Artificial Intelligence and the Uncertainty challenge in Fundamental Physics



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Simulation-Based Inference: Where Classical Statistics Meets Machine Learning

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Simulation-based inference (SBI) refers to situations where the likelihood function cannot be readily evaluated but a simulator is available to generate data from a parametric model for any value of the unknown parameter. In recent years, a wide range of machine learning-based techniques have been developed to enable classical statistical inference in the simulation-based setting. These methods enable learning likelihood functions, posteriors, likelihood ratios, confidence sets and other inferential quantities with very high-dimensional data spaces using only simulations from the statistical model. In this talk, I will give an overview of some of our recent work in this area. I will first present our work on learning likelihood functions of otherwise intractable models for spatial data, which is one of the first uses of SBI in the context of purely statistical models. While likelihood-based inference is conceptually simple and computationally efficient, it only offers approximate coverage guarantees. To obtain rigorous uncertainty quantification, one can combine SBI with Neyman inversion. From this class of techniques, I will present Waldo, a method that uses neural predictions to form a Wald-type test statistic which is inverted to obtain guaranteed-coverage confidence sets. Waldo provides an appealing way of obtaining frequentist uncertainty quantification based on outputs of predictive models, including deep neural networks and neural posteriors. I will conclude by outlining some future research directions in SBI which revolve around challenges related to model discrepancy and high-dimensional parameter spaces.

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