# Machine Learning to Investigate Material Properties: How to Improve Machine Performance

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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 this 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 skills. Improving these aspects require to go into the details of the machine 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, starting from some examples of ML applications to material science [3,4], several different strategies will be discussed to improve performances which span different feature vectors, regularization terms and augmented datasets.

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[2] G. Pilania, A. Mannodi-Kanakkithodi, B. P. Uberuaga, R. Ramprasad, J. E. Gubernatis & T. Lookman, Scientific Reports volume 6, Article number: 19375 (2016).
[3] J. Lederer, W. Kaiser, A. Mattoni and A. Gagliardi, Machine Learning based Charge Transport Computation for Pentacene, Advanced Theory and Simulations 2 (2), 1800136 (2019).
[4] J. Stanley, F. Mayr and A. Gagliardi, Machine Learning Stability and Bandgaps of Lead-Free Perovskites for Photovoltaics, Advanced Theory and Simulations (accepted) (2019)