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Machine learning in soil research: impact of model tuning on predictive uncertainty

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Machine learning algorithms are good in computing non-linear problems and fitting complex composite functions, which makes them an adequate tool to address multiple environmental research questions. Soil water retention data is often scarce. The landscape-scale spatial prediction may, therefore, require the application of pedotransfer functions (PTFs) to increase the input dataset. Machine learning algorithms are commonly involved in both, the spatial prediction of soil properties and the development of PTFs. In this context, any machine learning model has to be adjusted to the specific dataset. This makes parameter tuning a crucial point in model building. Concerning machine learning in soil research, we compare the commonly applied grid search tuning method to the differential evolution optimisation for the first time. The PTF development to predict soil water retention in two tropical mountain regions of different soil-landscapes shall serve as an application example. Results confirmed the differential evolution algorithm's high potential for tuning machine learning models. While models based on tuning by grid search roughly predicted the response variable' mean for both areas, models applying the differential evolution for model tuning explained up to 22 times more of the response variables' variance.