Reservoir Computing for Learning in Structured Domains

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Abstract

In many real world applicative domains (including e.g. Chemistry, Molecular Biology, Speech and Text Processing) the information of interest can naturally be organized in structured representations, such as sequences, trees and graphs. Such representations allow to effectively describe the relations among the entities involved. The possibility of inferring functions on structured domains by the means of neural network models is therefore of a great appeal.

Recurrent Neural Networks (RNNs) and Recursive Neural Networks (RecNNs) have been proposed for processing of sequence domains and hierarchical graph structures, respectively. In the context of sequence processing, Reservoir Computing (RC) in general, and Echo State Networks (ESNs) in particular, represent a novel and increasingly emerging paradigm for efficient modeling of RNNs.

In this talk we describe the results of our study on the development of new ESN-based models for learning in structured domains, progressively including sequences, trees and graph structures. The main focus is on the following research directions: extension of the class of data structures supported, efficiency of computation, generalization performance and adaptivity of the model. As regards the ESN model for sequence processing tasks, we propose an analysis of the main architectural factors of network design which influence the final model performance. Another important object of study is the Markovian characterization of the nature of ESN state dynamics, which influences its behavior and defines characteristics and limitations of the approach.
The extension of the class of data structures which can be processed by the means of RC models represents the main result of the presented work. In this regard, we introduce and analyze the TreeESN and the GraphESN models. TreeESN represents a generalization of the ESN approach for processing of hierarchical structures (e.g. rooted trees), and allows to extend the efficiency of RC models to RecNN modeling. GraphESNs, still preserving extreme efficiency of computation, further generalize the approach for directly processing both directed/undirected, cyclic/acyclic labeled graphs. The Markovian characterization of TreeESNs and GraphESNs dynamics, extended to the case of tree and graph structured state spaces, represents the basis for the good generalization performances in applications. In particular, TreeESNs and GraphESNs provide promising results in real-world tasks from relevant interdisciplinary domains, such as Cheminformatics. Ongoing work focuses on improving the adaptivity of the GraphESN model.