Learning-based representations of high-dimensional CAE models for automotive design optimization

de Jesus de Araujo Rios, T.

8 Conclusions and Outlook

Specialists in any field intuitively exploit experience when approaching new optimization problems. Experience allows us to propose better initial solutions and settings for optimization algorithms than starting without any information about the target problem. As a consequence, transferring experience allows us to accelerate the convergence of optimization problems and improve the quality of the optimized designs. However, if performed in an unsystematic fashion and by a small team of engineers, the exploitation of experience is limited and biased by the expertise of the team. Therefore, to exploit experience transfer in engineering optimization more efficiently, a systematic approach for learning a transferrable notion of experience is required, which starts by defining a method for representing different problem domains.

Engineering optimization data are high-dimensional, unstructured and have no canonical representation. Thus, classical machine learning algorithms have limited capability for abstracting engineering models into a common representation. However, a novel class of algorithms has been recently introduced, the so-called geometric deep learning (GDL), which extends the applications of machine learning to unstructured (geometric) data. In particular, point-based autoencoders are suitable for learning distributed low-dimensional representations of computer aided engineering (CAE) models. Furthermore, by sampling designs in the latent space, these autoencoders can perform as shape-generative models for automated frameworks. Hence, applying GDL techniques on engineering data is a promising approach for learning representations of CAE models for an experience-based engineering optimization framework, which is the main subject of this dissertation.

In the remainder of this chapter, the conclusions drawn from the findings of the research that led to this dissertation are presented (Section 8.1). Also, in Section 8.2, potential directions for future research that builds up on the work presented in this dissertation are discussed.

8.1 Conclusions

As the representation of CAE data is not canonical, a first step for learning design features from CAE data is to define which combination of data type and methods are the most suitable for the task. Hence, in Chapter 3, a review of the state of the art on geometric data and geometric deep learning is presented, which answers *RQ1*: *"How is geometric data defined in the context of design optimization problems?"*. In the context of this dissertation, the term *geometric data* refers to mathematical representations of 3D objects, which are utilized in simulation-based design optimization problems. The most widespread geometric representation in engineering is the polygonal mesh, which is utilized for simulating the performance of 3D designs. However, learning shape-generative models based on non-isomorphic meshes is a challenge and currently available approaches have limited generative capabilities.

Differently, 3D point clouds represent objects of different topology with more flexibility and their manipulation requires less processing effort than polygonal meshes. Therefore, from the reviewed representations, 3D point cloud data are the most suitable for learning compact representations of CAE models, which addresses the question *"How can compact representations of 3D designs for engineering optimization be learned from CAE data?"* (*RQ2*). Furthermore, based on the review on GDL techniques, point-based deep autoencoders learn distributed representations of high-dimensional data and have shown promising results as shape-generative models for 3D objects. Therefore, in this research, an autoencoder is utilized for learning compact latent representations of 3D point clouds sampled from CAE models.

In Chapter 4, an architecture of a 3D point cloud autoencoder (PC-AE-Rios) is proposed for learning design representations of CAE models. The shape-generative performance of PC-AE-Rios is comparable to state-of-the-art point-based networks and scalable to higher-dimensional models (10^5 points) than typically utilized in the literature. It is also shown that learning on organized point clouds using the mean-squared distance (MSD) between corresponding points as loss function improves the quality of the shapes generated by the PC-AE-Rios. Furthermore, learning on organized point clouds requires lower computational effort, preserves the capability of PC-AE-Rios to process unorganized point clouds after the training, and allows to generate simplified meshes (water-tight, genus-0) on the output point clouds.

In a first-of-its-kind framework for evolutionary design optimization using point cloud autoencoders (Section 4.6), the performance of PC-AE-Rios is compared to free-form deformation (FFD) in a set of target-shape matching optimizations (TSMOs). The experiments show that PC-AE-Rios is a suitable representation for design optimization and more efficient than FFD for generating shapes within the learned space of features. In extrapolation scenarios, as expected for machine learning models, the performance of PC-AE-Rios is less consistent and the quality of the generated objects decreases.

However, the TSMO experiments show that the features learned by PC-AE-Rios relate to the regions occupied by the designs, which leads to the question *"What is the geometric interpretation of the features learned by the selected deep-generative method?"* (*RQ3*). To answer this question, a novel feature visualization technique for 3D point cloud autoencoders is proposed (Section 5.2). The method exploits the properties of the 1D convolutional layers, which are utilized in the encoder of PC-AE-Rios, and projects the obtained activations onto the input 3D point cloud representation as color maps. Since the latent variables are obtained by processing the activations through a max-pooling operator, the regions in the point clouds that yield the highest activations correspond to the geometric structure of highest relevance to the visualized feature.

The proposed feature visualization method is utilized to evaluate the representations learned by PC-AE-Rios with respect to: Variations in the training data, shift-invariance, and the density with which the training data occupies different regions of the input space. Based on the results, the following geometric interpretation for the latent features learned by PC-AE-Rios is proposed, which answers *RQ3*: *The latent features represent the occupancy of fixed irregular volumes in the input space of PC-AE-Rios by the input shape, which indicate regions of design variations observed in the training data*. Hence, the features vary with the position, orientation and scale of the input shape. Furthermore, by increasing the dimensionality of the latent space, the volumes mapped by the latent variables become more refined, which improves the learning of shape details and, consequently, the quality of the generated models, as observed in the experiments.

To interpret the characteristics of the learned latent variables from a more practical perspective, the following question is stated: *"What are the advantages of learning design representations using a deep-generative model with respect to other suitable data-driven techniques?"* (*RQ4*). To answer *RQ4*, in Section 5.2, PC-AE-Rios is compared to PCA-based design representations as a data-driven representation for design optimization problems. The representations are compared based on three criteria: Data reconstruction quality, sensitivity of the output shapes to variations of the learned features, and capability to generate shapes through combinations of features. The main outcome of the experiments is that PC-AE-Rios learns a more diverse set of degrees of freedom, which allows one to modify local geometric features more efficiently than PCA-based representations. This property provides an advantage in nonlinear design optimization problems that require local design modifications, *e.g.*, the optimization of the aerodynamic downforce of vehicle designs, as also shown in the same chapter.

Once the architecture and capabilities of PC-AE-Rios are better understood, the following question targets the initial vision of an experience-based optimization framework: *How can the design space learned by deep generative models be utilized to transfer knowledge between design optimization problems?* (*RQ5*). To answer this question, a novel multi-task design optimization (MTO) framework is proposed, where the latent space of PC-AE-Rios is utilized to map the design features of 3D shapes utilized in different optimization problems to a common search space. In the framework, the multi-factorial optimization algorithm (MFEA) is adapted from the literature [68] and the proposed feature visualization technique is utilized for selecting the design features to be adapted and shared across the optimization tasks.

Based on a set of benchmark and vehicle aerodynamic design MTO problems, it is shown that PC-AE-Rios is a suitable method for mapping multiple design spaces to a common representation. Furthermore, by combining features of different designs in the latent space, which is interpreted as transfer of knowledge between tasks, the framework allows to accelerate and improve the solution of the optimization tasks. Although the problems are solved simultaneously, the experiment shows that PC-AE-Rios is a feasible approach for learning a transferrable representation of past optimized designs. These past solutions are biased by the designers' experience that can be utilized in new optimization problems, as targeted by the envisioned experience-based optimization framework. Nevertheless, the margin of improvement is limited by effects of negative knowledge transfer, which is not addressed in the present research.

Finally, despite the performance in the previous experiments, PC-AE-Rios generates output representations with low state-of-readiness for engineering simulations. Hence, *"How can the gap between the research on deep-generative models and their implementation for real-world engineering problems be narrowed?"* (*RQ6*). To address this challenge, a novel deep-generative model that builds upon the architecture of PC-AE-Rios is proposed: Point2FFD. The novel architecture combines a shape classifier and an FFD operator to the decoder of PC-AE-Rios, which predicts the deformation of simulation-ready mesh templates instead of the coordinates of mesh vertices.

In a set of experiments, it is shown that Point2FFD generates more realistic designs than obtained with PC-AE-Rios. Furthermore, compared to state-of-the-art point cloud (variational) autoencoders, Point2FFD provides competitive trade-off between accuracy and computational effort, despite the complexity of the network. In a set of vehicle aerodynamic optimization problems that compare Point2FFD to PC-AE-Rios, it is shown that Point2FFD improves the optimization performance (over 25% for the utilized shapes) and generates designs with characteristics that are in line with engineering solutions observed in similar problems.

8.2 Future Work

The contributions of the works in this dissertation cover a limited scope of the research on experience-based computation and cooperative intelligence for engineering systems. Thus, several challenges remain unsolved and the methods proposed in the present research have potential to be improved and adapted to a wider range of applications.

One of the limitations for further developing GDL methods for engineering is that the literature lacks engineering-tailored data sets. ShapeNetCore [23] allowed us to advance the state of the art, but the available information on the model properties is too limited for engineering tasks, *e.g.*, mass properties and aerodynamic performance. Recently, a data set of car hood models has been proposed [173], which is a step towards the proposed direction, but data sets with more complex objects and different types of data are still missing.

In line with the data set generation, the deep-generative models proposed in this research learn exclusively on geometric data. Yet, the synergies between optimization problems depend also on the domain of the optimization rather than exclusively the geometric properties. Hence, enabling these methods to learn simulation data, *e.g.*, flow and stress fields, along with the geometries has potential to increase the efficiency in the knowledge transfer between problems in different domains, such as from fluid dynamics to structural analyses. The currently available methods still depend on Euclidean representations [161], are defined in 2D domains [85] or learn based only on physical properties [63].

At last, neither of the methods proposed in this dissertation address the precision with which the shapes are modified. Event though the deep-generative models excel in design exploration, many engineering design tasks require the design modifications to be handled within a certain tolerance of values, which is not discussed in this work. Hence, a proper evaluation on the precision provided by the architectures and proposal of modifications to allow the deep-generative models to learn a latent space that accounts for design constraints are potential directions for improving the performance of the discussed methods.