Hands-on DMRG methods with ITensor

http://itensor.org
C++ library for tensor network wavefunctions

Includes tensor classes, matrix product states, DMRG

Useful for “post DMRG” methods:
  - MPS algorithms (time evolution, METTS)
  - MERA
  - PEPS

Contains both complete algorithms and “building blocks” - customizable at every level
Basic data types:

```c++
int i = 5;
Real r = 2.3456;
string s = "some string";
```

Printing:

```c++
println(i); //prints "5"
println(r); //prints "2.3456"
```
User defined types (objects)

Construct an object of type MyClass:

```cpp
MyClass m("MyClass m", 5);
```

Objects define various methods:

```cpp
m.doThing();

m.setValue(6);

println(m.name());
```
Some objects can be called like functions:

```cpp
FType f;

int j = f(5);
```

Other objects can be used like numbers:

```cpp
Numerical x(1.), y(2.);

Numerical r = x + y;

println(r.value());  //prints 3
```
One Site
Start with a single-site wavefunction, for example a spin $1/2$.

Single-site basis:

\[ |s=1\rangle = |↑\rangle \]
\[ |s=2\rangle = |↓\rangle \]
Most general wavefunction for a spin 1/2:

\[ |\psi\rangle = \sum_{s=1}^{2} \psi_s |s\rangle \]

The \( \psi_s \) are complex numbers.

Slight abuse of notation, may refer to either \( |\psi\rangle \) or \( \psi_s \) as the wavefunction.
Single-site wavefunction as a tensor:

\[ \psi_s \rightarrow \begin{pmatrix}
1 \\
2
\end{pmatrix} = \psi_1 \]
\[ = \psi_2 \]

**Using ITensor:**

Index \( s(“s”,2); \)

//"s" gives the name of the Index when printed
// 2 is the dimension/range of the Index

ITensor psi(s); //default initialized to zero
Now initialize $\psi_s$. First choose $|\psi\rangle = |\uparrow\rangle$

Index s("s",2);

ITensor psi(s); // Prints:

  // psi =

psi(s(1)) = 1; // ITensor r=1: s/Link-79180:2

  // (1) 1.0000000000

PrintData(psi);
Make some operators:

\[
\text{ITensor } Sz(s, \text{prime}(s)); \\
\text{ITensor } Sx(s, \text{prime}(s));
\]

New ITensors start out full out zeros

What does “prime” mean?

\text{prime}(s) \text{ returns copy of } s \text{ with a “prime level” of 1}

Could use different indices (say } s \text{ and } t), \text{ but } s’ \text{ convenient - can easily remove prime later}
Our operators:

\[
\text{ITensor } S_z(s, \text{prime}(s)), \\
S_x(s, \text{prime}(s));
\]

Set their components:

\[
\text{commaInit}(S_z, s, \text{prime}(s)) = 0.5, 0.0, \quad 0.0, -0.5; \\
\text{commaInit}(S_x, s, \text{prime}(s)) = 0.0, 0.5, \quad 0.5, 0.0;
\]
Let’s multiply $\hat{S}_x |\psi\rangle$

$$(\hat{S}_x)_{s'}^s \psi_s = \begin{array}{c}
\text{Index } s' \\
\text{Index } s
\end{array} = \begin{array}{c}
\text{Index } s' \\
\text{Index } s
\end{array}$$

In code,

```c
ITensor phi = Sx * psi;
```

Easy!

* operator contracts matching indices.

Indices $s$ and $s'$ don’t match because of different prime levels.
What state is \( \text{phi} \)?

\[
(\hat{S}_x)_{s'}^s \psi_s = \rho_s = \rho_{s'}
\]

\[
\text{ITensor phi = Sx * psi;}
\text{'PrintData(phi);'}
\]

Prints:

\[
\text{phi = \{ITensor r = 1: s'/Link'---####:2 (2) 0.50000}\}
\]
More interesting $\psi_s$: choose $\theta = \pi/4$ and

\[
\begin{align*}
1 & = \cos \theta/2 \\
2 & = \sin \theta/2
\end{align*}
\]

Real theta = Pi/4; // Prints:
// psi =
psi(s(1)) = cos(theta/2); // ITensor r = 1:
psi(s(2)) = sin(theta/2); // s/Link-1185:2
// (1) 0.9238795325
PrintData(psi); // (2) 0.3826834324
Diagrammatically, measurements (expectation values) look like:

\[ \langle \psi | \hat{S}_z | \psi \rangle \]

For convenience, make:

```cpp
ITensor cpsi = dag(prime(psi));
```

Calculate expectation values:

```cpp
Real zz = (cpsi * Sz * psi).toReal();
Real xx = (cpsi * Sx * psi).toReal();
```
Real zz = (cpsi * Sz * psi).toReal();
Real xx = (cpsi * Sx * psi).toReal();

Printing the results,

println("<Sz> = ", zz);
println("<Sx> = ", xx);

we get the output

<Sz> = 0.35355
<Sx> = 0.35355

\[
\sqrt{(0.35355)^2 + (0.35355)^2} = 1/2
\]
Take a closer look at the tensor contractions:

ITensor Zpsi = Sz * psi;

Zpsi =

Index s matches, so it’s automatically contracted.

Zpsi and cpsi share Index s’, * contracts it, leaving a scalar ITensor

ITensor expect = cpsi * Zpsi;
Real zz = expect.toReal();
Review:

• Construct an Index using

\[
\text{Index } a(“a”,4);
\]

• Construct ITensor using indices \(a, b, c\)

\[
\text{ITensor } T(a,b,c);
\]

• Set ITensor components using

\[
T(a(2),b(1),c(3)) = 5;
\]

• We can prime an Index \(b \rightarrow b'\) using

\[
\text{prime}(b)
\]

• The \(*\) operator automatically contracts matching Index pairs
Quiz:

If we * the following tensors, how many indices remain?

![Diagram with tensors]
Quiz:

If we * the following tensors, how many indices remain?
Code hands-on session:

<library folder>/tutorial/01_one_site

1. Compile by typing “make” then run by typing “./one”

2. Change psi to be an eigenstate of $S_x$

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$$

3. Compute overlap of $|\psi\rangle$ with $|\phi\rangle = \hat{S}_x |\psi\rangle$:

$$\text{Real olap} = (\text{dag(phi)*psi}).\text{toReal}();$$

Try also normalizing $|\phi\rangle$ first using the code

```java
phi *= 1/phi.norm();
```
Two Sites
Most general two-spin wavefunction is

$$\left| \Psi \right\rangle = \sum_{s_1, s_2 = 1}^{2} \psi_{s_1 s_2} \left| s_1 \right\rangle \left| s_2 \right\rangle$$

Amplitudes a rank-2 tensor

$$\psi_{s_1 s_2} =$$
Let's make a singlet

\[
\begin{align*}
1 & \quad 2 \\
\ &= \ 1/\sqrt{2} \\
2 & \quad 1 \\
\ &= \ -1/\sqrt{2}
\end{align*}
\]

Using ITensor:

Index s1("s1",2,Site), s2("s2",2,Site);
ITensor psi(s1,s2); //default initialized to zero
psi(s1(1),s2(2)) = 1./sqrt(2);
psi(s1(2),s2(1)) = -1./sqrt(2);
Why **Site** tag in Index constructor?

```cpp
Index s1("s1",2,Site),
     s2("s2",2,Site);
```

Two Index types: **Link** (default) and **Site**.

Useful for priming just one type of Index, for example.
Let’s make the Heisenberg Hamiltonian\[ \hat{H} = S_1 \cdot S_2 \]
\[ \hat{H} = S^z_1 S^z_2 + \frac{1}{2} S^+_1 S^-_2 + \frac{1}{2} S^-_1 S^+_2 \]

First create operators, for example $S^+$

```plaintext
ITensor Sp1(s1, prime(s1));
commaInit(Sp1, s1, prime(s1)) = 0, 1,
                      0, 0;
```

Multiply and add operators to make $H$:

```plaintext
ITensor H = Sz1*Sz2 + 0.5*Sp1*Sm2 + 0.5*Sm1*Sp2;
```
Tensor form of $H$

\[
\hat{H} = \quad + \frac{1}{2} \quad + \frac{1}{2} 
\]

Showing Index labels

\[
\hat{H} = \quad s_1' \quad s_2' \quad s_1 \quad s_2
\]
Compute singlet energy with this Hamiltonian:

\[
\hat{H} |\psi\rangle = s'_1 \hat{H} s'_2 = s'_1 \hat{H} s'_2
\]

ITensor Hpsi = H * psi;
Compute singlet energy with this Hamiltonian:

\[ \hat{H} |\psi\rangle = \begin{array}{c}
\hat{H} \\
\psi
\end{array} = \begin{array}{c}
\hat{H} \psi
\end{array} \]

```
ITensor Hpsi = H * psi;
Hpsi.mapprime(1, 0);
```
Compute singlet energy with this Hamiltonian:

\[
\hat{H} |\psi\rangle = \begin{pmatrix} s_1' & s_2' \\ s_1 & s_2 \end{pmatrix} \hat{H} \begin{pmatrix} s_1 \ s_2 \end{pmatrix} = \hat{H} \psi \quad ; \quad E = \begin{pmatrix} \psi^\dagger \\ s_1 & s_2 \end{pmatrix} \hat{H} \psi
\]

ITensor Hpsi = H * psi;

Hpsi.mapprime(1,0);

Real E = (dag(psi) * Hpsi).toReal();

Print(E);

//Prints:
//E = -0.75
Or compute energy in one shot:

\[ E_{\text{Sing}} = \text{Real } E = (\text{dag(prime(psi))} * H * \psi).\text{toReal}() \]

Real \( E = (\text{dag(prime(psi))} * H * \psi).\text{toReal}(); \)
Print(E);

//Prints:
//E = -0.75
We’ll use imaginary time evolution to find this Hamiltonian’s ground state

\[ e^{-\beta H/2} |0\rangle \propto |\Psi_0\rangle \]

1. Read through `two.cc`, compile and run by typing “make two” then run by typing “./two”

2. Open `imag_tevol.cc` and implement the code to make \( e^{-\beta H} \) using a Taylor series (summed using a recursive formula)

3. Try increasing \( \beta \), compile, and re-run the code until it converges to the ground state
for(int ord = max_order - 1; ord >= 1; --ord) {
    expH = expH * (x/ord);
    expH.mapprime(2,1);
    expH += I;
}

Solution for missing code (near line 120 of imag_tevol.cc):
The density matrix renormalization group (DMRG) works with a variational wavefunction known as a matrix product state (MPS).

Matrix product states arise from compressing one-dimensional wavefunctions through the singular-value decomposition (SVD).

Let’s see how this works...
Recall:
Singular-value decomposition

Given rectangular (4x3) matrix $M$

$$M = \begin{bmatrix}
0.435839 & 0.223707 & 0.10 \\
0.435839 & 0.223707 & -0.10 \\
0.223707 & 0.435839 & 0.10 \\
0.223707 & 0.435839 & -0.10
\end{bmatrix}$$

Can decompose as

$$\begin{bmatrix}
1/2 & -1/2 & 1/2 \\
1/2 & -1/2 & -1/2 \\
1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & -1/2
\end{bmatrix} \begin{bmatrix}
0.933 & 0 & 0 \\
0 & 0.300 & 0 \\
0 & 0 & 0.200
\end{bmatrix} \begin{bmatrix}
0.707107 & 0.707107 & 0 \\
-0.707107 & 0.707107 & 0 \\
0 & 0 & 1
\end{bmatrix}$$
Matrices $A$ and $B$ one-sided unitaries (isometries):

$$A^\dagger A = 1$$
$$BB^\dagger = 1$$

$D$ diagonal

Elements of $D$ can be chosen:

(I) Real
(II) Positive semi-definite
(III) Decreasing order
Keep fewer and fewer elements of D:

\[
\begin{bmatrix}
1/2 & -1/2 & 1/2 \\
1/2 & -1/2 & -1/2 \\
1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & -1/2
\end{bmatrix}
\begin{bmatrix}
0.933 & 0 & 0 \\
0 & 0.300 & 0 \\
0 & 0 & 0.200
\end{bmatrix}
\begin{bmatrix}
0.707107 & 0.707107 & 0 \\
-0.707107 & 0.707107 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

\[
= M =
\begin{bmatrix}
0.435839 & 0.223707 & 0.10 \\
0.435839 & 0.223707 & -0.10 \\
0.223707 & 0.435839 & 0.10 \\
0.223707 & 0.435839 & -0.10
\end{bmatrix}
\]

\[
\| M - M \|^2 = 0
\]
Keep fewer and fewer elements of $D$:

$$
\begin{align*}
A & = \begin{bmatrix}
1/2 & -1/2 & 1/2 \\
1/2 & -1/2 & -1/2 \\
1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & -1/2 \\
\end{bmatrix} \\
D & = \begin{bmatrix}
0.933 & 0 & 0 \\
0 & 0.300 & 0 \\
0 & 0 & 0 \\
\end{bmatrix} \\
B & = \begin{bmatrix}
0.707107 & 0.707107 & 0 \\
-0.707107 & 0.707107 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\end{align*}
$$

$$
= M_2 = \\
\begin{bmatrix}
0.435839 & 0.223707 & 0 \\
0.435839 & 0.223707 & 0 \\
0.223707 & 0.435839 & 0 \\
0.223707 & 0.435839 & 0 \\
\end{bmatrix}
$$

$$
\| M_2 - M \|^2 = 0.04 = (0.2)^2
$$
Keep fewer and fewer elements of $D$:

$$
\begin{bmatrix}
1/2 & -1/2 & 1/2 \\
1/2 & -1/2 & -1/2 \\
1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & -1/2 \\
\end{bmatrix}
\begin{bmatrix}
0.933 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0.707107 & 0.707107 & 0 \\
\end{bmatrix}
\begin{bmatrix}
0.707107 & 0.707107 & 0 \\
-0.707107 & 0.707107 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\begin{bmatrix}
0.329773 & 0.329773 & 0 \\
0.329773 & 0.329773 & 0 \\
0.329773 & 0.329773 & 0 \\
0.329773 & 0.329773 & 0 \\
\end{bmatrix}
= M_3 = 
\begin{bmatrix}
0.329773 & 0.329773 & 0 \\
0.329773 & 0.329773 & 0 \\
0.329773 & 0.329773 & 0 \\
0.329773 & 0.329773 & 0 \\
\end{bmatrix}

\|M_3 - M\|^2 = 0.13 = (0.3)^2 + (0.2)^2
Keep fewer and fewer elements of $D$:

\[
\begin{bmatrix}
1/2 & -1/2 & 1/2 \\
1/2 & -1/2 & -1/2 \\
1/2 & 1/2 & 1/2 \\
1/2 & 1/2 & -1/2 \\
\end{bmatrix}
\begin{bmatrix}
0.933 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
0.707107 & 0.707107 & 0 \\
-0.707107 & 0.707107 & 0 \\
0 & 0 & 0 \\
0 & 0 & 1 \\
\end{bmatrix}
\]

\[
M_3 = \text{Truncating SVD} = \text{Controlled approximation for } M
\]

\[
\|M_3 - M\|^2 = 0.13 = (0.3)^2 + (0.2)^2
\]
Recall:

Most general two-spin wavefunction

\[ \psi_{s_1 s_2} = \]

Can treat as a matrix:

\[ \psi_{s_1 s_2} = \]
SVD this matrix:

\[ \psi_{s_1 s_2} = s_1 \quad \text{(blue)} \quad s_2 \]

\[ = s_1 \quad \text{(yellow)} \quad \text{(red)} \quad \text{(purple)} \quad s_2 \]

Bend lines back to look like wavefunction:
Using ITensor:

//Say we have a two-site ITensor psi

//Declare ITensors
//to hold results
ITensor A(s1), D, B; //Indices of psi present
   //on A remain, others
   //put onto B

//Call svd method
svd(psi, A, D, B);
What have we gained from SVD?

Generic two-spin wavefunction (say spin $S$):

(2$S+1$)$^2$ parameters
Not clear which parameters important, unimportant

Compressed wavefunction:

SVD tells us which parameters are important, might be very few!

Later see that # parameters also scales much better
This form of wavefunction known as **matrix product state** (MPS)

Why? Amplitude a product of matrices:

\[
|\Psi\rangle = \sum_{s_1, \alpha, \alpha', s_2} A_{s_1 \alpha} D_{\alpha \alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle
\]

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

Canonical form

\[
|\Psi\rangle = \sum_{s_1, \alpha, \alpha', s_2} A_{s_1 \alpha} D_{\alpha \alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle
\]

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

$$|\Psi\rangle = \sum_{s_1,\alpha,\alpha',s_2} A_{s_1\alpha} D_{\alpha\alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle$$

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

\[ |\Psi\rangle = \sum_{s_1, \alpha', s_2} \psi_{s_1 \alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle \]

Left-canonical

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

Matrix $B$ is “right orthogonal” (from SVD)

$$BB^\dagger = I$$

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or "gauges"

Canonical form

\[ |\Psi\rangle = \sum_{s_1, \alpha, \alpha', s_2} A_{s_1 \alpha} D_{\alpha \alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle \]

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

\[
|\Psi\rangle = \sum_{s_1, \alpha, \alpha', s_2} A_{s_1 \alpha} D_{\alpha \alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle
\]

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

\[ |\Psi\rangle = \sum_{s_1, \alpha, \alpha', s_2} A_{s_1 \alpha} D_{\alpha \alpha'} B_{\alpha' s_2} |s_1\rangle |s_2\rangle \]

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

\[ |\Psi\rangle = \sum_{s_1, \alpha, s_2} A_{s_1 \alpha} \psi_{\alpha s_2} |s_1\rangle |s_2\rangle \]

Schollwöck, Ann. of Phys. 326, 96 (2011)
MPS have different equivalent forms, or “gauges”

Matrix $A$ is “left orthogonal” (from SVD)

$$A^\dagger A = I$$

Schollwöck, Ann. of Phys. 326, 96 (2011)
We’ll use the SVD to study the entanglement of a two-site wavefunction

<library folder>/tutorial/03_svd

1. Read through `svd.cc`; compile; and run

2. Make a *normalized* wavefunction that is the sum
   \[(1-\text{mix})\times\text{prod} + \text{mix}\times\text{sing}\]

3. SVD this wavefunction

   ```
   ITensor A(s1),D,B;
   Spectrum spec = svd(psi,A,D,B);
   ```

3. Compute the entanglement entropy using the eigenvalue spectrum “spec” returned by svd.

   *\(n^{th}\) eigenvalue:*
   ```
   spec.eig(n);
   ```

   *Number of eigenvalues:*
   ```
   spec.numEigsKept();
   ```
04 Four
Say we have a 4-site MPS. What can we do with it?

Depends on the gauge!

\[
\Psi = \sum_{\{s\}, \{\alpha\}} M_{\alpha_1}^{s_1} M_{\alpha_1 \alpha_2}^{s_2} M_{\alpha_2 \alpha_3}^{s_3} M_{\alpha_3}^{s_4} |s_1 s_2 s_3 s_4\rangle
\]
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:
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:

\[ \{ \begin{array}{c}
S_1 \\
S_2 \\
S_3 \\
S_4
\end{array} \]  

**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)

Contract, SVD & regroup
Can repeat gauge transformation (repeated SVD)

Contract, SVD & regroup

Contract, SVD & regroup
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:
What have we gained?

Consider measuring an operator on site 1

First, general wavefunction:

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

Cost scales exponentially!

2⁴ in this case
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

Site indices run from 1...d

Link index runs from 1...m (from SVD)

Computational cost \( \sim d^2 m \) (compared to \( d^4 \))
//Define lattice sites
SpinHalf sites(N);
Gauging an MPS Using ITensor:

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

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

Recall:

```
\[ = \]
```

```
\[ = \]
```
Recall:

Measuring an MPS Using ITensor:

//Measure Sz on second site
Measuring an MPS Using ITensor:

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

Recall:

![Graphical representation](image)
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

$$\hat{B}_{N/2} = S_{N/2} \cdot S_{N/2+1}$$

```cpp
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:

$$D = \langle \hat{B}_{N/2} \rangle - \frac{1}{2} \langle \hat{B}_{N/2-1} \rangle - \frac{1}{2} \langle \hat{B}_{N/2+1} \rangle$$
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();
Just as we can measure one-site operators, can measure two-site operators
Just as we can measure one-site operators, can measure two-site operators

Recall:
Since two “center” sites have orthogonal environment, ok to apply operators:
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\[
\text{SVD & regroup}
\]
Would NOT be ok on another bond without regauging

Truncating SVD not globally optimal except at orthogonality center
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Truncating SVD not globally optimal except at orthogonality center
Q: What can we do with this capability?

A: For short-ranged Hamiltonians, can time evolve
Trick is to use Trotter decomposition

Useful for Hamiltonians of the form

\[ H = H_1 + H_2 + H_3 + \ldots \]

For example

\[ H = \sum_j S_j \cdot S_{j+1} \]

\[ = (S_1 \cdot S_2) + (S_2 \cdot S_3) + (S_3 \cdot S_4) \]
For a small time step $\tau$

$$e^{-\tau H} \approx e^{-\tau H_1/2} e^{-\tau H_2/2} e^{-\tau H_3/2} \ldots$$

$$\ldots e^{-\tau H_3/2} e^{-\tau H_2/2} e^{-\tau H_1/2} + \mathcal{O}(\tau^3)$$
Diagrammatically,
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Apply to MPS as follows:
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Apply to MPS as follows:
Apply to MPS as follows:
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Interesting applications:  \[ |\psi'\rangle = e^{-\tau H} |\psi\rangle \]

If \( \tau \) real (imaginary time evolution), enough steps will give ground state

If \( \tau \) imaginary, evolve in real time, study dynamics \[1\]

Evolving through imaginary time \( \beta/2 = 1/(2T) \) simulates finite temperature \[2\]

We’ll implement time evolution for the Heisenberg chain

1. Read through `gates.cc`; compile; and run

2. Apply the gate G to the MPS bond tensor AA. The gate G can be multiplied times AA as if it’s an ITensor.

3. Reset the prime level back to zero using AA’s `.noprime()` class method.

3. Try increasing the total time “ttotal” to imaginary time evolve toward the ground state.
   (Exact energy for 20 sites: $E_0 = -8.6824733317$)
We have seen a Hamiltonian looks like this:
We have seen a Hamiltonian looks like this:

\[ \hat{H} |\Psi\rangle \]

Does a 1d Hamiltonian have a local form/factorization like an MPS?
Want something like

Operator (H) as product of “matrices”
matrix product operator
Focus on just one tensor
Focus on just one tensor
Focus on just one tensor

Specific values for horizontal bonds gives site operator
Focus on just one tensor

Specific values for horizontal bonds gives site operator
Focus on just one tensor

Specific values for horizontal bonds gives site operator

Each tensor a matrix of site operators!
Each tensor a matrix of site operators!

Hamiltonians can be written

$$\begin{bmatrix} 0 & 1 \\ \hat{\sigma}^z & \hat{I} \end{bmatrix} \begin{bmatrix} \hat{I} \\ \hat{\sigma}^z \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
Each tensor a matrix of site operators!

Multiply out

\[
\begin{bmatrix}
\hat{I} \\
\hat{\sigma}_z \\
\end{bmatrix}
\begin{bmatrix}
\hat{I} \\
\hat{I} \\
\end{bmatrix}
\begin{bmatrix}
1 \\
0 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
\hat{\sigma}_z \\
\hat{I} \\
\end{bmatrix}
\begin{bmatrix}
\hat{I} \\
\hat{\sigma}_z \\
\end{bmatrix}
\begin{bmatrix}
1 \\
0 \\
\end{bmatrix}
\]

\[
\hat{\sigma}_1 \otimes \hat{I}_2 + \hat{I}_1 \otimes \hat{\sigma}_2
\]
This Hamiltonian is

\[ H = \sum_i \hat{\sigma}_i^z \]
More complicated example

$$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}^T \begin{bmatrix} \hat{I} & \hat{\sigma}^z & 0 \\ \hat{\sigma}^z & 0 & \hat{I} \\ -h\hat{\sigma}^x & \hat{\sigma}^z & \hat{I} \end{bmatrix} \begin{bmatrix} \hat{I} & \hat{\sigma}^z & 0 \\ \hat{\sigma}^z & 0 & \hat{I} \\ -h\hat{\sigma}^x & \hat{\sigma}^z & \hat{I} \end{bmatrix} = 1$$

$$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$
More complicated example

\[
\begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix}^T \begin{bmatrix}
\hat{I} \\
\hat{\sigma}^z \\
-\hbar \hat{\sigma}^x \hat{\sigma}^z \\
\end{bmatrix} \begin{bmatrix}
\hat{I} \\
\hat{\sigma}^z \\
-\hbar \hat{\sigma}^x \hat{\sigma}^z \\
\end{bmatrix} 1 \\
\begin{bmatrix}
1 \\
0 \\
0
\end{bmatrix}
\]
More complicated example

\[
\begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix}^T \begin{bmatrix}
1 \\
\hat{\sigma}^z \\
-\hbar \hat{\sigma}^x
\end{bmatrix} + \begin{bmatrix}
2 \\
1 \\
0
\end{bmatrix} \begin{bmatrix}
\hat{I} \\
\hat{\sigma}^z \\
-\hbar \hat{\sigma}^x
\end{bmatrix} \begin{bmatrix}
1 \\
0 \\
0
\end{bmatrix}
\]
More complicated example

\[
\begin{pmatrix}
0 \\
0 \\
1
\end{pmatrix}^T \begin{pmatrix}
\hat{I} & \hat{\sigma}^z & 0 \\
\hat{\sigma}^z & \hat{\sigma}^z & \hat{I} \\
-h\hat{\sigma}^x & \hat{\sigma}^z & \hat{I}
\end{pmatrix} \begin{pmatrix}
\hat{I} \\
\hat{\sigma}^z \\
\hat{\sigma}^z \\
-h\hat{\sigma}^x \\
\hat{\sigma}^z \\
\hat{I}
\end{pmatrix} \begin{pmatrix}
1 \\
1 \\
0 \\
0
\end{pmatrix}
\]
More complicated example

\[
\begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix}^T
\begin{bmatrix}
\hat{I} & \hat{\sigma}^z & 0 \\
\hat{\sigma}^z & 0 & \hat{I} \\
-h\hat{\sigma}^x & \hat{\sigma}^z & \hat{I}
\end{bmatrix}
\begin{bmatrix}
\hat{I} \\
\hat{\sigma}^z & 0 \\
-h\hat{\sigma}^x & \hat{\sigma}^z & \hat{I}
\end{bmatrix}
\begin{bmatrix}
1 \\
0 \\
0
\end{bmatrix}
\]

\[
-h\hat{\sigma}^x
\]

\[
\bullet
\]

\[
\bullet
\]
More complicated example

\[
\begin{pmatrix}
0 \\
0 \\
1
\end{pmatrix}^T 
\begin{bmatrix}
1 &  \hat{I} \\
\hat{\sigma}^z & 0 \\
-h\hat{\sigma}^x & \hat{\sigma}^z & \hat{I}
\end{bmatrix}
\begin{pmatrix}
1 \\
\hat{I} \\
\hat{\sigma}^z & 0 \\
-h\hat{\sigma}^x & \hat{\sigma}^z & \hat{I}
\end{pmatrix}
\begin{pmatrix}
1 \\
1 \\
0 \\
0
\end{pmatrix}
\]

\[ -h\hat{\sigma}^x \]

\[ \hat{I} \]
The Hamiltonian is

$$\hat{H} = \sum_j \hat{\sigma}_j^z \sigma_j^z + 1 - \hbar \hat{\sigma}_j^x$$
DMRG is the best method for finding ground states of 1d Hamiltonians

Want to solve \( H|\Psi\rangle = E|\Psi\rangle \)

Think of H as MPO
Important: MPS should be in definite gauge
i.e. most tensors unitary
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i.e. most tensors unitary
This way, tensors left/right of center define orthonormal bases
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This way, tensors left/right of center define orthonormal bases
Can project Hamiltonian into this basis
Can project Hamiltonian into this basis
Doing the same on the right gives
Doing the same on the right gives
Doing the same on the right gives

\[ \tilde{H} | \tilde{\Psi} \rangle = \tilde{E} | \tilde{\Psi} \rangle \]
Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!
Can efficiently multiply effective $\hat{H}$ times $|\tilde{\Psi}\rangle$

Order important!
Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!

$2 \sim m^3$
Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!

$2 \sim m^3$

$3 \sim m^2$
Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!

$2 \sim m^3$

$3 \sim m^2$

$4 \sim m^2$
Can efficiently multiply effective $\tilde{H}$ times $|\tilde{\Psi}\rangle$

Order important!
Use Lanczos/Davidson to solve (sparse matrix eigensolver)
Now, with improved wavefunction, shift orthogonality center (using SVD)

Important to truncate to m singular values ("number of states kept" in DMRG)
Now, with improved wavefunction, shift orthogonality center (using SVD)

Important to truncate to m singular values ("number of states kept" in DMRG)
Grow projected Hamiltonian
Grow projected Hamiltonian
Grow projected Hamiltonian
Grow projected Hamiltonian

Recover older projected Hamiltonian saved in memory
Iterating leads to sweeping procedure
Iterating leads to sweeping procedure

1. Solve eigenproblem
Iterating leads to sweeping procedure

I. Solve eigenproblem
II. SVD wavefunction
Iterating leads to sweeping procedure

I. Solve eigenproblem
II. SVD wavefunction
III. Grow effective $H$
Iterating leads to sweeping procedure
Iterating leads to sweeping procedure
Iterating leads to sweeping procedure
Iterating leads to sweeping procedure
Iterating leads to sweeping procedure
Iterating leads to sweeping procedure
We’ll implement a key missing step of the DMRG algorithm

1. Read through `dmrg.cc`; compile; and run

2. SVD the two-site tensor phi into factors A, D, B
   The last argument to svd should be “opts” to pass through parameters controlling truncation:

   ```
   svd(phi, ... , opts);
   ```

3. Multiply the singular-value tensor D back into A or B as appropriate to shift orthogonality center of MPS.

4. Add code to print out the energy at each step (or even to measure other local operators).