Noncontextuality in variational quantum algorithms

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VQE: abstract view

$$\langle H \rangle = \sum_{P \in \mathcal{S}} h_P \langle P \rangle$$

$\mathcal{S}$ is the set of Pauli operators whose expectation values are estimated in the VQE procedure.

What can we learn about the procedure from $\mathcal{S}$?

Contextuality

$\mathcal{S}$, a set of Pauli operators, is contextual if it is impossible to assign simultaneous values to the operators without contradiction.

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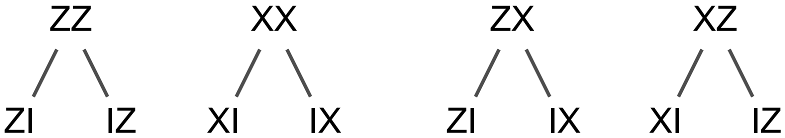

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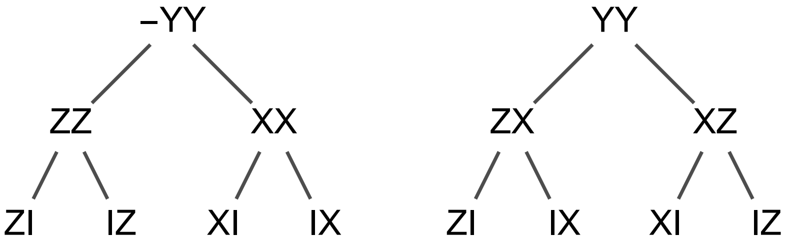

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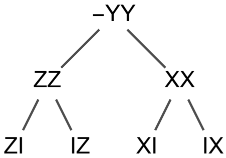

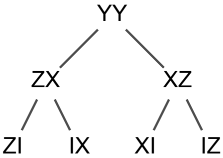

Value assignments:

$$\left.\begin{array}{l} ZI \mapsto V_{zi} \\ IZ \mapsto V_{iz} \\ XI \mapsto V_{xi} \\ IX \mapsto V_{ix} \end{array}\right\} \Longrightarrow \quad \boxed{-YY \mapsto V_{zi}V_{iz}V_{xi}V_{ix}} \qquad \boxed{YY \mapsto V_{zi}V_{iz}V_{xi}V_{ix}}$$

Necessary and sufficient condition for noncontextuality

A set $\mathcal{S}$ of Pauli operators is noncontextual if and only if it has the form

$$\mathcal{S} = \mathcal{Z} \cup C_1 \cup C_2 \cup \cdots \cup C_N,$$

where

- operators in $\mathcal{Z}$ commute with all operators in $\mathcal{S}$,
- operators in the same C_i commute, and
- operators in different C_i anticommute.[1]

[1] WMK and P. J. Love, Phys. Rev. Lett. **123**, 200501 (2019); arXiv:1904.02260.

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What can we do with this?

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Form of a noncontextual Pauli Hamiltonian

$$\mathcal{S} = \mathcal{Z} \cup C_1 \cup C_2 \cup \cdots \cup C_N,$$

Any Hamiltonian whose terms have this structure can be written in the form:

$$H = \underbrace{\sum_{B \in \overline{G}} h_B B}_{\text{terms in } \mathcal{Z}} + \underbrace{\sum_{B \in \overline{G}} \sum_{i=1}^{N} h_{B,i} B C_{i1}}_{\text{terms in } C_1 \cup C_2 \cup \cdots \cup C_N},$$

where

- $\{C_{i1} \mid i = 1, 2, ..., N\}$ is an anticommuting set of Pauli operators — one from each C_i,
- G is an independent, commuting set of Pauli operators that also commute with the C_{i1}, and
- $\overline{G}$ is the Abelian group generated by G.[2]

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So $\langle H \rangle$ is a function of the expectation values of G and $\{C_{i1} \mid i = 1, 2, ..., N\}$.

Allowed sets of expectation values: for each $G_j \in G$ and each C_{i1},

$$\langle G_j \rangle = q_j \text{ and } \langle C_{i1} \rangle = r_i, \quad \text{such that } q_j = \pm 1 \text{ and } |\vec{r}| = 1.$$

Noncontextual Pauli Hamiltonian as classical objective function

If we define $\mathcal{J}_B$ such that $B = \prod_{j \in \mathcal{J}_B} G_j$, then

$$\langle H \rangle_{(\vec{q},\vec{r})} = \sum_{B \in \overline{G}} \left(h_B + \sum_{i=1}^{N} h_{B,i} r_i \right) \prod_{j \in \mathcal{J}_B} q_j,$$

where $q_j = \pm 1$ and $|\vec{r}| = 1$.

For each eigenvalue E of H, there exists $(\vec{q}, \vec{r})$ such that $\langle H \rangle_{(\vec{q},\vec{r})} = E$.

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Consequences:

1. The NONCONTEXTUAL HAMILTONIAN PROBLEM is in NP, since for every eigenvalue there exists a classical witness $(\vec{q}, \vec{r})$.
2. Can classically simulate noncontextual VQE using this objective function. Number of parameters $(\vec{q}, \vec{r})$ is at most $2n + 1$ for n qubits. Not efficient in the worst case, but we can use heuristics as for other NP-complete problems.[3]

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A closing thought...

Noncontextual VQE looks like QAOA: a variational quantum algorithm to approximate a solution to an NP-complete problem.

So for noncontextual VQE, we should expect that the potential for quantum advantage reduces to choosing a clever ansatz, as in QAOA: there is no “quantumness” in the measurements.

Thank you!

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References:

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Thank you for your attention!