# How to truncate big Hilbert spaces?

Huan Q. Bui

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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 $N \lessapprox 20$ 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)**

*blah*

Low-rank approximation:

**Theorem (Low-rank approximation)**

Applications: image compression

# Compressing $|\Psi\rangle$ with SVD

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

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

$$|\Psi\rangle = \sum_{l,r} \psi_{lr} |l\rangle |r\rangle, \qquad |l\rangle \in \mathbb{H}_L$$

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

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

$\mathbf{U}, \mathbf{V}$ are unitary. $\mathbf{D} = \text{diag}(\lambda_1, \lambda_2, \dots)$:

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

# Compressing $|\Psi\rangle$ with SVD

After SVD:

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

Normalization:

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

# Compressing $|\Psi\rangle$ with SVD

Why SVD and Schmidt decomposition?

SVD compression $\equiv$ make states with low entanglement entropy

von Neumann entanglement entropy between $L$ and $R$:

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

$$[\rho_L]_{ll'} = \sum_r \psi^*_{lr}\psi_{l'r} \qquad [\rho_R]_{rr'} = \sum_l \psi^*_{lr}\psi_{lr'}$$

Fact: Eigenvalues of $\rho_L, \rho_R$ are exactly the $\lambda_i$'s. 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 $\lambda_i$'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/approximate such a $|\Psi\rangle$.

Insert chicken and egg here.

Solution:

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# MPS and DMRG

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