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Machine Learning in Chemistry and Materials Science: Achievements and Perspectives

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Machine learning (ML) methods have emerged as powerful chemistry and materials science tools. In several tasks, these methods can be used as surrogate or complementary models aiming to reduce the computational burden present in theoretical quantum chemistry approaches, such as DFT calculations. Instead of calculating material properties from first principles approaches, machine learning models learn the mapping function (structure to property) from available data. Once trained, the model can be used to predict the properties of out-of-sample compounds. Besides performing direct mapping, ML methods can also be applied in the inverse design process, in which the model learns to generate novel compounds from desired properties. Our group started contributing to this field early in 2019 in the context of the CINE project. Here, after a brief introduction to ML, I will summarize some of our recent achievements in several problems, such as i) representative molecule selection via unsupervised learning; ii) data mining analysis of quantum chemistry data; iii) molecular property prediction with supervised methods; iv) molecular design using variational autoencoders; and v) feature learning via contrastive learning from multiple molecular representations. Finally, future direction and challenges will be pointed out.

Keywords: machine learning; property prediction; molecular design; representation learning in chemistry.

Support/Acknowledgements: FAPESP and Shell (Proc. 2017/11631-2, 2020/05329-4, 2021/08852-2), CNPq (Proc. 313680/2021-3), and the strategic importance of the support given by ANP (Brazil's National Oil, Natural Gas and Biofuels Agency) through the R&D levy regulation.

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