Improving Variational Quantum Algorithms by Isolating Nonclassicality

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   - Pauli operators
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4. Noncontextual Hamiltonians [KL20]
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Qubits

Bit = two-state classical system:

$$\text{state space} = \{0, 1\}$$

Qubit = two-level quantum system:

$$\text{state space} \equiv \mathcal{H}_2 = \{a_0|0\rangle + a_1|1\rangle \ : \ |a_0|^2 + |a_1|^2 = 1\}$$

Classical computer of n bits:

$$\text{state space} = \{\text{length } n \text{ bitstrings}\} = \{0, 1\}^n$$

Quantum computer of n qubits $\Rightarrow$ 2^n-dimensional Hilbert space:

$$\text{s. s.} = \underbrace{\mathcal{H}_2 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_2}_{n \text{ copies}} = \left\{ \sum_b a_b|b\rangle \ : \ b = \text{length } n \text{ bitstrings} \right\}$$

Qubits

Example. A quantum computer with 3 qubits:

$$\begin{aligned}
\text{state space} = \mathcal{H}_2^{\otimes 3} = \Big\{ & a_{000}|000\rangle \\
& + a_{001}|001\rangle \\
& + a_{010}|010\rangle \\
& + a_{011}|011\rangle \\
& + a_{100}|100\rangle \\
& + a_{101}|101\rangle \\
& + a_{110}|110\rangle \\
& + a_{111}|111\rangle \ : \ \sum_b |a_b|^2 = 1 \Big\}
\end{aligned}$$

Gates (operations)

Can perform some set of unitary operations, which we often call *gates*.

Example. A quantum computer with 3 qubits:

$$\begin{aligned}\text{operations} &= \mathcal{U}(\mathcal{H}_2 \otimes \mathcal{H}_2 \otimes \mathcal{H}_2) \\ &= 8 \times 8 \text{ unitary matrices}\end{aligned}$$

Measurements

Measure each qubit in $\{|0\rangle, |1\rangle\}$ basis (*computational basis*).

For bitstrings b, given a state $\sum_b a_b|b\rangle$, we get outcome $|b\rangle$ with probability $|a_b|^2$ (Born rule).

Example quantum circuit: generate a random bit

Needs quantum computer with 1 qubit: computational basis $= \{|0\rangle, |1\rangle\}$.

Algorithm:

1. Prepare state $|\psi_0\rangle = |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.
2. Apply unitary operation $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle).$$

3. Measure in computational basis:
   - Prob. of outcome $|0\rangle$ is $|\langle 0|\psi_1\rangle|^2 = |1/\sqrt{2}|^2 = 0.5$.
   - Prob. of outcome $|1\rangle$ is $|\langle 1|\psi_1\rangle|^2 = |1/\sqrt{2}|^2 = 0.5$.

Pauli operators

For example, n qubit Pauli operator:

$$P = \underbrace{\sigma_z \otimes I \otimes \sigma_x \otimes I \otimes \cdots \otimes \sigma_y \otimes \sigma_z}_{n \text{ Pauli matrices}} \equiv ZIXI \cdots YZ.$$

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: e.g.,

$$(XXZI)(YYZX) = (X \otimes X \otimes Z \otimes I)(Y \otimes Y \otimes Z \otimes X) = -ZZIX.$$

Quantum Simulation

Usually means Hamiltonian simulation. Either...

1. simulate time-evolution under given H, or...
2. **calculate (part of) spectrum.**

Typical problem: given H, find ground state energy.

Example. Two-qubit Hamiltonian[1]:

$$H \approx 0.398ZI + 0.398IZ + 0.0113ZZ + 0.181XX.$$

$$\Rightarrow \quad \text{eigenvalues} \approx -0.805, -0.192, 0.170, 0.827.$$

[1] A. Kandala *et al.*, Nature **549**, 242 (2017).

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 CC, 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 $|\psi(\vec{\theta})\rangle = U(\vec{\theta}) |\psi_0\rangle$.

2. Iteration step: on QC, estimate $\langle \psi(\vec{\theta}) | P | \psi(\vec{\theta}) \rangle$ for each $P \in \mathcal{S}$.

Variational quantum eigensolver

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

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

$\Rightarrow$ Focus on the set $\mathcal{S}$ of terms in Hamiltonian.

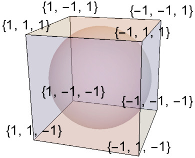
Contextuality of Pauli operators

Given $\mathcal{S}$, try to construct a classical, realistic model (think HVM):

1. joint value assignments to $\mathcal{S}$.
2. probability distributions over the joint value assignments.

Example. $\mathcal{S} = \{X, Y, Z\}$:

1. joint value assignment $= v = \{\pm1, \pm1, \pm1\}$.
2. probability distribution: $p(v) =$ point in sphere:



Definition. $\mathcal{S}$ is *contextual* if joint values cannot be self-consistent.

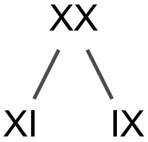
Contextuality of Pauli operators

How can a joint value assignment to $\mathcal{S}$ be inconsistent?

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

So if $P, Q \in \mathcal{S}$ and $[P, Q] = 0$, then from values assigned to P and Q we *infer* value assigned to PQ.

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



William M. Kirby and Peter J. Love, Phys. Rev. Lett. **123**, 200501 (2019).

Contextuality of Pauli operators

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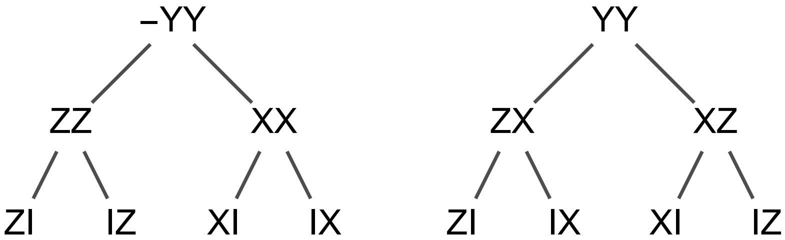
$\mathcal{S}$ is contextual if any joint values necessarily violate some such inference.

William M. Kirby and Peter J. Love, Phys. Rev. Lett. **123**, 200501 (2019).

Contextuality of Pauli operators

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



Means that for any joint value assignment to $\mathcal{S}$, we infer that YY and $-YY$ have the same value $\quad\Rightarrow\quad$ contradiction!

$\Rightarrow\quad$ This $\mathcal{S}$ is contextual.

A common misconception about noncontextuality

noncontextual $=$ commuting ✗

A set of observables...

- is noncontextual iff *no logical contradiction in assigning* joint values.
- commutes iff $\exists$ *quantum state that realizes* joint values (common eigenstate).

commuting $\Rightarrow$ noncontextual ✓

Contextuality of Pauli operators

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

$$\mathcal{S} = \mathcal{C} \cup \mathcal{T},$$

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

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Special cases of noncontextual sets:

1. any commuting set.
2. any anticommuting set.
3. any set in which commutation is an equivalence relation (includes cases 1 and 2): for example, $\{(XI, XZ), (YI, YZ), (ZI, ZZ)\}$.

Contextuality of Pauli operators

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

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

Noncontextual Hamiltonians

Noncontextual $\Rightarrow$ can build classical model!

1. phase space points = joint value assignments to $\mathcal{S}$.
2. states = probability distributions over phase space.

For n-qubit noncontextual Hamiltonian, probability distributions parametrized by $\vec{a}$ = at most $2n+1$ real parameters.

Can efficiently express expected energy as function of these:

$$\langle H \rangle = E(\vec{a}).$$

William M. Kirby and Peter J. Love, Phys. Rev. A **102**, 032418 (2020).

Noncontextual Hamiltonians

Noncontextual H...

$\Rightarrow$ Classical function for energy:

$$\langle H \rangle = E(\vec{a}).$$

$\Rightarrow$ Can replace quantum part of VQE with this function.
$\Rightarrow$ variational ~~quantum~~ eigensolver (with classical objective function of $\leq 2n+1$ real parameters).

What about contextual Hamiltonians?

Given arbitrary H, can partition:

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

for $H_{\text{n.c.}}$ noncontextual, as large as possible.

Ground state $\vec{a}_0$ of $H_{\text{n.c.}}$ corresponds to common eigenspace of $\mathcal{A}$, some commuting set of operators that we can derive from $H_{\text{n.c.}}$.

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

William M. Kirby, Andrew Tranter, and Peter J. Love, "Contextual subspace variational quantum eigensolver," arXiv preprint (2020), arXiv:2011.10027.

Contextual Hamiltonians

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

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

Each operator in $\mathcal{A}$ removes one qubit's worth of freedom, so $H_{\text{c.}}$ becomes a Hamiltonian on $n - |\mathcal{A}|$ qubits.

Example. If noncontextual ground state corresponds to common eigenspace of $\mathcal{A} = \{ZII, IZI\}$ with eigenvalues $\{1, -1\}$, then

$$\begin{aligned} H_{\text{c.}} &= h_1 IIZ + h_2 IZZ + h_3 ZIX + h_4 ZZX + h_5 XII \\ \mapsto \quad H_{\text{reduced}} &= (h_1 - h_2)Z + (h_3 - h_4)X. \end{aligned}$$

Contextual Hamiltonians

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

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

Each operator in $\mathcal{A}$ removes one qubit's worth of freedom, so $H_{\text{c.}}$ becomes a Hamiltonian on $n - |\mathcal{A}|$ qubits.

Can we use more quantum resources to improve accuracy?

Idea: stop fixing eigenvalues of some of operators in $\mathcal{A}$ to increase "resolution" of $H_{\text{c.}}$ $\Rightarrow$ set # of qubits for $H_{\text{c.}}$ to any desired value.

Application to molecules

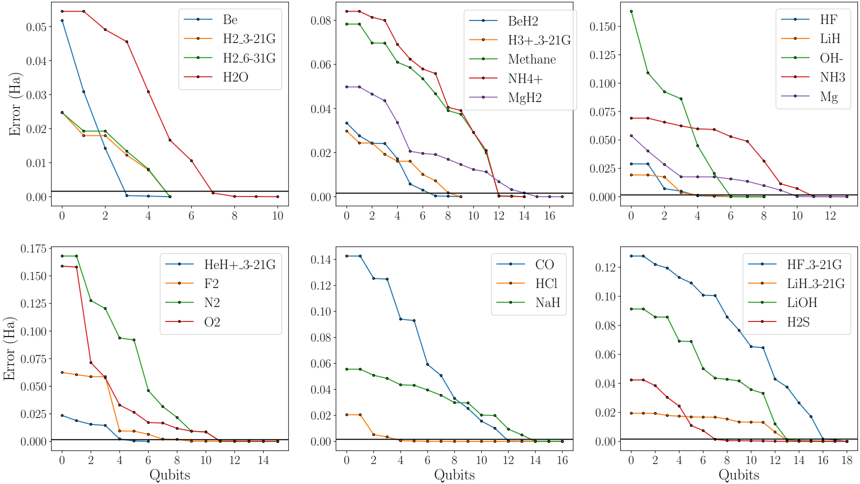

Figure: Approximation errors versus number of qubits used on the quantum computer, for molecular Hamiltonians. Black line is chemical accuracy.

Summary

1. Given H, can determine whether contextual [KL19].
2. If noncontextual, simulate classically [KL20].
3. If contextual, split into noncontextual part and contextual part, and trade off quantum resources for accuracy [KTL20].

Thank you! Any questions?

William M. Kirby and Peter J. Love. Contextuality test of the nonclassicality of variational quantum eigensolvers. *Phys. Rev. Lett.*, 123:200501, Nov 2019.

William M. Kirby and Peter J. Love. Classical simulation of noncontextual pauli hamiltonians. *Phys. Rev. A*, 102:032418, Sep 2020.

William M. Kirby, Andrew Tranter, and Peter J. Love. Contextual subspace variational quantum eigensolver. *arXiv:2011.10027*, 2020.