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A deep learning framework for causal shape transformation

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ABSTRACT

Recurrent neural network (RNN) and Long Short-term Memory (LSTM) networks are the common go-to architecture for exploiting sequential information where the output is dependent on a sequence of inputs. However, in most considered problems, the dependencies typically lie in the latent domain which may not be suitable for applications involving the prediction of a step-wise transformation sequence that is dependent on the previous states only in the visible domain with a known terminal state. We propose a hybrid architecture of convolution neural networks (CNN) and stacked autoencoders (SAE) to learn a sequence of causal actions that nonlinearly transform an input visual pattern or distribution into a target visual pattern or distribution with the same support and demonstrated its practicality in a real-world engineering problem involving the physics of fluids. We solved a high-dimensional one-to-many inverse mapping problem concerning microfluidic flow sculpting, where the use of deep learning methods as an inverse map is very seldom explored. This work serves as a fruitful use-case to applied scientists and engineers in how deep learning can be beneficial as a solution for high-dimensional physical problems, and potentially opening doors to impactful advance in fields such as material sciences and medical biology where multistep topological transformations is a key element.

1. Introduction

In the past years, hierarchical feature extraction has been very successful in accomplishing various computer vision tasks spanning over generic object detection, image enhancement, and medical imaging (Havaei et al., 2017; Larochelle & Bengio, 2008; Lore, Akintayo, & Sarkar, 2017; Redmon, Divvala, Girshick, & Farhadi, 2016; Ren, He, Girshick, & Sun, 2015). Aside from extracting image features typical of such applications, deep learning methods have also proved to be promising in engineering tasks such as multi-modal sensor fusion (Ngiam, Khosla et al., 2011; Srivastava & Salakhutdinov, 2012), prognostics (Akintayo, Lore, Sarkar, & Sarkar, 2016; Sarkar, Lore, & Sarkar, 2015), and robotic path planning (Hadsell et al., 2008; Levine, Pastor, Krizhevsky, Ibarz, & Quillen, 2016; Lore, Sweet, Kumar, Ahmed, & Sarkar, 2016). In this paper, we propose a methodology using the fusion of two deep learning architectures as an inverse mapping to solve a high-dimensional one-to-many problem typical to the engineering domain. Specifically, we apply the proposed framework on a flow sculpting problem, where a specific sequence of transformation steps is desired given the initial and final cross-sectional shape of the fluid flow. The same framework can be applied in other forms of design engineering problems such as manufacturing, chemical engineering, and biology where an unknown sequence of processing steps is desired to achieve the observable final product.

For sequence prediction, recurrent neural networks (RNN) (Mikolov, Karafiát, Burget, Cernockỳ, & Khudanpur, 2010) and long short-term memory (LSTM) networks (Hochreiter & Schmidhuber, 1997) are the common go-to architectures for exploiting sequential information where the output is dependent on previous computation. However, dependencies of the computation of such architectures typically lie in the latent domain. This becomes sub-optimal or even unsuitable for certain applications involving the prediction of a step-wise transformation sequence that is dependent on the previous computation only in the visible domain (Fig. 1).

As a solution, a framework is constructed to handle such a scenario by chaining two popular deep architectures into the pipeline and avoids tedious re-implementation for a complex model. In the context of the problem under study, the resultant framework simultaneously predicts the intermediate shape between two flow shapes and learns a sequence of causal actions contributing to the shape transformation in the visible domain. This topological transformation framework can be extended to other applications, for example, in learning to transform the belief space for robotic path planning (Zhang, Kahn, Levine, & Abbeel, 2016), sequential decision making in games (Silver et al., 2016), learning the material

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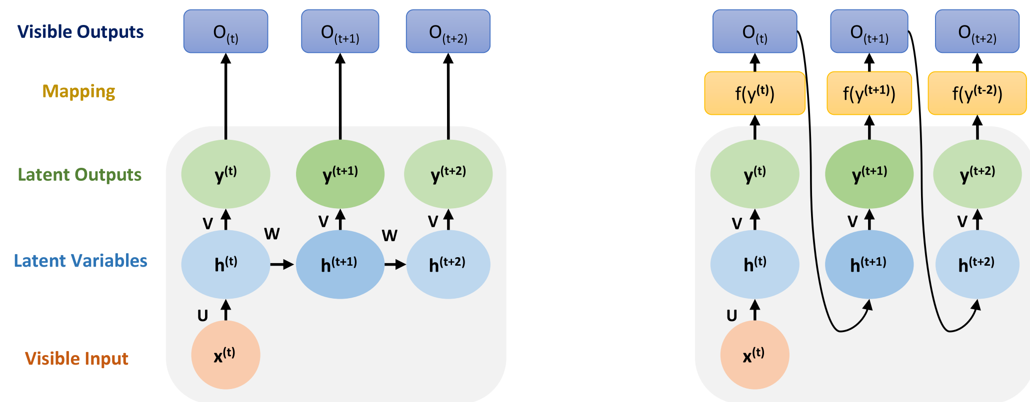

(a) Dependencies in the latent domain. (b) Dependencies in the visible domain.

Fig. 1. Difference between a typical problem using an RNN (left) and the problem considered here (right). Both frameworks take in input vector **x** at index t, pass it through the hidden layer **h** and produces a latent output **y**. The latent outputs **y** are mapped to visible outputs **o** via function $\boldsymbol{f}(\cdot)$. In RNN, there are dependencies in the latent layer. In our hybrid approach for the considered problem, the visible output is used as the input to the next (i.e. dependent on the visible outputs) without dependencies in the latent layer.

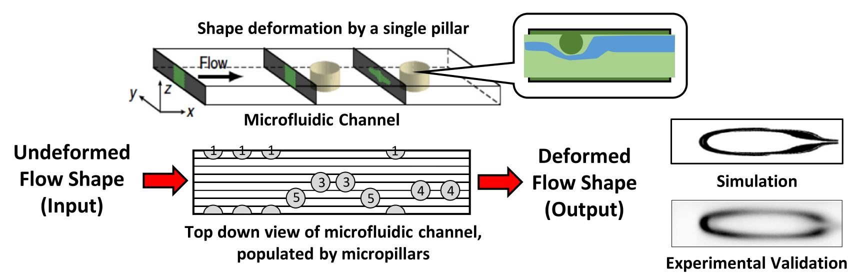

Fig. 2. Pillar programming. Each pillar contributes to the deformation of the flow. The position–diameter pair of each pillar is assigned an index which will be used as class labels for classification.

processing pathways to obtain desired microstructures starting from an initial microstructure (Wodo, Zola, Pokuri, Du, & Ganapathysubramanian, 2015), and learning a sequence of manufacturing steps in additive manufacturing (Paulsen, Di Carlo, & Chung, 2015), with *fast-design* being the main advantage without prolonged wait times in generating candidate solutions (see Section 6 for more elaborations). The contributions of the paper are outlined next:

1. A formulation of learning causal shape transformations to predict a sequence of transformation actions is presented, in the setting where only an initial shape and a desired target shape are provided.
2. An integrated hierarchical feature extraction approach using stacked autoencoders (SAE) (Vincent, Larochelle, Bengio, & Manzagol, 2008) with convolutional neural networks (CNN) (Krizhevsky, Sutskever, & Hinton, 2012) is proposed to capture transformation features to generate the associated sequence resulting in the transformation, specifically for problems where RNN and LSTM-based methods cannot be applied.
3. The proposed approach is tested and validated via numerical simulations on an engineering design problem (i.e. flow sculpting in microfluidic devices), with results showing much superior prediction accuracy over previously explored methods such as evolutionary algorithms and a multi-class, multi-label classification framework.

The rest of the paper is structured as follows: In Section 2, we discuss the problem setup and present some of the previous approach taken to solve the problem. Upon examining these previous approach, the motivation for a superior formulation is described in Section 3 . We present the proposed method in Section 4 and exhibit the results in Section 5. Finally, we outline other possible applications which can benefit from the proposed approach in Section 6 before concluding the paper in Section 7.

2. Problem setup and previous approach

In this section, we describe the problem setup for microfluidic flow sculpting and provide a brief background on previous approach in handling sequence prediction.

2.1. Microfluidic flow sculpting

Inertial fluid flow sculpting via micropillar sequences is a recently developed method of fluid flow control with a wealth of applications in the microfluidics community (Amini et al., 2013). This technique utilizes individual deformations imposed on fluid flowing past a single obstacle (pillar) in confined flow to create an overall net deformation from a rationally designed sequence of such pillars. If the pillars are spaced far enough apart (space $> 6D$, for a pillar diameter D), the individual deformations become independent, and can thus be pre-computed as building blocks for a highly efficient forward model for the prediction of sculpted flow given an input pillar sequence (Stoecklein, Wu, Kim, Di Carlo, & Ganapathysubramanian, 2016) (Fig. 2). Since its debut, flow sculpting via micropillar sequence design has been used in a diverse variety of applications like novel fiber and particle fabrication (Nunes et al., 2014; Paulsen & Chung, 2016; Paulsen et al., 2015; Wu, Owsley, & Di Carlo, 2015), biodiagnostics (Sollier et al., 2015), and tissue engineering (Hwang, Khademhosseini, Park, Sun, & Lee, 2008).