QC OPTIMIZATION CHALLENGE

Can variational quantum circuits model probability distributions? (Siemens)

Motivation

Similar to classical neural networks, variational quantum circuits (VQCs) [1] can be used to learn input-output relations from data, e.g., to learn a forecasting model of a technical plant.

In many applications, the technical plant, e.g., a wind or gas turbine, cannot be modeled deterministically. Instead, it is advantageous to model a stochastic process, for example to be able to use model-based reinforcement learning for control optimization [2].

This is possible with classical neural networks but requires some effort and the question arises as to whether this does not work just as well or better with quantum machine learning methods, which are inherently stochastic. Based on our very positive experience [3] with VQCs with data re-uploading [4] and proper target scaling, we are particularly interested in whether VQCs can be used to model probability distributions.

This project is a cooperation with Siemens.

Working plan

We suggest the following steps:

1. Literature research on what already exists on this topic
2. Selection of a simple benchmark
3. Perform own investigations into how VQCs can solve the task without modification
4. Develop suggestions for modifications to the VQCs, if possible, or test alternative methods described in the literature.

Success Measure

The aim of this modeling is both to learn the expected value of the forecast with the lowest possible error (e.g., RMSE) and at the same time to map the true probability distribution in a meaningful way, measured, for example, by the Kullback-Leibler divergence or the Hellinger distance.

[1] Maria Schuld & Francesco Petruccione, Variational circuits as machine learning models, 2021

[2] Stefan Depeweg et al., Learning and policy search in stochastic dynamical systems with Bayesian neural networks, 2017

[3] Simon Eisenmann et al., Model-based offline quantum reinforcement learning, 2024

[4] Maria Schuld et al., Effect of data encoding on the expressive power of variational quantum machine learning models, 2021