Entanglement witness by quantum circuits

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Machine learning algorithms are applied to the entanglement detection problem. We compare complexity and performance of different methods, including conventional methods, machine learning, quantum algorithms.

CONTENTS

I. INTRODUCTION

Entanglement [1] is the key ingredient of quantum computation [], quantum communication [], and quantum cryptography []. It is essential to benckmark (characterize) entanglement structures of target states.

II. PRELIMINARY

A. Notations

The (classical) training data is a set of m data points $\left\{(\mathbf{x}^{(i)}, y^{(i)})\right\}_{i=1}^{m}$ where each data point is a pair $(\mathbf{x}, y)$. Normally, the input $\mathbf{x} := (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$ is a vector where d is the number of *features* and its *label* $y \in \Sigma$ is a scalar with some discrete set Σ of alphabet/categories. For simplicity, we assume $\Sigma = \{-1, 1\}$ (binary classification).

Notations: a graph $G = (V, E)$ with vertices V and edges E; The hats on the matrices such as $\hat{A}$, $\hat{H}$, $\hat{\rho}$, $\hat{O}$, $\hat{W}$, emphasize that they play the roles of operators. denote vector (matrix) $\mathbf{x}$, $\mathbf{K}$ by boldface font.

For specific purpose, we use different basis (representations) for quantum states. One is the computational basis $\{|z\rangle\}$ with $z \in [2^n]$ where n is the number of qubits, while the other useful one is the binary representation of

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computational basis $\{|\mathbf{x}\rangle \equiv |x_1, x_2, \ldots, x_n\rangle\}$ with $x_j \in \{0,1\}$. For simplicity, we let $N \equiv 2^n$ and $|\mathbf{0}\rangle \equiv |0^n\rangle \equiv |0\rangle^{\otimes n}$ if no ambiguity. $|+\rangle := (|0\rangle + |1\rangle)/\sqrt{2}$

B. Entanglement detection

Definition 1 (Entangled state)**.** pure state; mixed state is convex combination of entangled ...

Definition 2 (Bipartite state)**.**

1. *entanglement structures*

Given a n-partite quantum system and its partition into m subsystems, the *entanglement structure* indicates how the subsystems are entangled with each other. In some specific systems, such as distributed quantum computing[] quantum networks[] or atoms in a lattice, the geometric configuration can naturally determine the system partition.

Remark 1. Compared with genuine entanglement, multipartite entanglement structure still lacks a systematic exploration, due to the rich and complex structures of N-partite system. Unfortunately, it remains an open problem of efficient entanglement-structure detection of general multipartite quantum states.

Definition 3 (Multi-partite state)**.**

Definition 4 (Fully separable state?)**.** An n-qubit pure state $|\psi_f\rangle$ is *P-fully separable* iff it can be written as $|\psi_f\rangle = \otimes_i^m |\phi_{A_i}\rangle$. An n-qubit mixed state $\hat{\rho}_f$ is P-fully separable iff it can be decomposed into a conex mixture of P-fully separable pure states

$$\hat{\rho}_f = \sum_i p_i \left|\psi_f^i\right\rangle\!\left\langle\psi_f^i\right|, (\forall i)(p_i \geq 0, \sum_i p_i = 1). \tag{1}$$

P-bi-separable... $S_f^P \subset S_b^P$

By going through all possible partitions, one can investigate higher level entanglement structures, such as entanglement intactness (non-separability), which quantifies how many pieces in the n-partite state are separated.

Definition 5 (Entanglement intactness, depth)**.** the entanglement intactness of a state $\hat{\rho}$ to be m, iff $\hat{\rho} \notin S_{m+1}$ and $\hat{\rho} \in S_m$.

Remark 2. When the entanglement intactness is 1, the state is genuine entangled; and when the intactness is N, the state is fully separable.

Example 1 (GHZ, W)**.** bipartite: Bell states; nontrivial multipartite: tripartite

Definition 6 (genuine entangled)**.** A state $\hat{\rho}$ possesses P-genuine entanglement iff $\hat{\rho} \notin S_b^P$. A state possesses P-genuine entanglement if it is outside of S_b^P. A state possesses *genuine multipartite entanglement* (GME) if it is outside of S_2, and is (fully) n-separable if it is in S_n.

2. *Graph state*

graph state is an important class of multipartite states in quantum information. cluster state is the special case of graph state. 2D cluster state is the universal resource for the measurement based quantum computation (MBQC) [2].

Definition 7 (graph state)**.** Given a graph $G = (V, E)$, a graph state is constructed as

- vertices: $|+\rangle^{\otimes n}$
- edges: apply controlled-Z to every edge, that is $|G\rangle = \prod_{(i,j)\in E} \mathsf{cZ}_{(i,j)} |+\rangle^{\otimes n}$

An n-partite graph state can also be uniquely determined by n independent stabilizers, $S_i := X_i \bigotimes_{j\in n} Z_j$, which commute with each other and $\forall i, S_i |G\rangle = |G\rangle$.

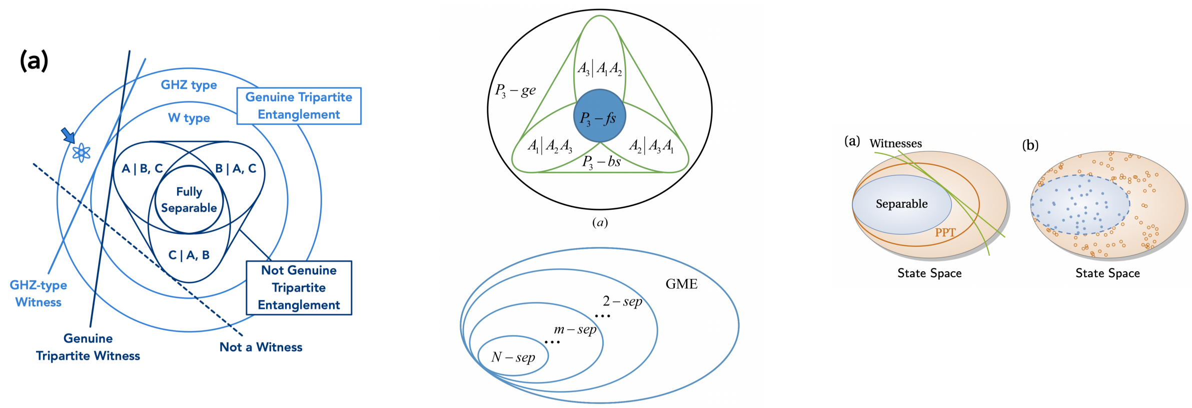

FIG. 1: (a) entanglement witness, PPT criteria, SVM (kernel)?. (c) convex hull...

Problem 1 (Certify entanglement)**.** Multipartite entanglement-structure detection

- **Input**: Given a state close to a **known** state $|\psi\rangle$,
- **Output**: the certified lower-order entanglement among several subsystems could be still useful for some quantum information tasks. entanglement structure

Remark 3. The graph state is the unique eigenstate wtih eignevalue of $+1$ for all the n stabilizers. As a result, a graph state can be writteb as a product of stailizer projectors, $|G\rangle\langle G| = \prod_{i=1}^{n} \frac{S_i+\mathbb{1}}{2}$. stabilizer formalism?;

Remark 4. The entanglement entropy $S(\hat{\rho}_A)$ equals the rank of the adjacency matrix of the underlying bipartite graph, which can be efficiently calculated.

Proposition 1 ([3])**.** *Given a graph state $|G\rangle$ and a partition $\mathcal{P} = \{A_i\}$, the fidelity between $|G\rangle$ and any Fully separable state? is upper bounded by*

$$\mathrm{Tr}(|G\rangle\langle G|\,\hat{\rho}_f) \leq \min_{\{A,\bar{A}\}} 2^{-S(\hat{\rho}_A)} \tag{2}$$

where $S(\hat{\rho}_A)$ is the von Neumann entropy of the reduced density matrix $\hat{\rho}_A = \mathrm{Tr}_{\bar{A}}(|G\rangle\langle G|)$.

Theorem 1. *k local measurements. Here, k is the chromatic number of the corresponding graph, typically, a small constant independent of the number of qubits.*

Proposition 2 (Entanglement of graph state)**.** *[4]. witness; bounds*

3. Entanglement witness

Theorem 2 ([5])**.** *The weak membership problem for the convex set of separable normalized bipartite density matrices is NP-Hard.*

- ***Input**: ??*
- ***Output**: ??*

Question 1. *specific cases? approximately correct? quantum computation? machine learning (data)?*

Theorem 3 (PPT criterion)**.** *the positive partial transpose (PPT) criterion, saying that a separable state must have PPT. Note, it is only necessary and sufficient when $d_A d_B \leq 6$.*

see Fig. 1

Definition 8 (Entanglement witness)**.** entanglement witness $\hat{W}$

$$\mathrm{Tr}\left(\hat{W}\hat{\rho}\right) \geq 0, \forall \text{ separable} \;; \quad \mathrm{Tr}\left(\hat{W}\hat{\rho}\right) < 0, \text{ for some entangled} \tag{3}$$

natural question: nonlinear EW [6] (kernel method)

Definition 9 (Fidelity)**.** Given a pair of states (target and real),

$$F(|\psi\rangle, |\psi'\rangle) := \tag{4}$$

Problem 2 (Fidelity estimate)**.** defined as follows

- **Input**: Given two density matrices $\hat{\rho}$ and $\hat{\rho}'$,
- **Output**: Fidelity with error ϵ

Problem 3 (Trace/expectaton estimate)**.** defined as follows

- **Input**: Given an observable $\hat{O}$ and a mixed state $\hat{\rho}$ in density matrix,
- **Output**: the expectation value $\mathrm{Tr}\left(\hat{O}\hat{\rho}\right) =$ with error ϵ (trace distance)

Problem 4 (Entanglement witness with prior)**.** with prior knowledge

- **Input**: a **known** state $|\psi\rangle$, with noise
- **Output**: ???

decision problem

C. Shadow tomography

Intuitively, a general tomography [7] that extract all information about a state requires exponential copies (samples/measurements). Inspired by Aaronson's shadow tomography [8], Huang et. al [9]

Problem 5 (Shadow tomography)**.** *shadow tomography*

- **Given (Input): unknown** D-dimensional mixed state ρ, known 2-outcome measurements $E_1, \ldots, E_M$
- **Goal (Output):** estimate $\mathbb{P}[E_i \text{ accept } \hat{\rho}]$ to within additive error ϵ, $\forall i \in [M]$, with $\geq 2/3$ success probability

Theorem 4 ([8])**.** *It is possible to do shadow tomography using* $\tilde{\mathcal{O}}(\frac{\log^4 M \cdot \log D}{\epsilon^4})$ *copies. [no construction algorithm?] sample complexity lower bound* $\Omega(\log M \cdot \epsilon^{-2})$*,*

random Pauli measurements

Definition 10 (classical shadow)**.** classical shadow

$$\hat{\rho}_{cs} = \mathcal{M}^{-1}\left(U^\dagger \left|\hat{b}\middle\rangle\middle\langle\hat{b}\right| U\right) \tag{5}$$

predict linear function with classical shadows

$$o_i = \mathrm{Tr}(O_i \hat{\rho}_{cs}) \text{ obeys } \mathbb{E}[o] = \mathrm{Tr}(O_i \hat{\rho}) \tag{6}$$

Lemma 1. *the variance*

$$\mathrm{Var}[o] = \mathbb{E}[(o - \mathbb{E}[o])^2] \leq \left\| O - \frac{\mathrm{Tr}(O)}{2^n}\mathbb{1} \right\|^2_{shadow} \tag{7}$$

sample complexity

$$N_{tot} = \mathcal{O}\left(\frac{\log(M)}{\epsilon^2} \max_{1\leq i\leq M} \left\| O_i - \frac{\mathrm{Tr}(O_i)}{2^n}\mathbb{1} \right\|^2_{shadow}\right) \tag{8}$$

Theorem 5 (Pauli/Clifford measurements)**.** *additive error* ϵ*,* M *arbitrary* k*-local linear function* $\mathrm{Tr}\left(\hat{O}_i\hat{\rho}\right)$, $\Omega(\log(M)3^k/\epsilon^2)$ *copies of the state* $\hat{\rho}$*.*

III. CLASSICAL AND QUANTUM ALGORITHMS

We consider the problem

Problem 6 (???)**.** problem without training data

- **Input**: a graph G encoding in a graph state $|G\rangle$
- **Output**: entanglement structure

with training data

- **features**:
- label:

A. Quantum-classical (ML) hybrid method

1. Classical machine learning

separability classifier by neural network [10]. rigorous quantum advantage of quantum kernel method in SVM [11]. classical machine learning with classical shadow [12].

Definition 11 (SVM)**.** find a hyperplane (a linear function)

nonlinear boundary. map to a higher dimensional (feature) space, in which data is linearly separable.

Definition 12 (Kernel method)**.** Gaussian kernel; graph kernel; shadow kernel

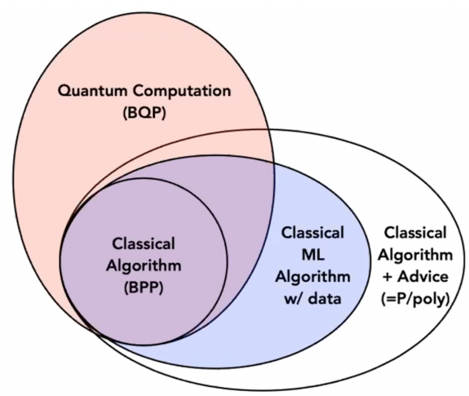

FIG. 2: computational model powered by training data

Theorem 6 (power of data)**.** *data learning*

2. Quantum trace estimation

The task of estimating quantities like

$$\mathrm{Tr}(\rho_1 \cdots \rho_m) \qquad \text{(multivariate traces)}$$

given access to copies of the quantum states ρ_1 through ρ_m.

Theorem 7 (Quantum trace estimation)**.** *multivariate trace estimation can be implemented in constant quantum depth, with only linearly-many controlled two-qubit gates and a linear amount of classical pre-processing*

B. Variational quantum circuits

1. Variational quantum kernel estimation

an ansatz

$$\hat{W}_a := \sum_i a_{..} \bigotimes \hat{\sigma}^{(n)}, \quad \hat{\sigma} \in \{\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z, I\} \tag{9}$$

Algorithm III.1: Entanglement witness by ...

```
input  : density matrix ρ̂
output: determine entangled structure??
for  i = 1, 2, ..., m do
    W_i                                  // this is a comment
    return "separable?"
return entangled ?
```

2. Variational trace estimate

find optimal entanglement witness (qunatum circuit?)

C. Theoretical upper bounds and lower bounds

Definition 13 (graph property)**.** monotone

Problem 7 (Graph property test)**.**

quantum advantage

- no input encoding problem [13]
- contrived problem? for exponential speedup
- convex body query? complexity

	gate/depth/computation	query?complexity	measurements/samples
shadow tomography: entanglement witness (no ML, data); classical machine learning; quantum (variational) circuits			$\mathcal{O}$, Ω

TABLE I: complexity measures of different methods

IV. NUMERICAL SIMULATION

A. Classification accuracy

performance of different methods:

B. Robustness to noise

tradeoff between (white noise) tolerance (robustness) and efficiency (number of measurements).

$$\hat{\rho}_{noise} = (1 - p_{noise}) |G\rangle\langle G| + p_{noise} \frac{\mathbb{1}}{2^n} \tag{10}$$

p_{noise} indicates the robustness of the algorithm (witness).

Remark 5. the largest noise tolerance p_{limit} just related to the **chromatic number** of the graph.[??] graph property

V. CONCLUSION AND DISCUSSION

todo

- experiment (generation, verification) [14]
- error correction?

Acknowledgements

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Appendix A: Machine learning background