

Article

Hybrid Machine Learning-Based Approach for Predicting the Poisson's Ratio of Mechanical Metamaterials

Hümeysra Şevval Balcı ^{1,2,*}, Furkan Balcı ^{3,4} , Hakkı Alparslan İlgin ⁵  and Daver Ali ⁶ 

¹ The Institute of Graduate Programs, Karabük University, Karabük 78050, Türkiye

² Department of Biomedical Device Technology, Yüksek İhtisas University, Ankara 06330, Türkiye

³ Department of Electrical and Electronics Engineering, Faculty of Technology, Gazi University, Ankara 06500, Türkiye; furkanbalci@gazi.edu.tr

⁴ Graduate School of Natural and Applied Sciences, Ankara University, Ankara 06100, Türkiye

⁵ Department of Electrical and Electronics Engineering, Faculty of Engineering, Ankara University, Ankara 06100, Türkiye; ilgin@eng.ankara.edu.tr

⁶ Department of Biomedical Engineering, Faculty of Engineering, Karabük University, Karabük 78050, Türkiye; daverali@karabuk.edu.tr

* Correspondence: humeyrasevval.balcı@yuksekihtisas.edu.tr

Abstract

This study proposes and validates a framework that integrates Grey Wolf Optimization (GWO) with Extreme Gradient Boosting (XGBoost) for estimating the Poisson's ratio of auxetic structures. First, for 320 models derived from Computer-Aided Design-based (CAD-based) unit-cell designs, a systematic sweep of diameter and cellular dimensions was conducted to obtain porosity coverage in the 45–85% range. Subsequently, elastic modulus and Poisson's ratio were computed via finite element analysis (FEA) at three mesh resolutions (0.20/0.25/0.30 mm), and relationships between design variables and outputs were examined using correlation heatmaps and Locally Weighted Scatterplot Smoothing (LOWESS) curves. GWO optimized the XGBoost hyperparameters through a multi-band narrowed search strategy; performance was evaluated using Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), Mean Squared Error (MSE), and Coefficient of Determination (R^2) metrics, as well as residual diagnostics and Ground Truth–Prediction alignments for Poisson's ratio. Across all configurations, $R^2 \geq 0.994$ and absolute errors are on the order of $\sim 10^{-3}$; the 0.25 mm mesh stands out in terms of overall balance with the lowest squared-error profile and the highest R^2 , the 0.30 mm mesh is practically equivalent in terms of MAE, and the 0.20 mm mesh is comparatively weaker. Residual diagnostics—comprising a pattern-free cloud around zero, slight right-skewness, and limited heteroskedasticity—indicate low bias and no substantive model-specification issues. The findings align with physical insight, confirming that Poisson's ratio shifts toward more negative values as porosity increases and toward less negative values as diameter increases. The proposed GWO–XGBoost framework provides a reliable pre-screening tool for rapid design exploration and Poisson's-ratio-targeted optimization, with the potential to reduce the need for additional FEA simulations and experimental iterations during early-stage design.



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1. Introduction

Mechanical metamaterials with a negative Poisson's ratio, which contract laterally under uniaxial compression [1], offer advantages such as high impact resistance, energy dissipation capacity, light weight, and low density [2–4]. In 1892, Love [5], based on Voigt's crystal-elasticity experiments [6], highlighted an early example indicating that negative Poisson's ratio responses may be observed in crystalline systems. Subsequently, Gibson et al. theoretically analyzed the elastic and plastic mechanical behavior of two-dimensional hexagonal honeycombs and compared their predictions with experiments, showing that negative Poisson's ratio behavior is not determined solely by the constituent material but is also influenced by the cellular geometry, and that this response can be well explained by bending and elastic buckling mechanisms of the cell-wall ligaments [7]. In 1991, Evans introduced the term 'auxetic' (from the Greek *auxetos*, 'that may be increased') to replace the phrase 'materials with a negative Poisson's ratio' and surveyed the key implications of this behavior, the main routes for fabricating auxetic polymers, and their potential engineering applications [8]. Several geometries have been proposed to achieve negative Poisson's ratio behavior, including re-entrant structures [9], chiral structures [10], star-shaped configurations [11], rotating squares and triangles [12], and sinusoidal ligaments [13]. One of the most prominent advantages of these structures lies in their ability not only to absorb externally applied stress more effectively than conventional materials but also to distribute it uniformly across a larger surface area [14]. This prevents stress concentrations from accumulating in specific regions, thereby mitigating adverse effects such as local fractures, crack propagation, or structural weakening, ultimately enhancing both impact resistance and long-term mechanical durability.

Due to the unique advantages they offer, auxetic structures have application potential across a wide range of fields, including biomedical applications [15,16], optics [17], automotive technologies [18], and aerodynamic applications [19]. In this context, ongoing research and development activities on auxetic materials have the potential not only to enhance the performance of existing technologies but also to provide innovative solutions that may guide the development of next-generation materials and products [20]. However, achieving a target Poisson's ratio in auxetic structures often relies on designer experience and repeated case-by-case analyses [21]. To address this limitation, the present study aims to predict Poisson's ratio directly from geometric design parameters, providing a faster, more systematic, and engineering-relevant modeling framework for early-stage design exploration.

Machine learning (ML)-based models have increasingly been used to accelerate meta-material design because they can learn nonlinear relationships between geometric parameters and mechanical responses from finite element analysis (FEA)- or experiment-based datasets [21]. Once trained, such models can rapidly estimate the response of previously untested design combinations, thereby reducing the number of costly numerical or experimental trials required during preliminary design optimization. Several recent studies have demonstrated the potential of ML- and optimization-assisted approaches for the prediction and inverse design of auxetic and mechanical metamaterials. For example, Chang et al. employed a back-propagation neural network (BPNN) combined with a genetic algorithm (GA) for the inverse design of auxetic metamaterials with a target Poisson's ratio [21]. Lyngdoh et al. used FEA and interpretable ML to investigate the auxetic behavior of cementitious cellular composites [22], while Oladipo et al. integrated experiments, FEA, and multilayer perceptron (MLP)-based learning to evaluate the auxetic response of 3D-printed re-entrant metamaterials [23]. Other studies have explored artificial neural network (ANN)-based surrogate models with evolutionary computation [24], kernel- and tree-based regression models such as support vector regression (SVR), k-nearest neighbors

(KNN), and Extreme Gradient Boosting (XGBoost) [25], as well as generative and inverse design strategies including convolutional neural network (CNN)–Cycle-Consistent Generative Adversarial Network (CycleGAN), few-shot learning with conditional variational autoencoders (cVAE), and diffusion-based models [26–28]. Although these approaches have shown promising results, their performance strongly depends on the dataset size, topology representation, target output, and optimization strategy.

In this study, a hybrid Grey Wolf Optimizer–XGBoost (GWO–XGBoost) framework is proposed for predicting the Poisson’s ratio of Cross-Chiral auxetic structures. The Poisson’s ratio was selected as the primary target output because it is the fundamental mechanical indicator used to determine whether a structure exhibits auxetic behavior, as auxeticity is directly characterized by a negative Poisson’s ratio. The FEA-derived dataset was used to train XGBoost regression models, while GWO was employed to optimize the model hyperparameters. In this way, the proposed framework combines the strong predictive capability of XGBoost for tabular FEA data with the global search ability of GWO, enabling accurate and computationally efficient Poisson’s ratio estimation [29,30]. The main contribution of this study is the development of a geometry-based predictive framework that estimates Poisson’s ratio without requiring additional FEA-derived response variables as model inputs. This provides a practical route for screening Cross-Chiral auxetic designs and identifying promising parameter combinations before performing more detailed numerical or experimental validation.

The remainder of this paper is organized as follows. Section 2 describes the computer-aided design (CAD)-based dataset generation, FEA procedure, GWO–XGBoost framework, and performance metrics. Section 3 presents the FEA-based observations and predictive model results. Section 4 summarizes the main findings, limitations, and future research directions.

2. Materials and Methods

This section describes the methodological workflow used to generate the dataset and develop the predictive model. First, the CAD-based design of the auxetic model, which is widely used in the literature, was carried out, and a comprehensive dataset was generated based on different geometric parameters. Then, the mesh structure was created, the boundary conditions of the models were defined, and their elastic properties under uniaxial loading were obtained using FEA. Finally, the GWO–XGBoost framework and the evaluation metrics used to assess the prediction performance are presented.

2.1. CAD-Based Design of the Auxetic Model and Development of a Parametric Dataset

In this study, the Cross-Chiral structure was selected due to the ease of varying its geometric parameters and the identifiable rotational–bending deformation mechanism, and was modelled using SOLIDWORKS software [31,32]. Figure 1 illustrates the geometric parameters of the unit cell in the xy -plane, where the independent design variables l_1 and h_1 denote the outer dimensions in the x and y directions, respectively, while the derived parameters l_2 and h_2 represent the inner opening dimensions.

To preserve symmetry, the inner opening dimensions were not selected independently; instead, they were derived using the relations $h_2 = \beta h_1$ and $l_2 = \beta l_1$, with $\beta \in \{0.35, 0.38\}$. The outer dimensions l_1 and h_1 were assigned values of $\{14, 16, 18, 20\}$ mm, and the circular ligament diameter d was varied over $\{1, 1.5, 2, 2.5, 3\}$ mm. Following the combination scheme shown in Figure 2, a total of 320 distinct Cross-Chiral geometrical models were generated by varying the selected design parameters within the predefined dimensional ranges. The rotation angle, which strongly influences auxetic behavior, was kept constant across all models to isolate the effects of the dimensional design variables on Poisson’s

ratio. Circular cross-sections were adopted to mitigate local stress concentrations arising from sharp corners.

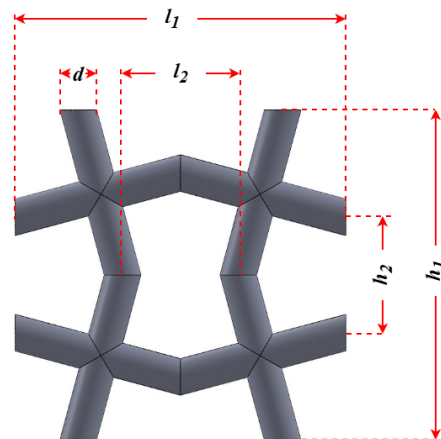


Figure 1. Two-dimensional geometric parameters of the Cross-Chiral structure unit cell.

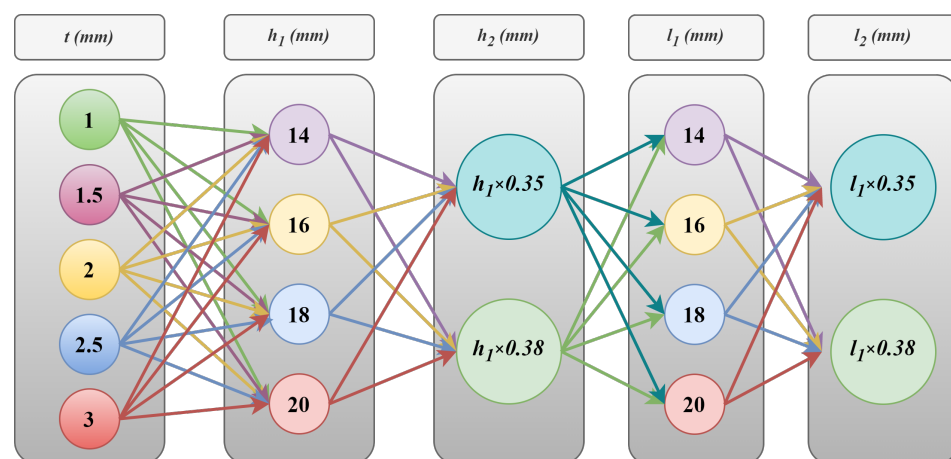


Figure 2. Parameter combination diagram of the diameter, height, and length variables used in the design of the Cross-Chiral model.

The primary objective of this study is to predict the mechanical responses of auxetic structures using artificial intelligence-based models; therefore, a large number of parameter combinations were explored in order to construct a sufficiently diverse dataset that enhances the generalizability and predictive accuracy of such data-driven approaches.

2.2. Calculation of Density and Porosity Ratios of the Models

In the field of metamaterials, it has been widely reported that a decrease in density leads to a corresponding reduction in the effective elastic modulus of porous structures [33]. Porosity is defined as the percentage of void volume present within a solid structure [34]. In addition to theoretical calculations, the use of CAD software such as SOLIDWORKS provides a practical approach for determining the volumetric properties of such structures. In this study, the density of the model (ρ_R) was calculated by dividing the solid volume obtained from SOLIDWORKS (V_s) by the total volume of the model (V_b), as given in Equation (1).

$$\rho_R = \frac{V_s}{V_b} \quad (1)$$

The porosity percentage is calculated as $(1 - \rho_R) \times 100$. The porosity ratios of the models used in this study range from 44.1% to 84.9% (Figure 3). In the graphs, the cell height (h_1) and cell length (l_1) were taken as design parameters, while the z-axis represents

the porosity values. This visualization demonstrates in three dimensions the effects of variations in the design parameters on the porosity ratio.

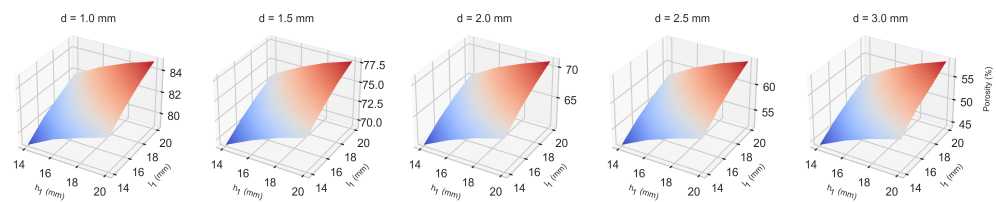


Figure 3. 3D surface plot of porosity ratios with respect to different diameter ratios (d).

2.3. Finite Element Analysis Modeling and Simulation

FEA is a numerical method that enables the solution of models with complex geometries, which are difficult to solve as a whole, by dividing them into a finite number of small and simple elements. Through this method, many problems encountered in physics and engineering can be approximately solved with reduced experimental requirements and lower costs. In this study, FEA was performed using ANSYS (Version 2022 R1) to predict the behavior of the designed models under specific loads. Larger repeating unit-cell systems can provide a more realistic evaluation of inter-cell interactions and deformation behavior, particularly in approximating bulk effective properties. Nevertheless, the use of a limited number of unit cells in FEA is a common approach to obtain computationally efficient yet representative results [35]. In this study, a 2×2 unit-cell configuration was selected because it keeps the computational cost at a reasonable level for a large number of parameter combinations while allowing the deformation interaction between neighboring Cross-Chiral cells to be captured. This enabled the generation of a consistent and comparable dataset across all designs. However, it should be noted that edge effects cannot be completely eliminated in a finite 2×2 model. Therefore, the obtained mechanical properties should be interpreted as the effective response of the investigated finite periodic configuration rather than as fully scale-independent bulk properties.

2.3.1. Mesh Sensitivity Analysis

In FEA, mesh sensitivity analysis is of critical importance for obtaining reliable and reproducible results. Mesh sensitivity is commonly assessed by comparing the numerical responses obtained at different element sizes and selecting a mesh configuration for which the solution shows only minor variations with further mesh refinement. In this study, an h-adaptive meshing strategy was not preferred because the main objective was to generate a consistent and comparable FEA database for model training rather than to resolve local stress concentrations in detail. Accordingly, three different element sizes, namely 0.20 mm, 0.25 mm, and 0.30 mm, were investigated to provide sufficient resolution for the smallest ligament diameter, and these element sizes were kept constant across all models to maintain consistency in the comparisons. This choice minimizes mesh-induced effects and enables a direct and consistent comparison of mechanical responses among different geometric configurations. The models were meshed with second-order quadratic tetrahedral 3D solid elements, as shown in Figure 4 [32]. As presented in Table 1, the Poisson's ratio and effective Young's modulus values exhibit only small variations among the investigated mesh sizes. Therefore, the selected mesh settings are considered sufficiently consistent for comparative evaluation within the investigated mesh range. It should be noted that this result indicates limited mesh sensitivity within the tested element-size range rather than proving a general mesh-independent behavior over all possible mesh refinements. Therefore, within the investigated mesh range, a single validated mesh configuration can be selected to provide a reasonable balance between numerical accuracy and computational cost.

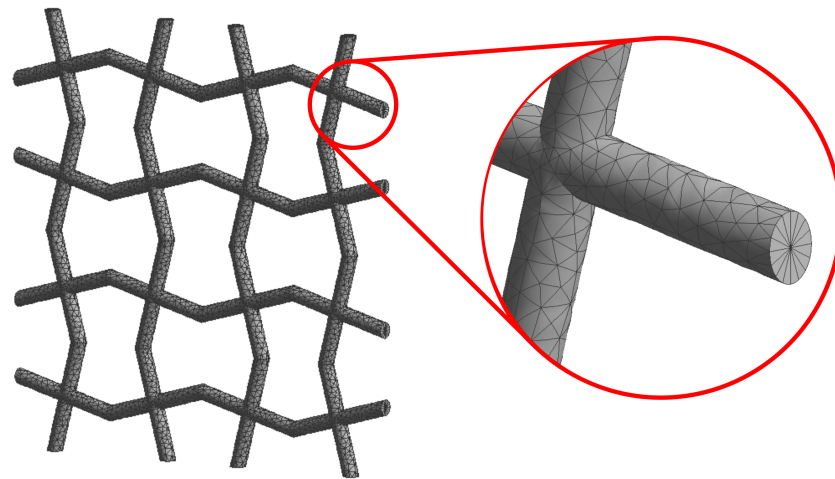


Figure 4. View of the mesh structure of the model used in the analyses, generated with tetrahedral 3D solid elements.

Table 1. Comparison of Poisson’s ratio and effective elastic modulus for different mesh sizes.

d (mm)	h_1 (mm)	h_2 (mm)	l_1 (mm)	l_2 (mm)	Mesh Size (mm)	Poisson’s Ratio	Effective Elastic Modulus (E_y /GPa)
1	14	14×0.35	16	16×0.35	0.20	−0.459	2.11
					0.25	−0.460	2.11
					0.30	−0.461	2.12
2	18	18×0.38	16	16×0.38	0.20	−0.425	10.41
					0.25	−0.425	10.43
					0.30	−0.425	10.44
3	20	20×0.35	14	14×0.38	0.20	−0.279	29.96
					0.25	−0.279	30.01
					0.30	−0.279	30.05

2.3.2. Definition of Boundary Conditions

In a FEA, the conditions that either constrain the values or apply effects to the selected surfaces and edges of the model are referred to as boundary conditions. As shown in Figure 5, the elastic response of the models was examined under uniaxial loading. A compressive load of 1 MPa was applied through a rigid (non-deformable) plate placed on top of the scaffolds. The displacements of the scaffolds were constrained in the z -direction on the front surfaces, in the x -direction on the left lateral surfaces, and in the y -direction on the bottom surfaces, while the right lateral surfaces were left free. The auxetic structure was modelled as a linear elastic, isotropic material with Young’s modulus of 1.2×10^{11} Pa, Poisson’s ratio of 0.36, and density of 4620 kg/m^3 . The loading plate was modelled using structural steel properties with an increased Young’s modulus (2×10^{15} Pa) to approximate rigid-body behavior during compression. Static structural analyses were performed in ANSYS with geometric nonlinearity enabled (Large Deflection ON) to accurately capture rotation-dominated deformation mechanisms.

A uniform pressure was applied to the upper surface of the loading plate. To prevent rigid-body motion while allowing realistic load transfer, frictionless support boundary conditions were assigned to the lateral faces of the loading plate. To validate the rigidity assumption of the loading plate, the difference between the maximum and minimum total displacement values within the plate was examined and found to be nearly zero. The results indicate that the plate undergoes nearly uniform translation without significant internal

bending. The significantly higher stiffness of the plate ensured negligible deformation compared to the auxetic structure during loading.

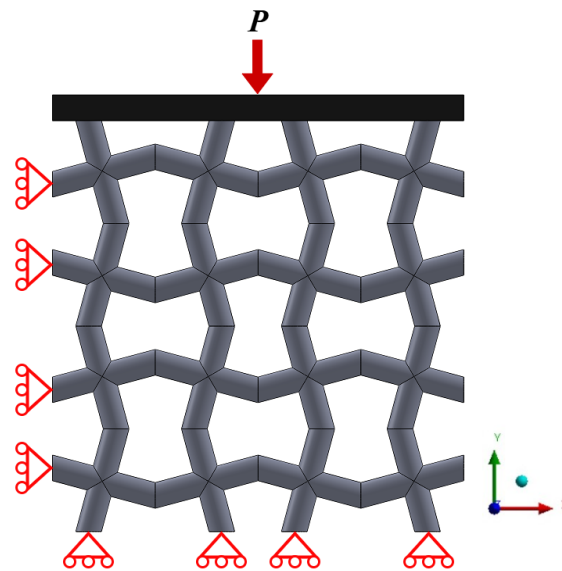


Figure 5. Illustration of the boundary conditions applied in the FEA of the Cross-Chiral model.

2.3.3. Determination of Elastic Properties: Elastic Modulus and Poisson's Ratio

Elastic deformation is defined as the reversible (recoverable) deformation in which a material, when subjected to an external load, undergoes a change in shape and fully returns to its original dimensions and configuration once the load is removed. In this region, the stress–strain relationship is generally linear, following Hooke's law, and the stored mechanical energy is completely released. When the elastic limit is exceeded, permanent, i.e., plastic deformation begins. A high elastic modulus (Young's modulus) indicates that the material is stiff, exhibiting less deformation under applied stress and therefore demonstrating higher resistance to deformation. In this study, the effective elastic modulus of the models was calculated using the expression given in Equation (2):

$$E_y = \frac{\sigma_y}{\varepsilon_y} \quad (2)$$

where E_y , σ_y , and ε_y denote the effective elastic modulus, the applied stress in the y -direction, and the strain in the y -direction, respectively.

The load was applied as a uniform pressure on the upper surface of the loading plate. The nominal stress in the loading direction was taken as equal to the applied pressure. The longitudinal strain was calculated as $\varepsilon_y = \Delta L_y / L_{y0}$. Here, ΔL_y was obtained from the ANSYS Directional Deformation (y Axis) output using the displacement of the top surface, since the bottom boundary was constrained in the y -direction.

Poisson's ratio was calculated from the ratio of transverse strain to longitudinal strain under uniaxial loading, as given in Equation (3):

$$\nu_{yx} = -\frac{\varepsilon_x}{\varepsilon_y} \quad (3)$$

where ν_{yx} , ε_x , and ε_y represent the Poisson's ratio, the strain in the x -direction, and the strain in the y -direction, respectively.

The longitudinal strain (ε_y) was calculated according to the engineering strain definition as the ratio of the vertical displacement difference between the top and bottom boundaries to the initial specimen height (L_{y0}). Since the bottom boundary was constrained

in the y -direction, the displacement difference (ΔL_y) was obtained from the Directional Deformation (y axis) output in ANSYS using the vertical displacement of the top surface. The longitudinal strain ε_y was then computed by dividing this displacement by the initial height.

Similarly, the transverse strain (ε_x) was determined as the ratio of the horizontal displacement difference between the right and left boundaries to the initial specimen width (L_{x0}). As the left boundary was constrained in the x -direction, the displacement difference (ΔL_x) was obtained from the Directional Deformation (x axis) output in ANSYS using the horizontal displacement of the right surface. The transverse strain ε_x was then calculated by dividing this displacement by the initial width. The Poisson's ratio was subsequently calculated using these strain values according to Equation 3.

Finite models may inherently exhibit edge effects; however, all geometries were analyzed using the same unit-cell configuration and identical boundary conditions. Therefore, edge-induced deviations are consistently present across the dataset. Since the strains were obtained from displacement differences between opposite boundaries, the reported effective material properties represent suitable and comparable responses for data-driven modeling.

2.4. Hybrid Grey Wolf Optimizer–XGBoost Framework

The hybrid method employed in this study is based on the integration of the GWO, a nature-inspired, non-parametric heuristic search algorithm, with XGBoost, a powerful predictor grounded on gradient-boosted decision trees. This approach aims to efficiently explore the hyperparameter space using multi-band narrowed intervals, thereby producing results that are both rapid and highly accurate. In the multi-band search strategy, the hyperparameter space is divided into distinct bands, each containing predefined intervals for parameters such as the learning rate (η), number of trees (n_{estim}), maximum tree depth (d_{tree}), sampling ratios (s, c), minimum child weight (m_{child}), and regularization parameters ($\lambda_2, \lambda_1, \gamma$). Here, λ_2 and λ_1 denote the L2 and L1 regularization coefficients, respectively. In this way, the search strategy encompasses not only conventional ranges but also uncommon parameter combinations overlooked in previous works. For each band b , the search space is defined as:

$$B^{(b)} = \{\theta \mid L^{(b)} \leq \theta \leq U^{(b)}\} \quad (4)$$

where $L^{(b)}$ and $U^{(b)}$ denote the lower and upper bound vectors of the band, respectively. The parameter vector is defined as:

$$\theta = [n_{\text{estim}}, d_{\text{tree}}, \eta, s, c, m_{\text{child}}, \lambda_2, \lambda_1, \gamma] \quad (5)$$

Integer-type parameters ($n_{\text{estim}}, d_{\text{tree}}, m_{\text{child}}$) are rounded to the nearest integer, while the others are treated as continuous variables. The GWO algorithm is a heuristic method inspired by the hunting strategy and hierarchical structure of grey wolf packs, widely applied for solving complex optimization problems [36]. Beginning with a randomly generated population in the search space, the top three individuals are identified as α , β , and δ , representing the leaders, while the remaining wolves update their positions based on these leaders. This process enables the approximation of the three best solutions at each iteration. To avoid notational ambiguity, the linearly decreasing control coefficient of GWO is denoted by a . The position update rules are expressed as:

$$A_m = 2ar_{1,m} - a, \quad C_m = 2r_{2,m}, \quad a = 2 - \frac{2t}{T_G - 1}, \quad m \in \{\alpha, \beta, \delta\} \quad (6)$$

$$D_\alpha = |C_\alpha \odot \theta_\alpha - \theta|, \quad D_\beta = |C_\beta \odot \theta_\beta - \theta|, \quad D_\delta = |C_\delta \odot \theta_\delta - \theta| \quad (7)$$

$$X_1 = \theta_\alpha - A_\alpha \odot D_\alpha, \quad X_2 = \theta_\beta - A_\beta \odot D_\beta, \quad X_3 = \theta_\delta - A_\delta \odot D_\delta \quad (8)$$

$$\theta^{(t+1)} = \text{clip}\left(\frac{X_1 + X_2 + X_3}{3}, L^{(b)}, U^{(b)}\right) \quad (9)$$

where $\odot$ denotes element-wise multiplication, and $r_{1,m}, r_{2,m} \sim U(0, 1)$ are independent random vectors. The algorithm iterates for T_G generations, with early stopping applied when a threshold criterion is met. For each band, an initial global GWO search is performed; subsequently, a refined local GWO is executed around the best solution by narrowing the band boundaries by $\pm 10\%$:

$$L_{\text{loc}} = \max(L^{(b)}, \theta_b^* - 0.1 \cdot (U^{(b)} - L^{(b)})) \quad (10)$$

$$U_{\text{loc}} = \min(U^{(b)}, \theta_b^* + 0.1 \cdot (U^{(b)} - L^{(b)})) \quad (11)$$

Finally, the optimal band and parameter set are selected as:

$$b^* = \arg \min_b Q(\theta_b^*) \quad (12)$$

where $Q(\theta_b^*)$ denotes the validation-based objective value of the best solution obtained for band b , and $\theta_{b^*}^*$ is used as the final hyperparameter configuration for XGBoost.

XGBoost is a robust ensemble learning technique based on gradient boosting [37]. Its core principle is to sequentially train multiple weak learners, namely decision trees, and combine them to form a strong predictor for regression or classification tasks. At each iteration, the model incorporates a new tree to minimize residual errors from prior iterations. The optimization objective is expressed as:

$$\hat{y}_i = \sum_{k=1}^K f_k(x_i), \quad f_k \in F \quad (13)$$

where f_k is a regression tree chosen from the set F . The overall objective function is

$$\mathcal{L} = \sum_{i=1}^n l(y_i, \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (14)$$

where $l(\cdot)$ is the loss function, such as squared error or absolute error, and $\Omega(f_k)$ is the regularization term penalizing model complexity:

$$\Omega(f) = \gamma J + \frac{1}{2} \lambda_2 \sum_{j=1}^J \omega_j^2 + \lambda_1 \sum_{j=1}^J |\omega_j| \quad (15)$$

Here, J denotes the number of leaves, ω_j is the prediction score of leaf j , λ_2 is the L2 regularization coefficient, λ_1 is the L1 regularization coefficient, and γ is the split penalty. This regularization prevents overfitting and enhances generalization. At the t^{th} iteration, the updated prediction is given by:

$$\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + f_t(x_i) \quad (16)$$

The second-order Taylor expansion of the loss function is

$$\mathcal{L}^{(t)} \approx \sum_{i=1}^n \left[g_i f_t(x_i) + \frac{1}{2} h_i f_t^2(x_i) \right] + \Omega(f_t) \quad (17)$$

with

$$g_i = \frac{\partial l(y_i, \hat{y}_i^{(t-1)})}{\partial \hat{y}_i^{(t-1)}}, \quad h_i = \frac{\partial^2 l(y_i, \hat{y}_i^{(t-1)})}{\partial (\hat{y}_i^{(t-1)})^2} \quad (18)$$

representing the first- and second-order gradients, respectively. This derivative-based optimization leverages second-order information, ensuring faster convergence and more stable learning compared to traditional gradient boosting.

By integrating GWO-optimized hyperparameters into XGBoost's learning framework, the hybrid method balances model complexity and generalization capacity automatically, while producing highly accurate predictions through sequential tree aggregation. In this study, the methodological framework of the proposed hybrid approach is summarized through a flowchart that illustrates the integrated structure of the hyperparameter search process and the XGBoost-based prediction mechanism (Figure 6). The diagram visualizes the partitioning of the hyperparameter space into multi-band narrowed intervals, the identification of leader solutions via the GWO algorithm, the local refinement steps, and the transfer of the optimal parameter set obtained to the XGBoost model.

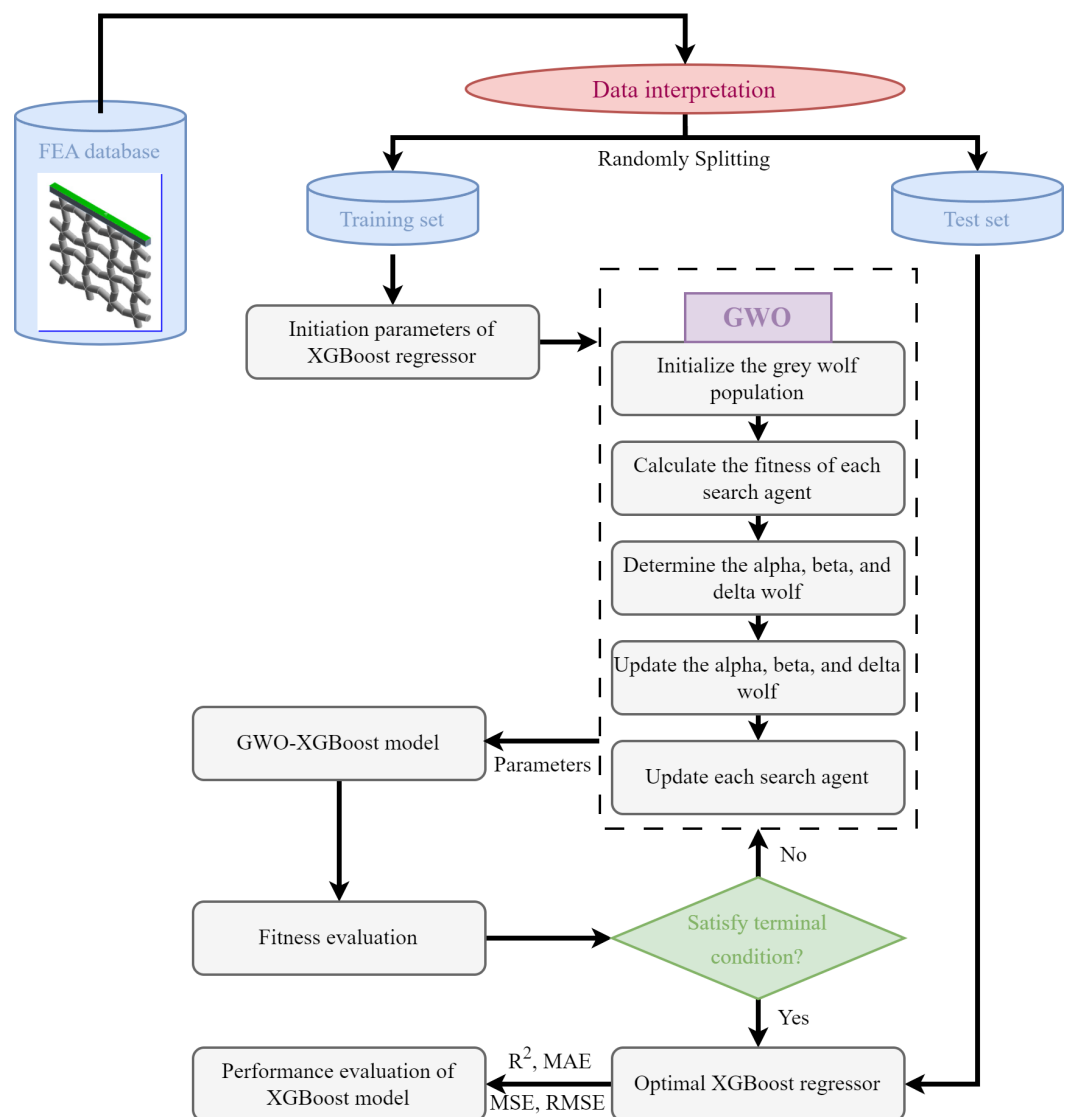


Figure 6. Flowchart illustrating the operational steps of the proposed hybrid Grey Wolf Optimizer–XGBoost model.

2.5. Metrics for Performance Evaluation

The predictive performance and robustness of the proposed hybrid GWO–XGBoost model were evaluated using widely adopted metrics in the literature, namely the coefficient of determination (R^2), mean squared error (MSE), root mean squared error (RMSE), and

mean absolute error (MAE). These metrics provide different perspectives on how accurately the model can predict the Poisson's ratio of Cross-Chiral structures.

The coefficient of determination (R^2) indicates the proportion of variance explained by the model. Although values closer to 1 indicate better predictive performance, R^2 may also take negative values when the model performs worse than the mean-based predictor. It is expressed as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (19)$$

where y_i denotes the actual values, $\hat{y}_i$ the predicted values, and $\bar{y}$ the mean of the actual values.

The MSE measures the average of the squared differences between the predicted and actual Poisson's ratio values. Since it penalizes larger errors more heavily, it is a critical metric for assessing the model's sensitivity to errors. A lower MSE indicates that the hybrid GWO–XGBoost model produces predictions that are generally closer to the actual values:

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (20)$$

The RMSE is obtained by taking the square root of the MSE and, unlike MSE, it has the same unit as the target variable. This makes it easier to interpret. Since RMSE is more sensitive to larger errors, it plays a significant role in evaluating the stability of the model. For variables with small value ranges, such as the Poisson's ratio, a low RMSE indicates high predictive accuracy:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (21)$$

The MAE represents the mean of the absolute differences between the predicted and actual values. Unlike RMSE, it is less sensitive to large errors and reflects the typical magnitude of prediction errors in a straightforward manner. A small MAE value indicates that the model's prediction performance is stable and reliable:

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (22)$$

3. Results and Discussion

In this section, first, in the subsection on the evaluation of FEA findings, the relationships between the design variables and Poisson's ratio are examined through correlation heatmaps and Locally Weighted Scatterplot Smoothing (LOWESS) trend curves to identify the dominant determinants. Subsequently, in the subsection on the performance results of the hybrid GWO–XGBoost model, MAE, RMSE, MSE, and R^2 metrics obtained under different mesh resolutions—together with residual diagnostics and Ground Truth vs. Predictions alignments are reported to assess the accuracy and robustness of the data-driven predictive framework. Finally, in the discussion, quantitative metrics and visual evidence are synthesized to address physical consistency, mesh sensitivity, limitations, and implications for design/optimization, thereby consolidating both FEA-based observations and GWO–XGBoost-based predictions within a common interpretive framework.

3.1. Evaluation of Finite Element Analysis Findings

The stress distributions obtained from the FEA provide an important indicator for evaluating the strength-related response of the designed structures under the applied loading conditions. In this context, the maximum von Mises stress values obtained from

the FEA analyses were compared with the tensile yield strength of the selected material. While the tensile yield strength defined in ANSYS Engineering Data is 930 MPa, the maximum von Mises stress values obtained from the analyses were found to vary between 11 and 172 MPa. These values remain well below the yield strength of the material for all models. This result indicates that, under the applied loading and boundary conditions, the models remained within the linear elastic region and did not reach the yielding/plastic deformation limit. However, this evaluation is valid only under the present linear elastic FEA conditions; fatigue, buckling, fracture, and nonlinear plastic behavior are beyond the scope of this study.

A correlation analysis was conducted to examine the relationships between the design parameters and Poisson's ratio. The correlation matrices obtained for different mesh sizes are presented in Figures 7–9. The results indicate a strong negative relationship between porosity and diameter ($r \approx -0.96$). Similarly, the high negative correlation between porosity and Poisson's ratio ($r \approx -0.88$ to -0.90) is notable. This finding indicates that the structure's auxetic behavior changes markedly with increasing porosity. On the other hand, the diameter parameter exhibits a high positive correlation with Poisson's ratio ($r \approx 0.84$ – 0.87), suggesting that diameter plays a critical role in the effectiveness of the auxetic mechanism. The correlations between Poisson's ratio and the cell height and length parameters are low ($|r| < 0.45$), indicating that the direct effects of these parameters are limited. The largely similar correlation patterns across the three mesh sizes indicate limited mesh sensitivity within the investigated mesh range.

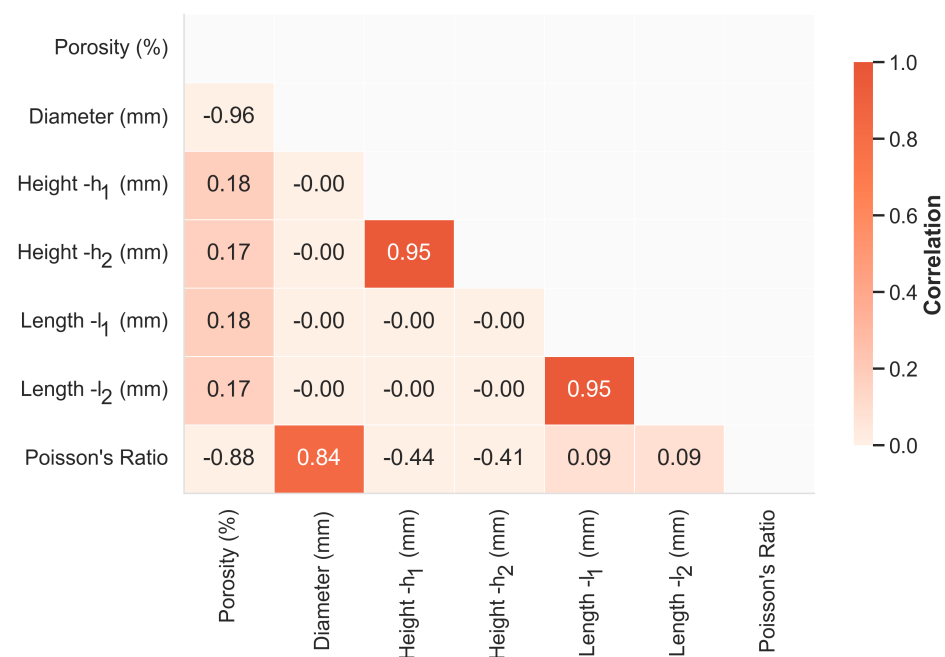


Figure 7. Correlation matrix for the 0.20 mm mesh size.

LOWESS was used to visualize local trends between the design parameters and Poisson's ratio. Figures 10–12 present the scatter plots and LOWESS curves for the FEA data used as input to the GWO algorithm. The points represent FEA results, whereas the curves indicate local regression trends. Porosity values are mostly concentrated between 45% and 85%. The LOWESS curve shows a clear negative trend, confirming that increasing porosity leads to more negative Poisson's ratio values. The wider scatter observed at high porosity levels suggests increased sensitivity of the auxetic response. In contrast, increasing diameter shifts Poisson's ratio toward less negative values. The Poisson's ratio reaches approximately -0.6 for models with a diameter of 1.0 mm, whereas it clusters around

−0.2 for models with a diameter of 3.0 mm. This indicates that diameter has a strong and systematic effect on auxetic behavior. Cell heights h_1 and h_2 show only a weak negative trend, while cell widths l_1 and l_2 exhibit only a weak positive trend. Considering the input parameters jointly, porosity and diameter emerge as the dominant determinants of Poisson's ratio. While an increase in porosity leads to stronger auxetic behavior (more negative Poisson's ratio), an increase in diameter acts in the opposite direction. Cell height and width exhibit limited and more scattered effects. These findings strongly support prioritizing porosity and diameter in the optimization process.

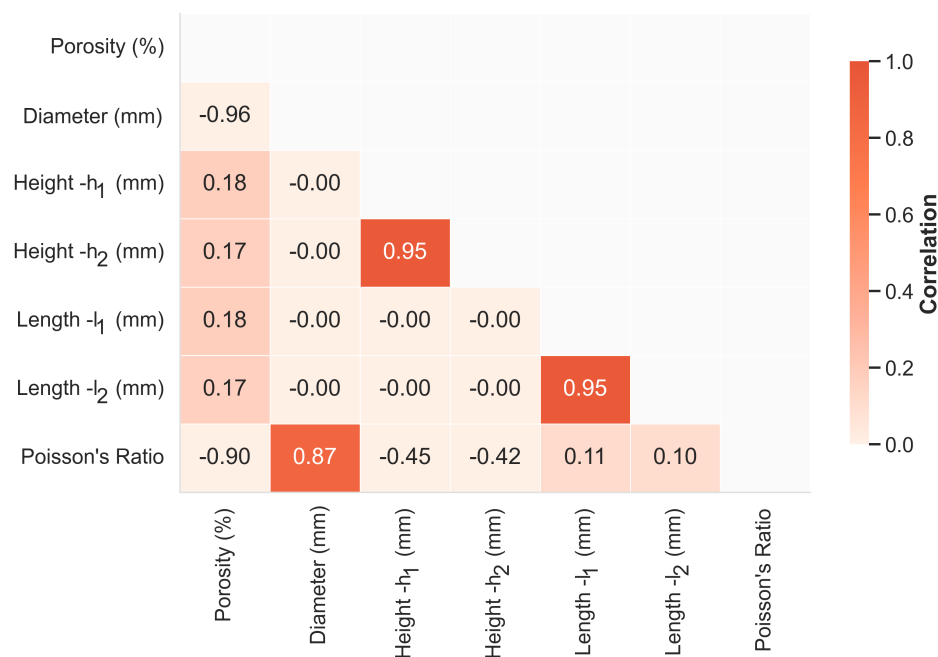


Figure 8. Correlation matrix for the 0.25 mm mesh size.

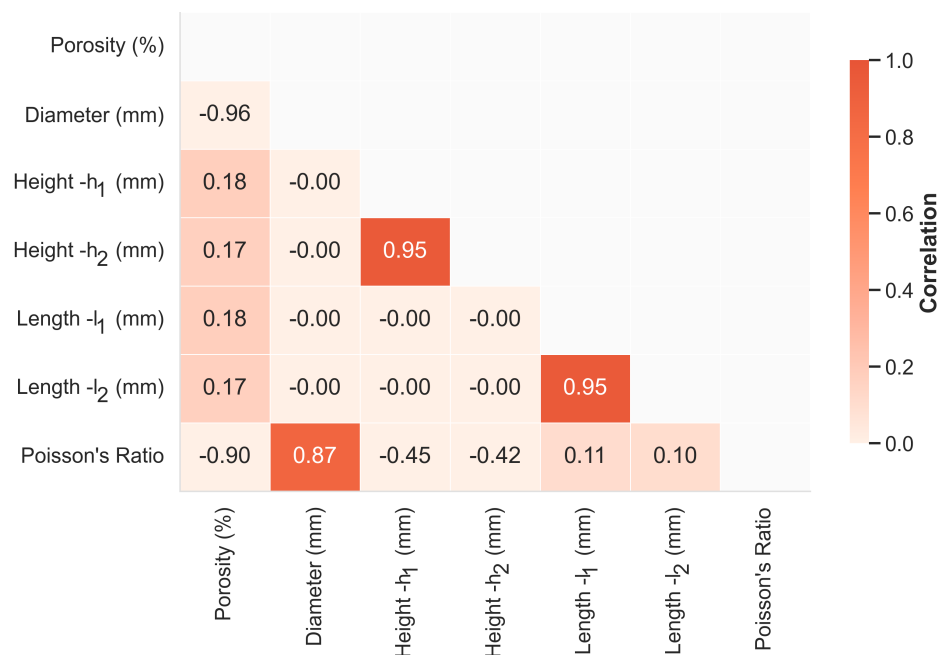


Figure 9. Correlation matrix for the 0.30 mm mesh size.

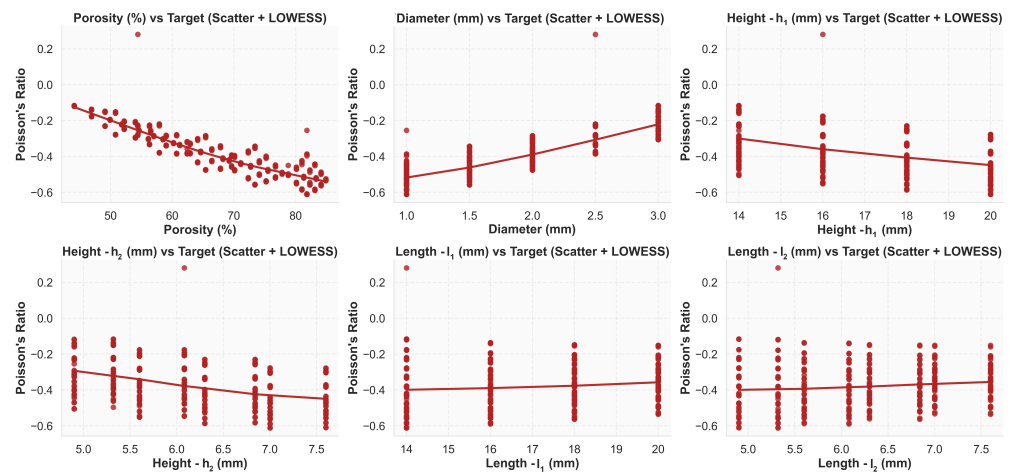


Figure 10. Scatter plots and LOWESS regression curves for the 0.20 mm mesh size: comparison of the effects of porosity, diameter, and unit-cell parameters on Poisson's ratio.

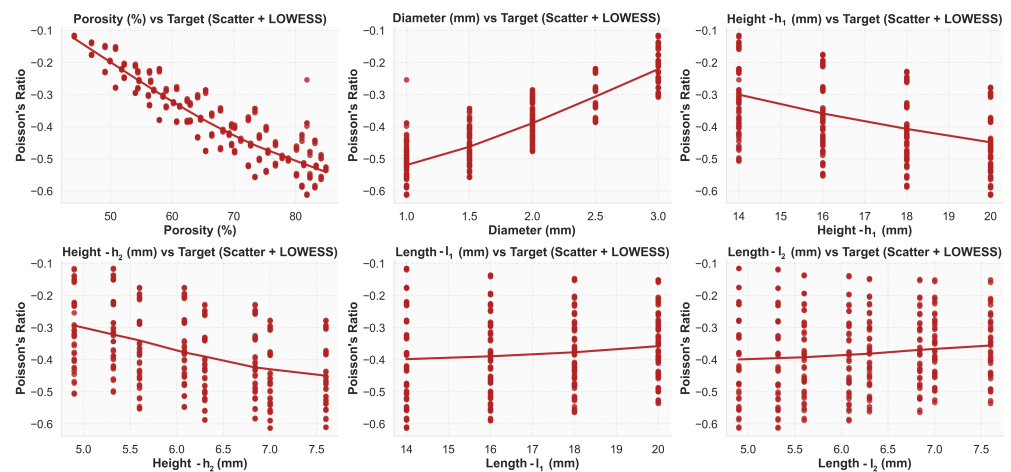


Figure 11. Scatter plots and LOWESS regression curves for the 0.25 mm mesh size: comparison of the effects of porosity, diameter, and unit-cell parameters on Poisson's ratio.

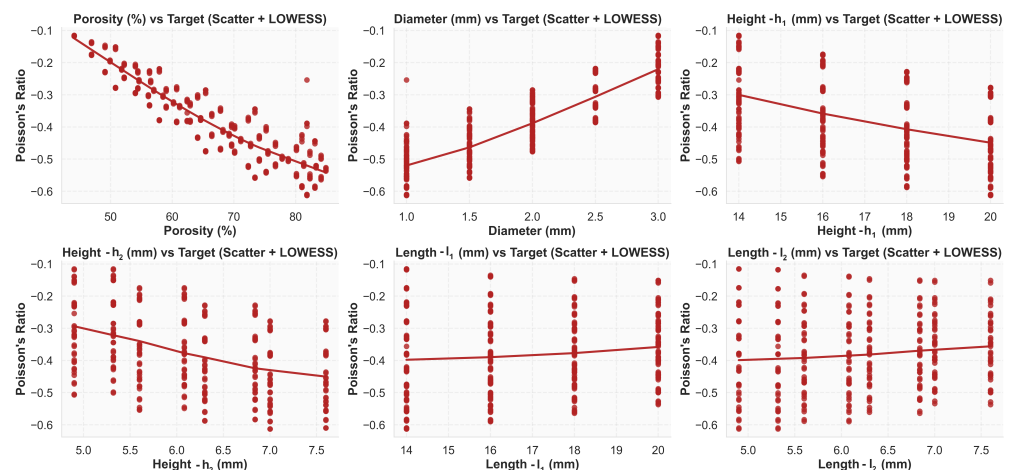


Figure 12. Scatter plots and LOWESS regression curves for the 0.30 mm mesh size: comparison of the effects of porosity, diameter, and unit-cell parameters on Poisson's ratio.

3.2. Performance Results of the Hybrid GWO–XGBoost Model

Residual plots were used to evaluate the model's predictive performance by visualizing, for each instance, the error difference between the true Poisson's ratio and the predicted Poisson's ratio ($e_i = y_i - \hat{y}_i$). In Figures 13–15, the panels on the right dis-

play the residuals–predictions scatter plots. In the ideal case, the expectation is that the points form an unpatterned cloud with approximately constant spread around the zero line. Importantly, three independent models were trained for three different mesh resolutions (0.20, 0.25, and 0.30 mm), allowing mesh density to be treated as a modeling parameter rather than a fixed numerical setting. This strategy enables an explicit assessment of whether the learning-based framework can generalize across discretization levels and provide reliable Poisson’s-ratio predictions without requiring repeated FEA at a converged mesh. In Figures 13–15, the panels on the left show the residual distributions, where the histogram and the kernel density curve (KDE) are presented together; the zero-error point ($e = 0$) is indicated by a vertical dashed line as a reference. From a performance perspective, the most important properties are that the residuals are centered around zero, indicating weak model bias, and that the histogram is symmetric, indicating the absence of a one-directional systematic error. Across the three mesh densities, the residuals are centered around $e \approx 0$, indicating that no global bias is observed. The consistency of the residual structure across different mesh resolutions demonstrates that the proposed GWO–XGBoost framework captures the underlying geometry–mechanics relationship in a mesh-robust manner, supporting its use as a surrogate model that can reduce the need for additional FEA runs during preliminary design screening. The distributions are slightly right-skewed with sparse yet relatively large positive residuals, indicating that in the prediction of Poisson’s ratio the GWO–XGBoost model, albeit rarely, underestimates some instances (with relatively larger errors). No discernible trend or curvature is observed in the residuals–predictions scatter plots; therefore, no pattern indicating a strong functional form misspecification is present. Evidence of heteroskedasticity is limited and mostly appears as a mild widening in the extreme prediction ranges. Table 2 summarizes the hyperparameter ranges and types used for the GWO–XGBoost optimization. Table 3 presents, for three mesh resolutions (0.20/0.25/0.30 mm), the cross-validation-based best hyperparameters (additionally α and γ) and a summary of performance on the holdout set. Although several mechanical response quantities—such as the effective elastic modulus, von Mises stress measures (maximum, minimum, and average), and total deformation metrics (maximum, minimum, and average)—were computed via FEA to characterize the structural behavior of the auxetic designs, these FEA-derived outputs were not used as input features in the ML model. In the proposed learning setup, the input vector consists exclusively of geometry- and dimension-based design parameters, while the target variable is the Poisson’s ratio obtained from FEA. This intentional separation ensures that the model learns a direct mapping from geometric descriptors to Poisson’s ratio, enabling prediction without requiring any additional FEA-derived quantities as inputs and preserving the framework’s role as a pre-FEA surrogate model.

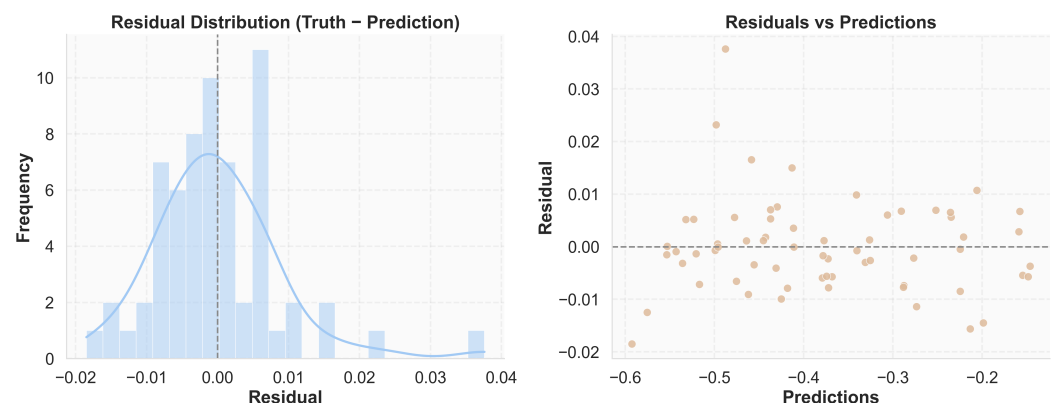
Table 2. Hyperparameter search space used for the GWO–XGBoost optimization.

Hyperparameter	Range	Type
$n_{\text{estimators}}$	[100, 1500]	int
max_depth	[2, 20]	int
η	[0.005, 0.1]	float
subsample	[0.5, 1.0]	float
colsample_bytree	[0.5, 1.0]	float
min_child_weight	[1, 20]	int
λ	[0.0, 15.0]	float

Table 3. Best cross-validation-selected hyperparameters (criterion: RMSE) and holdout performance for Poisson’s ratio prediction across mesh resolutions.

Quantity	0.20 mm Mesh	0.25 mm Mesh	0.30 mm Mesh
$n_{\text{estimators}}$	458	667	739
max_depth	9	9	13
η	0.0349	0.0460	0.0447
subsample	0.5280	0.5369	0.5721
colsample_bytree	0.5267	0.5513	0.5522
min_child_weight	6	8	6
λ	7.5417	7.1387	6.2617
α	0.0011	1.3389×10^{-5}	1.6407×10^{-9}
γ	0.0	0.0	0.0

In the overall comparison across meshes, the 0.25 mm mesh configuration stands out with the narrowest spread and the shortest positive tail. This observation further indicates that, despite being trained independently, models associated with different mesh resolutions converge toward similar predictive behavior, reinforcing the notion that mesh density does not fundamentally alter the learned mapping between geometric descriptors and Poisson’s ratio. In addition, its histogram is more tightly clustered around zero, the density of outliers is lower, and the residual–prediction point cloud appears more homogeneous and pattern-free. The 0.30 mm mesh configuration exhibits comparable performance, whereas its tail behavior is relatively longer than that of the 0.20 mm configuration. The 0.20 mm mesh configuration has the widest spread and several pronounced positive outliers; furthermore, the volatility of residuals increases relatively in the extreme prediction regions. This assessment indicates that the model operates generally without bias, is largely independent of mesh density, and is stable; apart from a limited number of under-prediction cases, no pattern indicating a significant systematic error is observed. From an application perspective, this mesh-independence implies that the trained GWO–XGBoost models can be employed to estimate Poisson’s ratio for new auxetic designs without requiring mesh-converged finite element simulations, thereby significantly reducing computational cost during early-stage design exploration. From the standpoint of diagnostic quality, the 0.25 mm mesh resolution provides the most balanced residual structure and was therefore selected as the preferred configuration for subsequent evaluation.

**Figure 13.** Residual diagnostics for Poisson’s ratio prediction with GWO–XGBoost for the 0.20 mm mesh size: (left), histogram + KDE ($e = y - \hat{y}$, dashed $e = 0$); (right), e – $\hat{y}$ scatter.

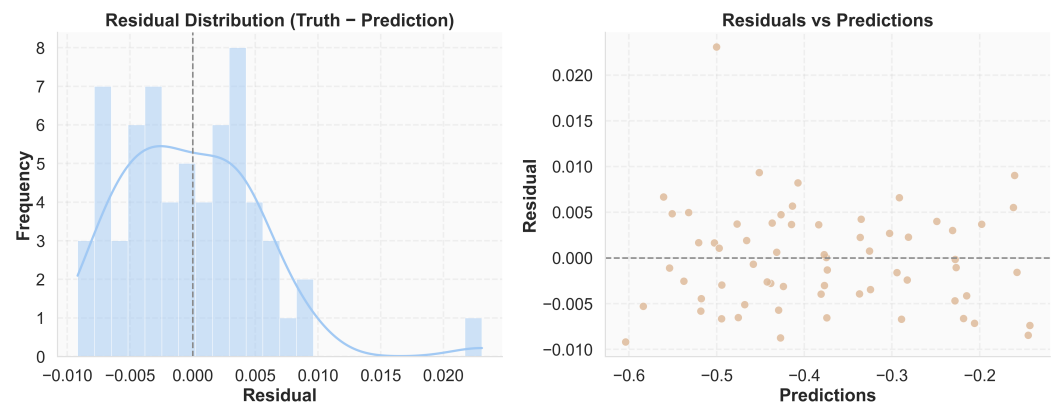


Figure 14. Residual diagnostics for Poisson's ratio prediction with GWO-XGBoost for the 0.25 mm mesh size: (left), histogram + KDE ($e = y - \hat{y}$, dashed $e = 0$); (right), $e-\hat{y}$ scatter.

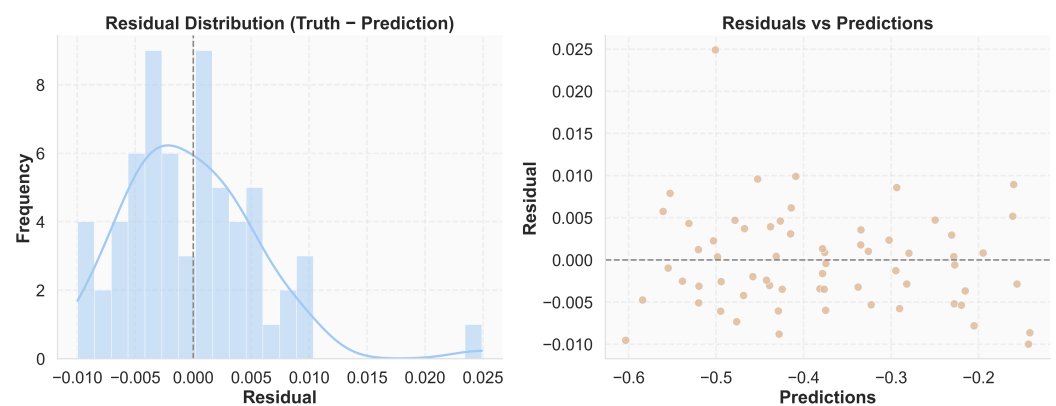


Figure 15. Residual diagnostics for Poisson's ratio prediction with GWO-XGBoost for the 0.30 mm mesh size: (left), histogram + KDE ($e = y - \hat{y}$, dashed $e = 0$); (right), $e-\hat{y}$ scatter.

Figure 16 presents the principal error metrics (MAE, RMSE, MSE) for the GWO-XGBoost model across different mesh resolutions on a logarithmic axis, together with the explained variance (R^2) on the right axis. The logarithmic scale renders even small differences in the metrics visible, facilitating relative comparisons across configurations. The model achieves high accuracy for all meshes: $R^2 \geq 0.994$ and absolute errors on the order of 10^{-3} ; on the Poisson's ratio scale, this corresponds to an absolute error level of $\lesssim 1\%$. Based on the lowest RMSE/MSE and the highest R^2 , the 0.25 mm mesh resolution provides the best overall balance. While the 0.30 mm mesh model is nearly equivalent to 0.25 mm in terms of MAE, its slightly higher RMSE/MSE indicates heavier error tails; the 0.20 mm mesh model is markedly weaker, with larger errors and lower R^2 , which may be attributable to finite element resolution noise or resolution-specific variation inadequately captured by the model. Overall, the GWO-XGBoost model estimates Poisson's ratio with high precision. For subsequent analyses, the 0.25 mm mesh model should be preferred, whereas the 0.30 mm mesh model is a practically equivalent alternative when MAE is prioritized.

Figures 17–19 present Ground Truth vs. Predictions plots that visually corroborate the test results from which the reported metrics were obtained. Across the three meshes, the prediction curve for Poisson's ratio closely follows the true Poisson's ratio curve even at peaks and troughs; rare local deviations—under-prediction near peaks and over-prediction near troughs—are consistent with the slight right-skew observed in the Poisson's ratio residuals; no pronounced trend or change in variance is detected along the sample index, as supported by the pattern-free cloud in the residual–prediction scatter and the limited

heteroskedasticity; furthermore, all Poisson's ratio estimates remain within the expected auxetic range $[-0.6, -0.18]$, confirming physical consistency.

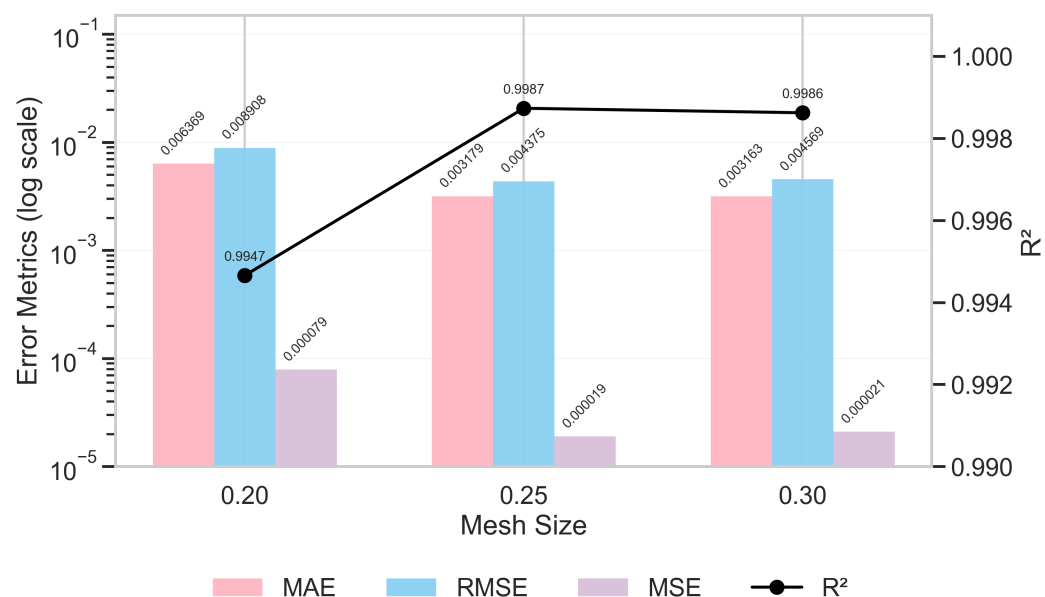


Figure 16. Performance metrics of the GWO-XGBoost model across different mesh sizes.

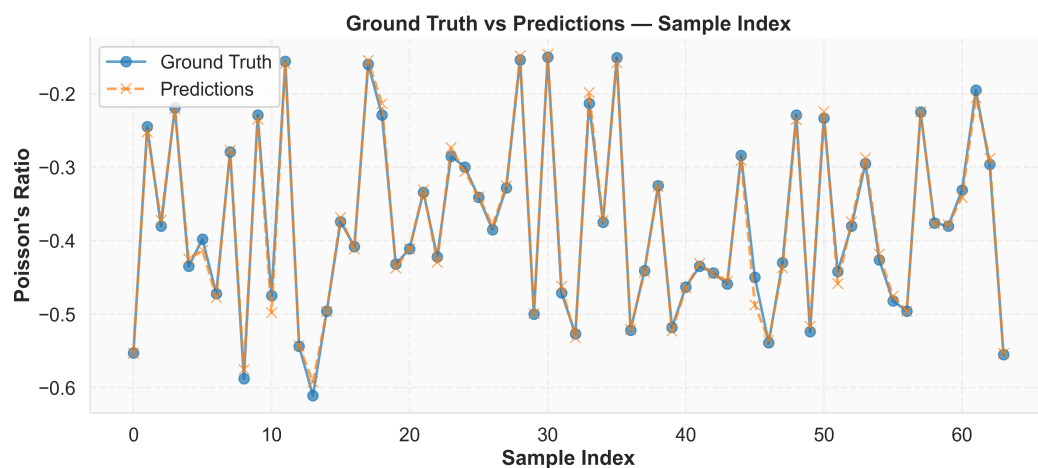


Figure 17. Ground Truth vs. Predictions for the 0.20 mm mesh size.

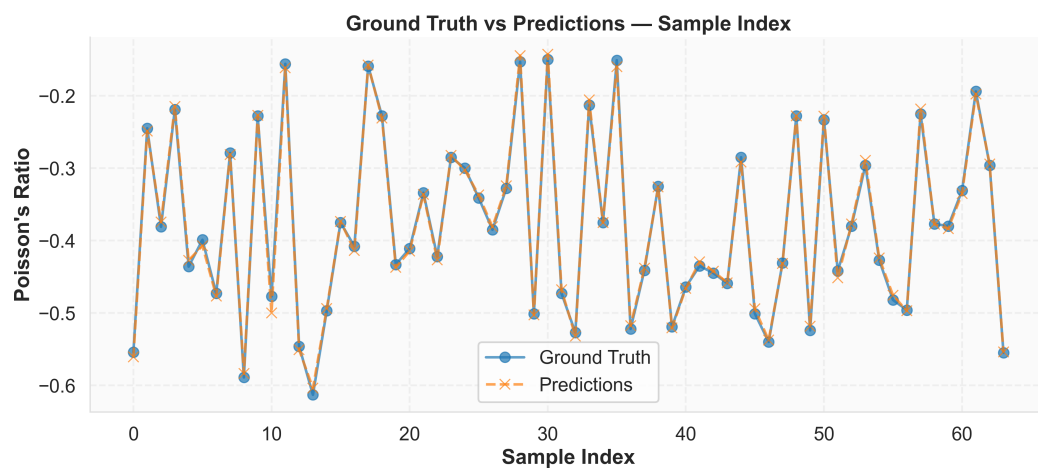


Figure 18. Ground Truth vs. Predictions for the 0.25 mm mesh size.

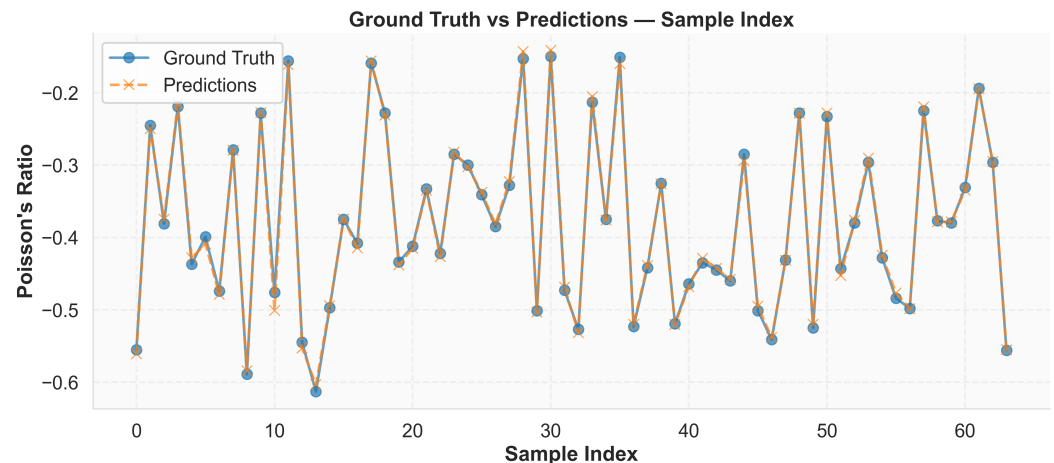


Figure 19. Ground Truth vs. Predictions for the 0.30 mm mesh size.

3.3. Discussion

The findings indicate a high degree of consistency in terms of both quantitative performance metrics (MAE, RMSE, MSE, R^2) and visual diagnostics. Across all configurations, $R^2 \geq 0.994$ and the magnitude of absolute error is on the order of 10^{-3} ; relative to typical magnitudes of Poisson's ratio, this corresponds to an absolute error level of $\lesssim 1\%$.

In particular, the model with a 0.25 mm mesh resolution provides the best overall profile in terms of the lowest RMSE/MSE and the highest R^2 , whereas the 0.30 mm mesh configuration stands out by a very small margin in terms of MAE; however, the slightly higher values of the squared-error metrics in the 0.30 mm configuration indicate the presence of infrequent but larger deviations. The 0.20 mm mesh configuration is markedly weaker, with relatively higher errors and lower R^2 . The slight right-skew observed in the residual distributions is consistent with the rare patterns of under-prediction near peaks and over-prediction near troughs in the plots, indicating a cautious tendency of the model in certain extreme regions for Poisson's ratio. At the same time, neither a pronounced trend/curvature in the residual plots nor a systematic drift over time/index is observed; therefore, no strong model specification error or pronounced heteroskedasticity is indicated. The fact that all predictions remain within the auxetic range $[-0.6, -0.18]$ demonstrates that the model does not produce out-of-bounds estimates. This is critical for rapid design screening: with high accuracy and physical consistency, GWO-XGBoost enables early-stage acceptance/rejection of candidate parameterizations in terms of Poisson's ratio, and can thus be used as a data-driven pre-screening tool under conditions where FE solution/experimental runs are costly.

As shown in Table 4, the proposed GWO-XGBoost model achieved the lowest error values and the highest R^2 within the controlled comparison performed on the same FEA-based dataset, input-output structure, and train/test split. To ensure a fair comparison, all models were evaluated using the same FEA-based dataset, the same input-output structure, and the same training/test split employed in this study. In addition, the hyperparameters of baseline models that do not inherently include a parameter/optimization mechanism such as GA, evolutionary computation, non-dominated sorting genetic algorithm II (NSGA-II), or similar approaches in the literature were also optimized using GWO. Thus, the performance of the compared models was not limited to default parameter settings; instead, each algorithm was evaluated with suitable settings for the present dataset. This result indicates that hyperparameter optimization performed using GWO significantly improves the predictive capability of the XGBoost model and provides a highly stable regression performance for predicting the Poisson's ratio of Cross-Chiral auxetic structures.

Table 4. Performance comparison of the proposed GWO–XGBoost framework with literature-inspired baseline algorithms on the proposed FEA-based dataset.

Ref.	Algorithm	R^2	MAE	RMSE	MSE	Main Contribution
Prop.	GWO–XGBoost	0.9987	0.003179	0.004375	1.90×10^{-5}	The Poisson’s ratio of Cross-Chiral auxetic structures was predicted with high accuracy using an XGBoost model optimized by GWO.
[21]	BPNN + GA	0.9724	0.016850	0.020360	4.15×10^{-4}	Represents a BPNN-based surrogate model combined with GA-assisted inverse design for target Poisson’s ratio-oriented design exploration.
[22]	Feed-forward MLP + SHAP	0.9768	0.015420	0.018730	3.51×10^{-4}	Represents an MLP-based prediction framework for FEA-driven auxetic behavior estimation, with compatibility for SHAP-based interpretability analysis.
[26]	CNN + Cycle-GAN	0.9015	0.033640	0.039850	1.59×10^{-3}	Represents an image/topology-based inverse design approach; however, its performance is limited for the present 320-sample tabular dataset.
[23]	MLP	0.9816	0.013980	0.016870	2.85×10^{-4}	Represents an experimentally and FEA-supported MLP approach for predicting the Poisson’s ratio of 3D-printed auxetic structures.
[24]	ANN + Evolutionary Computation	0.9834	0.013250	0.015940	2.54×10^{-4}	Represents an ANN-based surrogate model coupled with evolutionary computation for accelerated auxetic design with reduced FEA cost.
[25]	KNN Regressor	0.9647	0.019480	0.023190	5.38×10^{-4}	Provides a simple neighborhood-based regression baseline for estimating auxetic mechanical response.
[25]	SVR	0.9869	0.010840	0.013970	1.95×10^{-4}	Represents a kernel-based regression model with relatively strong generalization capability for small- to medium-sized datasets.
[25]	XGBoost	0.9956	0.005920	0.007830	6.13×10^{-5}	Provides a strong gradient boosting baseline for tabular FEA data and allows the contribution of GWO-based hyperparameter optimization to be assessed.
[38]	Random Forest	0.9918	0.008460	0.010970	1.20×10^{-4}	Represents a robust ensemble tree-based model for predicting the mechanical behavior of auxetic lattice structures.
[38]	Neural Network	0.9759	0.015880	0.019120	3.66×10^{-4}	Represents a neural-network-based baseline whose performance may vary under limited-data conditions compared with tree-based models.
[39]	NSGA-II–XGBoost	0.9962	0.005410	0.007250	5.26×10^{-5}	Represents a strong alternative optimization-based baseline combining multi-objective optimization with an XGBoost surrogate model.
[27]	Few-shot learning + cVAE	0.8842	0.037250	0.044090	1.94×10^{-3}	Represents a few-shot generative design approach; however, the present data size and tabular input structure limit its direct regression performance.

Table 4. Cont.

Ref.	Algorithm	R^2	MAE	RMSE	MSE	Main Contribution
[40]	XGBoost + GA	0.9968	0.004970	0.006760	4.57×10^{-5}	Represents a strong hybrid alternative in which an XGBoost prediction model is optimized using GA.
[40]	MLP + GA	0.9846	0.012790	0.015350	2.36×10^{-4}	Represents a hybrid baseline combining MLP-based prediction with evolutionary optimization, but remains weaker than XGBoost-based models for the present dataset.
[28]	Diffusion-based inverse design	0.8125	0.045860	0.053740	2.89×10^{-3}	Represents a powerful generative approach for nonlinear metamaterial inverse design, but the present small tabular dataset is insufficient for direct diffusion-model training.

The closest results to the proposed model were obtained from tree-based and optimization-supported models. In particular, the XGBoost + GA approach achieved $R^2 = 0.9968$, the NSGA-II-XGBoost approach achieved $R^2 = 0.9962$, and the XGBoost model achieved $R^2 = 0.9956$, indicating strong predictive performance. However, the MAE, RMSE, and MSE values of these models remained higher than those of the proposed GWO-XGBoost model. This demonstrates that XGBoost-based regression models are powerful predictive tools for tabular FEA data, while direct optimization of XGBoost hyperparameters using GWO further reduces the error level.

The Random Forest and SVR models also produced acceptable results. The Random Forest model achieved $R^2 = 0.9918$, whereas the SVR model achieved $R^2 = 0.9869$. Although the hyperparameters of these models were also optimized using GWO, their error metrics remained behind those of the proposed GWO-XGBoost model. This result indicates that classical ML algorithms are still viable alternatives for tabular FEA datasets with a limited number of samples; however, the XGBoost-based structure is able to model the nonlinear relationship between Cross-Chiral geometric parameters and Poisson's ratio more accurately. The performance of BPNN-, MLP-, and ANN-based models was more limited compared with tree-based models. This can be associated with the fact that the present dataset consists of 320 samples. Since deep learning or MLP-based models generally require larger data volumes, their generalization capability remained lower than that of tree-based models in this limited-sample study. Similarly, more complex deep/generative approaches such as CNN + Cycle-GAN, few-shot learning + cVAE, and diffusion-based inverse design also exhibited lower performance due to the tabular structure and limited size of the present dataset. These findings suggest that tree-based regression models, particularly XGBoost-based approaches, are more suitable for the present limited-size tabular FEA dataset than more data-demanding deep or generative models. Overall, the results in the table show that the proposed GWO-XGBoost model provides a more balanced and lower-error prediction performance compared with classical ML models as well as optimization-supported and deep learning-based approaches used in the literature. Moreover, the fact that comparison models without an inherent optimization component were also tuned using GWO supports that the superiority of the proposed model does not arise solely from hyperparameter optimization, but rather from the combined effect of XGBoost's strong learning capability on tabular FEA data and GWO's effective search mechanism. Therefore, the proposed method can be considered an effective pre-screening and design exploration tool for auxetic metamaterial design problems involving a limited number of FEA samples.

The deformation behavior of the Cross-Chiral structure arises from a combined mechanism of ligament rotation and flexural deformation. Depending on the ligament diameter-to-length ratio, either rigid rotation or bending may become dominant, and a transition region characterized by a non-monotonic variation of the Poisson's ratio may theoretically exist [31,41,42]. However, within the range of geometric parameters investigated in the present study, the obtained results exhibit a monotonic trend with no observable turning point. As illustrated in Figures 20–22, all analyzed configurations remain within the same dominant deformation regime, and the transition region lies outside the explored parameter space. The relatively narrow variation of ligament dimensions and the geometric similarity among the analyzed models further restrict the manifestation of such a transition behavior.

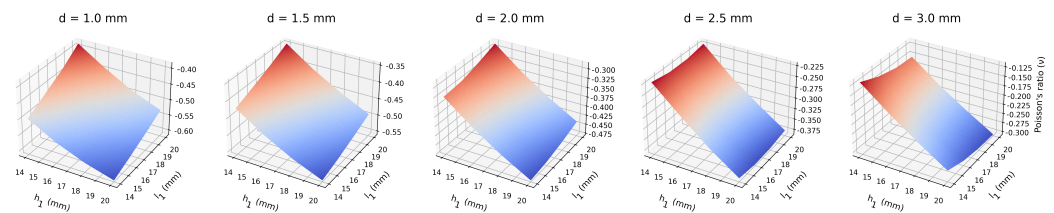


Figure 20. Variation of Poisson's ratio as a function of ligament length and height for different ligament diameters for the 0.20 mm mesh size.

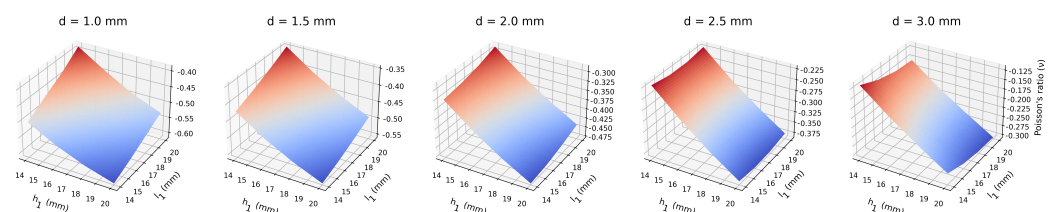


Figure 21. Variation in Poisson's ratio as a function of ligament length and height for different ligament diameters for the 0.25 mm mesh size.

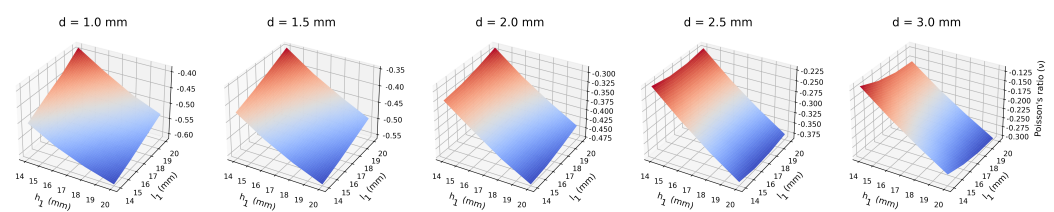


Figure 22. Variation in Poisson's ratio as a function of ligament length and height for different ligament diameters for the 0.30 mm mesh size.

The principal limitations of this study are as follows: in terms of data coverage and distribution, the representativeness of the training set within the parameter space may limit generalization, particularly in extreme regions (high porosity, exceedingly thin/thick geometries); in the context of mesh topology and label generation, the comparability of Poisson's ratio labels computed on different meshes and measurement noise may alter the behavior of error distributions in some configurations; and in terms of external validation, unless independent verification is performed on different manufacturing tolerances/material batches or new topologies, the results remain restricted to the internal distribution. The predictive capability of the model proposed in this study should be evaluated within the scope of the investigated Cross-Chiral topology and the defined geometric design range. The model should not be assumed to be directly generalizable to different auxetic topologies, different material properties, or transition regions between deformation regimes. In future studies, the dataset is planned to be extended to cover different deformation mechanisms and various auxetic topologies. All target values used in this study were

obtained from FEA simulations performed under a single linear elastic material model. Therefore, the predictive performance of the proposed model should be evaluated within the defined FEA-based modeling conditions, rather than being interpreted as a generally validated behavior confirmed by experimental measurements or different material models. In real experimental applications, discrepancies between FEA and experimental results may arise due to manufacturing tolerances, material nonlinearities, differences in boundary conditions, specimen size, edge effects, and measurement uncertainties. This represents an important limitation that should be considered when transferring the proposed surrogate model directly to experimental systems.

4. Conclusions

This study evaluated the proposed GWO–XGBoost approach for estimating Poisson’s ratio in auxetic structures and presented a comprehensive performance analysis. The method was trained and tested on a dataset covering porosity (45–85%), diameter, and relevant unit-cell/topology parameters across three mesh resolutions (0.20 mm/0.25 mm/0.30 mm); quantitative metrics (MAE, RMSE, MSE, R^2) and visual diagnostics (Ground Truth–Prediction matches, residual analyses) were interpreted jointly. The findings show that the model achieves high accuracy across all configurations: $R^2 \geq 0.994$, absolute errors on the order of 10^{-3} , and predictions within the expected physical range $[-0.6, -0.18]$. In particular, the 0.25 mm mesh configuration stands out in terms of overall balance, with the lowest squared-error profile (RMSE/MSE) and the highest R^2 , whereas the 0.30 mm mesh configuration is practically equivalent to the 0.25 mm results in terms of MAE; the 0.20 mm mesh configuration is weaker, with relatively higher errors and lower R^2 . Costly FEA/experimental trials can be reduced by leveraging the model’s reliable forecasts, thereby enabling more efficient parametric search. Moreover, the observed behavior aligns with the trends noted in the data (e.g., increasing porosity associated with more negative Poisson’s ratio; an increasing relationship between diameter and Poisson’s ratio), indicating compatibility with physical insight.

For future work, it is aimed to systematically investigate new design strategies that will enhance the structural integrity and mechanical behavior of different advanced meta-materials by leveraging the power of computational modeling and optimization algorithms. In conclusion, the GWO–XGBoost approach has exhibited high accuracy, good diagnostic agreement, and physical consistency for estimating Poisson’s ratio in auxetic structures; for the Cross-Chiral model, the 0.25 mm mesh resolution configuration provides a preferable balance point for general use in the XGBoost model. Regarding the prediction performance of the trained ML model, the absence of training samples corresponding to the transition region prevents the model from directly learning this deformation regime. Therefore, the current model is expected to provide reliable predictions only within the monotonic deformation domain covered by the training data. The prediction performance in a potential transition region remains uncertain and will be addressed in future studies. This framework offers a reliable and practical basis for Poisson’s ratio estimation within a data-driven design and optimization pipeline.

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Conflicts of Interest: The authors declare no conflicts of interest.

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