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

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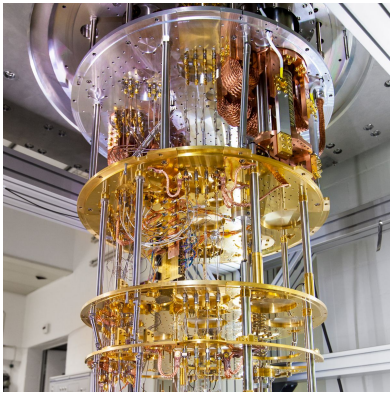
Background

Classical: $0, 1 \rightarrow$ bits
Quantum: $\alpha|0\rangle + \beta|1\rangle$ s.t. $|\alpha|^2 + |\beta|^2 = 1$
Qubit: unit of quantum information used to represent computational states

- n qubits $\rightarrow 2^n$ computational states
- quantum algorithms are operations on computational states



Background: Examples

$|0\rangle, |1\rangle$ are orthogonal basis vectors of $\mathbb{C}^2$: can consider the state

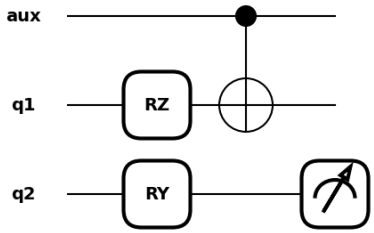
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \text{ as } |\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

- **NOT** has matrix form $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$: maps basis $|0\rangle \to |1\rangle$, $|1\rangle \to |0\rangle$
- **Hadamard** is a single qubit operation that outputs a sum of both basis states

$$H = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \quad H|0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

Background

- **Quantum circuit**: a sequence of operations (rotations, entanglements) on quantum states
- **Parametrized quantum circuit (PQC)**: a quantum circuit with operations depending on parameters (eg. rotation depending on θ)
- **Quantum machine learning**: applying a quantum circuit to a learning task. E.g. fitting a regressor via circuit implementation

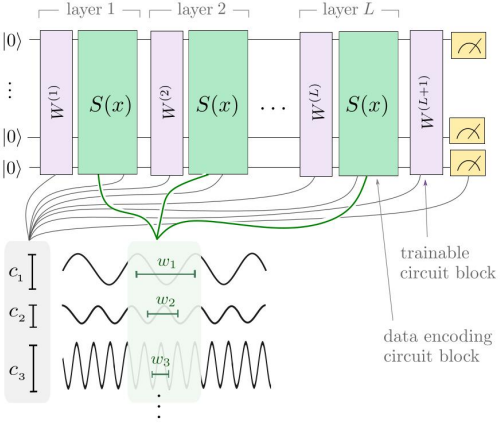


Regression PQC structure

1. **Encoding**: data x embedded in quantum state via rotations $S(x)$
2. **Param. Blocks**: embeddings $S(x)$ entangled and rotated with parameters θ_i in block W_i
3. **Measurement**: final state is measured

More encoding $\rightarrow$ more Fourier terms.

$$f_\theta(x) = W_{L+1} S(x) W_L S(x) \cdots S(x) W_1$$

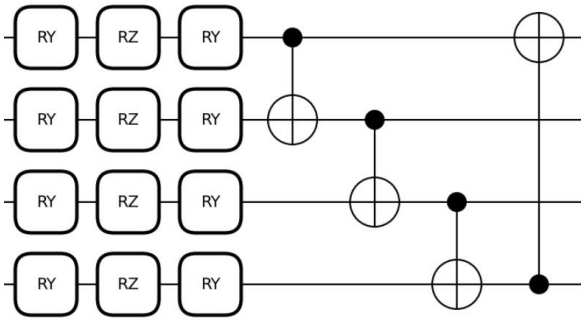


M. Schuld, 2020

How are W_i parametrized?

- follows a 'template' (ansatz) sequence of gates
- functional form f_θ determined by ansatz
- trainability, expressibility, generalizibility

θ are optimized wrt. loss as in usual ML



Hardware efficient ansatz block (HWE) in a 4 qubit system.

Project Goals

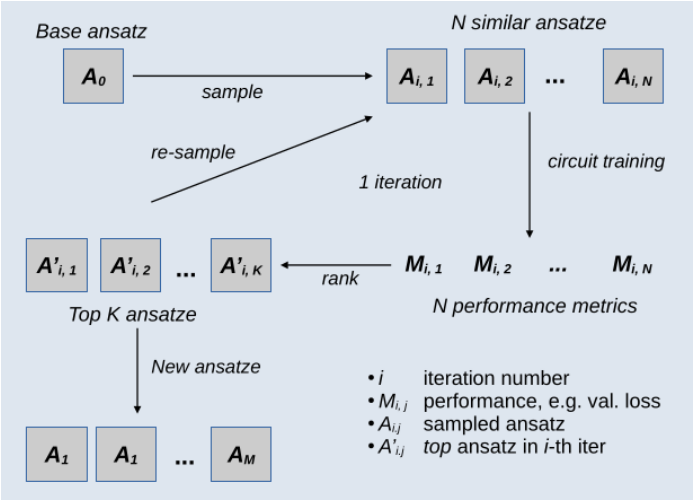
- Develop framework for architecture selection in quantum regression models
- Ensure scalability, flexibility, generalization
- Apply to BSE49 chemical dataset on larger qubit system

Strategy

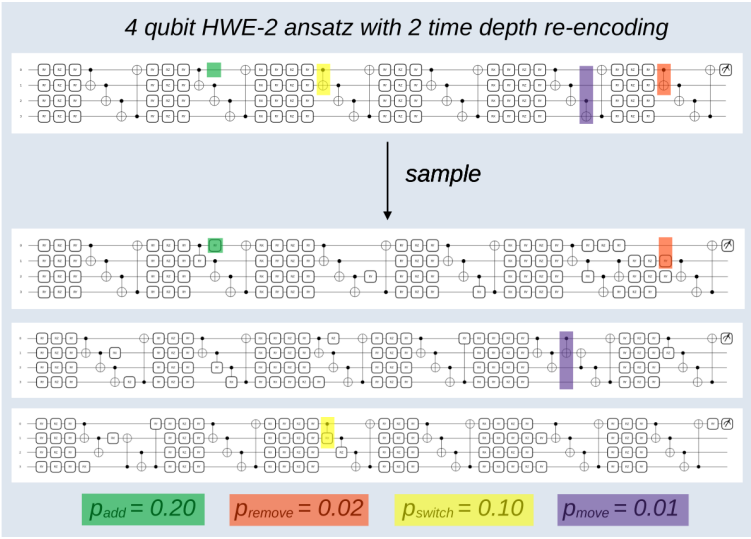
The gate sampling strategy is parametrized by four actions

- p_{add}: addition
- p_{remove}: removal
- p_{switch}: gate switch
- p_{move}: wire change

Probabilities may be decayed during training, number of samples controlled.



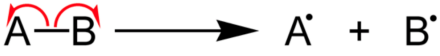
4 Qubit HWE-2 sampling



Data Application

The framework is used for circuit selection in

1. **4 Qubit Noisy quadratic**: $y = \|x\|^2 + \epsilon$, $x \in (-2, 2)^4$, $\epsilon \sim N(0, 0.5^2)$
2. **16 Qubit BSE49**: featurized bond separation energy dataset



Homolytic bond separation

Comparison

Local framework

- slightly modifies base ansatz
- sampling occurs locally
- flexible number of circuit executions
- iteration and algorithm level changes from base controlled
- no meta learning required
- unseen gate types in base may be incorporated

Other approaches

- aims for best global ansatz
- involves random sampling from exponential search space
- GNN-based approaches require non-sparse training data
- involves meta-learning (model on a model), incorporating lots of noise

Outlook

- local framework applicable to a general PQC task
- flexible, scalable, lots of control over computing resources
- a step towards automated circuit design for regression in quantum chemistry

Acknowledgements

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