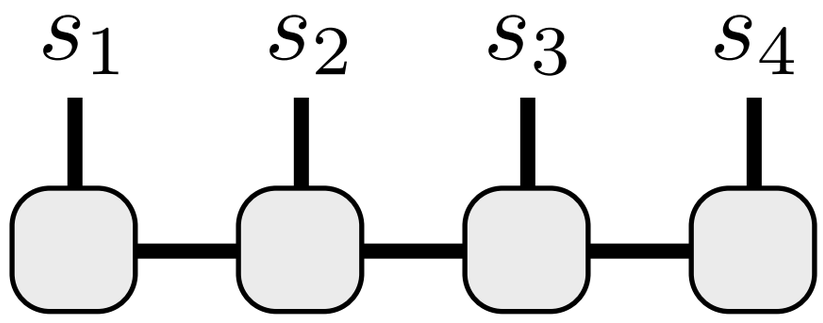
04 Four

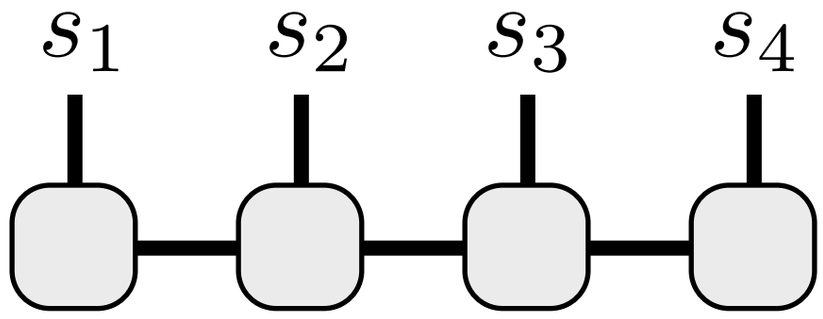
Say we have a 4-site MPS.
What can we do with it?



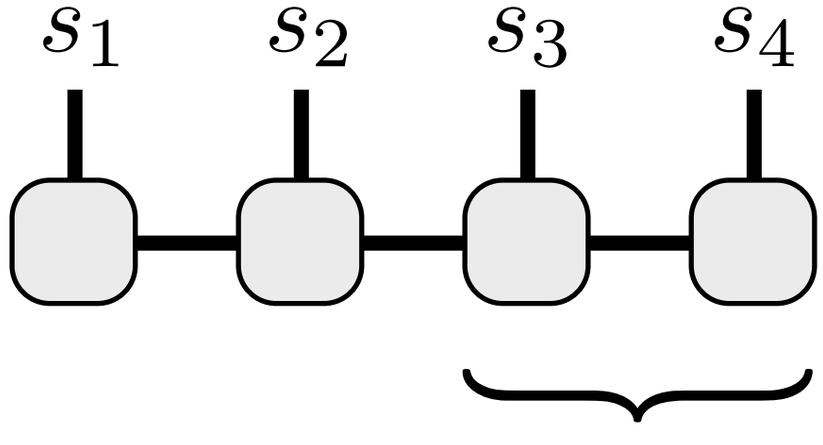
Depends on the gauge!

$$|\Psi\rangle = \sum_{\{s\},\{\alpha\}} M^{s_1}_{\alpha_1} M^{s_2}_{\alpha_1\alpha_2} M^{s_3}_{\alpha_2\alpha_3} M^{s_4}_{\alpha_3} |s_1 s_2 s_3 s_4\rangle$$

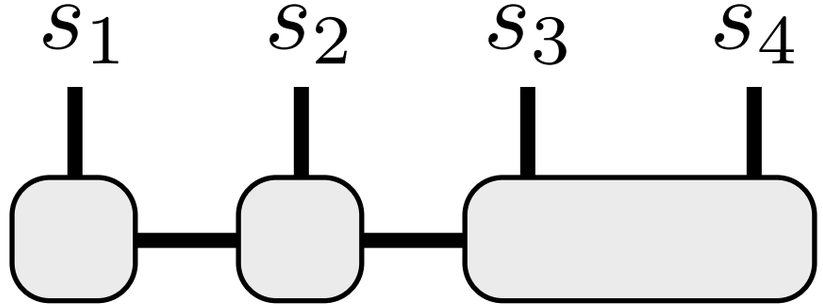
Assume we know nothing about the MPS
Put it in a useful gauge:



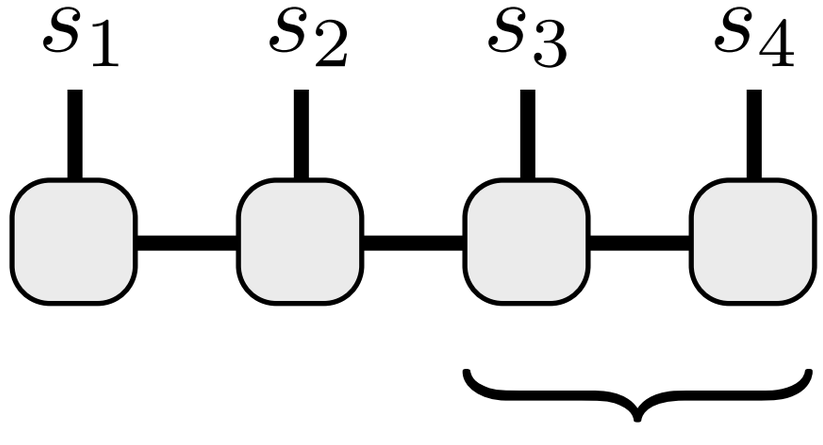
Assume we know nothing about the MPS
Put it in a useful gauge:



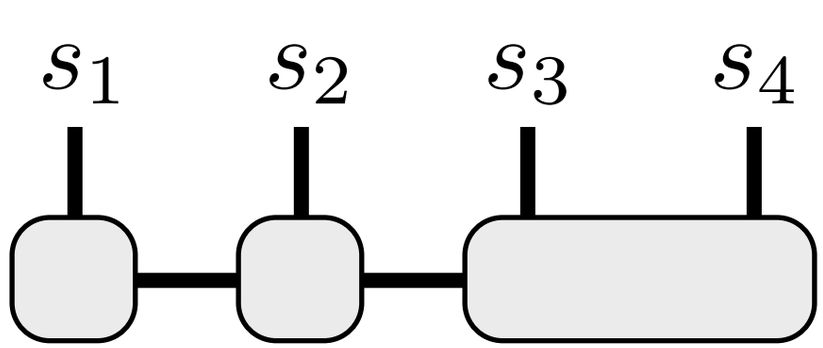
Contract



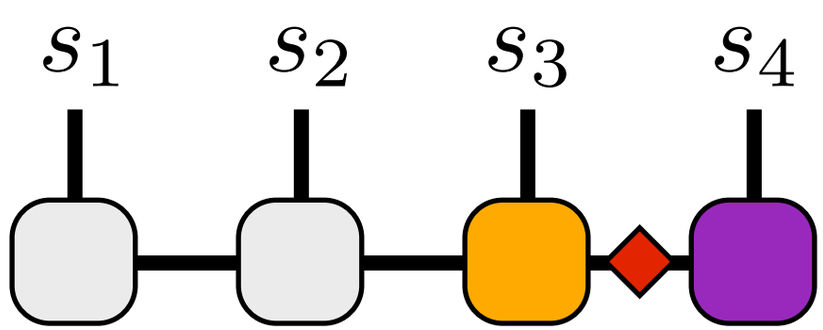
Assume we know nothing about the MPS
Put it in a useful gauge:



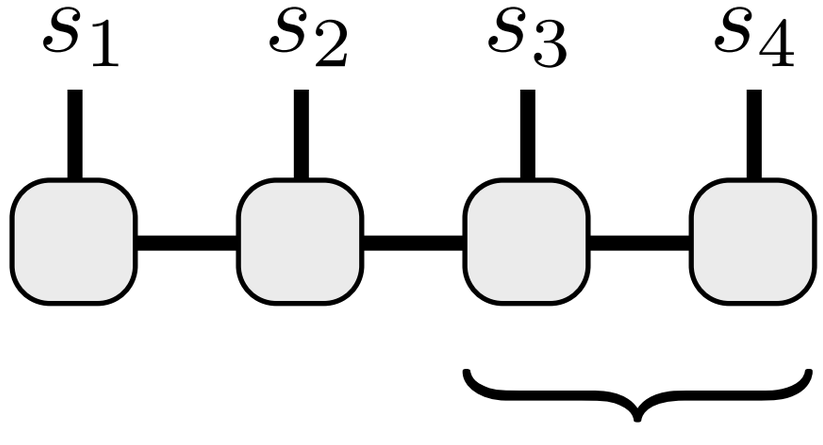
Contract



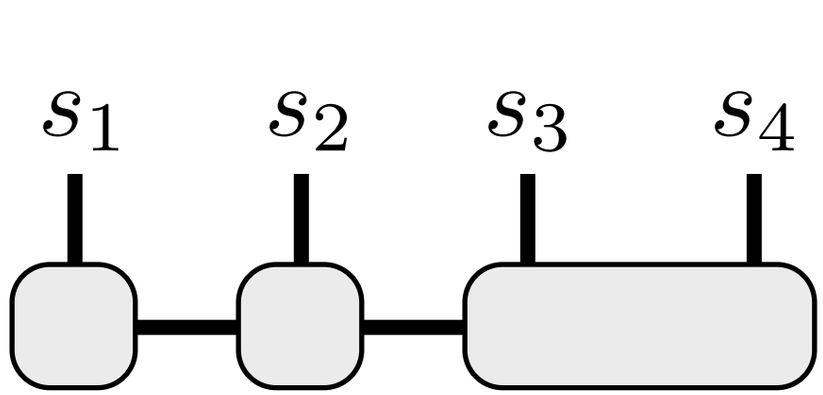
SVD



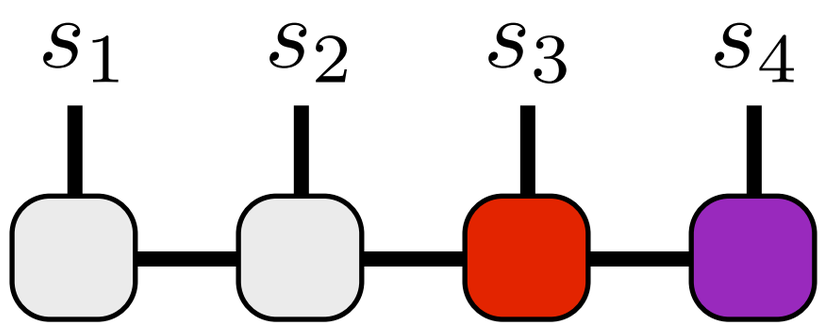
Assume we know nothing about the MPS
Put it in a useful gauge:



Contract

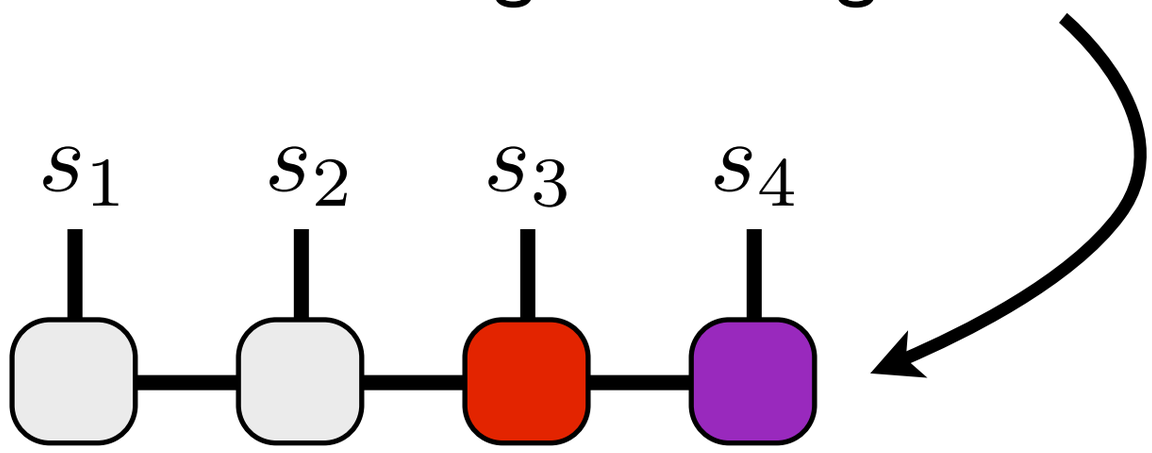


SVD

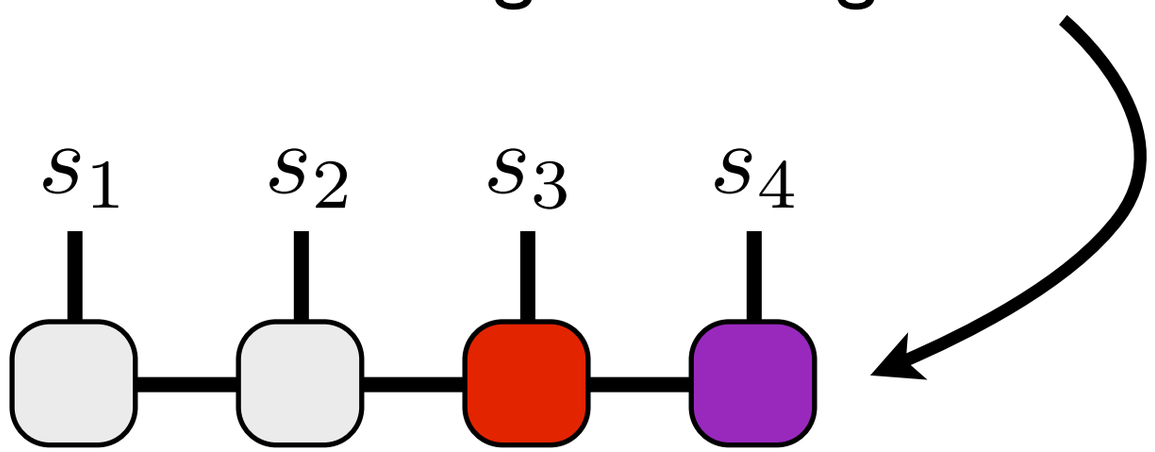


Group (AD) B

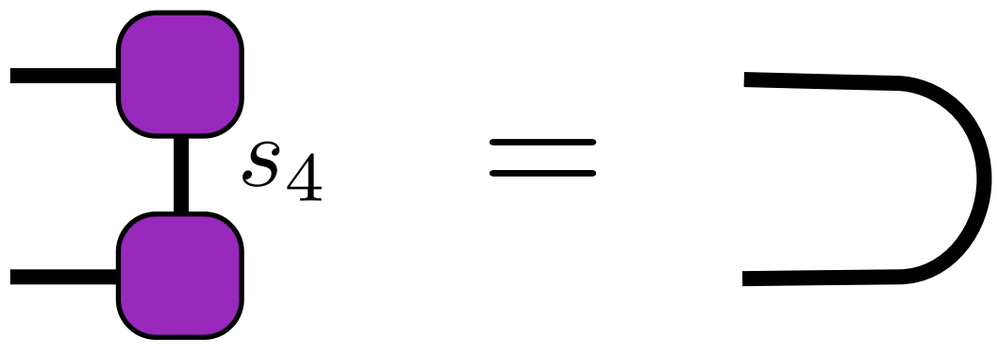
Note that site 4 tensor now right orthogonal



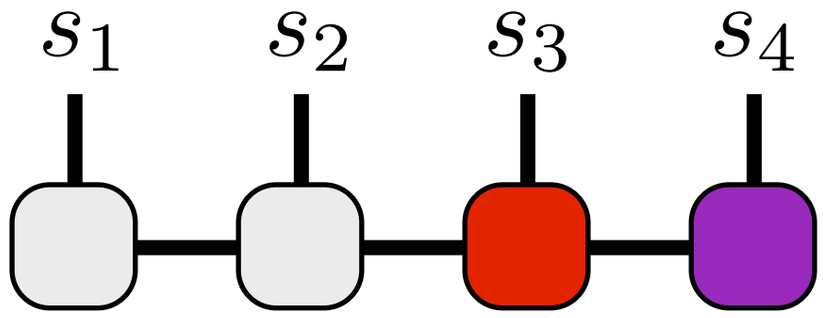
Note that site 4 tensor now right orthogonal



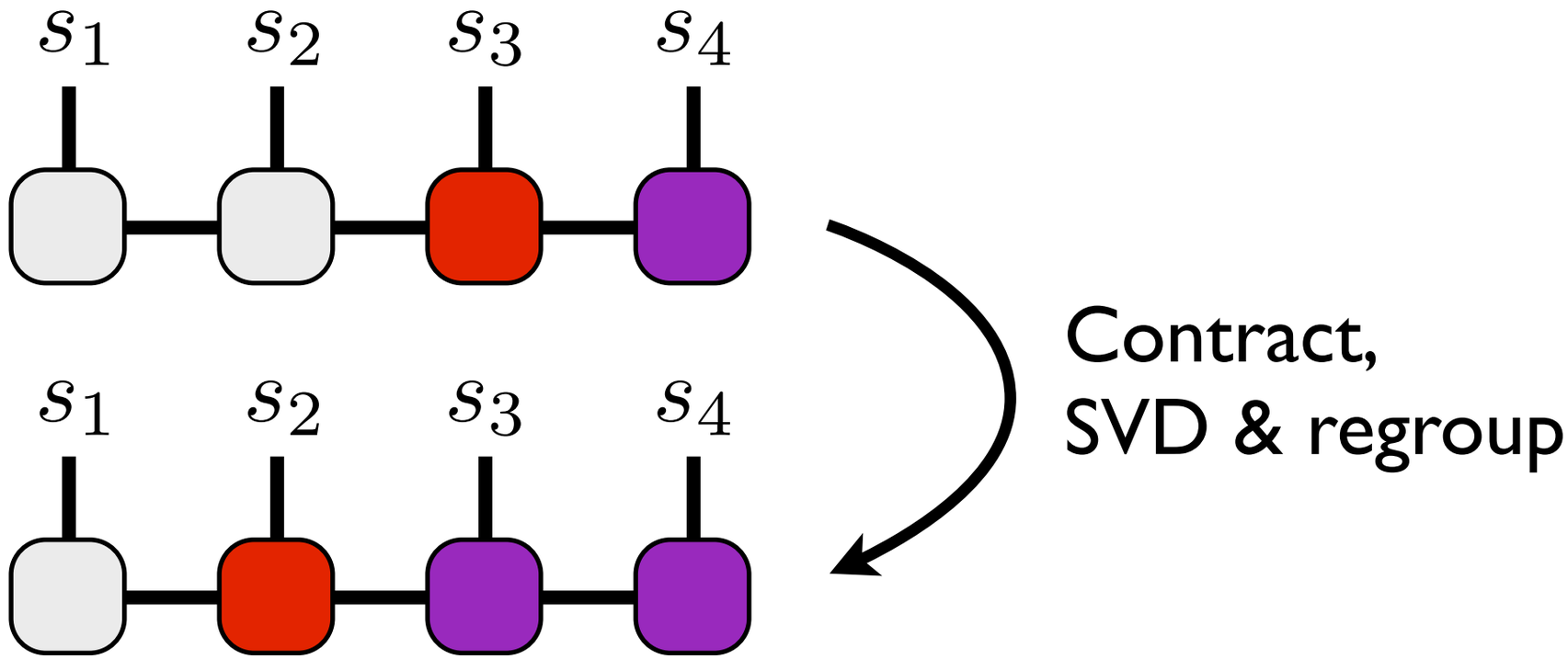
Recall this means



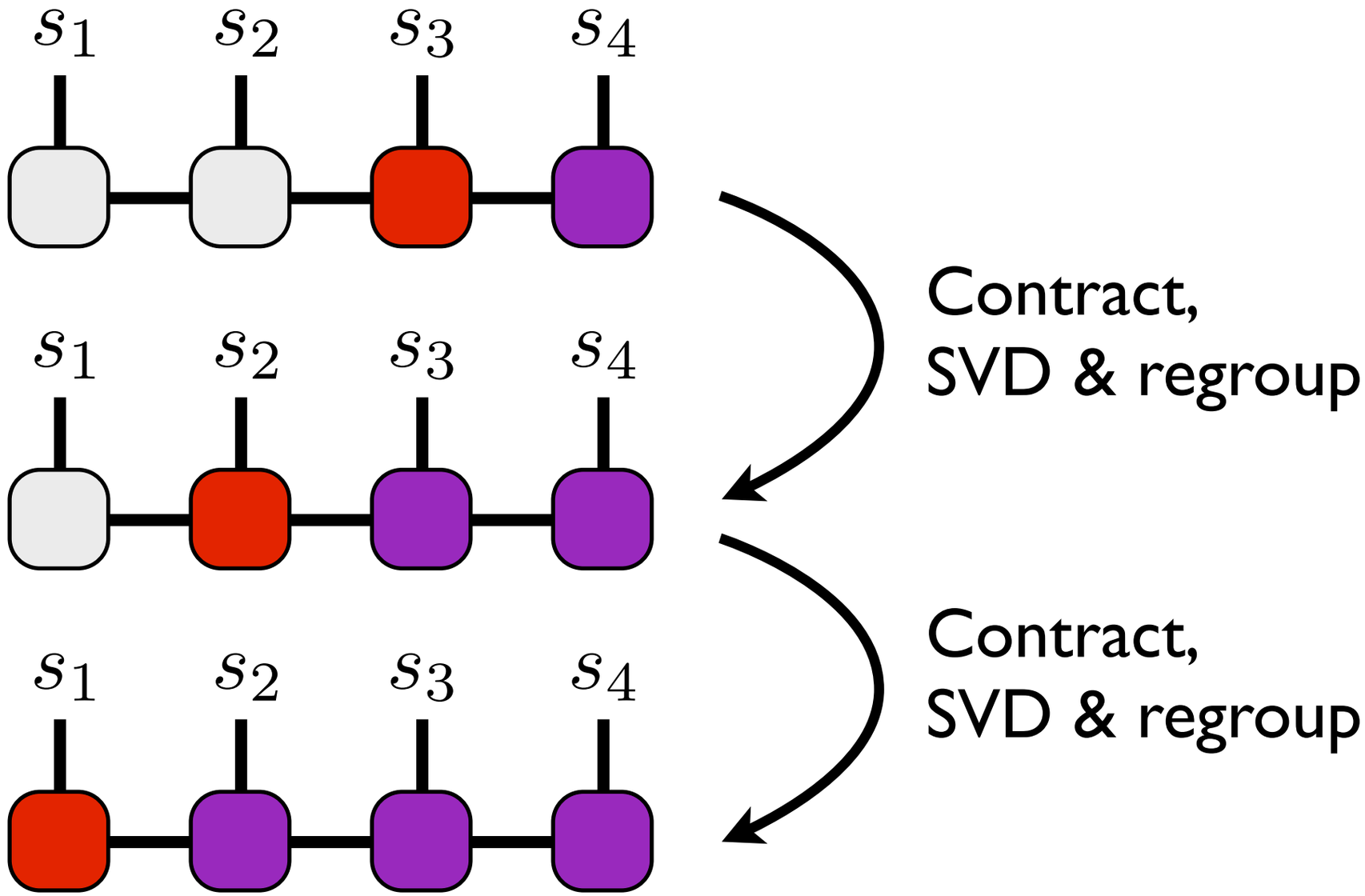
Can repeat gauge transformation (repeated SVD)



Can repeat gauge transformation (repeated SVD)

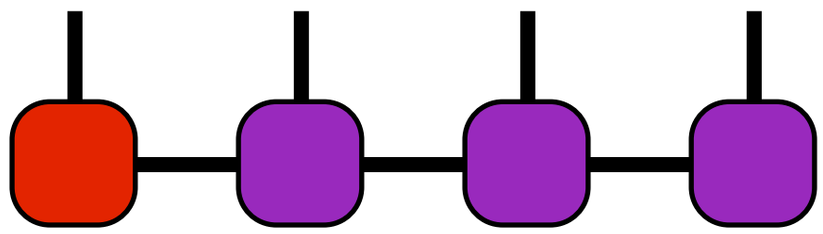


Can repeat gauge transformation (repeated SVD)



What have we gained?

Consider measuring an operator on site 1

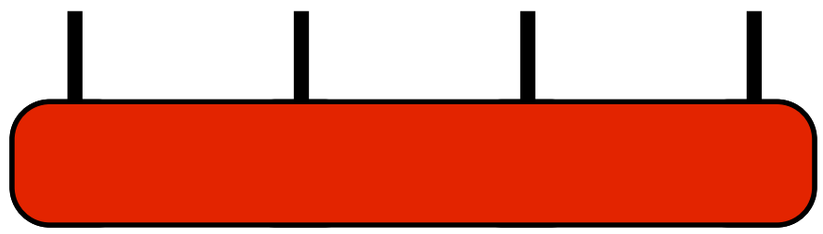


What have we gained?

Consider measuring an operator on site 1

First, general wavefunction:

$|\Psi\rangle$



What have we gained?

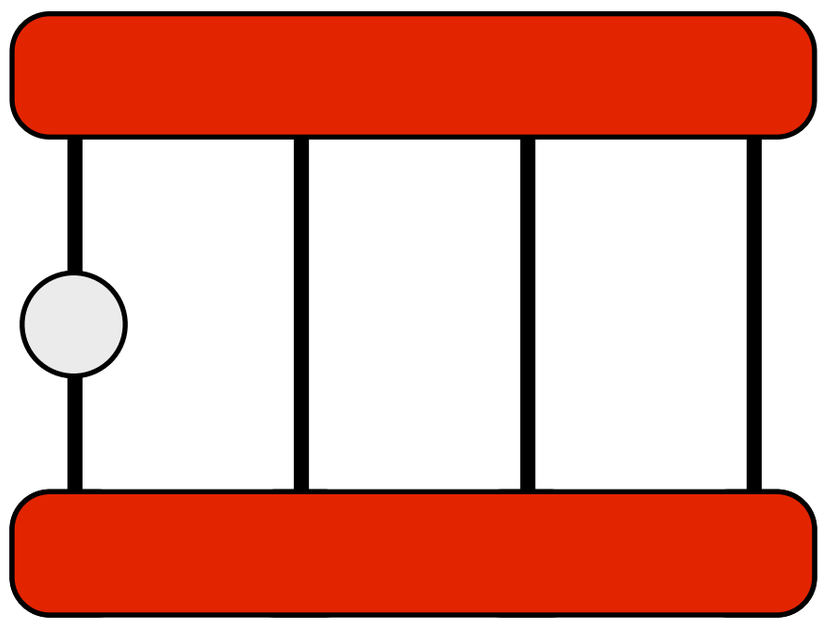
Consider measuring an operator on site 1

First, general wavefunction:

$\langle \Psi |$

$\hat{A}_1$

$|\Psi\rangle$



What have we gained?

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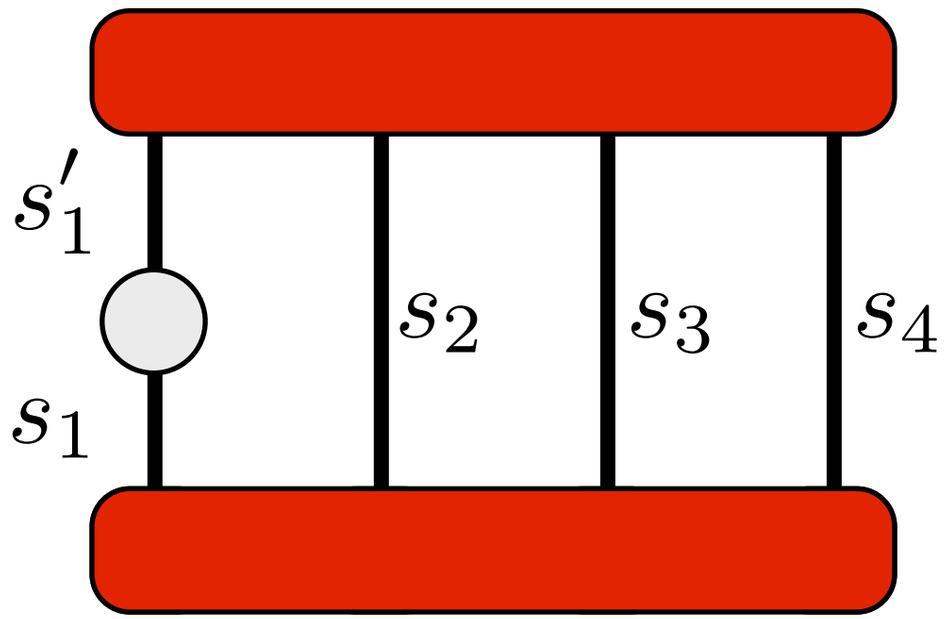
First, general wavefunction:

$\langle \Psi |$

$\hat{A}_1$

$|\Psi\rangle$



Cost scales exponentially!

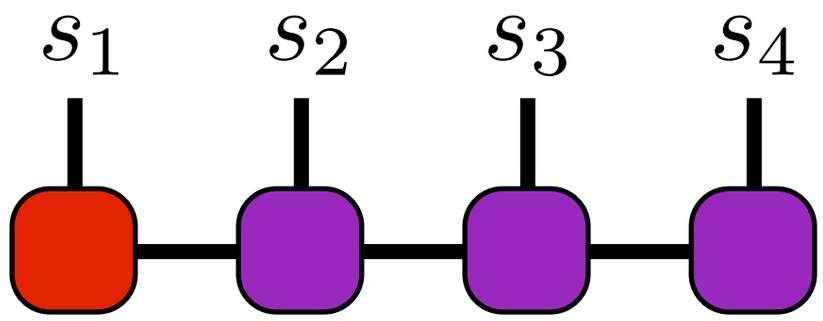
2^4 in this case

$$\langle \hat{A}_1 \rangle = \sum_{\{s\}} \bar{\psi}_{s_1' s_2 s_3 s_4} A_{s_1' s_1} \psi_{s_1 s_2 s_3 s_4}$$

What have we gained?

Consider measuring an operator on site 1

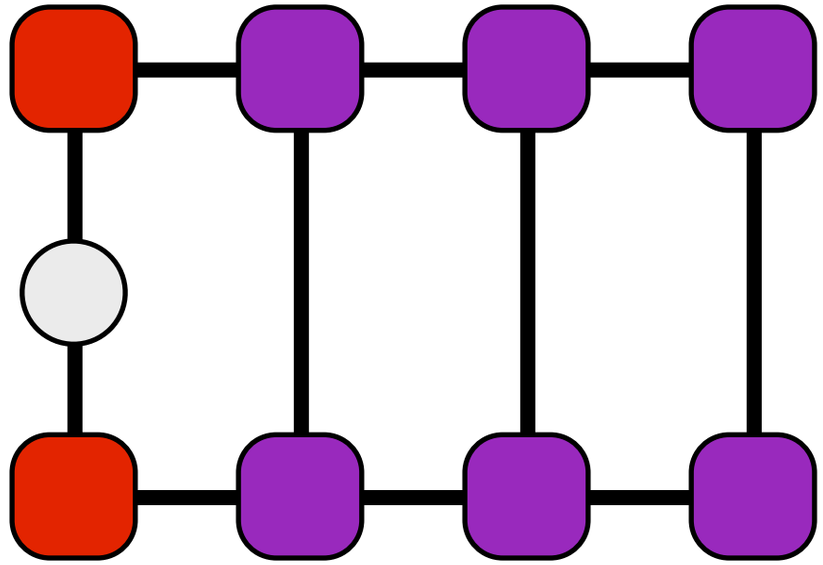
Now gauged MPS:



What have we gained?

Consider measuring an operator on site 1

Now gauged MPS:

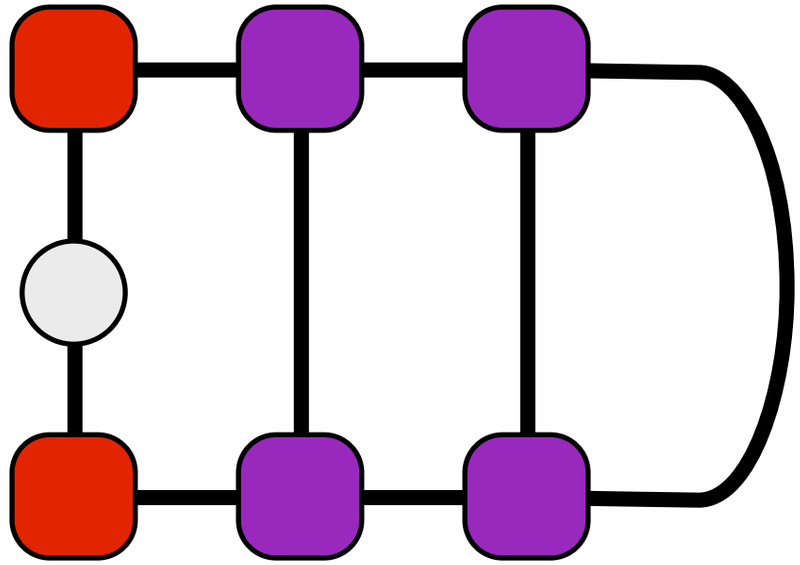


Use right orthogonality

What have we gained?

Consider measuring an operator on site 1

Now gauged MPS:

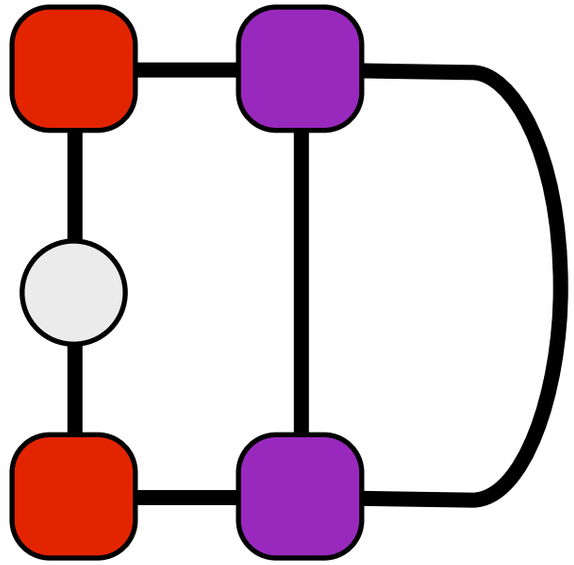


Use right orthogonality

What have we gained?

Consider measuring an operator on site 1

Now gauged MPS:

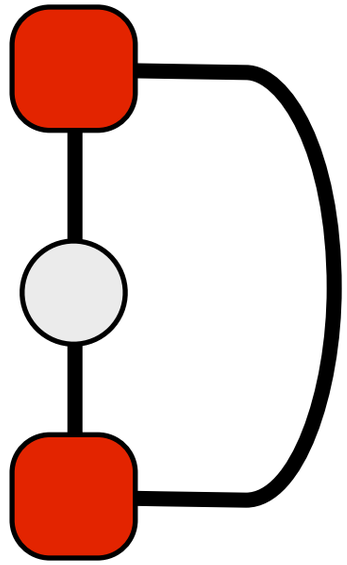


Use right orthogonality

What have we gained?

Consider measuring an operator on site 1

Now gauged MPS:



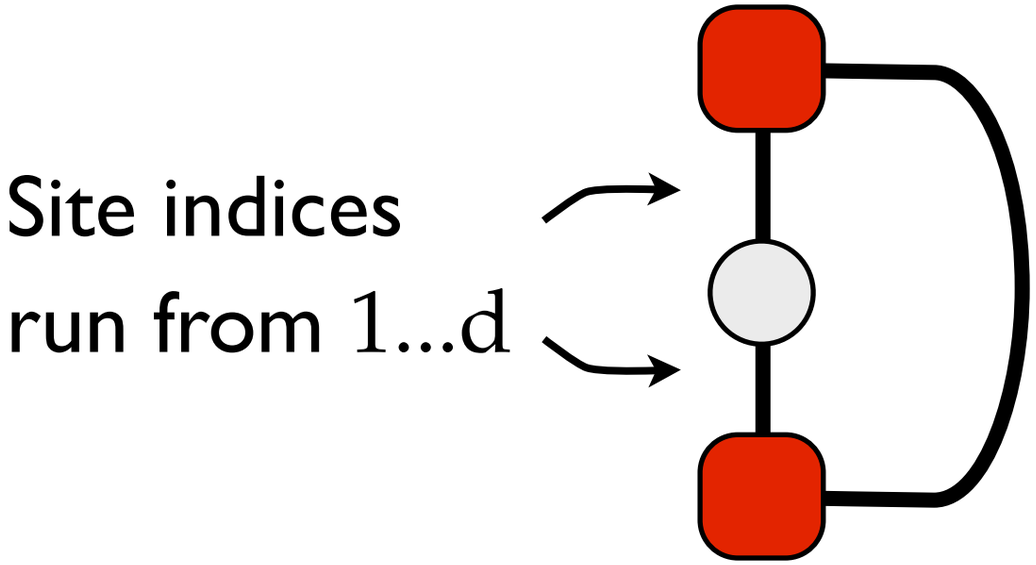
Use right orthogonality

Much simpler computation!

What have we gained?

How much simpler a computation?

Choose always $\leq m$ singular values
in each SVD



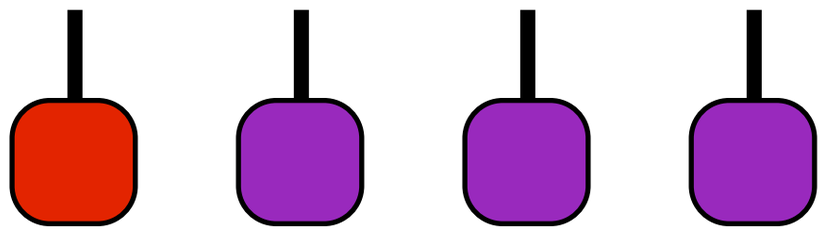
Computational cost ~ $d^2\, m$ (compared to d^4)

Gauging an MPS Using ITensor:

```
//Define lattice sites
SpinHalf sites(N);
```

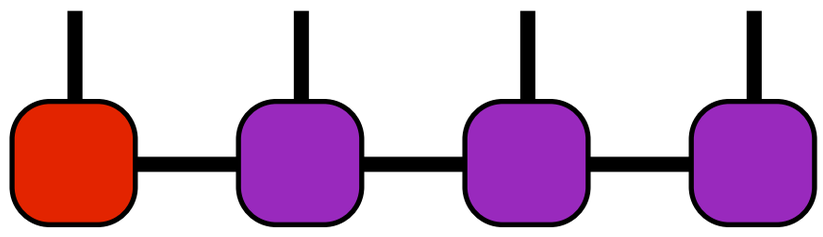
Gauging an MPS Using ITensor:

```
//Define lattice sites
SpinHalf sites(N);
MPS psi(sites);
```



Gauging an MPS Using ITensor:

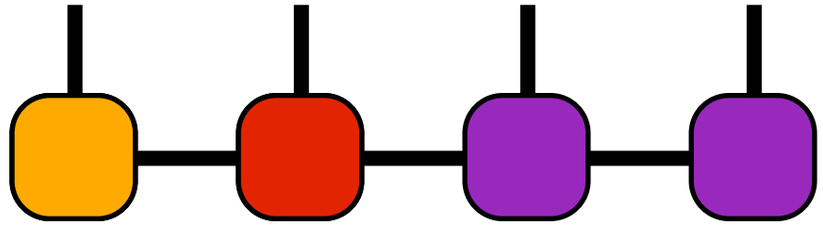
```
//Define lattice sites
SpinHalf sites(N);
MPS psi(sites);
computeGroundState(H,psi); //optimize psi
```



Gauging an MPS Using ITensor:

```
//Define lattice sites
SpinHalf sites(N);
MPS psi(sites);
computeGroundState(H,psi); //optimize psi


//Gauge MPS to second site
psi.position(2);
```

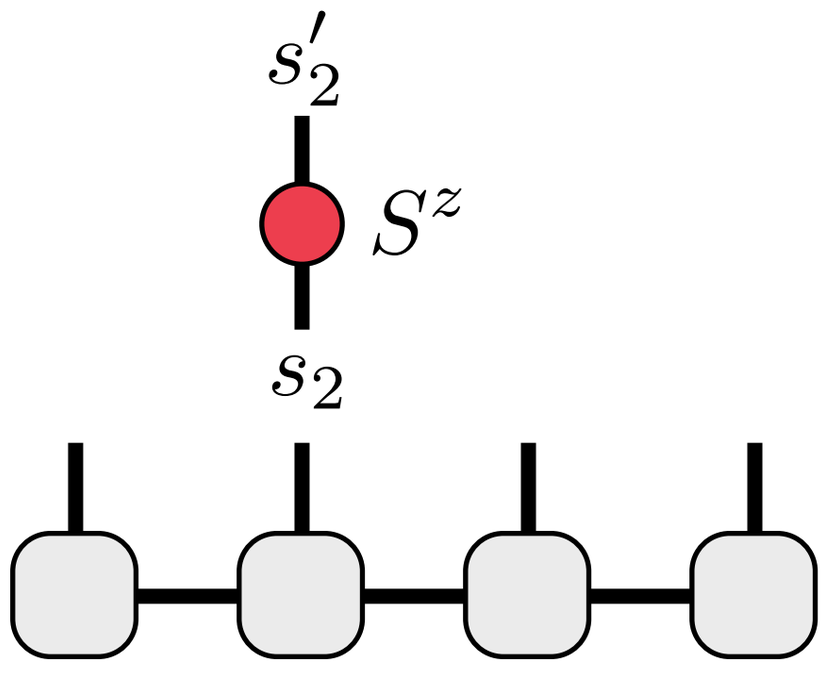


Measuring an MPS Using ITensor:

Can obtain single-site operators from "SiteSet" object:

```
//Obtain single-site operators
ITensor Sz = sites.op("Sz",2);
```

```
sites.op("Sz",2) ==
```

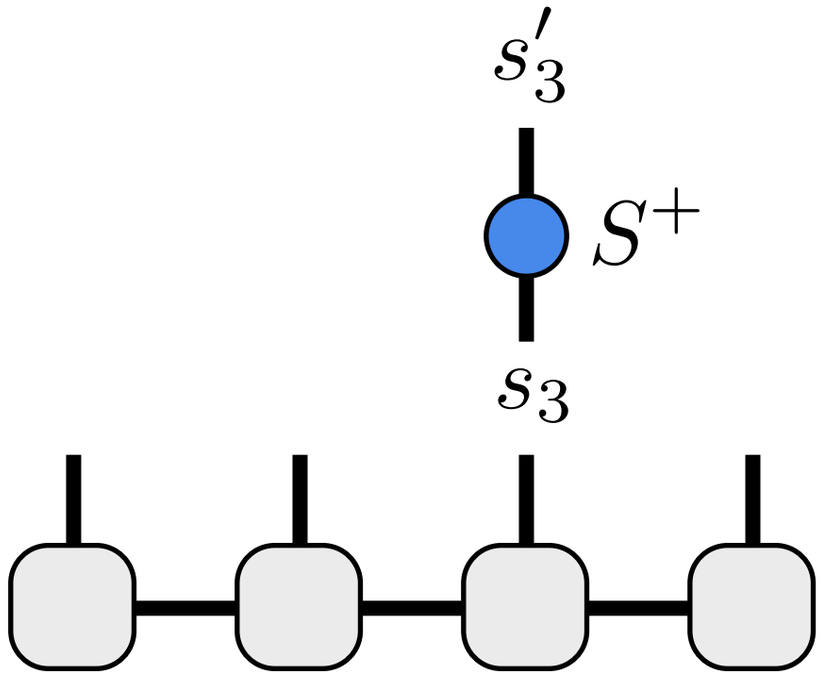


Measuring an MPS Using ITensor:

Can obtain single-site operators from "SiteSet" object:

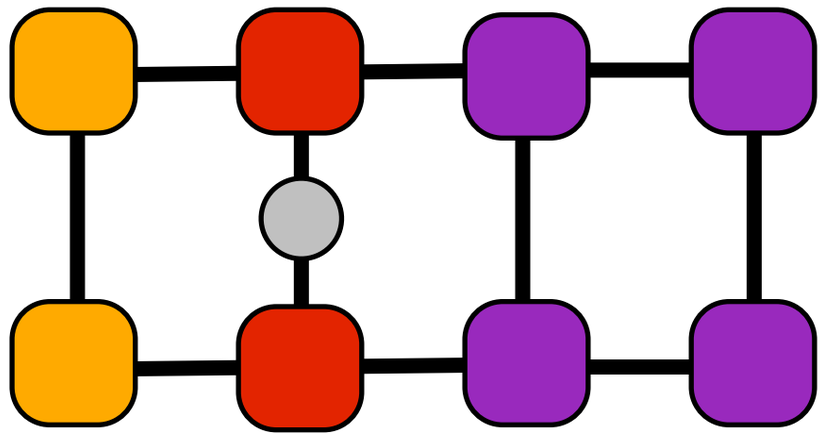
```
//Obtain single-site operators
ITensor Sz = sites.op("Sz",2);
ITensor Sp = sites.op("S+",3);
```

sites.op("Sp",3) ==

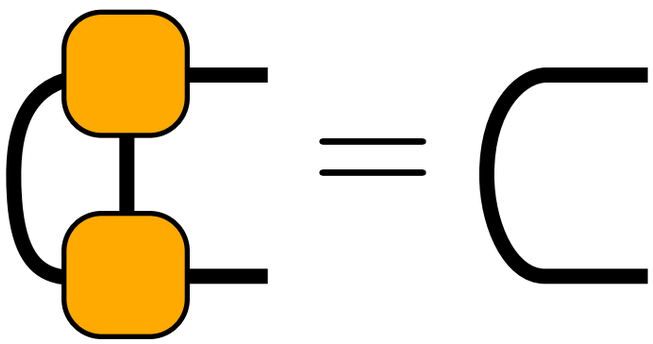


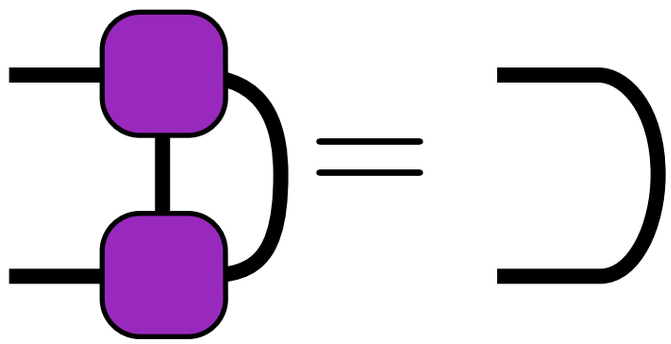
Measuring an MPS Using ITensor:

```
//Measure Sz on second site
```



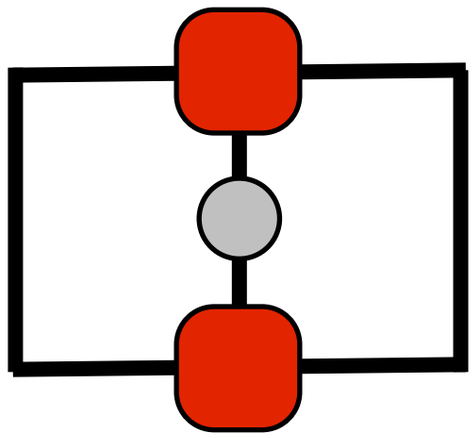
Recall:



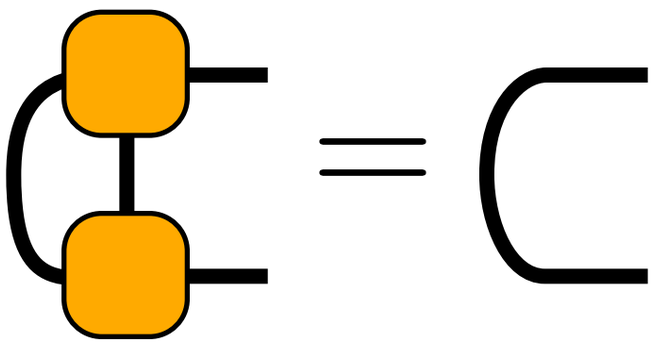


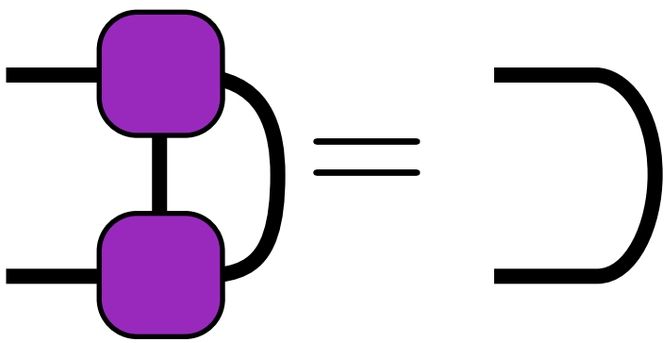
Measuring an MPS Using ITensor:

```
//Measure Sz on second site
```



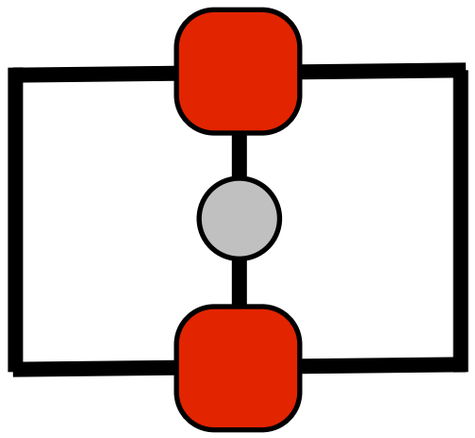
Recall:



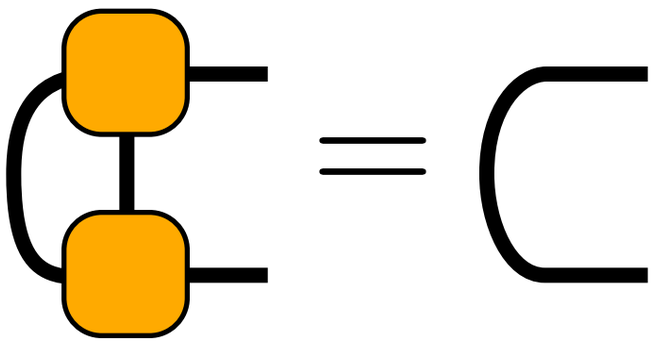


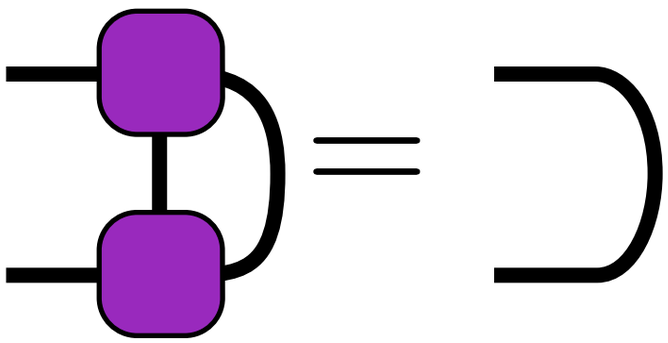
Measuring an MPS Using ITensor:

```
//Measure Sz on second site
Real sz_expect = (dag(prime(psi.A(2),Site))
                  * sites.op("Sz",2)
                  * psi.A(2)).toReal();
```



Recall:





We'll measure the dimer order of the J_1-J_2 model

`<library folder>/tutorial/04_mps`

1. Read through **`j1j2.cc`**; compile; and run

2. Call `psi.position(N/2);` to gauge the MPS to site `N/2`

3. Measure $\hat{B}_{N/2} = \mathbf{S}_{N/2} \cdot \mathbf{S}_{N/2+1}$

```
ITensor wf = psi.A(N/2)*psi.A(N/2+1);
Real b = (dag(prime(wf,Site))*B(sites,N/2)*wf).toReal();
```

4. Repeat for bonds (N/2-1) and (N/2+1). (Don't forget to call `psi.position(b);` to include the "gauge center" `b` in each bond!!) Use to compute and save dimer order parameter:

$$D = \langle \hat{B}_{N/2} \rangle - \frac{1}{2}\langle \hat{B}_{N/2-1} \rangle - \frac{1}{2}\langle \hat{B}_{N/2+1} \rangle$$

Solution for missing code (near line 40 of `j1j2.cc`):

```
psi.position(N/2-1);
ITensor wf = psi.A(N/2-1)*psi.A(N/2);
val += -0.5*(dag(prime(wf,Site))*B(sites,N/2-1)*wf).toReal();


psi.position(N/2);
wf = psi.A(N/2)*psi.A(N/2+1);
val += (dag(prime(wf,Site))*B(sites,N/2)*wf).toReal();


psi.position(N/2+1);
wf = psi.A(N/2+1)*psi.A(N/2+2);
val += -0.5*(dag(prime(wf,Site))*B(sites,N/2+1)*wf).toReal();
```