How to make big Hilbert spaces small

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Outline

- Motivation
- Compressing $|\Psi\rangle$ with SVD
- Matrix Product States (MPS)
- Density matrix renormalization group (DMRG), roughly

Motivation

N sites, each with spin-1/2. Find ground state of:

$$\mathcal{H} = -J\sum_{i=1}^{N}\sigma_i^z\sigma_{i+1}^z - h\sum_{i=1}^{N}\sigma_i^x$$

Hilbert space dimension $\sim 2^N$

Exact diagonalization O.K. for $N \lessapprox 20$ on laptop

$N \to \infty$: needle in the haystack

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$N \to \infty$: needle in the haystack

$\boxed{!!}$ For many relevant Hamiltonians, haystack $\ll$ full Hilbert space

e.g. haystack $\sim$ subspace of states with low entanglement entropy

$\implies$ Clever parameterization + efficient algorithms = ☺?

Compressing $|\Psi\rangle$?

$$|\Psi\rangle = \sum_{\{\sigma\}} \psi_{\sigma_1\sigma_2\ldots\sigma_N} |\sigma_1\sigma_2\ldots\sigma_N\rangle$$

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- How to approximate $|\Psi\rangle$ well without storing d^N coefficients?
- Possible to reduce entanglement entropy after approximation?

Compressing $|\Psi\rangle$ with SVD

Theorem (Singular value decomposition)

For any M, there are unitary U, V for which $M = USV^\dagger$, where $S = diag(s_1, s_2, \ldots)$.

s_i: singular values of $M \equiv$ eigenvalues of $\sqrt{M^\dagger M}$. $s_i \geq 0$

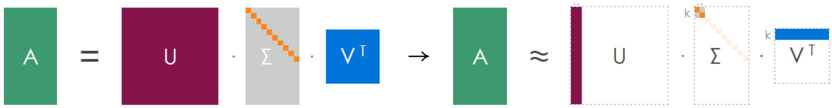
Theorem (Low-rank approximation)

The HS-distance from a rank-m matrix $A_{n\times n}$ to the nearest $n \times n$ matrix of rank $k \leq m$ is the square root of the sum of the squares of the smallest $n - k$ singular values of A.

Hilbert-Schmidt norm:

$$\|A\|_{HS} = \sqrt{\sum |A_{ij}|^2} = \sqrt{\mathrm{Tr}(A^\dagger A)} = \sqrt{\sum s_i^2}$$

Compressing $|\Psi\rangle$ with SVD



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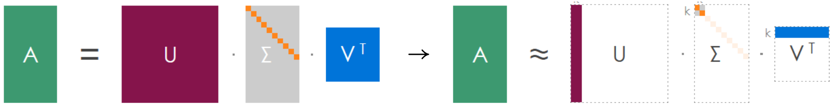
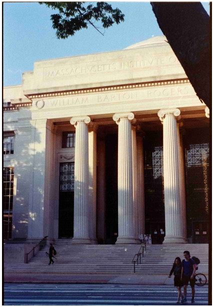


Application: image compression



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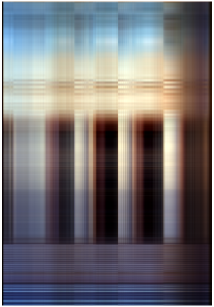

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Split N spins on a 1d chain into $L + R$:

$$|\Psi\rangle = \sum_{l,r}^{\min(N_L, N_R)} \psi_{lr} |l\rangle |r\rangle$$

ψ_{lr} has two indices $\implies$ treat as a matrix (NOT an operator!)

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Apply SVD: $\quad \psi_{lr} = [\mathbf{U}\ \mathbf{D}\ \mathbf{V}]_{lr}$

$\mathbf{U}, \mathbf{V}$ are unitary. $\mathbf{D} = \mathrm{diag}(s_1, s_2, \ldots)$:

$$\begin{aligned} s_i\text{'s} &= \text{singular values of } \psi_{lr} \\ &= \text{eigenvalues of } \sqrt{\psi^\dagger \psi} = \sqrt{\rho} \implies s_i^2 = \text{eigenvalues of } \rho \end{aligned}$$

Compressing $|\Psi\rangle$ with SVD

After SVD:

$$
\begin{aligned}
|\Psi\rangle &= \sum_{l,r} \sum_{i} \mathbf{U}_{li} \mathbf{D}_{ii} \mathbf{V}_{ir} |l\rangle |r\rangle \\
&= \sum_{i} \sum_{l,r} \mathbf{U}_{li} \mathbf{D}_{ii} \mathbf{V}_{ir} |l\rangle |r\rangle \\
&= \sum_{i} s_i |i\rangle_L |i\rangle_R \quad \leftarrow \text{ Schmidt decomposition}
\end{aligned}
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Can simply read off reduced density matrices:

$$\rho_L = \psi\psi^\dagger = \sum_i s_i^2\,|i\rangle_L\,\langle i|_L \qquad \rho_R = \psi^\dagger\psi = \sum_i s_i^2\,|i\rangle_R\,\langle i|_R$$

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$$

Normalization:

$$
\mathrm{Tr}\left(\psi^\dagger\psi\right) = \sum_i s_i^2 = 1 \implies s_i^2\text{: probability for i}^{\text{th}}\text{ Schmidt state pair}
$$

Example:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle - |\uparrow\downarrow\rangle\right)$$

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Matrixify and SVD:

$$|\Psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle \quad \text{with} \quad [\psi_{ij}] = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}$$

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How? von Neumann entanglement entropy between L and R:

$$S(\rho_L) = -\operatorname{Tr}[\rho_L \ln \rho_L] = -\operatorname{Tr}[\rho_R \ln \rho_R] = S(\rho_R)$$

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Eigenvalues of ρ_L, ρ_R are exactly $\{s_i\}$.

$$\rho_L = \psi\psi^\dagger = \sum_i s_i^2 \left|i\right\rangle_L \left\langle i\right|_L \qquad \rho_R = \psi^\dagger\psi = \sum_i s_i^2 \left|i\right\rangle_R \left\langle i\right|_R$$

So,
$$S = S(\rho_L) = S(\rho_R) = -\sum_i^{\sim 2^{N/2}} s_i^2 \ln s_i^2 \to -\sum_i^m s_i^2 \ln s_i^2$$

Drop small s_i's $\implies$ reduce S and exponential compression, $m \sim \mathcal{O}(100)$

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Entanglement entropy is 0 $\implies$ not entangled (makes sense)

But wait...

We need $|\Psi\rangle$ to compress. But we want to find such a $|\Psi\rangle$ for some H.

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DMRG:

- numerical variational technique for finding ground states
- works with MPS, not $|\Psi\rangle$
- most efficient method for 1d systems

MPS

Every $|\Psi\rangle$ can be written as an MPS. From Schmidt decomposition:

$$|\Psi\rangle = \sum_i s_i |i\rangle_L |i\rangle_R = \sum_{i_m} s_i |i_m\rangle_L |i_m\rangle_R$$

m : position on the 1d chain where the $L - R$ split occurs.

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$\underline{|i_m\rangle_L \text{ can be built recursively}}$:

$$|i_1\rangle_L = \sum_{\sigma_1} A^{\sigma_1}_{i_1} |\sigma_1\rangle$$

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$$|i_1\rangle_L = \sum_{\sigma_1} A^{\sigma_1}_{i_1} |\sigma_1\rangle$$

$$|i_2\rangle_L = \sum_{i_1,\sigma_2} A^{\sigma_2}_{i_2,i_1} |i_1\rangle_L |\sigma_2\rangle = \sum_{i_1,\sigma_1,\sigma_2} A^{\sigma_1}_{i_1} A^{\sigma_2}_{i_2,i_1} |\sigma_1\sigma_2\rangle = \sum_{\sigma_1,\sigma_2} (A^{\sigma_1} A^{\sigma_2})_{1,i_2} |\sigma_1\sigma_2\rangle$$

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$$|i_3\rangle_L = \sum_{\sigma_1,\sigma_2,\sigma_3} (A^{\sigma_1} A^{\sigma_2} A^{\sigma_3})_{1,i_3} |\sigma_1\sigma_2\sigma_3\rangle$$

$$\vdots$$

MPS

Schmidt states:

$$|i_m\rangle_L = \sum_{\{\sigma\}_1^N} (A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_m})_{1,i_m} |\sigma_1 \sigma_2 \dots \sigma_m\rangle$$

$$|i_m\rangle_R = \sum_{\{\sigma\}_{m+1}^N} (B^{\sigma_{m+1}} B^{\sigma_{m+2}} \dots B^{\sigma_N})_{i_m,1} |\sigma_{m+1} \sigma_{m+2} \dots \sigma_N\rangle$$

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Full wavefunction:

$$\boxed{|\Psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_m} \; S \; B^{\sigma_{m+1}} B^{\sigma_{m+2}} \dots B^{\sigma_N} |\sigma_1 \sigma_2 \dots \sigma_N\rangle}$$

Matrix dimensions:

$$\underbrace{(1 \times d), (d \times d^2), \dots,}_{A} \underbrace{(d^{N/2} \times d^{N/2})}_{S}, \underbrace{\dots (d^2 \times d), (d \times 1)}_{B}$$

MPS

Example:

$$|\mathrm{GHZ}_4\rangle = \frac{|0000\rangle + |1111\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \sum_{\{\sigma\}} A_1^{\sigma_1} A_2^{\sigma_2} A_3^{\sigma_3} A_4^{\sigma_4} |\sigma_1 \sigma_2 \sigma_3 \sigma_4\rangle$$

where

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where

$$A_1^0 = \begin{pmatrix} 1 & 0 \end{pmatrix}, \quad A_2^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad A_3^0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad A_4^0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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MPS & Hilbert space decimation

Idea: Motivated by, not allowing matrix dimensions exceed a fixed D

From:

$$(1 \times d), (d \times d^2), \ldots, (d^{N/2} \times d^{N/2}), \ldots (d^2 \times d), (d \times 1)$$

To:

$$(1 \times d), (d \times d^2), \ldots (D \times D), (D \times D), (D \times D) \ldots (d^2 \times d), (d \times 1)$$

To generalize, can make all matrices to $D \times D$, so that

$$\boxed{|\Psi\rangle = \sum_{\{\sigma\}} \mathrm{Tr}\left[A_1^{\sigma_1} A_2^{\sigma_2} \ldots A_m^{\sigma_m} A_{m+1}^{\sigma_{m+1}} A_{m+2}^{\sigma_{m+2}} \ldots A_N^{\sigma_N}\right] |\sigma_1 \sigma_2 \ldots \sigma_N\rangle}$$

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where

$$A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad A^1 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Can see that

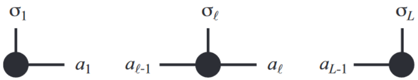
$$\mathrm{Tr}\left[A^{\sigma_1} A^{\sigma_2} A^{\sigma_3} A^{\sigma_4}\right] = 1 \iff \sigma_1 = \sigma_2 = \sigma_3 = \sigma_4$$

So far

- SVD & Schmidt decomposition allows for compressing $|\Psi\rangle$
- From Schmidt decomposition to MPS for general $|\Psi\rangle$
- Decimate Hilbert space by keeping matrices in MPS at $(D \times D)$
- Hilbert space "smaller" $(ND^2$ vs $d^N)$ and MPS corresponds to $|\Psi\rangle$ with lower entanglement entropy
- MPS: natural way to describe ground states of relevant Hamiltonians

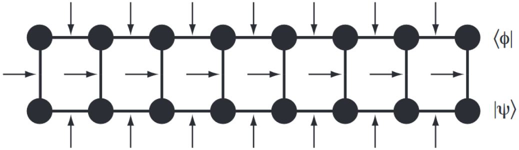
Graphical notation

Matrices:



MPS:

Overlap for two MPS's (arrows indicate sum over indices)



Graphical notation

MPO: Matrix product operators.

If $\langle \sigma_1 \sigma_2 \ldots \sigma_N | \Psi \rangle = A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_N}$, then

$$\langle \sigma_1 \ldots \sigma_N | \hat{O} | \sigma'_1 \ldots \sigma'_N \rangle = W^{\sigma_1 \sigma'_1} W^{\sigma_2 \sigma'_2} \ldots W^{\sigma_{N-1} \sigma'_{N-1}} W^{\sigma_N \sigma'_N}$$

or

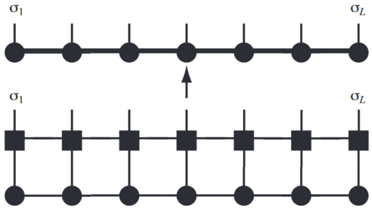
$$\hat{O} = \sum_{\{\sigma, \sigma'\}} W^{\sigma_1 \sigma'_1} W^{\sigma_2 \sigma'_2} \ldots W^{\sigma_{N-1} \sigma'_{N-1}} W^{\sigma_N \sigma'_N} |\sigma\rangle \langle \sigma'|$$

$\implies$ can calculate $\langle \Psi | H | \Psi \rangle$ in MPS language!

Graphical notation

MPO on MPS:

$$\hat{O}\,|\Psi\rangle = \sum_{\{\sigma,\sigma'\}} (W^{\sigma_1\sigma_1'}W^{\sigma_2\sigma_2'}\dots)(A^{\sigma_1}A^{\sigma_2}\dots)\,|\sigma\rangle = \sum_{\{\sigma\}} N^{\sigma_1}N^{\sigma_2}\dots|\sigma\rangle$$

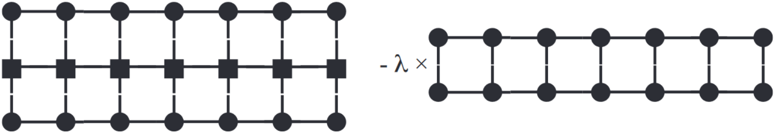


Ground state search

Variationally extremize

$$\langle\Psi| H |\Psi\rangle - \lambda \langle\Psi|\Psi\rangle, \text{ so that } |\Psi\rangle \to |\Psi_g\rangle, \ \lambda \to E_0$$

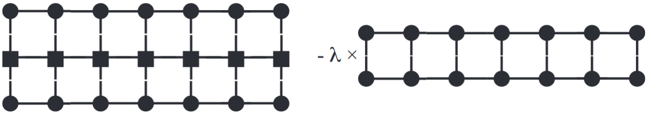
Graphically,



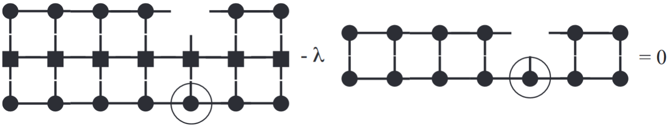
<u>Idea</u>: Keep matrices on all sites but one (l) constant, optimize elements of $A_l^{\sigma_l}$. Sweep through l.

Ground state search

Minimizing



≡ solving



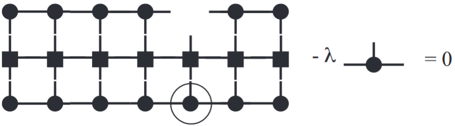
$\Longrightarrow$ a generalized eigenvalue problem, where we treat $A_l^{\sigma_l}$ as a vector v

Ground state search

<u>Aside</u>: left-/right-normalized

$$\sum_{\sigma_l} A^{\sigma_l \dagger} A^{\sigma_l} = I \qquad \sum_{\sigma_l} B^{\sigma_l \dagger} B^{\sigma_l} = I$$

If $|\Psi\rangle$ is both left- and right-normalized,



$\implies$ standard eigenvalue problem

Ground state search: DMRG

Algorithm (DMRG):

- Start with initial guess for $|\Psi\rangle$, which is right-normalized $|\Psi\rangle \sim BBBBB\ldots$
- Calculate current state of network for sites $N-1$ through 1
- *Right-sweep*: From $l=1$ through $L-1$: at l, solve for M^{σ_l} then left-normalize into A^{σ_l} by SVD; remaining matrices of the SVD are multiplied into $M^{\sigma_{l+1}}$
- *Left-sweep*: From $l=L$ through $l=2$: at l, solve for M^{σ_l} then right-normalize into $B^{\sigma_l} bySVD$; remaining matrices of the SVD are multiplied into $M^{\sigma_{l-1}}$
- Repeat right and left sweeps until convergence

Ground state search (DMRG)

Algorithm, formalized: Subscript denotes the number of updates

$$
\begin{aligned}
M_0 B_0 B_0 B_0 &\xrightarrow{\text{diag}} M_1 B_0 B_0 B_0 \xrightarrow{\text{SVD}} A_1 M_0 B_0 B_0 \\
&\xrightarrow{\text{diag}} A_1 M_1 B_0 B_0 \xrightarrow{\text{SVD}} A_1 A_1 M_0 B_0 \\
&\xrightarrow{\text{diag}} A_1 A_1 M_1 B_0 \xrightarrow{\text{SVD}} A_1 A_1 A_1 M_0 \\
&\xrightarrow{\text{diag}} A_1 A_1 A_1 M_1 \xrightarrow{\text{SVD}} A_1 A_1 M_1 B_1 \\
&\xrightarrow{\text{diag}} A_1 A_1 M_2 B_1 \xrightarrow{\text{SVD}} A_1 M_1 B_2 B_1 \\
&\xrightarrow{\text{diag}} A_1 M_2 B_2 B_1 \xrightarrow{\text{SVD}} M_1 B_2 B_2 B_1 \\
&\quad \vdots
\end{aligned}
$$

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