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Free-form Grid Structure Form Finding based on Machine Learning and Multi-objective Optimisation

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Abstract (250 words)

Free-form structural designs are reshaping modern architecture with their expressive aesthetics and novel spatial configurations. However, their digital transformation still encounters obstacles, particularly in aligning fluid geometries with rigorous structural requirements, and in assembling high-quality datasets suitable for advanced machine learning (ML) methods. Traditional form-finding approaches often neglect critical factors—such as material behavior, load paths, and construction logistics—resulting in discrepancies between conceptual 3D models and built outcomes. To overcome these challenges, this paper presents a novel pipeline that integrates ML with multi-objective evolutionary optimisation, using glued laminated timber (GLT) as a case study. Central to our method is a Transformer-based neural network that harnesses NURBS representations of 3D geometry, creating a structured dataset for curvature prediction. These ML-generated forms are then refined through an evolutionary optimisation process targeting minimal structural mass, stress, and strain energy. Experimental results show notable improvements in design performance, with reductions in mass (3.6%), stress (up to 15%), and strain energy (68% under mesh load). This synergy of ML-driven geometry and robust optimisation significantly advances digital construction practices by fostering a data-driven, automated workflow for complex free-form design. Practical implications extend across the building and infrastructure sectors, enabling better alignment between conceptual design and final construction, lowering material consumption, and mitigating deviations during fabrication. By coupling aesthetic exploration with structural rigour, the framework underlines a crucial step toward more sustainable, efficient, and constructible free-form structures.

Keywords: Free-form structure; Form-finding; Machine Learning; Multi-objective optimization; Material rationality

Highlights

- ML and optimisation enhance free-form design rationality, ensuring constructability in digital construction.
- Transformer-based NURBS prediction bridges aesthetic design with structural performance.
- Data-driven design fosters sustainability and precision in free-form timber construction.

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1 Section 1- Introduction

As the regular architecture form could not meet the up-to-date aesthetic requirements, the distinct architectural expression and engineering challenges of free-form grid structures place them at the forefront of spatial design innovation (Pottmann, Schiftner, and Wallner 2008). While aesthetically appealing, the inherent complexity of these designs presents significant challenges for traditional workflows. The irregular forms introduce new obstacles for conventional design paradigms, affecting everything from design methods to design tools. These structures defy traditional modelling with complex surfaces that cannot be succinctly expressed through simple analytic functions, departing from conventional architectural forms. Current form-finding methods often overlook critical constraints, such as material properties, fabrication tolerances, and construction logistics, leading to costly adjustments later in the process (Gramazio and Kohler 2014). Historically, the genesis of such structures relied heavily on physical experimentation methods, such as the inverse hanging method for compression structures and the soap film technique for pre-stressed shapes (Bletzinger and Ramm 2001; Otto and Rasch 1995). With the rise of digital transformation in the construction industry, there is an urgent need to develop intelligent, data-driven tools capable of handling this complexity efficiently and ensuring that free-form designs are both rational and constructible from the outset. The emergence of computational graphics technologies, notably Bezier surfaces, B-splines, and Non-Uniform Rational B-splines (NURBS), has revolutionised the field of complex geometry design and optimisation (Ghasemi et al. 2015; Vukašinović and Duhovnik 2019).

To achieve the complex form, some new criteria need to be met compared with traditional regular architectural design, such as smoothness and geometric dimensions (Pottmann et al. 2015). In addition, the deviation of the real project from the original design needs to be decreased if considering constraints like material, structural stiffness and manufacturing, which means that additional knowledge about geometry is essential in the optimum design (Wallner and Pottmann 2011). Existing approaches often fall short in integrating material properties and construction constraints into the design process, particularly in the early stages where decisions have the most significant impact on project outcomes. Traditional design and optimization approaches often fall short in addressing these complex requirements, spotlighting the necessity for sophisticated optimization techniques capable of untangling the complexities of free-form structure (Marano, Quaranta, and Greco 2009). The demand for new design techniques has led to the adoption and development of diverse computational methods and algorithms. Among these new techniques, optimisation algorithms (Xia et al. 2006) stand out due to their efficacy in addressing the multifaceted challenges inherent in the design and realisation of optimised structures. Related studies have shown that optimisation for structural performance effectively generates free-form structures with stable mechanical behaviour (Shimoda et al. 2016). Different algorithms have been applied and developed to the topology and shape optimisation (Çarbaş and Saka 2012), for example, gradient descent (Le, Bruns, and Tortorelli 2011), GA (Genetic Algorithm) (Goldberg 1989), evolution algorithm (Wang et al. 2021) and NGSA-II algorithm (Ma et al. 2019). Among the different algorithms, the optimisation objectives are various, including maximum displacement, element stress, overall quality of the structure, and strain energy (Ohmori, Kimura, and Maene 2009) by setting the coordinate of control points as the variable. However, in these multi-objective optimisation processes, the efficiency of the existing algorithm is not high, and the optimal results have low similarity to the initial surface before the optimisation (Wang et al. 2021).

Under the context of calling for new technologies for rational free-form structures, machine learning (ML) has also shown its potential to generate free-form structures based on its data processing

capability (Huang, Kalogerakis, and Marlin 2015). ML is a new ground-breaking technique that has been widely used in computer vision, image processes, natural language processes, and generative tasks (Shinde and Shah 2018). In (Aksöz and Preisinger 2020), augmenting finite element analysis for optimizing space frame structures, aiming to reduce computation times significantly through ML has been discussed. Based on the learning and analysis of the data from the collected data (e.g. images, graphics), ML can generate new data of the same type through deep neural networks (DNNs) (Larochelle et al. 2009) and generative adversarial networks (GAN) (Goodfellow et al. 2014) in generative floor plans (Huang and Zheng 2018). Other ML networks like long short-term memory (LSTM) can be applied to dealing with graphical information (Xie and Wen 2019). Since the complex geometric information of the free-form morphology cannot be fully represented through graphics or images, the 2D application of these ML methods is one main limitation.

Despite advances in ML form-finding and multi-objective optimisation, studies still treat geometry generation and structural tuning separately. None exploit sequential NURBS data while embedding GLT's orthotropic limits, leaving design-to-fabrication gaps. This paper unifies Transformer-based curvature prediction with evolutionary optimisation to produce constructible, performance-driven free-form timber grids.

In this study, ML is utilised to generate rational geometric information for free-form morphology, considering the constraints from material properties by taking timber as the building material. Based on the predicted geometric information, the free-form morphology is further optimised for structural performance through evolution algorithms.

2 Machine Learning Prediction for Material Rationality

Quantifying the impact of building material properties on free-form morphology is challenging. The primary approach to using ML to predict the geometric information of free-form morphology involves using real free-form grid structures as the learning input. This input encompasses data about the extent to which building materials can be shaped. After training, ML can predict new curves based on the range of achievable shapes, as learned from previous cases of free-form structures. One significant advantage of using ML for prediction is its ability to integrate the design with material considerations effectively.

2.1 Description for Free-form Morphology

The mathematical model serves as a superior approximation method due to its high efficiency and accuracy. Among the various mathematical models, B-splines and NURBS are the most commonly utilized. Based on the rational B-spline, NURBS is developed by adding an extra parameter called weights. NURBS offers greater flexibility and adaptability across diverse geometric types than B-splines. A p times NURBS curve is defined as:

$$C(U) = \frac{\sum_{i=0}^n N_{i,p}(u) \omega_i P_i}{\sum_{i=0}^n N_{i,p}(u) \omega_i}, a \leq u \leq b \quad (1)$$

where $C(u)$ is the coordinate of a random point on the NURBS curve in x-y-z space, $\{P_i\}$ is the control point, $N_{i,p}(u)$, $i = 0, 1, \dots, n$ is the i th p times B-spline base function, which is called B-spline. $\{\omega_i\}$ is the weight factor. The coordinate of a random point on the NURBS surface can be expressed in the below formulation:

$$S(u, v) = \frac{\sum_{i=0}^m \sum_{j=0}^n N_{i,p}(u) N_{j,q}(v) \omega_{i,j} P_{i,j}}{\sum_{i=0}^m \sum_{j=0}^n N_{i,p}(u) N_{j,q}(v) \omega_{i,j}}, a \leq u \leq b; c \leq v \leq d \quad (2)$$

where u, v are the parameters of the surface; p, q are the number of powers of the surface; the surface is the segmentation functions about u, v ; knot vectors U, V are combined by knots u, v . For curved surfaces, $\{P_{(i,j)}\}$ forms a control grid in two directions and the number of control points is $(n + 1) \times (m + 1)$; $N_{i,p}(u)$ and $N_{i,q}(v)$ are base functions of u and v directions; $\{\omega_{(i,j)}\}$ is the weight factor.

2.2 Learning Prediction Experiment

Selecting the appropriate ML method for prediction tasks is crucial as it determines the types of data used for training and testing. In (Meng, Sun, and Chang 2022), the free-form structure is depicted through curves, which are then transformed into sequential datasets. Building on this method of information transformation, the Transformer model is chosen for handling the transformed sequential data in this study. Originally designed for natural language processing (Lin et al. 2022), Transformers have been successfully adapted for various sequence modelling tasks across spatial domains (Zhu et al. 2021). Their self-attention mechanism provides a sophisticated means to model relationships between different points along a curve, effectively capturing both local and global dependencies.

To complete the prediction learning task, choosing the appropriate free-form case is critical. For this ML process, the Centre Pompidou-Metz Model is utilized as a case study to extract data for the Transformer. The structural design of the Centre Pompidou-Metz features a weave pattern, constructed from glue-laminated timber, making it an excellent source of learning input shown in Figure 1.

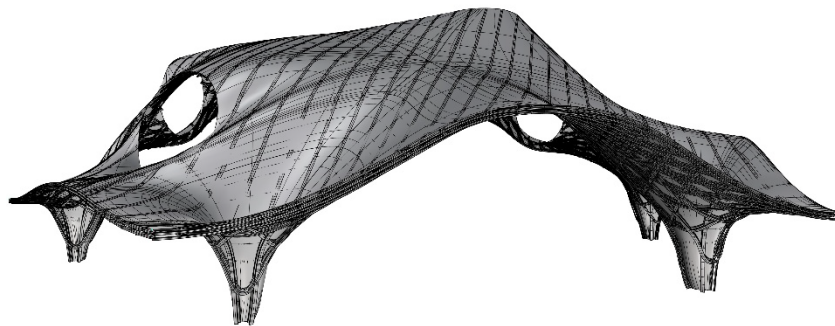


Figure 1 3D model of the Centre Pompidou-Metz case

2.2.1 Data Transformation

The main difficulty for ML prediction application in free-form structural morphology is the extraction of the information, as most of the ML deals with the data in 1 or 2 dimensions. In this model, all timber beams and columns are curved to create a distinctive free-form shape. An essential step following the 3D modelling process is to extract geometric information and convert it into discrete numerical values to serve as inputs for ML. Each beam or column in this model is characterised by six faces and 12 boundary lines, which include four critical curves that define the geometry necessary to generate this unique curved structure. The data transformation process is presented in Figure 2.

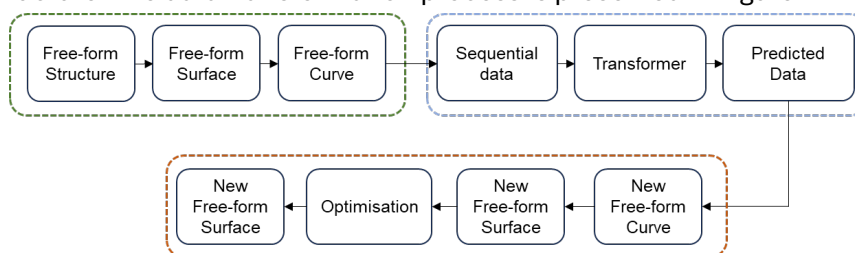


Figure 2 Data extraction and transformation process

2.2.2 Training and Learning

After establishing the dataset format, identifying the relevant features and the desired outputs is crucial for the prediction task. In this study, geometric information representing the free-form NURBS curve is extracted, including x-coordinate, y-coordinate, z-coordinate, position parameter, curvature, vector_x, vector_y, and vector_z. The features used to predict the curvature, vector_x, vector_y, and vector_z are the x-coordinate, y-coordinate, z-coordinate, and position parameters. For the pilot test, 16 curves are selected, each divided into 20 segments, resulting in 336 point samples. To enhance the dataset, K-fold validation is adopted, creating five folds with sample sizes of 3, 3, 3, 3, and 4, respectively. Following dataset preparation, the subsequent steps using the Transformer model include:

After preparing the dataset, the following steps of using Transformer are as follows:

- Positional encoding: This allows the model to recognize the position of each point in the sequence, crucial for maintaining the order of data in sequence processing;
- Transformer encoder layer: This layer, which can be stacked, forms the encoder part of the Transformer, essential for processing the sequence data;
- Modify the Transformer model: Adaptations are made so the model can take sequences of curve data as input and predict the desired geometric outputs;
- Train the model: The model is trained with a batch size of 32 and over 100 epochs to ensure adequate learning.
- Evaluation of the model: Performance is assessed on a test set to gauge the effectiveness of the model under evaluation conditions;
- Fine-tuning and Optimisation: Depending on initial results, adjustments are made to the model's architecture, training parameters, and learning rate to optimize performance.

3 Multi-objective Optimisation for Free-Form Morphology

Based on the tuned Transformer model, given the x-coordinate, y-coordinate, z-coordinate, and position parameter of the points, the NURBS curves meet the restrictions of the GLT and can be interpolated through curvature, vector_x, vector_y, and vector_z. In this case, three curves are selected to patch the free-form prototype surface in Figure 3 (a), which is arrayed to generate the surface shown in Figure 3 (b).

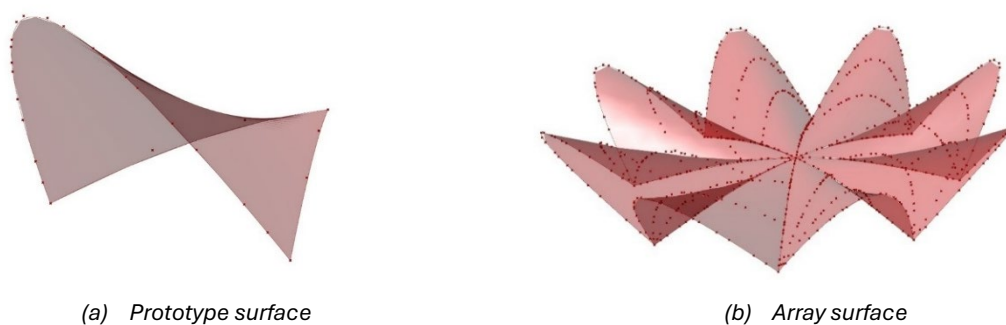


Figure 3 Example surface

3.1 Strain Energy for Structural Rationality

The optimisation method and objectives for structural mechanical rationality have a direct impact on the outcome of the morphology. The optimal objective is commonly set as displacement, stress, strain energy and others, and displacement and stress are vectors that reflect the structure's local characteristics, whereas strain energy is scalar.

The determination of the interrelationships between mechanical properties is a critical issue to address during the morphology creation process. The structural balance equation is:

$$F = K \cdot \delta \quad (3)$$

F – Force vector of structure nodes

K – Structural stiffness matrix

δ – Displacement vector of the structure

When the structure is subjected to small elastic deformation, the strain energy U is expressed as:

$$U = \frac{1}{2} F^T \delta \quad (4)$$

Eq (4) deduces the relationship between strain energy and structure internal force. Research has demonstrated that when strain energy is selected as the objective function, as the strain energy of the structure decreases, not only does the stiffness of the structure increase, but the bending moments are greatly reduced, increasing the ultimate load capacity. Assuming that the load is constant, the structure's strain energy is proportional to the displacement of the structural nodes; that is, decreasing the displacement results in decreasing the strain energy. The smallest strain energy, smallest structural displacement, and largest structural rigidity are all mutually unified.

The strain energy is a scalar, and its value can be thought of as the sum of the strain energies of all the elements in the structure. Besides, the strain energy is unrelated to the selected coordinate system. In the global coordinate system, the strain energy equals the strain energy in the local coordinate system. In complex structure systems, the finite element method is commonly used to divide the structure into several elements when calculating them.

$$U = \sum_{i=1}^N \bar{u}_i \quad (5)$$

Where \bar{u}_i is strain energy of every element, N is total number of the elements in the structure

3.2 Multi-objective Optimisation for Free-form Morphology

To conduct multi-objective optimisation for free-form surface in Figure 3, the optimal model can be expressed as a nonlinear function on multidimensional space formed by vector P :

$$\min \begin{cases} U(P) \\ Mass \\ \sigma \end{cases} \quad (6)$$

Finding the minimum of $U(P)$ can be seen as solving the extreme value problem for nonlinear multivariate functions. The solution to the extreme value problem can be achieved by a one-dimensional search, which means the direction of descent of the objective function $U(P)$, which is used to adjust the optimisation variables P to gradually converge to the optimal solution.

In the given free-form surface, the three curves are divided into 4 control points and 22 control points, respectively. The optimisation variables are chosen as the z-coordinate of the two control points of the two side curves and the weights of the 11th and 12th control points, and the optimal results are shown in Figure 4. The optimal value for the mass remained within a narrow range, indicating a consistent reduction of about 3.6% from the original value. The curve's trend, displaying convergence in oscillation, underscores the effectiveness of the multi-objective optimization process. The optimal stress value achieved was 0.005, marking a substantial decrease from the original value of 0.013. The results fluctuated within a range of 0.005 to 0.011, with a minimum reduction of 15%. While the reduction in strain energy under gravity load—from 0.02 to 0.018—was modest, the results for the mesh load were

more dramatic, with a decrease from nearly 3.5 to 1.1, corresponding to a 68% reduction. The visualised optimised results and comparisons of the initial, and 60th steps are compared in Figure 5 and Figure 6.

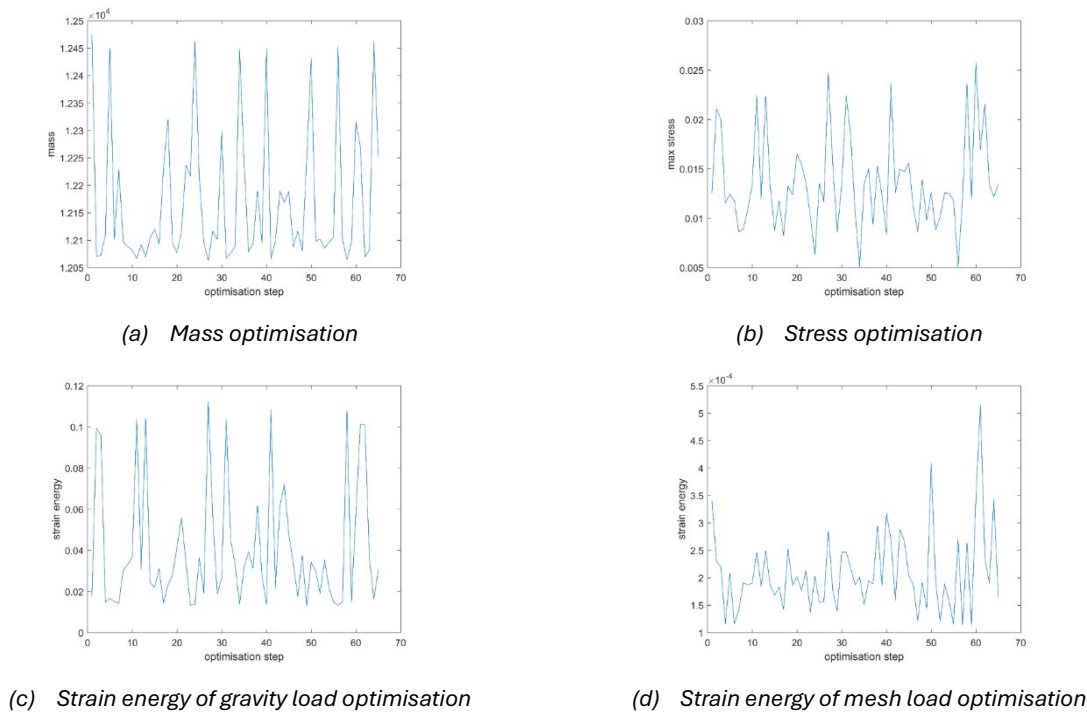


Figure 4 Optimisation results

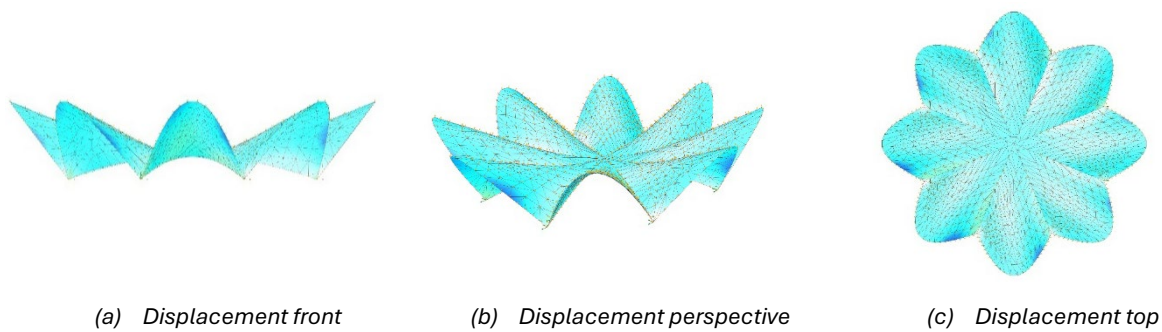


Figure 5 Displacement of original morphology

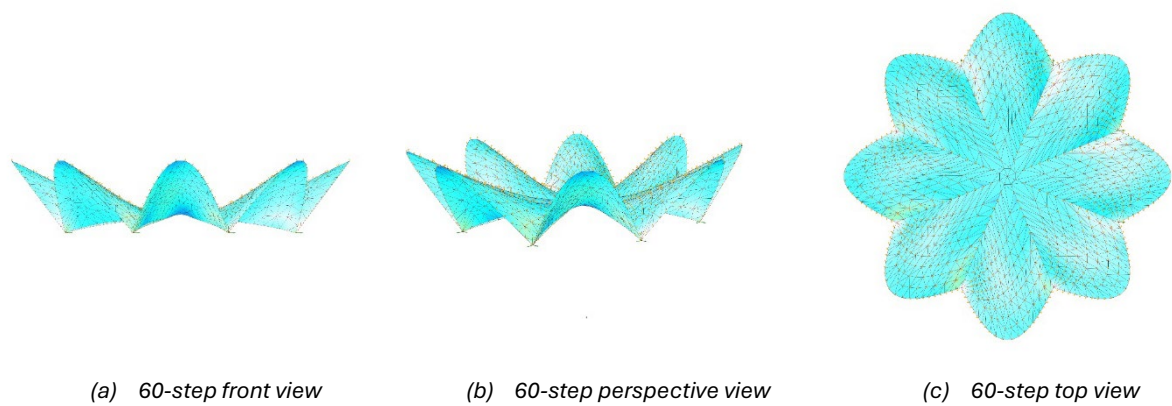


Figure 6 Displacement after 60-step evolution

4 Discussion

The Transformer model has demonstrated exceptional effectiveness in handling the complexities inherent in free-form designs. Its capacity to process sequential 3D geometric data enables accurate predictions of structural forms, showcasing its potential beyond traditional natural language processing tasks and extending its utility to spatial and geometric data analysis. Despite some variation between predicted and actual values, this does not significantly detract from the Transformer's utility in predictive tasks. These discrepancies are largely due to the inherent complexities of free-form structures and the challenges in capturing the nuances of three-dimensional geometry through machine learning.

The integration of evolutionary algorithms was pivotal in refining the Transformer-generated designs to meet specific structure performance criteria. Significant improvements were observed in multi-objective optimization concerning mass, stress, and strain energy, validating the multifaceted capabilities of these algorithms. The evolutionary approach effectively enhanced the exploration and exploitation phases of the optimization process, leading to more efficient and robust design solutions. Beyond technical validation, the findings carry meaningful implications for architectural and construction practice. The proposed framework offers a scalable tool for early-stage design automation of free-form timber structures, helping architects and engineers reduce costly design iterations. By minimizing mass and improving structural efficiency, it contributes to sustainable building practices. The ability to align ML-driven form-finding with material and fabrication constraints supports more precise, constructible outcomes—particularly valuable for digital fabrication and robotic timber assembly workflows.

However, this research faces several notable limitations that could influence the applicability and effectiveness of the proposed methodologies in various free-form structure scenarios. Firstly, the quality and quantity of data are crucial for training the machine learning models, and any inadequacies in this regard can significantly impair model accuracy. Ensuring a comprehensive and high-quality dataset is paramount for achieving reliable predictions and robust optimization results.

Furthermore, the generalizability of the model when applied to structures or materials different from those used in this study is a concern. Adapting the model to accommodate larger or more intricate designs necessitates complex modifications, which may pose challenges in terms of computational resources and the need for tailored adjustments. This highlights the importance of further research into developing more adaptable and scalable models that can handle a broader range of free-form structure designs without compromising performance.

5 Conclusions

This study represents a significant advancement in the field of architectural design by integrating machine learning and evolutionary algorithms to generate and optimise free-form morphology. This approach successfully addresses the dual challenges of adhering to building material limitations and enhancing structural stiffness, which are critical in the construction of viable and sustainable architectural structures. By extracting geometric information from free-form surfaces and translating these into sequential data, the use of advanced machine learning techniques is facilitated, specifically the Transformer model, to predict and optimise structural forms. This approach not only streamlines the initial stages of design but also ensures that the final forms are both feasible and structurally rational. Despite some deviations from the actual values, the Transformer's predictive outputs are promising. The model has effectively demonstrated its applicability to geometric form prediction in the

context of free-form surface analysis, marking a significant step forward in the intersection of machine learning and architectural design. This research contributes to the digital transformation of architectural design by providing a data-driven, automated workflow for generating and optimizing free-form structures. By bridging the gap between aesthetic design and practical construction constraints, our methodology offers a scalable framework for the design of complex geometries, ensuring that the final structures are not only visually compelling but also structurally efficient and constructible. The integration of ML and optimization in this work represents a significant step forward in the field of digital construction, paving the way for more sustainable and innovative architectural solutions. Still, there are limitations in the application of the methodology. The primary constraint is the reliance on the precision of 3D geometric models as learning inputs, which may not capture the full complexity of real construction projects. Further research is needed to expand the capabilities of the algorithms used, incorporating more dynamic and real-time data inputs involving variations in material properties, construction tolerances, and environmental impacts. The oscillatory convergence patterns of the multi-objective evolutionary optimisation suggest that the stability of the algorithms could be further improved to ensure smoother progression towards the optimum.

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Data Availability Statement

Data could be requested from the authors.

Conflicts of Interest

The authors declare no conflict of interest.

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