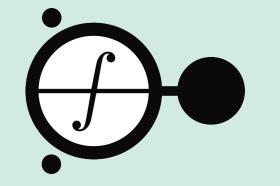
# Challenges and Issues on Artificial Hydrocarbon Networks: The Chemical Nature of Data-Driven Approaches

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### **BACKGROUND AND SCOPE**

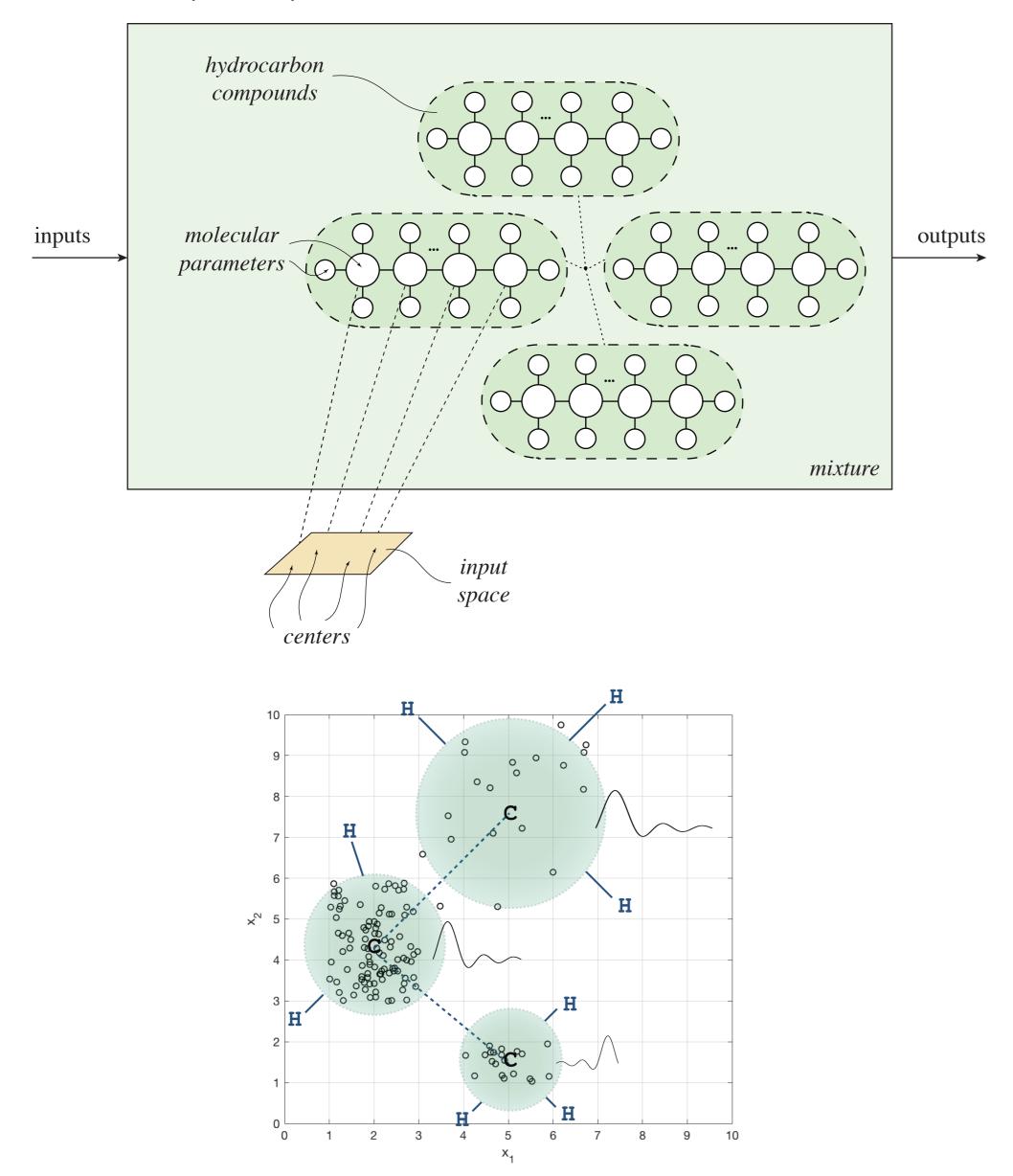
Recently, artificial hydrocarbon networks (AHN), a supervised learning method inspired in the inner structures and mechanisms of chemical compounds, have been proposed as a data-driven approach. AHN have proved to be efficient in predictive power when modeling a data-based problem. However, it stills require more studies on its challenges, issues and applications.

This work aims to discuss challenges and trends of AHN as a data-driven method. It also 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 AHN**

#### **APPLICATIONS & HIGHLIGHTS OF AHN**

The goal of the AHN method is to package information, from a set of instances, in basic units known as molecules. Then, create compounds (nonlinear) and mixtures (linear).

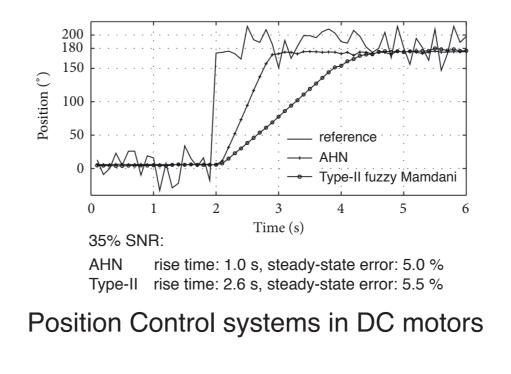


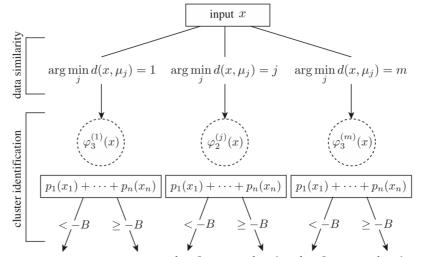
– Key features in supervised ML.

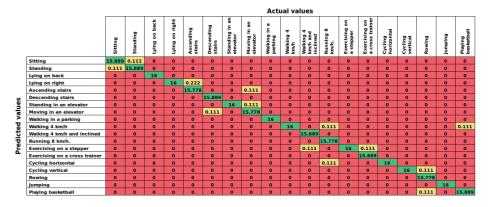
Features	AHN	DT	NN	NB	kNN	SVM
Accuracy	$\checkmark \checkmark \checkmark$	$\checkmark\checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark$	$\checkmark\checkmark$	$\checkmark \checkmark \checkmark$
Tolerance (missing values)	$\checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark$	$\checkmark\checkmark$
Tolerance (noise)	$\checkmark \checkmark \checkmark$	$\checkmark\checkmark$	$\checkmark\checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark$	$\checkmark\checkmark$
Variety of attributes	$\checkmark\checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark\checkmark$	$\checkmark\checkmark$	$\checkmark\checkmark$	$\checkmark\checkmark$
Regression	$\checkmark \checkmark \checkmark$	$\checkmark$	$\checkmark\checkmark$	$\checkmark$	$\checkmark\checkmark$	$\checkmark\checkmark$
Classification	$\checkmark \checkmark \checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark\checkmark$	$\checkmark \checkmark \checkmark$
Interpretability	$\checkmark\checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark$	$\checkmark \checkmark \checkmark$	$\checkmark\checkmark$	$\checkmark$

Symbols: low ( $\checkmark$ ), medium ( $\checkmark \checkmark$ ) and high ( $\checkmark \checkmark \checkmark$ ) satisfaction

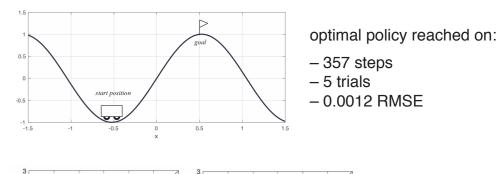
# - Some applications and case studies.

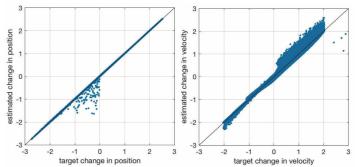






AHN accuracy 99.49(0.44) % deep-RNN accuracy 99.27(0.16) % statistical equivalent (*p* = 0.109); AHN 6.98*x* less parameters Human activity recognition





# The inspiration in organic compounds to develop a ML method considers three facts observed from nature:

- Stability

- Organization
- Multi-functionality

if d(x, 0) < 2.63 and  $g_1(x) < 0.57$ , then sample = *benign*, or if d(x, 0) < 2.63 and  $g_1(x) \ge 0.57$ , then sample = *malignant*, or if  $d(x, 0) \ge 2.63$  and  $g_2(x) < 1.12$ , then sample = *benign*, or if  $d(x, 0) \ge 2.63$  and  $g_2(x) \ge 1.12$ , then sample = *malignant* 

Interpretability of AHN-based classifier

Reinforcement learning from scratch

# TRENDS AND ISSUES OF AHN

- New training algorithms
- Big data processing
- Kernels and relations in molecules
- Hybrid approaches with AHN
- Transfer learning



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