Exploiting Contextuality in Variational Quantum Algorithms

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Outline

1. Background
2. Contextuality of VQE [KL19]
3. Quasi-quantized (phase-space) model for noncontextual VQE [KL20]
4. Approximation method for contextual VQE [KTL20]

Variational quantum eigensolver

Goal: find ground state energy of H.

Method:

1. preprocess

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

   for Pauli operators P in some set $\mathcal{S}$, and real coefficients h_P.

2. given ansatz $|\psi(\vec{\theta})\rangle$, estimate expectation values of each $P \in \mathcal{S}$ separately.
3. given results, classically evaluate $\langle H \rangle$, and update ansatz parameters $\vec{\theta}$ to minimize.

Variational quantum eigensolver

Want to understand where "quantumness" appears in this algorithm.

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

$\Rightarrow$ Focus on the set of measurements $\mathcal{S}$.

Pauli operators

For example, n qubit Pauli operator:

$$P = \underbrace{Z \otimes I \otimes X \otimes I \otimes \cdots \otimes Y \otimes Z}_{n \text{ Pauli matrices}} \equiv ZIXI \cdots YZ.$$

Facts:

1. Hermitian, eigenvalues $= \pm 1 \quad \Rightarrow \quad$ self-inverse.
2. Basis for Hermitian operators on n qubits.
3. Paulis P, Q either commute or anticommute.
4. P, Q commute $\quad \Leftrightarrow \quad PQ = \pm R$ for Pauli R.

Contextuality of Pauli operators

Given $\mathcal{S}$, suppose you want to construct a classical, realistic model (think HVM). This consists of:

1. joint value assignments to $\mathcal{S}$: "ontic states."
2. probability distributions over the joint value assignments: "epistemic states."
3. need to impose uncertainty relation, i.e., restriction on which measurements can be performed simultaneously.

For example, suppose $\mathcal{S} = \{X, Y, Z\}$.

1. joint value assignment $= v = \{\pm 1, \pm 1, \pm 1\}$.
2. probability distribution: $p(v) = \prod_{i=1}^{3} \frac{1}{2}(1 + v_i r_i)$ for $|\vec{r}| \leq 1$.

Contextuality: when is it possible versus impossible to construct such a model?

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Strong contextuality: when is it possible versus impossible to construct the joint value assignments?

Contextuality of Pauli operators

Focus on joint value assignments (strong contextuality).

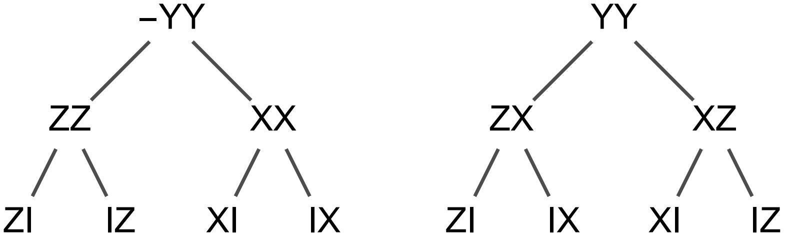
Any commuting subset of $\mathcal{S}$ is simultaneously measurable.

So if $P, Q \in \mathcal{S}$ and $[P, Q] = 0$, and joint value assignment is classical, "real" values for $\mathcal{S}$, then by measuring P and Q we infer value assigned to PQ.

For example, $\mathcal{S} = \{XI, IX\} \quad \Rightarrow \quad$ for assignment $\{\pm 1, \pm 1\}$ to $\mathcal{S}$, can infer assignment to XX.

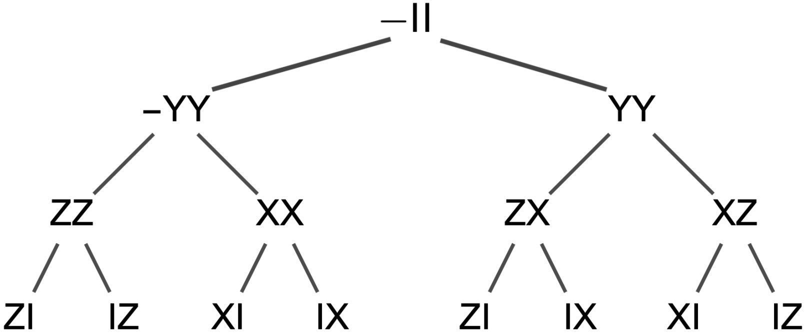
Contextuality of Pauli operators

Example: $\mathcal{S} = \{XI, IX, ZI, IZ\}$.



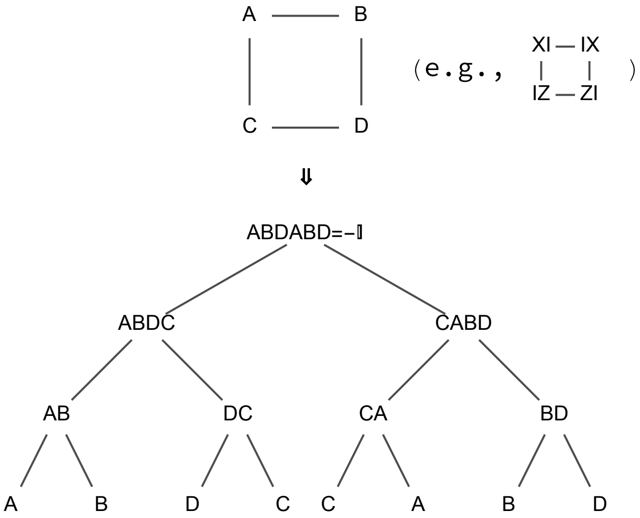
Contextuality of Pauli operators

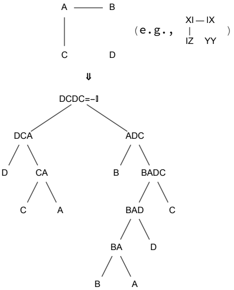
Example: $\mathcal{S} = \{XI, IX, ZI, IZ\}$.



Contextuality of Pauli operators

Generalize: tree depends only on commutation relations. E.g.,




A — B
C D
(e.g., XI — IX
IZ YY)
⇓
DCDC=−𝕀
DCA
ADC
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BAD
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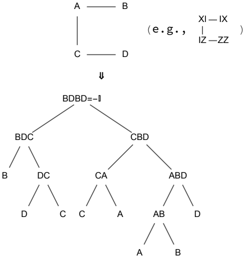
A — B
C — D
(e.g., XI — IX
IZ — ZZ)
⇓
BDBD=−𝕀
BDC
CBD
B
DC
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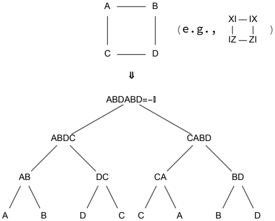
C
C
A
AB
D
A
B


A — B
C — D
(e.g., XI — IX
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⇓
ABDABD=−𝕀
ABDC
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C
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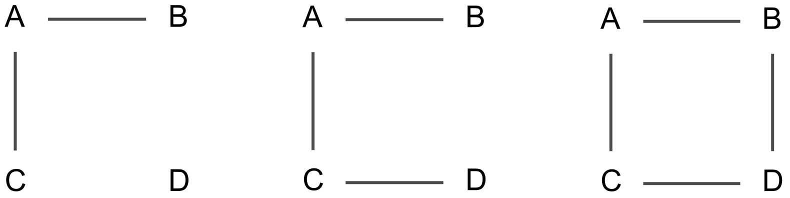
Contextuality of Pauli operators



$\mathcal{S}$ is noncontextual iff it contains none of these commutation subgraphs.

$\Leftrightarrow$ $\mathcal{S}$ is noncontextual iff it has the form

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

where $A \in \mathcal{Z}$ commutes with any $P \in \mathcal{S}$, and $B_i \in C_i$ commutes with $B_j \in C_j$ iff $i = j$.

Up to this point: [KL19].

Noncontextual Hamiltonians

Hamiltonian H is noncontextual iff its set of Pauli terms has the form

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

Therefore, $A, B \in C_i \quad \Rightarrow \quad AB$ commutes with everything $\quad \Rightarrow \quad$ can add AB to $\mathcal{Z} \quad \Rightarrow \quad$ can remove B from C_i and recover by inference on A, AB: $A \cdot AB = B$.

Therefore, can recover Hamiltonian terms by inference on

$$\mathcal{S}' = \mathcal{Z}' \cup \{C_{11}\} \cup \{C_{21}\} \cup \cdots \cup \{C_{N1}\},$$

where $\mathcal{Z} \subset \mathcal{Z}'$, $\mathcal{Z}'$ still commutes with everything, and $C_{i1} \in C_i$.

Noncontextual Hamiltonians

Can recover Hamiltonian terms by inference on

$$\mathcal{S}' = \mathcal{Z}' \cup \{C_{11}\} \cup \{C_{21}\} \cup \cdots \cup \{C_{N1}\}.$$

Let G be a set of generators for the Abelian group $\overline{\mathcal{Z}'}$. Can recover Hamiltonian terms by inference on

$$G \cup \{C_{11}\} \cup \{C_{21}\} \cup \cdots \cup \{C_{N1}\},$$

which is independent, i.e., all outcome assignments are allowed.

Every noncontextual Hamiltonian has the form:

$$H = \sum_{B \in \overline{G}} \left(h_B B + \sum_{i=1}^{N} h_{B,i} B C_{i1} \right).$$

Noncontextual Hamiltonians

Every noncontextual Hamiltonian has the form:

$$H = \sum_{B \in \overline{G}} \left(h_B B + \sum_{i=1}^{N} h_{B,i} B C_{i1} \right).$$

What are the allowed probability distributions (epistemic states)? Turn out to lead to the following sets of expectation values:

$$\langle G_j \rangle = q_j = \pm 1, \quad \langle C_{i1} \rangle = r_i$$

for $|\vec{r}| = 1$. Can prove that these are enough to generate all possible expectation values of the Hamiltonian.

Quasi-quantized model (Robert Spekkens [Spe16]): equivalent to a classical phase-space model with an uncertainty relation.

Noncontextual Hamiltonians

Every noncontextual Hamiltonian has the form:

$$H = \sum_{B \in \overline{G}} \left(h_B + \sum_{i=1}^{N} h_{B,i} C_{i1} \right) B.$$

$$\langle G_j \rangle = q_j = \pm 1, \quad \langle C_{i1} \rangle = r_i$$

for $|\vec{r}| = 1$.

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

for $\mathcal{J}_B$ s.t. $B = \prod_{j \in \mathcal{J}_B} G_j$.

Classical objective function of $O(n)$ real parameters!

Noncontextual Hamiltonians

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for $\mathcal{J}_B$ s.t. $B = \prod_{j \in \mathcal{J}_B} G_j$.

Classical objective function of $O(n)$ real parameters $(\vec{q}, \vec{r})$!

Immediate consequences:

1. "dequantization" of noncontextual VQE.
2. noncontextual Hamiltonian problem is in NP (hence NP-complete).

Up to this point: [KL20].

What about contextual Hamiltonians?

Given any arbitrary H, can partition:

$$H = H_{\text{n.c.}} + H_{\text{c.}},$$

where $H_{\text{n.c.}}$ is noncontextual and as large as possible.

Ground state $(\vec{q}, \vec{r})_0$ of $H_{\text{n.c.}}$ corresponds to subspace of quantum states: the common eigenspace of the G_j (eigenvalues q_j) and the single operator

$$\mathcal{A} \equiv \sum_{i=1}^{N} r_i C_{i1} \qquad \text{(eigenvalue } +1\text{)}.$$

If this eigenspace is > 1 dimensional, can minimize expectation value of $H_{\text{c.}}$ within this subspace on quantum computer to obtain correction to noncontextual ground state energy.

Contextual Hamiltonians

$$H = H_{\text{n.c.}} + H_{\text{c.}}$$

Noncontextual ground state $\leftrightarrow$ subspace stabilized by $q_j G_j$ for $j = 1, 2, ..., m$ and $\mathcal{A} \equiv \sum_{i=1}^{N} r_i C_{i1}$ (rotated Pauli).

$\langle H_{\text{n.c.}} \rangle$ is determined classically, $\langle H_{\text{c.}} \rangle$ is determined quantumly.

Each "stabilizer" G_j and $\mathcal{A}$ removes one qubit's worth of freedom from the quantum search space, so $H_{\text{c.}}$ becomes a Hamiltonian on $n - m - 1$ qubits.

Can we use more quantum resources to improve accuracy?

Contextual Hamiltonians

Can we use more quantum resources to improve accuracy?

Idea: drop some of the G_j (and inferred terms) from noncontextual part, simulating them instead on the quantum computer.

$\Rightarrow$ reduces m, hence $H_{\text{c.}}$ becomes a Hamiltonian on more qubits $(n - m - 1)$, and accuracy of overall approximation improves.

whole method = Contextual Subspace VQE (CS-VQE)

Up to this point: [KTL20].

Applying Contextual Subspace VQE to molecules

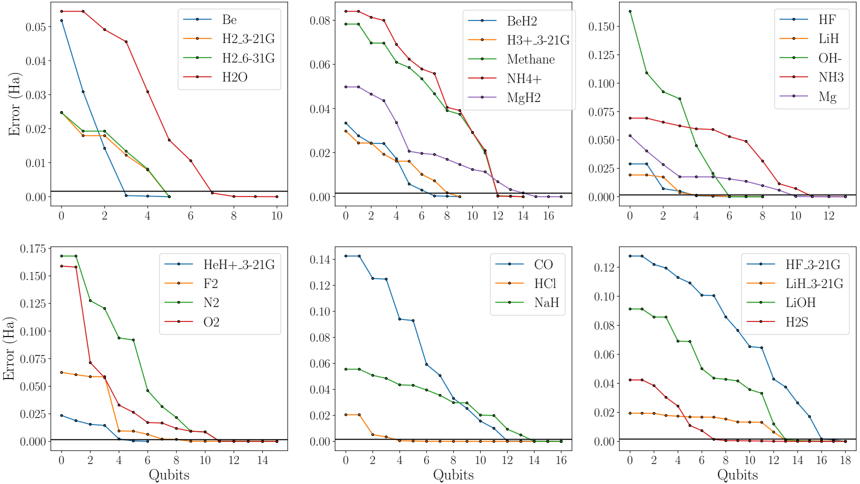

Figure: CS-VQE approximation errors versus number of qubits used on the quantum computer, for tapered molecular Hamiltonians. Black line is chemical accuracy.

Applying Contextual Subspace VQE to molecules (cont'd)

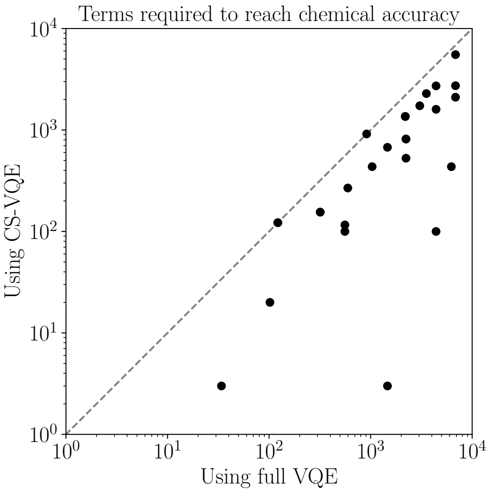

Figure: Number of terms to simulate on the quantum computer in order to reach chemical accuracy using CS-VQE versus standard VQE.

What is being swept under the rug?

1. Maximum noncontextual part of a Hamiltonian is worst-case hard to find (but greedy heuristic works well for molecules).
2. Noncontextual ground state is worst-case hard to find, but isn't worse than original VQE (and Monte Carlo + optimization seems to work well).
3. Order to move qubits from noncontextual part to quantum part might be worst-case hard to find (but greedy heuristic works well for molecules).

Thank you! Any questions?

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