DMRG Steps

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1- A warm up for future steps in DMRG:

Consider a one dimensional chain of fermions described by the below Hamiltonian. This Hamiltonian commutes with the total number operator, $[H, N] = 0$. Use this property to block diagonalize the Hamiltonian. Then diagonalize each block in Hamiltonian (by exact diagonalization technique) and find the energy spectrum. Compare the results and run time with the original method when we diagonalize the entire non-block diagonal Hamiltonian. (assume t = 1 and $\mu = 0.1$)

$$H = -t \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) - \mu \sum_i (-1)^i c_i^\dagger c_i$$

$$N = \sum_i c_i^\dagger c_i$$

Hint: sort the values in the number operator, use the sorted indices to find a permutation matrix (a unitary matrix) then use this permutation to transform the Hamiltonian to the desired basis.

*Use the same approach to diagonalize the Hamiltonian for one dimensional Heisenberg model. ($[H, L_z] = 0$).

2- Finite DMRG for Heisenberg Model.

Instruction: Run the infinite-size algorithm until the desired system size is reached. During this process, store all the left and right blocks, with their corresponding operators and basis transformations (this step is called “warmup”). Once the desired system size is reached you should start performing “DMRG sweeps”, from right-to-left, and left-to-right to improve accuracy.

Description of a Left to Right sweep:

- Add a site to the left block using the same idea of the infinite-size DMRG. Since the total size of the system needs to be kept fixed, we need to “shrink” the right block. This is done by using the smaller right block from the infinite-size step, or from the previous right-to-left sweep.
- Diagonalize the superblock Hamiltonian of the two blocks combined, same as for the infinite DMRG.
- Calculate the reduced density matrix of the left block.
- Diagonalize the density matrix to obtain the full spectrum and eigenvectors.
- Truncate the basis by keeping only the m eigenvectors with the largest eigenvalues.
- Rotate the Hamiltonian and the operators of the left block involved in the interactions between blocks to the new basis.
- Iterate until reaching the far right end of the system, with a right block containing a single site. This completes the left-to-right sweep.

3- Infinite and finite DMRG for Hubbard Model (even sites spin up / odd sites spin down or vice versa)

Hint: Consider annihilation operator (c) as σ_- and creation operator ($c^\dagger$) as σ_+ then assume that each site is a unit cell containing two electrons:

4- Imposing symmetry in DMRG for Hubbard model, considering that [H,N] = 0, where $N = N_{up} + \lambda * N_{down}$.

Hint: Now we want to preserve system's symmetry, meaning that the superblock Hamiltonian should remain block-diagonal in every iteration and the number of up and down spins is conserved in the ground state wave function. (Hamiltonian Commutes with Number operator). For this purpose, we should calculate number operator defined as $N = N_{up} + \lambda * N_{down}$ for left and right block, then we sort its diagonal values. After finding the sorted indices we can find the transformation which permutes all other operators with respect to these indices. We build Hamiltonian with these permuted operators and it will be block-diagonal. Diagonalizing this Hamiltonian with a proper initial vector for Lanczos algorithm will keep the ground state wave function in the desired basis so the reduced density matrix will also be block diagonal and the system's symmetry in conserved in next iteration. This approach is much faster and the results are also more accurate.

5 - Implement a more optimized Lanczos diagonalization function and calculate all the correlation functions in Hubbard model (in the left block, right block, and between the left and right block). [To get familiar with the Lanczos diagonalization technique, study the "Obtaining the ground-state: Lanczos diagonalization" in the DMRG lecture notes.]

Instruction: In the traditional implementation, the superblock Hamiltonian is needed. But here we don't have the superblock Hamiltonian matrix, instead we have the left & right block operators that by calculating their Kronecker product we can get the superblock Hamiltonian matrix. We don't want to use Kronecker product because it's not efficient, instead we reshape v_prev (initial vector for Lanczos) into Dim_L & Dim_R (Dimension of left and right operators respectively) then take the i^{th} component of O_L and O_R lists (left block and right block operators respectively), and multiply O_L{i} from the left and transpose of O_R{i} from the right and then take sum over i's. This yields the reshape of v_next (as a matrix) by an additional reshape we can change its dimension to be a vector. You may need to use the Gram-Schmidt method to re-orthogonalize vectors. Finally, construct the tri-diagonal matrix (T) and Compute the eigenvalues and eigen-vectors of Hamiltonian using those of T.

6- Use the wavefunction transformation to obtain the initial Lanczos vector from the ground state wavefunction in the previous iteration. (for finite DMRG)

Instruction: For the left to right sweep (as an example): In the first iteration use the last ground state wavefunction form the infinite DMRG, but in the next iterations use the wavefunction from the previous iteration. Reshape it to $(2\chi, 2\chi)$. Call it ψ_{last}.

- Load the right block truncation matrices from the infinite algorithm. (T_R)
- Use ψ_{last} to calculate the reduced density matrix for the left block and find the left block truncation matrix. (T_L)
- Calculate $T_L^{\dagger} * \psi_{\text{last}}$(Undo the truncation), Call it ψ_{left}.
- Reshape ψ_{left} to $(\chi_L, \chi_R, 2)$ then permute it by the following order (0,2,1). (This is because we want to move the spin from right block to left block). Note: the mentioned permutation order follows the python syntax.
- Reshape ψ_{left} to $(2\chi_L, \chi_R)$ where χ_L and χ_R are bound dimension for left and right block respectively.
- Calculate $\psi_{\text{left}} * T_R^{\dagger}$, Call it ψ_{right}.
- Finally reshape it to be a vector, call it ψ_{init}.

Use this vector as the initial guess in Lanczos diagonalization algorithm, after finding the ground state wavefunction (ψ_g), calculate fidelity which is defined as $\left|\langle\psi_{\text{init}}|\psi_g\rangle\right|^2$. It should be almost zero, in other words, $1 - \left|\langle\psi_{\text{init}}|\psi_g\rangle\right|^2$should be almost 1. For the right to left sweep, a similar approach can be taken.

7- Follow instructions in the previous step, but this time preserve the system's symmetry (as indicated in part 4). This also can be done for Heisenberg model.

8- Wavefunction transformation for infinite DMRG.

Instruction:

- After the second iteration in infinite DMRG, save wavefunctions from the last two and the last iteration, call them $\psi_{n-1.n-1}$ and $\psi_{n,n}$,repectively. Reshape them to $(\text{Dim}_L, \text{Dim}_R)$, call these matrices as $\Lambda_{n-1.n-1}$ and $\Lambda_{n,n}$. In fact, if we are in the iteration with n+1 spins in left block and n+1 spins in right block, then $\psi_{n-1.n-1}$is the wavefunction for the iteration with n-1 spins in left block and n-1 spins in right block, and $\psi_{n,n}$ is the wavefunction for the iteration with n spins in left block and n spins in right block.
- Choose a very small value λ (say $\lambda = 10^{-12}$) and add an identity matrix of λ values to $\Lambda_{n-1,n-1}$. (That's because we need to calculate $\Lambda^{-1}_{n-1,n-1}$ and this noise is required to avoid any none value).
- Use the reduced density matrix of $\psi_{n,n}$ to calculate the left block truncation matrix.
- Use the reduced density matrix of $\psi_{n-1.n-1}$ to calculate the left block truncation matrix.
- Move one spin from right block to left block, meaning $\Lambda_{n,n} \rightarrow \Lambda_{n+1,n-1}$. Follow the instructions from part 6, but ignore the last step.

- We have now obtained the left side basis in SVD, use a similar approach to obtain the right side basis. (Move one spin from left block to right block $\Lambda_{n,n} \rightarrow \Lambda_{n-1.n+1}$).

- Calculate $\Lambda_{n+1,n+1} = \Lambda_{n+1,n-1} * \Lambda^{-1}_{n-1,n-1} * \Lambda_{n-1.n+1}$.

- Finally reshape it to be a vector, call it ψ_{init}

Use this vector as the initial guess in Lanczos diagonalization algorithm, after finding the ground state wavefunction, calculate fidelity to check the result.

9- Impose symmetry in the previous part.