

# [Tutorial T09.2] DMRG: subspace expansion and error estimation

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## Exercise (a): Complete the subspace expansion feature of `DMRG_3S_Ex.m`

There is a function `DMRG_3S_Ex.m` which is placed in the same subdirectory together with this tutorial material. This function partially implements subspace expansion in the single-site update for searching the ground state. The subspace expansion prevents the single-site DMRG algorithm to get stuck in local minima and in principle allows to dynamically adjust the bond-dimension, similar to the 2-site DMRG. Nevertheless, it remains a strictly single-site (3S) update, which has performance advantages in case the local dimension  $d$  becomes large.

**Complete the parts which are enclosed by the comments `TODO - Exercise 1`.**

## Majumdar-Ghosh model

We have already encountered the Majumdar-Ghosh model in T07. The Majumdar-Ghosh model is a spin-1/2 chain with nearest-neighbor and next-nearest-neighbor interactions,

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

It has the exact ground state, with energy  $E_0 = -3N/8$  and the bond dimension  $N_{\text{keep}} = 2$ . In the following, we will compare the ground-state search of the single-site DMRG with and without subspace expansion using  $N_{\text{keep}} = 10$  and a series of special initial states for which the single-site DMRG algorithm is prone to getting stuck. Note that the option 'noex' switches off the subspace expansion.

```
clear

% system parameter
J1 = 1; % nearest-neighbour coupling strength
J2 = 1/2; % next-nearest-neighbour coupling strength
N = 40; % number of sites in a chain

% DMRG parameter
Nkeep = 10; % bond dimension
Nsweep = 5; % number of pairs of left+right sweeps

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

% Hamiltonian tensor for each chain site
Hloc = cell(8,8);
Hloc(:) = {zeros(size(I))};
Hloc{1,1} = I;
Hloc{2,1} = squeeze(S(:,1,:));
Hloc{3,1} = squeeze(S(:,2,:));
Hloc{4,1} = squeeze(S(:,3,:));
Hloc{5,2} = I;
Hloc{6,3} = I;
```

```

Hloc{7,4} = I;
Hloc{8,2} = J1*(Hloc{2,1}');
Hloc{8,3} = J1*(Hloc{3,1}');
Hloc{8,4} = J1*(Hloc{4,1}');
Hloc{8,5} = J2*(Hloc{2,1}');
Hloc{8,6} = J2*(Hloc{3,1}');
Hloc{8,7} = J2*(Hloc{4,1}');
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

E0_exact = -3*N/8; % exact value

```

After setting up the Hamiltonian and choosing our parameters, we choose an initial state with  $A_{11}^\uparrow = A_{22}^\downarrow = 1$  while all other entries are set to zero. At the left boundary, we choose all entries zero except  $A_{11}^\uparrow = A_{12}^\downarrow = 1$  while on the right boundary, only  $A_{11}^\uparrow = A_{21}^\downarrow = 1$  are non-zero. (**Quick question:** what kind of state does this represent?) We then perturb this state by adding small random numbers to the  $A$ -matrices. We iterate over several randomly generated perturbations and keep track how single-site DMRG converges compared to DMRG3S.

```

del = 1e-8; % small number
Nr = 10; % number of DMRG runs with random perturbation
MA = cell(1,N);
A = zeros(Nkeep,2,Nkeep);
A(1,1,1) = 1;
A(2,2,2) = 1;
MA(:) = {A};
MA{1} = A(1,:,:) + A(2,:,:) ;
MA{end} = A(:, :, 1) + A(:, :, 2);

% worst difference between GS energy and mean energy of the optimized MPS:
dEGS = 0;
MR = cell(1,N); % corresponding random perturbation
Eiter_1site = cell(1,Nr);
Eiter_3S = cell(1,Nr);

for itr = 1:Nr
    Minit = cell(1,N);
    for itN = 1:N
        if itN == 1
            Minit{itN} = rand(1,2,Nkeep)*del+MA{itN};
        elseif itN == N
            Minit{itN} = rand(Nkeep,2,1)*del+MA{itN};
        else
            Minit{itN} = rand(Nkeep,2,Nkeep)*del+MA{itN};
        end
    end
end

```

end

```
[~,~,Eiter_1site{itr}] = DMRG_3S_Ex(Hs,Nkeep,Nsweep,'Minit',Minit,'noex');  
[~,~,Eiter_3S{itr}] = DMRG_3S_Ex(Hs,Nkeep,Nsweep,'Minit',Minit);
```

end

```
DMRG3S: search for the ground state  
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2  
21-05-28 18:09:25 | Initial MPS given as input. Energy = 14.5  
21-05-28 18:09:25 | Sweep #1/10 (right -> left) : Energy = -12.82955  
21-05-28 18:09:25 | Sweep #2/10 (left -> right) : Energy = -14.51584  
21-05-28 18:09:25 | Sweep #3/10 (right -> left) : Energy = -14.63316  
21-05-28 18:09:25 | Sweep #4/10 (left -> right) : Energy = -14.66828  
21-05-28 18:09:25 | Sweep #5/10 (right -> left) : Energy = -14.68312  
21-05-28 18:09:25 | Sweep #6/10 (left -> right) : Energy = -14.69264  
21-05-28 18:09:25 | Sweep #7/10 (right -> left) : Energy = -14.69809  
21-05-28 18:09:25 | Sweep #8/10 (left -> right) : Energy = -14.70151  
21-05-28 18:09:25 | Sweep #9/10 (right -> left) : Energy = -14.70223  
21-05-28 18:09:25 | Sweep #10/10 (left -> right) : Energy = -14.70248  
Elapsed time: 0.4811s, CPU time: 0.68s, Avg # of cores: 1.414  
DMRG3S: search for the ground state  
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2  
21-05-28 18:09:25 | Initial MPS given as input. Energy = 14.5  
21-05-28 18:09:25 | Sweep #1/10 (right -> left) : Energy = -12.95394  
21-05-28 18:09:25 | Sweep #2/10 (left -> right) : Energy = -14.70772  
21-05-28 18:09:25 | Sweep #3/10 (right -> left) : Energy = -14.99612  
21-05-28 18:09:25 | Sweep #4/10 (left -> right) : Energy = -15  
21-05-28 18:09:25 | Sweep #5/10 (right -> left) : Energy = -15  
21-05-28 18:09:25 | Sweep #6/10 (left -> right) : Energy = -15  
21-05-28 18:09:26 | Sweep #7/10 (right -> left) : Energy = -15  
21-05-28 18:09:26 | Sweep #8/10 (left -> right) : Energy = -15  
21-05-28 18:09:26 | Sweep #9/10 (right -> left) : Energy = -15  
21-05-28 18:09:26 | Sweep #10/10 (left -> right) : Energy = -15  
Elapsed time: 0.6017s, CPU time: 1.95s, Avg # of cores: 3.241  
DMRG3S: search for the ground state  
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2  
21-05-28 18:09:26 | Initial MPS given as input. Energy = 14.5  
21-05-28 18:09:26 | Sweep #1/10 (right -> left) : Energy = -13.5627  
21-05-28 18:09:26 | Sweep #2/10 (left -> right) : Energy = -14.5798  
21-05-28 18:09:26 | Sweep #3/10 (right -> left) : Energy = -14.64701  
21-05-28 18:09:26 | Sweep #4/10 (left -> right) : Energy = -14.67348  
21-05-28 18:09:26 | Sweep #5/10 (right -> left) : Energy = -14.70216  
21-05-28 18:09:26 | Sweep #6/10 (left -> right) : Energy = -14.83186  
21-05-28 18:09:26 | Sweep #7/10 (right -> left) : Energy = -14.98587  
21-05-28 18:09:26 | Sweep #8/10 (left -> right) : Energy = -14.99991  
21-05-28 18:09:26 | Sweep #9/10 (right -> left) : Energy = -15  
21-05-28 18:09:26 | Sweep #10/10 (left -> right) : Energy = -15  
Elapsed time: 0.4311s, CPU time: 0.55s, Avg # of cores: 1.276  
DMRG3S: search for the ground state  
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2  
21-05-28 18:09:26 | Initial MPS given as input. Energy = 14.5  
21-05-28 18:09:26 | Sweep #1/10 (right -> left) : Energy = -13.29028  
21-05-28 18:09:26 | Sweep #2/10 (left -> right) : Energy = -14.71421  
21-05-28 18:09:26 | Sweep #3/10 (right -> left) : Energy = -14.99829  
21-05-28 18:09:26 | Sweep #4/10 (left -> right) : Energy = -15  
21-05-28 18:09:26 | Sweep #5/10 (right -> left) : Energy = -15  
21-05-28 18:09:26 | Sweep #6/10 (left -> right) : Energy = -15  
21-05-28 18:09:27 | Sweep #7/10 (right -> left) : Energy = -15  
21-05-28 18:09:27 | Sweep #8/10 (left -> right) : Energy = -15  
21-05-28 18:09:27 | Sweep #9/10 (right -> left) : Energy = -15  
21-05-28 18:09:27 | Sweep #10/10 (left -> right) : Energy = -15  
Elapsed time: 0.5698s, CPU time: 1.8s, Avg # of cores: 3.159  
DMRG3S: search for the ground state
```

```

# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:27 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:27 | Sweep #1/10 (right -> left) : Energy = -13.24031
21-05-28 18:09:27 | Sweep #2/10 (left -> right) : Energy = -14.87531
21-05-28 18:09:27 | Sweep #3/10 (right -> left) : Energy = -14.99851
21-05-28 18:09:27 | Sweep #4/10 (left -> right) : Energy = -14.99999
21-05-28 18:09:27 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:27 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:27 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:27 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:27 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:27 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.4324s, CPU time: 0.6s, Avg # of cores: 1.388
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:27 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:27 | Sweep #1/10 (right -> left) : Energy = -13.66152
21-05-28 18:09:27 | Sweep #2/10 (left -> right) : Energy = -14.99908
21-05-28 18:09:27 | Sweep #3/10 (right -> left) : Energy = -15
21-05-28 18:09:27 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:27 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:27 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:27 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:28 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:28 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:28 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5136s, CPU time: 1.46s, Avg # of cores: 2.843
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:28 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:28 | Sweep #1/10 (right -> left) : Energy = -13.00055
21-05-28 18:09:28 | Sweep #2/10 (left -> right) : Energy = -14.17836
21-05-28 18:09:28 | Sweep #3/10 (right -> left) : Energy = -14.2476
21-05-28 18:09:28 | Sweep #4/10 (left -> right) : Energy = -14.32591
21-05-28 18:09:28 | Sweep #5/10 (right -> left) : Energy = -14.53697
21-05-28 18:09:28 | Sweep #6/10 (left -> right) : Energy = -14.6295
21-05-28 18:09:28 | Sweep #7/10 (right -> left) : Energy = -14.63513
21-05-28 18:09:28 | Sweep #8/10 (left -> right) : Energy = -14.6411
21-05-28 18:09:28 | Sweep #9/10 (right -> left) : Energy = -14.64535
21-05-28 18:09:28 | Sweep #10/10 (left -> right) : Energy = -14.64998
Elapsed time: 0.4761s, CPU time: 0.51s, Avg # of cores: 1.071
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:28 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:28 | Sweep #1/10 (right -> left) : Energy = -13.43255
21-05-28 18:09:28 | Sweep #2/10 (left -> right) : Energy = -14.89786
21-05-28 18:09:28 | Sweep #3/10 (right -> left) : Energy = -14.99999
21-05-28 18:09:28 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:28 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:28 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:28 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:29 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:29 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:29 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5418s, CPU time: 1.79s, Avg # of cores: 3.304
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:29 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:29 | Sweep #1/10 (right -> left) : Energy = -13.11274
21-05-28 18:09:29 | Sweep #2/10 (left -> right) : Energy = -14.82466
21-05-28 18:09:29 | Sweep #3/10 (right -> left) : Energy = -14.99678
21-05-28 18:09:29 | Sweep #4/10 (left -> right) : Energy = -14.99998
21-05-28 18:09:29 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:29 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:29 | Sweep #7/10 (right -> left) : Energy = -15

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21-05-28 18:09:29 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:29 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:29 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.4311s, CPU time: 0.48s, Avg # of cores: 1.113
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:29 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:29 | Sweep #1/10 (right -> left) : Energy = -12.83582
21-05-28 18:09:29 | Sweep #2/10 (left -> right) : Energy = -14.97359
21-05-28 18:09:29 | Sweep #3/10 (right -> left) : Energy = -15
21-05-28 18:09:29 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:29 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:29 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:29 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:29 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:30 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:30 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5305s, CPU time: 1.5s, Avg # of cores: 2.827
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:30 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:30 | Sweep #1/10 (right -> left) : Energy = -13.24998
21-05-28 18:09:30 | Sweep #2/10 (left -> right) : Energy = -14.54472
21-05-28 18:09:30 | Sweep #3/10 (right -> left) : Energy = -14.65565
21-05-28 18:09:30 | Sweep #4/10 (left -> right) : Energy = -14.67918
21-05-28 18:09:30 | Sweep #5/10 (right -> left) : Energy = -14.68903
21-05-28 18:09:30 | Sweep #6/10 (left -> right) : Energy = -14.69468
21-05-28 18:09:30 | Sweep #7/10 (right -> left) : Energy = -14.69608
21-05-28 18:09:30 | Sweep #8/10 (left -> right) : Energy = -14.69896
21-05-28 18:09:30 | Sweep #9/10 (right -> left) : Energy = -14.70089
21-05-28 18:09:30 | Sweep #10/10 (left -> right) : Energy = -14.70141
Elapsed time: 0.5389s, CPU time: 0.63s, Avg # of cores: 1.169
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:30 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:30 | Sweep #1/10 (right -> left) : Energy = -12.34949
21-05-28 18:09:30 | Sweep #2/10 (left -> right) : Energy = -14.95709
21-05-28 18:09:30 | Sweep #3/10 (right -> left) : Energy = -15
21-05-28 18:09:30 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:31 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:31 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:31 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:31 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:31 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:31 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5769s, CPU time: 1.67s, Avg # of cores: 2.895
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:31 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:31 | Sweep #1/10 (right -> left) : Energy = -13.27051
21-05-28 18:09:31 | Sweep #2/10 (left -> right) : Energy = -14.17137
21-05-28 18:09:31 | Sweep #3/10 (right -> left) : Energy = -14.28558
21-05-28 18:09:31 | Sweep #4/10 (left -> right) : Energy = -14.62146
21-05-28 18:09:31 | Sweep #5/10 (right -> left) : Energy = -14.98586
21-05-28 18:09:31 | Sweep #6/10 (left -> right) : Energy = -14.99993
21-05-28 18:09:31 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:31 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:31 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:31 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.451s, CPU time: 0.64s, Avg # of cores: 1.419
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:31 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:31 | Sweep #1/10 (right -> left) : Energy = -13.14793
21-05-28 18:09:31 | Sweep #2/10 (left -> right) : Energy = -14.99262

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21-05-28 18:09:31 | Sweep #3/10 (right -> left) : Energy = -15
21-05-28 18:09:31 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:31 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:32 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:32 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:32 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:32 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:32 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5645s, CPU time: 1.58s, Avg # of cores: 2.799
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:32 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:32 | Sweep #1/10 (right -> left) : Energy = -12.98761
21-05-28 18:09:32 | Sweep #2/10 (left -> right) : Energy = -14.51001
21-05-28 18:09:32 | Sweep #3/10 (right -> left) : Energy = -14.64852
21-05-28 18:09:32 | Sweep #4/10 (left -> right) : Energy = -14.68049
21-05-28 18:09:32 | Sweep #5/10 (right -> left) : Energy = -14.69281
21-05-28 18:09:32 | Sweep #6/10 (left -> right) : Energy = -14.70093
21-05-28 18:09:32 | Sweep #7/10 (right -> left) : Energy = -14.70408
21-05-28 18:09:32 | Sweep #8/10 (left -> right) : Energy = -14.70537
21-05-28 18:09:32 | Sweep #9/10 (right -> left) : Energy = -14.70763
21-05-28 18:09:32 | Sweep #10/10 (left -> right) : Energy = -14.70882
Elapsed time: 0.4736s, CPU time: 0.69s, Avg # of cores: 1.457
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:32 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:32 | Sweep #1/10 (right -> left) : Energy = -13.42186
21-05-28 18:09:32 | Sweep #2/10 (left -> right) : Energy = -14.86197
21-05-28 18:09:32 | Sweep #3/10 (right -> left) : Energy = -14.99999
21-05-28 18:09:32 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:33 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:33 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:33 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:33 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:33 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:33 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5154s, CPU time: 1.5s, Avg # of cores: 2.91
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:33 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:33 | Sweep #1/10 (right -> left) : Energy = -13.08705
21-05-28 18:09:33 | Sweep #2/10 (left -> right) : Energy = -14.61728
21-05-28 18:09:33 | Sweep #3/10 (right -> left) : Energy = -14.92881
21-05-28 18:09:33 | Sweep #4/10 (left -> right) : Energy = -14.99808
21-05-28 18:09:33 | Sweep #5/10 (right -> left) : Energy = -14.99998
21-05-28 18:09:33 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:33 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:33 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:33 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:33 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.4212s, CPU time: 0.51s, Avg # of cores: 1.211
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:33 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:33 | Sweep #1/10 (right -> left) : Energy = -13.21654
21-05-28 18:09:33 | Sweep #2/10 (left -> right) : Energy = -14.81125
21-05-28 18:09:33 | Sweep #3/10 (right -> left) : Energy = -14.99998
21-05-28 18:09:33 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:33 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:34 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:34 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:34 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:34 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:34 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5492s, CPU time: 1.69s, Avg # of cores: 3.077

```

```

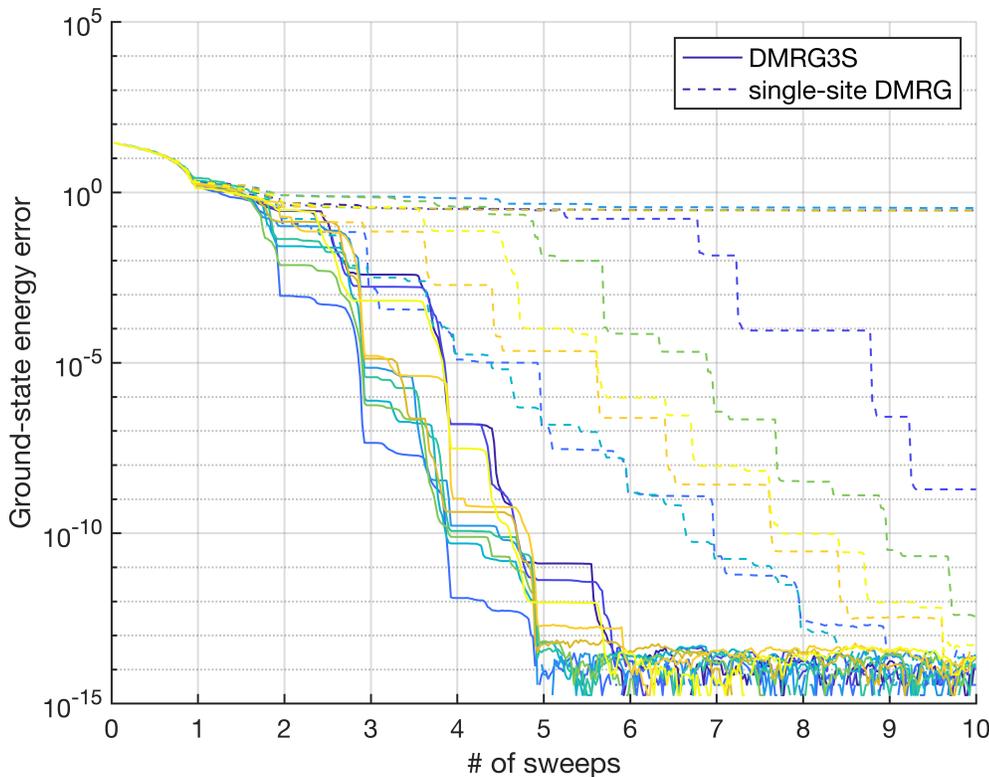
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:34 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:34 | Sweep #1/10 (right -> left) : Energy = -12.98723
21-05-28 18:09:34 | Sweep #2/10 (left -> right) : Energy = -14.54968
21-05-28 18:09:34 | Sweep #3/10 (right -> left) : Energy = -14.63237
21-05-28 18:09:34 | Sweep #4/10 (left -> right) : Energy = -14.9259
21-05-28 18:09:34 | Sweep #5/10 (right -> left) : Energy = -14.9999
21-05-28 18:09:34 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:34 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:34 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:34 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:34 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.4428s, CPU time: 0.54s, Avg # of cores: 1.219
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 10, # of sweeps = 5 x 2
21-05-28 18:09:34 | Initial MPS given as input. Energy = 14.5
21-05-28 18:09:34 | Sweep #1/10 (right -> left) : Energy = -13.6708
21-05-28 18:09:34 | Sweep #2/10 (left -> right) : Energy = -14.69626
21-05-28 18:09:34 | Sweep #3/10 (right -> left) : Energy = -14.99933
21-05-28 18:09:34 | Sweep #4/10 (left -> right) : Energy = -15
21-05-28 18:09:34 | Sweep #5/10 (right -> left) : Energy = -15
21-05-28 18:09:35 | Sweep #6/10 (left -> right) : Energy = -15
21-05-28 18:09:35 | Sweep #7/10 (right -> left) : Energy = -15
21-05-28 18:09:35 | Sweep #8/10 (left -> right) : Energy = -15
21-05-28 18:09:35 | Sweep #9/10 (right -> left) : Energy = -15
21-05-28 18:09:35 | Sweep #10/10 (left -> right) : Energy = -15
Elapsed time: 0.5645s, CPU time: 1.74s, Avg # of cores: 3.083

```

```

% visualize:
figure;
hold on;
Cls = parula(Nr);
for itr = 1:Nr
    plot((1:numel(Eiter_3S{itr}))/N,abs(Eiter_3S{itr}(:)-E0_exact),...
        'LineWidth',1,'Color',Cls(itr,:));
    plot((1:numel(Eiter_1site{itr}))/N,abs(Eiter_1site{itr}(:)-E0_exact),...
        '--','LineWidth',1,'Color',Cls(itr,:));
end
legend({'DMRG3S','single-site DMRG'},'FontSize',13);
set(gca,'FontSize',13,'LineWidth',1,'YScale','log');
xlim([0 2*Nsweep]);
grid on;
xlabel('# of sweeps');
ylabel('Ground-state energy error');
hold off;

```



We see that DMRG3S converges up to numerical precision after around 6 sweeps while conventional single-site DMRG takes more sweeps to converge. For some of the random perturbations, single-site DMRG does not converge to the ground-state at all, opposed to DMRG3S.

### Exercise (b): Complete the function `twoSiteVariance_Ex.m`

There is a function `twoSiteVariance_Ex.m` which is placed in the same subdirectory together with this tutorial material. This function partially implements the calculation of the two-site variance as an error measure.

**Complete the parts which are enclosed by the comments `TODO - Exercise 2`.**

### Heisenberg chain: error estimation

To test `twoSiteVariance_Ex.m` we consider a Heisenberg spin chain and calculate its ground-state. Its Hamiltonian is given by

$$H = \sum_{l=1}^{N-1} \vec{S}_l \cdot \vec{S}_{l+1}.$$

In the following, we will compare the two-site variance of the optimized GS obtained by DMRG3S and two-site DMRG for different bond dimensions.

```
clear
```

```

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

% DMRG parameter
Nsweep = 10; % number of pairs of left+right sweeps

% magnitude of local spin
s = 1/2;
% Local operators
[S,I] = getLocalSpace('Spin',s);

```

We set up the MPO of the Heisenberg chain as given in the lecture:

```

% % MPO formulation of Hamiltonian
% Hamiltonian tensor for each chain site
Hloc = cell(5,5);
Hloc(:) = {zeros(size(I))};
Hloc{1,1} = I;
Hloc{2,1} = squeeze(S(:,1,:));
Hloc{3,1} = squeeze(S(:,2,:));
Hloc{4,1} = squeeze(S(:,3,:));
Hloc{end,2} = J*(Hloc{2,1}');
Hloc{end,3} = J*(Hloc{3,1}');
Hloc{end,4} = J*(Hloc{4,1}');
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 DMRG for different bond dimensions.

```

Nkeeps = [5,10,20,40,80,160]; % bond dimensions
var_2site = zeros(1,numel(Nkeeps));
var_3S = zeros(1,numel(Nkeeps));
for itK = 1:numel(Nkeeps)
    Nkeep = Nkeeps(itK);

    % first 2-site DMRG:
    [MGS_2site,~,~] = DMRG_2site(Hs,Nkeep,Nsweep);
    var_2site(itK) = twoSiteVariance_Ex(MGS_2site,Hs);

    % DMRG3S
    [MGS_3S,~,~] = DMRG_3S_Ex(Hs,Nkeep,Nsweep);
    var_3S(itK) = twoSiteVariance_Ex(MGS_3S,Hs);
end

```

Two-site DMRG: search for the ground state

```
# of sites = 40, Nkeep = 5, # of sweeps = 10 x 2
21-05-28 18:09:35 | Initialize with iterative diagonalization. Energy = -16.8593
21-05-28 18:09:35 | Sweep #1/20 (right -> left) : Energy = -17.48374
21-05-28 18:09:35 | Sweep #2/20 (left -> right) : Energy = -17.48719
21-05-28 18:09:35 | Sweep #3/20 (right -> left) : Energy = -17.4882
21-05-28 18:09:36 | Sweep #4/20 (left -> right) : Energy = -17.48858
21-05-28 18:09:36 | Sweep #5/20 (right -> left) : Energy = -17.48872
21-05-28 18:09:36 | Sweep #6/20 (left -> right) : Energy = -17.48877
21-05-28 18:09:36 | Sweep #7/20 (right -> left) : Energy = -17.4888
21-05-28 18:09:36 | Sweep #8/20 (left -> right) : Energy = -17.48881
21-05-28 18:09:36 | Sweep #9/20 (right -> left) : Energy = -17.48881
21-05-28 18:09:36 | Sweep #10/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #11/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #12/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #13/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #14/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #15/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #16/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #17/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #18/20 (left -> right) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #19/20 (right -> left) : Energy = -17.48882
21-05-28 18:09:36 | Sweep #20/20 (left -> right) : Energy = -17.48882
Elapsed time: 1.065s, CPU time: 1.18s, Avg # of cores: 1.108
```

DMRG3S: search for the ground state

```
# of sites = 40, Nkeep = 5, # of sweeps = 10 x 2
21-05-28 18:09:36 | Initialize with iterative diagonalization. Energy = -16.8593
21-05-28 18:09:36 | Sweep #1/20 (right -> left) : Energy = -17.48149
21-05-28 18:09:37 | Sweep #2/20 (left -> right) : Energy = -17.48739
21-05-28 18:09:37 | Sweep #3/20 (right -> left) : Energy = -17.48862
21-05-28 18:09:37 | Sweep #4/20 (left -> right) : Energy = -17.48897
21-05-28 18:09:37 | Sweep #5/20 (right -> left) : Energy = -17.48908
21-05-28 18:09:37 | Sweep #6/20 (left -> right) : Energy = -17.48911
21-05-28 18:09:37 | Sweep #7/20 (right -> left) : Energy = -17.48911
21-05-28 18:09:37 | Sweep #8/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #9/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #10/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #11/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #12/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #13/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #14/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #15/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:37 | Sweep #16/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #17/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #18/20 (left -> right) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #19/20 (right -> left) : Energy = -17.48912
21-05-28 18:09:38 | Sweep #20/20 (left -> right) : Energy = -17.48912
Elapsed time: 1.327s, CPU time: 1.62s, Avg # of cores: 1.22
```

Two-site DMRG: search for the ground state

```
# of sites = 40, Nkeep = 10, # of sweeps = 10 x 2
21-05-28 18:09:38 | Initialize with iterative diagonalization. Energy = -17.17619
21-05-28 18:09:38 | Sweep #1/20 (right -> left) : Energy = -17.5396
21-05-28 18:09:38 | Sweep #2/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #3/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #4/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #5/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #6/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #7/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #8/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #9/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #10/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #11/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #12/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:38 | Sweep #13/20 (right -> left) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #14/20 (left -> right) : Energy = -17.53968
21-05-28 18:09:39 | Sweep #15/20 (right -> left) : Energy = -17.53968
```

21-05-28 18:09:39 | Sweep #16/20 (left -> right) : Energy = -17.53968  
21-05-28 18:09:39 | Sweep #17/20 (right -> left) : Energy = -17.53968  
21-05-28 18:09:39 | Sweep #18/20 (left -> right) : Energy = -17.53968  
21-05-28 18:09:39 | Sweep #19/20 (right -> left) : Energy = -17.53968  
21-05-28 18:09:39 | Sweep #20/20 (left -> right) : Energy = -17.53968  
Elapsed time: 1.113s, CPU time: 1.92s, Avg # of cores: 1.726

DMRG3S: search for the ground state

# of sites = 40, Nkeep = 10, # of sweeps = 10 x 2

21-05-28 18:09:39 | Initialize with iterative diagonalization. Energy = -17.17619  
21-05-28 18:09:39 | Sweep #1/20 (right -> left) : Energy = -17.53856  
21-05-28 18:09:39 | Sweep #2/20 (left -> right) : Energy = -17.53966  
21-05-28 18:09:39 | Sweep #3/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:39 | Sweep #4/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:39 | Sweep #5/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:39 | Sweep #6/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:39 | Sweep #7/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:39 | Sweep #8/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #9/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #10/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #11/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #12/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #13/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #14/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #15/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #16/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #17/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #18/20 (left -> right) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #19/20 (right -> left) : Energy = -17.5397  
21-05-28 18:09:40 | Sweep #20/20 (left -> right) : Energy = -17.5397  
Elapsed time: 1.28s, CPU time: 1.91s, Avg # of cores: 1.492

Two-site DMRG: search for the ground state

# of sites = 40, Nkeep = 20, # of sweeps = 10 x 2

21-05-28 18:09:40 | Initialize with iterative diagonalization. Energy = -17.32798  
21-05-28 18:09:40 | Sweep #1/20 (right -> left) : Energy = -17.54142  
21-05-28 18:09:40 | Sweep #2/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #3/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #4/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #5/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #6/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #7/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #8/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #9/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:41 | Sweep #10/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #11/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #12/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #13/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #14/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #15/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #16/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #17/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #18/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:42 | Sweep #19/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:43 | Sweep #20/20 (left -> right) : Energy = -17.54145  
Elapsed time: 2.337s, CPU time: 19.22s, Avg # of cores: 8.223

DMRG3S: search for the ground state

# of sites = 40, Nkeep = 20, # of sweeps = 10 x 2

21-05-28 18:09:43 | Initialize with iterative diagonalization. Energy = -17.32798  
21-05-28 18:09:43 | Sweep #1/20 (right -> left) : Energy = -17.54141  
21-05-28 18:09:43 | Sweep #2/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:43 | Sweep #3/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:43 | Sweep #4/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:43 | Sweep #5/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:43 | Sweep #6/20 (left -> right) : Energy = -17.54145  
21-05-28 18:09:44 | Sweep #7/20 (right -> left) : Energy = -17.54145  
21-05-28 18:09:44 | Sweep #8/20 (left -> right) : Energy = -17.54145

```
21-05-28 18:09:44 | Sweep #9/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #10/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #11/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #12/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #13/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #14/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #15/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:44 | Sweep #16/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #17/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #18/20 (left -> right) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #19/20 (right -> left) : Energy = -17.54145
21-05-28 18:09:45 | Sweep #20/20 (left -> right) : Energy = -17.54145
Elapsed time: 2.116s, CPU time: 14.64s, Avg # of cores: 6.919
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 40, # of sweeps = 10 x 2
21-05-28 18:09:45 | Initialize with iterative diagonalization. Energy = -17.4161
21-05-28 18:09:45 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:45 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:45 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:46 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:47 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:48 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 3.579s, CPU time: 30.17s, Avg # of cores: 8.43
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 40, # of sweeps = 10 x 2
21-05-28 18:09:49 | Initialize with iterative diagonalization. Energy = -17.4161
21-05-28 18:09:49 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:49 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:49 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:49 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:50 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:51 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:52 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 3.625s, CPU time: 31.9s, Avg # of cores: 8.801
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 80, # of sweeps = 10 x 2
21-05-28 18:09:53 | Initialize with iterative diagonalization. Energy = -17.5012
21-05-28 18:09:53 | Sweep #1/20 (right -> left) : Energy = -17.54147
```

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21-05-28 18:09:53 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:54 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:54 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:55 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:55 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:55 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:56 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:56 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:56 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:57 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:57 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:58 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:58 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:58 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:09:59 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:09:59 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:00 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:00 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:01 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 8.33s, CPU time: 66s, Avg # of cores: 7.923
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 80, # of sweeps = 10 x 2
21-05-28 18:10:01 | Initialize with iterative diagonalization. Energy = -17.5012
21-05-28 18:10:02 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:02 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:02 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:03 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:03 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:04 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:04 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:04 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:05 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:05 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:05 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:06 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:06 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:07 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:07 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:07 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:08 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:08 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:08 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:09 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 7.739s, CPU time: 63.06s, Avg # of cores: 8.148
Two-site DMRG: search for the ground state
# of sites = 40, Nkeep = 160, # of sweeps = 10 x 2
21-05-28 18:10:10 | Initialize with iterative diagonalization. Energy = -17.51978
21-05-28 18:10:12 | Sweep #1/20 (right-> left) : Energy = -17.54147
21-05-28 18:10:13 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:15 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:16 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:17 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:19 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:20 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:21 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:23 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:24 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:25 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:27 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:28 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:29 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:31 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:32 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:33 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:35 | Sweep #18/20 (left -> right) : Energy = -17.54147

```

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21-05-28 18:10:36 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:37 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 28.55s, CPU time: 187.7s, Avg # of cores: 6.573
DMRG3S: search for the ground state
# of sites = 40, Nkeep = 160, # of sweeps = 10 x 2
21-05-28 18:10:40 | Initialize with iterative diagonalization. Energy = -17.51978
21-05-28 18:10:41 | Sweep #1/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:42 | Sweep #2/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:43 | Sweep #3/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:45 | Sweep #4/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:46 | Sweep #5/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:47 | Sweep #6/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:48 | Sweep #7/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:49 | Sweep #8/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:50 | Sweep #9/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:51 | Sweep #10/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:52 | Sweep #11/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:53 | Sweep #12/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:54 | Sweep #13/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:55 | Sweep #14/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:56 | Sweep #15/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:57 | Sweep #16/20 (left -> right) : Energy = -17.54147
21-05-28 18:10:58 | Sweep #17/20 (right -> left) : Energy = -17.54147
21-05-28 18:10:59 | Sweep #18/20 (left -> right) : Energy = -17.54147
21-05-28 18:11:00 | Sweep #19/20 (right -> left) : Energy = -17.54147
21-05-28 18:11:01 | Sweep #20/20 (left -> right) : Energy = -17.54147
Elapsed time: 22.93s, CPU time: 154.1s, Avg # of cores: 6.719

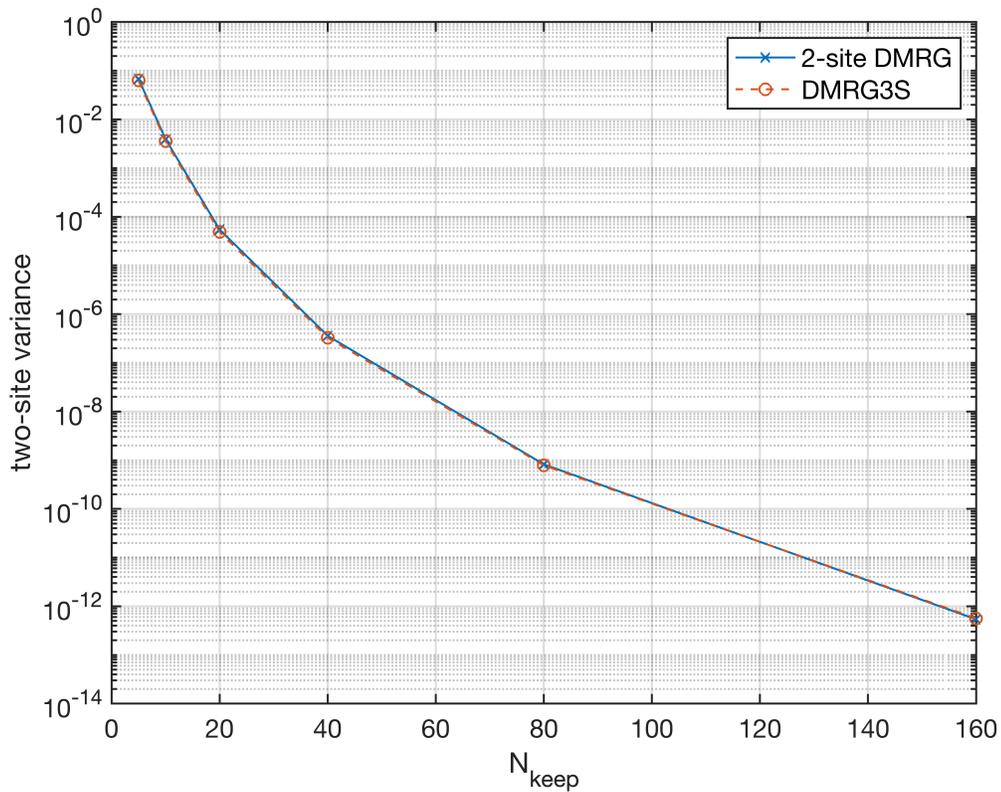
```

Plot how the two-site variance decreases with the bond dimension:

```

figure;
semilogy(Nkeeps,var_2site,'-x','LineWidth',1);
hold on;
semilogy(Nkeeps,var_3S,'--o','LineWidth',1);
set(gca,'FontSize',13,'LineWidth',1);
xlim([0 max(Nkeeps)]);
grid on;
legend({'2-site DMRG','DMRG3S'},'FontSize',13)
xlabel('N_{keep}');
ylabel('two-site variance');
hold off;

```



As expected, the variance decreases with  $N_{\text{keep}}$ . Two-site DMRG and DMRG3S yield almost identical variances. Note however that DMRG3S is only marginally faster for  $s = 1/2$  than 2-site DMRG. This is because of the small physical dimension  $d = 2$ . If  $s$  is increased,  $d$  increases and the DMRG3S eventually becomes faster. However, calculations also become quite a bit heavier. But if your computer is able to handle it, give larger  $s$  a try!