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Upscaling optimal topology multimaterials structures using Deep Neural Networks

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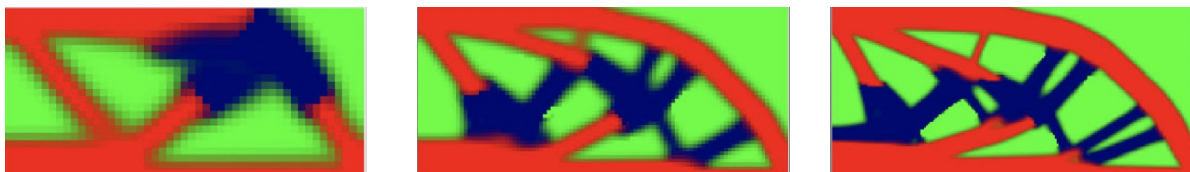
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Abstract: The problem of Topology Optimization aims to solve the question of the optimal material distribution subjected to known boundary and load conditions subject to a target volume fraction. In this study, we present a machine learning framework to tackle the problem of Multi Material Topology upscaling, i.e., the prediction of a higher resolution topology with just the low-resolution input. A Convolutional Deep Neural network was trained with a data set generated from an iterative code found in the existing literature. The network architecture implemented in this study is a modified version of SRGAN which has proven capabilities in upscaling complex real-world images. In this study, the perceptual loss function was used as the loss function in order to not penalize the network for its predictions that are off by a couple of pixels while simultaneously rewarding the network for its outputs that yield accurate compliance. The paper aims to present a novel approach to the problem of Topology Upscaling of 2x by mapping local features of the low-resolution topology to their higher resolution counterparts.

Key Words — Multi-Material Topology Optimization, Deep Neural Networks, Image Super Resolution, Physics Informed Neural Networks.

1. Introduction

The problem of optimal topology has existed for at least a century now. One of the most elegant solutions was given by O. Sigmund in his landmark paper proposing an iterative method to solve the problem of topology optimization called SIMP, where he introduced a penalty on intermediate densities to obtain optimal topology [1]. However, the quality of the output depends highly on the mesh size. The time for convergence, is low at lower mesh densities, and exponentially increases by the power of two as the mesh size increases (Figure 1). Thus, if the code was used for an industrial application, the simulation time would be significantly higher. Although many efforts have been made to improve O Sigmund's approach, the gains have been marginal [2].



(a) Mesh 50x25, 408 it, 24 sec

(b) Mesh 100x50, 408 it, 106 sec

(c) Mesh 200x100, 408 it, 414 sec

Figure 1 Evolution of optimal topology with mesh size on an MBB test case using a multimaterials approach [6]

Generative Adversarial Networks have had great success in the realm of Image Processing. However, their implementation to tackle the problem of Topology optimization has had limited success. [3], [4] proposed solutions through image processing techniques to upscale the optimal topology. [3] describes the implementation of a Pixelwise loss function and [4] locally refined the mesh and extrapolated the features directly from the low-resolution (LR) topology output to a higher resolution (HR) output. Both studies in essence assume that the features of the optimal topology at lower and higher resolution are identical. However, this is most certainly not the case. This is because, by the very nature of the classical problem definition, the iterative algorithm tries to converge to a local minimum and not the global minimum. This results in vastly different structures for the same input condition as can be seen in figure 1. Thus, the assumption that the Higher and Lower topology will have identical features is not ideal if we are tackling the problem of upscaling the topology. This is the problem that this study tries to address. The more general question we want to tackle is “Can we infer High Resolution optimal topology from a set of HR/LR relationships?”. We choose here to use classical Deep Learning techniques.

2. Network Architecture

For the reasons described above, the goal of the Neural Net should be to predict the *ideal optimal high-resolution topology* for the *true low-resolution* input. The solution to such an objective is described in the paper by [5]. In the paper they propose a ‘*SRGAN – Super Resolution Generative Adversarial Network*’ that is capable of upscaling the input image to 4x with the definition of a custom loss function that they called ‘*Perceptual Loss function*’. The network architecture used in this study is the exact same as the ones they used however with a slight difference in both the network architecture as well as the characteristics of the training and validation data.

The generator (Figure 2) consists of 16 residual blocks (B=16) with identical layout (not visualized in figure 2). In each block we have two convolutional layers each followed by a Batch Normalization layer and Parametric ReLU as the activation function. The image resolution is increased by 2x by using an Up-sampling Layer.

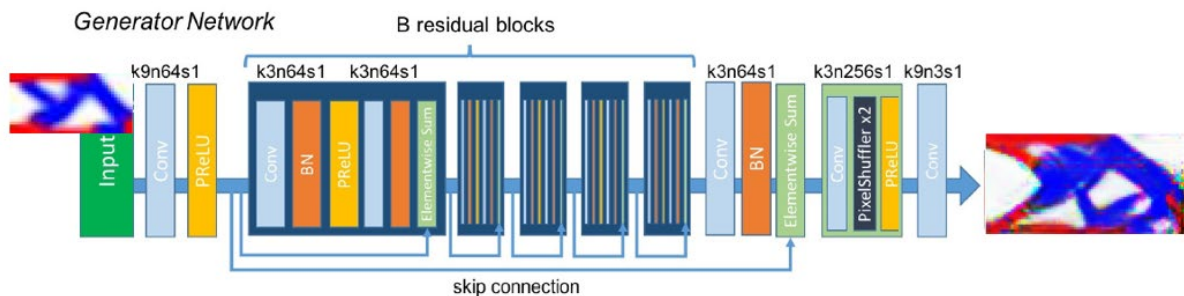


Figure 2 Generator Network Diagram

The discriminator (Figure 3) consists of 6 convolution layers with an increasing number of 3x3 filters increasing from 64 up to 256. The resulting feature maps are then followed by two dense layers and a final sigmoid activation to obtain the probability for sample classification.

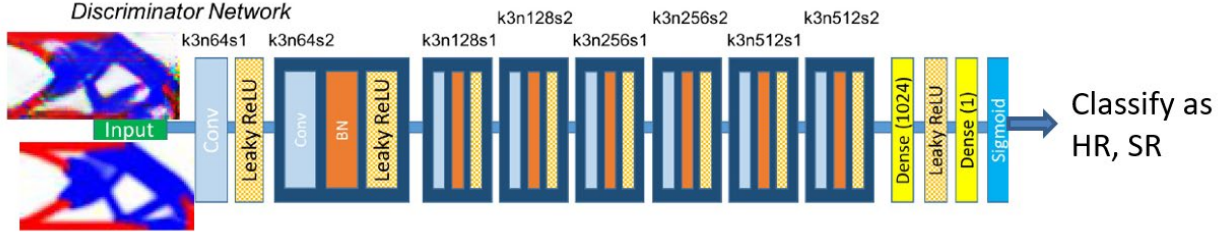


Figure 3 Discriminator Network Diagram

3. Loss Function

The loss function in this study consists of two parts. The ‘*Content Loss*’ and the ‘*Adversarial Loss*’. The content loss or the VGG loss is based on the ReLU activation layers of the nineteen-layered, pre-trained VGG Network. Mathematically the VGG Loss can be described as follows (equation 1)

$$l_{VGG/i,j}^{SR} = \frac{1}{W_{i,j}H_{i,j}} \sum_{x=1}^{W_{i,j}} \sum_{y=1}^{H_{i,j}} (\phi_{i,j}(I^{HR})_{x,y} - \phi_{i,j}(G_{\theta_G}(I^{LR}))_{x,y})^2 \quad (1)$$

Where, $\phi_{i,j}$ represents the feature map obtained by the j^{th} convolution before the i^{th} max pooling layer in the trained VGG19 network. Then the VGG loss can be defined as the Euclidean distance between the feature representations of a reconstructed image $G_{\theta_G}(I^{LR})$ and the reference image I^{HR} . $W_{i,j}$ and $H_{i,j}$ represent the respective dimensions of the feature maps in the VGG network.

The ‘*Adversarial Loss*’, as described below drives the generator in the direction where it can reach a point where its outputs can fool the discriminator. This is done to favor the solutions that lie on the manifold of the true optimal topologies. The generative loss can be described as

$$l_{Gen}^{SR} = \sum_{n=1}^N -\log D_{\theta_D}(G_{\theta_G}(I^{LR})) \quad (2)$$

Where $D_{\theta_D}(G_{\theta_G}(I^{LR}))$ is the probability that the reconstructed image $G_{\theta_G}(I^{LR})$ is a true optimal topology.

4. Data Set Characteristics and Experimental Setup

The dataset used in this study was a custom *labelled* dataset that was created using the Multi-Material Topology Optimization code described in [6]. The data set consists of optimized topologies of three materials whose Young's modulus ratio was defined as 3:2:1. The optimal topologies were generated with void volume fractions ranging from 0.2 to 0.5 with a 0.01 increment. The material volume fraction was divided into the ratios given in table 1.

Table 1 Material Distribution Ratios of Optimal Topologies in the Dataset

1 Material		
1		
	2 Material	
	1:01	2:01
	1:02	2:03
	1:03	3:02
		3 Materials
	1:01:01	2:01:01
	1:01:02	2:01:02
	1:01:03	2:01:03
	1:02:01	2:02:01
	1:02:02	2:02:03
	1:02:03	2:03:01
	1:03:01	2:03:02
	1:03:02	2:03:03
	1:03:03	

With the above-described material ratios and the void volume fraction sweep, there were 589 unique input data points. Of these 589 input data points, 250 *equi-spaced* data points were selected and optimal topologies were generated for *Cantilever and MBB* boundary conditions. The mesh size that is used in the individual experiment is described in table 2. The data set was split into two independent sets. Testing data that consists of 80% of the data and the validation containing the remaining 20% of the data. The environment that was used for the study is as follows: *Python – 3.8.8, TensorFlow – 2.4.1*, Training was performed on an *Nvidia GPU*.

The objective of this study was to evaluate the Network Architecture to predict the optimal topology in its existing state. So, as an initial proof-of-concept, three experiments were performed as described in the table below.

Table 2 Description of Experiments Performed.

Experiment	Boundary Conditions	Mesh Size input	Number of Epochs	Time till Training Completion	Number of data Points
Exp-1	Cantilever	40x20	5000	22 Hrs	251
Exp-2	Cantilever	100x50	5000	24 Hrs	251
Exp-3	Cantilever + MBB	40x20	6000	30 Hrs	502

5. Preliminary Results

The preliminary results (shown in the appendix) of the experiments performed clearly demonstrate the network's capability to map the features of the low-resolution input image to the corresponding features in the high-resolution image. The best results obtained were from Exp-1 in the single material case where, the optimal topology prediction visually matches the target topology. In the two- and three-material cases, there is still excess noise which is the case in Exp 1, Exp 2, Exp 3. Based on the preliminary results it can be concluded that, despite the networks capabilities, it struggles to handle multiple boundary conditions as seen from the results of Exp -3. Furthermore, the presence of noise within the predicted topology and outside, indicates the inadequacies of only using loss functions from the literature from Image Processing. A *physics-based loss function* in tandem with the existing loss function might improve the quality of the results.

Acknowledgments

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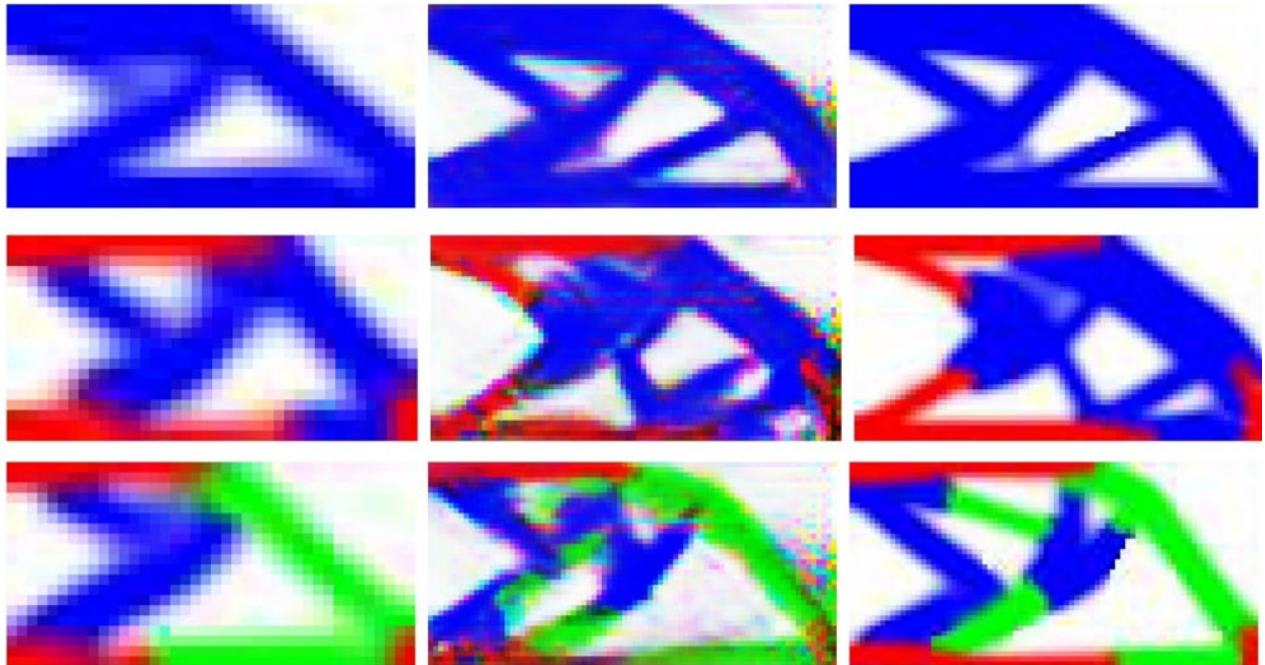
Annex

Experiment-1

Low-Resolution Input

Generator Output

True High-Resolution Output

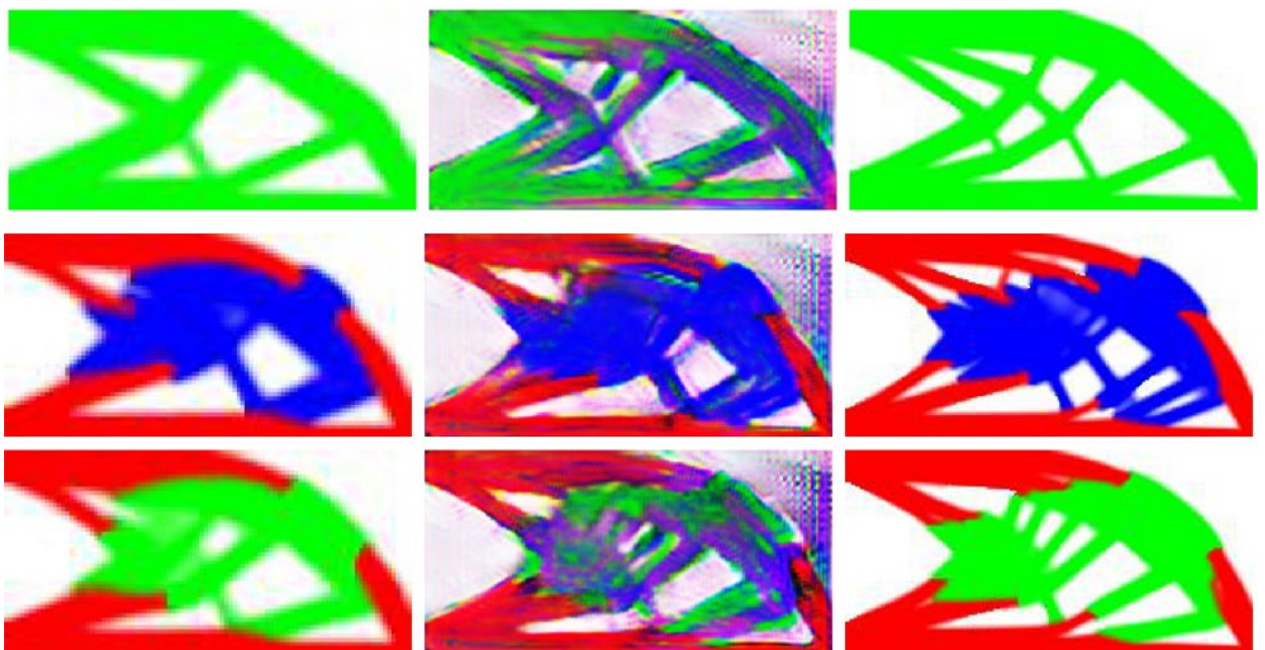


Experiment-2

Low-Resolution Input

Generator Output

True High-Resolution Output

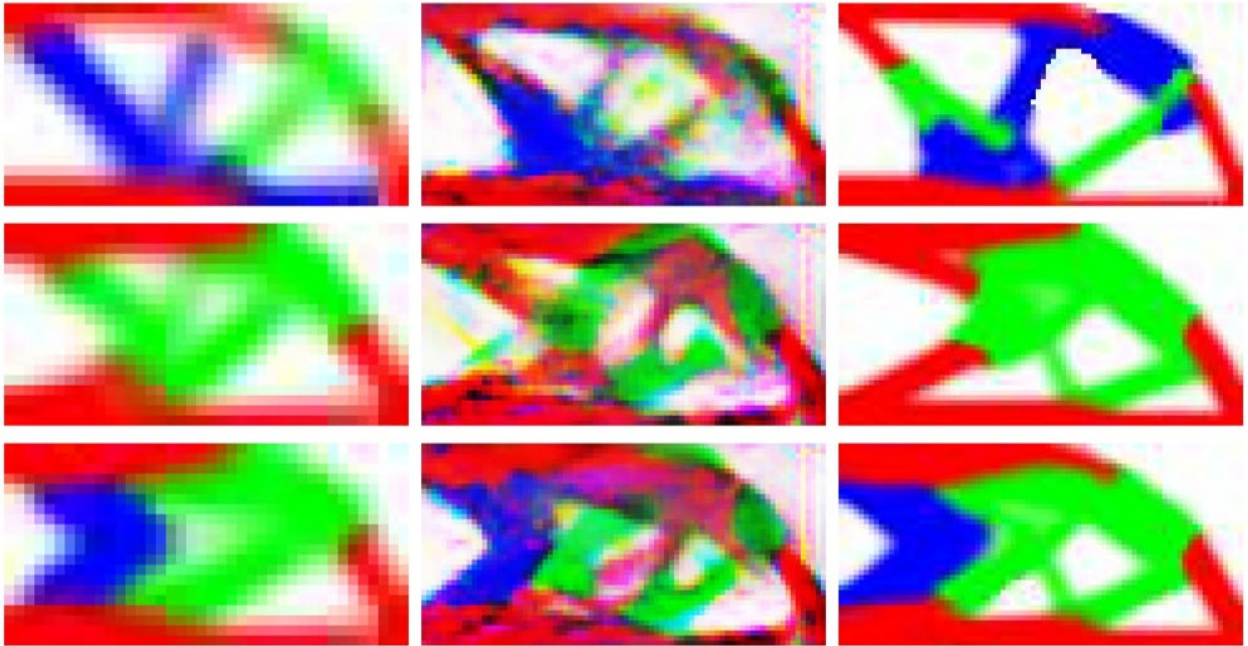


Experiment-3

Low-Resolution Input

Generator Output

True High-Resolution Output



GitHub Repository: <https://github.com/Anirudh-Kanthamraju/Multi-Material-Topology-Optimisation>