Variational Quantum Eigensolver introduction

- **Ansatz**: a parameterized circuit used as Ansatz for the wave function
- **Optimizer**: a classical optimizer. Can either be a Qiskit optimizer or a callable that takes an array as input and returns a Qiskit or SciPy optimization result
- **Initial points**: an optional initial point (i.e. initial parameter values) for the optimizer. If *None* then VQE will look to the ansatz for a preferred point, and if *Not* will simply compute a random one
- **Callback**: a callback that can access the intermediate data during the optimization
- **Quantum instance**: the backend

https://qiskit.org/documentation/stubs/qiskit.algorithms.VQE.html
VQE setup: ansatz determination

**Operator:** finite-size spin $\frac{1}{2}$ Heisenberg chains

$$\mathcal{H} = 2J \sum_{i=1}^{4} \vec{s}_i \cdot \vec{s}_{i+1} + B \sum_{i=1}^{4} s_i^z$$

**Ansatz:** parametrized circuit

**Initial points:** initial parameters

**Rotations layer**

**Entanglement layer**

$$V_j(\tilde{\theta}_j) = \theta_1, \theta_2, \ldots$$
IBM Quantum Simulations


VQE setup: ansatz determination

Heuristic Ansatz – HA

Pros:
- Easily fitted with hardware configuration
- Can in principle reproduce very well the target waveform

Cons:
- The number of layers needed could easily increase

\[ V_j(\tilde{\theta}_j) = \begin{bmatrix} q_0 & R_y \theta_1 & + & + & + \\ q_1 & R_y \theta_2 & + & + & + \\ q_2 & R_y \theta_3 & + & + & + \\ q_3 & R_y \theta_4 \\ \end{bmatrix} \]

Rotations layer Entanglement layer


Pros:
- Preservation of $S$ and $m$ quantum numbers
- More scalable, and should take less iterations to converge

Cons:
- Not so easy to apply on hardware

\[ W_{ij}(\theta) = \begin{bmatrix} q_0 & R_x \frac{\theta_{ij}}{2} & H & H & R_x \frac{\theta_{ij}}{2} \\ q_1 & + & + & + & + \\ q_2 & + & + & + & + \\ q_3 & + & + & + & + \\ \end{bmatrix} \]

Ansatz initialisation required:
- Low B: $S = 0$, $m = 0$
- Intermediate B: $S = 1$, $m = -1$

Four spin $\frac{1}{2}$ Heisenberg closed ring

Noisy simulated VQE results

\[ \mathcal{H} = 2J \sum_{i=1}^{4} \vec{s}_i \cdot \vec{s}_{i+1} + B \sum_{i=1}^{4} s_i^z \]

Custom noise model derived from QV 128 IBM Quantum chip (early 2021)
Kraus decomposition used by Qiskit to model errors
Six spin ½ Heisenberg closed ring

Noisy simulated VQE results

\[ \mathcal{H} = 2J \sum_{i=1}^{6} \vec{s}_i \cdot \vec{s}_{i+1} + B \sum_{i=1}^{6} s_i^z \]

**Simulating Static and Dynamic Properties of Magnetic Molecules with Prototype Quantum Computers** – L. Crippa et al., Magnetochemistry 7, 117 (2021)

Custom noise model derived from QV 128 IBM Quantum chip (early 2021)

Kraus decomposition used by Qiskit to model errors