Learning to detect entanglement

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Abstract

Classifying states as entangled or separable is a fundamental, but expensive task. This paper presents a method, the forest algorithm, to improve the amount of resources needed to detect entanglement. Starting from “optimized” methods for using geometric criterion to detect entanglement, specific steps are replaced with machine learning models. Tests using numerical simulations indicate that the model is able to declare a state as entangled in fewer steps compared to existing methods. This improvement is achieved without affecting the correctness of the original algorithm.

1 Introduction

Entanglement is a defining feature of quantum information. Detection algorithms are typically based on either quantum state tomography or entanglement witnesses [1, 2]. Witnesses can reveal entanglement in a single measurement, but only for a small portion of states. This drawback makes witnesses difficult to use without prior information about the underlying state. Tomography does not require prior information, but the number of measurements quickly becomes unreasonable as the number of qubits increases.

In this paper, pure states are denoted by $|\varphi\rangle$ and mixed states by $\rho$. A separable pure state admits the factorization: $|\varphi\rangle = |\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_N\rangle$, where $N$ is the number of qubits. Similarly, separable mixed states can be expressed in the following form:

$$\rho = \sum_i p_i \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_N$$

where $\sum_i p_i = 1$. Non-separable states are entangled.

Quantum state tomography is the following problem: given a set of measurement results on sets of positive operator value measures, infer the state $\rho$. Given a source producing an unknown quantum state, to determine whether the state is entangled, one could observe the source, infer the state’s description via tomography, and compute whether the state can be written in the form of Eq. (1).

Consider the space of linear operators acting on a $D$-dimensional Hilbert space. This space has an orthonormal basis, $\{B_i\}$, for the inner product $\langle B_1, B_2 \rangle = \text{tr}(B_1^\dagger B_2)$. Under this basis, the state $\rho$ can be represented as:

$$\rho = \frac{1}{D} \cdot \text{id} + \sum_{i=1}^{D^2-1} x_i B_i$$

where $\text{id}$ is the identity operator and $B_0$ is taken to be $\text{id}/\sqrt{D}$. Here, $x_i = \text{tr}(\rho^i B_i)$, is the expected value of the measurement associated with $B_i$. This paper uses $\{B_i\}$, with the state $\rho$ implicit, to represent this expectation.

For $N$-qubit quantum states, it is customary to use tensor products of Pauli matrices, $\{\text{id}, \sigma_1 = \sigma_x, \sigma_2 = \sigma_y, \sigma_3 = \sigma_z\}$, as the basis. According to the geometric criterion [3], a state is entangled if:

$$\sum_{a_1=1}^{3} \sum_{a_2=1}^{3} \cdots \sum_{a_N=1}^{3} (\sigma_{a_1} \otimes \sigma_{a_2} \otimes \cdots \otimes \sigma_{a_N})^2 > 1$$

For a state $\rho$, write $\pi(\rho)$ as the vector of expectations corresponding to measurements associated with elements of the improper basis consisting of tensor products of Pauli matrices excluding the identity. For vectors of reals, $\pi \cdot \varpi < \pi \cdot \varpi$ implies $\pi \neq \varpi$. Thus, a state cannot be equal to a separable state if:

$$\pi(\rho) \cdot \pi(\rho) > \max_{\text{separable}|\varphi\rangle} \pi(\rho) \cdot \pi(|\varphi\rangle \langle \varphi|)$$

It can be shown that the right hand side of Eq. (4) is less or equal to 1.

There are $2^{2N} - 1$ elements in the Pauli basis and as many parameters for quantum state tomography to infer. This is prohibitively expensive. With the geometric criterion, only a (often much smaller) subset, such that the inequality in Eq (3) is violated, is required. Following the convention in [3], an measurement is “large” or “small” based on the the contribution it makes to violating the geometric criterion.

Laskowski et al proposed a method that eliminates measurements that are likely to be small by exploiting correlation complimentarity [4, 5], which states, for a mutually anti-commuting set of operators, $S$:

$$\sum_{B \in S} \langle B \rangle^2 \leq 1$$

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This method, the tree algorithm, uses a search tree to navigate mutually anti-commuting subsets of the improper basis. If an inferred \((B)^2\) is large, \((i.e., > 0.16)\) the tree moves onto a different subset.

The main idea of this paper is to replace the search tree with a random forest, a type of machine learning model. The training process to build the model and how the model can be used to select which expectation to infer next is described. The model does not make decisions about whether a state is entangled and thus any state that violates the geometric criterion will be declared as entangled. Numerical evidence is presented to indicate that the model is more likely to select more helpful measurements.

2 Forest Algorithm

In (supervised) machine learning, the input can be described by a vector \(x\) and the output by \(y\). Given a training set of \((x, y)\) samples, the machine learning algorithm learns the input-output relationship, \(f(x)\), by fitting \(f\) to the training set. A more comprehensive and detailed treatment is presented in \[6\].

When using the geometric criterion, the entanglement detection procedure is:

1. There is a source producing a quantum state. Initially, nothing is known about the state.
2. Choose \(B\) from the improper basis, using a score based on the expected value of \((B)^2\).
3. Repeatedly make the measurement associated with \(B\) to determine \((B)\). The knowledge obtained from these measurements are used to update the scores.
4. Repeat steps 2 and 3 until the sum of inferred \((B)^2\)s exceeds 1.

As there is no initial information about the state, the natural choice of how to obtain the training set is by sampling pure states using the Haar measure.

The challenge of expressing step 2 in the machine learning framework is that the amount of information to available predict a given \((B)^2\) changes. For now, consider the “last iteration”. As an example, using \((ab)\) as a shorthand for \(\sigma_a \otimes \sigma_b\), the model could be asked to make a judgement about \((xx)^2\). At the last iteration, all the information that could be used to predict \((xx)^2\), namely, \{\((xy)^2, (xz)^2, \cdots, (zz)^2\}\, would be known (assuming the geometric criterion has not yet been satisfied). However, any element of the improper basis could be the last to be selected. Thus, for two qubits, 9 models need to be trained:

\[
\begin{align*}
    f_{xx} : \pi_{xx} &= \langle xy \rangle^2, \langle xz \rangle^2, \cdots, \langle zz \rangle^2, \\
    y_{xx} &= 1\, (\langle xx \rangle^2 \geq \max_i(\pi_{xx})) \\
    f_{xy} : \pi_{xy} &= \langle xy \rangle^2, \langle xz \rangle^2, \cdots, \langle zz \rangle^2, \\
    y_{xy} &= 1\, (\langle xy \rangle^2 \geq \max_i(\pi_{xy})) \\
    \ldots
    f_{zz} : \pi_{zz} &= \langle xy \rangle^2, \langle xz \rangle^2, \cdots, \langle zz \rangle^2, \\
    y_{zz} &= 1\, (\langle zz \rangle^2 \geq \max_i(\pi_{zz}))
\end{align*}
\]

where \(1\) is the indicator function. Generalizing:

\[
f_j \sim 1 \left[ x_j = \max_i \pi(\rho), \text{ given } \pi(\rho)_{-j} \right]
\]

where \(\pi_{-j}\) is the vector \(\pi\) without entry \(j\). The notation \(f \sim g\) indicates \(f\) is trained to learn \(g\).

The choice of \(y\) as the maximum reflects the fact that the algorithm only considers which choice is best, not how much better the best choice is compared to the second-best choice.

It remains to choose a functional form for \(f\) and fit \(f\) to the data. A random forest, which is a collection of decision trees, is used here. Formally, a decision tree partitions the input space into regions, \(r_1, r_2, \cdots, r_k\), with associated output values, \(y_1, y_2, \cdots, y_k\), and

\[
f_{\text{tree}}(\pi) = \sum_{i=1}^k y_i \cdot 1(\pi \in r_i)
\]

The forest’s output is the average (or majority vote) of its constituent decision trees.

The training procedure is discussed extensively in \[6\]. A sketch of the construction for binary classification problems, where \(y \in \{0, 1\}\), is as provided. To train a tree, the tree initially has one region containing the entire input space. Samples falling into a region is viewed as a data producing 1s and 0s and entropy can be calculated for this source.

During each iteration, each region is split by a decision rule \(x_j < \theta\). Let \(p(r)\) and \(n(r)\) be the number of \(y = 1\) and \(y = 0\) samples in the training set falling, respectively, into region \(r\), and write \(t(r)\) for \(p(r) + n(r)\). Then let \(L(p(r), n(r))\) be an impurity measure (entropy is used, but the Gini Index is also popular). Now let \(r\) be the original region and \(r_1\) and \(r_2\) be the regions after the split, define the (ascending) impurity gain for a split as:

\[
G(r, j, \theta) = t(r)L(r) - [t(r_1)L(r_1) + t(r_2)L(r_2)]
\]

Since the goal is for the tree to become more pure when descending the tree, the decision rule is chosen to maximize the impurity gain going downwards.

Iterative splitting continues until all regions are (mostly) pure. To build a forest, train many trees on carefully selected subset of the training data such that
Figure 1: A “toy” tree. A decision rule \( < \theta \) is represented as a node \( ab \) with \(< \) and \( \geq \) edges for each possibility. A terminal node represents a region defined \( r \) defined by the decision rules on the path leading to the node and the node is labelled with the pair \( p(r), n(r) \).

With the trained model in hand, it is time to tackle the problem of updating the scores based on the measurement results. Let \( R_j \) be the set of input vectors for model \( f_j \) that agree with the known information. Define the tree’s score as:

\[
s_j^{\text{tree}} = \frac{\sum_{r_i \cap R_j \neq \emptyset} p(r_i)}{\sum_{r_i \cap R_j \neq \emptyset} t(r_i)} \tag{10}
\]

The forest’s score is the average of its constituent decision trees’ scores. To explain the notation \( r_i \cap R_j \neq \emptyset \), suppose the only known measurement so far is \( \langle zz \rangle^2 = 0.25 \). Now consider a region is defined by the decision rule \( \langle zz \rangle^2 \geq 0.16 \) and vectors with \( \langle zz \rangle^2 = 0.25 \) is all quantum states with \( \langle zz \rangle^2 = 0.25 \), a non-empty set. However, the other subdivided region with \( \langle zz \rangle^2 < 0.16 \) does have an empty intersection. When the denominator of the Eq \[10\] is 0, then \( s_j^{\text{tree}} \) is defined as 1.

For a more complete example, consider a “toy” tree for \( f_{xx} \), represented as a graph in Fig. 1. Suppose, so far, the results are \( \langle yy \rangle^2 = 0.36 \) and \( \langle zz \rangle^2 = 0.01 \). Then, the tree’s score is: \( 3/(3+2) = 0.6 \) as only the centre node is reachable.

3 Numerical Experiment

The performance of the forest algorithm is analyzed by generating two to six qubit states and running both the forest and tree algorithms on the same states. Since the tree algorithm requires \( \langle xx \cdots x \rangle \) to be large, a rotation is applied to enforce this criterion. Also included in the comparison are: “optimal” and “random”. Optimal always makes the largest unknown measurement, whereas random chooses an unknown measurement at random, but starting with \( \langle xx \cdots x \rangle \).

Source code for the numerical experiments is available at [7]. The forests were generated using the scikit-learn package [8] and Eigen package [9] was used for matrix computations. Due to practical limitations, 30000 states were used to train each model and 1500 states were tested for each qubit. Machine learning models generally “get better” with more training data and having more data could improve the result.

The test sets of \( N \)-qubit states were constructed using the following procedure:

\[
|\varphi\rangle = R \cdot G_1 G_2 \cdots G_n (|0\rangle^\otimes N) \tag{11}
\]

where \( n \) is a random integer between \( K = 3 \cdot N^2 + 27 \) and \( 2 \cdot K \) and each \( G_i \) is a quantum gate operating on 1 or 2 chosen qubits from the universal gate set [10]:

\[
\begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}, \begin{bmatrix} 1 & 0 \\
0 & e^{i\pi/4}
\end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0
\end{bmatrix} \tag{12}
\]

The final rotation, \( R \), ensures \( \langle xx \cdots x \rangle \) is the largest measurement. Finally, rejection sampling is applied to discard states that cannot be declared entangled by the geometric criterion, as all of the measurements would need to be made regardless of algorithm.

This roundabout construction (as opposed to sampling over a uniform measure) is to verify how well the forests “generalize” to a generic test distribution of states that is different to the distribution that it was trained on. The final rotation making \( \langle xx \cdots x \rangle \) the largest measurement is a major concession to the tree algorithm that allows the mutually anti-commuting subset strategy to be applied to its fullest extent. Despite this concession, the average number of measurements taken before the geometric criterion is violated is:

| Qubits | Forest | Tree | Δ | Optimal | Random |
|--------|--------|------|---|---------|--------|
| 2      | 4.41   | 4.44 | 0.03 | 2.96    | 4.85   |
| 3      | 5.91   | 6.06 | 0.16 | 3.01    | 7.52   |
| 4      | 10.65  | 10.94| 0.29 | 3.80    | 13.77  |
| 5      | 21.83  | 23.14| 1.31 | 5.43    | 27.29  |
| 6      | 48.91  | 50.80| 1.89 | 8.65    | 57.21  |

Detailed results for three to six qubits are presented in Fig. 2.

These results indicate that the forest algorithm is an improvement over the tree algorithm. The advantage of the forest algorithm over the tree algorithm increases with the number of qubits, possibly exponentially. Both algorithms are better than random, suggesting that the mathematical structure of entanglement is being exploited. It is unclear if anything close to the “optimal” performance can be achieved without further experimental assumptions.
Figure 2: The performance of the tree and forest algorithms on sample of 1500 entangled states. “Optimal” refers to the number of measurements required to prove entanglement via the geometric criterion if there were an oracle for the largest measurement. “Random” refers to making measurements at random. The forest algorithm is able to declare states as entangled with fewer measurements than the tree algorithm on average. Its edge grows with the number of qubits.
4 Discussions

This section aims to provide intuition for the forest algorithm. Following the work of Hayden, Leung, and Winter in \cite{hayden2000comparing}, concentration of measure arguments indicate random forests are well suited to capture the relationships between the measurements.

It is well known that a continuous measure that is invariant under unitary transformations is a uniform measure. For a group, $(G, \otimes)$, the Haar measure, $\mu$, is the measure such that, for any $S \subseteq G$ and $g \in G$, $\mu(S) = \mu((g \otimes s | s \in S)) = \mu(\{s \otimes g | s \in S\})$. Sampling unitary matrices from its Haar measure is unitary invariant by definition. As expected, the prior represents a uniform distribution on the $2^N$ unitary matrices from its Haar measure is unitary invariant under unitary transformations is a uniform measure such that, for any $S \subseteq G$ and $g \in G$, $\mu(S) = \mu((g \otimes s | s \in S)) = \mu(\{s \otimes g | s \in S\})$. Sampling unitary matrices from its Haar measure is unitary invariant by definition. As expected, the prior represents a uniform distribution on the 2-dimensional sphere. Sampled according to the uniform distribution. However, Lévy’s Lemma \cite{levy1925additions} states: if $f$ has Lipschitz constant $\eta$ (that is, $|f(x) - f(y)| \leq \eta |x - y|$) and $X$ is sampled according to the uniform measure on the k-dimensional sphere, then:

$$\Pr(|f(X) - m_f| > \varepsilon) \leq \exp\left[-(k - 1)\varepsilon/(2\pi^2\eta^2)\right]$$

where $m_f$ is the median of $f$ under the same measure.

Consider the expectation as a function. First, convert $|\varphi\rangle$ into the real vector, $\varphi = [\varphi^r, \varphi^i]^T$, where $\varphi^r$ and $\varphi^i$ are the vectors containing the real and imaginary parts of $|\varphi\rangle$ respectively. Then, for a Pauli matrix, $B$:

$$f(\varphi)(B) = \text{tr}[|\varphi\rangle\langle \varphi| \cdot B] = \sum_{jk} (\varphi^r_j - i\varphi^i_j)(\varphi^r_k + i\varphi^i_k)B_{kj}$$

Lévy’s Lemma can be applied to $f$, as $\varphi$ is now uniformly distributed on the $2^{N+1}$ dimensional sphere. The partial derivatives of $f$ are:

$$\frac{\partial f}{\partial \varphi^r_m} = 2\varphi^r_mB_{mm} + \sum_{j \neq m} \varphi^r_jB_{mj} + \sum_{k \neq m} \varphi^r_kB_{km}$$

$$\frac{\partial f}{\partial \varphi^i_m} = 2\varphi^i_mB_{mm} + \sum_{j \neq m} \varphi^i_jB_{mj} - \sum_{k \neq m} \varphi^i_kB_{km}$$

Now, bound $(\nabla f)^T(\nabla f)$:

$$(\nabla f)^T(\nabla f) = \sum_m \left( \frac{\partial f}{\partial \varphi^r_m} \right)^T \left( \frac{\partial f}{\partial \varphi^r_m} \right) + \left( \frac{\partial f}{\partial \varphi^i_m} \right)^T \left( \frac{\partial f}{\partial \varphi^i_m} \right)$$

$$= 2 \sum_m |\varphi_m|^2 \cdot |B_{mm}|^2 + 2 \sum_{jk} \varphi^r_j\varphi^r_k \sum_m B_{km}B_{mj}$$

The sum has been simplified by noting that the Pauli matrices are Hermitian. The first term is bounded by $2 \sum_m |\varphi_m|^2 = 2$ and the second is $\text{tr}[|\varphi\rangle\langle \varphi| \cdot B^2] = 1$, as Pauli matrices square to identity. This bound is an appropriate value for $\eta^2$. Finally, Applying Lévy’s Lemma shows that $(B^i)^2 < \varepsilon$ with high probability, that is, with probability $1 - \alpha(1)$.

This result indicates that for a given state, most observables are small, but a subset of observables are very large (in order to violate the geometric criterion). For different states, different observables are large. This large/small behaviour is easily captured by the decision rules, making random forests a good machine learning algorithm for this task.

The impurity gain of each node indicates that the model captures the concept of correlation complementarity. Recalling Eq. (6), the importance of $\langle B_j \rangle$ for determining the size of, say, $\langle xz \cdots x \rangle$ can be computed as the fraction of impurity gain on nodes split using the $\langle B_j \rangle$ in the forest for $\langle xz \cdots x \rangle$ compared to the impurity gain of all nodes in the tree. In the two qubit case of determining whether $\langle xx \rangle$ is going to be large, the forest assigns $\approx 16\%$ importance to $\langle xy \rangle, \langle xz \rangle, \langle yx \rangle$ and $\langle xx \rangle$ but only $\approx 9\%$ importance to the other four features. The heavier emphasis of anti-commuting measurements is true for other models and for more qubits.

Further evidence that the forests “learned” correlation complementarity can be seen in example traces. Let $|D_1^2\rangle = \frac{[|001\rangle + |010\rangle + |100\rangle]}{\sqrt{3}}$ and $|D_2^2\rangle = \frac{[|011\rangle + |101\rangle + |110\rangle]}{\sqrt{3}}$. Consider the execution trace of the forest algorithm on the following state with $\alpha = 5\pi/71$, from the experiments in \cite{4}.

$$|G(\alpha)\rangle = \cos(\alpha)|D_2^2\rangle + \sin(\alpha)|D_1^2\rangle$$

This trace shows that the forest algorithm follows the tree algorithm’s strategy of scanning measurements from a mutually commuting subset until correlation complementarity indicates switching to a different subset. However, the random forest’s thresholds for switching are more finely tuned compared to an arbitrary constant value of $(B^i)^2 > 0.4^2$ for the tree algorithm. In the example, even though the first measurement is slightly above the threshold of $0.4^2$, the forest algorithm comes back to measurements that anti-commute with $xx$ and finds three large measurements to declare the state entangled. However, once the forest algorithm finds $xxz$ and $xxz$, it avoids measurements that anti-commute with them.

In some sense, the collection of forests is a set of non-parametric models capturing correlation complementarity through the joint probability distribution of $\pi(\rho)$. Then, the tree scoring function can then be viewed as a conditional expectation. This is more clear when rewrit-
ing Eq. (10) as:

\[
\frac{1}{\sum_{r_i \cap R_i \neq \emptyset} p(r_i) + n(r_i)} \left( \sum_{r_i \cap R_i \neq \emptyset} 1 \cdot p(r_i) + 0 \cdot n(r_i) \right)
\]

(19)

Since the expectation of an indicator is the probability of the indicated event. Thus, the scores represent a direct estimate of the probability that an unknown measurement would be the best at declaring entanglement in fewer steps.

5 Conclusion

This paper presents an example usage of machine learning in entanglement detection. Empirical evidence shows that the forest algorithm is an improvement, for two to six qubits, over the existing tree algorithm. The forest algorithm achieved this without sacrificing “correctness”: every state the forest algorithm declares entangled is guaranteed to be entangled, even though it may take longer or fail to detect entanglement.

Developments in machine learning provide non-parametric methods for analysing quantum systems. Non-parametric methods can eliminate arbitrary parameters in analyses. The success of the forest algorithm is an example where the analysis was improved by eliminating the threshold to move onto a different mutually commuting subset. It is possible this approach can be applied to other problems in quantum information processing.

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