Tensor Networks

How physicists can tackle exponentially hard problems

March 5, 2019  |  Patrick Emonts  |  Max Planck Institute of Quantum Optics
Motivation

- experiment
- model
- hypothesis
- nature
How complex is this problem?

We take a system that can take two states \( \uparrow \) and \( \downarrow \).

Number of possibilities

\[ Z = 2^N \]
How bad is exponential scaling?

Physical example
- $10^{23}$ Number of atoms in 12 g of carbon
- $10^{80}$ Number of atoms in the visible universe
Quantum Mechanics in 2 slides – Slide 1

Hilbert space $\mathcal{H}$  vector space of all possible configurations

state $|\psi\rangle$ vector in $\mathcal{H}$ that describes the state of the system

Hamilton operator $H$ Linear operator that describes the energy of the system

Note on Notation: Bra and Ket vectors

$|\psi\rangle$ is a column vector

$\langle \psi |$ is a row vector
Quantum Mechanics in 2 slides – Slide 2

<table>
<thead>
<tr>
<th>Schrödinger equation</th>
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<td>[ i \frac{d}{dt}</td>
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<th>time-independent Schrödinger equation (time-ind. Hamiltonian)</th>
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<th>Expectation values</th>
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<td>Probability theory</td>
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<td>[ \langle X \rangle = P(X) X ]</td>
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### Expressing spins with matrices

#### Definitions

|\(\uparrow\rangle\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} |

|\(\downarrow\rangle\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} |

\[ S_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

#### Calculating with spins

\[ S_z |\uparrow\rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2} |\uparrow\rangle \]
Combining multiple spins

Consider a system consisting of two spins that can take two values (\(\downarrow\) and \(\uparrow\)).

**Hilbert space \(\mathcal{H}\)**

\[\mathcal{H} = \text{span}\{ |\downarrow_1\rangle |\downarrow_2\rangle, |\downarrow_1\rangle |\uparrow_2\rangle, |\uparrow_1\rangle |\downarrow_2\rangle, |\uparrow_1\rangle |\uparrow_2\rangle\}\]

Spins on different sites are combined by tensor products:

\[
|\downarrow_1\rangle |\downarrow_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
\]

\[
|\downarrow_1\rangle |\uparrow_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}
\]

\[
|\uparrow_1\rangle |\downarrow_2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}
\]

\[
|\uparrow_1\rangle |\uparrow_2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\]
Letting spins interact

Interaction of two spins

\[ H = -J (S_1^z \otimes S_2^z) \]

Matrix representation

\[ H = -J \left( \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \otimes \left( \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \]

\[ = \frac{J}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]
Calculating an expectation value

**Preparation of a state**

\[
|\psi\rangle = \sqrt{0.5} |\uparrow_1\rangle |\downarrow_2\rangle + \sqrt{0.5} |\downarrow_1\rangle |\uparrow_2\rangle \\
= \sqrt{0.5} |\uparrow_1 \downarrow_2\rangle + \sqrt{0.5} |\downarrow_1 \uparrow_2\rangle \\
= \sqrt{0.5} |\uparrow\downarrow\rangle + \sqrt{0.5} |\downarrow\uparrow\rangle \\
= \begin{pmatrix}
0 \\
\sqrt{0.5} \\
\sqrt{0.5} \\
0
\end{pmatrix}
\]

**Expectation value**

\[
\langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \\
= \langle \psi | H | \psi \rangle \\
= \frac{J}{4} \begin{pmatrix}
0 & \sqrt{0.5} & \sqrt{0.5} & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & -1 \\
0 & 0 & 0 & 1
\end{pmatrix} \begin{pmatrix}
0 \\
\sqrt{0.5} \\
\sqrt{0.5} \\
0
\end{pmatrix} \\
= -\frac{J}{4}
\]
Computational complexity of many-body systems scales exponentially with the system size. We cannot solve those systems exactly and have to use approximate methods.

Quantum mechanical systems evolve according to the Schrödinger equation. We are interested in the ground-state $|\Psi\rangle$ and expectation values $\langle E \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$.
Tensor Networks

Idea

Use an Ansatz with polynomially many parameters although the Hilbert space has exponentially many states

Hilbert space

We explore only a small part of the Hilbert space
What is a Tensor Network?

A general quantum mechanical state

\[ |\psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1...\sigma_n} |\sigma_1\sigma_2...\sigma_n\rangle \]

Example: \( |\psi\rangle = \sqrt{0.5} |\uparrow_1\rangle |\downarrow_2\rangle + \sqrt{0.5} |\downarrow_1\rangle |\uparrow_2\rangle \)

\[ \mathcal{H} = \text{span}\{ |\downarrow_1\rangle |\downarrow_2\rangle, |\downarrow_1\rangle |\uparrow_2\rangle, |\uparrow_1\rangle |\downarrow_2\rangle, |\uparrow_1\rangle |\uparrow_2\rangle \} \]

\[ c_{\downarrow_1,\downarrow_2} = 0 \]

\[ c_{\downarrow_1,\uparrow_2} = \sqrt{0.5} \]

\[ c_{\uparrow_1,\downarrow_2} = \sqrt{0.5} \]

\[ c_{\uparrow_1,\uparrow_2} = 0 \]
What is a Tensor Network?

A general quantum mechanical state

\[ |\psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1...\sigma_N} |\sigma_1\sigma_2...\sigma_n\rangle \]

Problem

The coefficients depend on the configuration of all spins. Thus, there are exponentially many coefficients.

A fancy way to write a quantum mechanical state

\[ |\psi\rangle = \sum_{\sigma_1...\sigma_n} \sum_{a_1,...,a_{n-1}} A_{a_1}^{\sigma_1} A_{a_2}^{\sigma_2} ... A_{a_{n-2}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_{n-1}} A_{a_n}^{\sigma_n} c_{\sigma_1...\sigma_n} |\sigma_1\sigma_2...\sigma_n\rangle \]
A Tensor Network State

\[ |\psi\rangle = \sum_{\sigma_1...\sigma_n} \sum_{a_1,...,a_{n-1}} A^{\sigma_1}_{a_1,a_2} A^{\sigma_2}_{a_2,a_3} \cdots A^{\sigma_{n-1}}_{a_{n-2},a_{n-1}} A^{\sigma_n}_{a_{n-1}} |\sigma_1\sigma_2...\sigma_n\rangle \]

Dimensions of object \( A \)

- \( \sigma \): physical index: (↑, ↓)
- \( a \): virtual index

- Dimension of physical index: \( d \approx 10 \)
- Dimension of virtual index: \( D \approx 100 \)
The number of legs determines the number of indices of the object

- A connection $\Leftrightarrow$ Contraction of indices
## Pictorial representation as Arrays

The pictorial representation of arrays is shown in a grid format, with indices `i`, `j`, and `k`. Each element of the array is represented by (i, j, k) coordinates. The grid structure helps visualize the arrangement of elements in a three-dimensional space.
Calculations with pictures

Matrix-Vector Multiplication

\[ v_i = \sum_{i,j} A_{ij} b_j \]

Matrix-Matrix Multiplication

\[ C_{kl} = \sum_{i,k,l} A_{ki} B_{li} \]
Calculations with pictures – Quiz

Trace

\[ c = \sum_{i,j} A_{ij}B_{ji} \]

= Tr[AB]
Calculations with pictures – Quiz

\[ c = \sum_{i,j} A_{ij} B_{ji} \]

= \text{Tr}[AB]
Tensor manipulations – Grouping

Tensor to Matrix

\[ A_{i,j,k} = A_{i,(jk)} = A_{i,m} \]

Pictorial language

\[ i \rightarrow j = j \rightarrow k = i \rightarrow m \]
Splitting of tensor

\[ A = U \cdot S \cdot V^\dagger \]
**Singular Value Decomposition**

$$M = U \cdot S \cdot V^\dagger,$$

- $M$ arbitrary $mxn$ matrix
- $U$ unitary $mxm$ matrix
- $S$ diagonal $mxn$ matrix
- $V$ unitary $nxn$ matrix
SVD – Truncation

Note

The shape of $M$ does not change since we are only manipulating an index which we contract.
SVD – Example

Original Image

Truncated Image (20 SV)
Matrix Product States

A Tensor Network State

\[ |\psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} \sum_{a_1, \ldots, a_{n-1}} A_1^{\sigma_1} A_{a_1}^{\sigma_2} \cdots A_{a_{n-2}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_n} |\sigma_1 \sigma_2 \ldots \sigma_n\rangle \]

- Dimension: 1D
- Typical quantities
  - correlations
  - expectation values of observables
Matrix Product States – Bra, Ket and Norms

\[ |\Psi\rangle = \quad \langle \Psi| = \quad \langle |\Psi\rangle = \]

\[ \langle \Psi|\Psi\rangle = \]

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Matrix Product States – How to get the Tensors?

A general quantum mechanical state

\[ |\psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} c_{\sigma_1, \sigma_2, \ldots, \sigma_N} |\sigma_1 \sigma_2 \ldots \sigma_n\rangle \]

Matrix Product state

\[ |\psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} \sum_{a_1, \ldots, a_{n-1}} A_{a_1}^{\sigma_1} A_{a_1, a_2}^{\sigma_2} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_n} |\sigma_1 \sigma_2 \ldots \sigma_n\rangle \]
Matrix Product States – Why contraction order matters!

Different contraction orders yield different contraction complexities

\[ \langle \psi | \psi \rangle = \]
Matrix Product States – Why contraction order matters!

The number of matrix elements needed scales exponentially with the number of sites $N$.

\[ \mathcal{O}(D^2d^2) \]
\[ \mathcal{O}(D^2d^3) \]
\[ \mathcal{O}(D^2d^4) \]
\[ \mathcal{O}(Dd^5) \]
\[ \mathcal{O}(D^2d^2) \]
\[ \mathcal{O}(D^2d^3) \]
\[ \mathcal{O}(D^2d^4) \]
\[ \mathcal{O}(Dd^5) \]
\[ \mathcal{O}(d^6) \]
Matrix Product States – Why contraction order matters!

Complexity

The number of matrix elements does not depend on the number of sites $N$ at all and the procedure scales linear in time with $N$.
Matrix Product States – Calculation of an expectation value

**Expectation values**

\[
\langle O \rangle = \frac{\langle \psi | O | \psi \rangle}{\langle \psi | \psi \rangle}
\]

\[
\langle O_i \rangle = \frac{\langle \psi | O_i | \psi \rangle}{\langle \psi | \psi \rangle}
\]

\[
\langle \psi | O | \psi \rangle =
\]

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MPS is an Ansatz to describe many-body states with polynomially many parameters

- The pictorial description simplifies the formulation of calculations and algorithms
- We have to be careful about the order of contractions
Minimization of energy

Goal
Find the groundstate of a Hamiltonian $H$, i.e. find the state with the smallest energy eigenvalue.

Classical mechanics

Quantum mechanics
Find $|\psi_{\text{min}}\rangle$ such that

$$E_{\text{min}} = \frac{\langle \psi_{\text{min}} | H | \psi_{\text{min}} \rangle}{\langle \psi_{\text{min}} | \psi_{\text{min}} \rangle}$$
is minimal.
Tensor network notation

A Tensor Network State

\[ |\psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} \sum_{a_1, \ldots, a_{n-1}} A_{\sigma_1}^{a_1} A_{\sigma_2}^{a_1, a_2} \ldots A_{\sigma_{n-1}}^{a_{n-2}, a_{n-1}} A_{\sigma_n}^{a_{n-1}} |\sigma_1 \sigma_2 \ldots \sigma_n\rangle \]
Calculation of energies

Expectation value

$$\langle E \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Calculation of an observable

$$\langle \Psi | O | \Psi \rangle =$$
Energy minimization via imaginary time evolution

Motivation

The ground state is the state with the smallest energy. All other states are suppressed more quickly by an exponential.

Time evolution in imaginary time

\[
\langle \psi_0 \rangle = \lim_{\delta \to \infty} \frac{\exp(-H\delta) \langle \psi \rangle}{\|\exp(-H\delta) \langle \psi \rangle\|} = \lim_{\delta \to \infty} \frac{U(\delta) \langle \psi \rangle}{\|U(\delta) \langle \psi \rangle\|}
\]
Trotterization of an operator

Evolution operator

\[ U(\delta) = e^{-\delta H} \]

Ising Model

\[ H = \sum_i S_i^z S_{i+1}^z = \sum_i h_{i,i+1} \]

\[ H_{\text{even}} = \sum_{i \text{ even}} h_{i,i+1} \quad H_{\text{odd}} = \sum_{i \text{ odd}} h_{i,i+1} \]

\[ H = H_{\text{even}} + H_{\text{odd}} \]
Trotterization of an operator

Evolution operator

\[ U(\delta) = e^{-\delta H} \]

Trotterization of an operator

\[ U(\delta) = e^{-\delta H} \]
\[ = e^{-\delta H_{\text{even}}} e^{-\delta H_{\text{odd}}} e^{-\delta^2 [H_{\text{even}}, H_{\text{odd}}]} \]
\[ \approx e^{-\delta H_{\text{even}}} e^{-\delta H_{\text{odd}}} \]

Pictorial representation
Making life easy: infinite systems

General MPS

Translationally invariant MPS
Back to the start: An MPS with diagonal matrices

We started with

\[ c_{\sigma_1,\sigma_2,\ldots,\sigma_N} = \]

and got

\[ c_{\sigma_1,\sigma_2,\ldots,\sigma_N} = \]
The iTEBD algorithm

We start with an infinite system that consists of two sites A and B

Disclaimer
This algorithm is proven to be numerically unstable. You should NOT use it in research, it is shown here due to its simplicity.
The iTEBD algorithm

We start with an infinite system that consists of two sites A and B

Disclaimer
This algorithm is proven to be numerically unstable. You should NOT use it in research, it is shown here due to its simplicity.
The iTEBD algorithm

1. Apply the operator $U$ to sites $A$ and $B$
2. Contract all indices and group indices (blue and green)
3. Compute SVD of the tensor
4. Reintroduce $\lambda_B$
5. Update $\Gamma_A$ and $\Gamma_B$
6. Repeat the procedure with the sites $B$ and $A$
Results for an Ising spin system

Parameters

- $D = 10$
- $\delta = 0.001$
Outlook

PEPS

MERA
Tensor Networks

How physicists can tackle exponentially hard problems

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References I

**Basics**


**iTEBD**