Contribution ID: **22**   Type: **Talk**

Shallow Ensembles: Simple, Scalable and Size-Extensive Uncertainty Estimates for Atomistic Modelling

Friday 30 August 2024 11:00 (30 minutes)

Statistical learning algorithms provide a generally-applicable framework to sidestep time-consuming experiments, or accurate physics-based modeling, but they introduce a further source of error on top of the intrinsic limitations of the experimental or theoretical setup. Uncertainty estimation is essential to quantify this error, and make application of data-centric approaches more trustworthy. To ensure that uncertainty quantification is used widely, one should aim for algorithms that are reasonably accurate, but also easy to implement and apply. In particular, including uncertainty quantification on top of an existing model should be straightforward, and add minimal computational overhead. Furthermore, it should be easy to process the outputs of one or more machine-learning models, propagating uncertainty over further computational steps. We compare several well-established uncertainty quantification frameworks against these requirements, and propose a practical approach, which we dub shallow ensemble propagation, that provides a good compromise between ease of use and accuracy. We present applications to the field of atomistic machine learning for chemistry and materials, which provides striking examples of the importance of using a formulation that allows to propagate errors without making strong assumptions on the correlations between different predictions of the model.

Primary authors: KELLNER, Matthias (EPFL); Prof. CERIOTTI, Michele (EPFL)

Presenter: KELLNER, Matthias (EPFL)