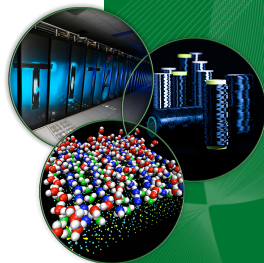


DMRG Algorithm

September 22, 2016



Let us define *block* to mean a finite set of sites. Let $N > 0$ be called the total number of sites. Let C denote the states of a single site. This set is model dependent. For the Hubbard model it is given by: $C = \{e, \uparrow, \downarrow, (\uparrow, \downarrow)\}$, where e is a formal element that denotes an empty state. For the t-J model it is given by $C = \{e, \uparrow, \downarrow\}$, and for the spin 1/2 Heisenberg model by $C = \{\uparrow, \downarrow\}$, for the Hubbard model with 2 orbitals, C is composed of 16 elements. A *real-space-based Hilbert space* \mathcal{V} on a block B and set C is a Hilbert space with basis C^B . I will simply denote this as $\mathcal{V}(B)$ and assume that C is implicit and fixed. This is a Hilbert space because (i) it is a vector space over \mathbb{C} , and (ii) it has a norm.¹ It is a vector space: The elements $\psi \in C^B$ are endowed² of a formal sum and multiplication. It has a norm: Because it has an inner product: for every $\psi, \psi' \in C^B$ as $(\psi, \psi') = 0$ if ψ and ψ' are different and 1 if equal.³

¹Or it has the topology induced by the norm, making the space separable also.

²Elements of the Hilbert space are usually noted with the so-called Dirac notation as $|\psi\rangle$.

³The inner product (ψ, ψ') is usually noted in the so-called Dirac notation as $\langle\psi|\psi'\rangle$.

Notation

A *real-space-based Hilbert space* can also be thought of as the external product space of $\#C$ Hilbert spaces on a site, one for each site in block B . The basis $\psi \in C^B$ of \mathcal{V} is called the *computational basis* of \mathcal{V} . $C^B = \bigotimes B$, so that $\psi \in C^B$ can be written as $\psi_{i_0} \otimes \psi_{i_1} \otimes \cdots \otimes \psi_{i_{N-1}}$ where ψ_{i_n} is in the n -th space B , and it is the i_n -th element of that space.

I give a procedural description of the DMRG algorithm[1, 2] in the following. We start with an initial block S (the initial system) and E (the initial environment). Consider two sets of blocks X and Y . We will be adding blocks from X to S , one at a time, and from Y to E , one at a time. Again, note that X and Y are sets of blocks whereas S and E are blocks. Now we start a loop for the DMRG “infinite” algorithm by setting $step = 0$ and $\mathcal{V}_R(S) \equiv \mathcal{V}(S)$ and $\mathcal{V}_R(E) \equiv \mathcal{V}(E)$. The system is grown by adding the sites in X_{step} to it, and let $S' = S \cup X_{step}$, i.e. the $step$ -th block of X to S is added to form the block S' ; likewise, let $E' = E \cup Y_{step}$. Let us form the following product Hilbert spaces: $\mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$ and $\mathcal{V}(E') = \mathcal{V}_R(E) \otimes \mathcal{V}(Y_{step})$ and their union $\mathcal{V}(S') \otimes \mathcal{V}(E')$ which is disjoint.

Notation

We will consider now operators acting on \mathcal{V} . A special operator is called the Hamiltonian. Consider $\hat{H}_{S' \cup E'}$, the Hamiltonian operator, acting on $\mathcal{V}(S') \otimes \mathcal{V}(E')$. We diagonalize $\hat{H}_{S' \cup E'}$ (using Lanczos) to obtain its lowest eigenvector:

$$|\psi\rangle = \sum_{\alpha \in \mathcal{V}(S'), \beta \in \mathcal{V}(E')} \psi_{\alpha, \beta} |\alpha\rangle \otimes |\beta\rangle, \quad (1)$$

where $\{|\alpha\rangle\}$ is a basis of $\mathcal{V}(S')$ and $\{|\beta\rangle\}$ is a basis of $\mathcal{V}(E')$.

Let us define the density matrices for system:

$$(\hat{\rho}_S)_{\alpha, \alpha'} = \sum_{\beta \in \mathcal{V}(E')} \psi_{\alpha', \beta}^* \psi_{\alpha, \beta} \quad (2)$$

in $\mathcal{V}(S')$, and environment:

$$(\hat{\rho}_E)_{\beta, \beta'} = \sum_{\alpha \in \mathcal{V}(S')} \psi_{\alpha, \beta'}^* \psi_{\alpha, \beta} \quad (3)$$

in $\mathcal{V}(E')$.

Notation

We then diagonalize $\hat{\rho}_S$, and obtain its eigenvalues and eigenvectors, $W_{\alpha,\alpha'}^S$ in $\mathcal{V}(S')$ ordered in decreasing eigenvalue order.

We change basis for the operator $H^{S'}$ (and other operators as necessary), as follows:

$$(H^{S' \text{ new basis}})_{\alpha,\alpha'} = (W^S)^{-1}_{\alpha,\gamma} (H^{S'})_{\gamma,\gamma'} W_{\gamma',\alpha'}^S. \quad (4)$$

We proceed in the same way for the environment, diagonalize $\hat{\rho}_E$ to obtain ordered eigenvectors W^E , and define $(H^{E' \text{ new basis}})_{\alpha,\alpha'}$.

Let m_S be a fixed number that corresponds to the number of states in $\mathcal{V}(S')$ that we want to keep. Consider the first m_S eigenvectors W^S , and let us call the Hilbert space spanned by them, $\mathcal{V}_R(S')$, the DMRG-reduced Hilbert space on block S' . If $m_S \geq \#\mathcal{V}(S')$ then we keep all eigenvectors and there is effectively no truncation. We truncate the matrices $(H^{S' \text{ new basis}})$ (and other operators as necessary) such that they now act on this truncated Hilbert space, $\mathcal{V}_R(S')$. We proceed in the same manner for the environment.

Notation

Now we increase *step* by 1, set $S \leftarrow S'$, $\mathcal{V}_R(S) \leftarrow \mathcal{V}_R(S')$, $H_{S'} \leftarrow H_S$, and similarly for the environment, and continue with the growth phase of the algorithm.

In the infinite algorithm, the number of sites in the system and environment grows as more steps are performed. After this infinite algorithm, a finite algorithm is applied where the environment is shrunk at the expense of the system, and the system is grown at the expense of the environment. During the finite algorithm phase the total number of sites remains constant allowing for a formulation of DMRG as a variational method in a basis of matrix product states.

Why the DMRG works?

The advantage of the DMRG algorithm is that the truncation procedure described above keeps the error bounded and small. Assume $m_S = m_E = m$. At each DMRG step [3] the truncation error $\epsilon_{tr} = \sum_{i>m} \lambda_i$, where λ_i are the eigenvalues of the truncated density matrix ρ_S in decreasing order. The parameter m should be chosen such that ϵ_{tr} remains small, say [3] $\epsilon_{tr} < 10^{-6}$. For critical 1D systems ϵ_{tr} decays as a function of m with a power law, while for 1D system away from criticality it decays exponentially. For a more detailed description of the error introduced by the DMRG truncation in other systems see [3, 4, 5, 6].

DMRG step by step

❶ $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

DMRG step by step

1 $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

2

$$S' = S \cup X_{step}, \mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$$

$$E' = E \cup Y_{step}, \mathcal{V}(E') = \mathcal{V}_R(E) \otimes \mathcal{V}(Y_{step})$$

DMRG step by step

① $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

②

$$S' = S \cup X_{step}, \mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$$

$$E' = E \cup Y_{step}, \mathcal{V}(E') = \mathcal{V}_R(E) \otimes \mathcal{V}(Y_{step})$$

③ Diagonalize $\hat{H}_{S' \cup E'}$ over $\mathcal{V}(S') \otimes \mathcal{V}(E')$ to obtain ψ

DMRG step by step

① $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

②

$$S' = S \cup X_{step}, \mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$$

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③ Diagonalize $\hat{H}_{S' \cup E'}$ over $\mathcal{V}(S') \otimes \mathcal{V}(E')$ to obtain ψ

④ Obtain Density Matrix $\hat{\rho}_S$ from ψ

DMRG step by step

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$$S' = S \cup X_{step}, \mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$$

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③ Diagonalize $\hat{H}_{S' \cup E'}$ over $\mathcal{V}(S') \otimes \mathcal{V}(E')$ to obtain ψ

④ Obtain Density Matrix $\hat{\rho}_S$ from ψ

⑤ Diagonalize Density Matrix $\hat{\rho}_S$ to obtain $W_{\alpha, \alpha'}^S$ (similar for E)

DMRG step by step

① $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

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⑤ Diagonalize Density Matrix $\hat{\rho}_S$ to obtain $W_{\alpha, \alpha'}^S$ (similar for E)

⑥ Truncate W^S if necessary (similar for W^E)

DMRG step by step

① $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

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③ Diagonalize $\hat{H}_{S' \cup E'}$ over $\mathcal{V}(S') \otimes \mathcal{V}(E')$ to obtain ψ

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⑤ Diagonalize Density Matrix $\hat{\rho}_S$ to obtain $W_{\alpha, \alpha'}^S$ (similar for E)

⑥ Truncate W^S if necessary (similar for W^E)

⑦ $H^{S'}$ into $W^{S\dagger} H^{S'} W^S$ (similar for E)

DMRG step by step

① $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

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③ Diagonalize $\hat{H}_{S' \cup E'}$ over $\mathcal{V}(S') \otimes \mathcal{V}(E')$ to obtain ψ

④ Obtain Density Matrix $\hat{\rho}_S$ from ψ

⑤ Diagonalize Density Matrix $\hat{\rho}_S$ to obtain $W_{\alpha, \alpha'}^S$ (similar for E)

⑥ Truncate W^S if necessary (similar for W^E)

⑦ $H^{S'}$ into $W^{S\dagger} H^{S'} W^S$ (similar for E)

⑧ Auxiliary matrices $c_{\gamma}^{S'}$ into $W^{S\dagger} c_{\gamma}^{S'} W^S$ (similar for E)

DMRG step by step

① $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

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$$S' = S \cup X_{step}, \mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$$

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⑦ $H^{S'}$ into $W^{S\dagger} H^{S'} W^S$ (similar for E)

⑧ Auxiliary matrices $c_{\gamma}^{S'}$ into $W^{S\dagger} c_{\gamma}^{S'} W^S$ (similar for E)

⑨ $step++$, $S \leftarrow S'$, $\mathcal{V}_R(S) \leftarrow \mathcal{V}_R(S')$, $H_{S'} \leftarrow H_S$ (similar for E)

DMRG step by step

① $step = 0, \mathcal{V}_R(S) \equiv \mathcal{V}(S), \mathcal{V}_R(E) \equiv \mathcal{V}(E).$

②

$$S' = S \cup X_{step}, \mathcal{V}(S') = \mathcal{V}_R(S) \otimes \mathcal{V}(X_{step})$$

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③ Diagonalize $\hat{H}_{S' \cup E'}$ over $\mathcal{V}(S') \otimes \mathcal{V}(E')$ to obtain ψ

④ Obtain Density Matrix $\hat{\rho}_S$ from ψ

⑤ Diagonalize Density Matrix $\hat{\rho}_S$ to obtain $W_{\alpha, \alpha'}^S$ (similar for E)

⑥ Truncate W^S if necessary (similar for W^E)

⑦ $H^{S'}$ into $W^{S\dagger} H^{S'} W^S$ (similar for E)

⑧ Auxiliary matrices $c_{\gamma}^{S'}$ into $W^{S\dagger} c_{\gamma}^{S'} W^S$ (similar for E)

⑨ $step++$, $S \leftarrow S'$, $\mathcal{V}_R(S) \leftarrow \mathcal{V}_R(S')$, $H_{S'} \leftarrow H_S$ (similar for E)

⑩ Goto 2

See [2](#). Implementation details in [7](#).

“Infinite” DMRG



system



environment

“Infinite” DMRG



system



environment

“Infinite” DMRG



system



environment

“Infinite” DMRG

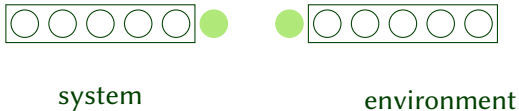


system



environment

“Infinite” DMRG



“Finite” DMRG



“Finite” DMRG



“Finite” DMRG



“Finite” DMRG



“Finite” DMRG



“Finite” DMRG



“Finite” DMRG



How do we shrink a basis?

“Finite” DMRG



How do we shrink a basis? **Answer:** We just use a previously saved one.

“Finite” DMRG



How do we shrink a basis? **Answer:** We just use a previously saved one.

Each vertical dashed line defines a **center of orthogonality**, and defines a Hilbert space basis, referred to as the DMRG basis at that center.

Hamiltonian Construction

The left block linear or Hilbert space has size n_l , and the right block n_r . The left block plus right block space, the so-called superblock linear space, is the *outer* or *Kronecker* product of left and right spaces, and has size $n_l \times n_r$.

$$H' = H_L \otimes I_R + I_L \otimes H_R + \sum_{\gamma=0}^{\gamma < \Gamma} c_L^\gamma \otimes c_R^\gamma,$$

where H'_L is a $n_l \times n_l$ CRS matrix, H'_R a $n_l \times n_r$ CRS matrix, $c_L'^\gamma$ are Γ CRS matrices of rank n_l , and $c_R'^\gamma$ are Γ CRS matrices of rank n_r .

Hamiltonian With Symmetries

The square matrix H' of rank $n_l \times n_r$, when written in an appropriate basis, is block diagonal. Only one of those blocks need to be diagonalized, the needed block is usually known through the use of quantum numbers. A more accurate expression of H' is then

$$H = P_{SE}^{-1} \left(H_L \otimes I_R + I_L \otimes H_R + \sum_{\gamma=0}^{\gamma < \Gamma} c_L^\gamma \otimes c_R^\gamma \right) P_{SE}, \quad (5)$$

where P_{SE} is a permutation of indices in the superblock basis.

For a fully stored approach we need to compute the matrix block for H .

show where this is done in the code

For a fully on-the-fly approach (normally used) we need to compute the vector x given a vector y , where $x = Hy$. *show where this is done in the code*

Is there more structure to the P_{SE} permutation?

States in S each has a quantum number (non-negative integer) q_i , i a state in $\mathcal{V}(S)$,⁴ q_i are ordered in increasing number. States in E each has a quantum number (non-negative integer) q_j , j a state in E , q_j are ordered in increasing number. We construct the space in $SE = \text{space in } S \text{ cartesian product with space in } E$. In other words (i, j) is a state in SE iff i is a state in S , and j a state in E . We assign the quantum number $q_{(i,j)} = q_i + q_j$ to state (i, j) in SE . By construction, you can see that $q_{(i,j)}$ is not (necessarily) ordered in increasing number. We define the permutation P_{SE} that orders $q_{(i,j)}$.

⁴Let me call the Hilbert space $\mathcal{V}(S)$ just S only for the purposes of this answer.

How big is a single diagonal block of H matrix compared full H' matrix

This is model dependent. *If there is truncation what follows will be bounds, not actual sizes.* Let's say we have N sites. For the Hubbard model, blocks are labeled by a pair $(N_{\uparrow}, N_{\downarrow})$ such that $0 \leq N_{\uparrow} \leq N$ (same for N_{\downarrow}). There are then $(N+1)^2$ blocks I think. Each block has size $C(N, N_{\uparrow})C(N, N_{\downarrow})$. The block we are usually interested in is the largest, the one with

$$N_{\uparrow} = N_{\downarrow} = N/2.$$

For the Heisenberg model, blocks are labeled by N_{\uparrow} such that $0 \leq N_{\uparrow} \leq N$. There are then $(N+1)$ blocks I think. Each block has size $C(N, N_{\uparrow})$. The block we are usually interested in is the largest, the one with $N_{\uparrow} = N/2$.

For the t-J model, blocks are labeled by $(N_{\uparrow}, N_{\downarrow})$ such that $0 \leq N_{\uparrow} \leq N$, $0 \leq N_{\downarrow} \leq N$, and $N_{\uparrow} + N_{\downarrow} \leq N$. There are then FIXME blocks. Each block has size $C(N, N_{\uparrow})C(N - N_{\uparrow}, N_{\downarrow})$. The block we are usually interested in is the largest, the one with $N_{\uparrow} = N_{\downarrow} = N/4$. Etc, for other models.

Can you comment on the sizes and sparseness of H_L , H_R , C_L , C_R and whether there are further structure or pattern in these matrices?

I'll be using L and S as synonyms, same for R and E ⁵ Anyway, States in L each has a quantum number (non-negative integer) q_i , $i \in L$, q_i are ordered in increasing number. States in R each has a quantum number (non-negative integer) q_j , $j \in R$, q_j are ordered in increasing number. H_L is a matrix in space L , with the property that $H_L(i1, i2) = 0$ if $q_{i1} \neq q_{i2}$. That is, H_L is said to respect symmetry. H_R is a matrix in space R , with the property that $H_R(j1, j2) = 0$ if $q_{j1} \neq q_{j2}$. That is, H_R also respects symmetry. C_L and C_R are model dependent, and in general do not respect symmetry. Different C s might have different symmetries also.

⁵But please don't confuse sites with states in spaces constructed in or out of a block of sites. I don't think I have to mention blocks of sites at all, so all these letters can be used to refer to the vector spaces.

Can you comment on...? (continued)

For the Hubbard model, C_s are destruction operators. Therefore, $C_L(i1, i2) = 0$ unless $q_{i1} \neq f_C(q_{i2})$ where $f_C : \{0, 1, \dots\} \rightarrow \{0, 1, \dots\}$ is the function associated with the symmetry of C .

For the Heisenberg model, there are two kinds of C_s : spin down-flip (let's call them $C1$) and S_z operators (let's call them $C2$). $C1_L(i1, i2) = 0$ if $q_{i1} \neq f_{C1}(q_{i2})$ where $f_{C1} : \{0, 1, \dots\} \rightarrow \{0, 1, \dots\}$ is the function associated with the symmetry of $C1$. $C2_L(i1, i2) = 0$ if $q_{i1} \neq q_{i2}$, that is, $C2$ respects symmetry.

For the Heisenberg model, there are 3 kinds of C_s , let's call them $C1$ and $C2$ and $C3$. Therefore, $CX_L(i1, i2) = 0$ if $q_{i1} \neq f_{CX}(q_{i2})$ where $f_{CX} : \{0, 1, \dots\} \rightarrow \{0, 1, \dots\}$ is the function associated with the symmetry of CX , for $X=1,2,3$. Also, f_{C3} is the identity, because $C3$ is the density operator, which (like the Hamiltonian) respects quantum numbers. I guess the model dependence of symmetries can be encoded in the f_C functions.



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