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Clustering Topologically-Optimized Designs based on Structural Deformation

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Abstract. Topology optimization can be used to generate a large set of lightweight structural solutions either by changing the constraints or the weights for different objectives in multi-objective optimization. Engineers must analyze and review the designs to select solutions according to their preference towards objectives such as structural compliance and crash performance. However, the sheer number of solutions challenge the engineers' decision-making process. An automated way of summarizing solutions is to cluster groups of similar designs based on a suitable metric. For example, with the Euclidean metric in the objective vector, design groups with similar performance can be identified and only the representative designs from the different clusters may be analyzed. Since the deformation behavior of a structure is an important design feature, in this work, we investigate the use of manifold learning algorithms to identify and group similar designs using the nodal displacement data. The proposed approach can process the volumetric deformation of geometries with completely different topologies. In this study, we couple the manifold learning techniques, t-distributed Stochastic Neighbor Embedding (t-SNE) and Uniform Manifold Approximation and Projection (UMAP), with the clustering algorithms, k-means and Ordering Points To Identify the Clustering Structure (OPTICS), to identify the representative deformation modes. Using Gaussian Random Fields (GRF) to create artificial displacement fields, we generate a labeled dataset with different modes, which enabled us to evaluate our method using classification accuracy, precision, recall, and F1-score. Finally, using our approach, we successfully distinguished between similar and non-similar designs in the results from topology optimization.

Keywords: deformation behavior, topology optimization, manifold learning, Gaussian random field, classification metrics

1 Introduction

Topology Optimization (TO) [1] is a mathematical method that optimizes material layout within a given design space for a given set of loads, boundary conditions, and constraints, with the goal of maximizing the performance of a structure. Thanks to the progress in the manufacturing technologies, like 3D-printing,

as well as the latest research developments in the TO field, these methods are increasingly used across different disciplines, including civil engineering [2] and vehicle crashworthiness [3, 4, 5, 6, 7, 8, 9]. When conflicting objectives such as crash energy absorption and structural compliance are used, a multi-objective TO approach creates a Pareto front of optima, from which engineers need to select solutions using additional criteria such as appearance [10].

A large set of solutions might impede the engineers' decision-making process. To mitigate this problem, Hagg et al. [11] cluster similar solutions and obtain a representative solution from each group. They use machine learning methods, such as Principal Component Analysis (PCA) [12], autoencoder [13], t-distributed Stochastic Neighbor Embedding (t-SNE) [14], kernel-PCA [15], and Isomap [16] to map the set of solutions to a similarity space and cluster similar solutions into different classes. Similarly, Dommaraju et al. [10] use PCA to develop a metric for geometrical differences and identify prototypical designs in the Pareto front. In a separate research paper [17], they use an autoencoder, a non-linear dimensionality reduction method, to identify geometrical prototypes.

Since the deformation behavior of a structure is important, we investigate methods to cluster based on deformation modes. Garcke et al. [18] and Sible et al. [19] demonstrate the use of non-linear dimensionality reduction methods on the displacement fields of a set of structures to find designs with similar deformation modes, including complex deformations from crash simulations. However, their approaches might not be suitable for TO designs since they assume isometric deformation. Furthermore, we want to analyze TO designs with very different topologies. Another interesting approach, proposed by Diez et al. [20], combines decision tree and rule mining to identify different deformation behaviors in crash simulation results but it requires labeled datasets.

In this study, we propose the use of manifold learning methods, t-SNE and Uniform Manifold Approximation and Projection (UMAP) [21], to perform dimensionality reduction on the nodal displacement data. The resultant data can then be processed by clustering algorithms such as k-means [22] and OPTICS (Ordering Points To Identify the Clustering Structure) [23] to identify structures with similar deformation behavior. Dimensionality reduction methods require that the nodal displacement data is consistent across the structures. So, we retain the elements that are allotted very small densities by the TO method.

To evaluate the performance of the proposed methods, we use two types of datasets. The first dataset is created by applying artificial displacement fields on cube-shaped structures to obtain different deformation modes. We can then investigate if our proposed approach correctly identifies the different modes. The second dataset contains TO results. While the first labeled dataset allows us to evaluate our approach using classification metrics, the second dataset allows only visual evaluation.

This paper is structured as follows. In Section 2, we briefly discuss the proposed workflow of our method. In Section 3, we discuss the two types of datasets and how to generate them while the results and conclusions are presented in Section 4 and Section 5, respectively.

2 Method

Figure 1 shows the proposed workflow to find the deformation modes where N is the number of structures in the set, M is the dimension of the nodal displacement field, and P is the number of dimensions in the similarity space produced by the manifold learning algorithm.

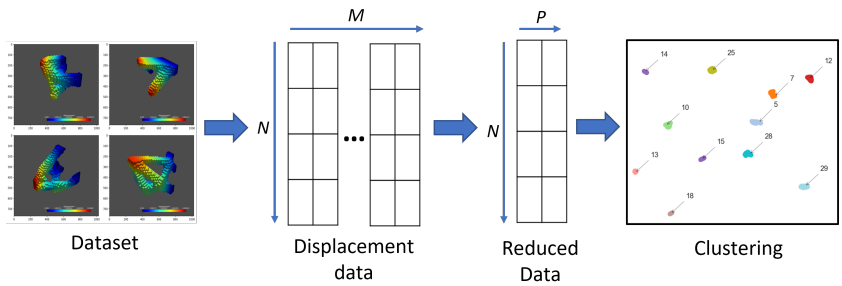


Fig. 1: General workflow to obtain design clusters. Displacement data are preprocessed into a matrix of size $N \times M$, then a manifold learning algorithm reduces the size of the matrix to $N \times P$. Finally, a clustering algorithm tries to find clusters and obtain representative designs from each cluster.

Instead of removing the low-density elements, data of all the nodes in the cube is used as input for the dimensionality reduction method to ensure consistency of data across all designs. Therefore, with our approach, we can compare the deformation behavior of topologically different structures, as shown in Section 4.

To reduce the dimensionality of the nodal displacement field, we use the manifold learning methods, UMAP, and t-SNE, which non-linearly reduce the data. We consider two different clustering algorithms: k-means [22], a popular inexpensive clustering algorithm, and OPTICS [23], a density-based clustering algorithm. Silhouette method [24] is used to set the appropriate number of clusters for k-means algorithm.

3 Dataset Generation

In this section, we discuss the datasets used to test our approach, namely the artificial and topology optimization datasets. The initial finite element mesh that we use for both types of dataset is shown in Figure 2.

3.1 Labeled Test Dataset

3.1.1 Gaussian Random Field To generate a labeled test dataset of deformed structures, we apply displacement fields generated by Gaussian Random

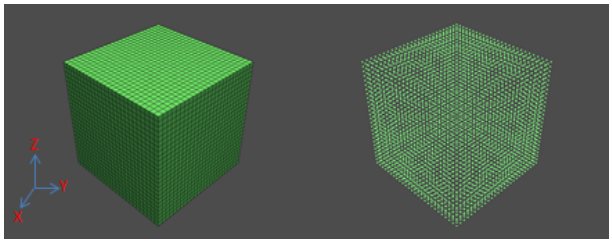


Fig. 2: Finite element model in a cube domain, each side is 1 m in length, with 15,625 elements. The material properties are mass density=7.83 10^{-9} ton mm^{-3}, Young's modulus=2.07 10^5 MPa, and Poisson's ratio=0.33.

Field (GRF) [25] on cube-shaped structures. GRF determines the displacement field using the mean and the covariance function. Given the displacements of specified nodes, the mean function determines the most probable positions of the unspecified nodes while the covariance function incorporates the uncertainty associated with the field. Using GRF, we can easily specify the deformation mode and generate the corresponding deformed structures much more quickly compared to finite element simulations.

3.1.2 Dataset Generation To generate the displacement fields seen in mechanical structures, we compose the displacement field using the main field and the noise field. We also add randomness to the selected node positions, displacement magnitudes, and displacement directions to increase the variation across designs and to challenge our approach.

To apply main field on an undeformed cube structure, we randomly select one or more nodes on the surface of the cube. A few examples are shown in the top row of Figure 3. The selected two nodes act as specified nodes while the remaining nodes act as unspecified nodes. After that, we can calculate the mean displacement of the structures using the mean of GRF. The resulting set of structures are shown in the bottom row of Figure 3.

To generate a noise field, it is possible to use the covariance matrix of a GRF. However, due to the large number of nodes in our cube structure, it is too expensive to create the covariance matrix. Therefore, we use a different approach to create the noise field. We randomly select 100 nodes on the cubic surface, which are then assigned displacement vectors with random magnitudes and directions. To deform the structure, we can compute the mean node positions using GRF. The resulting cube structure with noise field is shown in Figure 4. By adding different noise fields to the main field, multiple deformations of a single mode can be obtained. The resulting structures are shown in Figure 5.

To make the separation of the deformation modes more challenging, the amount of noise level for each mode can be varied. Noise level is defined as the ratio between the maximum displacement of the noise field and the maximum displacement of the main field. Deformed models with different noise levels are

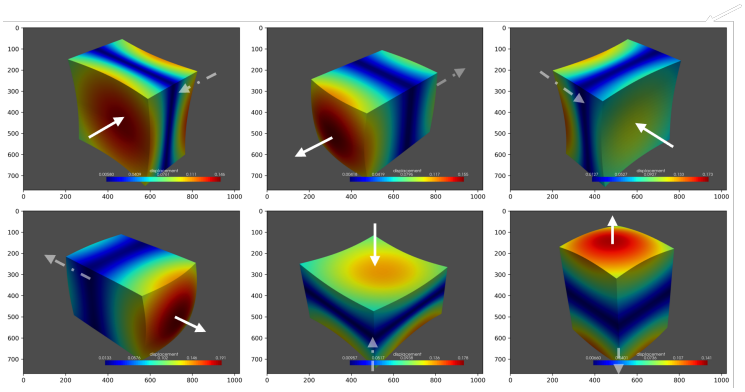
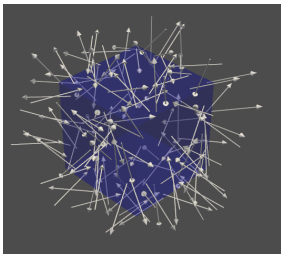
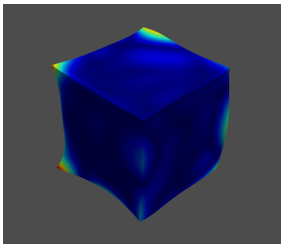


Fig. 3: Examples of our labeled test dataset. We apply displacement vectors on two opposing faces of the cube.

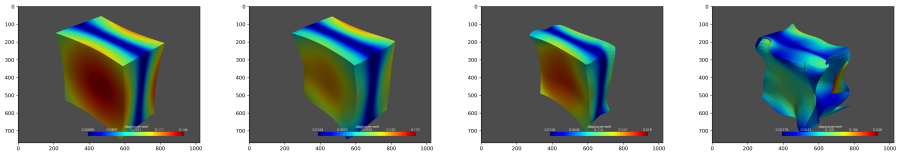


(a) Select random nodes on the surface



(b) Deformed cube model

Fig. 4: Deforming model with noise field



(a) Noise level=0% (b) Noise level=20% (c) Noise level=50% (d) Noise level=100%

Fig. 5: Models deformed using different noise levels

shown in Figure 5 where the maximum displacement of the main field is 0.2 m. For visualization purpose, the displacement is scaled up by a factor of two. For higher noise levels, the deformations become less realistic. So a noise level of 50% is chosen.

In total, there are 5 sets of node selections. Each set of node selections produces 6 different deformation modes, with 20 structures for each mode. Therefore, we have 600 structures in this dataset with 30 deformation modes.

3.2 Topology Optimization Design Dataset

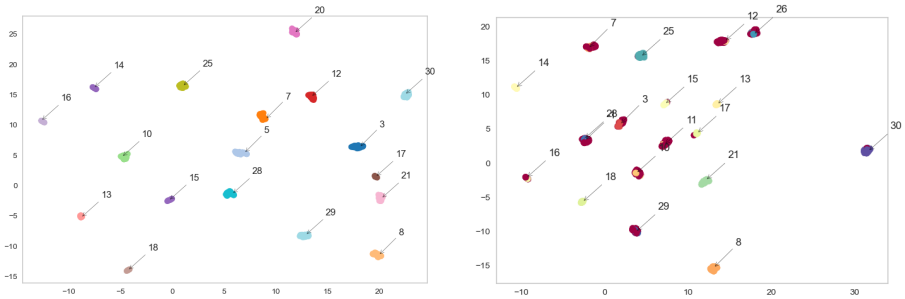
The dataset of TO designs used in this paper are the results of Solid Isotropic Material with Penalization (SIMP) TO [1]. Move limit parameter used is 0.1 while the filter radius and volume fraction are 0.1 and 0.3, respectively. For each optimization, one of the faces is fixed and the cubic structure is optimized for two arbitrarily applied loads. In total, there are 100 topologically different structures in this dataset. Several structures in the TO design set can be seen in Figures 9 and 10.

4 Results and Analysis

4.1 Results on Labeled Test Dataset

In this subsection, we show the results of applying our approach on the labeled test dataset with a noise level of 50%. In Figure 6, we show the plots of using UMAP with k-means (Figure 6a) and OPTICS (Figure 6b). As seen in Figure 6, both k-means and OPTICS could easily cluster the structures in our dataset, although k-means does not perform well when the clusters are located very close to each other.

We investigate the clustering accuracy obtained using UMAP to other dimensionality reduction methods: PCA, k-PCA, and t-SNE. For reference, results with no dimensionality reduction are also used. With k-means clustering, there is no noticeable difference in classification accuracy (0.6) between the reduction methods for this dataset. However, with OPTICS as the clustering method, UMAP outperforms other methods (Figure 7).



(a) Clusters labeled by k-means

(b) Clusters labeled by OPTICS

Fig. 6: Identified clusters in the artificial dataset using UMAP.

4.2 Results on TO Design Dataset

In this subsection, we apply UMAP with k-means clustering on the TO design dataset. Using the silhouette method, we select 18 as the proper number of clusters. To show that our proposed cluster designs with similar deformation behavior, we visualize four structures from two clusters numbered 11 and 2 (Figure 8).

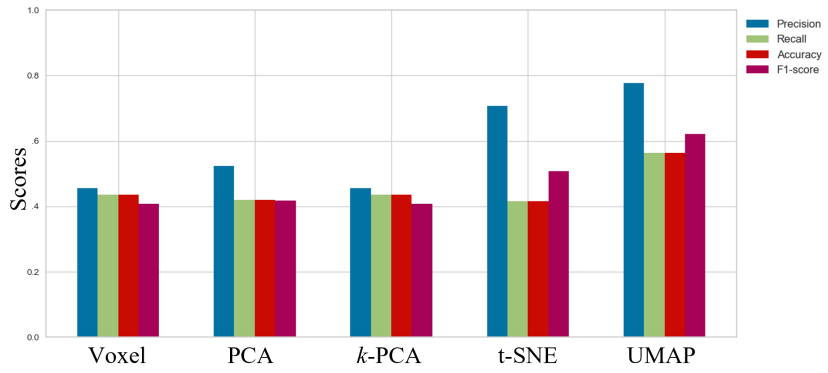


Fig. 7: Comparison of different dimensionality reduction methods based on precision, recall, accuracy, and F1-score. OPTICS is used for clustering designs.

Figure 9 shows four structures in cluster 11 which have similar circular deformation pattern in the middle, despite having different underlying topologies. Figure 10 shows another example cluster. Here, the structures have pronounced deformation in the fore-most corner.

5 Conclusion and Future Work

In this paper, we address the problem of clustering a large set of topologically different TO designs, based on the deformation behavior. We use manifold learning methods to perform dimensionality reduction and then use clustering algorithms to cluster designs with similar deformation behaviors. For a consistent node-to-node comparison, we retain the low-density elements of the TO designs. The main methods that we use for our work are t-SNE and UMAP for dimensionality reduction, and k-means and OPTICS to perform clustering.

To test our approach, we generated two datasets: a labeled dataset generated with GRF and a TO design dataset. With our approach, we successfully identified structures with similar deformation behavior on both datasets.

Future work may explore the applicability of our approach using different mechanical features, methods, or datasets. Interesting mechanical features to

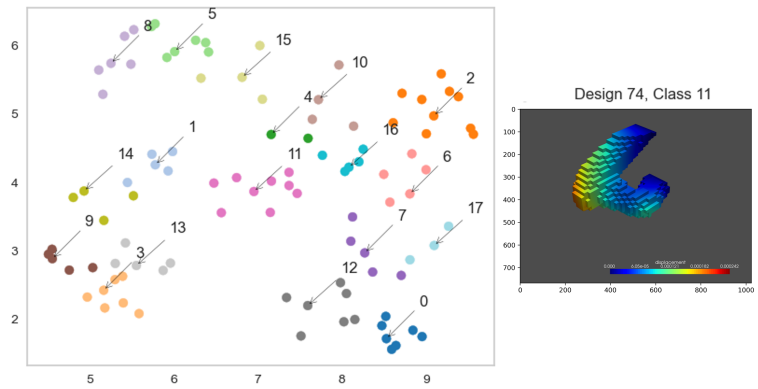
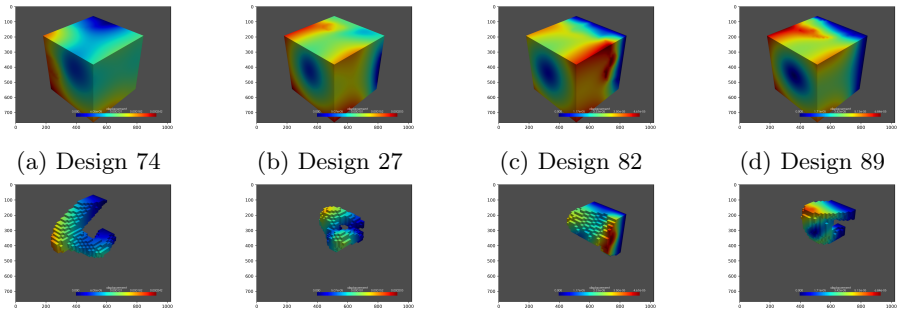


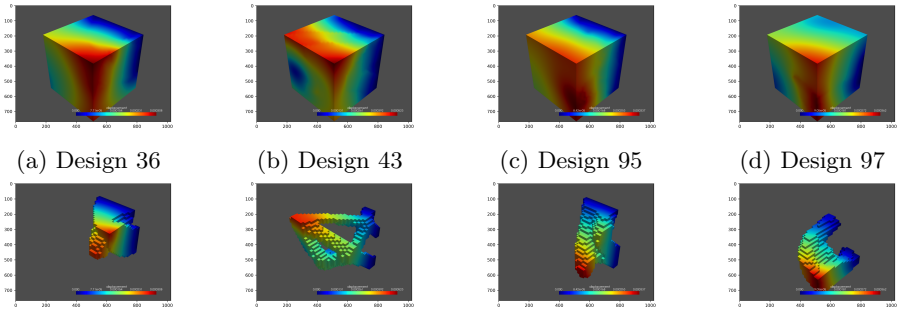
Fig. 8: TO designs mapped to 2-D by UMAP



(a) Design 74 (b) Design 27 (c) Design 82 (d) Design 89

(e) Design 74 (f) Design 27 (g) Design 82 (h) Design 89

Fig. 9: Different designs from class 11



(a) Design 36 (b) Design 43 (c) Design 95 (d) Design 97

(e) Design 36 (f) Design 43 (g) Design 95 (h) Design 97

Fig. 10: Different designs from class 1

explore are stress, strain, geometries, and displacement as time series. We might also explore other methods which could potentially separate different deforma-

tion behavior better than manifold learning methods, such as tree-based algorithms or neural-networks. If available, we could test our approach on larger datasets with more diverse TO designs to further test its performance.

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