

# Quantum Machine Learning Matrix Product States

Jacob D Biamonte<sup>1,2,\*</sup>

<sup>1</sup>Deep Quantum Labs, Skolkovo Institute of Science and Technology, 3 Nobel Street, Moscow, Russia 121205

<sup>2</sup>Institute for Quantum Computing, University of Waterloo, 200 University Ave West, Waterloo, Canada ON N2L 3G1

\*jacob.biamonte@qubit.org

## ABSTRACT

Matrix product states minimize bipartite correlations to compress the classical data representing quantum states. Matrix product state algorithms and similar tools—called tensor network methods—form the backbone of modern numerical methods used to simulate many-body physics. Matrix product states have a further range of applications in machine learning. Finding matrix product states is in general a computationally challenging task, a computational task which we show quantum computers can accelerate. We present a quantum algorithm which returns a classical description of a  $k$ -rank matrix product state approximating an eigenvector given black-box access to a unitary matrix. Each iteration of the optimization requires  $O(n \cdot k^2)$  quantum gates, yielding sufficient conditions for our quantum variational algorithm to terminate in polynomial-time. Implications include:

- (i) Applications of quantum random access memory are severely limited from the general restriction imposed by quantum theory in which a quantum memory itself is modified by access. Our method recursively optimizes a rank- $k$  description of a quantum state: this in turn can be accessed *in situ* and hence our results augment the efficiency of quantum random access memory.
- (ii) Recently low-depth quantum circuits for various tasks have taken center stage. We augment these studies by providing a missing theoretical backbone, both quantifying algorithms in terms of entanglement and providing lower bounds for the gate-depth needed to for a computation to generate specific quantities of entanglement.
- (iii) Matrix product structure allows many operations to be done efficiently classically (provided one has the matrix product state to begin with). Hence, our method opens the door for hybrid quantum/classical algorithms which utilize quantum effects to determine a matrix product state and then utilizes various classical/quantum subroutines to calculate properties of matrix product states. This brings with it a host of applications in the simulation of physics and chemistry as well as in machine learning.

## Introduction

There is contemporary interest in near term quantum computing demonstrations of *quantum supremacy*—in which a quantum computer outperforms a classical one at some task. There is likewise ample interest in understanding the effectiveness of low-depth quantum circuits for e.g. machine learning<sup>1</sup> and quantum simulation. Missing in this theory is a quantification of the entanglement that a given quantum computation can support<sup>2</sup>. Using a quantum computer to determine a matrix product state provides a means to fill in this missing theory, as the degree of entanglement is specified in the description of the matrix product state. Indeed, the quantum algorithm we present minimizes bipartite entanglement across step-wise partitions of a quantum state, returning the classical description of a rank- $k$  approximation to an eigenvector of a unitary matrix.

Matrix product states are interesting for their vast range of practical applications. There is a growing and active community exploring the use of tensor network algorithms as a means to discover and un-

derstand new properties of quantum systems<sup>3–11</sup>. Additionally, machine learning has been merged with matrix product states and other tensor network methods<sup>12–14</sup>. Our algorithm opens the door to accelerate these classical algorithms by utilizing quantum computers.

An additional advantage of our framework is that it provides a practical route towards quantum supremacy. One can more directly compare the performance of a quantum vs. classical computer, paired-off on the same functional task. A classical tensor network contraction engine hence provides a gold-standard as a quantum computer will need to outperform these methods to constitute a meaningful demonstration.

Our own approach to tensor network states centered initially around casting an algebraic theory of logic gates into the setting of tensor network states—as used at the crossroads of condensed matter theory and quantum computation—by myself with several colleagues<sup>2, 15, 16</sup>. We adapted these tools and discovered efficient tensor network descriptions of finite Abelian lattice gauge theories<sup>17</sup>. These tools also lead to the discovery of a wide class of efficiently contractable tensor networks, representing counting problems<sup>18</sup>. The present paper connects these results as well as a vast range of tensor networks literature directly and definitively, providing a new bidirectional bridge between tensor network methods and practical quantum computation.

Quantum random access memory (qRAM) is a cornerstone of several quantum algorithms including quantum principle component analysis<sup>19</sup>. The fact remains that qRAM is difficult to realize and when realized always suffers from the inherent and unavoidable peculiar feature of quantum mechanics where states are modified through measurement. Quantum algorithms that make ample use of qRAM hence stand to greatly benefit by incorporating aspects of our methods. The reason is that we minimize the quantum resources needed to store a given state in qRAM and hence provide more efficient *in situ* quantum data-storage and quantum data-retrieval methods (both named as a tantamount practical challenge faced by quantum machine learning algorithms in<sup>1</sup>).

The algorithm is general in that it works given only black-box access to a unitary matrix. In the discussion however, we drop this restriction and cast the steps needed to perform a meaningful near-term demonstration of this algorithm on a quantum computer, providing a low-rank approximation to eigenvectors of the quantum computers free- (or closely related effective) Hamiltonian, taking a large step towards a practically useful task with low gate counts.

## Results

We work in the standard mathematical setting of quantum computing. We define  $n$  qubits arranged on a line and fix the standard canonical (computational) basis.

We consider the commutative Hermitian subalgebra generated by the  $n$ -projectors  $P_i = |0\rangle\langle 0|_i$  where the subscript  $i$  denotes the corresponding  $i$ th qubit acted on by  $P_i$ , with the remainder of the state-space acted on by the identity. These form our observables.

Rank is the maximum Schmidt number (the non-zero singular values) across any of the  $n - 1$  step-wise partitions of the qubits on a line. Rank provides an upper-bound on the bipartite entanglement that a quantum state can support—as will be seen, a rank- $k$  state has at most  $\ln_2(k)$  ebits of entanglement. The quantum algorithm we present works by finding a sequence of  $k$ -rank approximations, where the  $k$ th approximation can be used to seed the  $k + 1$ th approximation.

We parameterize a circuit family generating matrix product states with  $\theta$  a real vector with entries in  $[0, 2\pi)$ . We consider action on the initial rank-1 state  $|\mathbf{0}\rangle = |0\rangle^{\otimes n}$  and define two states  $|\psi(\theta)\rangle = U^\dagger(\theta)QU(\theta)|\mathbf{0}\rangle$  and  $|\tilde{\psi}(\theta)\rangle = U(\theta)|\mathbf{0}\rangle$ , both of yet to be specified rank.

We will construct an objective function (2) to minimize and hence to recover our approximate eigen-

vector. The choice of this function provides a desirable degree of freedom to further tailor the algorithm to the particular quantum processor at hand. We choose

$$p_i(\theta) = \langle \psi(\theta) | P_i | \psi(\theta) \rangle \quad (1)$$

and call

$$\mathcal{L}(\theta) = \sum_{i=1}^n \ln p_i(\theta) \quad (2)$$

the loglikelihood function of the  $n$ -point correlator  $\prod_{i=1}^n p_i(\theta)$ . The minimization of (2) corresponds to maximizing the probability of measuring each qubit in  $|0\rangle$ . This minimization can be done using a variety of optimization and machine learning algorithms.

As mentioned, our algorithm works given only oracle access to a unitary  $Q$ . The spectrum of  $Q$  is necessarily contained on the complex unit circle and so we note immediately that

$$1 = \max_{\phi} |\langle \phi | Q | \phi \rangle|^2 \geq \max_{\theta} |\langle 0 | \psi(\theta) \rangle|^2 = \max_{\theta} |\langle \tilde{\psi}(\theta) | Q | \tilde{\psi}(\theta) \rangle|^2 \quad (3)$$

with equality of the left-hand-side if and only if  $|\phi\rangle$  is an eigenvector of  $Q$ .

Importantly, the maximization of  $\theta$  on the right-hand-side of (3) corresponds to the minimization of the loglikelihood (2). We will then parameterize  $\tilde{\psi}(\theta_k)$  where  $k$  denotes a  $k$ -rank matrix product state of interest. Learning this matrix product state recovers an approximation to an eigenvector of  $Q$ . With a further promise on  $Q$  that all eigenvectors have a rank- $p$  matrix product state representation, then we conclude that  $k < p$  implies a fundamental error in our approximation. We consider then that the  $k$ th singular value of the state takes the value  $\varepsilon$ . It then follows that the one-norm error scales with  $O(\varepsilon)$  and the two-norm error scales only with  $O(\varepsilon^2)$ . In general we arrive at the monotonic sequence ordered by the following relation

$$\max_{\theta_{k+1}} |\langle \tilde{\psi}(\theta_{k+1}) | Q | \tilde{\psi}(\theta_{k+1}) \rangle|^2 \geq \max_{\theta_k} |\langle \tilde{\psi}(\theta_k) | Q | \tilde{\psi}(\theta_k) \rangle|^2 \quad (4)$$

valid for  $k = 1$  to  $\lceil 2^{n/2} \rceil$  (minimum to maximum possible rank).

Indeed, increasing the rank of the matrix product state approximation can improve the eigenvector approximation. Yet it should be noted that ground state eigenvectors of physical systems are in many cases known to be well approximated with low-rank matrix product states<sup>3–11</sup>. This depends on further properties of  $Q$  and is a subject of intensive study in numerical methods, further motivating the quantum algorithm we present here. We will develop our algorithm agnostic to  $Q$ , leaving a more specific near-term demonstration (in which  $Q$  is implemented by e.g. a free-Hamiltonian) to the Discussion. Generally we will express  $|\tilde{\psi}(\theta)\rangle$  as a matrix product state as

$$|\tilde{\psi}(\theta)\rangle = \sum_{q,r,s,\dots,n} A_q^{[\theta_q]} A_r^{[\theta_r]} A_s^{[\theta_s]} \dots A_n^{[\theta_n]} |q, r, s, \dots, n\rangle \quad (5)$$

In (5) the rank ( $k$ ) of the representation is embedded into the realization of the  $A$ 's. Quantum mechanics allows the deterministic generation of a class of isometries, where an isometry that is also an endomorphism on a particular space is called unitary— $\text{End}(\mathbb{C}_2^{\otimes n}, \mathbb{C}_2^{\otimes n})$ . Matrix product states (5) are isometries—hence correlation functions are readily calculated from them. Furthermore, matrix product states can

be deterministically generated by the uniform quantum circuit given in Figure 1. Other isometric structures of interest include trees and so-called, Multiscale Entanglement Renormalization Ansatz (MERA) networks<sup>5,20–22</sup>.

The algorithm begins with rank-1 qubit states.

$$|\tilde{\psi}(\theta)\rangle = \bigotimes_{i=1}^n (\cos \theta_1^i |0\rangle + e^{-i\theta_2^i} \sin \theta_1^i |1\rangle) \quad (6)$$

Minimization of the objective function (2) returns  $2n$  real numbers describing a local matrix product state. Approximations of higher rank are made by utilizing the quantum circuit structure given in Figure 1.

Consider then a rank- $k$  approximation to an eigenvector of  $Q$ . The blocks in Figure 1 represent unitary maps. These circuits act on at most  $\lceil \ln_2(k) \rceil$  qubits. Hence, each of these blocks has at most  $k^2$  real degrees of freedom in  $[0, 2\pi)$ . The general realization of these blocks using the typical basis of CNOT gates and arbitrary local unitaries can be done by a range of methods, see i.e.<sup>23</sup>. A commonly used theoretical lower bound requires  $\frac{1}{4}(k^2 - 3\ln_2 k - 1)$  CNOT gates, where the method in<sup>23</sup> requires  $k^2$  local qubit gates and did not reach this theoretical lower bound of CNOT gates. The total number of single qubit and CNOT gates nevertheless scales as  $O(k^2)$  for each block, where the number of blocks is bounded by  $n$ . Hence the implementation complexity scales as  $O(l \cdot n \cdot k^2)$ , where the optimization routine terminates after  $l$  steps.

Evident alternative methods to realize circuits exist. For example, a heuristic circuit realization can be preformed by adjusting controllable Hamiltonian parameters realizing each block, subject again to minimization of (2). Provided these sequences are localized appropriately, the matrix product structure still remains. To further quantify the presented quantum algorithm, we will show that the contemporary theory considering low-depth quantum circuits should be course grained by considering the maximum amount of entanglement a circuit of depth  $m$  on  $n$  qubits can realize. Our results are independent of the exact measure of entanglement used.

An ebit is the amount of entanglement contained in a maximally entangled two-qubit (Bell) state. A quantum state with  $q$  ebits of entanglement (quantified by some entanglement measure) has the same amount of entanglement (in that measure) as  $q$  Bell states. If a task requires  $r$  ebits, it can be done with  $r$  or more Bell states, but not with fewer. Maximally entangled states in  $\mathbb{C}^d \otimes \mathbb{C}^d$  have  $\ln_2(d)$  ebits of entanglement. The maximum possible ebits supported by a rank- $k$  matrix product state is of course bounded above by  $k$ . The question is then to upper bound the maximum amount of entanglement a given quantum computation can generate, provided a course graining to classify quantum algorithms in terms of both the circuit depth, as well as the maximum ebits possible. For low-depth circuits, these arguments are surprisingly relevant.

We then consider vertical partitions of a quantum circuit with the  $n$  qubits place horizontally on a line. For an  $m$ -depth quantum circuit (where  $m$  is presumably bounded above by a low-order polynomial in  $n$ ), the maximum number of two-qubit gates crossed in a vertical partition is never more than  $m$ . The maximum number of ebits generated by a fully entangling two-qubit gate is never more than a single ebit. We then consider the  $n - 1$  partitions of the qubits, the maximum partition with represent to ebits is into two (ideally) equal halves, which is never more than  $\lceil n/2 \rceil$ . We then arrive at the general result that an  $m$ -depth quantum circuit on  $n$  qubits never applies more than  $\min\{\lceil n/2 \rceil, m\}$  ebits of entanglement. This immediately puts a lower-bound of  $\sim n/2$  on the two-qubit gate-depth for  $Q$  to potentially drive a system into a state supporting the maximum possible ebits of entanglement.

## Discussion

We now turn to the realization of  $Q$  and sketch a meaningful demonstration for a near-term device. Polynomial time simulation of Hamiltonian evolution is well known to be **BQP**-hard. This provides an avenue for  $Q$  to represent a problem of significant computational interest, as simulating quantum evolution and quantum factoring are in **BQP**.

Let  $Q(t)$  be the one-parameter unitary group generated by  $\mathcal{H}$ , where  $\mathcal{H}$  represent a 3-SAT instances. Given access to an oracle computing  $\langle \tilde{\psi}(\theta_1) | \mathcal{H} | \tilde{\psi}(\theta_1) \rangle$ , we can minimize over all eigenvectors, which is **NP**-hard. Hence, finding even rank-1 states can be **NP**-hard.

When  $\mathcal{H}$  is a general quantum Hamiltonian, minimization of  $\langle \tilde{\psi}(\theta_k) | \mathcal{H} | \tilde{\psi}(\theta_k) \rangle$  is in turn, **QMA**-hard. For example, pairing our procedure with an additional procedure (quantum phase estimation) to minimize  $Q$  over all eigenvectors would hence provide rank- $k$  variational states and hence our methods provide a new research direction which incorporates tensor network methods in works such as e.g.<sup>24–26</sup>. It should however be noted that phase estimation adds significant experimental difficulty compared with the algorithm presented here.

For a near-term demonstration, we envision  $Q$  to be realized by bootstrapping the underlying physics of the system realizing  $Q$ . For instance, one can realize  $Q$  as a modification of the system's free-Hamiltonian using effective Hamiltonian methods (modulating local gates). This greatly reduces practical requirements on  $Q$ .

The interaction graph of the Hamiltonian generating  $Q$  can be used to define a tensor network state (as it will have the same structure as the layout of the chip, it will no longer have the contractable properties of a matrix product state but is still of interest). The algorithm works otherwise unchanged, but the circuit acts on this interaction graph (instead of a line) to create a corresponding tensor network state. Tailored free-evolution of the system Hamiltonian generates  $Q$ . Our algorithm returns a tensor network approximation of an eigenstate of  $Q$ . The first interesting demonstrations of the quantum algorithm we have presented should realize rank-2 tensor networks, and the corresponding tensor network can be realized with a few hundred gates for a system with a few hundred qubits.

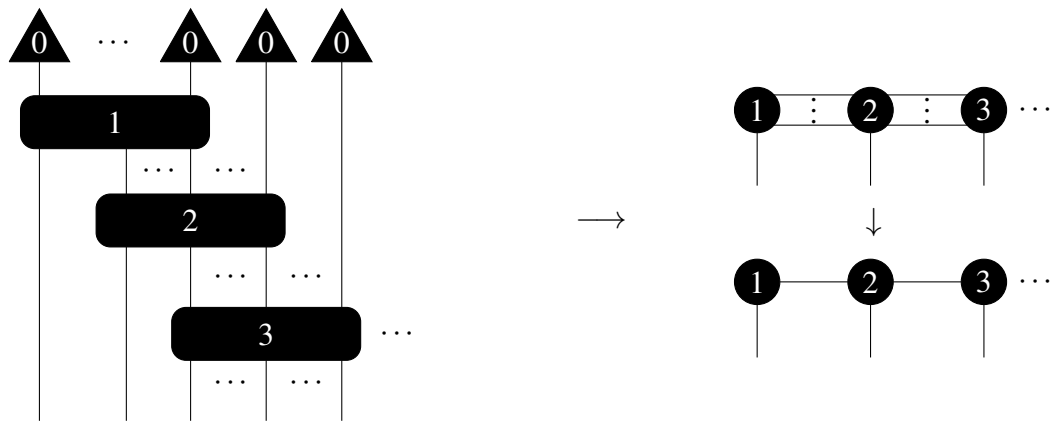
## References

1. Biamonte, J. *et al.* Quantum machine learning. *Nat.* **549**, 195–202 (2017). DOI 10.1038/nature23474. [1611.09347](#).
2. Biamonte, J., Bergholm, V. & Lanzagorta, M. Tensor network methods for invariant theory. *J. Phys. A Math. Gen.* **46**, 475301 (2013). DOI 10.1088/1751-8113/46/47/475301. [1209.0631](#).
3. Biamonte, J. Charged String Tensor Networks. *Proc. Natl. Acad. Sci.* **114**, 2447 (2017). [1703.01302](#).
4. Orús, R. A practical introduction to tensor networks: Matrix product states and projected entangled pair states. *Annals Phys.* **349**, 117–158 (2014). DOI 10.1016/j.aop.2014.06.013. [1306.2164](#).
5. Vidal, G. Entanglement renormalization: an introduction. In Carr, L. D. (ed.) *Understanding Quantum Phase Transitions* (Taylor & Francis, Boca Raton, 2010).
6. Verstraete, F., Murg, V. & Cirac, J. I. Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems. *Adv. Phys.* **57**, 143–224 (2008). DOI 10.1080/14789940801912366. [0907.2796](#).
7. Cirac, J. I. & Verstraete, F. Renormalization and tensor product states in spin chains and lattices. *J. Phys. A Math. Theor.* **42**, 504004 (2009). DOI 10.1088/1751-8113/42/50/504004. [0910.1130](#).



8. Schollwöck, U. The density-matrix renormalization group in the age of matrix product states. *Annals Phys.* **326**, 96–192 (2011). DOI 10.1016/j.aop.2010.09.012. [1008.3477](#).
9. Orús, R. Advances on tensor network theory: symmetries, fermions, entanglement, and holography. *Eur. Phys. J. B* **87**, 280 (2014). DOI 10.1140/epjb/e2014-50502-9. [1407.6552](#).
10. Eisert, J. Entanglement and tensor network states. *Model. Simul.* **3**, 520 (2013). [1308.3318](#).
11. Evenbly, G. & Vidal, G. Tensor Network States and Geometry. *J. Stat. Phys.* **145**, 891–918 (2011). DOI 10.1007/s10955-011-0237-4. [1106.1082](#).
12. Cichocki, A. *et al.* Tensor networks for dimensionality reduction and large-scale optimization: Part 1 low-rank tensor decompositions. *Foundations Trends Mach. Learn.* **9**, 249–429 (2016). DOI 10.1561/22000000059. [1609.00893](#).
13. Cichocki, A. *et al.* Tensor networks for dimensionality reduction and large-scale optimization: Part 2 applications and future perspectives. *Foundations Trends Mach. Learn.* **9**, 431–673 (2017). DOI 10.1561/22000000067.
14. Clark, S. R. Unifying neural-network quantum states and correlator product states via tensor networks. *J. Phys. A: Math. Theor.* **51**, 135301 (2018). URL <http://stacks.iop.org/1751-8121/51/i=13/a=135301>.
15. Biamonte, J. D., Clark, S. R. & Jaksch, D. Categorical Tensor Network States. *AIP Adv.* **1**, 042172 (2011). DOI 10.1063/1.3672009. [1012.0531](#).
16. Bergholm, V. & Biamonte, J. D. Categorical quantum circuits. *J. Phys. A Math. Gen.* **44**, 245304 (2011). DOI 10.1088/1751-8113/44/24/245304. [1010.4840](#).
17. Denny, S. J., Biamonte, J. D., Jaksch, D. & Clark, S. R. Algebraically contractible topological tensor network states. *J. Phys. A Math. Gen.* **45**, 015309 (2012). DOI 10.1088/1751-8113/45/1/015309. [1108.0888](#).
18. Biamonte, J. D., Morton, J. & Turner, J. Tensor Network Contractions for #SAT. *J. Stat. Phys.* **160**, 1389–1404 (2015). DOI 10.1007/s10955-015-1276-z. [1405.7375](#).
19. Lloyd, S., Mohseni, M. & Rebentrost, P. Quantum principal component analysis. *Nat. Phys.* **10**, 631–633 (2014). DOI 10.1038/nphys3029. [1307.0401](#).
20. Vidal, G. Entanglement renormalization. *Phys. Rev. Lett.* **99**, 220405 (2007). DOI 10.1103/PhysRevLett.99.220405. [cond-mat/0512165](#).
21. Giovannetti, V., Montangero, S. & Fazio, R. Quantum Multiscale Entanglement Renormalization Ansatz Channels. *Phys. Rev. Lett.* **101**, 180503 (2008). DOI 10.1103/PhysRevLett.101.180503. [0804.0520](#).
22. Vidal, G. Class of quantum many-body states that can be efficiently simulated. *Phys. Rev. Lett.* **101**, 110501 (2008). DOI 10.1103/PhysRevLett.101.110501. [quant-ph/0610099](#).
23. Möttönen, M., Vartiainen, J. J., Bergholm, V. & Salomaa, M. M. Quantum Circuits for General Multiqubit Gates. *Phys. Rev. Lett.* **93**, 130502 (2004). DOI 10.1103/PhysRevLett.93.130502. [quant-ph/0404089](#).
24. McClean, J., Romero, J., Babbush, R. & Aspuru-Guzik, A. The theory of variational hybrid quantum-classical algorithms. *New J. Phys.* **18**, 023023 (2016). URL <http://dx.doi.org/10.1088/1367-2630/18/2/023023>.

25. Peruzzo, A. *et al.* A variational eigenvalue solver on a photonic quantum processor. *Nat. Commun.* **5**, 4213 (2014). DOI 10.1038/ncomms5213. [1304.3061](#).
26. Kandala, A. *et al.* Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. *Nat.* **549**, 242–246 (2017). DOI 10.1038/nature23879. [1704.05018](#).



**Figure 1.** (left) Quantum circuit realization of a matrix product state with open boundary conditions. (right) Using standard graphical rewrite rules—or by manipulating equations—one readily recovers the familiar matrix product state depiction as a ‘train of tensors’.