

Single-site DMRG for the ground and first excited states

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In this tutorial, we will obtain the ground state and the first excited state of spin chain systems, by using the **density-matrix renormalization group (DMRG)**. Though this is one of the simplest applications of the DMRG, it still needs a bit of machinery. There is a new directory `DMRG` for the functions for the DMRG methods. We also introduce new functions:

- `DMRG/eigs_1site.m`: At each iteration of the single-site DMRG, one needs to update the ket tensor (acting on one site) to minimize the expectation value of the Hamiltonian. Or, if a reference MPS is given to introduce the orthogonality constraint to the variational MPS, the orthogonality should hold at each iteration as well. This function does that job by using the Lanczos method.
- `Tensor/svdTr.m`: This function performs the singular value decomposition (SVD) of a tensor. It supports the bond space truncation, keeping the largest singular values and the corresponding singular vectors. However, the single-site DMRG does not truncate the bond space via SVD; the truncation feature will be used for later topics.

Please review these newly added functions, since they will be used for the following exercises.

Exercise (a): Complete the ground state search feature of `DMRG_1site_Ex.m`

There is a function `DMRG_1site_Ex.m` which is placed in the same subdirectory together with this tutorial material. This function partially implements the single-site update for searching the ground state and the first excited state. **Complete the parts which are enclosed by the comments `TODO - Exercise 1`**, for the ground state search. Ignore the other parts enclosed by `TODO - Exercise 2` for now, since they are for Exercise 2 about the first excited state search. As long as these parts for Exercise 2 are complete, the function will run for the demonstration below, without trouble.

XY spin chain: Ground state search

Once you finish Exercise 1, the function `DMRG_1site_Ex.m` is ready to obtain the ground state of spin chain systems. For demonstration, we consider the XY spin chain, where spin-1/2's lie along a one-dimensional lattice of length N and the spins have nearest-neighbor interaction. The name "XY" comes from that only the x and y components of the neighboring spins are coupled:

$$\begin{aligned}\hat{H}_{XY} &= - \sum_{\ell=1}^{N-1} (\hat{S}_{\ell}^x \hat{S}_{\ell+1}^x + \hat{S}_{\ell}^y \hat{S}_{\ell+1}^y) \\ &= - \frac{1}{2} \sum_{\ell=1}^{N-1} (\hat{S}_{\ell}^{+} \hat{S}_{\ell+1}^{-} + \hat{S}_{\ell}^{-} \hat{S}_{\ell+1}^{+}).\end{aligned}$$

By using the Jordan-Wigner transformation, the XY model is mapped onto free spinless fermions in one dimension. So it is exactly solvable, in the sense that the ground-state energy for even N has explicit expression,

$$E_0 = \frac{1}{2} - \frac{1}{2 \sin \frac{\pi}{2(N+1)}}.$$

(In previous tutorials on the iterative diagonalization of non-interacting tight-binding chain, we have obtained the ground-state energy in a semi-analytic way.) The correlation function of nearest-neighbor spins with respect to the ground state has also,

$$\langle \Psi_0 | \hat{S}_\ell^+ \hat{S}_{\ell+1}^- | \Psi_0 \rangle = \langle \Psi_0 | \hat{S}_\ell^- \hat{S}_{\ell+1}^+ | \Psi_0 \rangle = -\frac{1}{2(N+1)} \left[\frac{(-1)^\ell}{\sin \frac{(2\ell+1)\pi}{2(N+1)}} - \frac{1}{\sin \frac{\pi}{2(N+1)}} \right],$$

where $|\Psi_0\rangle$ means the ground state of the XY model. Note that the above equations only apply for even N . For odd N , there are degenerate ground states while the ground state is unique for even N .

Let's focus on even N for this tutorial. The goal is to verify the implementation of the single-site DMRG, by comparing with the exact result. First, set the parameters for the Hamiltonian and the DMRG routine.

```
clear

% system parameter
J = -1; % coupling strength
N = 40; % number of sites in a chain

% DMRG parameter
Nkeep = 30; % bond dimension
Nsweep = 4; % number of pairs of left+right sweeps

% Local operators
[S,I] = getLocalSpace('Spin',1/2);
```

In the lecture, the MPO representation of the Heisenberg interaction is given. Here the MPO has a simpler form, which can be obtained by removing $\hat{S}_\ell^z$ terms from the Heisenberg case. Note that each local part of MPO has four legs which are ordered as left-bottom-right-top. The bottom (top) leg is to be contracted with the third leg of bra (ket) tensor.

```
% % MPO formulation of Hamiltonian
% Hamiltonian tensor for each chain site
Hloc = cell(4,4);
Hloc(:) = {zeros(size(I))};
Hloc{1,1} = I;
Hloc{2,1} = squeeze(S(:,1,:));
Hloc{3,1} = squeeze(S(:,2,:));
Hloc{4,2} = J*(Hloc{2,1}');
Hloc{4,3} = J*(Hloc{3,1}');
Hloc{end,end} = I;
Hloc = cell2mat(reshape(Hloc,[1 1 size(Hloc,1) size(Hloc,2)]));
Hloc = permute(Hloc,[3 1 4 2]); % leg order: left-bottom-right-top

% full chain
Hs = cell(1,N);
```

```
Hs(:) = {Hloc};
Hs{1} = Hs{1}(end,:,:,); % choose the last components of the left leg
Hs{end} = Hs{end}(:,:,1,:); % choose the first components of the right leg
```

Run the single-site DMRG.

```
[M_GS,E_GS,Eiter] = DMRG_1site_Ex (Hs,Nkeep,Nsweep);
```

```
Single-site DMRG: search for the ground state
# of sites = 40, Nkeep = 30, # of sweeps = 4 x 2
21-05-14 16:53:45 | Initialize with iterative diagonalization. Energy = -12.31553
21-05-14 16:53:45 | Sweep #1/8 (right -> left) : Energy = -12.55386
21-05-14 16:53:45 | Sweep #2/8 (left -> right) : Energy = -12.5539
21-05-14 16:53:45 | Sweep #3/8 (right -> left) : Energy = -12.5539
21-05-14 16:53:45 | Sweep #4/8 (left -> right) : Energy = -12.5539
21-05-14 16:53:45 | Sweep #5/8 (right -> left) : Energy = -12.5539
21-05-14 16:53:46 | Sweep #6/8 (left -> right) : Energy = -12.5539
21-05-14 16:53:46 | Sweep #7/8 (right -> left) : Energy = -12.5539
21-05-14 16:53:46 | Sweep #8/8 (left -> right) : Energy = -12.5539
Elapsed time: 1.198s, CPU time: 12.01s, Avg # of cores: 10.02
```

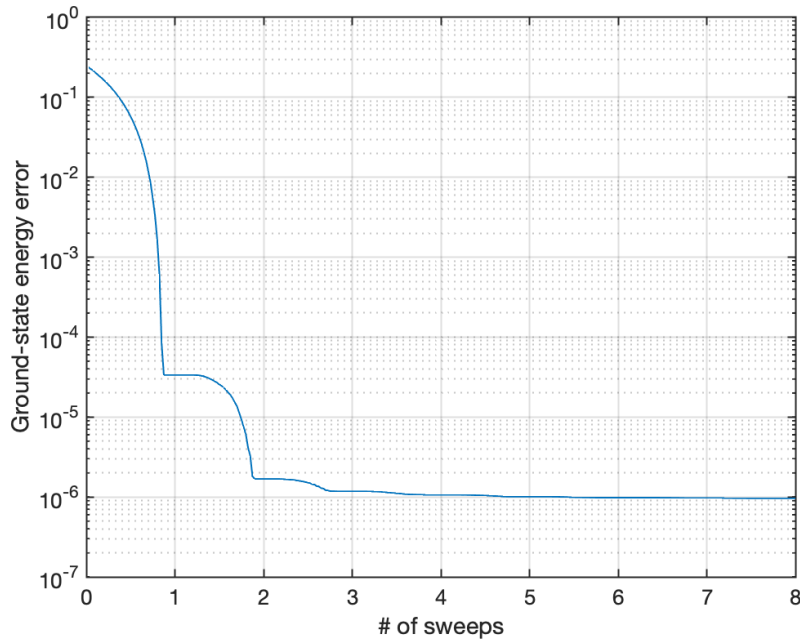
Compare the ground-state energy with the exact value.

```
E0_exact = 0.5 - (1/2/sin(pi/2/(N+1))); % exact value
disptime(['Exact GS energy = ',sprintf('%.5g',E0_exact),', DMRG = ', ...
        sprintf('%.5g',E_GS),', error = ',sprintf('%.5g',E_GS-E0_exact)]);
```

```
21-05-14 16:53:46 | Exact GS energy = -12.554, DMRG = -12.554, error = 9.6234e-07
```

Plot how the energy expectation value converge to the exact value as the iteration proceeds.

```
figure;
semilogy((1:numel(Eiter))/N,Eiter(:)-E0_exact,'LineWidth',1);
set(gca,'FontSize',13,'LineWidth',1);
xlim([0 2*Nsweep]);
grid on;
xlabel('# of sweeps');
ylabel('Ground-state energy error');
```



The error is $O(10^{-6})$. The error can be further decreased by increasing bond dimension N_{keep} . Indeed, the accuracy is bound by finite bond dimension, since the system is gapless. Consider a bipartition of the chain, into left and right halves. The entanglement between two parts in the ground state increases with the system size N logarithmically, for the gapless systems. Thus, to achieve the same accuracy, we should use larger bond dimension that increases as the power law of N .

On the other hand, for the gapped systems, high accuracy can be achieved with small bond dimensions. For example, the AKLT model needs only the bond dimension 2.

Spin-spin correlation function

Compute the spin-spin correlation function $\langle \hat{S}_{\ell}^{+} \hat{S}_{\ell+1}^{-} \rangle$, i.e., the expectation value of the product of spin-raising and -lowering operators at nearest-neighbor sites. Be aware of that the result MPS M is in left-canonical form, as mentioned in the documentation of `DMRG_1site_Ex.m`.

```
% compute correlation function for the nearest-neighbour spins
SS = zeros(1,N-1);
for itN = (2:N)
    T = updateLeft([],[],M_GS{itN-1},S(:,1,:),3,M_GS{itN-1});
    T = updateLeft(T,3,M_GS{itN},S(:,2,:),3,M_GS{itN});

    for itN2 = ((itN+1):N)
        T = updateLeft(T,2,M_GS{itN2},[],[],M_GS{itN2});
    end

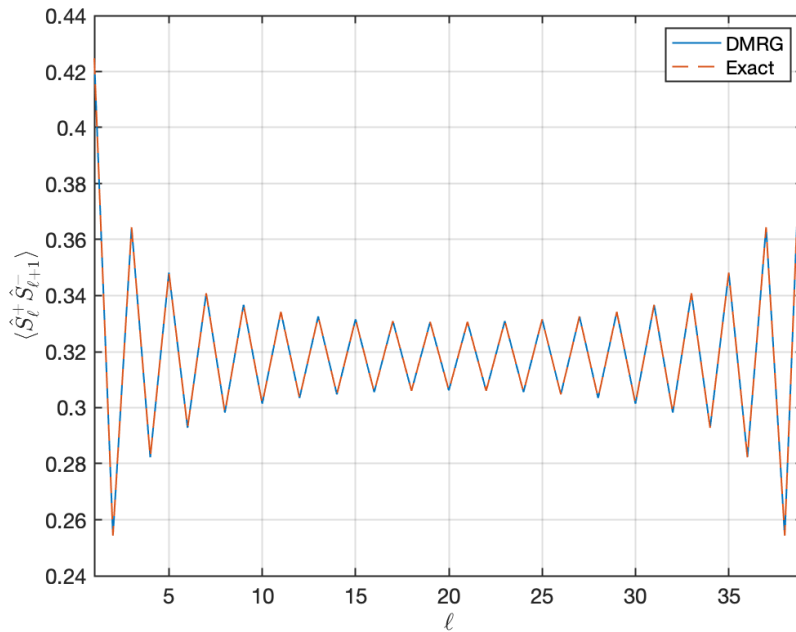
    SS(itN-1) = T;
end
SS = SS*2; % *2 due to 1/sqrt(2) in S(:,1,:) and S(:,2,)
```

```

% exact relation
SS_exact = (((-1).^(1:N-1))./sin((2*(1:N-1)+1)*pi/2/(N+1)) - ...
            1./sin(pi/2/(N+1)))/(-2*(N+1));

figure;
plot((1:N-1),SS,'-',(1:N-1),SS_exact,'--','LineWidth',1);
legend({'DMRG','Exact'});
set(gca,'FontSize',13,'LineWidth',1);
xlabel('$\ell$', 'Interpreter','latex');
ylabel('$\langle \hat{S}_\ell^+ \hat{S}_{\ell+1}^- \rangle$', ...
        'Interpreter','latex');
xlim([1 N-1]);
grid on;

```



The numerical result and the exact result coincide nicely!

Exercise (b): First excited state search

Further complete `DMRG_1site_Ex.m`, for the parts enclosed by the comments `TODO` - Exercise 2.

These parts consider an optional input `Morth` to the function `DMRG_1site_Ex`. When given, the function will search for the MPS within the subspace orthogonal to `Morth`, while minimizing the energy expectation value. For this, (i) we need to consider the overlap between `Morth` and `M` (variational MPS considered within the routine). And (ii) we optimize a local ket tensor which minimizes energy within the subspace orthogonal to the tensor obtained by computing the overlap. It can be done by using the function `eigs_1site` with an optional input.

After completing the function (finally!), obtain the first excited state $|\Psi_1\rangle$ of the XY model. Its energy is analytically given by

$$E_1 = E_0 + \sin \frac{\pi}{2(N+1)}.$$

Compare with your DMRG result. And compute the spin-spin correlation function $\langle \Psi_1 | \hat{S}_\ell^+ \hat{S}_{\ell+1}^- | \Psi_1 \rangle$ for the first excited state, and compare it with the correlation function for the ground state.

Exercise (c): Majumdar-Ghosh model

Find **the ground state and the spin-spin correlation function** $\langle \hat{S}_\ell^+ \hat{S}_{\ell+1}^- \rangle$ **for the Majumdar-Ghosh model.** The Majumdar-Ghosh model is a spin-1/2 chain with nearest-neighbor and next-nearest-neighbor interactions,

$$H = \sum_{\ell=1}^{N-1} \vec{\hat{S}}_\ell \cdot \vec{\hat{S}}_{\ell+1} + \frac{1}{2} \sum_{\ell=1}^{N-2} \vec{\hat{S}}_\ell \cdot \vec{\hat{S}}_{\ell+2}.$$

It has the exact ground state, with energy $E_0 = -3N/8$ and the bond dimension $N_{\text{keep}} = 2$. Compare your DMRG result with these exact values.