

How to make big Hilbert spaces small

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Outline

- Motivation
- Compressing $|\Psi\rangle$ with SVD
- MPS and DMRG

Motivation

N sites, each is a 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 $N \lesssim 20$ on laptop

$N \rightarrow \infty$ (thermodynamic limit): needle in the haystack

!! For most relevant Hamiltonians, haystack \ll full Hilbert space
e.g. haystack \sim subspace of states with low entanglement entropy
 \implies Clever parameterization + efficient algorithms = ☺?

Compressing $|\Psi\rangle$ with SVD

Theorem (Singular value decomposition)

For any $M \in \mathbb{M}_{A \times B}$, there are "unitary" U, V for which $M = USV^\dagger$, where $S = \text{diag}(s_1, s_2, \dots, 0, 0)$.

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 $A \in \mathbb{M}_{n \times n}$ 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 .

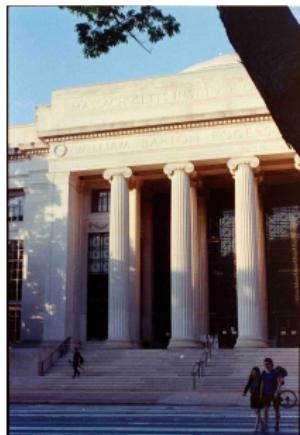
Hilbert-Schmidt norm:

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

Compressing $|\Psi\rangle$ with SVD

Application: image compression

$$A = U \cdot \Sigma \cdot V^T \rightarrow A \approx U \cdot \Sigma \cdot V^T$$



→



Compressing $|\Psi\rangle$ with SVD

Idea: represent $|\Psi\rangle$ as a matrix, then SVD

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!)

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

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

s_i 's = singular values of ψ_{lr}

= eigenvalues of $\sqrt{\psi^\dagger \psi} = \sqrt{\rho} \implies s_i^2$ = eigenvalues of ρ

Compressing $|\Psi\rangle$ with SVD

After SVD:

$$\begin{aligned} |\Psi\rangle &= \sum_{l,r} \sum_i \mathbf{U}_{li} \mathbf{D}_{ii} \mathbf{V}_{ir} |l\rangle |r\rangle \\ &= \sum_i \sum_{\substack{l,r}} \mathbf{U}_{li} \mathbf{D}_{ii} \mathbf{V}_{ir} |l\rangle |r\rangle \\ &= \sum_i s_i |i\rangle_L |i\rangle_R \leftarrow \text{Schmidt decomposition} \end{aligned}$$

Can simply read off reduced density matrices:

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

Normalization:

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

Compressing $|\Psi\rangle$ with SVD

Example:

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

Matrixify and SVD:

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

$$[\psi_{ij}] = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}}_D \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

Compressing $|\Psi\rangle$ with SVD

Why SVD and Schmidt decomposition?

SVD compression \equiv make states with low entanglement entropy

i.e., SVD gives *low-entanglement approximation*

How? von Neumann entanglement entropy between L and R :

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

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

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

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

Compressing $|\Psi\rangle$ with SVD

Example:

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Matrixify and SVD

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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 .



MPS and DMRG

MPS: Matrix product state ←

DMRG: Density matrix renormalization group

MPS:

- expresses wavefunctions in terms of products of matrices
- natural way to generate states with low entanglement entropy

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.

$|i_m\rangle_L$ can be built recursively:

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

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

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

⋮

MPS

Schmidt states:

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

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

Full wavefunction:

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

Matrix dimensions?

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

Example:

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

where

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

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MPS & Hilbert space decimation

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

From:

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

To:

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

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

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

MPS

Example:

$$|\text{GHZ}_4\rangle = \frac{|0000\rangle + |1111\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}} \sum_{\{\sigma\}} \text{Tr}[A^{\sigma_1} A^{\sigma_2} A^{\sigma_3} A^{\sigma_4}] |\sigma_1 \sigma_2 \sigma_3 \sigma_4\rangle$$

where

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

Can see that

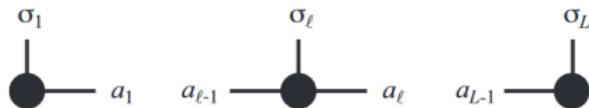
$$\text{Tr}[A^{\sigma_1} A^{\sigma_2} A^{\sigma_3} A^{\sigma_4}] = 1 \iff \sigma_1 = \sigma_2 = \sigma_3 = \sigma_4$$

So far

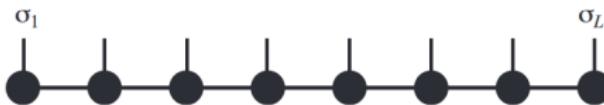
- SVD & Schmidt decomposition allows for compressing $|\Psi\rangle$
- From Schmidt decomposition to MPS for general $|\Psi\rangle$
- Decimate Hilbert space by keeping matrices in MPS at $(D \times D)$
- Hilbert space “smaller” (ND^2 vs d^N) and MPS corresponds to $|\Psi\rangle$ with lower entanglement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

Graphical notation

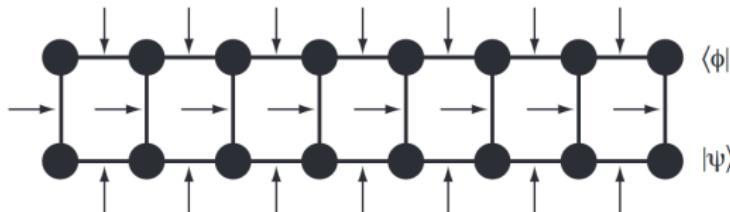
Matrices:



MPS:



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



Graphical notation

MPO: Matrix product operators.

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

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

or

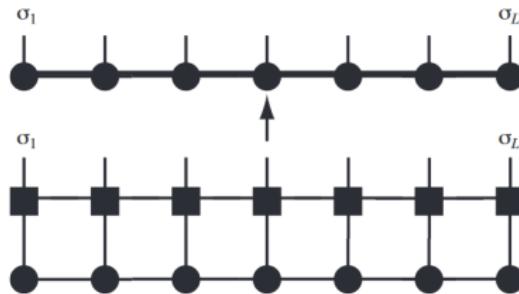
$$\hat{O} = \sum_{\{\sigma, \sigma'\}} W^{\sigma_1 \sigma'_1} W^{\sigma_2 \sigma'_2} \dots W^{\sigma_{N-1} \sigma'_{N-1}} W^{\sigma_N \sigma'_N} |\sigma\rangle \langle \sigma'|$$

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

Graphical notation

MPO on MPS:

$$\hat{O} |\Psi\rangle = \sum_{\{\sigma, \sigma'\}} (W^{\sigma_1 \sigma'_1} W^{\sigma_2 \sigma'_2} \dots) (A^{\sigma_1} A^{\sigma_2} \dots) |\sigma\rangle = \sum_{\{\sigma\}} N^{\sigma_1} N^{\sigma_2} \dots |\sigma\rangle$$

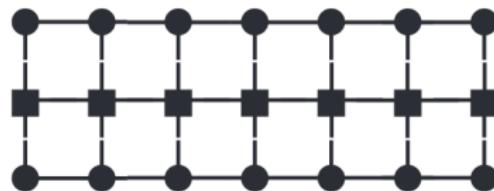


Ground state search

Variationally extremize

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

Graphically,



Idea: Keep matrices on all sites but one (I) constant, optimize elements of $A_I^{\sigma_I}$. Sweep through I .

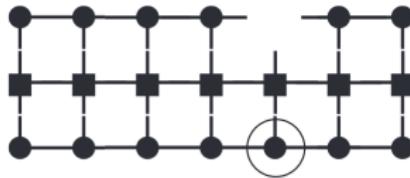
Ground state search

Minimizing



$$-\lambda \times \text{[lattice diagram]} = 0$$

\equiv solving



$$-\lambda \times \text{[lattice diagram with a gap]} = 0$$

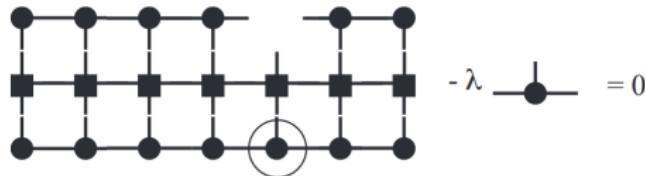
\implies a generalized eigenvalue problem, where we treat $A_I^{\sigma I}$ as a vector v

Ground state search

Aside: left-/right-normalized

$$\sum_{\sigma_I} A^{\sigma_I \dagger} A^{\sigma_I} = I \quad \sum_{\sigma_I} B^{\sigma_I \dagger} B^{\sigma_I} = I$$

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



⇒ standard eigenvalue problem

Ground state search: DMRG

Algorithm (DMRG):

- Start with initial guess for $|\Psi\rangle$, which is right-normalized
 $|\Psi\rangle \sim BBBB\dots$
- 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^{σ_l} by SVD; 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

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

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