A Data-Driven Investigation and Estimation of Optimal Topologies Under Variable Loading Configurations

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Abstract. We explore the feasibility and performance of a data-driven approach to topology optimization problems involving structural mechanics. Our approach takes as input a set of images representing optimal 2-D topologies, each resulting from a random loading configuration applied to a common boundary support condition. These images represented in a high dimensional feature space are projected into a lower dimensional space using component analysis. Using the resulting components, a mapping between the loading configurations and the optimal topologies is learned. From this mapping, we estimate the optimal topologies for novel loading configurations. The results indicate that when there is an underlying structure in the set of existing solutions, the proposed method can successfully predict the optimal topologies in novel loading configurations. In addition, the topologies predicted by the proposed method can be used as effective initial conditions for conventional topology optimization routines, resulting in substantial performance gains. We discuss the advantages and limitations of the presented approach and show its performance on a number of examples.

Keywords: Data-driven design, topology optimization, dimensionality reduction

1 Introduction

Efficient use of material is a key priority for designers in many industries including automotive, aerospace and consumer product industries [1–3]. Optimizing material layout to satisfy a specific performance criteria, i.e. topology optimization is thus a crucial part of engineering design process. With recent advances in manufacturing technologies, topology optimization now attracts even more attention [2]. So far, various optimization algorithms including genetic algorithms, method of moving asymptotes, level sets and topological derivatives have been studied for structural topology optimization [1, 4–8].

Although structural optimization algorithms are becoming computationally more efficient with time, the need for a large number of iterations can rarely be avoided due to the essence optimization theory. Even with very small alterations in the design constraints, a structurally optimum topology can not be predicted
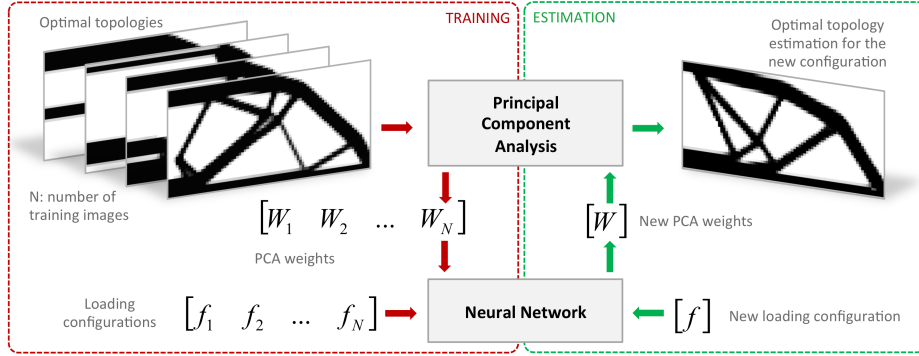
Fig. 1. Overview of our approach for optimal topology estimation.

directly by a human from physical principles due to the complex nature of the problem. Based on this observation, we explore how known solutions to topology optimization problems can be exploited to generate a new design for a novel set of loading configurations. Here, the main challenge is to find a mapping between design constraints and the resulting optimal topologies. With this motivation, we present a data-driven approach to topology optimization involving structural mechanics and explore its feasibility and performance.

Our approach takes as input a set of images representing optimal 2D topologies, each resulting from a conventional optimization method, and generates an optimal topology estimation for a novel set of design constraints (Fig. 1). In this study, only the variation in loading configurations is explored under a fixed set of structural boundary conditions. In the proposed method, the set of input images (known optimal topologies) which are represented in a high dimensional image space are projected onto a lower dimensional space using Principal Component Analysis (PCA). Once the dimensionality is reduced, a mapping between the loading configurations and the optimal topologies represented as PCA component weights is computed using a feed-forward neural network. Using the trained mapping, we estimate the PCA component weights for a novel loading configuration, and use the resulting estimation to synthesize a solution in the image space. This image represents our estimation of the optimal topology, given a novel loading configuration.

The primary goal of this study is to explore the feasibility and effectiveness of a data-driven approach to structural topology optimization problems. Our results show that the proposed method can successfully predict the optimal topologies in different problem settings, but the results are sensitive to the complexity and the size of the design space dictated by the loading configurations. However, independent of the problem complexity, a practical advantage of the proposed system is that the resulting topology estimations serve as effective initial conditions that facilitate faster convergence in conventional topology optimization problems.

2   Related Work

In this section, we review the literature on structural topology optimization techniques, use of data analysis and dimensionality reduction approaches as well as mapping methods.

Structural Topology Optimization: Topology optimization is one of the most powerful technologies in structural design [1, 7]. It optimizes the shape and material connectivity of a domain through the use of finite element methods together with various optimization techniques [8].

Density-based topology optimization approaches including homogenization methods [9, 10] and solid isotropic microstructure with penalty (SIMP) methods [11, 12] are one of the most popular methods in the literature. These methods approach topology optimization in a way that defines geometry by optimizing material distribution in the domain. A detailed review on density based topology optimization methods can be found in [13–15]. Another approach for structural topology optimization is based on topological derivatives and level-sets [8, 16, 17]. The optimization process utilizes the implicit description of the boundary to numerically represent the geometry. A recent work [7] discusses the level-set based topology optimization methods more deeply. In [15], topological derivative and level-set based methods in the literature are claimed to be very promising although they are not widely embraced by industries. Aside from the above methods, evolutionary approaches are also used for topology optimization, e.g. [4, 5]. However, the use of genetic algorithms are computationally expensive, thus they are suitable for only small scale problems [15].

Since topology optimization is an iterative and computationally demanding process, an efficient implementation of the above mentioned methods in various programming languages is also important for designers. In [18, 19], authors present two different versions of an efficient MATLAB code for structural topology optimization of classical Messerschmitt-Blkow-Blohm (MBB) beam problem. As an optimization technique, they implemented an available SIMP approach with slight modifications involving filters. In our approach, we utilize the available code in [18] to generate the initial optimized topologies for different loading conditions as a way to generate the pool of training data.

Data Analysis and Dimensionality Reduction: In data-driven methods, a pre-analysis of available data to extract informative characteristics is essential, especially for large multivariate data sets. To the best of our knowledge, there is no use of dimensionality reduction methods for structural topology optimization in the literature. Such methods are commonly used in engineering design and computer science (e.g. [20–25]). Commonly used dimensionality reduction methods include principal component analysis (PCA) [26], multidimensional scaling (MDS) [27], Isomaps [28] and locally linear embedding (LLE) [29].

PCA is an eigenvector based approach that uses an orthogonal transformation to convert the original data into linearly independent components. Dimensionality reduction is accomplished by representing data in terms of the linearly independent components that best explain the variance in the data. In MDS, high dimensional data is embedded into low dimensional space in such
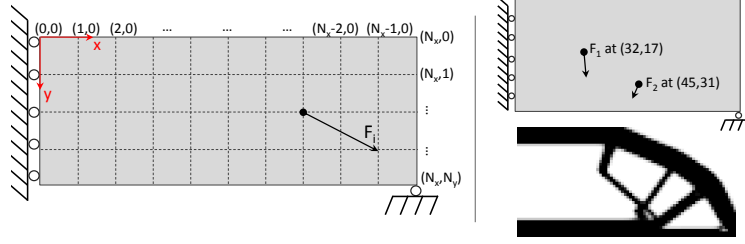
Fig. 2. Left: Design domain for topology optimization problem. Right: Example loading configuration and resulting optimal topology.

a way that pairwise distances between data points are preserved. Isomaps aim to preserve the geodesic distances in the manifold formed by the data. LLE is a neighborhood-preserving dimensionality reduction method. It projects high-dimensional data into lower dimensional global coordinates by utilizing different linear embeddings for each data point locally. In the proposed work, we use PCA to analyze the dominant characteristics of our data set and to reduce the dimensionality accordingly. However, the aforementioned dimensionality reduction methods could be adopted into the workflow of the proposed techniques without loss of generality.

One important aspect of the proposed work is the mapping between an input configuration (in our case the loading configuration) and the resulting optimal topology. Note that a PCA-based learning and topology reconstruction is readily implementable with the available training images. However, the key need is to be able to specify a novel loading configuration, from which the optimal topology can be estimated. In previous work, most methods employ a linear mapping between the input feature vectors and the resulting PCA reconstructions [23, 30]. However, the relationship between the input loading configurations and the resulting topology reconstructions in our domain is highly non-linear as demonstrated in the following sections. To address this challenge, we present a mapping technique that uses feed-forward neural networks. This generative method provides a significant improvement over linear regression models.

3   Problem Formulation

We illustrate our approach using the Messerschmitt-Blkow-Blohm (MBB) beam problem, a classical problem in topology optimization. The rectangular beam is represented by an N_x-by-N_y image as illustrated in Fig.2. The design domain is discretized by square finite elements each of which corresponds to a pixel in the gray-scale images. A number of external forces, F_i $(i = 1, ..., k)$, can be applied to the beam at the nodes represented by (x_i, y_i) coordinates. Applied forces can be in any direction, i.e. they can have both horizontal and vertical components with magnitudes ranging between $[0, 1]$. Boundary support conditions are shown in Fig.2. Note that this model is used to facilitate discussions; the following sections
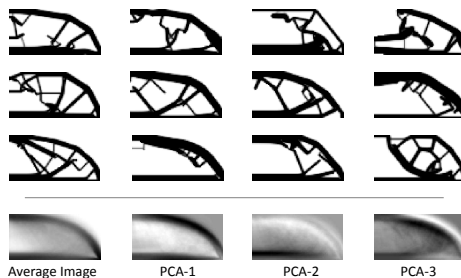
Fig. 3. Top: Example training samples. Bottom: Average image and first three PCA images.

will demonstrate results on variations of the domain, boundary conditions and loading configurations.

Our aim is to estimate the optimal topology for such problems when a novel loading condition is prescribed. For this, we generate a pool of training data where each training sample consists of a known loading configuration, and a corresponding optimal topology. To compute the optimal topologies given the loads, we use a density-based topology optimization algorithm given in [18]. The method assigns a density value between $[0, 1]$ to each pixel in the domain that dictates the Young's modulus for that particular pixel with lighter colors representing weaker portions. The optimization works toward minimizing the compliance resulting from the generated gray-scale structure. Resulting images with a varying Young's modulus field represent the optimal topologies for corresponding loading configurations. Collection of these images establish an input database to our method.

4   Component Analysis

Principal component analysis is useful for analyzing the input data to identify the significant features inherent in the data, as a way to facilitate dimensionality reduction with minimal information loss.

Suppose we have M images each with N_x-by-N_y resolution in our dataset. Then, gray-scale density values for images are stacked into M column vectors $\mathbf{t_j}$ $(j = 1, ..., M)$ of length $l = N_x \times N_y$ to form the high-dimensional image space feature vectors. To mean-shift the data, the average image $\mathbf{\bar{t}}$ is calculated and subtracted from each sample in the training dataset, i.e. $\mathbf{t_j} - \mathbf{\bar{t}}$. In Fig.3, a randomly selected subset of the example training dataset (with 1000 samples), the resulting mean image, and the first three PCA component images are shown.

Let the mean centered image be $\mathbf{u_j} = \mathbf{t_j} - \mathbf{\bar{t}}$, we can store our entire data set into lxM matrix $\mathbf{U}$ to perform principal component analysis. Each column of $\mathbf{U}$ represents one mean centered image. In order to obtain the eigenvectors (i.e. principal components), the covariance matrix can then be constructed as $\mathbf{C} = \mathbf{UU^T}$. However, size of the matrix $\mathbf{C}$ is l-by-l and calculating l eigenvectors
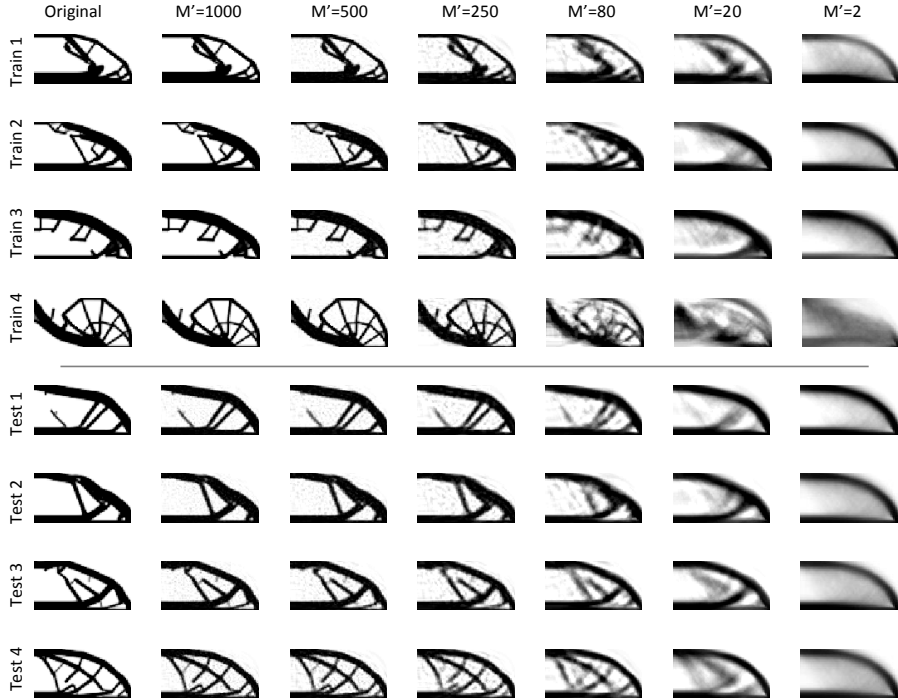
Fig. 4. Reconstruction of example samples relative to the different number of eigencomponents used. Each row corresponds to a different example. The upper half illustrates reconstructions for sample training images. The lower half shows the same for test images (i.e., images not involved in the construction of PCA).

may not be practical. As mentioned in [22], if the number of features is larger than the number of training images ($l >> M$), there can be at most ($M - 1$) useful eigenvectors (corresponding to non-zero eigenvalues) instead of l. These eigenvectors of l-by-l $\mathbf{UU^T}$ matrix can be determined from the eigenvectors of M-by-M matrix $\mathbf{U^T U}$ as $\mathbf{c_j} = \mathbf{Uv_j}$ where $\mathbf{v_j}$ is eigenvectors of $\mathbf{U^T U}$. In this paper, $\mathbf{c_j}$'s will be referred to as eigen-images. Each input topology optimization image can then be represented as a linear combination of these M eigen-images, resulting in a PCA weight vector of $\mathbf{W_i} = [w_1, w_2, ..., w_M]^T$. Even using only a few number of eigen-images, M', associated with the largest eigenvalues, a good approximation of an image can be obtained. In Fig.4, reconstruction of sample topology optimization images with different number of eigen-images are illustrated. In this example images are 80-by-40 pixels. There are 1000 training images generated by random assignments to the loading configurations and solving for the corresponding optimal topologies. Since PCA is limited by the number of training samples ($1000 < 3200$), the number of non-zero eigen-images is 1000. Here, it can be observed that a remarkably small number of eigen-images are sufficient for a high-fidelity reconstruction of the original images. Note that
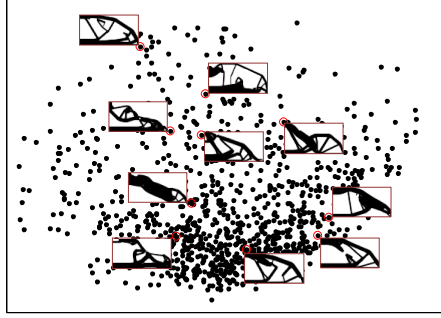
Fig. 5. Training images projected into the 2D space created by the first two PCA components.

Fig.4 shows example reconstructions of samples that were used during training (train), as well as for novel samples that were not part of the training (test). In remainder of the paper, we will use the first 80 eigen-images in our examples.

Fig.5 shows the dataset of 1000 training images when projected to the space created by the first two eigen-vectors.

To quantify the mismatch between an original image and its reconstruction, we use the L_1 distance between the two images:

$$d(t_1, t_2) = \frac{\|t_1 - t_2\|_{L1}}{length(t)} \tag{1}$$

Fig.6 illustrates this difference. This metric provides a value between $[0, 1]$ where 0 represents identical images.
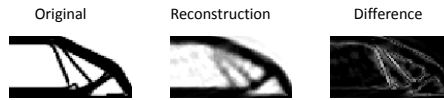

Fig. 6. Difference between an example topology and its reconstruction using first 80 eigen-images.

When properly weighted, eigen-images can be linearly combined to create an approximation to a new image representing a new optimized topology. For this purpose, a set of PCA weights associated with the corresponding loading configuration should be estimated. We deal with this problem by introducing a mapping function between the loading configurations, **F** and the PCA weights, **W** of the training samples. Details of this process will be described in the next section.

5   Mapping Load Configurations to Optimal Topologies

A useful application of PCA decomposition is that with a low dimensional data, a mapping between the original input and the PCA vector space can be created. In this section, we present a neural network approach to generate this mapping, specifically between the force vector indicating load conditions ($\mathbf{F_i}$) and the PCA weights ($\mathbf{W_i}$).

Theoretically, a neural network with sufficiently complicated structure and training samples is able to learn any input-output relationship for regression. However, with high dimensional data, such regression would require considerably high number of training samples and number of hidden layer nodes resulting in impractical convergence time in the training stage [31]. We present results that indicate with limited amount of data and empirically determined number of hidden layer nodes, the neural network can learn the structure of the topology optimization gracefully.

In our experiments, we utilize a fully-connected feed-forward single hidden layer neural network [31] as the learner with the following input and output configurations:

1. The input vector of the neural network is composed of four real numbers (x and y positions and magnitudes) for each force in the problem.
2. The output vector of the neural network is composed of 80 real numbers corresponding to the PCA weights.

We train the resulting neural network with scaled conjugate gradient algorithm [31], we use 80 nodes in the hidden layer for all examples presented in the results section.

6   Results and Discussions

With a sufficient number of training samples, the neural network can generate a precise mapping between the loading configurations and the corresponding PCA weights. However, the resulting estimation can be affected by the number of eigen-images used to express that image. Fig.7 illustrates the performance of our approach on several test samples for a specific design domain (middle configuration in Fig.9. In this configuration, PCA and neural network are trained with 400 samples and tested with randomly generated loading configurations. As previously mentioned , only the first 80 eigen-vectors with highest variances are used for reconstruction and estimation. Fig.7 shows the original samples and their corresponding estimations using our method. Note that estimation involves using the neural network to map the loading configuration into the PCA weight vector, followed by a PCA based reconstruction using 80 samples.

As a convenient method, linear regression is one of the most favored approaches for learning the mapping between a set of feature vectors [23]. However, the relationship between the loading configurations and the PCA weights in such a high dimensional space may not be accurately predicted by this approach. In
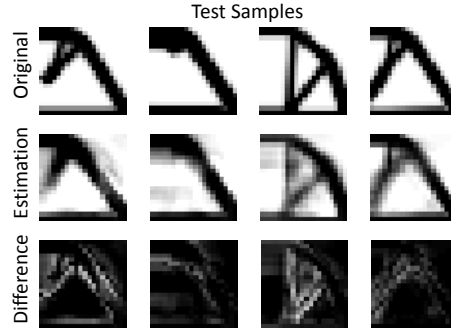
Fig. 7. Difference between example topologies and their neural network estimations using the first 80 eigen-images.

Fig.8, we compare the performance of neural network versus linear regression on a sample test image. Both mapping methods are trained with 400 samples. Note that linear regression fails to reproduce some of the details in the optimal topology.
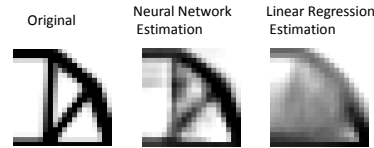

Fig. 8. Comparison of neural network estimation with linear regression estimation of an example topology.

Fig.9 illustrates the performance of our algorithm on several test configurations. In the top row, basic representations of the design problems are illustrated. Here, boundary conditions and loading configurations are shown. Red areas represent spaces where forces can be placed. In the following row, reconstructions of several test samples using eigen-images are presented. Since only the first 80 eigen-images are used to construct an image, there are slight differences from the original optimal topologies. We compare our estimation results with the optimal topologies in the third row. As the design problem becomes more complex, the accuracy of resulting estimations reduces since the number of training samples for neural network may fail to be sufficient. Better estimations can be made using a higher number of training samples for more complex problems. In the last row of Fig.9, a histogram showing the distribution of error between the optimal topology and the estimation result of our approach among 100 test samples is given for each design configuration. Although we use a limited number of train-
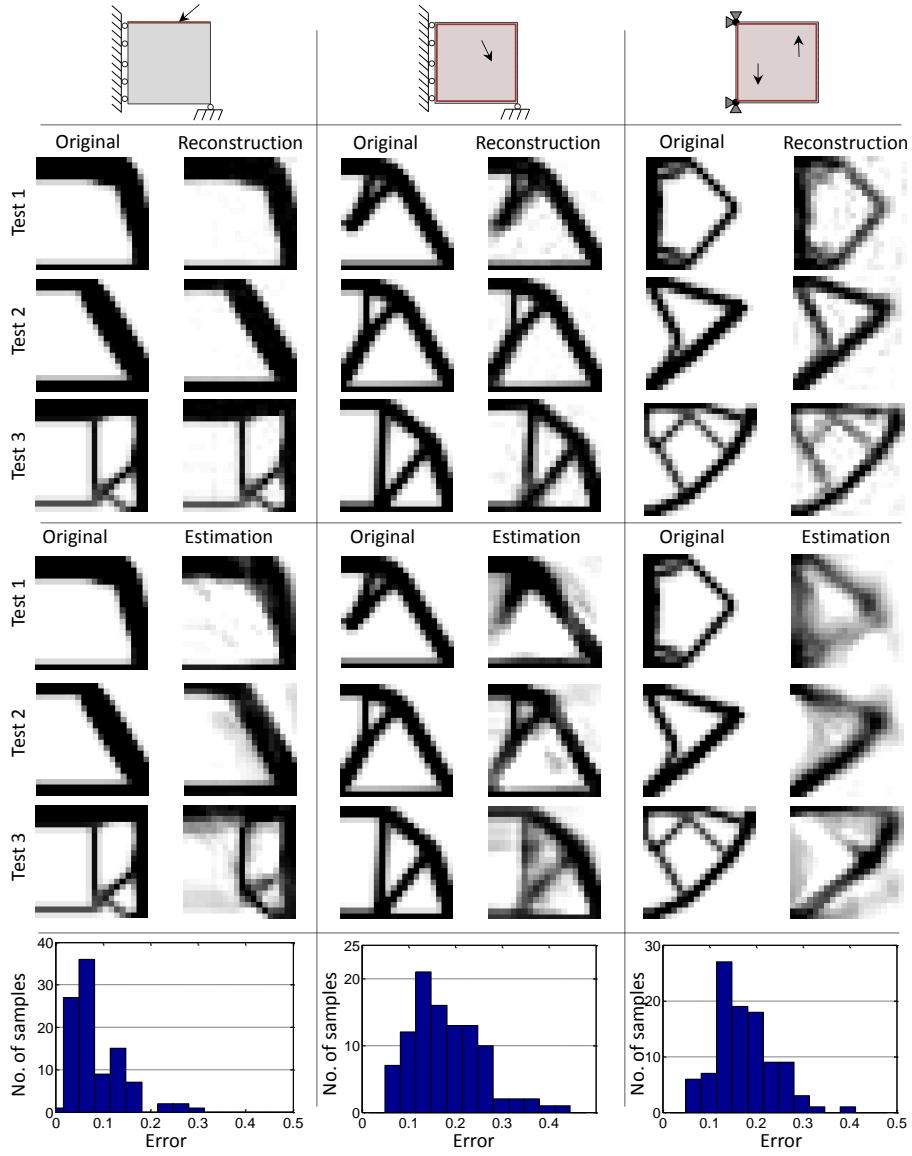
Fig. 9. Performance of our method for different design configurations. Left: single force anywhere on the top surface in any direction and magnitude. Middle: single force anywhere in the domain in any direction and magnitude. Right: two vertical forces anywhere in the domain in any magnitude. Reconstruction refers to the PCA reconstruction of the sample using the eigen-images. Estimation uses the proposed neural network, followed by PCA reconstruction.
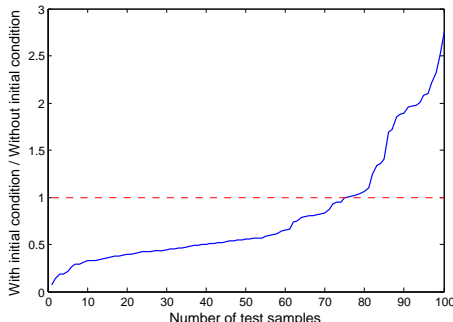
Fig. 10. Convergence time ratio of 100 samples with and without using the neural network result as an initial condition to subsequent optimization. Configuration used: Fig.9 (left).

ing samples and PCA components, the main structure for optimal topologies can be estimated.

In design problems involving complex loading configurations, the reconstruction accuracy may decrease visually (e.g., estimations in the last column of Fig.9). However, even in those cases, our optimal topology estimates can be used as an initial condition for a conventional topology optimization algorithm, e.g. [18, 19], to reduce the convergence time. Fig.10 shows the effect of using our estimation as an initial condition. For around 70% of 100 test samples, reduction in convergence time is observed for the posed problems. This gain can be even more significant for larger and more complex design domains.

7   Conclusions

We explore the feasibility and performance of a data-driven approach to topology optimization problems involving structural mechanics. We take a set of optimal topology examples for a given configuration, and project them into a lower dimensional space with PCA analysis. We then learn a mapping from loading configurations to optimal topologies using neural networks. Using the trained network, we studied the performance of estimating optimal topologies for novel loading configurations. Our results show that the proposed method can successfully predict the optimal topologies in different problem settings. Moreover, we also prove that the topologies predicted by the proposed method are effective initial conditions for faster convergence in subsequent topology optimization. We believe such time and computational power savings will be greater as the problem size and complexity increase. Thus, a valuable future direction is the application of the proposed method for 3D topology optimization.

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