Contribution ID: **61** Type: **Invited talk**

Machine Learning applied to Material Science

Tuesday, 9 April 2024 16:00 (30 minutes)

Machine learning (ML) is emerging as a new tool for many different fields which now span, among the others, chemistry, physics and material science [1,2]. The idea is to use ML algorithms as a powerful machinery to identify, starting from big data analysis, subtle correlations between simple elemental quantities and complex material properties and then use these to predict them. This approach can help to screen many material properties directly in-silico avoiding more computational expensive ab-initio calculations and experimental measurements.
However, adapting existing ML architectures to problems in chemistry, physics and material science is not straightforward. Several aspects need to be addressed to improve machine performance which can be summarized into prediction accuracy and generalization. Improving these aspects require to go into the details of the algorithm and analyze the way they learn from a training dataset. This allows to identify which architecture, training algorithm and dataset are relevant for the problem at hand.
In the present talk I will give an overview about several techniques and algorithms spanning from domain adaptation to autoencoders to enhance the performance of machine learning applied to experimental and simulation data analysis.

[1] Wei Li, Ryan Jacobs, Dane Morgan Computational Materials Science 150, 454-463 (2018)
[2] G. Pilania, A. Mannodi-Kanakkithodi, B. P. Uberuaga, R. Ramprasad, J. E. Gubernatis & T. Lookman, Scientific Reports volume 6, Article number: 19375 (2016).

Primary author: Prof. GAGLIARDI, Alessio (Technical University Munich)

Presenter: Prof. GAGLIARDI, Alessio (Technical University Munich)

Session Classification: Session 8

Track Classification: MLC