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Inverse machine learning framework for optimizing lightweight metamaterials

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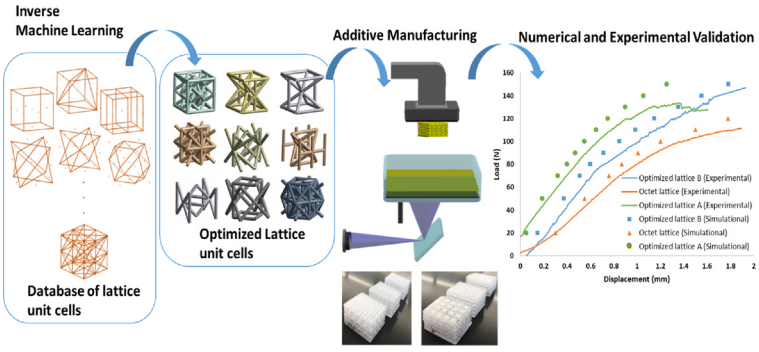
HIGHLIGHTS

- New inverse design ML framework for the optimization of lattice unit cells is proposed.
- Along with optimal lattice unit cells, desired mechanical properties can be obtained.
- compression strength of the new unit cells shows 40–120% better than octet unit cell.
- The lattice cored sandwiches show excellent mechanical properties.
- This framework can be applied to optimize other load bearing structures.

GRAPHICAL ABSTRACT

The pipeline of the inverse design framework.



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ABSTRACT

Structure scouting and design optimization for superior mechanical performance through inverse machine learning is an emerging area of interest. Inverse machine learning can be a substantial approach in structural design to explore complex and massive numbers of geometrical patterns within short periods of time. Here, an inverse design framework using generative adversarial networks (GANs) is proposed to explore and optimize structural designs such as lightweight lattice unit cells. Lightweight lattice structures are widely accepted to have excellent mechanical properties and have found applications in various engineering structures. Using the proposed framework, different lattice unit cells that are 40–120% better in load carrying capacity than octet unit cell are discovered. These new lattice unit cells are analyzed numerically and validated experimentally by testing 3D printed lattice unit cells and lattice cored sandwiches. The proposed inverse design framework can be applied to the design and optimization of other types of load bearing structures.

1. Introduction

Machine learning is being widely used in various engineering applications such as discovery of new polymers, chemicals, and structures. [1–5] Forward regression and classification in machine learning are implemented in material, medical, chemical, and structural engineering, which surpass highly expensive and time-consuming simulations and experimental validations. Machine

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learning algorithms such as Convolutional Neural Network (CNN) has been used to discover new thermoset shape memory polymers with high recovery stress. [4] Kernel Ridge Regression (KRR) has been used in the property predictions of polymers to handle nonlinear relations and to establish a material design protocol that accelerates the discovery of new polymers. [6] Gaussian Process Regression (GPR) has been studied, indicating that it is more suitable for predicting a better uncertain/confidence interval of polymers and their properties. [7] The mechanical properties of cement are predicted by using Support Vector Machines (SVM) which are found to be very effective in real value function estimation. [8,9] Several other machine learning techniques like Decision Trees, K-nearest Neighbors, and Gradient Boosting Algorithms have been proven to be effective in predicting structural properties with great accuracy. [10] Stress distributions in the aortic wall based on finite element analysis (FEA) results with an average discrepancy of 0.492% are estimated using neural networks. [11] The longitudinal and transverse elastic modulus and shear modulus of carbon fibers are predicted by using the data generated from finite element modeling. [12] Support Vector Regression models are used to propose direct relationship between the input and output of the elements. This avoids the complex numerical iterations involved in finding the internal displacement field. [13]

In our previous studies, we demonstrated the advantage of applying machine learning techniques to predict the structural properties and propose novel biomimetic rods with better buckling resistance and optimal lattice unit cells than their nature counterparts. [5] We proposed optimal rods inspired from their biological counterparts based on plant stems and animal quills. Forward machine learning was used to extract hidden features in the biomimetic rods and expedite the computation process. [5] In a similar manner, we proposed symmetric optimal lattice unit cells. Using a forward machine learning model, we predicted the structural properties of a huge data set of lattice unit cells whose properties were unknown. Later, this data set was filtered to select optimal lattice unit cells. Although, through this forward machine learning technique, superior rods and lattice unit cells were discovered, there are certain limitations. The data filtering process is semi-optimal and it is cumbersome to filter huge output datasets. The procedure followed for fetching the optimized designs in the data filtering process is similar to hard coding and involves a great deal of manual efforts. This is time consuming and also it is observed that, especially with huge data sets that contain millions of data points, some of the optimal designs may be missed out. Through this forward process it is also impossible to achieve the purpose of "structures by design", i.e., given the desired structural properties, find the optimal structures. That is, although optimal designs can be proposed that are better than those in the training dataset, it is not feasible to propose certain optimal designs that are within a set of structural boundary conditions like mass, volume, strength, etc. Hence, this demands a better machine learning technique that is capable of handling huge datasets with minimal time consumption and manual effort, and one that is able to predict targeted optimal designs based on a set of desired design constraints.

For this purpose, an inverse machine learning framework using Generative Adversarial Networks (GANs) is adopted in this study. Unlike forward machine learning, where certain desired properties of a chemical or physical structure are predicted, the idea of inverse machine learning is to predict an optimal structure, given the desired properties. While forward machine learning prediction is a straight forward process where we predict numerical data (output) based on categorical data (input), inverse machine learning is the *vice versa* of the previous process, but can be complicated. Inverse design networks using two deep neural networks have led to faster and accurate results compared to other numerical techniques. [14] GANs are used to design photonic crystals based on the data from a supervised machine learning model. [14] Novelty of 92.53% is achieved in designing hypothetical inorganic materials using GANs in which 84.5% are chemically valid. [15] A new regression and conditional generative adversarial network (RCGAN) are proposed for the inverse design of two-directional graphene and boron-nitride hybrids. [16] The advantage of using RCGANs is the application of supervised regressive networks which compensate for the inability of GANs to generate data samples when fed with continuous and quantitative labels. GANs are also used to design *meta*-surfaces to match the required optical spectra by substituting complex conventional prediction models. [17]

Although the application of machine learning techniques like GANs and regression have been proven to be very advantageous in discovering new patterns in various fields over the recent years, application of inverse design in structural design optimization based on mechanical properties has not been explored. For example, sandwich structures with lightweight core such as lattice core can be designed in numerous combinations to exhibit a wide variety of properties based on the connectivity and orientation of truss elements they are made of. The lattice core plays an important role in the overall load carrying capacity and lightweight feature of the sandwich structures. Lattice unit cells like octet, Kagome and tetrahedron structures were designed with various advantages in structural performance, impact absorption, damping features and acoustic insulation. [18–22] These structures were proposed based on several thorough numerical and experimental validations by various groups. Linear and nonlinear effective properties of lattice structures using continuum theory models were proposed. [19,23–26] With the advancement in manufacturing technologies like 3D or 4D printing, lattice core with very complex geometrical configurations can be manufactured to amplify the performance of these lightweight sandwich structures. [27]

Topology optimization technique was also used to develop new optimal lattice unit cells (ORC, OQSO) which were 5% and 38% stiffer compared to octet lattice unit cell in standard (001) direction. [21] Elastic and isotropic unit cells were designed by merging different basic unit cells such as simple cubic unit cell, octet unit cell, etc., to compensate for the elastic anisotropic nature of octet lattice unit cell. [22] Topology optimization techniques were developed to design and automatically generate truss structures within given design constraints. [28] Although classical topology optimization has been used to optimize lattice unit cell, it may be difficult to implement in designing and optimizing lattice structures with given structural boundary conditions or constraints, or difficult to conduct inverse design. This method relies on mass reduction to design optimal structures which can overlook structures with sensitive mass dependency. Therefore, although decent research contributions in topology optimization have been made in proposing novel optimal lattice unit cells, a wide range of unexplored space in lattice unit cell designs is proven to exist and inverse design remains a challenge.

In this paper, we propose the first inverse machine learning framework to identify, predict and optimize targeted lattice unit cell designs that can be used to manufacture high performance sandwich structures. To create the inverse design framework, GANs are used to generate many potential lattice unit cells and the rest of the inverse design framework consists of the forward regression model and boundary conditions. The combination of all these components forms the single inverse design framework, leading to design of lattice unit cells with desired properties. In this study, we first generated a dataset of several lattice unit cells and converted them in to fingerprints (numerical representation). These fingerprints are used to 1) train forward regression models to predict the structural properties of given lattice unit cells, and 2) input to the GANs to generate new lattice unit cells. The optimal lattice unit cells predicted using the inverse design framework are

then used to design sandwich structures and evaluated with numerical and experimental methods. Detailed illustration on the methods, results and discussion are presented in the following sections.

The predicted lattice unit cells exhibit compression strength of 40–120% higher than octet unit cell with the same overall volume under uniaxial compression. With minor adjustments in the initial and boundary conditions, this framework can be easily implemented in designing various structures with given properties. The implementation of GANs and machine learning regression models to optimize the structural performance of metamaterials opens up new possibilities to discover novel optimal structures with minimal computational time and effort through inverse design. The optimized lattice unit cells and sandwich structures can be used for lightweight applications in aerospace, automobile and navel structural components.

2. Methods

2.1. Inverse machine learning framework

Fig. 1 shows the framework for inverse design of lattice unit cells used in this study. The framework is composed of a training dataset fed to the discriminator which trains to differentiate between real and fake data generated by the generator. The real data then passes through the set of initial conditions, boundary conditions and forward regression to obtain a new set of lattice unit cells with superior properties. This new dataset is used to discover further optimized lattice unit cells by iteratively training the GAN network (manually updating the discriminator with latest datasets). Here, once the inverse design framework is ready with trained GAN network and regression models, the input will be the desired properties in a lattice unit cell (for example, low mass, high compression strength or symmetric truss distribution). The output will be a set of optimal lattice unit cells in the form of fingerprints that fall within the fixed input conditions. Therefore, the desired inverse design, i.e., prediction of optimal lattice structures as output with given properties as input, is achieved.

2.2. Data generation and fingerprinting

For any machine learning modeling, the data handling and fingerprinting play a prominent role in effectively predicting the required attributes. In this study, the data consists of several 3D lattice unit cells formed by using cylindrical elements with corresponding cross-sectional areas. In order to maintain consistency among all the data samples, a Representative Volume Element (RVE) is considered with 27 vertices. All the lattice unit cells data used in this study is generated by forming several combinations of the cylindrical elements, whereas each element is formed by connecting two neighboring vertices within the RVE (Refer to Fig. A1). These lattice unit cells are tested for uni-axial compression using ANSYS simulation software. [29] Uniform load is applied on all the lattice unit cells by fixing one surface. Finally, a database of around 1500 different lattice unit cells (Refer to Table S3 in Excel file) with their mass and compression stresses obtained from the ANSYS-Model interface. Once the dataset is formed, for the machine learning algorithms to understand the data, each data point, i.e., each lattice unit cell within the dataset must be converted into a machine-readable format. For this purpose, initially, all the 27 vertices in the RVE are numbered from 1 to 27 and each element that is possible in the RVE is named by the two vertices it connects. Now any lattice unit cell in the dataset is represented by forming a vector of numbers consisting all the element names that the particular unit cell is constructed from. This way of fingerprinting the lattice unit cells will be convenient in designing the structures based on the element numbers and further interpretation of designs predicted by the inverse design framework by any user. For machine learning algorithms, these fingerprints are further converted into a vector of 1′s and 0′s. By fixing one constant position to each element, the fingerprint vector is formed by having 1′s where there is an element in the design and 0′s for the rest of the positions; see Table S3. While the vector representation of the lattice unit cells by the names of the elements will be convenient for human interpretation, further modification of these vectors in 1′s and 0′s is more appropriate for AI systems.

Froward regression analysis is an integrated component in the inverse design framework. Employing the fingerprints of the lattice unit cells as input data, forward regression models are developed to predict the mass and compression strength of untrained lattice unit cell designs. The models developed in forward regression can only predict the mechanical properties like the compression strength, etc. It is not feasible to use the forward regression models to predict new fingerprints, given the mechanical properties as inputs. This is due to the few input variables, i.e., mass and compression strength while the desired output will be a huge vector

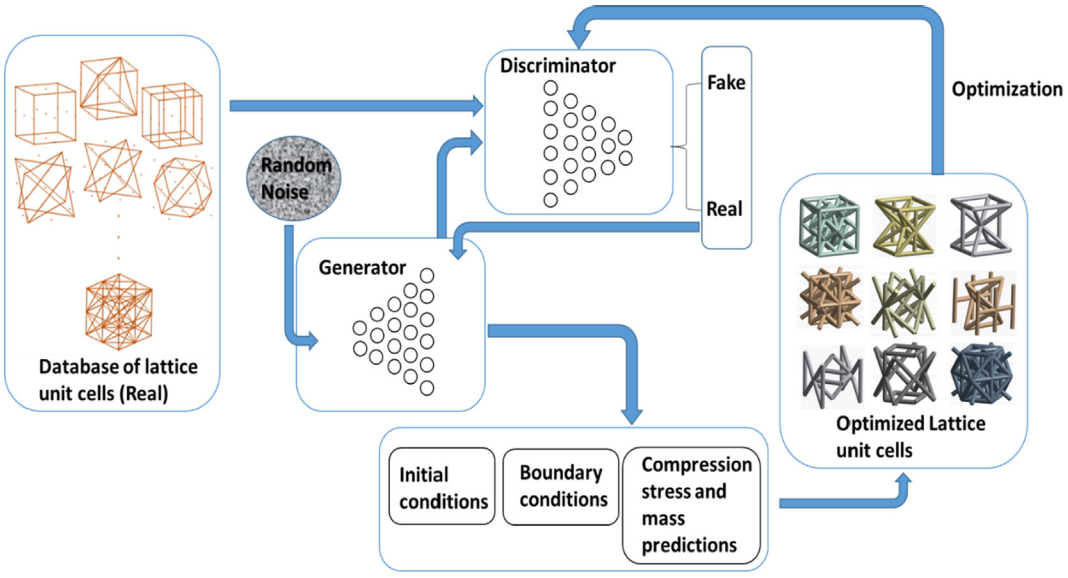

Fig. 1. The pipeline of the inverse design framework.

of elements that can vary over a wide range of 20–100 variables. The dataset size and the sensitive dependency of the mechanical properties of the unit cell on its structural orientation makes it extremely difficult to backpropagate a forward regression model. Therefore, in order to predict new structures based on required properties and other boundary conditions, inverse machine learning techniques should be developed. For this purpose, GANs, a new class of machine learning technique is employed. GANs are a type of machine learning which use two neural networks to generate new data based on a given training data set. While one of the neural networks, the generator generates new data, the other neural network, the discriminator, differentiates the newly generated data from the existing training data. The GAN runs till the discriminator neural network cannot identify the difference between the existing training data and the newly generated data. This newly generated data will be the desired output.

In this study, the data available in the training database of 1500 lattice unit cells is fed to the discriminator of the GANs system. Based on this, the generator tries to learn from the discriminator and keeps on generating new fingerprints until the discriminator fails to identify fake data from real data. The final output will be a set of unique fingerprints that have very close resemblance to the fingerprints for the original 1500 training dataset. Now, the initial training datasets have several fingerprints of lattice unit cells which are good structures in terms performance under uni-axial compression while others perform poorly compared to octet lattice or other superior structures. The GANs can only generate several new structures based on the training data that have similar but not the same features. Hence, once the GANs generate new data, the new fingerprints should be validated if they satisfy the required criteria. This includes optimal compression strength, mass, whether the fingerprints generated can form an authentic structure or not, and whether it is a bending dominated or stretching dominated structure. For this purpose, the newly generated dataset is passed through several boundary conditions to check for the above stated criteria. The mass and compression strength of the generated fingerprints can be tested quickly by performing forward regression using the model generated in the previous section. Maxwell's criterion can be used to differentiate if a structure is bending or stretching dominated. [25] In this study, all the joints are considered to be rigid. To validate whether a proposed lattice unit cell form a structure or not, it is done by placing another condition that only considers fingerprint for which at least one end of each individual element is connected to any other element. This will eliminate fingerprints with truss elements without joints.

2.3. Experimental and numerical validation

All the lattice unit cells predicted and evaluated in this study are modeled using 3D CAD design software, SolidWorks. ANSYS Workbench is used to simulate the compression behavior of these CAD designs for linear and non-linear analysis. The CAD designs from SolidWorks are converted into a vendor-neutral file format (IGES) and imported into ANSYS platform for simulations. VeriGuide (tensile strength 28.5 MPa, elastic modulus 1.14 GPa), a commercially available photo-polymerizable and 3D printable resin is used as the base material for all the numerical and experimental validations. For simulations, the structures are meshed using tetrahedron elements and large deflections is checked for non-linear analysis. Mesh convergence is validated for various mesh sizes and an adaptive sizing with resolution order 4 (~900,000 elements) is considered for balancing speed of simulations and convergence (See Fig. A2 for meshed lattice unit cells and deformed shapes under uniaxial compression loading). For the experimental validation, stereolithographic (STL) files of the three-dimensional lattice structures are generated using SolidWorks. These STL files can be read by any type of 3D printers. A professional 3D printer (Pico 2), which uses vat photopolymerization technique to cure materials is used for manufacturing the lattice structures (some of the printed unit cells can be found in Fig. S1). All the unit cells are manufactured using VeriGuide, a commercial polymer with an overall volume of $20 \times 20 \times 20$ mm. Once the postprocessing is complete, the mass of each unit cell is measured using a dual range XS105 balance and an MTS machine (ADMET eXpert 2610 Table Top 5kN Universal Test System) is used to conduct uniaxial compression test on all the samples. The compression tests are conducted at a speed of 1 mm/min and the load and displacement for each sample are recorded to get the load vs. displacement curves. All the structures failed due to brittle fracture at low strain. It can be observed from Fig. 2 that the simulation results are in good agreement with the experimental data. The slight deviation in the experimental and simulation results may be due to imperfections in the 3D printed parts or due to improper removal of uncured resin and support parts.

2.4. Comparison based on the Gibson-Ashby model

Gibson and Ashby [31] developed a model for the modulus of cellular structures based on the linear-elastic properties at various relative densities:

$$\frac{E^*}{E_s} = c_1 \left(\frac{\rho^*}{\rho_s}\right)^2 \quad (1)$$

where E^* is the Young's modulus of the porous structure, $E_s$is the Young's modulus of the base material, $\rho^*/\rho_s$is the relative density of the unit cell and c_1 is the geometric constant of proportionality that can be obtained from the experimental data. [31] c_1 value for octet, lattices A and B unit cells in Fig. 2 are found to be 0.09, 0.1 and 0.125 based on the experimental results at various densities as shown in Fig. 3. Based on Fig. 3, it is clear that the relative modulus of the octet unit cell is less dependent on the relative density of the unit cell. In other words, with the same relative density, the unit cells A and B have higher modulus ratio. If the same material is used for the unit cells octet, A, and B, this result translates to unit cells A and B have higher stiffness than the octet unit cell, which is a desired feature for load carrying structures.

3. Results and discussions

3.1. Forward regression analysis

MATLAB Regression Learner module containing various types of regression models is used to correlate the data. [30] Multiple machine learning algorithms like Random Forest, Support Vector Models and Gaussian Process Regression models are tested with the initial dataset for their performance. Rational Quadratic GPR model performed best with a low root-mean-square deviation (RMSE) of 0.20912. From the predicted vs. true response plots for mass and compression strength (Fig. 4), it can be perceived that the machine learning predictions match quite well with the true values with the line being predictions and the dots being the observations. The plots should be interpreted by considering that the closer the observations are to the prediction line, the better the model is.

3.2. Inverse machine learning using GANs

By passing the fingerprints generated by the GANs through the conditions defined in Section 2.2, we can filter as many structures that perform better than a set datum point, octet lattice unit cell in this case. All the fingerprints that pass the condition sets perform

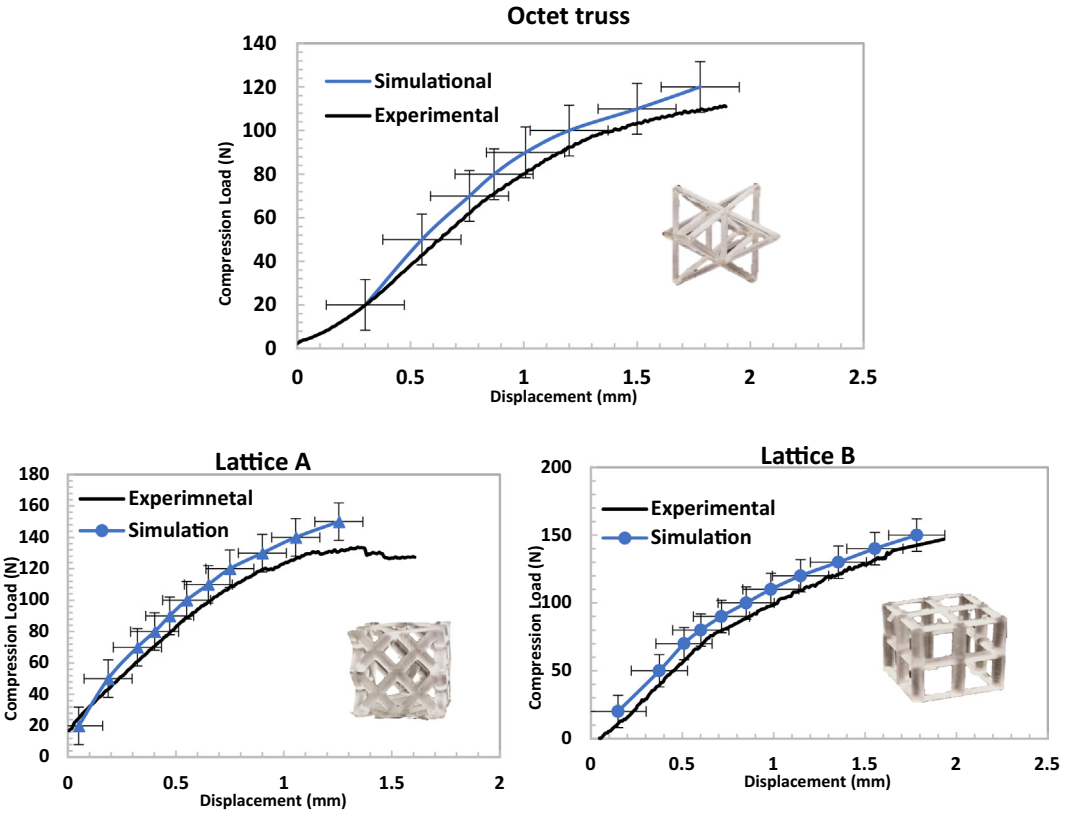

Fig. 2. Experimental vs. simulation comparison for lattice unit cells under uni-axial compression.

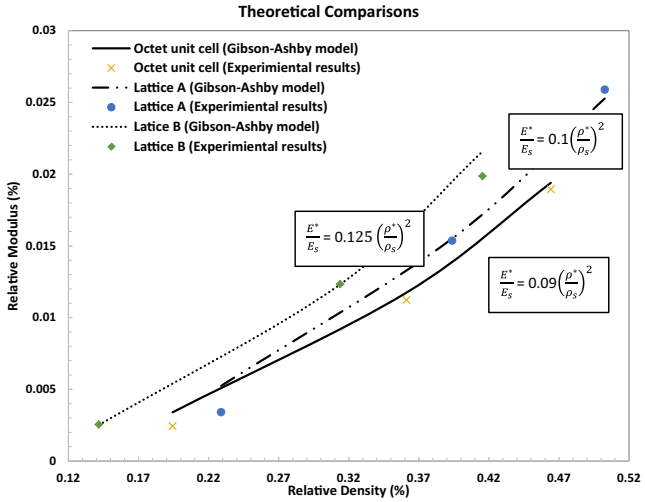

Fig. 3. Experimental vs. Gibson-Ashby model predictions of the relative modulus of lattice unit cells.

better than octet unit cell. As yet, the inverse design is used to generate structures that perform better than octet unit cell training on the initial dataset of 1500 fingerprints. A few sample fingerprints tested for uniaxial compression that pass the set conditions are evaluated through ANSYS simulations in Fig. 5. It can be observed that the predicted lattice unit cells vary at different range of compression loads (40–120%) while all of them obeying the focus objective, i.e., better than the octet unit cell. Although there is no one common factor among the optimal structures that explains their better performance than the octet lattice, several features such as low mass in some lattices like lattices A and B, parallel orientation of truss members in lattices B, C, and D, and stronger joint connectivity in lattices C and D, could account for their better performance as compared to the octet lattice.

Now, to obtain further optimized structures, the newly generated fingerprints that perform better than the octet unit cell shall be considered. Using the above stated inverse design technique, a new data of about 500 lattice unit cells that perform better than the octet unit cells is formed. Now this latest dataset is fed to the discriminator, and the generator is trained to generate new fingerprints by training on the new dataset. The GAN will generate novel fingerprints close to the new sample space and this data can be passed through the set of boundary conditions. By setting the target for mass and compression strength to be much higher than those from the previous learning cycles, i.e., even lower mass and higher compressive strength than the octet unit cell, further optimized lattice unit cells can be predicted that perform better than the octet unit cell at a higher order. Table A1 lists the images of 16 optimized lattice unit cells.

3.3. Continuous optimization of the lattice unit cells by inverse design

The inverse design framework in this study allows continuous optimization of the lattice unit cells by iteratively utilizing the framework in Fig. 1. To quantify the capability of the inverse machine learning framework, several cycles of optimized lattice unit cells are generated by optimizing the structures for each cycle. Four sets or generations of these unit cells and their performances under uniaxial compression loading are presented in Fig. 6. Initially the boundary conditions of the inverse design framework are set to predict lattice unit cells that are better than the octet unit cell by constraining the mass and compressive strength of the predicted unit cells. As stated in the inverse machine learning section, each new set of optimal lattice unit cells obtained is generated by training the GANs with new optimal dataset generated from the previ-

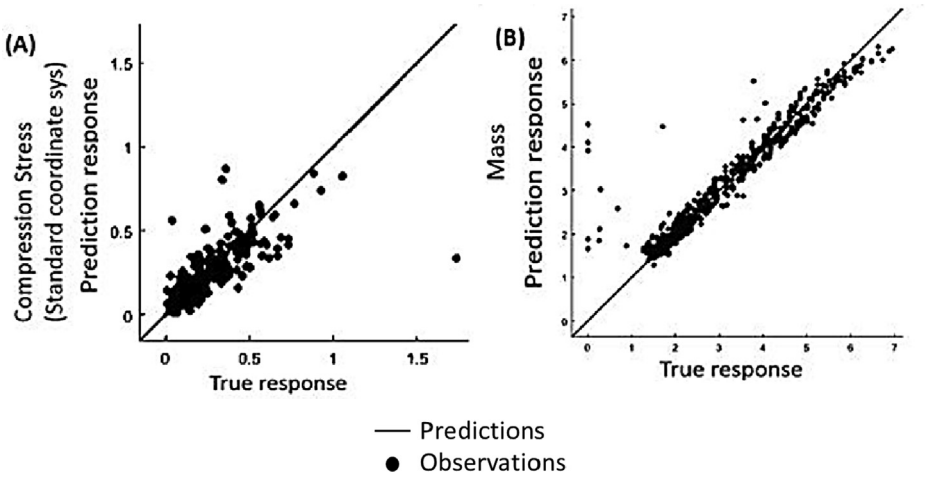

Fig. 4. True response by ANSYS finite element analysis versus prediction by GPR machine learning algorithm for (A) Uniaxial compression stress and (B) Mass.

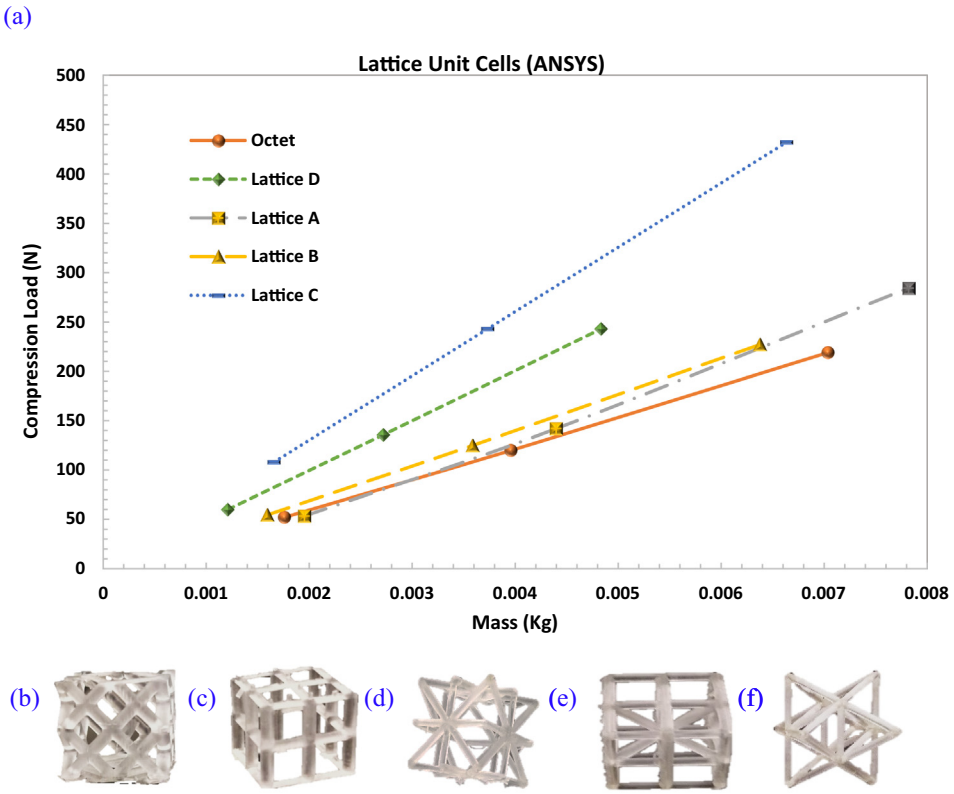

Fig. 5. (a) ANSYS simulation caparisons for uniaxial compression of various optimal unit cells predicted through inverse design, (b) Lattice A, (c) Lattice B, (d) Lattice C, (e) Lattice D, (f) Octet lattice unit cell.

ous set. From the ANSYS simulation results in Fig. 6, the improvement in the structural performance from the first generation (set 1) to the fourth generation (set 4) can be clearly observed to be increased by 50%. The results have been summarized in Table S1.

3.4. Compression analysis of lattice cored sandwich structures

One potential application of lattice unit cells is to construct lattice cored sandwich panels. In this study, the optimal lattice unit cells predicted by the inverse machine learning framework were used to construct several sandwich structures with varying densities. Lattice core sandwich structures are constructed by sandwiching the lattice core in between two thin plates on the top and bottom. The core is made by stacking lattice unit cells side by side. Thin sheets with 10% of the thickness of the core are used to laminate the 4 by 4 unit cells, forming several sandwich structures with varying dimensions (see Fig. S2 for several 3D printed lattice cored sandwich panels). Testing procedures similar to the lattice unit cells were performed on the sandwich structures and the results can be observed in the comparison of compression strength with densities in Fig. 7. The compressive strengths of the sandwich structures are obtained by dividing the maximum compressive loads of the unit cells by the cross-sectional area. The sandwich structures performed in a similar pattern to those observed in the single unit cell comparisons. Under uniaxial compression, the sandwich structures constructed using optimal lattice unit cells

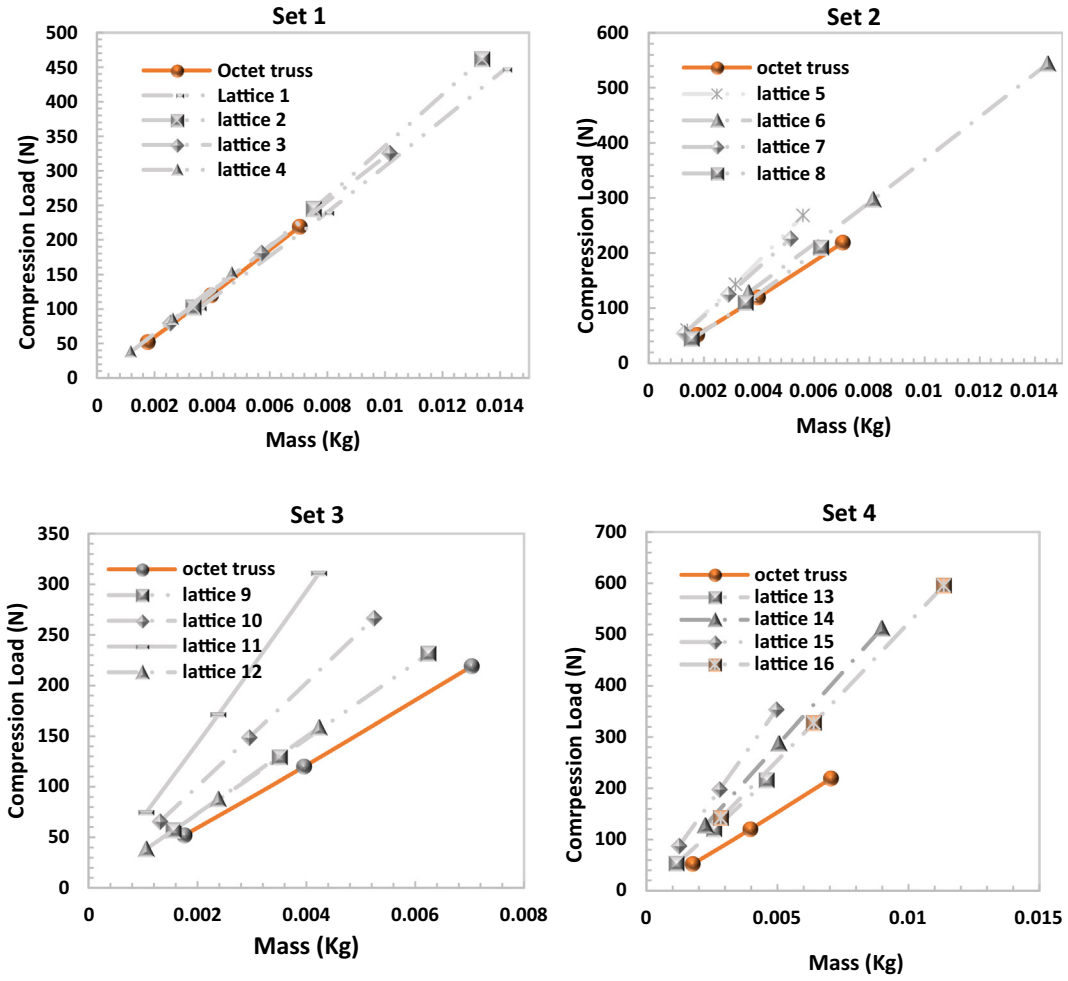

Fig. 6. ANSYS simulations for compression load vs. mass of several optimized lattice unit cells optimized for each generation (Set 1 to Set 4) (Refer to Table S1 and Table A1 for more information and images of lattice unit cells).

perform 60% better as compared to the octet lattice cored sandwich structures.

4. Conclusion

The design space in metamaterials like lightweight and multifunctional cellular structures is huge. With the advancement in novel simulation and manufacturing techniques, bringing these structures into practical applications is getting much easier. Although remarkable work on studying various cellular structures and their behavior has been done, there is still a vast volume unexplored in the design space. In this work, machine learning techniques are used to propose an inverse design framework to explore a wider range of structural designs. GANs and forward regression techniques are used to propose novel lattice unit cells that perform better than the octet unit cell. The predicted unit cells are validated through numerical and experimental testing and proved to be 40–120% better than the octet unit cell under uniaxial compression. We also used the optimized unit cells as sandwich cores, and compared favorably between the test results and simulations. One feature of the inverse machine learning framework is that it allows continuous optimization of the lattice unit cells, by iteratively utilizing the newly created unit cells as training dataset for next generation predictions. This framework can be used to optimize other types of structural design and to propose novel structures with a desired range of mechanical properties. Based on the excellent performance of the optimized lattice unit cells

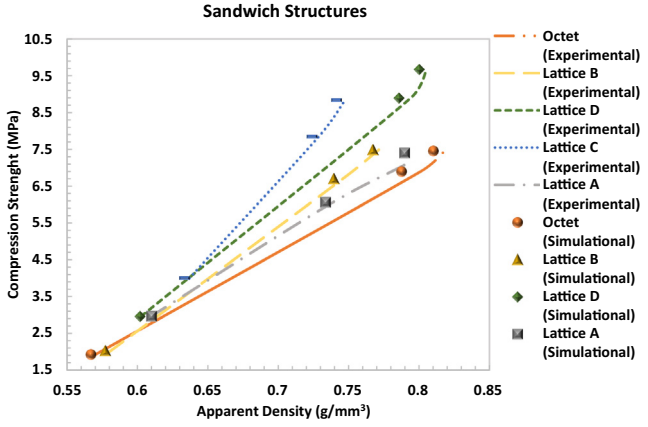

Fig. 7. Compression strength vs. apparent density comparisons between ANSYS simulation and experimental testing of several lattice cored sandwich panels in Fig. S2.

and adequate prediction accuracy of the regression models and inverse design framework, it can be seen that this technique can be applied to design and further optimize various biomimetic metamaterials with different properties like shock absorption, higher bending or buckling strengths and shape recovery. In our future works, we intend to improve the prediction and generative

accuracy of the machine learning models by improving data generation and fingerprinting. These models shall be used to design novel metamaterials with superior shock absorption capacities compared to biomimetic counterparts like honeycomb and other cellular structures.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A

Here each point of the entire RVE is numbered from 1 to 27. Each pair of numbers represents the element connecting the respective points. For example (12) is an element formed by connecting point 1 and 2. Likewise all the elements in the RVE can be represented by the two points it connects. Now by using the "combnk" function, various combinations of the elements can be generated. To form direction dependent optimal asymmetric lattice unit cells, the cuboid with 27 points is considered as a RVE. Hence the number of elements to form a particular lattice unit cell are predefined and various combinations are generated using the same "combnk" function. For example (12 13 15 213 1314 1415 1015 910 39 519 1316 1625 1518 1827 911 1121 1922 2225 2526 2627 1920 2021 2124 2427 18 89 813 815 819 821 825 82,725 23 35 28 58 46 47 67 46 68 78 45 27) is a lattice unit cell

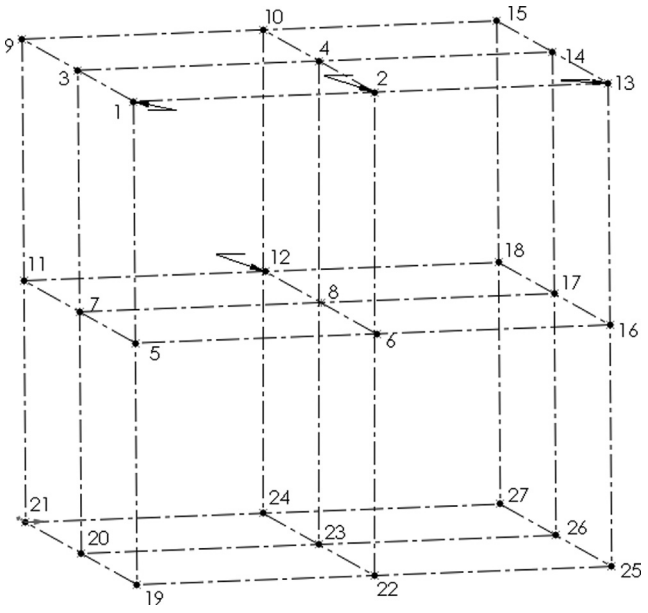


Fig. A1. Procedure to form different lattice unit cells based on representative volume element (RVE).

formed by the 43 elements represented in the fingerprint. Here elements with two digits (12, 13, 15 etc.) means the element is formed by connecting two points, the first digit represents one point and the second digit represents the other point. For the elements with three digits (213, 519, 911 etc.) the first digit represents one point and second two digits are the number of other points. In case of elements with four digits (1314, 1415, 1015, etc.), the first two digits represent one point and the second two digits represent the other point forming the elements. These fingerprints are further converted into vectors of 1's and 0's, for better results while using the machine learning algorithms. For this purpose, every element in the RVE is given a fixed position in the fingerprint vector. Now for a particular fingerprint, all the positions where there is an element is names as 1 and the rest of the posi-

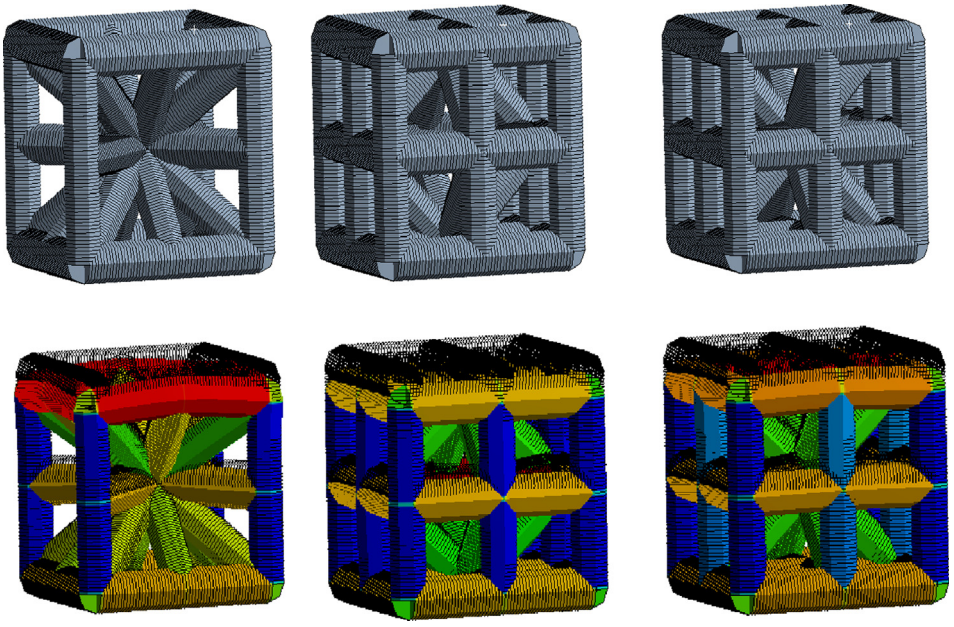
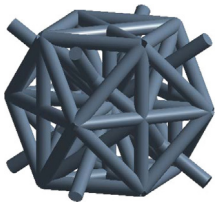
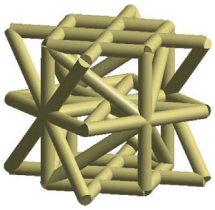
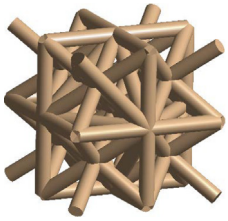
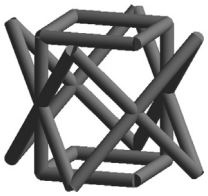
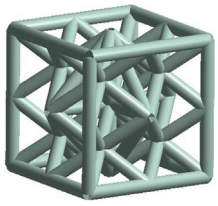
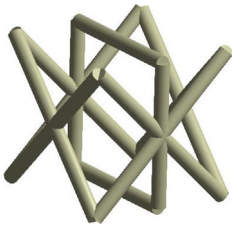
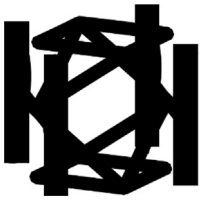
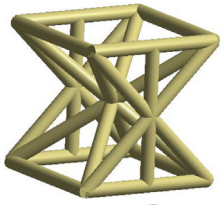
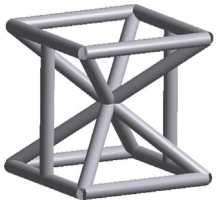
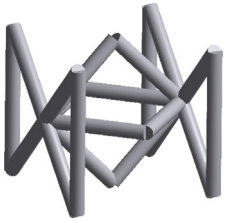
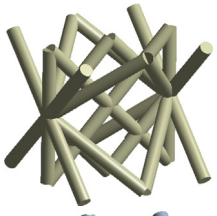
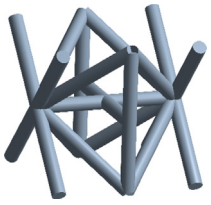
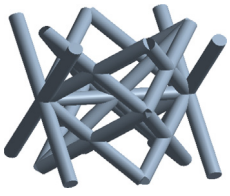
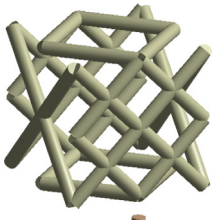
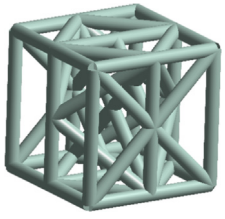
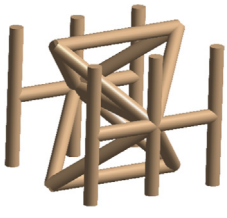


Fig. A2. ANSYS mesh and deformation contours of few lattice unit cells.

Table A1
Images of several optimal lattice unit cells.

	Lattice 1		Lattice 2
	Lattice 3		Lattice 4
	Lattice 5		Lattice 6
	Lattice 7		Lattice 8
	Lattice 9		Lattice 10
	Lattice 11		Lattice 12
	Lattice 13		Lattice 14
	Lattice 15		Lattice 16

tions are names as 0. For example, assume a sample RVE consists of only 10 element in total. Then a unit cell fingerprint consisting all the 10 elements is represented as (1 1 1 1 1 1 1 1 1 1). For a unit cell consisting of 4 elements whose positions are defined as 1, 3, 5 and 7 will look like (1 0 1 0 1 0 1 0 0 0). Example of a fingerprint from the actual RVE defined in this study will look like (1 1 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0 0 0 0 0 0 0 1 1 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0).

Appendix B. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.matdes.2021.109937.

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