Quantum circuit architecture selection via local optimization towards quantum machine learning of bond dissociation energy chemical data

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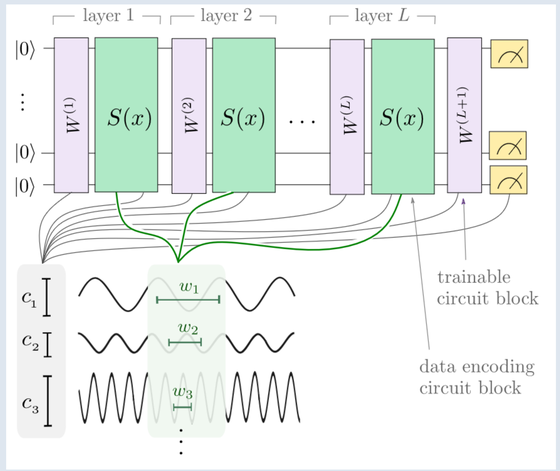
Abstract

The trainability and expressibility of quantum regression models is determined by the sequence of gate operations (ansatz) of the model circuit implementation. Standard circuit ansatze are used for QML, yet the optimal ansatz is completely regression task dependent. We propose a local search approach towards task-specific ansatz selection from a candidate ansatz.

1. Background

Quantum machine learning (QML) or parametrized quantum circuits (PQC) for regression are a growing research area with immense impact for chemical applications. QML models are implemented in sequences of operations on quantum states.

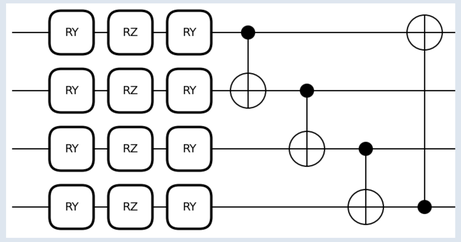
- Expressible quantum circuits feature repeated data encoding blocks ***S(x)***
- Functions implemented via quantum circuit are truncated Fourier series (M. Schuld, 2020)



Source: M. Schuld, 2020

i. Input *x* encoded into quantum state via rotations ***S(x)***.
ii. State is entangled and rotated with parameters $\boldsymbol{\theta}_i$ via W_i between encoding steps.
iii. Circuit trained by minimizing $\boldsymbol{\theta}$ wrt. objective function, e.g. MSE.

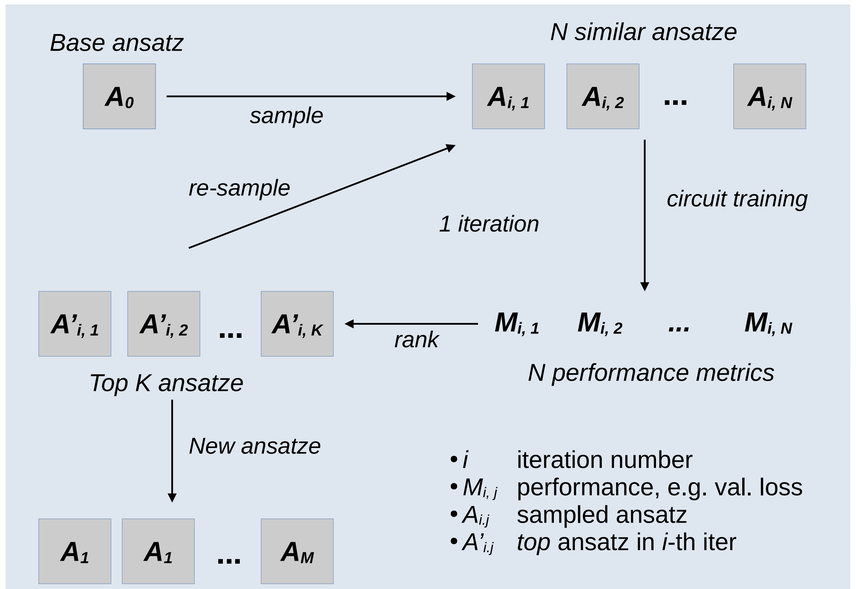
Circuits can be trained with gradient-based methods. The parametrized blocks $\boldsymbol{W}_i$ often follow a standard template of rotation and entanglement operations and are not regression task specific.



- 4 qubit circuit
- Hardward Efficient (HWE) block with rotation and entangling layers
- HWE-*k* ansatz repeats this block *k* times

2. Method

From a candidate structure, e.g. HWE-2, we apply an iterative framework to efficiently yield circuits beginning from the base ansatz.
1) the sequence of gate operations is probabilistically altered to yield a sample of similar ansatze
2) new circuits are re-sampled from top circuits, the sample is then trained and best circuits are selected
3) process yields improved ansatze each iteration, terminates on convergence



Sampling occurs with four actions on gates in temporal order, given by

- p_{add}: *probability of gate addition*
- p_{remove}: *probability of gate removal*
- p_{switch}: *probability of switching type*
- p_{move}: *probability of wire change*
- N_{sample}: *sample size*

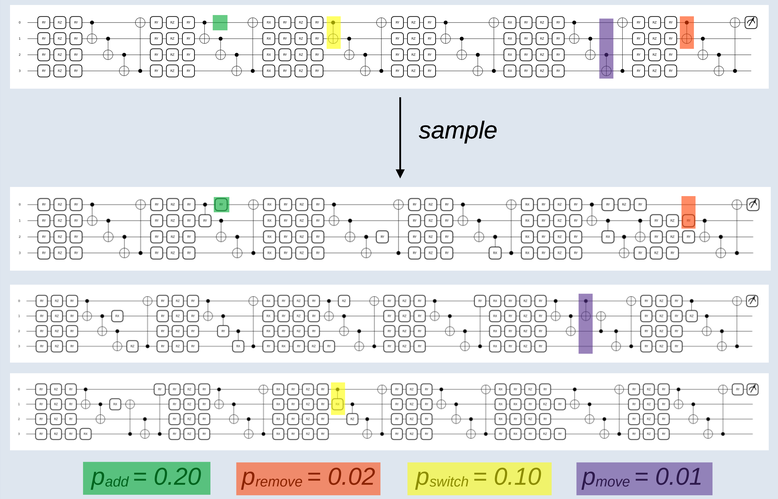
The probabilities $\boldsymbol{p}_i$ parametrize a ***Bernoulli(p_i)*** variable indicating a change in the circuit. These affect iteration step changes in the base ansatz. Given ***g*** gates and setting $\boldsymbol{p_{add} = 1 / g}$, 1 gate is added on average in each iteration step. $\boldsymbol{p}_i$ can be decayed for changes to occur less frequently with each iteration, controlling deviation from $\boldsymbol{A_0}$. Training and circuits are implemented with PennyLane differentiable QC package.

The local optimization approach is first applied to 4 qubit noisy regression data following

$$y = x_1^2 + x_2^2 + x_3^2 + x_4^2 + \varepsilon, \qquad x \in (-2, 2)^4 \quad \text{and} \quad \varepsilon \sim N(0, 0.5^2)$$

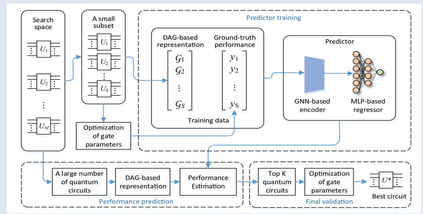
Architecture selection is next applied to BSE49 chemical bond separation energy data (V. K. Prasad, 2021) for a 16 qubit regression.

4 qubit HWE-2 ansatz with 2 time depth re-encoding



3. Outlook

Current approaches randomly sample from the search space of ansatze and train a neural net (NSGA-II, GNN) to predict performance performance given structure of observed circuits (Y. Du, 2022 and Z. He, 2023).



- Z. He, 2023
- GNN GRU message passing for generalizing performance to search space of circuits

Our framework:
- avoids circuit representation, meta-learning of circuit models
- scalable to larger ansatze: avoids sparse sampling, training data
- applicable to general PQC-based task

4. Acknowledgements

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5. Citations

I. Schuld, M., Sweke, R. and Meyer, J.J. (2021) *https://doi.org/10.1103/PhysRevA.103.032430*
II. Prasad, V.K. et al. (2021) *https://doi.org/10.1038/s41597-021-01088-2*
III. Du, Y. et al. (2022) *https://doi.org/10.1038/s41534-022-00570-y*
IV. He, Z. et al. (2023) *https://doi.org/10.1007/s11128-023-03881-x*