Simulating Stochastic Processes with Variational Quantum Circuits

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Introduction

Quantum devices are seen as a disruptive technology with the potential to speed up many applications in science and technology. Therefore, sophisticated algorithms are needed to exploit its potential. Within this work, we consider one area of possible quantum advantage [1] – the simulation of stochastic processes – and propose a hybrid quantum-classical learning algorithm for simulation models, that can be run on near-term devices.

Stochastic Processes

As a toy problem, we consider an iconic stationary discrete-time stochastic process – the period-N uniform renewal process, that produces bitstrings for which the number of 0s between two consecutive 1s is uniformly distributed between 0 and $N-1$. Such a process features N internal states:

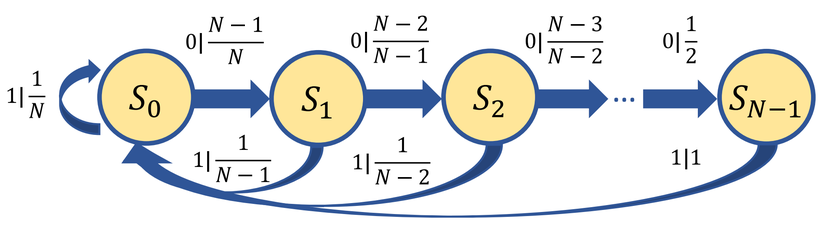

Figure 1: Illustration of the period-N uniform renewal process. The labels $x|P(x)$ indicate an emission of x with probability $P(x)$ while transitioning to some state S_i.

Quantum Computing

Unlike Classical Computing, Quantum Computers utilize quantum mechanical properties like the spin as their domain of computation. Exploiting quantum effects such as superposition and entanglement grants these devices a particular advantage over their conventional counterparts.

Simulation Models

Classical simulation models initialize their memory M_c to some internal state $E(\overleftarrow{x})$ based on a past observation $\overleftarrow{x}$ and emit an output symbol x_i, while updating their memory M_c for the next simulation step:

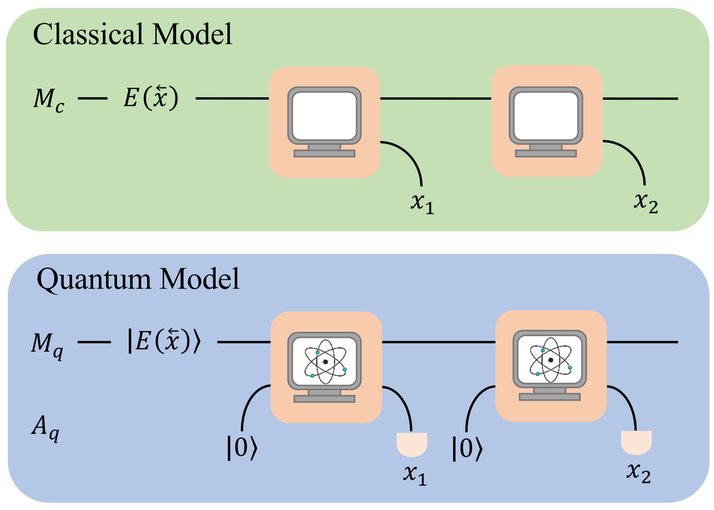

Figure 2: Comparison of classical and quantum simulation models.

By contrast, quantum models feature two quantum registers M_q and A_q, where M_q is initialized to some suitable quantum state $|E(\overleftarrow{x})\rangle$ while a measurement of A_q reflects the first simulation step.

Learning Algorithm

Formulated as a classical optimization procedure, the learning algorithm features a classical pre-processing step and a quantum sub-routine within a hybrid optimization loop. The latter also includes a quantum post-processing step to compute a regularization term. Classical optimizer such as ADAM [2] can be used to update the training parameters.

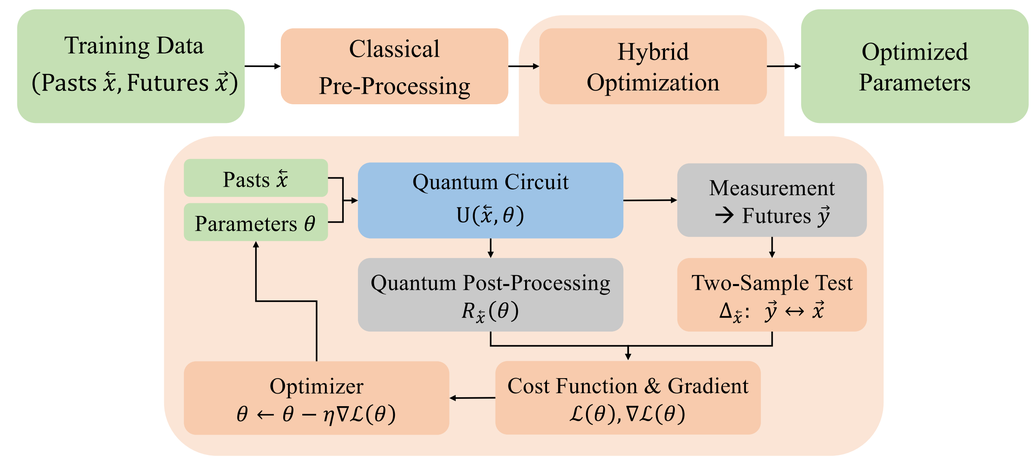

Figure 3: Schematic illustration of the hybrid quantum-classical learning algorithm.

The cost function is composed of two parts – one that measures the difference $\Delta_{\overleftarrow{x}}$ between the model's and the true sample distribution, and one regularization term $R_{\overleftarrow{x}}$ that originates from the quantum post-processing step and that penalizes models with a rich set of internal states:

$$\mathcal{L}(\theta) = \sum_{\overleftarrow{x}} \left[\Delta_{\overleftarrow{x}}(\theta) + \lambda \, R_{\overleftarrow{x}}(\theta) \right].$$

Validation

Validating the learned models is done via calculating the Kullback-Leibler (KL) divergence and the total variation (TV) distance over several simulation steps, showing a superior accuracy for models with the regularization compared to models without this term:

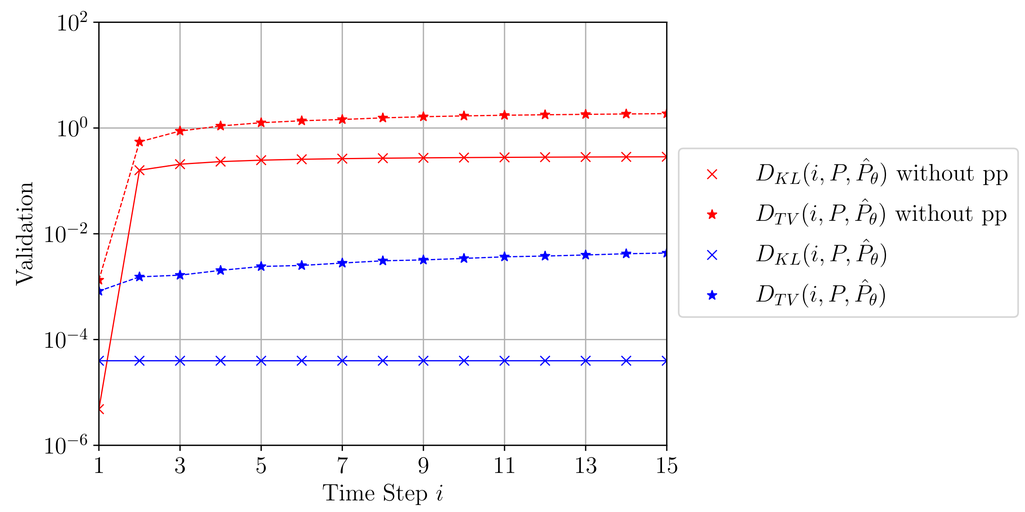

Figure 4: KL divergence and TV distance between the model's distribution and the true sample distribution over 15 simulation steps.

Furthermore, the internal quantum states of the register M_q are analyzed for a randomly initialized model (left), a learned model without regularization (center) and a learned model with regularization (right), where the same states should be observed over and over again.

Figure 5: Comparison of the internal states of different quantum simulation models.

Tools & Methods

- Python
- ADAM
- Qiskit
- QuTiP

References

[1] Chengran Yang, Andrew Garner, Feiyang Liu, Nora Tischler, Jayne Thompson, Man-Hong Yung, Mile Gu, and Oscar Dahlsten.
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[2] Diederik Kingma and Jimmy Ba.
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