Unraveling topology of Dynamic Neural Networks

Chinmay Datar[1,2], Felix Dietrich[2], Wil Schilders[1,3]

[1] Institute of Advanced Study, Technical University of Munich
chinmay.datar@tum.de
[2] Department of Computer Science, Technical University of Munich, Germany
felix.dietrich@tum.de
[3] Department of Mathematics and Computer Science, Eindhoven University of Technology, Netherlands
w.h.a.schilders@tue.nl

Deep learning has advanced scientific fields like physics [1], mathematics [2], and material science [3]. Nevertheless, multiple mysteries and challenges remain, and the difficulties are becoming apparent. Firstly, the predictions obtained from deep neural networks are usually hard to explain. Secondly, deep learning approaches require a large amount of data, which is seldom available in science and engineering applications. Thirdly, finding a suitable neural network architecture generally involves the exploration of many different architectures. This results in high computational costs.

We aim to tackle these challenges for a particular class of problems, namely Linear Time-Invariant (LTI) systems. For this class, we derive the architectures of dynamic neural networks from the properties of the LTI system and demonstrate that they are explainable. The main difference between a dynamic and a classical neural network is that the output of each neuron is a solution of an ordinary differential equation rather than a simple evaluation of an activation function.

The architecture and weights of dynamic neural networks are constructed in two steps. First, we transform the state-space model into a suitable form. Second, we derive a mapping from the LTI system matrices to the trainable parameters of the dynamic neural network. The mapping unravels the topology of the dynamic neural network, thereby eliminating the need for architecture search. Moreover, the mapping facilitates incorporating information in the LTI system into the trainable parameters of the dynamic neural network. Thus, the dynamic neural network can numerically simulate the underlying LTI system accurately in the forward propagation step without any optimization algorithm.

We demonstrate a proof-of-concept of this approach and show that the dynamic neural network makes accurate predictions on two numerical examples. The mapping derived in this work and the vast literature on model order reduction of LTI systems opens up a possibility to develop a theory of model order reduction for dynamic neural networks. Moreover, given the principled mapping from LTI systems to dynamic neural networks, an important future direction is to explore which nonlinear systems correspond to nonlinear networks.

References

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