Digest DMRG algorithm in the age of MPS

Empter

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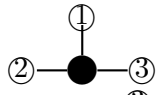
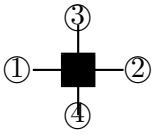
1 Indices definition in Mathematica code

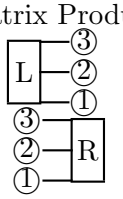
Single Matrix Product State (MPS):



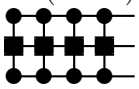


Single Matrix Product Operator (MPO):

L matrix:

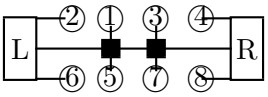


in details



R matrix:

Effective Hamiltonian H_{eff}:



2 DMRG in MPS[2]

1. Build up MPO from the Hamiltonian $H = W_1 W_2 \cdots W_N$, $W_1 = W^{\sigma_1,\sigma_1'}_{1,b_1}$ $W_l = W^{\sigma_l,\sigma_l'}_{b_{l-1},b_l}$ $W_N = W^{\sigma_L,\sigma_l'}_{b_{L-1},1}$, here 1 is a dummy index. Constructing MPO for short-range interacting H is quite easy, see Ref [2] 6.1 for example. For more complex systems, one can find general construction algorithm in Ref.https://dx.doi.org/10.1103/PhysRevB.91.165112 Sec.II, exponential decaying long-range interactions can be found in Ref.[3].

2. Initial guess, a result from iDMRG would be great, but one can also use a random renormalized mps. $|\psi_{init}\rangle = \sum_\sigma \sum_a M^{\sigma_1}_{1,a_1} M^{\sigma_2}_{a_1,a_2} \cdots M^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} M^{\sigma_L}_{a_{L-1},1} |\sigma\rangle$, mix-canonical is OK. Note that the MPS state can be split into three parts (left-canonical part A, Center and right-canonical part B):

$$|\psi\rangle = \sum_{\sigma_1 \cdots \sigma_L} (M^{\sigma_1} \cdots M^{\sigma_{l-1}})_{1,a_{l-1}} M^{\sigma_l}_{a_{l-1},a_l} (M^{\sigma_{l+1}} \cdots M^{\sigma_L})_{a_l,1} |\sigma_1 \cdots \sigma_L\rangle ,$$

or more compactly

$$|\psi\rangle = \sum_{a_{l-1},\sigma_l,a_l} M^{\sigma_l}_{a_{l-1},a_l} |a_{l-1}\rangle_A |\sigma_l\rangle |a_l\rangle_B . \tag{1}$$

Bring the intial state into the mix-canonical form with canonical center at site 1.

3. Build up R matrix recursively (from L-1 to 1):

$$R_{L-1} = \sum_{\sigma_L, \sigma'_L} M^{*\sigma_L}_{a_{L-1},1} W^{\sigma_L,\sigma'_L}_{b_{L-1},1} M^{\sigma'_L}_{a'_{L-1},1}$$

$$R_l = R^{a_l,a'_l}_{b_l} = \sum_{a_i,b_i,a'_i;i>l} \left(\sum_{\sigma_{l+1},\sigma'_{l+1}} M^{*\sigma_{l+1}}_{a_l,a_{l+1}} W^{\sigma_{l+1},\sigma'_{l+1}}_{b_l,b_{l+1}} M^{\sigma'_{l+1}}_{a'_l,a'_{l+1}} \right) R_{l+1} \cdots R_{L-1}$$

notice that indices $a'_{l+1}, b_{l+1}, a_{l+1}$ will be contracted with R_{l+1} leaving only three indices a'_l, b_l, a_l referring ① ② ③ respectively.

4. Right sweep, l run from 1 to L-1: Ground state research, to find the MPS $|\psi\rangle$ that minimizes $\langle\psi|\hat{H}|\psi\rangle / \langle\psi|\psi\rangle$. Introduce a Lagrangian multiplier λ, and extremize $\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle$, then we can get energy λ and state $|\psi\rangle$.

   In the mps representation, we can calculate the overlap in site l by using Eq. 1

$$\langle\psi|\psi\rangle = \sum_{\sigma_l} \sum_{a_{l-1}a_l} \sum_{a'_{l-1}a'_l} \Psi^A_{a_{l-1},a'_{l-1}} M^{*\sigma_l}_{a_{l-1},a_l} M^{\sigma_l}_{a'_{l-1},a'_l} \Psi^B_{a_l,a'_l}, \tag{2}$$

   here

$$\Psi^A_{a_{l-1},a'_{l-1}} = \sum_{\sigma_1 \cdots \sigma_{l-1}} (M^{\dagger\sigma_{l-1}} \cdots M^{\dagger\sigma_1} M^{\sigma_1} \cdots M^{\sigma_{l-1}})_{a_{l-1},a'_{l-1}}$$

$$\Psi^B_{a_l,a'_l} = \sum_{\sigma_{l+1} \cdots \sigma_L} (M^{\sigma_{l+1}} \cdots M^{\sigma_L} M^{\dagger\sigma_L} \cdots M^{\dagger\sigma_{l+1}})_{a'_l,a_l}.$$

   If we keep left-normalized from 1 to $l-1$ ($\sum A^\dagger A = I$) and right-normalized from $l+1$ to L ($\sum BB^\dagger = I$), it will be more simple, namely

$$\Psi^A_{a_{l-1},a'_{l-1}} = \delta_{a_{l-1},a'_{l-1}}, \ \Psi^B_{a_l,a'_l} = \delta_{a_l,a'_l}.$$

   Consider $\langle\psi|\hat{H}|\psi\rangle$ in MPO language

$$\langle\psi|\hat{H}|\psi\rangle = \sum_{\sigma_l,\sigma'_l} \sum_{a'_{l-1},a'_l} \sum_{a_{l-1},a_l} \sum_{b_{l-1},b_l} L^{a_{l-1},a'_{l-1}}_{b_{l-1}} W^{\sigma_l,\sigma'_l}_{b_{l-1},b_l} R^{a_l,a'_l}_{b_l} M^{*\sigma_l}_{a_{l-1},a_l} M^{\sigma'_l}_{a'_{l-1},a'_l},$$

   if we take equation 2 with respect to $M^{*\sigma_l}_{a_{l-1},a_l}$, one have

$$\sum_{\sigma'_l} \sum_{a'_{l-1},a'_l} \sum_{b_{l-1},b_l} L^{a_{l-1},a'_{l-1}}_{b_{l-1}} W^{\sigma_l,\sigma'_l}_{b_{l-1},b_l} R^{a_l,a'_l}_{b_l} M^{\sigma'_l}_{a'_{l-1},a'_l} - \lambda \sum_{a'_{l-1}a'_l} \Psi^A_{a_{l-1},a'_{l-1}} \Psi^B_{a_l,a'_l} M^{\sigma_l}_{a'_{l-1},a'_l} = 0,$$

   to write it in matrix equation form, we rewrite $H_{eff} = H_{(\sigma_l a_{l-1} a_l),(\sigma'_l a'_{l-1} a'_l)} = \sum_{b_{l-1},b_l} L^{a_{l-1},a'_{l-1}}_{b_{l-1}} W^{\sigma_l,\sigma'_l}_{b_{l-1},b_l} R^{a_l,a'_l}_{b_l}$, $N_{(\sigma_l a_{l-1} a_l),(\sigma'_l a'_{l-1} a'_l)} = \Psi^A_{a_{l-1},a'_{l-1}} \Psi^B_{a_l,a'_l} \delta_{\sigma_l,\sigma'_l}$ and a vector $\nu_{\sigma_l a_{l-1} a_l} = M^{\sigma_l}_{a_{l-1},a_l}$, a generalized eigenvalue equation then reached

$$H\nu - \lambda N\nu = 0. \tag{3}$$

$$H_{eff} = \sum_{b_{l-1}b_l} L^{a_{l-1},a'_{l-1}}_{b_{l-1}} W^{\sigma_l\sigma'_l}_{b_{l-1},b_l} R^{a_l,a'_l}_{b_l}$$

If $l = 1$, there is no L matrix so $H_{eff} = \sum_{b_l} W^{\sigma_1\sigma_1'}_{1,b_1} R^{a_1,a_1'}_{b_1}$. If the MPS is always kept in the mix-canonical form, then one can just ignore the N matrix because it only convert prime indices into non-prime ones.

Solver equation 3 to optimize the wavefunction in site l, use old M_l as initial guess for the Davison eigen solver, reshape the result ν to M_l form. In order to keep all M in normalized form, $SVD(M_{a_l,(\sigma_l,a_{l+1})}) = USV^\dagger$, $M_l = U, M_{l+1} = SV^\dagger M_{l+1}$. Note that the eigen solver does not need to give a result as accurate as possible because DMRG algorithm itself will drive the MPS to the ground state.

5. Generate/Update L matrix at site l from the new calculated M_l:

$$L_1 = \sum_{\sigma_1,\sigma_1'} M^{*\sigma_1}_{1,a_1} W^{\sigma_1,\sigma_1'}_{1,b_1} M^{\sigma_1'}_{1,a_1'},$$

$$L_l = L^{a_l,a_l'}_{b_l} = \sum_{a_i,b_i,a_i';i>l} \left(L_1 \cdots L_{l-1} \sum_{\sigma_l\sigma_l'} M^{*\sigma_l}_{a_{l-1},a_l} W^{\sigma_l,\sigma_l'}_{b_{l-1},b_l} M^{\sigma_l'}_{a_{l-1}',a_l'} \right) \tag{4}$$

6. Left sweep l from L to 2: Solver equation 3 in each step, right-normalize M_l, $SVD(M_{(\sigma_l,a_{l-1}),a_l}) = USV^\dagger$, $M_l = V^\dagger, M_{l-1} = USM_{l-1}$. Update R matrix.

7. Return to step 4 unless reach a convergence energy.

3 iDMRG[1]

Infinite algorithm of DMRG represented by matrix product state, serve as the initial input for finite MPS algorithm.

1. Build initial states for $l = 0$ and $l = 1$:

   $l = 0$: $\sum A^{\sigma_0}\Lambda^0 B^{\sigma_0'} |\sigma_0\sigma_0'\rangle$, this can be calculated directly from the SVD of the ground state. Reshape the ground state $\Psi^{\sigma_0\sigma_0'} = \Psi_{\sigma_0,\sigma_0'} \xrightarrow{SVD} U_{(\sigma_0,1),a_1} S_{a_1,a_1} V^\dagger_{a_1,(1,\sigma_0')} \xrightarrow{Reshape} A^{\sigma_0}_{1,a_1}\Lambda^0_{a_1,a_1} B^{\sigma_0'}_{a_1,1}$.

   $l = 1$: $\sum A^{\sigma_0}A^{\sigma_1}\Lambda^1 B^{\sigma_1'}B^{\sigma_0'} |\sigma_0\sigma_1\sigma_1'\sigma_0'\rangle$, construction L and R matrix from $l = 0$, calculate effective Hamiltonian

   $H_{eff} =$  $\xrightarrow{Reshape} H_{a_1\sigma_1\sigma_1'a_1,a_1\sigma_1\sigma_1'a_1} \xrightarrow{Eig} \Psi^{a_1\sigma_1\sigma_1'a_1} = \Psi_{(\sigma_1,a_1),(\sigma_1',a_1)} \xrightarrow{SVD} U_{(\sigma_1,a_1),a_2} S_{a_2,a_2} V^\dagger_{a_2,(a_1,\sigma_1')}$
   $\xrightarrow{Reshape} A^{\sigma_1}_{a_1,a_2}\Lambda^1_{a_2,a_2} B^{\sigma_1'}_{a_2,a_1}$.

2. At stage n $|\psi_n\rangle$ reads $\cdots A^{\sigma_n}\Lambda^n B^{\sigma_n'} \cdots$, right rotate $|\psi_n\rangle$, e.g., $A^{\sigma_n}_{a_{n-1},a_n}\Lambda^n_{a_n,a_n} = M_{a_{n-1},(\sigma_n,a_n)} \xrightarrow{SVD}$ $USV^\dagger = \Lambda^L_n V^\dagger = \Lambda^L_n B^{\sigma_{n+1}'}$, the state becomes $\cdots A^{\sigma_{n-1}}\Lambda^L_n B^{\sigma_{n+1}'} B^{\sigma_n'} \cdots$.

3. Also left rotate $|\psi_n\rangle$, $\Lambda^n_{a_n,a_n} B^{\sigma_n'}_{a_n,a_{n-1}} = M_{(\sigma_n',a_n),a_{n-1}} \xrightarrow{SVD} USV^\dagger = U\Lambda^R_n = A^{\sigma_{n+1}}\Lambda^L_n$, the state becomes $\cdots A^{\sigma_n}A^{\sigma_{n+1}}\Lambda^R_n B^{\sigma_{n-1}'} \cdots$.

4. The trial wave-function for next step is $|\psi^{trial}_{n+1}\rangle = \cdots A^{\sigma_{n+1}}\Lambda^R_n\Lambda^{-1}_{n-1}\Lambda^L_n B^{\sigma_{n+1}'} \cdots$.

5. Calculate the effective Hamiltonian for step $n + 1$, use $|\psi^{trial}_{n+1}\rangle$ as initial guess for an eigen-solver, update $A^{\sigma_{n+1}}\Lambda^{n+1}B^{\sigma_{n+1}'}$ (see step 1, $l = 1$, in that case the dimension is not large and do not need an initial ground state guess).

6. Truncation happened if dimension Λ^{n+1} is larger than D preset.

7. If Λ^{n+1} is sufficiently close to Λ^n then stop else return to step 2.

References

[1] I. P. McCulloch, Infinite size density matrix renormalization group, revisited. (2008). http://arxiv.org/abs/0804.2509

[2] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states. Ann. Phys. (N. Y). 326, 96–192 (2011).

[3] Crosswhite, et al., Applying matrix product operators to model systems with long-range interactions. Physical Review B 78, 035116 (2008).