How to truncate big Hilbert spaces?

Huan Q. Bui

ZGS, Oct 6, 2022

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 $N \lessapprox 20$ on laptop

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

$\boxed{!!}$ 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 $S = diag(s_1, s_2, \ldots, 0, 0)$.

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

Theorem (Low-rank approximation)

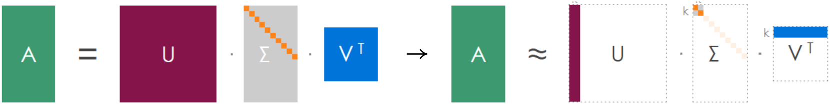
The HS-distance from a rank-m matrix $A \in \mathbb{M}_{n\times n}$ to the nearest $n \times n$ matrix of rank $k \leq m$ is the square root of the sum of the squares of the smallest $n - k$ singular values of A.

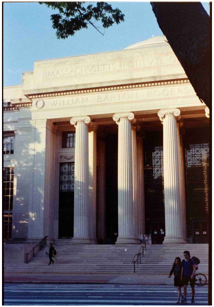
Hilbert-Schmidt norm:

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

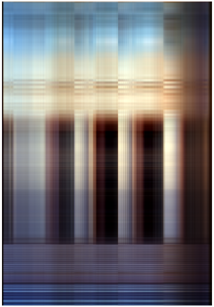
Compressing $|\Psi\rangle$ with SVD

Application: image compression





$\rightarrow$



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. $\mathbf{D} = \mathrm{diag}(\lambda_1, \lambda_2, \dots)$:

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

Compressing $|\Psi\rangle$ with SVD

After SVD:

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

Can simply read off reduced density matrices:

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

Normalization:

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

Example:

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

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:

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

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

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

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

Compressing $|\Psi\rangle$ with SVD

Example:

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

Matrixify and SVD:

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

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

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 $\leftarrow$

DMRG: Density matrix renormalization group

Matrix product state