study, K-Nearest Neighbors and CatBoost have provided the most accurate predictions, while tree-based algorithms showed minimal error distribution. In terms of computational efficiency CatBoost model displayed the best performance. Armanfar et al. (2024) have studied G-lattices. They employed a two-step process involving the classification of G-lattice type and cluster-specific trained regression models for precise prediction. In their study, mechanical properties were predicted under defined loading conditions.

The predictive performance of ML algorithms has also been studied on large-scale datasets. Hooshmand et al. (2023) applied several regression algorithms to predict stiffness. In their evolution, ANN outperformed other algorithms. Zhang et al. (2021) used Adaboost, Random Forest, and XGBoost to predict the elastic modulus of triply periodic minimal surface (TPMS) structures. All of these applied methods performed impressively, particularly Adaboost performed best. Their work testifies that the integration of machine learning models can enhance computational efficiency to a greater extent. Zhang et al. (2023) employed a Bayesian-optimized XGBoost algorithm to predict the maximum stress of lattice structures with manufacturing defects. Through computer tomography, they obtained the types and number of defects and included them in prediction datasets. They considered four types of defects, and

among these thick strut defect was the most influential. In another study, Jiang et al. (2024) trained neural networks to predict compressive strength of strut-based lattice structures. They achieved a mean absolute percentage error (MAPE) of 8.82 % on test sets, demonstrating the excellent generalization ability of their model.

The studies on comparative modelling further illustrate the efficiency of machine learning based prediction frameworks. Pasini et al. (2025) investigated four approaches (analytical model, semi-empirical model, ANN, and FEA) to predict mechanical properties of different types of lattice structures, which were fabricated through fused deposition modelling (FDM). Among these four methods, ANNs performed best using only experimental data. In another comparative study, Saleh et al. (2023) predicted compressive modulus (E), strength, and specific energy absorption (SEA) of triply periodic minimum surface (TPMS) lattice structures. Prediction performance comparison was done between the mathematical and the ANFIS models. For the training dataset, both of these models performed well. However, in the testing dataset, ANFIS outperformed the mathematical model.

Li et al. (2025) used a back-propagation neural network (BPNN) to predict and optimize the yield strength of a hybrid Gyroid–Diamond TPMS. In that Hybrid Gyroid–Diamond Structure (HGDS), two geometrical topologies were blended within a single structure to enhance mechanical performance. The model achieved an adequate correlation coefficient between predicted and experimental values. After optimization, the yield strength of HGDS increased by more than 100% compared to the original HGDS. This demonstrates that BPNN can effectively enhance the mechanical properties of hybrid TPMS structures. In another study, Liu et al. (2025) have introduced a novel neural network based framework integrating unit-cell images with auxiliary matrices to make simultaneous predictions of discrete mechanical indices (elastic modulus, energy absorption, stiffness, Poisson's ratio) and full force–displacement (F–D) curves.

Seid Ahmed et al. (2025) have predicted ultimate tensile strength by utilizing ten machine learning models. For their work, they compiled 422 samples from various sources, and they evaluated the performance of machine learning algorithms on this data. They used a 70/30 train-test split for model development. With 309 external samples, they performed external validation to confirm the model's generalization ability. They also performed experimental testing and FEA simulations to confirm the robustness of their models. In their study, TabNet showcased the best individual prediction performance, while the ensemble model improved the prediction performance further. Kartal and Kaptan (2025) compared the effectiveness of Response Surface Methodology (RSM), Analysis of Variance (ANOVA), and ANN in the prediction of tensile strength of PLA components. They found that RSM and ANOVA were more accurate, but ANN was more effective in nonlinear parameter effects. In the other research, Singh et al. (2022) trained an ANN to investigate the effects of FDM printing process parameters on tensile strength, material consumption, build time and surface quality. Their findings revealed that small and well-tuned networks have the ability to deliver accurate predictions with a limited amount of data.

Hou et al. (2023) compared six single machine-learning models and an ensemble model in terms of predicting ultimate tensile strength, yield strength and elongation in magnesium alloys. They obtained better performance with the ensemble model compared to single models. Predictions by the ensemble model were very close to experimental values. This demonstrates the effectiveness of ML models for mechanical properties prediction. Wu et al. (2023) encoded lattice morphology using D2 shape descriptors and trained a deep neural network on 210 FEA-generated datasets to predict energy absorption. Reddy et al. (2025) utilized ML models for surface roughness prediction of additively manufactured lattices. ML models were applied to analyze the impact of post-processing techniques on surface roughness. Random Forest performed better in terms of robustness, and the ANN could identify nonlinear relationships, as was noted in model evaluation.

All of these studies affirm the fact that machine learning has grown into a fundamental predictive instrument of mechanical performance. Our applications are inspired by the developments described above, and we use related ML systems to predict the elastic modulus (EM), energy absorption (EA), and peak stress (PS) of multi-material gyroid lattices, thus making it possible to quickly and accurately design next-generation metamaterials.

3. Methods

This section describes data collection and processing, ML models, and the model evaluation strategies employed in this study.

3.1 Data Collection and Processing

The dataset used in this study was collected from (Teawdeswan and Dong 2024). It contains five columns. The former two are design parameters: PLA percentage (x1) and relative density (x2). The other three columns are mechanical properties, namely, elastic modulus (EM, y1), energy absorption (EA, y2) and peak stress (PS, y3) respectively. In this study, we consider design parameters as features (inputs) as well as the mechanical properties as targets (outputs). TPU content is a complement to PLA and, therefore, we did not include it as an individual input feature.

Data processing was done using pandas in Python. The feature set and target set were separated into X and y matrices, respectively. Random seeding was used to ensure that all model runs were reproducible. For algorithms sensitive to feature scaling (e.g., SVR and ANN), both the feature set and the target set were standardized using:

$$X' = \frac{(X - \mu_x)}{\sigma_x}, \quad y' = \frac{(y - \mu_y)}{\sigma_y}$$

Here, μ and σ are the mean and standard deviation of each variable, respectively. This normalization was done to make all the variables equally important to model training.

3.2 Machine Learning Models

Five regression models were implemented to predict mechanical properties. All implementations were done in Python on the Google Colaboratory platform. The models were trained and evaluated separately to have a fair comparison.

3.2.1 Artificial Neural Network (ANN)

We utilized TensorFlow to implement the ANN. It was a 10-10-3 architecture with the input layer of two neurons. ReLU was used as the activation function in the hidden layers, while the output layer employed a linear activation.

In hidden layers, each neuron computes a weighted sum of its inputs followed by a ReLU activation:

$$z_j = \Sigma_{i=1}^{d} w_{ij} x_i + b_j$$
$$a_j = ReLU(z_j) = max(0, z_j)$$

Here, x_i represent input features, w_{ij} are connection weights, b_j denotes the bias term, and a_j stands for the activated output of neuron j.

The output layer performs a linear transformation to produce the final prediction vector:

$$\hat{y} = W_2 a + b_2$$

Here, W_2 is the weight matrix and b_2 denotes the bias vector of the output layer, whereas a is the vector of activations from the preceding hidden layer.

The network was trained by minimizing the Mean Squared Error (MSE) between predicted and actual values:

$$MSE = \left(\frac{1}{n}\right) \Sigma_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Training was done using the Adam optimization algorithm with a learning rate of 0.0045. In order to avoid overfitting and improve generalization, early stopping was implemented by continually tracking the validation loss and storing model weights of the epoch with the lowest validation error. The dataset was split into the training (70%), validation (10%), and testing (20%) sets. Training data were utilized to update model parameters. The early stopping criterion was determined by the validation set. Finally, the test set was utilized to measure model performance.

3.2.2 Support Vector Regression (SVR)

SVR was implemented using the scikit-learn library within a MultiOutputRegressor framework to make predictions and to optimize hyperparameters for each property independently. The algorithm approximates a regression function that predicts the target with a specified tolerance ε and also minimizes the complexity of the model.

The fundamental regression equation can be stated as follows:

$$f(x) = w^T \varphi(x) + b$$

Here, w represents the weight vector and b denotes the bias term. φ(x) is a mapping function which maps the input variables to a higher-dimensional feature space. The optimization problem aims to minimize the weight norm:

$$minimize \left(\frac{1}{2}\right) \|w\|^2$$

Subject to:

$$|y_i - (w^T\varphi(x_i) + b)| \leq \varepsilon, \quad for\ all\ i$$

To efficiently handle nonlinear relationships, the algorithm employs kernel functions defined as:

$$K(x_i, x_j) = \varphi(x_i)^T\varphi(x_j)$$

GridSearchCV with 10-fold cross-validation was employed for tuning the hyperparameters of each property. For each property, best parameters determined were: {'regressor__svr__epsilon': 0.01, 'regressor__svr__gamma': 'auto', 'regressor__svr__kernel': 'rbf'}. After fixing these parameters model was applied to the test set (size=0.2) for performance measurements.

3.2.3 Decision Tree Regression (DT)

Like SVR, DT was also implemented using the scikit-learn library with MultiOutputRegressor. Unlike SVR, DT has an inherent capability to handle multiple outputs. Despite this capability, we applied the MultiOutputRegressor wrapper to DT. This was done because this wrapper enables tuning hyperparameters for each output independently. If the MultiOutputRegressor wrapper was not applied, then there would be one hyperparameter setting for all outputs instead of target target-specific hyperparameter setting. Hence, the MultiOutputRegressor wrapper gives us more flexibility.

A decision tree splits the feature space into smaller, disjointed subsets according to feature thresholds, which reduce prediction error. At each internal node, the algorithm selects the feature x_j and threshold t that best divide the data into two subsets according to:

$$x_j \leq t \rightarrow left\ node$$
$$x_j > t \rightarrow right\ node$$

Each leaf node stores the average of all target values belonging to that subset, which serves as the model's prediction:

$$\hat{y}_L = \left(\frac{1}{N_L}\right) \Sigma_{\{i \in L\}}\, y_i$$

Here, y_i are target values and $\hat{y}_L$ represents prediction at leaf L. N_L denotes the number of training samples within the leaf. The splitting process continues until a termination criterion has been satisfied. Termination criteria are often defined by maximum depth or minimum number of samples per leaf.

GridSearchCV with the same setup as SVR was utilized in our DT. For the elastic modulus (EM) best parameters obtained were: {'max_depth': 10, 'min_samples_leaf': 2, 'min_samples_split': 2}. Best parameters set for the energy absorption (EA) were: {'max_depth': 10, 'min_samples_leaf': 1, 'min_samples_split': 2}. Whereas, default settings performed best for the peak stress (PS). The optimized DT model was implemented on test set and performance was measured.

3.2.3 Random Forest Regression (RF)

The RF is an ensemble learning algorithm which combines the outputs of numerous decision trees to improve on the aggregate accuracy and stability of a model. All the trees in the ensemble are trained using a random sample of the training data and also using a random sample of input features. This feature randomness, coupled with bootstrap sampling, assures that the trees are diverse and the trees are not closely related to each other, which helps to avoid overfitting. The ensemble prediction is obtained by averaging the outputs of all individual trees:

$$\hat{y}(x) = \left(\frac{1}{T}\right) \Sigma_{\{t=1\}}^{\{T\}}\, f_{t(x)}$$

where T is the total number of trees in the forest and $f_t(x)$ is the prediction from the t-th tree.

MultiOutputRegressor and GridSearchCV were utilized in our RF implementation. GridSearchCV used MAE to select the best parameters for each target. After parameter tuning, the model was applied to the test set and its performance was measured.

3.2.4 CatBoost Regression

The CatBoost is a gradient boosting algorithm which develops a sequential ensemble of decision trees. Every new tree is trained to fix the residuals of the last ensemble, and the model is improved with each additional training to achieve high predictive accuracy with a high level of generalization.

At iteration t, the ensemble prediction is updated according to:

$$F_t(x) = F_{t-1}(x) + \eta \cdot h_t(x)$$

where $F_t(x)$ represents the cumulative prediction after t iterations, η is the learning rate controlling the contribution of each new tree, and $h_t(x)$ denotes the weak learner fitted to the residuals.

We trained a separate model for each target using MultiOutputRegressor in our implementation, as it enables independent parameter tuning. The tree depth, learning rate and number of iterations were tuned through GridSearchCV with ten-fold cross-validation. MAE was used as the metric of cross-validation sets to identify best performing configurations. Like other models, the performance of CatBoost was measured on the test set.

3.3 Performance Measurement

To evaluate the performance of ML models on the test set, three metrics were considered for each property. They are: mean absolute error (MAE), root mean squared error (RMSE), and mean arctangent absolute percentage error (MAAPE).

The MAE is a measure of the average magnitude of errors, without consideration of direction and is represented by:

$$MAE = \left(\frac{1}{n}\right) \Sigma \, |y_i - \hat{y}_i|$$

MAE has the same units as the target variable, and it is not as affected by extreme outliers, so it is appropriate where both large and small errors are equally significant.

The RMSE is a measure of the standard deviation of the residuals (prediction errors) and is calculated as:

$$RMSE = \sqrt{\left[\left(\frac{1}{n}\right) \Sigma \, (y_i - \hat{y}_i)^2\right]}$$

RMSE is highly sensitive to outliers. The squaring term disproportionately increases the penalty for larger errors. A single large error (outlier) can significantly inflate the RMSE. It is utilized when large errors are particularly undesirable.

MAAPE is a scale-independent metric that assesses relative error on a percentage scale. It is an alternative to the popular mean absolute percentage error (MAPE). When the actual value y_i is zero, MAPE faces a division by zero problem. Again, when the actual value y_i is very close to zero, MAPE become extremely large, or even infinite. To address this, the alternative metric MAAPE uses the arctangent function to cap large percentage errors smoothly. This makes MAAPE advantageous to MAPE. Mathematically, MAAPE is defined as follows:

$$MAAPE = \left(\frac{1}{n}\right) \Sigma \, arctan\left(\left|\frac{(y_i - \hat{y}_i)}{y_i}\right|\right)$$

Together, MAE, RMSE, and MAAPE provide a holistic evaluation framework. MAE represents the average deviation between predictions and actual values, RMSE emphasizes the effect of large outliers by more severely penalizing them, and MAAPE represents the performance in a percentage relative form; this performance is resilient to the small magnitude of targets.

4. Results and Discussion

This section represents findings obtained from this study. At first, we present the training set cross-validation results of all applied models except ANN. Then, the early stopping result of the ANN is presented. At last, we present test set results to compare the performance of all applied algorithms.

4.1 Cross-validation Results

Ten-fold cross-validation was applied to SVR, DT, RF and CatBoost models. MAE was used as the cross-validation metric. The average cross-validation score with standard deviation is shown in Table 1 for each of the properties of all cross-validated algorithms.

Table 1. Cross-validation MAE (mean ± standard deviation)

Model	Elastic Modulus	Energy Absorption	Peak Stress
SVR	3.1035 ± 0.9259	**0.0367 ± 0.0051**	**0.0832 ± 0.0188**
DT	9.6107 ± 1.8112	0.2702 ± 0.0601	0.4352 ± 0.0511
RF	4.9739 ± 1.0040	0.1476 ± 0.0245	0.2384 ± 0.0406
CatBoost	**2.4793 ± 0.4068**	0.0633 ± 0.0131	0.1015 ± 0.0178

We can see that CatBoost performed best in terms of elastic modulus (EM), followed by SVR. On the other hand, in terms of energy absorption (EA) and peak stress (PS), SVR demonstrates the lowest error, followed by CatBoost. In all cases, DT showed poor performance.

4.2 Regularization of the ANN

The convergence behaviour and regularization of the ANN during training are illustrated in Figure 1, which presents the variation of training and validation losses with the number of epochs on a logarithmic scale.

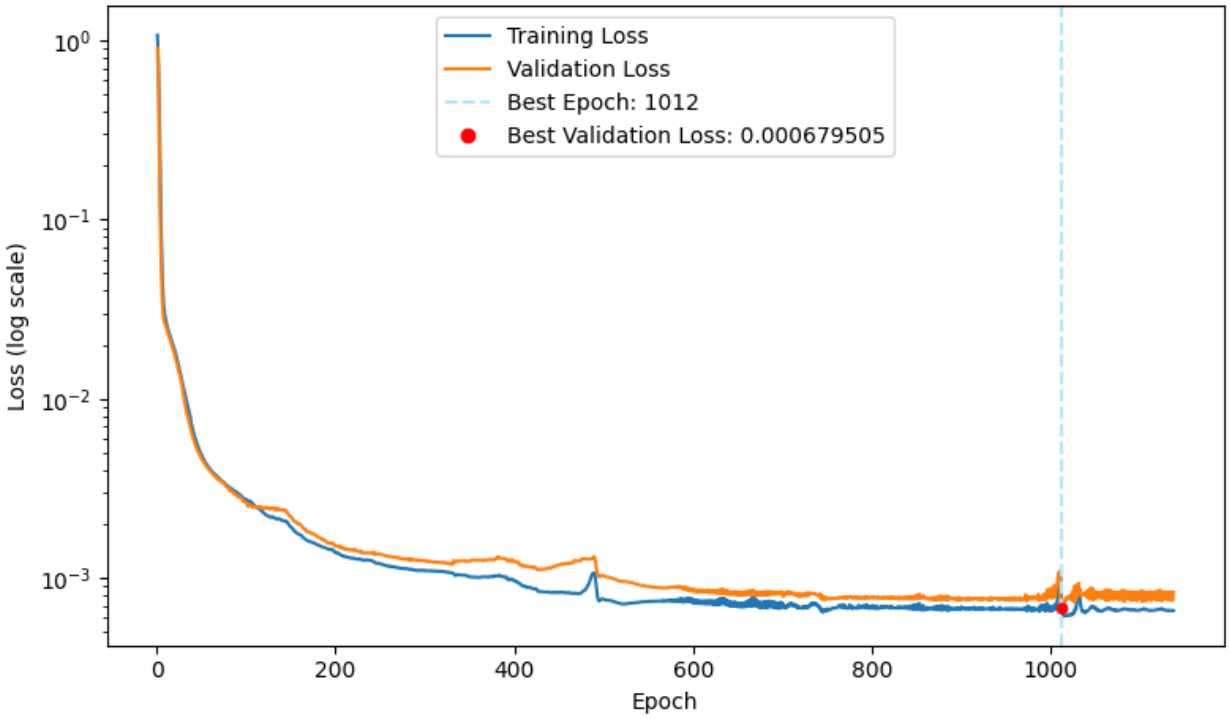

Figure 1. Training and validation loss curves for the ANN with early stopping

The loss curves show a steady reduction in both training and validation errors, followed by stabilization as the model approaches convergence. Early stopping was triggered at epoch 1012, corresponding to the minimum validation loss of 0.00068, marking the optimal balance between underfitting and overfitting. The close alignment of the two curves indicates that the ANN maintained stable learning without significant divergence between training and validation performance.

This confirms that the early stopping criterion acted as an effective regularization mechanism, ensuring that the model achieved high predictive accuracy while avoiding overfitting.

4.3 Test Set Evaluation

Table 2 shows how each model performed on the independent test set. When comparing the five machine learning models, it's clear that their prediction accuracy differs depending on which mechanical property is being tested. Models with smaller deviations and more consistent predictions are considered to have higher accuracy and better generalization capability (Table 2).

Table 2. Test-set performance of machine learning models

Metric	Model	Elastic Modulus	Energy Absorption	Peak Stress
MAE	ANN	2.5599	0.0995	0.1086
	SVR	3.104	**0.0344**	**0.0799**
	DT	8.7125	0.2466	0.3353
	RF	4.5108	0.1145	0.1648
	CatBoost	**1.8968**	0.0581	0.0898
RMSE	ANN	**3.3403**	0.1333	**0.1341**
	SVR	14.3397	**0.0751**	0.2903
	DT	17.3368	0.4645	0.6792
	RF	10.1143	0.2377	0.3017
	CatBoost	4.0405	0.0973	0.153
MAAPE	ANN	0.0839	0.1415	0.1417
	SVR	0.0429	0.0776	0.0625
	DT	0.0755	0.095	0.0835
	RF	**0.0407**	**0.0567**	**0.0539**
	CatBoost	0.0435	0.0655	0.0598

In elastic modulus (EM) prediction, the CatBoost demonstrated the highest level of accuracy and consistency in the form of the lowest MAE, which implies that there are smaller average errors in the entire range of observations. Conversely, the ANN model, although with a lesser degree of consistency, had the smallest number of large deviations as demonstrated by the lowest RMSE, indicating greater control in extreme prediction errors.

In terms of energy absorption (EA), the SVR has demonstrated the highest predictive accuracy and generalization ability, as indicated by the lowest MAE and RMSE values. This performance profile implies that the SVR model consistently produces reliable predictions while effectively reducing significant deviations. The CatBoost ranked second, exhibiting slightly higher error values yet maintaining competitive predictive reliability.

For peak stress, the SVR provides the most accurate predictions in terms of MAE, closely followed by CatBoost. However, the ANN demonstrates superiority in terms of RMSE, where CatBoost again comes second. This implies that CatBoost will always have good results in either of the two error measures, whereas SVR is superior in reducing average deviations, and ANN is superior in reducing larger deviations.

Interestingly, the Random Forest model demonstrates strong robustness, evidenced by its lowest MAAPE values across all properties. This consistency shows that RF maintains reliable proportional accuracy even when the magnitude of target values varies widely. Its stability in relative errors indicates resilience to outliers and strong generalization across different data ranges. Although it may not minimize RMSE or MAE, its balanced performance across varying scales underscores its robustness and dependability, making it a trustworthy choice when consistent predictive behaviour is prioritized over absolute precision.

Lastly, test-set MAEs of all cross-validated models (SVR, DT, RF, and CatBoost) were in the range of cross-validation results, which validates the high generalization.

5. Conclusion

This study compared five machine learning algorithms (ANN, SVR, DT, RF, and CatBoost) for predicting the mechanical properties of PLA/TPU gyroid lattice structures.

Among the evaluated models, CatBoost consistently demonstrated strong and balanced predictive performance across all mechanical properties. The SVR performed exceptionally well for energy absorption and peak stress. The RF model exhibited the most robust and scale-independent behaviour. In contrast, the DT performed poorly.

For all cross-validated models (SVR, DT, RF, and CatBoost), the test-set predictions were consistent with their cross-validation results, confirming strong model generalization. For the ANN, the use of early stopping strategy effectively prevented overfitting and ensured stable convergence, as evidenced by the close alignment between training and validation losses.

Overall, these findings suggest that ML can be used as a powerful method for mechanical property prediction of lattice structures with high accuracy and robustness. At the same time, the various algorithms offer complementary advantages in accuracy, robustness, and consistency.

For future work, different lattice geometries, different material combinations, or different ML models, especially physics-informed ML algorithms, can be studied to further improve predictive reliability, interpretability, and generalization for data-driven design in advanced manufacturing applications.

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