Exploiting Contextuality in Variational Quantum Eigensolvers

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Outline

1. Contextuality of VQE [KL19]
2. Quasi-quantized (phase-space) model for noncontextual VQE [KL20]
3. Approximation method for contextual VQE [KTL21]

Variational quantum eigensolver

Goal: find ground state energy of

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

for Pauli operators P in some set $\mathcal{S}$.

Method:

1. Main process: on classical computer, minimize

$$E(\vec{\theta}) = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle = \sum_{P \in \mathcal{S}} h_P \langle \psi(\vec{\theta}) | P | \psi(\vec{\theta}) \rangle$$

   for ansatz $|\psi(\vec{\theta})\rangle$.

2. Iteration step: on quantum computer, estimate $\langle P \rangle$ for each $P \in \mathcal{S}$.

Variational quantum eigensolver

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

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

$\Rightarrow$ Focus on $\mathcal{S}$.

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 $\mathcal{S}$ (the "classical, real" values).
2. probability distributions over the joint value assignments:
   - need to impose uncertainty relation, i.e., restriction on which values can be known simultaneously $\Leftrightarrow$ *quasi-quantization* [Spe16].

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

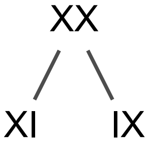
Contextuality of Pauli operators

Focus on joint value assignments (strong contextuality).

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

$P, Q \in \mathcal{S}$ and $[P, Q] = 0 \quad \Rightarrow \quad$ by measuring P and Q *infer* value assigned to PQ (since joint value assignment interpreted as "real" values for $\mathcal{S}$).

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

Focus on joint value assignments (strong contextuality).

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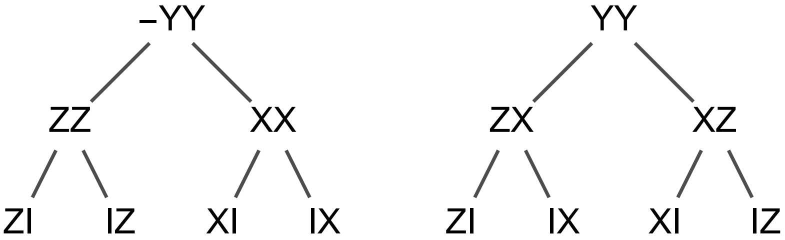
$P, Q \in \mathcal{S}$ and $[P, Q] = 0 \quad \Rightarrow \quad$ by measuring P and Q *infer* value assigned to PQ (since joint value assignment interpreted as "real" values for $\mathcal{S}$).

$\mathcal{S}$ is contextual if any joint values necessarily violate some such inference.

Contextuality of Pauli operators

Example: Peres-Mermin square $\Leftrightarrow \mathcal{S} = \{XI, IX, ZI, IZ\}$.



$\Rightarrow$ $\forall$ joint value assignments to $\mathcal{S}$, we infer that YY and $-YY$ have the same value $\Rightarrow$ contradiction! $\Rightarrow$ $\mathcal{S}$ is contextual.

Contextuality of Pauli operators

Result [KL19]. $\mathcal{S}$ is *noncontextual* iff it has the form

$$\mathcal{S} = \mathcal{Z} \cup \mathcal{T} = \mathcal{Z} \cup \mathcal{C}_1 \cup \mathcal{C}_2 \cup \cdots \cup \mathcal{C}_N,$$

where commutation is an equivalence relation on $\mathcal{T}$ ($\mathcal{C}_i$ = equivalence classes), and any $A \in \mathcal{Z}$ commutes with any $B \in \mathcal{S}$.

Definition. Hamiltonian H (VQE instance) is noncontextual iff its set $\mathcal{S}$ of Pauli terms is noncontextual.

Classical simulation of noncontextual Hamiltonians

$\Rightarrow$ can recover Hamiltonian terms by inference on

$$G \cup \{A_1\} \cup \{A_2\} \cup \cdots \cup \{A_N\},$$

where G is independent generating set for $\mathcal{Z}$, and $A_i \in C_i$.

$\Rightarrow$ every noncontextual Hamiltonian has the form:

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

Allowed probability distributions lead to following sets of expectation values:

$$\langle G_j \rangle = q_j = \pm 1, \quad \langle A_i \rangle = r_i$$

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

Classical simulation of noncontextual Hamiltonians

Given any noncontextual H...

Result [KL20]. For parameters $q_j = \pm 1$ and $|\vec{r}| = 1$.

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

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

Classical objective function of at most $2n + 1$ real parameters.

Immediate consequences:

1. "dequantization" of noncontextual VQE.
2. noncontextual Hamiltonian problem is in NP.

Hybrid simulation of 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.

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

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

On quantum computer, can minimize expectation value of $H_{\text{c.}}$ within this subspace to obtain correction to noncontextual ground state energy.

Contextual Subspace VQE (CS-VQE)

Result [KTL21].

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

$\langle H_{\text{n.c.}} \rangle$ 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 Hamiltonian on $n - 1 - |G|$ qubits.

Can we use more quantum resources to improve accuracy?

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

Applying Contextual Subspace VQE to molecules

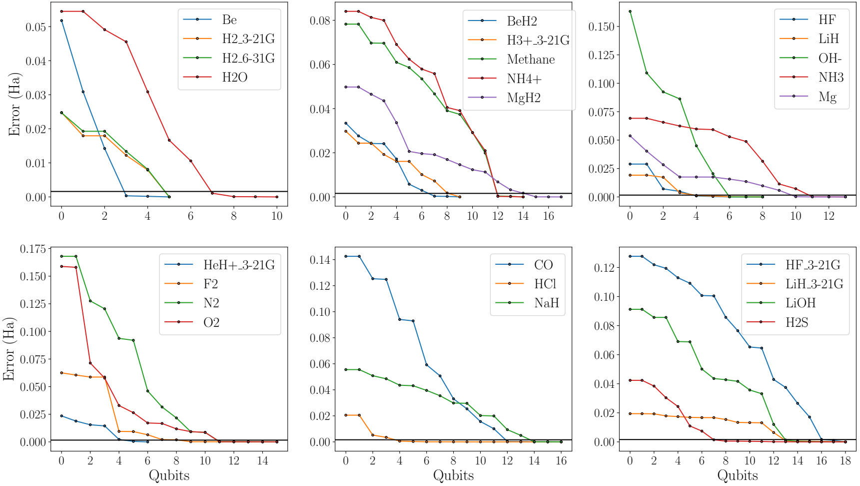


Figure: CS-VQE approximation errors versus number of qubits used on the quantum computer, for tapered Hamiltonians. Black line is chemical accuracy.

Thank you! Any questions?

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- Robert W. Spekkens. *Quasi-Quantization: Classical Statistical Theories with an Epistemic Restriction*, pages 83–135. Springer Netherlands, Dordrecht, 2016.

Code: `https://github.com/wmkirby1/ContextualSubspaceVQE`

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