# Computing the Geometric Measure of Entanglement with Matrix Product States

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In this paper we present a new algorithm to compute the Geometric Measure of Entanglement (GME) for pure quantum states. Using the Matrix Product State decomposition, our method avoids the approximations used for known numerical solutions. We prove that our new method for computing the GME with tensor networks is equivalent to the classical definition of the GME, and verify our algorithm for over 800 simulated quantum states. Our method computes the GME with an average error of $1.43 \times 10^{-10}$ runtime of 0.3s, which is both more accurate and faster than known semi-numerical results.

## 1. Introduction

Quantum entanglement is one of the most fascinating features of quantum mechanics. Its discovery lead to a revolution in the math and physics communities and transformed our understanding of physical systems at the particle level. Due to the complexity of quantum systems, the quantification of quantum entanglement remains challenging for most quantum states. This problem has been shown to be NP-Hard for most systems [1, 2].

As a result, while various measures have been proposed to quantify entanglement [3], most incur a large computational cost when analytic solutions are unknown.

For one such measure, the Geometric Measure of Entanglement (GME), recent work by Zhang et. al [4] shows how to efficiently estimate the GME using a semi-numerical algorithm originally proposed by Watrous [5]. This method uses the *Perez criterion* [6] to approximate GME with a more tractable semi-definite program. Similar work by Strestlov et. al [7, 8] uses the same technique to provide upper and lower bounds to the GME for symmetric quantum states.

In this paper, we how to directly measure the GME for pure quantum states by first decomposing the quantum wavefunction into its Matrix Product State representation. In doing so, we reduce the computational cost associated to computing the GME. The structure inherent to MPS decompositions allows for a more efficient computation of the GME, and avoids the need for approximations.

The rest of this paper is divided as follows: we first review some important definitions and results about tensor netowrks and quantum information theory, before examining the Matrix Product State and showing how to compute the GME via the MPS-GME algorithm. We then verify our proposition with over 800 simulated quantum states and compare our results to known analytic solutions.

## 2. Preliminaries

### 2.1. *Tensor Networks*

In this section we introduce some basic definitions and concepts related to tensor networks. Generally speaking, a *tensor* is defined as a collection of numbers labelled by $N$ indices, where $N$ is the *rank*, or *order*, of the tensor. The smallest tensors are scalars (zero order tensors), vectors (first order tensors), and matrices (second order tensors).

To combine tensors, we perform a *tensor contraction*, a summation over common indices. For small tensors (eg, vectors and matrices), this reduces to the vector dot product and matrix multiplication

operations. For vectors $x_i, y_i \in \mathbb{R}^n$ and matrices $A_{ij} \in \mathbb{R}^{n\times m}, B_{jk} \in \mathbb{R}^{m\times l}$ we write their contraction as

$$x_i y_i = \sum_{i=1}^{n} x_i y_i$$
$$A_{ij} B_{ik} = \sum_{j=1}^{m} a_{ij} b_{jk}.$$

On the left hand side, we've introduce the *Einstein summation notation*, where we contract over indices which share the same label. Importantly, we require that the dimension of the common index be the same for tensors to be contracted (for example, we cannot contract vectors $x \in \mathbb{R}^m$ and $y \in \mathbb{R}^n$ when $m \neq n$).

For higher order tensors $T_{ijk} \in \mathbb{R}^{d_1\times d_2\times d_3}$ and $U_{klm} \in \mathbb{R}^{d_3\times d_4\times d_5}$, we may contract them along a third axis:

$$T_{ijk} U_{klm} = \sum_{k=1}^{d_3} t_{ijk} u_{klm},$$

which results in a fourth order tensor. If $d_2 = d_4$, then we can also perform contractions over multiple indices

$$T_{ijk} U_{klm} = \sum_{j=1}^{d_2} \sum_{k=1}^{d_3} T_{ijk} U_{kjm}, \tag{2.1}$$

which results in a second order tensor.

The contraction of multiple tensors forms a *tensor network*. As shown in the previous example, the use of indices can become quite cumbersome very quickly, and it is often useful to express tensor networks with diagrams instead.

### 2.1.1. Tensor Network Notation

An elegant way to obtain intuition about tensor network operations is to use the graphical notation initially proposed by Roger Penrose [9]. In its basic form, tensors are represented as simple geometric shapes (e.g. circles, squares) with indices, or 'legs', attached to them. The number of indices corresponds to the order of the tensor.

Contractions are represented by two tensors that share a common index (also called a *bond*) as shown in Figure 1. Importantly, the dimension of each index is not expressed in tensor network diagrams, and it is implied that two indices that share a bond have the same dimension.

Indices which are contracted over are called *virtual indices*, while indices which do not share any bonds are called *free* or *physical* indices. The number of physical indices in a tensor network corresponds to the rank of the resulting tensor after it has been contracted.

The interpretation of free indices as being 'physical' comes from physics literature, where tensor networks are used to represent quantum wavefunctions.

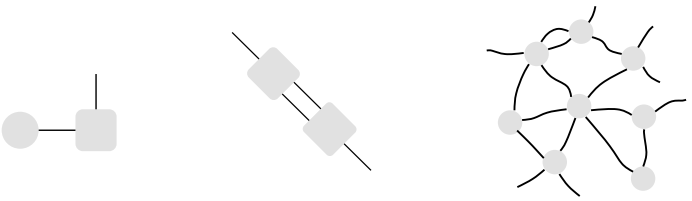

Figure 1. Contraction of a vector and a matrix (left) results in a vector with one physical index. Contracting two rank-3 tensors over two indices (such as Eq. 2.1) results in a second order tensor (middle). Tensor network notation can illustrate complex contractions, such as the contraction over 8 tensors to form a 7th order tensor (right).

### 2.2. *(Pure) Quantum Systems and Entanglement*

To understand how tensor networks are used to compute quantum entanglement, let's first review some basic concepts of quantum information theory (QIT). In its full glory, QIT is developed for *mixed* quantum states, for which the exact wavefunction may not be known. We restrict ourselves to QIT for *pure* quantum states, where we do have an expression for the wavefunction, since we interested in applying tensor network decompositions these wavefunctions.

To any physical system, we prescribe a Hilbert space $\mathcal{H}$, known as the *state space* of the system. Any unit vector $|\psi\rangle \in \mathcal{H}$ represents one of the possible states of the system and is known as a *state vector*. The state space $\mathcal{H}$ is a vector space over the complex numbers $\mathbb{C}$ endowed with the standard dot product,

$$\langle x, y\rangle = \sum_{i=1}^{n} x_i \bar{y}_i.$$

Thus, any finite $d$-dimensional physical system can be identified with the Hilbert space $\mathcal{H} = \mathbb{C}^d$. We represent the basis vectors of $\mathbb{C}^d$ as $|0\rangle, |1\rangle, \ldots, |d-1\rangle$, often called the *computational basis*.

*Example* 2.1. The simplest representation of a quantum system is the *qubit*. In this model, there are two possible observable states, labelled by the basis vectors $|0\rangle$ and $|1\rangle$. Thus a qubit $|\psi\rangle \in \mathbb{C}^2$ can be written as

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \tag{2.2}$$

where $\alpha, \beta \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1$. This additional requirement has the interpretation that the sum of the probabilities of ending up in state $|0\rangle$ and $|1\rangle$ should be equal to one.

*Example* 2.2. More generally, for quantum systems with finitely many observable states, say $d < \infty$, we can represent any possible state of the system as a *qudit*,

$$|\psi\rangle = \sum_{i=0}^{d-1} \alpha_i |i\rangle,$$

where $\alpha_i \in \mathbb{C}$ for $0 \leq i < d$ and $\sum_{i=0}^{d-1} |\alpha_i|^2 = 1$.

To model more complex quantum systems, we *compose* systems together via the tensor product. Thus the composition of two quantum systems with state spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, is represented by unit vectors

in the space $\mathcal{H}_1 \otimes \mathcal{H}_2$. Basis vectors in $\mathcal{H}_1 \otimes \mathcal{H}_2$ are abbreviated to

$$|ij\rangle \equiv |i\rangle \otimes |j\rangle.$$

*Example* 2.3. We can model a system of two qubits as

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle, \tag{2.3}$$

again requiring that $\sum_{i,j=0}^{1} |\alpha_{ij}|^2 = 1$. We can interpret $|\psi\rangle$ as a quantum system with four observable states.

Given a composite quantum system, one natural question would be to ask whether or not it can be factored into a product state. This is the fundamental question of quantum entanglement.

**Definition 2.1.** A composite quantum state $|\psi\rangle \in \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$ is *separable* if it factors as a product state, i.e. if it can be written as

$$|\psi\rangle = \bigotimes_{i=1}^{n} |\psi_i\rangle \in \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n, \tag{2.4}$$

where $|\psi_i\rangle \in \mathcal{H}_i$ for all $1 \leq i \leq n$. Otherwise, $|\psi\rangle$ is *entangled*.

*Example* 2.4. The *Bell states* are the simplest examples of entangled quantum systems. They are pairs of qubits which are not separable:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$
$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$
$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$
$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle).$$

One can check that none of these states factor as product states and are thus each entangled.

2.2.1. Quantifying Entanglement

With a qualitative description of entanglement, a variety of qualitative measures (reviewed in [3]) have been used to measure entanglement. For our results, we use two measures of quantum entanglement: the entanglement entropy and the geometric measure of entanglement, both of which been widely studied [10, 7, 8, 5, 11]. Again, we do not describe them in their full generality, but only for separable states.

Suppose we are interested in the entanglement between two sub-systems of $|\psi\rangle \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, where $\dim\mathcal{H}_1 = n$, $\dim\mathcal{H}_2 = m$, and $n \geq m$. We can quantify the entanglement between these two systems by applying the *Schmidt decomposition*.

**Theorem 2.1** (Schmidt Decomposition)**.** *For any vector* $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ *, there exists orthonormal sets* $\{|\psi_i\rangle\}_{i=1}^m \subset \mathcal{H}_1$ *and* $\{|\phi_i\rangle\}_{i=1}^m \subset \mathcal{H}_2$ *such that*

$$|\Psi\rangle = \sum_{i=1}^{m} \alpha_i |\psi_i\rangle \otimes |\phi_i\rangle, \tag{2.5}$$

*where* $\alpha_i \in \mathbb{C}$ *are all non-negative and unique up to re-ordering.*

*Proof* If we write $|\Psi\rangle$ in matrix form (it is a rank-2 tensor), this is essentially a restatement of the singular value decomposition, where the $\alpha_i$ are the singular values. □

**Definition 2.2.** The $\alpha_i$'s are called the *Schmidt coefficients*. The number of non-zero Schmidt coefficients (i.e. nonzero singular values) is the *Schmidt rank*.

The Schmidt decomposition of a bipartite system gives rise to our first measure of entanglement.

**Definition 2.3.** Given a pure state $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$, we define its *entanglement entropy* as

$$S(|\psi\rangle) = -\sum_i |\alpha_i|^2 \log(|\alpha_i|^2), \tag{2.6}$$

where $\alpha_i$ are the Schmidt coefficients of $|\psi\rangle$.

Note that if a quantum state is separable then $\alpha_i = 1$ and $S(|\psi\rangle) = 0$.

**Corollary 2.1.** $|\Psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ *is entangled if and only if it has Schmidt rank strictly greater than 1.*

*Proof* Applying the Schmidt decomposition to $|\Psi\rangle$ gives us a representation of the form in Eq. 2.5 with a single summand, which is a separable state. □

Corollary 2.1 gives us a way to identify the set of all separable states to the set of states which have Schmidt rank equal to one. An analogous result for tensor networks will help improve the computational efficiency for computing the next measure of entanglement.

**Definition 2.4.** For a pure quantum state $|\psi\rangle \in \mathcal{H}$, the *Geometric Measure of Entanglement* (GME) is defined as

$$E_{\sin^2}(|\psi\rangle) = 1 - \max_{\phi \in \mathcal{S}} |\langle \psi | \phi \rangle|^2, \tag{2.7}$$

where $\mathcal{S} \subset \mathcal{H}$ is the set of all separable states.

Note that $\max_{\phi\in\mathcal{S}} |\langle\psi|\phi\rangle|^2$ maximizes the squared cosine of the angle between $|\psi\rangle$ and any separable state. Hence $E_{\sin^2}(|\psi\rangle)$ minimizes the squared sine of the angle between $|\psi\rangle$ and all separable states.

When dealing with complex systems with large numbers of qubits, analytic solutions to the GME can only be obtained under certain simplifying assumptions[11, 12]. Hence, there have been several attempts to approximate the GME with numerical methods [4, 7, 8]. These methods rely on the *Peres criterion* [6] which provides necessary (and computationally efficient) conditions for separability. A numerical lower bound on the GME can thus be obtained by computing the maximum in Eq. 2.7 over all states that satisfy the Peres criterion (a superset of $\mathcal{S}$).

## 3. Entanglement in Tensor Networks

To reduce the computational costs of determining separability, we turn to the Matrix Product State (MPS) decomposition. The MPS has been studied widely in both math and physics literature [13, 14, 10, 15], as it reduces the space complexity of many-body wavefunctions and has some interesting entanglement properties.

We will provide some background on the MPS before proving how to compute the GME for pure quantum states efficiently via the MPS decomposition.

**Definition 3.1.** For an arbitrary rank-$n$ tensor $U_{d_1,\ldots,d_n} \in \bigotimes_{i=1}^{n} \mathbb{C}^{d_i}$, we define its *Matrix Product State* representation as

$$U_{d_1,\ldots,d_n} = A^{(1)}_{d_1,m_1} A^{(2)}_{m_1,d_2,m_2} A^{(3)}_{m_2,d_3,m_3} \cdots A^{(n)}_{m_{n-1},d_n}, \tag{3.1}$$

where we use Einstein summation notation to denote contractions over the indices $m_1,\ldots,m_{n-1}$. The number of sub-tensors $n$ is the *length* of the MPS.

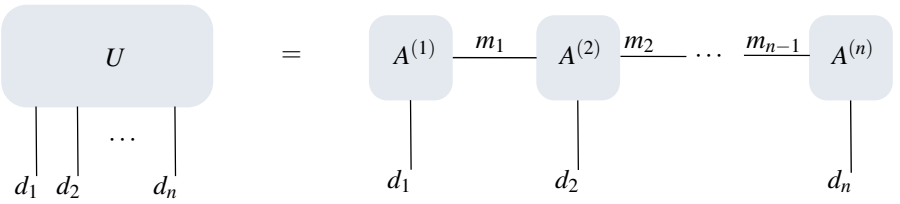


Figure 2. MPS decomposition of $U_{d_1,\ldots,d_n}$ written in tensor network notation. Note that we contract over each index $m_i$, and the rank of the MPS decomposition is equal to the number of open indices (in this case, $n$) as expected.

In their review [14], Szalay et. al describe a procedure through which we can obtain expressions for the $A^{(i)}$'s by iteratively reshaping the tensor and applying a singular value decomposition. Here we highlight one theorem from their work.

**Theorem 3.1** (Separation Theorem)**.** *For any tensor $U_{d_1,\ldots,d_n} \in \bigotimes_{i=1}^n \mathbb{C}^{d_i}$, there exists a minimal MPS representation, thus called the MPS decomposition, such that for any $i = 1,\ldots,n-1$ the dimensions of $\chi_i$ of the contractions $m_i$ are minimal and given by*

$$\chi_i = rank([U]^{d_{i+1},\ldots,d_n}_{d_1,\ldots,d_i}).$$

$[U]^{d_{i+1},\ldots,d_n}_{d_1,\ldots,d_i} \in \mathbb{C}^{d_1\times\cdots\times d_i} \otimes \mathbb{C}^{d_{i+1}\times\cdots\times d_n}$ *is a reshaping, or matricization of $U_{d_1,\ldots,d_n}$.*

The next result is one of the most useful results of tensor network applications in quantum physics, establishing a relationship between the dimensions $\chi_i$ of the MPS and the entanglement entropy of a quantum system [16, 13, 10, 17].

**Theorem 3.2** (Area law of entanglement)**.** *For a pure state vector $|\psi\rangle$, if $\chi$ is the maximum dimension of the contractions in the MPS decomposition for $|\psi\rangle$, then the entanglement entropy is bounded by*

$$S(|\psi\rangle) \leq 4\log(\chi). \tag{3.2}$$

The area law of entanglement shows that weakly-entangled systems can be represented with low-dimensional MPS representations. In particular, it allows us to determine the dimensions of MPS decompositions for separable states.

**Proposition 3.1.** *Any separable state vector $|\psi\rangle \in \bigotimes_{i=1}^n \mathbb{C}^{d_i}$ admits an MPS decomposition such that $\chi = 1$. Moreover, any tensor network of the form*

$$A^{(1)}_{d_1,m_1} A^{(2)}_{m_1,d_2,m_2} A^{(3)}_{m_2,d_3,m_3} \cdots A^{(n)}_{m_{n-1},d_n},$$

*where the dimension of the contractions $m_i$ is 1 for all $1 \leq i < n$, is the MPS decomposition of an (unnormalized) separable state vector in $\bigotimes_{i=1}^n \mathbb{C}^{d_i}$.*

*Proof* First let some tensor $U = A^{(1)}_{d_1,m_1} A^{(2)}_{m_1,d_2,m_2} A^{(3)}_{m_2,d_3,m_3} \cdots A^{(n)}_{m_{n-1},d_n}$ be given. Contracting over each $m_i$, we are left with some vector $|\phi\rangle \in \bigotimes_{i=1}^n \mathbb{C}^{d_i}$. This is the definition of an unnormalized state vector in the state space $\bigotimes_{i=1}^n \mathbb{C}^{d_i}$.

Since $\chi = 1$, by the area law of entanglement, the entanglement entropy is bounded by

$$S(|\phi\rangle) \leq 4\log(1) = 0.$$

Next, let some separable state vector $|\psi\rangle \in \bigotimes_{i=1}^n \mathbb{C}^{d_i}$ be given. Since it is separable, it factors as a product state

$$|\psi\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_n\rangle.$$

In particular, the rank the matricization $[|\psi\rangle]^{d_{i+1},\ldots,d_n}_{1,\ldots,d_i}$ is equal to one for any $1 \leq i \leq n$. Hence, by the Separation Theorem, $|\psi\rangle$ admits an MPS decomposition with

$$\chi = \max_{1\leq i<n} \chi_i = 1.$$

□

Using this proposition, we can redefine the Geometric Measure of Entanglement as follows. For notation, let $\langle A|B\rangle$ denote the full contraction between tensors $A$ and $B$.

**Definition 3.2** (Geometric Measure of Entanglement - MPS-GME)**.** For a pure quantum state $|\psi\rangle \in \mathcal{H} = \bigotimes_{i=1}^n \mathbb{C}^{d_i}$,

$$E_{\sin^2}(|\psi\rangle) = 1 - \max_{M\in\mathcal{M}_1(\mathcal{H})} |\langle \mathrm{MPS}(|\psi\rangle), M\rangle|^2, \tag{MPS-GME}$$

where $\mathrm{MPS}(|\psi\rangle)$ is the MPS decomposition of $|\psi\rangle$ and $\mathcal{M}_1(\mathcal{H})$ is the set of all MPS representations associated to $\mathcal{H}$ with $\chi = 1$.

## 4. Numerical Results

To implement the (MPS-GME), we used the `quimb` Python package [18], which has functionality for decomposing quantum wavefunctions into their MPS decompositions. It also provides a framework for tensor network optimization using `tensorflow` [19].

We verified (MPS-GME) with over 800 quantum states, using two families of states which have known analytic solutions to the GME (see [11]).

1. The first of these families is the *permutation invariant state* $|S(n,k)\rangle$, defined as:

$$|S(n,k)\rangle = \sqrt{\frac{k!(n-k)!}{n!}} \sum_{\text{permutations}} |\underbrace{0\cdots0}_{k}\underbrace{1\cdots1}_{n-k}\rangle. \tag{4.1}$$

   This corresponds to a system of $n$ qubits with $\binom{n}{k}$ possible measured states, each with an equally likely probability of being observed. The GME for permutation invariant states is:

$$E_{\sin^2}(|S(n,k)\rangle) = 1 - \frac{n!}{k!(n-k)!}\left(\frac{k}{n}\right)^k \left(\frac{n-k}{n}\right)^{n-k}.$$

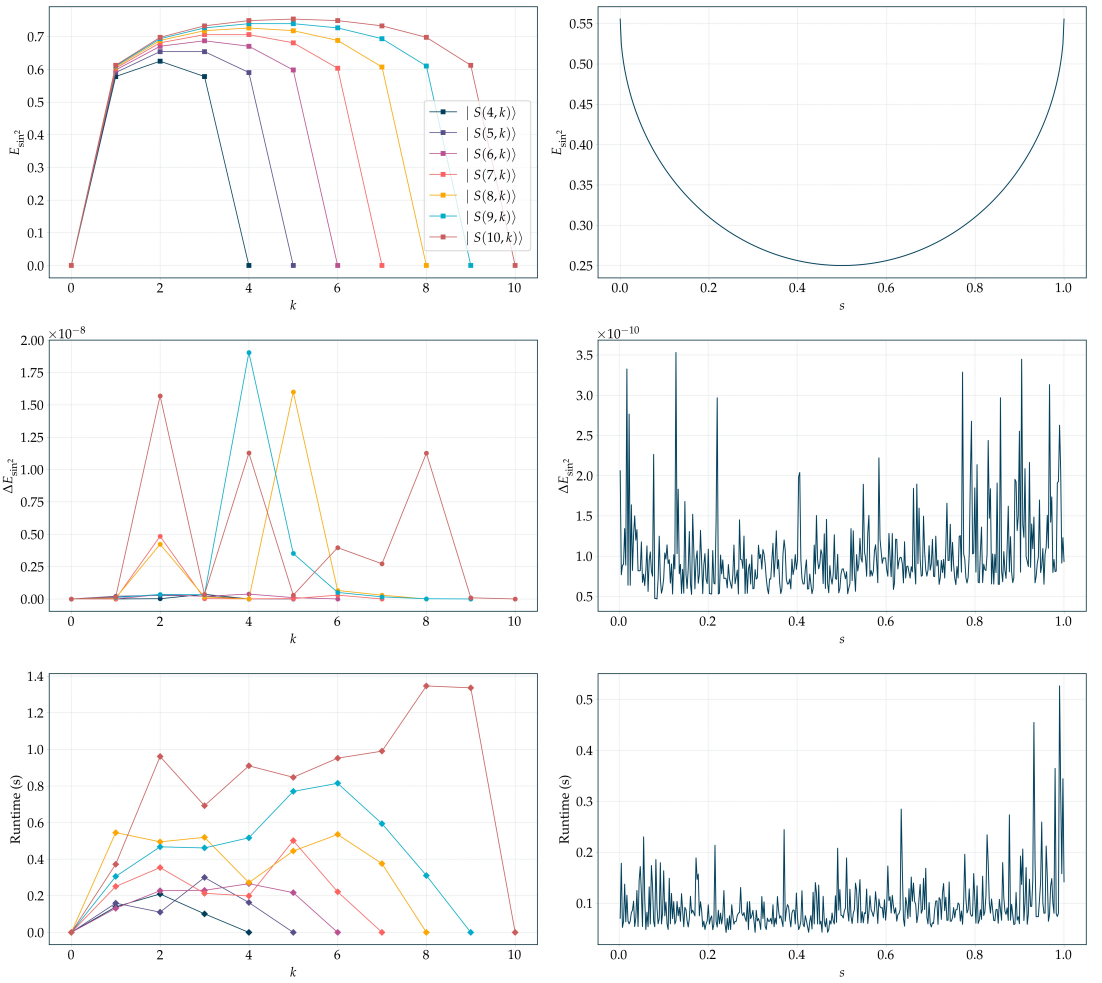


Figure 3. Numerical results for the entanglement curves for permutation invariant states (Eq. 4.1) on the left and superimposed 3-GHZ states (Eq. 4.2) on the right. Absolute errors and average runtime are shown in the second and third rows.

We tested 57 permutation invariant states, with $4 \leq n \leq 10$ and $0 \leq k \leq n$.

2. Next we considered a superposition of permutation invariant states, constructed as follows. We first define the 3-qubit states

$$|W\rangle := |S(3,2)\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$$
$$|\widetilde{W}\rangle := |S(3,1)\rangle = (|110\rangle + |101\rangle + |011\rangle)/\sqrt{3},$$

and then superimpose them to create a new state, parameterized by $(s,\phi) \in [0,1] \times [-\pi,\pi]$:

$$|W\widetilde{W}(s,\phi)\rangle = \sqrt{s}|W\rangle + \sqrt{1-s}e^{i\phi}|\widetilde{W}\rangle. \tag{4.2}$$

The value for $E_{\sin^2}$ is independent of the phase factor $\phi$, depending only on $s \in [0,1]$. The analytical solution can be derived by solving for the particular solution of a cubic polynomial (see [11] for details).
To test (MPS-GME) for these states, we used 400 $|W\widetilde{W}(s,0)\rangle$ superpositions, and 400 $|W\widetilde{W}(s,\pi)\rangle$ superpositions.

The numerical results for permutation invariant states and $|W\widetilde{W}(s,\phi)\rangle$ superpositions are shown in Figure 3. The error and runtime analysis is shown in Table 1.

| | $\lvert S(4,k)\rangle$ | $\lvert S(10,k)\rangle$ | $\lvert W\widetilde{W}(s,0)\rangle$ | $\lvert W\widetilde{W}(s,\pi)\rangle$ |
|---|---|---|---|---|
| $\Delta E_{\sin^2}$ | $1.2\times10^{-11}$ | $1.0\times10^{-10}$ | $2.6\times10^{-10}$ | $2.0\times10^{-10}$ |
| $\Delta t$ (s) | $0.4\pm0.2$ | $0.6\pm0.2$ | $0.10\pm0.01$ | $0.09\pm0.01$ |

TABLE 1 *Summary of error and runtime averages for each set of experiments. The highest and lowest errors ($|S(10,k)\rangle$ and $|S(4,0)\rangle$) are quoted for the permutation invariant states. Absolute error and runtime improve upon previous numerical approximations [4].*

## 5. Discussion

Our numerical results confirm that the Geometric Measure of Entanglement can be computed efficiently and with high accuracy with (MPS-GME). Unlike previous known estimates [4, 7, 8], our method avoids having to approximate the set of all separable states, instead minimizing Eq. 2.7 over $\mathcal{M}_1(\mathcal{H})$. The equivalence between $\mathcal{M}_1(\mathcal{H})$ and the set of separable states is formalized by Proposition 3.1, and allows us to compute the GME directly.

The improvements of this method over previous attempts is highlighted in Table 1 and Figure 3, which show the average runtime and absolute error for each simulation. Both the runtime and error improve upon the best known results from Zhang et. al [4].

While (MPS-GME) is a promising candidate for measuring entanglement in many-body quantum systems, it does introduce new challenges. First, the initial MPS decomposition is itself implemented as an optimization routine, and thus may introduce small numerical fluctuations that are difficult to quantify. Second, while optimizing over $\mathcal{M}_1(\mathcal{H})$ is computationally efficient, the underlying optimization routine can be sensitive to initial estimates, requiring a few attempts to converge in some cases. This problem persisted with several gradient-based optimization methods, including the Newton-CG, Nelder-Mead, and Nesterov Accelerated Gradient Descent.

## 6. Conclusion

In this paper, we presented an efficient method to measure the GME directly for pure quantum states. By decomposing quantum states into Matrix Product State decompositions, we are able to express the set of all separable states as Matrix Product State decompositions with bond dimension equal to one. This avoids having to approximate the set of separable states, which can only provide upper and lower bounds to the GME.

We verified our algorithm with over 800 quantum simulations of permutation invariant and superimposed 3-GHZ states, providing quick and accurate estimates to known analytic solutions.

While these results are promising, there are still some implementation details to consider before (MPS-GME) can be used to compute exact numerical solutions. One possible improvement would be to investigate higher order optimization methods for more precise estimates.

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