TOWARDS DEEP ACTIVE LEARNING USING RELIABLE UNCERTAINTY ESTIMATES

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Good machine learning models require a large set of labeled training data. Deciding which labeled data is most essential can be done on-the-fly using a technique called active learning. Using active learning both the predictions as the uncertainty on the predictions are combined to direct the data collection algorithms towards a desired objective, implicitly defining a good balance between exploration and exploitation. In this way, it is possible to optimize the properties one is interested in, while improving the model performance.

In previous work, we focused on using Gaussian Processes in an active learning framework to predict ab initio formation energies of geometrically similar structures, which lead to great speedups in discovering new quaternary materials. Deep graph learning offers new potential, by allowing us to incorporate the geometric structure of the atomic systems into the model. Unlike Gaussian processes, however, deep learning methods do not have implicit access to uncertainty quantification. The following question thus arises: "How can reliable uncertainty estimates be included in a deep graph learning model without significantly affecting either performance or training time?". We explicitly demand that the training time does not increase too much as, in active learning, the model has to be completely retrained on a regular basis. This implies that a purely Bayesian approach, which would be the preferred approach to deal with this issue, is not a real option as it quickly becomes too slow for large datasets.

Uncertainty estimation in deep neural networks is a hot topic in current machine learning literature, but so far no clear answer has emerged. We discuss different state-of-the-art approaches, which rely either on explicitly modeling the uncertainty on the predictions or ensemble methods and compare how well they perform in discovering new materials.