

Uncertainty quantification for neural network models

Monday 6 December 2021 11:00 (15 minutes)

This talk gives a brief introduction to uncertainty quantification (UQ) for neural networks. We investigate these methods as part of a Helmholtz AI voucher in collaboration with the MALA [1,2] project, where we build surrogate models to speed up demanding density functional theory calculations. In this context, UQ methods can be used to assess the validity of model predictions and can also serve to detect out-of-distribution data.

[1] <https://github.com/mala-project/mala>

[2] J. A. Ellis et al., Phys. Rev. B 104, 035120, 2021

Physical Presentation

I would not feel comfortable to present in front of an audience and prefer a video (call) presentation.

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Session Classification: Parallel Session