Artificial Hydrocarbon Networks: Chemical Nature Inspiration in Machine Learning

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Abstract– Inspiration in nature has been widely explored, from macro to micro-scale. When looking into chemical phenomena, stability and organization are two properties that emerge. Recently, artificial hydrocarbon networks (AHN), a supervised learning method inspired in the inner structures and mechanisms of chemical compounds, have been proposed by as a data-driven approach in artificial intelligence. AHN have been successfully applied in data-driven approaches, such as: regression and classification models, control systems, signal processing, and robotics. To do so, molecules –the basic units of information in AHN– play an important role in the stability, organization and interpretability of this method. Interpretability, saving computing resources, and predictability have been handled by AHN, as any other machine learning model. This short paper aims to highlight the challenges, issues and trends of artificial hydrocarbon networks as a data-driven method. Throughout this document, it presents a description of the main insights of AHN and the efforts to tackle interpretability and training acceleration. Potential applications and future trends on AHN are also discussed.

Keywords– machine learning, supervised learning, artificial organic networks, modeling, learning task

Introduction

Recently, artificial hydrocarbon networks (AHN), a supervised learning method inspired in the inner structures and mechanisms of chemical compounds, have been proposed as a data-driven approach in artificial intelligence [1]. This algorithm, inspired by nature, loosely mimics stability and organization of molecules in order to build organized structures made of packages of information. AHN have proved to be efficient in predictive power when modeling a data-based problem. However, the organizational property has not been strongly analyzed. If this organization capability is conducted in AHN, the output response in data-driven models will reveal, at least in a partial view, the inner structure and functionality of the systems model. So, new ways in building and training AHN are required. Thus, this paper aims to discuss challenges and trends of AHN as a data-driven method, with emphasis on interpretability and training acceleration. This document lays the foundations on AHN for implementing new training algorithms and the way to reveal the chemical nature of data-driven problems.

Key Concepts of Artificial Hydrocarbon Networks

AHN method was firstly proposed by Ponce and Ponce [2] as an implementation of their more general technique namely artificial organic networks (AON) [1]. In a nutshell, the purpose of the AHN method is to package information, from a set of instances, in basic units known as molecules. These molecules – composed of hydrogen and carbon atoms– are described by nonlinear functions, and they can be related among them using chemical heuristics resulting in complex units of information so-called compounds. Moreover, a set of compounds can be combined together, linearly, producing mixtures. To this end, the mixture constitutes a model [1]. Thus, the inspiration in organic compounds to develop a machine learning method considers three facts observed from nature [3]: (i) stability as the property of compounds to maintain their geometric configurations; (ii) organization based on the ground-state principle aiming to preserve energy minimization within the compounds; and (iii) multi-functionality for promoting transfer learning.
For training purposes, the method considers the simple AHN training algorithm [1] which is based on the gradient descent and the numerical solution of least squares estimates via QR-factorization. This training

algorithm has reported well performance in predictive power for low-dimensional input spaces, and large training time for computing suitable parameters in the model [4]. Currently, new training methods have been proposed based on hierarchical training [3] or using stochastic-parallel metaheuristic optimization [4]. The later, accelerating training in more than 3,500 times the simple AHN training algorithm.

Applications of Artificial Hydrocarbon Networks

Literature reports many different applications of AHN. Those can be classified as follows: function approximation and modeling [1]; robust human activity recognition systems [5]; signal processing in denoising audio and face recognition [1,6]; online advertising [6]; intelligent control systems for robotics [1,7,8,11] and mechatronics [1,9,10]; bio/medical applications [5,6,12]; and, theoretical approaches such as hybrid fuzzy-molecular inference systems [8], interpretability of the model [12] and training algorithms [3,4].

Highlights of Artificial Hydrocarbon Networks

In these years of AHN, this method has reached notable contributions, as those highlighted following:

- ***Type-II fuzzy inference like behavior –*** AHN have proved to be significantly similar to type-II fuzzy inference systems, handling noise and allowing experts to tune fuzzy partitions/rules [8].
- ***Competitive as deep learning –*** In [5], AHN reported to be significantly similar in performance as deep neural networks (DNN). This suggests that AHN can be trained with less data and obtaining comparable results as DNN.
- ***Interpretability of the model –*** In contrast to neural networks, AHN can be partially interpreted and converted into decision trees or rules-based models. This interpretability was implemented for medical diagnosis systems [12].
- ***Reinforcement learning for continuous domains –*** AHN have been applied for continuous reinforcement learning approaches, in both states and actions, typically found in robotics [11,13]. This approach has also revealed insights on using it as a transfer learning method.

Challenges and Trends of Artificial Hydrocarbon Networks

Until now, AHN have been successfully applied to different problems and different learning tasks. However, there still are challenges and issues about AHN that have to be faced. Trends in the development and application of AHN can be listed as follows: (i) new training algorithms for AHN are required for better computational performance mainly in time; (ii) the next big step in AHN is parallel computing that opens the possibility for parallel processing and big data analysis; (iii) since the predictive power of AHN is well accurate, it is important to study other functions as kernels and relationships in molecules aiming to perform other approximations; (iv) hybrid approaches with AHN might improve solutions to very complex problems, such as robotics, business intelligence, healthcare, and others; (v) few efforts in dynamic modeling using AHN are reported in literature, so it is important to focus some research in this direction; (vi) transfer learning using pre-defined molecules can be done, but more studies are necessary; (vii) interpretability of machine learning models and specifically of AHN models, are of great importance for knowledge extraction, thus automatic procedures for this task are required; and (viii) open-source coding of AHN is specially required for fast adoption, as the first efforts reported in [14].

Conclusions

In this short paper, we summarized the challenges, issues and trends of AHN as a data-driven method. Despite this method was proposed recently, it has been successfully applied to many different intelligent systems. However, there is a need to explore new ways on how this method can be useful. Important issues like interpretability, training acceleration and open-source efforts are also required. Finally, we believe that this method can be added as another powerful tool for practitioners, scientists and researchers in artificial intelligence community.

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