

How to make big Hilbert spaces small

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Outline

- Motivation
- Compressing $|\Psi\rangle$ with SVD
- Matrix Product States (MPS)
- Ground state calculation (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 $N \lesssim 20$ on laptop

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

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

!! For many relevant Hamiltonians, haystack \ll full Hilbert space

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

⇒ Clever parameterization + efficient algorithms = ⊙?

Compressing $|\Psi\rangle$?

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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 $S = \text{diag}(s_1, s_2, \dots)$.

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:

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

Compressing $|\Psi\rangle$ with SVD

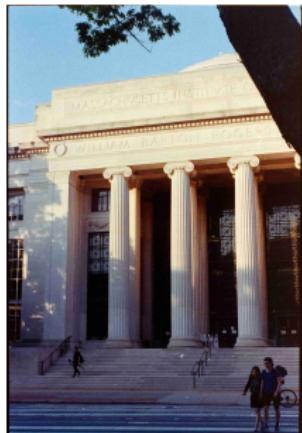
$$A = U \cdot \Sigma \cdot V^T \rightarrow A \approx U \cdot \Sigma \cdot V^T$$

The diagram illustrates the Singular Value Decomposition (SVD) of a matrix A . On the left, A is shown as a green rectangle. An equals sign follows, then U (a maroon rectangle), a dot, a grey rectangle containing a red diagonal line labeled Σ , another dot, and V^T (a blue rectangle). An arrow points to the right, followed by an approximation symbol (\approx). To the right of the approximation symbol, A is shown as a green rectangle, followed by a maroon rectangle U , a dot, a grey rectangle containing a red diagonal line labeled Σ with a small orange square at the top-left corner labeled k , another dot, and a blue rectangle V^T with a small orange square at the top-left corner labeled k .

Compressing $|\Psi\rangle$ with SVD

The diagram shows the decomposition of a matrix A into U , Σ , and V^T . On the left, A is shown as a green rectangle. An equals sign follows. To the right is a purple rectangle labeled U , followed by a dot. Next is a gray rectangle containing a red diagonal line from top-left to bottom-right, labeled Σ below it. Another dot follows. Then is a blue rectangle labeled V^T . An arrow points to the right. On the far right, the word "approximate" is followed by a purple rectangle labeled U , a dot, a gray rectangle with a red diagonal line labeled Σ , a dot, and a blue rectangle labeled V^T . The gray rectangle has a dashed border, and the blue rectangle has a dashed border.

Application: image compression



→



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

\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:

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

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Can simply read off reduced density matrices:

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

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Normalization:

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

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

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How? von Neumann entanglement entropy between L and R :

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

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

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

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, $m \sim \mathcal{O}(100)$

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

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

⋮

MPS

Schmidt states:

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

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

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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:

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

MPS

Example:

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

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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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To:

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

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

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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

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

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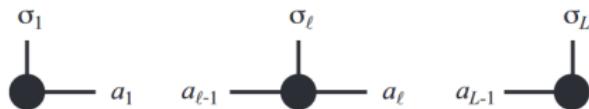
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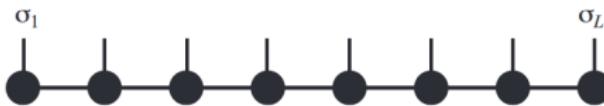
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- MPS: natural way to describe ground states of relevant Hamiltonians

Graphical notation

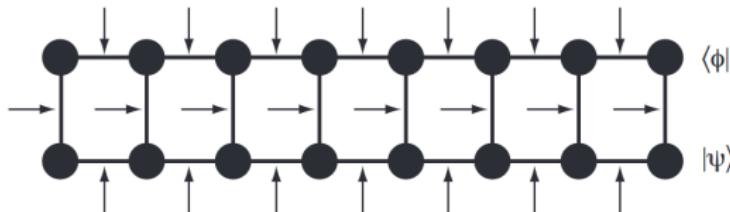
Matrices:



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

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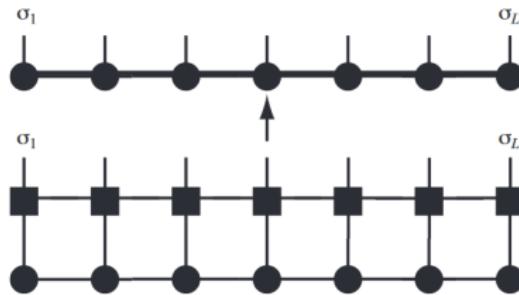
$$\hat{O} = \sum_{\{\sigma, \sigma'\}} W^{\sigma_1 \sigma'_1} W^{\sigma_2 \sigma'_2} \dots W^{\sigma_{N-1} \sigma'_{N-1}} W^{\sigma_N \sigma'_N} |\sigma\rangle \langle \sigma'|$$

⇒ 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

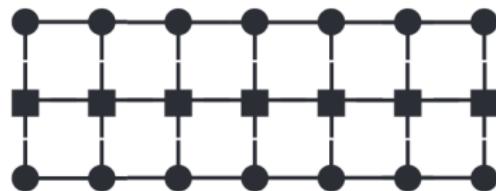
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Idea: Keep matrices on all sites but one (ℓ) constant, optimize elements of $A_{\ell}^{\sigma_{\ell}}$. Sweep through ℓ .

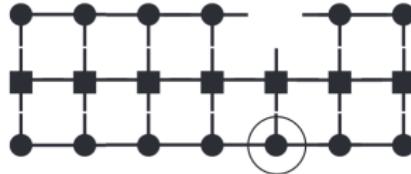
Ground state search

Minimizing



$$-\lambda \times$$

\equiv solving (gradient descent)



$$-\lambda$$

$$= 0$$

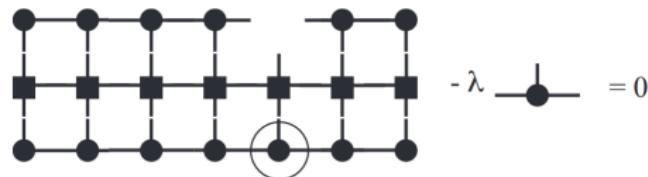
\implies a generalized eigenvalue problem, where we treat $A_\ell^{\sigma\ell}$ as a vector v

Ground state search

Aside: left-/right-normalized

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

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



⇒ standard eigenvalue problem

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- *Right-sweep*: From $\ell = 1$ through $N - 1$: at ℓ , solve for M^{σ_ℓ} then left-normalize into A^{σ_ℓ} by SVD; remaining matrices of the SVD are multiplied into $M^{\sigma_{\ell+1}}$

Ground state search

Algorithm:

- Start with initial guess for $|\Psi\rangle$, which is right-normalized
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- *Left-sweep*: From $\ell = L$ through $\ell = 2$: at ℓ , solve for M^{σ_ℓ} then right-normalize into B^{σ_ℓ} by SVD; remaining matrices of the SVD are multiplied into $M^{\sigma_{\ell-1}}$

Ground state search

Algorithm:

- Start with initial guess for $|\Psi\rangle$, which is right-normalized
 $|\Psi\rangle \sim BBBB\dots$
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- *Right-sweep*: From $\ell = 1$ through $N - 1$: at ℓ , solve for M^{σ_ℓ} then left-normalize into A^{σ_ℓ} by SVD; remaining matrices of the SVD are multiplied into $M^{\sigma_{\ell+1}}$
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- Repeat right and left sweeps until convergence

Ground state search

Algorithm, formalized: Subscript denotes the number of updates

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

DMRG

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DMRG

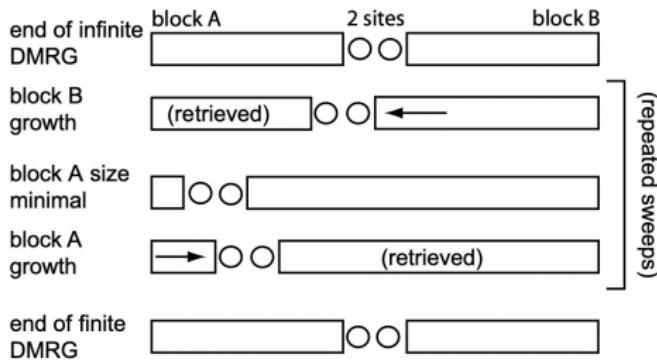
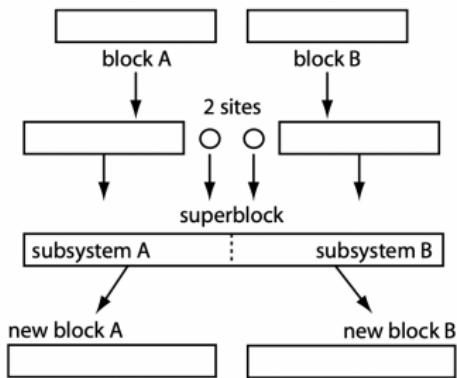
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- Repeat

DMRG



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