Contextual Subspace Variational Quantum Eigensolver

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APS March Meeting 2021

March 18, 2021

Outline

1. Contextuality of VQE [KL19]
2. Noncontextual Hamiltonians [KL20]
3. CS-VQE: a new hybrid quantum-classical algorithm [KTL20]

Variational quantum eigensolver (VQE)

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 $P \in \mathcal{S}$.

Contextuality of VQE

Noncontextual model = type of classical HVM.

Given $\mathcal{S}$, noncontextual model 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].

$\mathcal{S}$ is *noncontextual* iff possible to construct such a model.

(Set of all Pauli operators is *contextual*, i.e., no noncontextual model for it exists $\Rightarrow$ separation between classical and quantum.)

Contextuality of Pauli operators

Result [KL19]. $\mathcal{S}$ 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 $B \in \mathcal{S}$.

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

Result [KL20]. 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:

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

$\Rightarrow$ "dequantization" of noncontextual VQE.

Hybrid algorithm for arbitrary Hamiltonians

Contextual subspace VQE [KTL20].

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.

Hybrid algorithm for arbitrary Hamiltonians

Contextual subspace VQE [KTL20].

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

$\langle H_{\text{n.c.}} \rangle$ 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.

Applying Contextual Subspace VQE to molecules

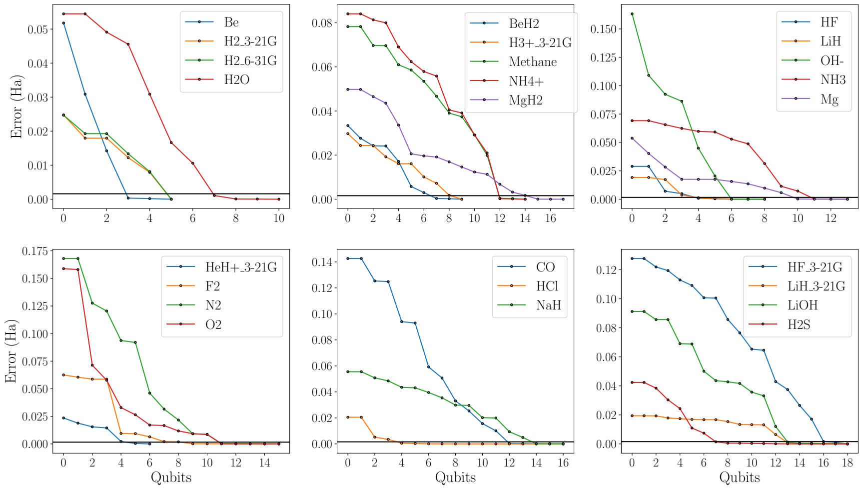

Figure: CS-VQE approximation errors versus number of qubits used on the quantum computer, for tapered Hamiltonians. Black line is chemical accuracy.

Thank you! Any questions?

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

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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`

Funding: NSF Grants No. DGE-1842474, PHY-1720395, PHY-1818914, and Google Inc.