Noncontextuality as Classicality in Variational Quantum Eigensolvers

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Abstract

Contextuality is an indicator of non-classicality in quantum systems. We use contextuality to evaluate the variational quantum eigensolver (VQE), a promising tool for near-term quantum simulation. We present an efficiently computable test to determine whether or not the Hamiltonian in a VQE procedure is contextual. Using the resulting structure for noncontextual Hamiltonians, we give a quasi-quantized model for variational quantum eigensolvers whose Hamiltonians are noncontextual, and use the model to show that the noncontextual Hamiltonian problem is NP-complete. These results support the notion of noncontextuality as classicality in quantum systems.

VQE

The goal of a variational quantum eigensolver is to approximate the ground state energy of some Hamiltonian, represented as a linear combination of Pauli operators:

$$H = \sum_{P\in\mathcal{S}} h_P P, \qquad (1)$$

where $\mathcal{S}$ is the set of Pauli terms P, and h_P are real coefficients. We find the expected energy by preparing an ansatz quantum state, and evaluating the expectation value of each Pauli term in $\mathcal{S}$ separately on our quantum device. We then treat their weighted sum (1) as the objective function for a classical optimization that updates the parameters of the ansatz.

Contextuality

A Pauli Hamiltonian is *contextual* if there are no consistent assignments of simultaneous values (± 1) to its terms [1]. The classic example of an obstacle to such assignments is the Peres-Mermin (PM) square [2]:

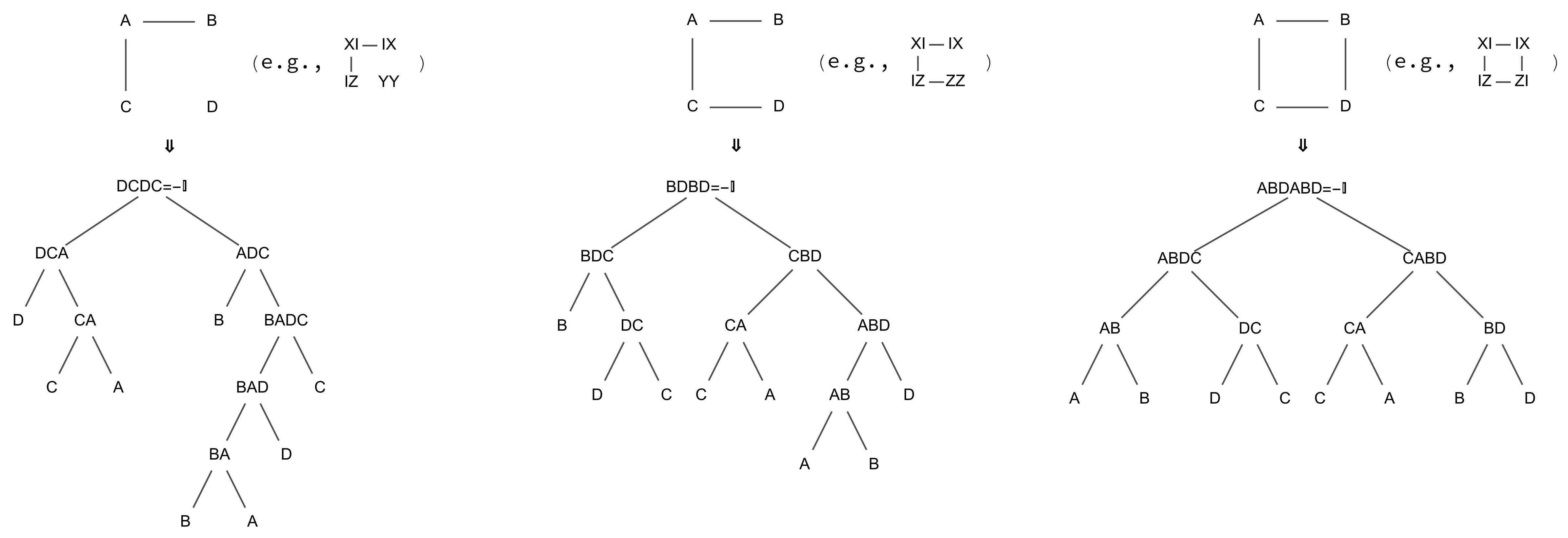
XI	IX	XX	$+1$
IZ	ZI	ZZ	$+1$
XZ	ZX	YY	$+1$
$+1$	$+1$	-1	

The product of any row or column (including the ± 1 at its end) is 1, so since the operators in any row or column can be measured simultaneously, any assignment of values to the operators must satisfy these products. However, no such assignment exists: the PM square is contextual.

Criterion for contextuality

If A, B are commuting Pauli operators, then they can be measured simultaneously, so from the values assigned to them we can infer the value assigned to AB. In each diagram below, the upper graph shows commutation relations amongst a set of four Pauli operators A, B, C, D (edges indicate commutation). Each lower graph shows a tree of inferences following from value assignments to A, B, C, D: each parent node is the product of its children, which commute.

Thus the implication of each lower graph is that the value assigned to its root is the product of the values assigned to the leaves, but since each leaf appears twice and each assigned value is ± 1, the value assigned to the root is $+1$. Since the root of each tree is $-\mathbb{1}$, this is a contradiction, so each of these commutativity graphs is contextual.



Hence, a set of Pauli operators is contextual if it contains a subset with one of the commutation graphs above. In [1], we show that the reverse implication also holds, i.e., the absence of these commutation graphs indicates noncontextuality.

Structure of a noncontextual Hamiltonian

From the above test, it follows that a Hamiltonian is *noncontextual* iff its Pauli terms $\mathcal{S}$ have the following structure:

$$\mathcal{S} = \mathcal{Z} \cup C_1 \cup C_2 \cup \cdots \cup C_N, \qquad (2)$$

where $\mathcal{Z}$ is the set of operators in $\mathcal{S}$ that commute with all others in $\mathcal{S}$, operators in the same C_i commute, and operators in different C_i anticommute [1]. Thus we can see that $\mathcal{S}$ is noncontextual iff, after identifying the fully-commuting subset $\mathcal{Z}$ (which takes $O(|\mathcal{S}|^2)$ classical operations), commutation is transitive on the remainder of $\mathcal{S}$ (which we can check in $O(|\mathcal{S}|^3)$ classical operations by testing all triples in $\mathcal{S}$).

Let $C_i \equiv \{C_{ij} | j = 1, 2, ..., |C_i|\}$ for each i; then for each j, $C_{i1}C_{ij}$ commutes with all operators in $\mathcal{S}$. Thus, let G be a generating set for the commuting set $\mathcal{Z} \cup \{C_{i1}C_{ij} | i, j\}$, and let $\overline{G}$ be the Abelian group generated by G. Then the Hamiltonian may be written:

$$H = \sum_{P\in\mathcal{S}} h_P P = \sum_{P\in\mathcal{Z}} h_P P + \sum_{i=1}^{N}\sum_{j=1}^{|C_i|} h_{ij} C_{ij} = \sum_{P\in\mathcal{Z}} h_P P + \sum_{i=1}^{N}\sum_{j=1}^{|C_i|} h_{ij} \underbrace{C_{i1}C_{i1}}_{\text{insert identity}} C_{ij}$$

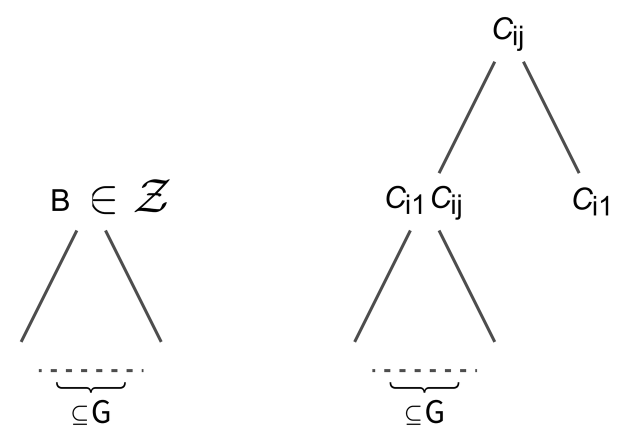
$$\Rightarrow \quad H = \sum_{B\in\overline{G}} \left(h_B + \sum_{i=1}^{N} h_{B,i} C_{i1} \right) B, \qquad (3)$$

where each step simply involves reorganizing the expression and/or relabeling the coefficients.

Quasi-quantized model

A *quasi-quantized model* is a classical statistical model with a classical uncertainty relation. It comprises a set of "actual" states of the system, called *ontic states*, and a set of allowed probability distributions, called *epistemic states* [3].

In our case, the ontic states are the joint assignments of values (± 1) to G (the generating set for the commuting components of the Hamiltonian) and $\{C_{i1} | i = 1, 2, ..., N\}$. Each such assignment induces an assignment to each operator in $\mathcal{S}$, as shown in the following diagrams (parent nodes are products of their children, which commute):



The epistemic states over these ontic states may be expressed as sets of expectation values for $G \cup \{C_{i1} | i = 1, 2, ..., N\}$: the set of allowed epistemic states is

$$\left\{ (\vec{q}, \vec{r}) \in \{\pm 1\}^{|G|} \times \mathbb{R}^N \mid |\vec{r}| = 1 \right\}, \qquad (4)$$

where

$$\langle G_j \rangle = q_j \text{ for each } G_j \in G, \text{ and } \langle C_{i1} \rangle = r_i \ \forall i. \qquad (5)$$

Via (3), each epistemic state gives an expectation value for the Hamiltonian:

$$\langle H \rangle_{(\vec{q},\vec{r})} = \sum_{B\in\overline{G}} \left(h_B + \sum_{i=1}^{N} h_{B,i} r_i \right) \prod_{j\in\mathcal{J}_B} q_j, \qquad (6)$$

for $\mathcal{J}_B$ such that $B = \prod_{j\in\mathcal{J}_B} G_j$. In our forthcoming work, we show that the expectation values thus generated always correspond to valid quantum states, and that they include all eigenstates of the Hamiltonian.

We may treat (6) as a classical objective function of an epistemic state $(\vec{q}, \vec{r})$, and implement any classical optimization procedure we like to find its minimum. As shown below, this implies that the associated local Hamiltonian problem is NP-complete, so it is not guaranteed to be classically tractable: however, it is unambiguously a classical problem.

The noncontextual Hamiltonian problem is NP-complete

Using (6), we can any expectation value of the noncontextual Hamiltonian given the set of classical parameters $(\vec{q}, \vec{r})$. Thus $(\vec{q}, \vec{r})$ can serve as a classical witness for any eigenvalue of the Hamiltonian. In particular, if the ground state energy of the Hamiltonian is below some value a, there exists $(\vec{q}, \vec{r})$ such that $\langle H \rangle_{(\vec{q},\vec{r})} < a$. This proves that the noncontextual Hamiltonian problem is in NP, up to some details, which are given in our forthcoming work. Since diagonal Hamiltonians are both NP-complete and noncontextual, the noncontextual Hamiltonian problem is NP-complete.

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