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Multi-scale structural design considering cellular connectivity using machine learning approaches

L. Meng[1], C. Yang[1,2], Y.L. Hou[3], T. Gao[1], J.H. Zhu[1,4] and W.H. Zhang[1]

[1]State IJR Centre of Aerospace Design and Additive Manufacturing
Northwestern Polytechnical University, Xi'an, China
[2]TSMC Nanjing Company Limited
Nanjing, China
[3]School of Mechanical and Power Engineering,
Zhengzhou University, Zhengzhou, China
[4]Institute of Intelligence Material and Structure, Unmanned System Technologies
Northwestern Polytechnical University, Xi'an, China

Abstract

Accompanied by the fast evolution of additive manufacturing, multi-scale porous structures are gaining ever-increasing popularity in high-performance structure design. Given the connectivity requirement imposed on neighbouring cellular microstructures for their successful printing, we propose in the current work a criterion for connectivity evaluation based on Dijkstra's shortest path algorithm, and a unit cell generation model is established with the aid of the Generative Adversarial Network (GAN) approach. A family of 9 lattice units satisfying a prescribed connectivity condition is subsequently optimized under various load conditions. Lastly, a multi-scale structural optimization design approach is developed under the neural network framework, and the best combination of the *a priori* optimized lattice units is found. The effectiveness of the proposed protocol is verified on a series of numerical examples considering structural stiffness/toughness.
Keywords: Additive manufacturing, multi-scale, connectivity, GANs, structural optimization.

1 Introduction

It is well recognized that multi-scale porous structure outperforms mono-scale ones in the sense of stability and multi-functionality, and is thus enjoying overwhelming popularity in structural design. Early works in multi-scale structure design generally requires prohibitive computational cost since local materials are optimized concurrently according to the local stress states. To circumvent this issue, Xia constructed a reduced-order database model viewing the local material optimization process as a generalized constitutive behaviour using separated representations [1]. It is however noticed that the geometric connectivity was not guaranteed by the optimized local microstructure. Later, Duriez addressed this issue through adaptive transmission zones which limit the loss of performance [2].

These days, along with the rapid development of computer science, machine learning algorithms find a more in-depth application recently in the field of computational mechanics, ranging from structural analysis to optimal design. Ulu et al. established a mapping between the loading configurations and the optimal topologies [3]. Most recently, Zhang et al. developed a framework for topology optimization via neural reparameterization (TONR), and dealt with such optimization problems as stress-constraint design, natural frequency maximization, and heat conduction system design [4].

In this current work, the authors intend to couple the machine learning algorithm with the multi-scale structure design, and the capability of machine learning algorithms in dealing with image information is leveraged for imposing geometric connectivity of cellular materials. The proposed method also takes advantage of neural networks in accelerating mechanical analysis.

2 Methods

2.1 Connectivity characterization via the Dijkstra's shortest path algorithm

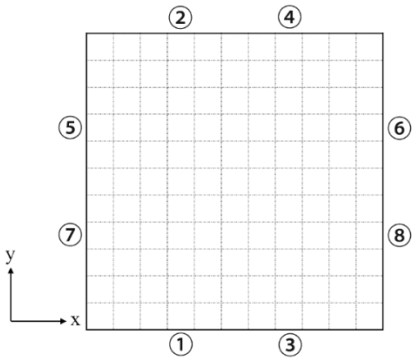


Figure 1. Schematic of microstructure discretization and transmission points.

Most conventional topology optimization approaches rest on the Solid Isotropic Material with Penalization (SIMP) material assumption, which may lead to undesired "gray elements". To alleviate the resulting uncertainty in the fabrication process, the current work focuses on the 0-1 solution of topology optimization, and the continuity of the structure is readily assessed. Borrowing the Dijkstra's algorithm, we define the

distance between two neighbouring elements as 1 if both elements are solid (with a material pseudo density of 1), whilst being INF (a relatively large value) if otherwise. Supposing a discrete finite element model composed of N elements, a $N \times N$ initial distance matrix D is set according to the prescribed element densities. By referring to the Dijkstra's shortest path algorithm, the entry D_{ij} is finally updated by the Dijkstra's shortest path between two elements, e_i and e_j. The matrix should hence be able to characterize the connectivity status of the cellular structure.

Figure 1. presents a microstructure design domain discretized by a 11×11 grid, and two transmission points are assigned on each edge where the connectivity constraints are imposed between neighbouring microstructures. For instance, to ensure the X-direction connectivity, the transmission points numbered by ②/⑦must be accessible to ⑥/⑧. Figure 2. showcases two Dijstra's distance calculations on two Chinese characters "西" and "北". It is found that transmission points ②-③ in "西" is connective since the Dijstra's shortest distance is 20, while transmission points②-⑥ in "北" is disconnected given the infinitive value.

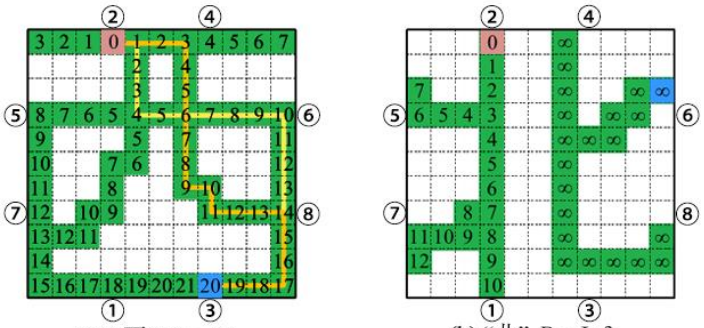


Figure 2. Schematic of the Dijkstra's distance calculation on two of the transmission points on two Chinese characters.

2.2 Generative adversarial network.

The generative adversarial networks are composed of a generative and a discriminative network. Its core idea lines in the adversarial training process in which the former network intends to increase the error rate of the discriminative network, and the latter seeks to distinguish candidates produced by the generator from the true data distribution. In the current work, the generator G takes a vector of random noise as the input and upsamples it to an image, i.e., a 0-1 valued microstructure image. The discriminator D, on the other hand, is a convolutional network that categorizes the images fed to it. In this current work, this binomial classifier labels images as "connective" or "disconnected". In the training process, both networks try to optimize a different and opposing objective function, or loss function, in a zero-sum game. Readers are noticed that, while training a GAN we do not train the generator and discriminator simultaneously. In real practice, when the discriminator is trained, the generator values are held constant, and vice versa. Figure 3. displays the structure of the GANs.

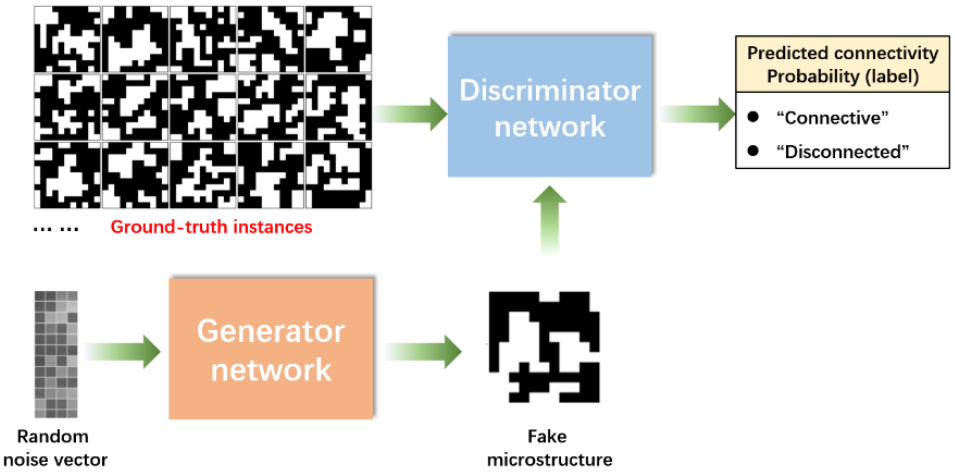


Figure 3. Schematic of GANs for microstructure connectivity prediction.

3 Results

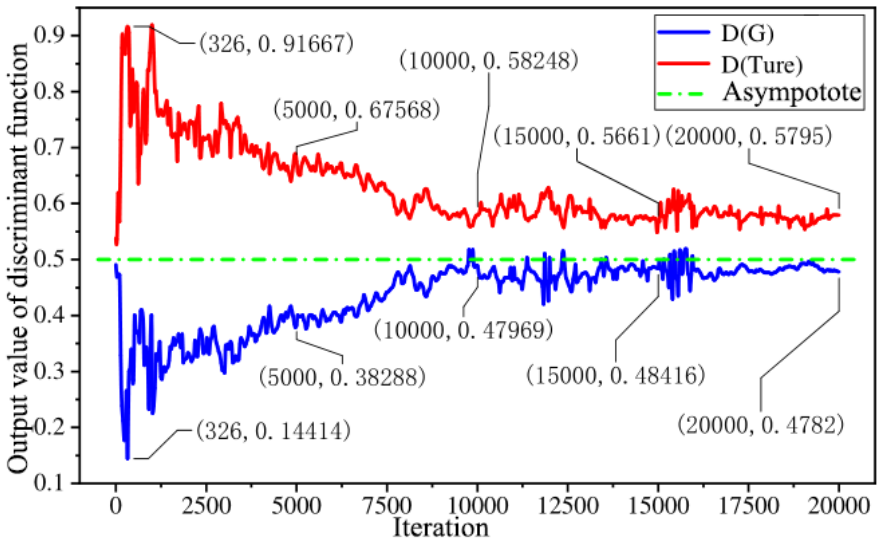


Figure 4: Generate adversarial networks' training curve.

In Figure 4., the red line depicts the averaged value of the predicted authenticity by the discriminator D, with the ground truth instances being the lattice unit cells satisfying the connectivity constraint. Contrarily, the blue line refers to the predicted authenticity where the generated sample from G is inputted. Theoretically, the closer the output of the discriminator D is to 1, the better the training effect is. However, the two networks are in general desired to perform almost equally such that neither of the networks overpowers the other. As clearly observed, with the continuous improvement of the quality of the samples generated by the generator G, the discriminator D encounters more and more challenges to distinguish the fed sample from G, i.e., D(G) to the authenticity, and the training of the networks stops is finally stopped at the Nash equilibrium asymptote 0.5 (theoretical solution). Figure 5 demonstrates a group of 15 samples obtained from the trained generator, and it is noted that the connectivity constraint is automatically imposed.

Figure 5. Microstructures randomly generated by the trained Generator G.

Despite the connectivity ensured by the GANs, the best topology of cellular lattice needs to be found such that the load-bearing capacity can be ultimately achieved at a structural level. In this work, we have adopted the top-99 line MATLAB codes for the prediction of the mechanical performance, i.e., the flexibility/stiffness, of each lattice structure [5]. By combining with the trained neural network, the optimal design of the lattice unit is carried out. Figure 6. illustrates the optimization procedure in which the stiffness along the longitude direction of the lattice cell is maximized.

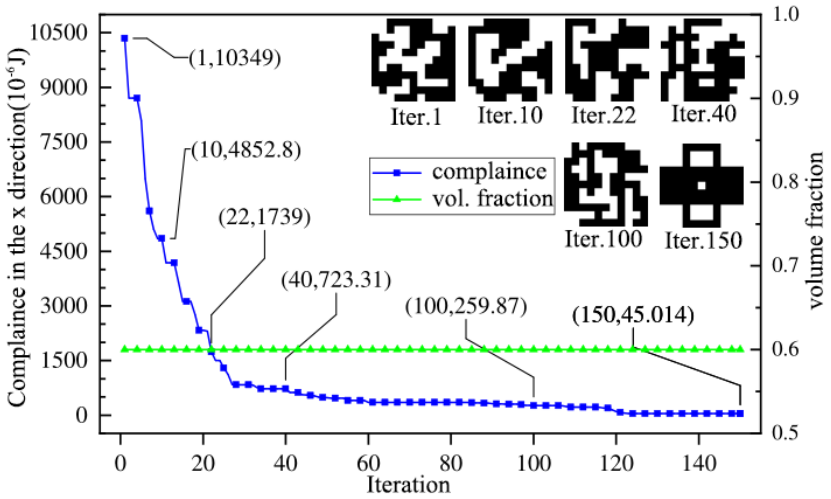
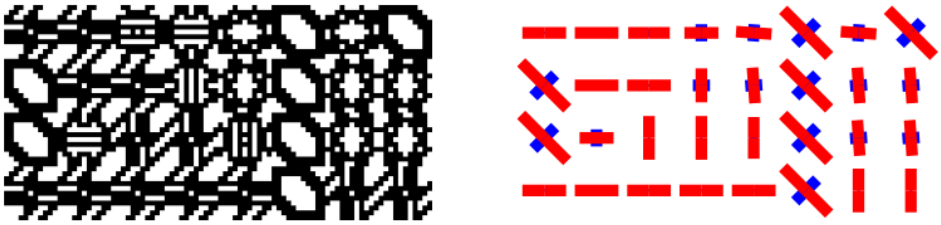


Figure 6. Iteration histories of compliance and volume fraction during optimization.

In real structural design, a part must experience different stress/load conditions at different locations. For this reason, we intend to generate a group of lattice cells that can be optimal in different cases. Choosing the compliance ratio of two orthogonal directions as a key factor, a group of 9 optimal unit cells is obtained a priori. Each lattice unit cell will be indexed by an integer from 1 to 9. The corresponding equivalent elastic matrices are pre-calculated and called during the optimization. Figure 7 (a) demonstrates the right half part of an optimized MBB beam using the 9 connectable lattice units, under a vertical traction force at the midspan of the beam.

The red lines in (b) demonstrate the principal stiffness directions of each lattice unit cell, and this is in perfect accordance with the load path.



(a) Multi-scale MBB beam (half part) (b) Principal stiffness direction

Figure 7 Optimal multi-scale MBB beam based on connectable lattice cluster.

4 Conclusions and Contributions

We report in this work a systematic approach to the optimal design of multi-scale lattice structures, considering the connectivity of neighbouring unit cells. The Dijkstra's shortest path algorithm is firstly coupled with the Generative Adversarial Networks in the design of microstructures, alleviating readily the long-standing disconnectivity issue that causes the failure of 3D printing. We then established a neural network metamodel for structural analysis, and sensitivity information is derived by the back propagation algorithm once the network is trained. The optimized cellular structures satisfying the connectivity constraints are finally employed for macroscopic structure design. The manufacturability of the final design has been lastly confirmed by additive manufacturing.

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