Applying MPO onto MPS

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We demonstrate that the application of matrix product operator (MPO) onto a matrix product state (MPS) results in another MPS. In this tutorial, we consider an MPO representation of the Hamiltonian and its ground state(s) as the MPO and the MPS, respectively.

To start with, we consider the spin-1/2 Heisenberg model on a short chain,

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

The chain length $N = 6$ is chosen to be short so that we can obtain the full Hamiltonian and the exact ground state by using iterative diagonalization. Here at all iterations before the last iteration, we do not rotate the basis into the energy eigenbasis and do not truncate the Hilbert space. It is necessary to compare the Hamiltonian constructed within iterative diagonalization (represented by a matrix `Hnow` below) with the MPO form of the Hamiltonian (to be obtained in the next section).

```
clear

N = 6; % chain length
M = cell(1,N); % MPS

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

H0 = I*0; % Hamiltonian for only the 1st site
M{1} = getIdentity(1,2,I,2); % 1st leg is dummy leg (vacuum)

for itN = (1:N)
    if itN == 1
        Hnow = H0;
        Anow = M{1};
    else
        % % add new site
        Anow = getIdentity(Hprev,2,I,2);
        Hnow = updateLeft(Hprev,2,Anow,[],[],Anow);
        % update the Hamiltonian up to the last sites
        % to the enlarged Hilbert space

        % % spin-spin interaction
        % Hermitian conjugate of the spin operator at
        % the current site
        Sn = permute(conj(S),[3 2 1]);
        HSS = updateLeft(Sprev,3,Anow,Sn,3,Anow);
        Hnow = Hnow+HSS;
    end

    if itN < N % no rotation, no truncation
        M{itN} = Anow;
        Hprev = Hnow;
```

```
        % spin operator at the current site; to be used for
        % generating the coupling term at the next iteration
        Sprev = updateLeft([],[],M{itN},S,3,M{itN});
    else
        [V,D] = eig((Hnow+Hnow')/2);
        [E_GS,minid] = min(diag(D));
        % select only the ground state
        M{itN} = contract(Anow,3,3,V(:,minid),2,1);
    end

    disptime(['#',sprintf('%02i/%02i',[itN,N]),' : ', ...
        'NK=',sprintf('%i/%i',[size(M{itN},3),size(Hnow,2)])]);
end
```

```
21-04-22 15:16:34 | #01/06 : NK=2/2
21-04-22 15:16:34 | #02/06 : NK=4/4
21-04-22 15:16:34 | #03/06 : NK=8/8
21-04-22 15:16:34 | #04/06 : NK=16/16
21-04-22 15:16:34 | #05/06 : NK=32/32
21-04-22 15:16:34 | #06/06 : NK=1/64
```

The ground-state energy is:

```
E_GS
```

```
E_GS = -2.4936
```

Currently, `M` is in a left-canonical form. By bringing it into a right-canonical form, the size of the constituent tensors can be decreased.

```
M
```

```
M = 1×6 cell
```

	1	2	3	4	5	6
1	1×2×2 double	2×2×4 double	4×2×8 double	8×2×16 double	16×2×32 dou...	32×2 double

```
M = canonForm(M,0) % right-canonical form
```

```
M = 1×6 cell
```

	1	2	3	4	5	6
1	1×2×2 double	2×2×4 double	4×2×8 double	8×2×4 double	4×2×2 double	[-1,0;0,...

MPO representation of Heisenberg chain Hamiltonian

We construct the MPO representation of the chain Hamiltonian, following the recipe given in a lecture. The MPO consists of the same tensor, called bulk tensor, except for the first and the last sites. A bulk tensor is rank-4, and its legs are as left-bottom-right-top. The bottom (top) leg is to be contracted with the second leg of bra (ket) tensor.

Let's first generate a bulk tensor.

```
% bulk tensor for each chain site
Hloc = cell(5,5);
```

```
Hloc(:) = {zeros(size(I))};
Hloc{1,1} = I;
for ito = (1:size(S,2)) % different components of spin operators
    Hloc{ito+1,1} = squeeze(S(:,ito,:));
    Hloc{end,ito+1} = squeeze(S(:,ito,:))';
end
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
```

For the tensors at the first and the last sites, we project the bulk tensor onto a specific index of its left and right legs, respectively. So the left and right legs, respectively, become dummy legs with singleton dimension.

```
% MPO for the full chain
Hs = cell(1,N);
Hs(:) = {Hloc};
Hs{1} = Hs{1}(end,:,:,:); % choose the last index of the left leg
Hs{end} = Hs{end}(:,:,1,:); % choose the first index of the right leg
```

The indices are chosen such that the pair of spin operators (which make up the interaction term) are complete, without unpaired operators remaining.

To check whether the MPO construction is right, we compare the MPO and the Hamiltonian from iterative diagonalization (represented by `Hnow`) We first contract the tensors of `Hs` to make a high-rank tensor acting onto all the chain sites. And we permute and reshape the high-rank tensor into a big matrix, which can be directly compared with `Hnow`.

```
Hs_tot = permute(Hs{1},[1 2 4 3]); % leg order: left-bottom-top-right
for itN = (2:N)
    Hs_tot = contract(Hs_tot,2*itN,2*itN,permute(Hs{itN},[1 2 4 3]),4,1);
end
Hs_tot = permute(Hs_tot,[(2:2:2*N) (3:2:2*N+1) 1 2*N+2]);
% permute singleton dimensions (= dummy legs) to the end
Hs_tot = reshape(Hs_tot,(size(I,1)^N)*[1 1]);
```

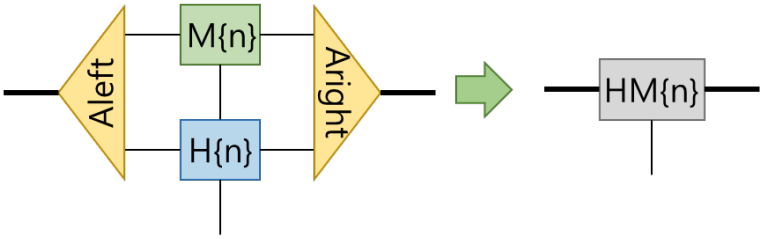
The two forms of the Hamiltonian are equivalent.

```
max(abs(Hs_tot(:)-Hnow(:)))
```

```
ans = 0
```

Application of MPO onto MPS

We apply the MPO representation of Hamiltonian H (represented by a cell array `Hs`) onto the ground state $|\psi\rangle$ (by a cell array `M`). The tensors at each site, `Hs{n}` and `M{n}`, are contracted, and their horizontal legs are merged by using isometries. The result is a rank-3 tensor `HM{n}`, which constitutes a MPS form of $H|\psi\rangle$.




```
HM = cell(1,N);
for itN = (1:N)
    HM{itN} = contract(Hs{itN},4,4,M{itN},3,2);
    % leg order: Hleft-Hbottom-Hright-Mleft-Mright

    % isometry to merge left legs
    if itN == 1
        Aleft = getIdentity(HM{itN},1,HM{itN},4);
    else
        % use Aright from the previous iteration,
        % to be a valid insertion of identity
        Aleft = conj(Aright);
    end

    % isometry to merge right legs
    Aright = getIdentity(HM{itN},3,HM{itN},5);

    % contract isometries
    HM{itN} = contract(Aleft,3,[1 2],HM{itN},5,[1 4]);
    % leg order: left-Hbottom-Hright-Mright
    HM{itN} = contract(HM{itN},4,[3 4],Aright,3,[1 2]);
end
```

As shown in the above tensor diagram, the bond dimensions have increased.

```
HM
```

```
HM = 1×6 cell
```

	1	2	3	4	5	6
1	1×2×10 double	10×2×20 dou...	20×2×40 dou...	40×2×20 dou...	20×2×10 dou...	10×2 double

The bond dimensions in the MPS form of $H|\psi\rangle$ can be compressed by performing a "round trip" of bringing into canonical forms; first into left-canonical, then into right-canonical.

```
[HM,HMnorm] = canonForm(HM,N) % left-canonical
```

```
HM = 1×6 cell
```

	1	2	3	4	5	6
1	1×2×2 double	2×2×4 double	4×2×8 double	8×2×16 double	16×2×10 dou...	10×2 double

```
HMnorm = 2.4936
```

```
HM = canonForm(HM,0) % here the second output should be 1
```

```
HM = 1×6 cell
```

	1	2	3	4	5	6
1	1×2×2 double	2×2×4 double	4×2×8 double	8×2×4 double	4×2×2 double	[-1,0;0,1]

Now, the tensors have the same sizes as those in `M`.

```
M
```

```
M = 1×6 cell
```

	1	2	3	4	5	6
1	1×2×2 double	2×2×4 double	4×2×8 double	8×2×4 double	4×2×2 double	[-1,0;0,...

The value of the norm `HMnorm` (which means $\|H|\psi\rangle\|$) is equal to the absolute value of the ground-state energy (represented by `E_GS`).

```
HMnorm - abs(E_GS) % zero up to numerical noise
```

```
ans = 1.7764e-15
```

For later purpose, we let the first tensor `HM{1}` absorb `HMnorm`.

```
HM{1} = HM{1}*HMnorm;
```

We can also check that $\langle\psi|H|\psi\rangle$ gives the ground-state energy, by contracting `HM` and `M`.

```
MHM = updateLeft([],[],M{1},[],[],HM{1});
for itN = (2:N)
    MHM = updateLeft(MHM,2,M{itN},[],[],HM{itN});
end
MHM - E_GS % zero up to numerical noise
```

```
ans = -3.1086e-15
```

Here we know that `M` represents the ground state, since the Hamiltonian can be exactly diagonalized, thank to small system size. For general systems, however, there is no straightforward way to verify whether a given state $|\psi\rangle$ is the true ground state of the system, not being a local mimima.

Still, we can verify whether $|\psi\rangle$ is an eigenstate of the Hamiltonian H by confiming $\langle\psi|H|\psi\rangle^2 - \langle\psi|H^2|\psi\rangle = 0$. The first term $\langle\psi|H|\psi\rangle^2$ can be computed as the square of `MHM` and the second term $\langle\psi|H^2|\psi\rangle$ as the squared norm $\|H|\psi\rangle\|^2$. We see that the equality is satisfied, meaning that $|\psi\rangle$ is an eigenstate.

```
MHM^2 - HMnorm^2
```

```
ans = 7.1054e-15
```

Exercise (a): MPO representation of the AKLT Hamiltonian

We have studied the AKLT states in the previous tutorials. The AKLT states are the ground states of the AKLT model, which is a chain of spin-1's that interact via nearest-neighbor interactions,

$$\hat{H} = \sum_{\ell=1}^{N-1} \left[(\hat{\vec{S}}_\ell \cdot \hat{\vec{S}}_{\ell+1}) + \frac{1}{3} (\hat{\vec{S}}_\ell \cdot \hat{\vec{S}}_{\ell+1})^2 \right].$$

The first term on the right-hand side is the Heisenberg interaction. The second term is a biquadratic term that has a form of the squared Heisenberg interaction. We consider an open boundary condition.

(i) Construct a bulk tensor of an MPO representation of the AKLT model Hamiltonian. The tensors of the MPO at the first and the last sites can be obtained in the same way as above, by projecting onto specific indices.

(ii) Check whether your construction of the MPO is correct, by comparing with the Hamiltonian from iterative diagonalization of a short chain, e.g., $N = 4$.

Exercise (b): Confirm the AKLT states are the eigenstates of the AKLT Hamiltonian

In a previous tutorial, we have learned that there are four AKLT states $|\psi(\alpha, \beta)\rangle$ $(\alpha, \beta = 1, 2)$ in case of the open boundary condition. For **all** these AKLT states $|\psi(\alpha, \beta)\rangle$, (i) compute the expectation values $\langle\psi(\alpha, \beta)|H|\psi(\alpha, \beta)\rangle$ and (ii) confirm $\langle\psi|H|\psi\rangle^2 - \langle\psi|H^2|\psi\rangle = 0$. For this exercise, consider a long chain of length $N = 50$.