On the Difficulty of Epistemic Uncertainty Quantification in Machine Learning: The Case of Direct Uncertainty Estimation through Loss Minimization

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Without any doubt, the notion of uncertainty is of major importance in statistics as well as machine learning and constitutes a key element of modern machine learning methodology. In recent years, it has gained in importance due to the increasing relevance of machine learning for practical applications, many of which are coming with safety requirements. In this regard, new problems and challenges have been identified by machine learning scholars, many of which call for novel methodological developments. Indeed, while uncertainty has a long tradition in statistics, and many useful concepts for representing and quantifying uncertainty have been developed on the basis of probability theory, recent research has gone beyond traditional approaches and also leverages more general formalisms and uncertainty calculi.
In the statistics literature, two inherently different sources of uncertainty are commonly distinguished, referred to as *aleatoric* and *epistemic*. While the former refers to variability due to inherently random effects, the latter is uncertainty caused by a lack of knowledge and hence relates to the epistemic state of an agent. Thus, epistemic uncertainty can in principle be reduced on the basis of additional information, while aleatoric uncertainty is non-reducible. Nevertheless, the objective quantification or measurement of aleatoric uncertainty is much easier than for epistemic uncertainty due to the lack of an objective ground truth for the latter.
In this talk, we analyse a recent proposal for epistemic-uncertainty-aware learning based on the idea of a second-order learner, which yields predictions in the form of distributions over probability distributions. While standard (first-order) learners can be trained to predict accurate probabilities, namely by minimising suitable loss functions (so-called proper scoring rules) on sample data, we will see that many of the recently proposed approaches based on loss minimisation do not work for second-order predictors in the sense that the loss functions proposed for inducing such predictors do not incentivise the learner to represent its epistemic uncertainty in a faithful way.

Biography:
Viktor Bengs obtained his Ph.D. in 2018 in Statistics at the Philipps-Universität Marburg. He is currently an interim professor at the Chair of Statistical Learning and Data Science of the Department of Statistics at the LMU Munich. Before he was affiliated with the Chair of Artificial Intelligence and Machine Learning of the Institute of Informatics at the LMU Munich. He is part of the editorial board of the Machine Learning Journal and has served for several top-tier conferences in Machine Learning as an invited reviewer, which was honored by being selected as a top reviewer at UAI 2021 and AISTATS 2022. His main research areas are multi-armed bandits, automated algorithm configuration, preference learning and uncertainty quantification.