Computational Difficulty of Global Variations in the Density Matrix Renormalization Group

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The density matrix renormalization group (DMRG) approach is arguably the most successful method to numerically find ground states of quantum spin chains. It amounts to iteratively locally optimizing matrix-product states, aiming at better and better approximating the true ground state. To date, both a proof of convergence to the globally best approximation and an assessment of its complexity are lacking. Here we establish a result on the computational complexity of an approximation with matrix-product states: The surprising result is that when one globally optimizes over several sites of local Hamiltonians, avoiding local optima, one encounters in the worst case a computationally difficult NP-hard problem (hard even in approximation). The proof exploits a novel way of relating it to binary quadratic programming. We discuss intriguing ramifications on the difficulty of describing quantum many-body systems.

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“How difficult is it to describe quantum systems in classical terms”? This question in its various variants has manifold implications to several fields of theoretical physics: to the context of numerically studying many-body systems of condensed-matter physics in their ground-state properties, to the question of the superiority of a quantum compared to a classical computer, and others. Recently, a renewed interest in questions of classically simulating quantum many-body systems [1–3] gave rise to a number of new results and simulation methods, a large number of them motivated or in their approach by ideas of quantum information theory [2–8]. The arguable workhorse of numerically finding ground states of many-body systems, the DMRG method [1–3], was recently reassessed and in some ways improved. It seems fair to say that the problem of finding ground states of systems with periodic boundary conditions or higher-dimensional systems is now much better understood than not very long ago [6]. The performance of DMRG-type methods has also been quantitatively related to entanglement scaling in ground states: One should expect an approximation in terms of matrix-product states – as DMRG is generating – to be most faithful, if an “entanglement area-theorem” holds, which in turn is typically the case in non-critical systems [8, 10].

Now, even if matrix product states form the right set of states that well-describe the true ground state properties, and one can expect MPS to faithfully represent the ground state [10]: “How difficult is it then to find the truly best approximation to the ground state”? This is the key question of the computational complexity of any method to find ground states. Quite surprisingly, given the maturity of the field and the significance of such simulations, this question is essentially open. In practice, DMRG produces very good results, despite of the possibility of getting stuck in local minima in the optimization. However, it is not certifiable: one never can be entirely sure whether one has indeed found a state close to the true ground state of the system. Hence, to find certifiable methods to get ground states seems very timely and important [11].

In this work, we present a first rigorous analysis of the complexity of finding ground states using variations over matrix-product states as in DMRG. As such, DMRG essentially amounts to a local variation of matrices in the matrix-product states [2, 3]. This is made most explicit in the variant of Ref. [5]. Here, we show that if we allow for a global variation over several sites at once – to find the globally best approximation in this set and to avoid local optima – one encounters a problem which is computationally hard, even in approximation. Or, actually more strongly: for any instance of a binary quadratic problem (including the NP hard exact satisfiability, or the maximum clique or independent set problems) one has an identical instance, realized with local translationally invariant hamiltonians [14]. To prove that this is true, we need 4-level systems, 6-local hamiltonians, and a variation over two sites. This is much stronger than merely saying that polynomially constrained problems of high degree as such are computationally hard, as it could a priori of course well be that these hard instances never occur in the specific context under consideration. Moreover, this reduction can be found with polynomial effort. So one faces the ironic and interesting situation that when locally varying matrix product states, one has an efficient subproblem, but may not get the certifiable true ground state of the system. In turn, when aiming at avoiding the problem of local minima and varying matrices of several sites at once, one encounters a hard problem.

Local hamiltonians. – The considered hamiltonians are r-
local and translationally invariant,

\[ H = \sum_{i=1}^{n-r+1} h(i), \]  

up to open boundary conditions (see Fig. 1), where the local interaction is governed by some general hamiltonian \( h(i) = \sum_{\alpha, \beta, \ldots, \xi} h_{\alpha, \beta, \ldots, \xi} (\sigma^{(i)}_\alpha \otimes \sigma^{(i+1)}_\beta \otimes \cdots \otimes \sigma^{(i+r-1)}_\xi). \) Here, \( \{\sigma^{(i)}_\alpha\} \) denotes any local operator basis for site \( i = 1, \ldots, n, \) such as Pauli operators in case of spin-1/2 systems. This insistence on local hamiltonians renders the assessment of the computational complexity fair, as in non-local models, one has the freedom to incorporate frustrated higher-dimensional systems.

\textit{Matrix product states.} – The density matrix renormalization group methods – in several variants – essentially produce a sequence of matrix product states (MPS) that better and better approximate the true ground state. These matrix product states correspond to non-translationally invariant versions of the finitely correlated states \([3]\), which were historically developed and studied independently from the DMRG context.

We consider chains of \( n \) sites and \( d \)-level constituents, so \( d = 2 \) for a spin chain. The local basis is denoted by \( \{|1\rangle, \ldots, |d\rangle\}. \) Then, MPS take the standard form \( |\psi\rangle = \sum_{i_1, \ldots, i_n=1}^d A^{(1)}_{i_1} A^{(2)}_{i_2} \cdots A^{(n)}_{i_n} |i_1, i_2, \ldots, i_n\rangle. \) Here, \( A^{(j)}_{i} \in \mathbb{C}^{D_j \times D_{j+1}}, \ j = 1, \ldots, n, \) are complex matrices. These matrices, depending on the auxiliary dimension \( D_j = \max_j D_j \) (the \textit{MPS dimension}), characterize the MPS. For simplicity, we impose open boundary conditions. This means that \( D_1 = D_{n+1} = 1 \), i.e., \( A^{(n)}_{i} \in \mathbb{C}^{D_n \times 1} \) and \( A^{(1)}_{i} \in \mathbb{C}^{1 \times D_2} \) are taken to be vectors. We consider normalized MPS, meaning that \( \langle \psi | \psi \rangle = 1. \) This is notably achieved by using the \textit{gauge condition} that \( \sum_i (A^{(j)}_{i})^\dagger A^{(j)}_{i} = 1 \) for each site \( j \) \([13]\). This condition can always be satisfied up to similarity transformations \([7]\), and is in numerical methods, most explicitly in Ref. \([5]\), insisted upon for numerical stability.

We look at optimizations over MPS, as it is explicitly or implicitly being done in DMRG approaches. Needless to say, there are many variants. The local variational method for finite-size DMRG involves optimizations over single sites \([5]\), essentially equivalent to the \( B \circ B \)-method of DMRG in case of open boundary conditions: For any site \( j = 1, \ldots, n, \) one keeps all matrices \( A^{(j)}_{i} \) of the sites \( i \) different from \( j \) fixed. Then, one finds the optimal MPS by varying over the matrices \( A^{(j)}_{1}, \ldots, A^{(j)}_{d} \) of site \( j \), satisfying normalization, to minimize the energy \( E = \langle \psi | H | \psi \rangle. \) Then, one takes the next site, optimizes over the matrices of that site, and “sweeps”, until a fixed point is reached \([2, 5, 6]\). In fact, assertions that in gapped systems, DMRG does find the ground state, implicitly assume that the globally optimal MPS can be found.

\textit{Main result.} – Yet, the problem one actually intends to solve is the full problem, so the global optimization problem of finding the best matrix product state. Or, if one has an infinite system, one should at least be able to solve the problem over several sites at once, in one run, solving the problem over these sites, say, of the length scale of the classical correlation length. Obviously, we have to allow for sequences of larger and larger systems in \( n, \) as otherwise, the complexity question and the one of finding the ground state no longer makes sense: for finite systems, there is always a finite \( D \) to exactly write out the true ground state. We will now see that there are hard instances in the class of variations over several sites at once.

\textbf{Problem 1 (DMRG with global variation over several sites)}

Consider a family of translationally invariant hamiltonians \( H \) of the form as in Eq. \( 1, \) with \( n = aD + b \) (\( a, b \in \mathbb{R} \) are fixed numbers). Let \( I \subset \{1, \ldots, n\} \) some finite subset of sites of the hamiltonian. Then, find for any MPS dimension \( D \) the optimal matrix product state

\[ |\psi\rangle = \sum_{i_1, \ldots, i_n=1}^d A^{(1)}_{i_1} A^{(2)}_{i_2} \cdots A^{(n)}_{i_n} |i_1, i_2, \ldots, i_n\rangle \]

by simultaneously varying the matrices \( A^{(j)}_{i} \) of sites \( j \in I \) satisfying the above gauge condition to achieve normalization \( \langle \psi | \psi \rangle = 1, \) to minimize the energy \( E = \langle \psi | H | \psi \rangle. \)

This is the very reasonable and natural variation over several sites to minimize the energy, aiming at avoiding local minima. Yet, surprisingly, one arrives at the subsequent observation:

\textbf{Theorem 1 (Hardness of DMRG with global variations)}

Finding the best MPS with varying over several sites is NP-hard in \( D. \) Moreover, the ground state energy \( \langle \psi | H | \psi \rangle \) can not be \( 1/D \)-approximated in polynomial time.

The latter statement is meant unless \( P = \text{NP}\) \([16, 18, 19]\). What we aim for is a reduction of this problem to a general binary quadratic problem. We start by abstract considerations, and then flush out how we can incorporate this in the MPS setting. To simplify the notation, we will first consider a setting involving \( N \) real variables, \( N \) even, and will later relate this to the dimension \( D. \) What follows is not a standard polynomial reduction to an NP-complete problem: we are heavily restricted by the specific form offered by MPS. Yet, it will turn out that the freedom that we have is just so sufficient for our purposes. We will introduce some new techniques. Readers only interested in the physical implications may read on the with the further discussion of simulatability issues.

\textit{Idea of relating optimization problems.} – We start by relating a certain class of quadratic continuous problems to a general binary quadratic problem, where variables can only take values in \( \{0, 1\}, \) which includes problems as the max clique problem. This will be the final form that we want to achieve with MPS, when minimizing the energy \( \langle \psi | H | \psi \rangle. \) The argument is as follows: For every real \( (N - 1) \times (N - 1) \)-matrix \( M \) with entries having absolute values smaller or equal to unity there exists an \( N \times N \)-matrix \( Y \) such that every problem of finding the minimal value of \( b M b^T \) for binary variables \( b_1, \ldots, b_{N-1} \in \{0, 1\} \) can be written as a problem of finding the minimal value of \( x^T y^T \) for \( x_1, \ldots, x_N, y_1, \ldots, y_N \in \)
[0, 1]. To see this, we may identify the first $N - 1$ variables $x_1, \ldots, x_{N-1}$ with $b_1, \ldots, b_{N-1}$. Now, for $x, y \in \{0, 1\}^N$,
\[
2 \sum_{k=1}^{N-1} x_k y_k - \sum_{k=1}^{N-1} (x_k + y_k) - x_N y_N
+ (x_1, \ldots, x_{N-1})^T M (x_1, \ldots, x_{N-1})^T / (2 (N - 1)^2)
\]
takes its minimal value exactly if (i) $y_k = 1 - x_k$, $x, y \in \{0, 1\}^N$, (ii) $x_N = y_N = 1$ hold, and (iii) $(x_1, \ldots, x_{N-1}) M (x_1, \ldots, x_{N-1})^{\dagger T}$ takes its minimal value over binary variables. Eq. (2) can clearly be incorporated in a single matrix $Y$ [17]. In this form, we are in the position to actually generate exactly this situation in the MPS setting when minimizing the energy. Also, the above approximation statement follows from results in Ref. [18], and using estimates for the deviation from binary variables, once we are in the position of formulating the problem as a minimization over $x y^T$.

**Incorporating this in MPS.** – In order to generate a fair worst-case scenario, we are free to take any variational set $I$, fix the other matrices of sites not contained in $I$ appropriately, and may take any local Hamiltonian $H$ and local physical dimension. Then, energy minimization amounts to solving the optimization problem. We will make use of a 6-local Hamiltonian, so $h$ acts non-trivially on 6 subsystems, $h \sim = |1\rangle \langle 1| \otimes I^6 + |2\rangle \langle 2| \otimes I^6 + |3\rangle \langle 3| \otimes I^6 + |4\rangle \langle 4| \otimes I^6$ for all $i$. The idea now is to think of four “regions” of the matrix product chain: To the left and to the right, there will be $m = \lceil \log_2 D \rceil$ sites, forming a “tail” to accumulate the proper range of the matrices. The left center consists of 6 sites, and the system will be constructed in a way such that the Hamiltonian acts only non-trivially on these sites. The right center is a chain of sites generating “indicator matrices”. This means that the chain consists for integer $N$ of $N^2 + 6 + 2 m$ sites, and $D = 2 N^2 + N$. $N$ labels both the auxiliary matrix dimension and the system size (we can always pad the system to get $n = a D + b$ for $a, b \in N$).

Let us first focus on the left center, embodying 6 sites: Sites $m + 3$ and $m + 5$ will form the set $I$, and we keep the other matrices fixed, respecting the gauge condition. We take $A_i^{(m+4)} = \sum_{l=1}^{N^2} E_i(l, 1) / \otimes 0_{D-N}$, and $A_i^{(m+4)}$ such that the gauge condition is satisfied, the other two matrices of this site being zero. Here, we use of the notation $E_i(l, j)$ for a matrix, all entries of which are zero, except that $E_i(l, j)_{i,j} = 1$. This matrix $A_i^{(m+4)}$ has the purpose of selecting appropriate parts of $A_i^{(m+3)}$ and $A_i^{(m+5)}$: the matrices $A_i^{(m+3)}$ and $A_i^{(m+5)}$ will later incorporate the variables $x_k$ and $y_k$, respectively. It is not difficult to see that for any complex $c_k, d_k$ satisfying $|c_k| \leq 1$ and $|d_k| \leq 1$, $k = 1, \ldots, N$, we can find $D \times D$-matrices satisfying $(A_i^{(m+3)})^\dagger A_i^{(m+3)} \leq I_D$ and $(A_i^{(m+5)})^\dagger A_i^{(m+5)} \leq I_D$, such that
\[
A_i^{(m+3)} A_i^{(m+4)} A_i^{(m+5)} = [c_1, \ldots, c_N]^\dagger [d_1, \ldots, d_N] / N.
\]
(2)

Conversely, for any solution of Eq. (2) we find $|c_k|, |d_k| \leq 1$ for all $k$. This follows from exploiting the gauge conditions for $A_i^{(m+5)}$ and making use of the specific form of $A_i^{(m+3)}$ that has been chosen. These numbers $c_1, \ldots, c_N$ and $d_1, \ldots, d_N$ are still complex: the key idea we use at this point is that we can appropriately combine them such that only absolute values remain: the role of the binary variables will be taken over by $x_k = |c_k|^2, y_k = |d_k|^2$.

**Generating indicator matrices from matrix products.** – To the right of the left center, we will append the right center, so appropriately chosen $N^2$ matrices. As we insist on a local Hamiltonian, we have no freedom to select only certain products: we will always have to deal with all possible products. We hence have to exploit a certain structure, such that from all exponentially many products, we can generate polynomially many indicator matrices, which are zero except from a single non-zero element. These indicator matrices will be used in the MPS construction to single out certain elements. It is not at all obvious that such matrices generating indicator matrices even exist: Yet, for any $N \times N$ matrix $Y$ with entries $Y_{k,l} \in \{0, 1\}$, one can indeed construct $D \times D$-matrices $M_i^{(j)} M_i^{(j)}$ for $j = 1, \ldots, N^2$ with this property [20]: For every binary word $(i_1, i_2, \ldots, i_{N^2}) \in \{0, 1\}^N$, we find
\[
P \prod_{j=1}^{N^2} M_i^{(j)} = \begin{cases} Y_{k,l} \left[ \begin{array}{cc} E(k,l) & 0 \\ 0 & 0 \end{array} \right] \text{ or,} \\ 0, \end{cases}
\]
for $k, l = 1, \ldots, N$, where $P \in \mathbb{R}^{D \times D}$ is defined as $P = \sum_{i=1}^{N^2} \sum_{j=1}^{N^2} E_i(k,l, N+l)$. Also, each non-zero matrix in Eq. (3) corresponds to a single binary word. In more colloquial and intuitive terms: we can take an arbitrary product of these matrices with lower index 1 or 2 defined by the binary word, and multiply it from the left with $P$, acting here as a shift operator. We will then always obtain a matrix with a single non-zero element. This single element can be arbitrary, forming the desired matrix $Y$. To check in retrospect that the given construction [20] has this property is straightforward.

**Combining results and minimizing the energy.** – We are now in the position to put the previous results together, and see that the binary optimization problem can indeed be encoded in energy minimization. Concerning the further matrices of the left center, we simply put $A_i^{(m+1)} = A_i^{(m+6)} = I_D$, and $A_i^{(m+2)} = 0_N \otimes 0_{D-N}, A_i^{(m+2)} = 0_N \otimes 1_{D-N}$. All other matrices of sites $m + 1, m + 2, m + 6$ are set to zero. The matrices forming the right center are identified with $A_i^{(m+6+l)} = M_i^{(l)}$, for $l = 1, \ldots, N^2$, $i = 1, 2$, and $A_i^{(m+6+l)} = A_i^{(m+6+l)} = 0_D$ for all $l = 1, \ldots, N^2$. The left and right tails are simply padded with matrices such that the product of them gives rise to an identity matrix [22]. Now, we find that we have satisfied the gauge condition for all matrices of sites $\{1, \ldots, n\} \setminus I$. Finally, we can combine all this: Let the matrices associated with sites $\{1, \ldots, n\} \setminus I$ be as chosen above, and the Hamiltonian as in Eq. (1). Then, energy minimization becomes
\[
\langle \psi | H | \psi \rangle = \sum_{k,l} |\text{tr}[A_i^{(m+3)} A_i^{(m+4)} A_i^{(m+5)} Y_{k,l} E(k,l)]|^2 = x y^T / N.
\]
This follows now from a direct evaluation of the overlap of the MPS, making use of the above results. This proves the validity of the theorem: the optimization problem encountered in the variation over matrix-product state is in this form identical to solving the respective instance of the binary quadratic problem, and for the very same Hamiltonian, for every instance of this problem, as in an instance of the max clique problem, one can find a D such that the variational problem becomes identical. This shows that indeed: even within the setting of varying over several sites simultaneously when finding optimal matrix-product states to approximate ground states, one encounters computationally difficult NP hard problems.

Further discussion of the simulatability of quantum many-body problems. – In this work, we have addressed the question of finding quantum ground states of one-dimensional many-body systems on a classical computer, as far as the complexity of local variations is concerned. This is a question that has not explicitly been addressed so far: even if MPS are a set faithfully representing the true ground state, how difficult is it to find the optimal one? It turns out that in the class of problems where one reasonably varies over several sites at once contains provably computationally difficult instances, even for local one-dimensional Hamiltonians. By no means should this be be read as a statement that DMRG does not work: In practice, DMRG obviously gives typically rise to very good results. But rather as a warning sign, that to find best approximations of many-body systems can be computationally hard. Moreover, it suggests that to further look for new certifiable algorithms to find ground states, including “error bars”, at least for non-critical systems, should be a very fruitful task. A number of questions are implicitly raised here: What is the significance of breaking the translational symmetry in MPS for ground state approximations? What role does the gauge freedom play? Also, what is the exact relationship to QMA completeness $^{[23]}$ of local hamiltonian problems? Can good bounds be found via polynomial relaxations $^{[24]}$? It would be exciting to further look at truly optimal translationally invariant MPS as approximations of translationally invariant ground states, to see under what conditions such approximations are truly efficient. It is the hope that the present work further fosters such considerations.

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17. If one has $x,y \in \{0,1\}^{N-1}$ that satisfy $\sum_{k=1}^{N-1} x_k y_k - \sum_{k=1}^{N-1} (x_k + y_k) = -(N-1)$, then $x_k, y_k \in \{0,1\}$ for all $k = 1,\ldots,N-1$. Hence, the binary character can be enforced via a single quadratic constraint: The first term ensures that for each $k$ at least one of the variables $x_k$ or $y_k$ must vanish. The second constraint is extremal, and can only be satisfied if for each $k$ either $x_k = 1$ or $y_k = 0$.
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20. Very explicitly, the construction is as follows: Let $M_1^{N(k-1)+1} = \begin{bmatrix} 0_N & 0_{N,D-N} \\ G_{k,l} & 0_{N,D-N} \\ H_{k,l} & 0_{N,D-N} \end{bmatrix}$, for $k,l = 1,\ldots,N$, where $G_{k,l} = Y_{k,l} E(k(N-1) + l, l)$ $\in \mathbb{R}^{N^2 \times N}$, and
\[ M_2^{(N(k-1)+l)} = 0_N \oplus I_{D-N}. \] The matrices \( H_{k,l} \in \mathbb{R}^{N^2 \times N} \) can be chosen such that \( (M_1^{(i)})^\dagger M_1^{(i)} + (M_2^{(i)})^\dagger M_2^{(i)} = I_D \) for all \( i \).

[21] The product \( M_1^{(i)} M_1^{(j)} \) vanishes whenever \( i \neq j \). Hence, the only contributing binary words are of the form \((1, \ldots, 1, 0, 1, \ldots, 1)\) with a single zero element, and \((1, \ldots, 1)\).

[22] Take \( A_3^{(k)} = \sum_{l=1}^{2^{k-1}} E(l, l) \) and \( A_4^{(k)} = \sum_{l=1}^{2^{k-1}} E(2^{k-1} + l, l) \) for \( k = 1, \ldots, m \), the other matrices of sites \( 1, \ldots, m \) being zero. The same matrices are taken in reverse order for \( n-m, \ldots, n \).

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