Contraction of finite PEPS

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In this tutorial, we will implement a scheme to measure correlation functions with respect to a projected entangled-pair state (PEPS) on a square lattice with open boundary conditions.

Resonating valence bond (RVB) state

Let's first identify which kind of tensor networks need to be contracted to measure correlation functions. For this, we take an example of the RVB state, which allows compact PEPS representation, and the correlation function of spin-z operators at nearest neighbors.

Each PEPS tensor at a lattice site consists of (i) two valence bond (or dimer) tensors defined on the right and down edges from the site and (ii) the projector onto a physical space.

The valence bond tensor represents a state $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle + |00\rangle$, where the first labels inside $|\cdot\rangle$ indicate the states of the left (upper) "virtual particle" for a horizontal (vertical) dimer. The leg order and directions are chosen as left (incoming)-right (outgoing) for a horizontal dimer and up (incoming)-down (outgoing) for a vertical dimer. Moreover, we use the ordered basis $\{|\uparrow\rangle, |\downarrow\rangle, |0\rangle\}$ for the bond spaces.

```
clear
VB = blkdiag([0,1;-1,0],1);
```

The projector is rank-5, with legs sorted as left (incoming)-up (incoming)-physical (incoming)-down (outgoing)-right(outgoing). The projector has an element 1 if and only if only one bond carrys spin $|\uparrow\rangle$ or $|\downarrow\rangle$ while the other three bonds are empty $|0\rangle$, and the bond spin equals to the physical spin. Accordingly, the projector is constructed as

```
[S,I] = getLocalSpace('Spin',1/2);
P = zeros(3,3,2,3,3);
for it1 = (1:size(I,2))
    P(it1,3,it1,3,3) = 1;
    P(3,it1,it1,3,3) = 1;
    P(3,3,it1,it1,3) = 1;
    P(3,3,it1,3,it1) = 1;
end
```

We obtain a rank-5 tensor by contracting the dimer tensors and the projector.

```
M = contract(P,5,4,VB,2,1);
M = contract(M,5,4,VB,2,1);
```

For contractions, we derive two types of reduced tensors, one made of `M` and its complex conjugate only, and the other made of `M`, its complext conjugate, and the spin-z operator.

```
MM = contract(conj(M),5,3,M,5,3);
for itl = (1:4)
```

```
    MM = contract(MM,8-(itl-1),[1 5-(itl-1)], ...
        getIdentity(MM,1,MM,5-(itl-1)),3,[1 2]);
end
MSM = contract(conj(M),5,3,S(:,:,2),2,1);
MSM = contract(MSM,5,5,M,5,3);
for itl = (1:4)
    MSM = contract(MSM,8-(itl-1),[1 5-(itl-1)], ...
        getIdentity(MSM,1,MSM,5-(itl-1)),3,[1 2]);
end
```

To the spin-spin correlation function, we consider two different square-lattice networks of the reduced tensors. To be more concrete, let's consider a lattice of 11 rows and 12 columns, and consider putting the spin-z operators at the "center," i.e., sites (6,6) and (6,7). The correlation function is written as $\langle\psi|\widehat{S}^z_{(6,6)}\widehat{S}^z_{(6,7)}|\psi\rangle/\langle\psi|\psi\rangle$. First, the network for the denominator is given by

```
Nrow = 11;
Ncol = 12;
Tden = cell(Nrow,Ncol);
Tden(:) = {MM};
Tden(:,1) = cellfun(@(x) x(end,:,:,:), Tden(:,1), 'UniformOutput',false);
Tden(1,:) = cellfun(@(x) x(:,end,:,:), Tden(1,:), 'UniformOutput',false);
Tden(end,:) = cellfun(@(x) x(:,:,end,:), Tden(end,:), 'UniformOutput',false);
Tden(:,end) = cellfun(@(x) x(:,:,:,end), Tden(:,end), 'UniformOutput',false);
```

Here we have projected the legs along the lattice boundary onto the last basis of $|0\rangle$ (for the bond space sfor kets) $\otimes|0\rangle$ (for the bonds spaces for bras). The network for the numerator is defined in a similar way,

```
Tnum = Tden;
Tnum(6,[6 7]) = {MSM};
```

Exercise (a): Complete the function for the MPO-MPS method of PEPS contraction

There is a function `contract_finPEPS_Ex.m`, which is in the same sub-directory with this script. It is supposed to contract tensor networks on a square lattice, such as `Tden` and `Tnum` above. Complete the parts enclosed by the comments `TODO (start)` and `TODO (end)`.

Once you complete the function, you can verify your implementation by running the following script.

```
Nkeep = 30;
Nsweep = 5;
Tnum_res = contract_finPEPS_Ex (Tnum,Nkeep,Nsweep);
```

```
22-11-13 17:10:22 | Contract tensors on a 11 x 12 lattice, with Nkeep = 30
Elapsed time: 6.323s, CPU time: 60.83s, Avg # of cores: 9.62
```

```
disp(Tnum_res);
```

```
  -2.6028e+41
```

```
Tden_res = contract_finPEPS_Ex (Tden,Nkeep,Nsweep);
```

```
22-11-13 17:10:28 | Contract tensors on a 11 x 12 lattice, with Nkeep = 30
Elapsed time: 5.684s, CPU time: 55.36s, Avg # of cores: 9.74
```

```
disp(Tden_res);
```

```
   3.5944e+42
```

```
disp(Tnum_res/Tden_res);
```

```
   -0.0724
```

As we see, the contraction results can be very small or large, since each tensor is not normalized and one contracts many of such tensors. Thus it is crucial to properly treat the normalization within the contraction scheme.

Exercise (b): Spin-spin correlation function of the RVB state with different lattice sizes

Consider the RVB state on a square lattice of "almost square" sizes, i.e., $N_{\mathrm{row}} = N_{\mathrm{col}} \pm 1$, for different odd numbers N_{row}. And put a pair of spin-z operators at the "center" of the lattice, i.e., sites $((N_{\mathrm{row}}+1)/2, N_{\mathrm{col}}/2)$, $((N_{\mathrm{row}}+1)/2, N_{\mathrm{col}}/2+1)$. Compute the spin-spin correlation functions for different lattice sizes.

Exercise (c): Ground state of Kitaev's toric code

Construct the ground state of Kitaev's toric code on a square lattice with open boundary conditions, as a PEPS. Compute the correlation function of two spin-z operators. What do you get? Can you explain the reason?