Multi-dimensional feature and data mining
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Summary

In this thesis we explore machine and deep learning approaches that address key challenges in high dimensional problem areas and also in improving accuracy in well known problems. In high dimensional contexts, we have focused on computational fluid dynamics (CFD) simulations. CFD simulations are able to produce complex and large outputs that accurately describe the physical properties of fluids and gases in various domains and they are frequently used for studying the effects of flow patterns and design choices on many engineering designs, such as wing, car and engine shapes. Due to the high dimensional aspect of the data, it is difficult to model toward achieving critical goals such as optimizing lift and drag forces. The key research question addressed in this thesis is whether we develop automated approaches that accurately abstract this information? We tackle these issues by studying a closely related field, 3D computer vision, and adapt approaches to the particular data type. Moreover, inspired by this data type we propose new, deep learning, approaches that are also applied to traditional computer vision.

The first part of this thesis focuses on understanding how computer vision deals with higher dimensional data than the traditional 2D image. We identify several categories of approaches as well as a generalization of methods from 2D to higher dimensions. We identify two main types of generalization, i.e. generalization to higher physical dimensions and generalization to more information per physical point, i.e. increasing the number of modalities. As the benchmarks and datasets are key components that drive the research questions and proposed approaches we also include a categorization of the available big scale dataset and benchmarks.

The second part of this thesis focuses on adapting computer vision approaches to
CFD simulation output. More specifically, combinations of CNNs and auto-encoders are used to learn to represent as well as perform model based prediction conditioned to CFD simulation output. Moreover, the more traditional feature engineering approach is tested as well and compared to the aforementioned deep learning approaches. We propose two different large scale datasets of CFD simulation output, i.e. a 3D simulation domain of the air around passenger vehicles in a virtual wind tunnel and a 2D simulation domain of the air around airfoils, which are used for training models and benchmarking their performance. With extensive experimentation, we conclude that deep learning and traditional approaches have different strengths and weaknesses and thus, according to the application in mind, a different approach might be favorable. Moreover, we concluded that, for generalization purposes, deep learning approaches outperform the hand crafted feature based ones. Finally, a common trend in most computer vision applications is that hand crafted features can provide complementary information to the deep learning approaches and a combination of the two produces higher performance models than any of the individual parts. A similar approach is considered very promising and is left for future work.

In the third, and final, part of the thesis, inspired by a large proportion of the CFD simulation output, i.e. the velocity vector fields, a new approach is proposed which focuses on vector fields and it is generalized back to traditional computer vision to create rotation invariant and equivariant deep learning models. These approaches are tested on standard benchmarks in the field, i.e. the MNIST-rot and a vehicle orientation benchmark. Finally, a weight regularization approach is defined and tested on the standard computer vision large scale image classification benchmarks and models, i.e. CIFAR-10, CIFAR-100 and ImageNet.