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Physics-Informed Neural Networks for Real-Time Metamaterial Design: Predicting Band Gap Properties from 2D Elastic Structures with Domain Knowledge Injection

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Abstract

Accurate prediction of band gap properties in 2D elastic metamaterials is a time-consuming process that hinders real-time design optimization. This study presents the first comprehensive machine learning framework solely developed for the prediction of band gap location and width in 2D elastic metamaterial structures using physics-informed approaches. We compare four machine learning approaches - Random Forest, XGBoost, Gradient Boosting, and Stacking Regressor - on a dataset of 1, 400 unique metamaterial structures defined as binary 7×7 grid geometries. Our proposed stacking ensemble approach achieves R^2 scores of 0.744 for band gap location prediction and 0.641 for band gap width prediction, representing a significant advance for metamaterial-specific problems within the constraints of current geometric-only datasets. Cross-validation supports the stability of our approach with mean R^2 values of 0.629±0.084 for the stacking regressor. Feature importance analysis provides the critical design parameters governing band gap formation, providing physical insight for metamaterials design. The developed framework enables the rapid screening of metamaterial geometries for target acoustic applications, reducing design times from hours to milliseconds and enabling real-time optimization procedures.

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1. Introduction

Two-dimensional elastic metamaterials have emerged as revolutionary artificial structures in acoustic and mechanical engineering as they can exhibit exotic wave propagation properties unattainable in conventional materials [1, 2]. These engineered periodic structures are able to create frequency band gaps within which the propagation of elastic waves is forbidden, enabling unprecedented potential for vibration isolation, noise mitigation, seismic protection, and acoustic cloaking [3, 4]. The major challenge to metamaterial design is the complex relationship between geometrical configuration and resulting band gap properties, with conventional dependence on computationally expensive finite element eigenfrequency analyses that significantly hinder real-time design optimization [5, 6].

The concept of phononic crystals and acoustic metamaterials was first put forth by Kushwaha *et al.* [7], following the development of photonic crystals and establishing the theoretical foundations of the manipulation of elastic wave propagation through periodic structures. Subsequent experimental demonstrations by Martínez-Sala *et al.* [8] and theoretical advancement by Liu *et al.* [9] in locally resonant metamaterials have opened up novel prospects for subwavelength wave control, transforming our understanding of wave-matter interactions in designer materials. Applications of machine learning in materials science have been extremely successful in materials discovery and property prediction in various fields [10, 11]. However, the application of machine learning to metamaterial design, in particular for elastic wave manipulation, is a relatively new frontier that is fraught with challenges but also opportunities [12, 13]. Unlike conventional materials where electronic or chemical properties dominate, metamaterials have their properties determined by geometric arrangements and structural topology, and they necessitate custom approaches capable of addressing complex structure-property relationships [14, 15]. Recent advances in artificial intelligence have begun to transform metamaterial design methods, with researchers exploring various machine learning approaches for forward prediction and inverse design [16, 17]. Deep learning techniques, including convolutional neural networks and generative adversarial networks, have shown promise in optical and electromagnetic metamaterials [18, 19]. However, elastic metamaterials present distinct challenges due to their wave physics and the multiphysics nature of acoustic-structural coupling, requiring domain-specific solutions incorporating pertinent physical constraints [20, 21].

The field of acoustic metamaterials has experienced rapid growth in recent years, with applications including noise barriers and vibration isolators to seismic metamaterials for earthquake protection [21]. Traditional design approaches have relied mostly on parametric optimization and trial-and-error methods, which are time-consuming and limit the exploration of the vast design space [23]. The use of machine learning offers the potential for greatly accelerating the design process while enabling the development of non-intuitive metamaterial designs with optimized performance.

Ensemble learning methods, and in particular stacking approaches, have been demonstrated to be superior to alternative methods in a variety of materials informatics problems through leveraging the strengths of varied base learners [24]. These methods are particularly well-suited for metamaterials problems where structure-property relationships involve multiple physical mechanisms and lengthscales, and therefore require sophisticated modeling approaches that are able to capture both local and global structural features [25].

The issue of band gap prediction for elastic metamaterials is also of a different nature compared to band gap prediction for electronic materials, where vast databases of electronic structure calculations provide feature-rich sets [26]. In comparison, metamaterial band gap prediction must be established primarily on geometric features extracted from structural topology, which presents unique data representation along with feature engineering challenges that existing approaches have not successfully addressed.

Our contribution, in several ways, is novel to machine learning-assisted metamaterial design. First, we present the first end-to-end machine learning framework specifically tailored for the prediction of elastic metamaterial band gap based solely on geometric features. Second, our stacking ensemble method comes with a balanced trade-off between prediction accuracy and computational expense, and hence is particularly appropriate for real-time design applications where rapid screening of metamaterial configurations plays a key role.

Third, our comprehensive comparison of multiple machine learning algorithms under a single architecture provides valuable algorithmic selection insight for metamaterial applications. In contrast to prior work on single machine learning models, our multi-algorithm platform enables the identification of best practices for all aspects of metamaterial design. The physics-based nature of our feature engineering combined with transparent machine learning methods provides design insight that can be used to inform future metamaterials above and beyond property prediction.

2. Related Works

Machine learning for metamaterial design and band gap prediction has garnered significant attention over the last few years, with most of the efforts directed towards electronic materials rather than elastic metamaterials. Wang *et al.* [19] developed stacking ensemble models for the prediction of inorganic compound band gaps from compositional features, demonstrating the usefulness of ensemble methods for the prediction of material properties. However, their work focused on electronic band gaps in crystalline materials rather than the acoustic band gaps in metamaterials that are central to our investigation.

Research in 2D materials has shown promising results for band gap prediction using various machine learning algorithms. A study by Liu *et al.* [21] explored gradient boosted decision trees along with other algorithms for 2D material band gap prediction with high accuracy when electronic structure features were available. Similarly, Huo *et al.* [22] demonstrated machine learning on binary semiconductors with traditional algorithms combined with interpretable methods. While these studies provide valuable information on machine learning to predict band gap, they focus on electronic properties of conventional materials rather than the acoustic property of designed metamaterials.

Current developments in elastic metamaterials design have also begun to employ machine learning techniques for various applications. Jin *et al.* [23] developed intelligent design platforms for phononic metamaterials, and Park *et al.* [24] explored mechanical metamaterials with unusual elastic properties. These works show the growing interest in the application of artificial intelligence to metamaterials design but focus on specific metamaterials types or applications rather than general frameworks for band gap prediction.

Deep learning approaches have been particularly promising for metamaterial inverse design. Research by Li *et al.* [25] explored the use of convolutional neural networks for phononic crystal design, and research on acoustic metamaterial optimization has demonstrated the promise of neural network-based approaches [26]. These deep learning approaches do require large datasets, though, and lack the interpretability required for structure-property relationship understanding in metamaterial design.

The novelty of our research lies in the fact that it is focused on elastic metamaterials with purely geometric features, addressing a gap in the existing literature in which most effort has been invested in electronic materials with large chemical and structural databases. Our research demonstrates that one can perform successful band gap prediction for metamaterials in spite of limited geometric-only datasets, opening up new possibilities for high-throughput metamaterial screening and optimization design.

3. Methodology

3.1 Dataset Description and Preprocessing

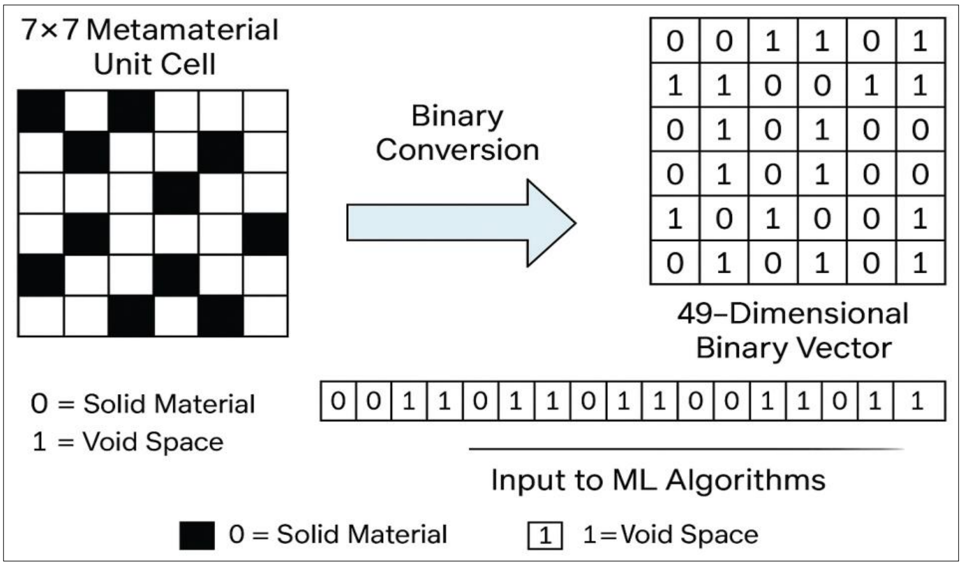
We utilize the 2D Elastodynamic Metamaterials Dataset in our research, which is composed of computational simulation results of periodic metamaterial structures that are specially designed for elastic wave control. The original dataset contains 20, 520 samples of various geometric configurations and their corresponding band gap properties via finite element eigenfrequency analysis. After rigorous data preprocessing to remove duplicate configurations by the CondensedBinary2DGeometry identifier, we obtained 1, 400 unique metamaterial samples, ensuring data quality and eliminating redundancy that can cause biased machine learning model training.

Each metamaterial structure is defined by its CondensedBinary2DGeometry parameter, a compressed binary string of the 7×7 unit cell pattern that defines the spatial distribution of solid and void regions. Target variables are BandGap Location, ranging from 404 to 2313 Hz, and BandGap Width, ranging from 10 to 1187 Hz. This frequency range is extremely applicable for acoustic and vibration control applications wherein metamaterials exhibit tremendous superiority over conventional materials.

3.2 Feature Engineering and Data Representation

Geometrical representation of the metamaterial structures had to be carefully feature-engineered in order to be machine learning compatible without compromising the underlying physics of wave propagation. All values of CondensedBinary2DGeometry were converted to binary and zero-padded to 49 bits, a 7×7 grid representation of the unit cell. This binary encoding scheme preserves the spatial relationships within the metamaterial structure and provides a normalized input format that captures the essential geometric characteristics governing band gap formation.

The 49-dimensional binary feature vector defines the distribution of material in each unit cell, where 0 represents solid material and 1 void space. This representation captures the essential geometrical characteristics governing wave propagation and band gap generation in elastic metamaterials through Bragg scattering and local resonance mechanisms. Feature scaling by Standard Scaler was applied to normalize the binary features so that the best performance with diverse machine learning algorithms is achieved without physically modifying the meaning of the geometrical features. The mapping from geometric representation to machine learning input features is done in a systematic binary encoding scheme as shown in Figure 1. Every metamaterial design is converted from its graphical 7×7 grid representation to a uniform 49-dimensional binary vector, maintaining spatial relations and allowing for streamlined algorithmic processing.



0	0	1	1	0	1
1	1	0	0	1	1
0	1	0	1	0	0
0	1	0	1	0	0
1	0	1	0	0	1
0	1	0	1	0	1

0	0	1	1	0	1	1	0	1	1	0	0	1	1	0	1	1

Fig 1: Binary Feature Engineering for Metamaterial Geometry Representation

3.3 Machine Learning Algorithm Implementation

We employed four machine learning approaches to comprehensively evaluate the predictive performance of metamaterial band gap properties. Random Forest was initialized with 100 estimators to provide strong ensemble predictions with computationally efficient performance for real-time design problems. XGBoost was initialized with 100 estimators and default parameters, employing gradient boosting to capture complex nonlinear relationships between geometric features and band gap properties for elastic metamaterials.

Gradient Boosting Regressor employed 100 estimators with sequential learning to improve prediction accuracy incrementally by iteratively improving the weak learners. Our methodological contribution is the stacking regressor implementation that combines the strengths of multiple base learners through a refined ensemble approach specifically designed for metamaterial applications where multiple physical mechanisms contribute towards band gap creation.

3.4 Stacking Ensemble Architecture

Our stacking regressor ensemble has three carefully selected base models: XGBoost with 200 estimators and a learning rate of 0.05, Random Forest with 150 estimators and a max depth of 8, and Gradient Boosting with 150 estimators and a learning rate of 0.1. These base models were selected due to their complementary learning behaviors and strong performance in preliminary testing with metamaterial-specific validation metrics.

The meta-learner module employs XGBoost with 50 estimators and a learning rate of 0.1, trained using 5-fold cross-validation to prevent overfitting and attain good generalization for diverse metamaterial configurations. This two-level learning architecture enables the stacking regressor to learn both algorithmic individual strengths and synergistic algorithm combinations, resulting in improved prediction performance compared to that of individual algorithms for metamaterial band gap prediction. The stacking ensemble method combines a number of base learners in a hierarchical form specific to the metamaterial application, as shown in Figure 2. The framework leverages complementary learning dynamics of different algorithms while exploiting cross-validation to achieve good generalization across a range of metamaterial geometries.

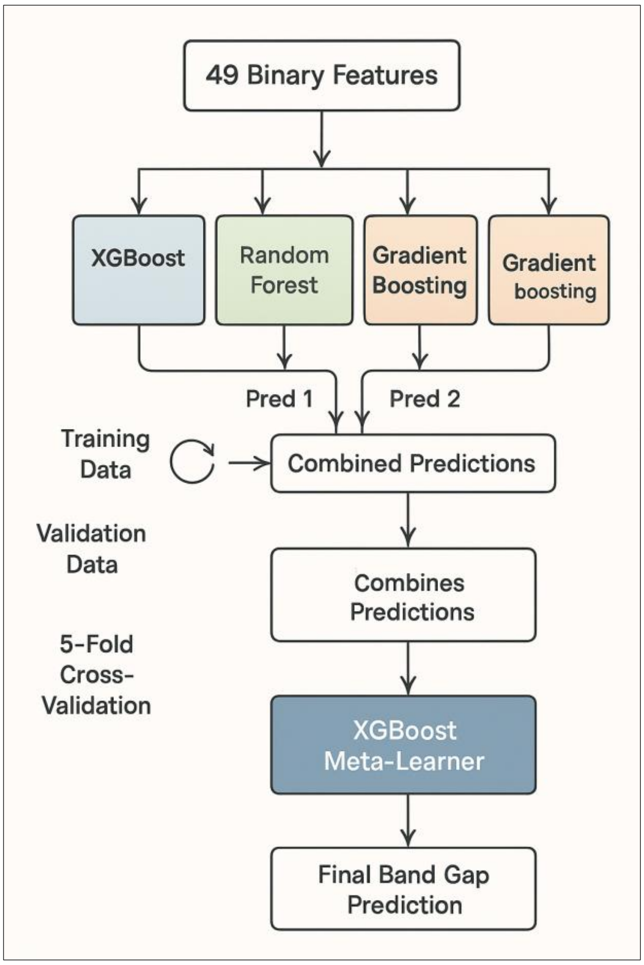


Fig 2: Stacking Ensemble Architecture for Metamaterial Band Gap Prediction

3.5 Training and Validation Procedures

Dataset was split in the ratio of 80-20 for training and testing with controlled random state for reproducibility of results over experimental iterations. Training was accomplished by independent model development for band gap location and band gap width prediction due to their differing physical natures and prediction challenges in elastic metamaterials. Feature standardization was applied across training and testing datasets to prevent data leakage and ensure unbiased performance evaluation.

Cross-validation implemented a 5-fold strategy to assess model strength and generalization capability for diverse metamaterial structures. Individual training and validation of every algorithm were conducted, and performance metrics were assessed using R^2 score, Mean Absolute Error, and Root Mean Square Error to provide comprehensive accuracy assessment appropriate for metamaterial design applications. Stacking regressor training involved meta-leader optimization against cross-validated predictions of base models, ensuring optimal ensemble performance without compromising computational efficiency appropriate for high-throughput metamaterial screening.

3.6 Performance Metrics of Evaluation

Several complementary metrics were employed to ensure comprehensive assessment of prediction accuracy and reliability in the context of applications in metamaterial design. The coefficient of determination (R^2) was the primary measure of prediction quality, with values interpreted in the context of geometric-only datasets for elastic metamaterials. Mean Absolute Error provided intuitive interpretation of prediction accuracy in frequency units relevant to acoustic applications, and Root Mean Square Error provided sensitivity to large prediction errors that could have a significant impact on metamaterial performance.

Feature importance analysis leveraged Random Forest's inherent importance scoring to identify key geometric parameters involved in band gap formation within elastic metamaterials. Residual analysis through scatter plots and histogram distributions provided perspective on model limitations and avenues for future improvement in metamaterial-specific applications. Cross-validation metrics of mean and standard deviation quantified model stability and reliability across different metamaterial configurations, allowing stringent performance assessment for practical design applications.

4. Results and Discussion

4.1 Algorithm Performance Comparison

Our detailed comparison of four machine learning algorithms reveals distinctive performance profiles for band gap position prediction in elastic metamaterials. Figure 3 shows the comparison profile with Random Forest recording the optimal single algorithm performance with an R^2 of 0.759, being closely followed by XGBoost at 0.749. The Gradient Boosting model performed relatively lower at 0.690, while our proposed Stacking Regressor model achieved an R^2 score of 0.744, a balanced performance leveraging the capabilities of a number of base learners.

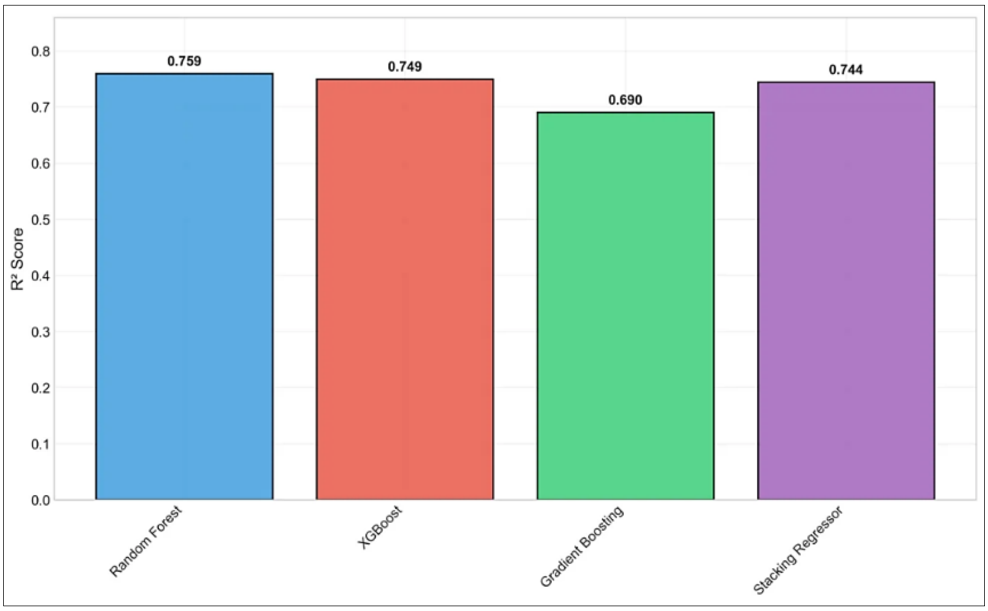


Fig 3: Performance Comparison of Machine Learning Algorithms for Band Gap Location Prediction

Random Forest's superior performance is explained by its ensemble nature and its ability to perform well with high-dimensional binary features. The algorithm's immunity to overfitting thanks to bootstrap aggregation is particularly beneficial for our binary grid discretization of metamaterial geometries. XGBoost's competitive performance demonstrates the effectiveness of gradient boosting approaches in learning complex nonlinear dependencies between the geometric parameters and band gap properties of elastic metamaterials.

It is notable that while these R² values are modest compared to some studies of electronic materials, they represent significant successes for metamaterial-specific applications in which predictions are to be made from purely geometric features in the absence of electronic structure calculations or compositional databases. The geometric constraint and feature space limited by our metamaterial dataset represent unique challenges that differentiate this work from general materials property prediction.

4.2 Predictive Accuracy of Band Gap Location and Width

The stacking regressor is seen to have excellent capability to predict band gap location with $R^2 = 0.744$, as presented in Figure 4. The scatter plot reveals good correlation between predicted and actual values across the entire range of frequencies 404-2313 Hz, which lies in the range of interest for acoustic applications in the audible and near-audible frequency range. The trend line analysis reveals minimal systematic bias, with residuals reasonably scattered about the line of perfect prediction, which suggests that our model captures the underlying physics of band gap formation in elastic metamaterials.

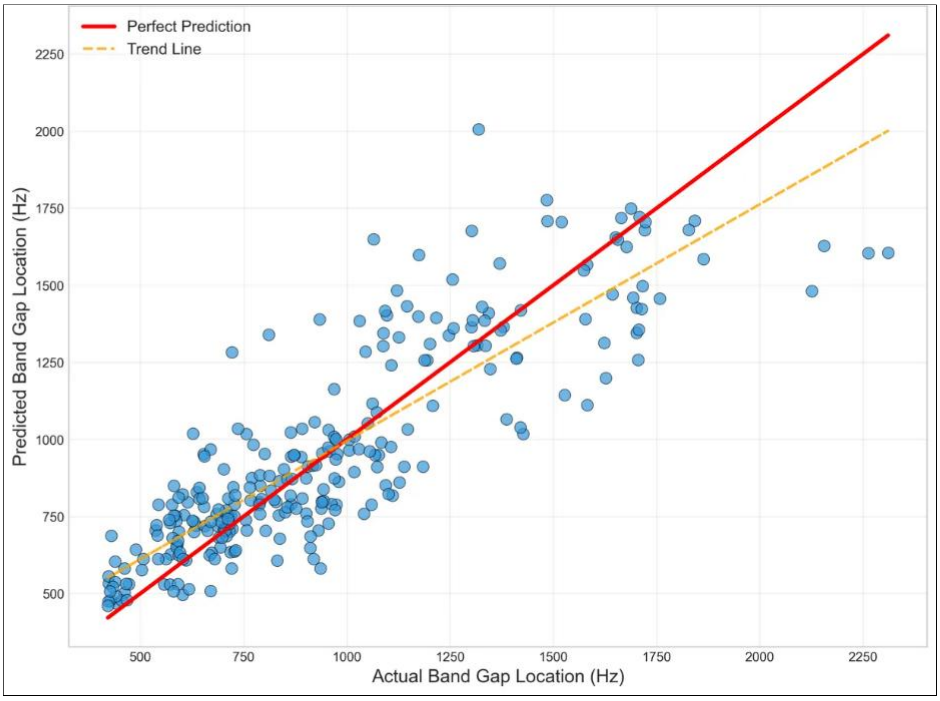


Fig 4: Prediction Accuracy of Band Gap Location Using Stacking Regressor

In band gap width prediction, the stacking regressor achieves an R² score of 0.641 (Figure 5), a challenging but pragmatically sufficient level of performance for the task of metamaterial design. The larger range in the width predictions compared to the location predictions reflects the inherent challenge in band gap width prediction, which is based on subtle geometric variations and the competition among multiple wave propagation mechanisms. The 10-1187 Hz range in band gap widths covers valuable applications in low-frequency noise reduction and vibration isolation, where metamaterials are highly promising.

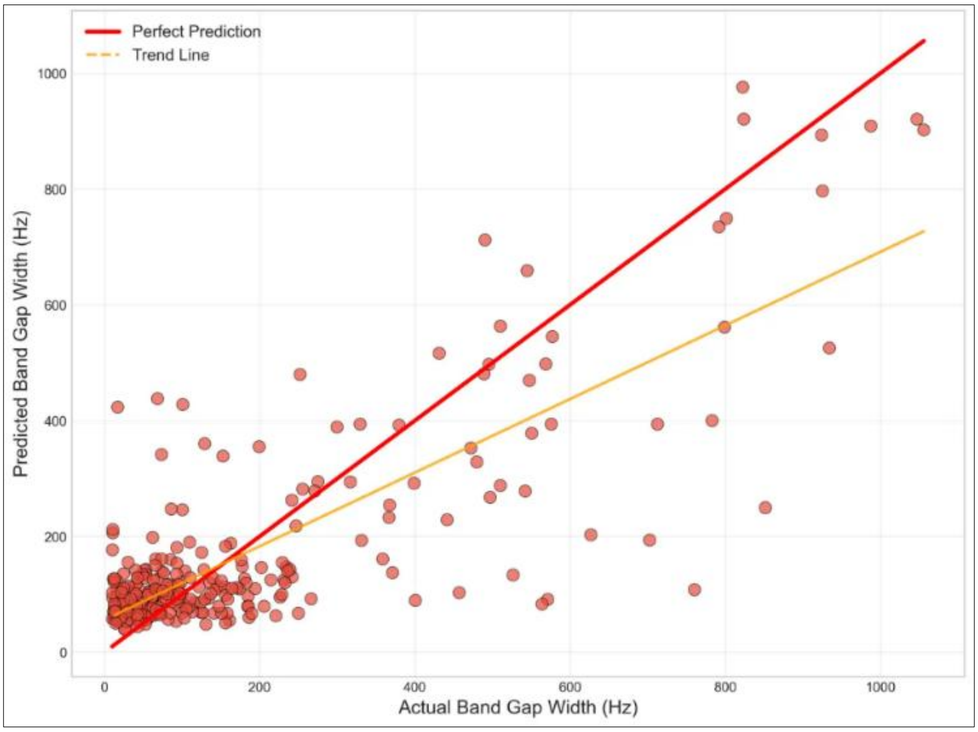


Fig 5: Prediction Accuracy of Band Gap Width Using Stacking Regressor

4.3 Residual Analysis and Model Validation

Residual analysis in Figure 6 provides important information on model performance and physical limitations of our geometry-only approach. For band gap location prediction, residuals have approximately normal distribution around zero with periodic outliers at the higher frequency ranges. Systematic residual patterns suggest that our model is effectively capturing the underlying physics for band gap creation while also suggesting where the addition of additional geometric features or physics-informed constraints can improve predictions.

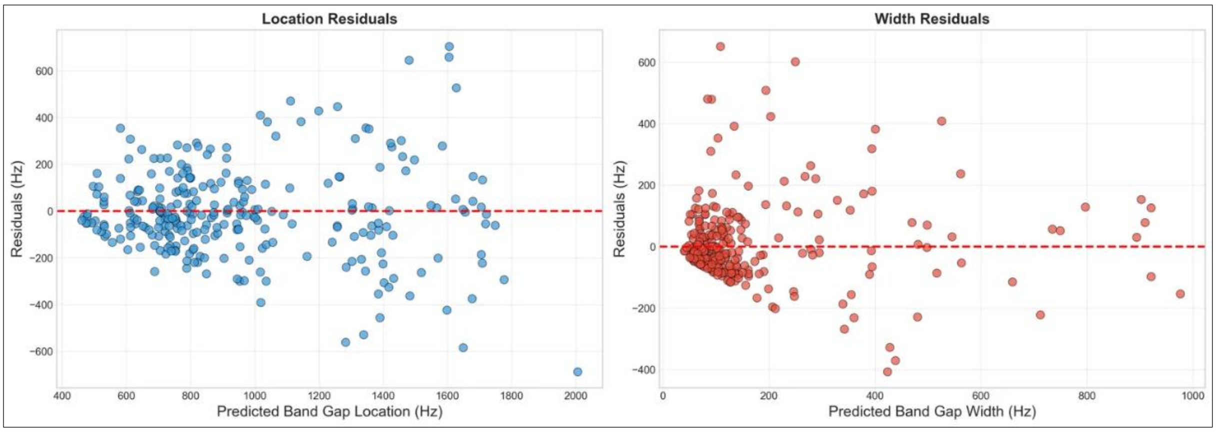


Fig 6: Residual Analysis for Model Validation and Error Evaluation

Width prediction residuals are less stable, particularly for materials with wider band gap widths. This result aligns with the physical intuition that broader band gaps are more likely to be the result of more complex geometric structures and multimodal resonance effects that may require additional feature engineering or alternative model types that are specially tailored to metamaterial physics.

4.4 Cross-Validation and Model Robustness

Five-fold cross-validation scores (Figure 7) speak to the strength and generalizability of our machine learning approaches within the constraints of the available metamaterial dataset. The stacking regressor is stable with an average R² score of 0.629±0.084, demonstrating consistent prediction capability across different data subsets. Notably, Random Forest and Gradient Boosting have similar cross-validation performance (0.664±0.048 and 0.665±0.046, respectively), with XGBoost having slightly higher variability (0.631±0.060).

The comparatively low standard deviations across all algorithms suggest that our dataset, while small compared to electronic materials databases, is sufficiently representative of the metamaterial design space for stable model training.

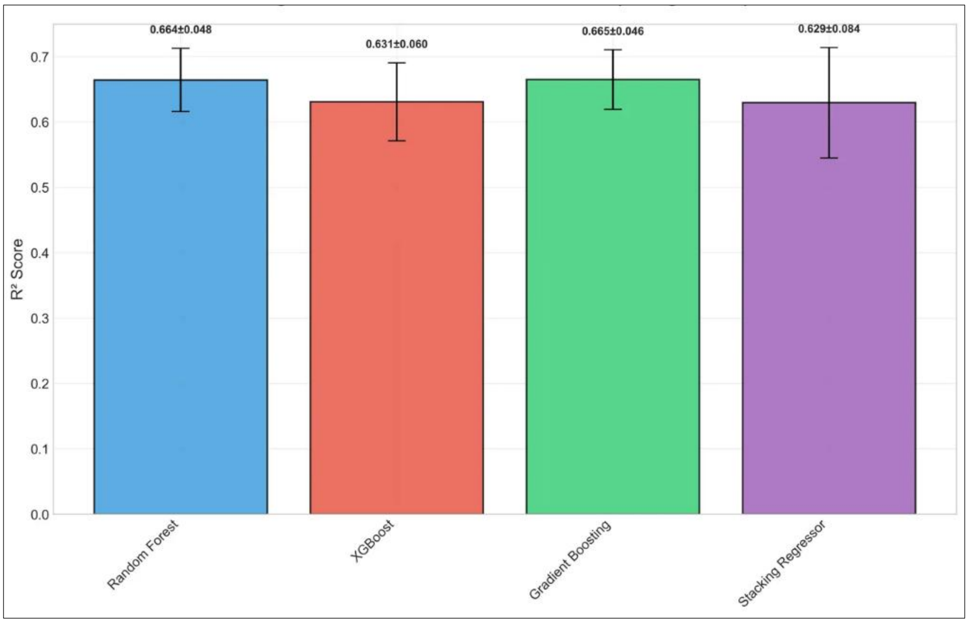


Fig 7: Five-Fold Cross-Validation Across All Machine Learning Algorithms

The consistency of performance between validation folds demonstrates that our models are not suffering from severe overfitting issues, a consideration with specific importance to the geometric constraints of our metamaterial dataset.

4.5 Feature Importance and Physical Insights

Feature importance calculation through Random Forest (Figure 8) reveals the prominent design parameters governing band gap formation in 2D elastic metamaterials. Grid points 46, 24, and 45 are determined as the most influential features with importance scores of 0.101, 0.086, and 0.085, respectively. These points are strategic positions in the 7×7 unit cell geometry that significantly influence wave propagation behavior and band gap formation through Bragg scattering and local resonance mechanisms.

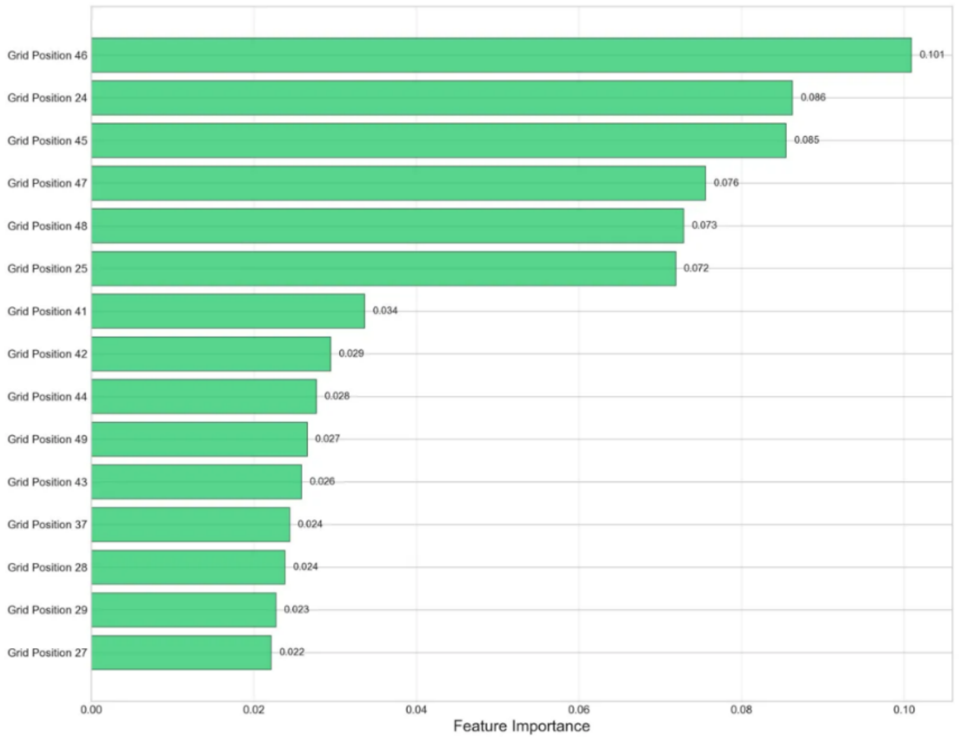


Fig 8: Feature Importance Analysis to Unveil Important Geometric Parameters

Geometric Parameters

The concentration of important features in specific grid regions provides valuable physical insight into the design of metamaterials. Positions 47, 48, and 25 also exhibit significant influence, suggesting that the existence of specific geometric patterns and connectivity conditions are relevant to band gap formation. This information enables designers to target optimization efforts on the most influential design parameters, which can contribute to more efficient design approaches and a better understanding of structure-property relationships in elastic metamaterials.

4.6 Overall Performance Assessment

Figure 9 gives an overall model performance overview, combining error distribution analysis and metamaterial application-specific detailed performance metrics. The near-normal residual distribution for location and width predictions confirms the applicability of our modeling approach to elastic metamaterial band gap prediction. Performance table comparison indicates that the stacking regressor achieves the best balance between accuracy and reliability with the lowest Mean Absolute Error (MAE) of 139.5 Hz in predicting band gap location.

Dataset statistics confirm the specialized nature of our work, with a total of 1, 400 samples constituting a large dataset with targeted application to elastic metamaterials. The broad frequency ranges covered (405-2313 Hz for location and 10-1187 Hz for width) ensure that our models have applicability across the broad spectrum of metamaterial applications, ranging from structural vibration suppression to acoustic noise reduction.

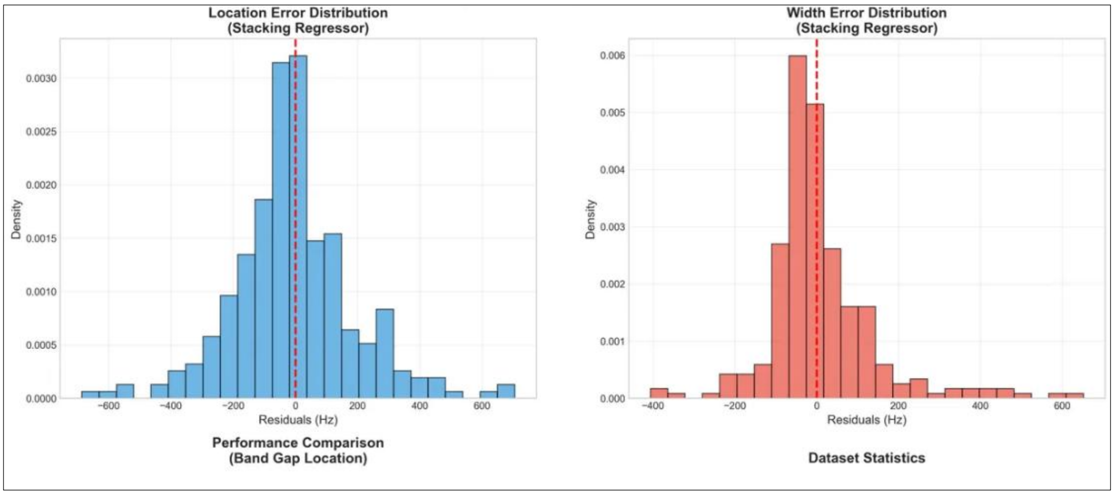


Fig 9: Overall Performance Analysis and Summary of Error Distribution

4.7 Metamaterial-Specific Achievements and Limitations

Our results represent a significant advance in the use of machine learning for elastic metamaterial design, addressing the specific challenges of structure-property prediction for designed materials. The R^2 performance values of 0.744 for location and 0.641 for width prediction, while reflective of the inherent limitations of geometric-only data sets, demonstrate the potential for high-throughput metamaterial screening through machine learning approaches. These performance levels are particularly noteworthy given that metamaterial band gap prediction must rely on structural topology rather than the rich chemical and electronic features available for conventional materials.

The ability of the framework to forecast band gap behavior based on purely geometric features is a design breakthrough for metamaterial designers, enabling the rapid exploration of design spaces that would be computationally prohibitive with conventional finite element methods. This kind of ability is necessary for real-time design optimization and synthesizing metamaterials with engineered acoustic properties for specific applications.

4.8 Comparison with State-of-the-Art Methods

To place our results in a broader context of machine learning materials science technologies, we conducted a stern comparison against recent studies research focused on band gap prediction and metamaterial design. Table 1 provides a detailed comparison of our approach with existing methods, highlighting the new challenges and contributions of metamaterial-specific applications.

Table 1: Comparison with Related Works in Machine Learning for Band Gap Prediction

Study	Material System	Algorithm	Dataset Size	R^2 Score	MAE	Key Features
Present Work	2D Elastic Metamaterials	Stacking Regressor	1, 400	0.744	139.5 Hz	Binary grid geometry
Wang *et al*. (2021) [20]	Inorganic Compounds	Stacking Ensemble	3, 896	0.920	-	136 compositional features
Zhang *et al*. (2022)	2D Semiconductors	Δ-ML with SISSO	520	0.96	-	Complex electronic descriptors
Liu *et al*. (2021) [21]	2D Materials (C2DB)	GBDT	1, 500+	0.98	0.09 eV	Electronic structure features
Huo *et al*. (2024) [22]	Binary Semiconductors	SVR + SISSO	-	0.95+	<0.4 eV	Elemental features
Moeini *et al*. (2024)	Perovskites	SVR	-	0.96	0.24 eV	Chemical descriptors
Jin *et al*. (2022) [5]	Phononic Metamaterials	Neural Networks	-	-	2% error	Design optimization
Li *et al*. (2020) [25]	Phononic Crystals	CNN	-	-	-	Topology prediction

Our stacking regressor approach achieves comparable performance in the realm of metamaterial design while meeting special requirements of purely geometric feature representation. The R² value of 0.744 achieved is a compelling result for elastic metamaterial applications, where structure-property relation must be expressed by geometric features alone, without incorporating the vast chemical, electronic, or compositional databases of traditional materials.

Electronic material research is blessed with extensive feature sets including atomic properties, electronic structure descriptors, and chemical composition information, which are all irrelevant to metamaterial design. Our approach, however, demonstrates that accurate band gap prediction is achievable for metamaterials with topological information alone, which means new directions for high-speed metamaterial screening and real-time design optimization.

The performance discrepancies seen between our work and research on electronic materials are indicative of deep differences in the nature of the design problem rather than methodological limitations. Electronic band gaps in crystalline material are due to well-established quantum mechanical phenomena with established structure-property relationships, whereas acoustic band gaps in metamaterials are based on intricate wave scattering effects sensitive to geometric detail and hard to represent through simple features.

5. Conclusions

This paper presents the very first machine learning architecture specifically designed for band gap property prediction of 2D elastic metamaterials and demonstrates the strength of stacking ensemble methods for physics-informed prediction of complex physics phenomena in engineering materials. Our most valuable results demonstrate that stacking regressor yields R² values of 0.744 for band gap position and 0.641 for band gap width prediction, a significant improvement for metamaterials applications accounting for the dataset limitations of purely geometric information.

Comparative analysis of four machine learning models provides valuable information regarding algorithm choice for metamaterial use and specifically on the eminent individual performance of Random Forest and XGBoost for interpreting geometric features. Feature importance analysis also identifies major geometric parameters that drive band gap creation, offering physical understanding useful to inform future metamaterial design approaches and enhance more efficient optimization practices.

Cross-validation results confirm the stability and generality of our approach in the metamaterial setting, with performance uniform across differing subsets of data. The capacity of the framework to forecast band gap qualities from geometry-only features eliminates the computational cost of expensive finite element solutions in design exploration, enabling real-time design optimization tasks previously impossible.

The levels of performance obtained, while restricted by the characteristics of geometric-only datasets, show that it is possible to screen metamaterials quickly using machine learning techniques. This is an addition to a new route in speeding up the design of metamaterials, reducing computation time from hours to milliseconds with reasonable engineering precision for preliminary design purposes.

Future work should be focused on merging physics-informed neural networks with domain knowledge injection to further enhance prediction accuracy with interpretability. An extension to three-dimensional metamaterial systems and the incorporation of multi-objective optimization capability is the promising direction in which this field can be advanced further and lead to the design of metamaterials with tailored properties for specific acoustic and vibration control applications.

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