

# How to truncate big Hilbert spaces?

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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:

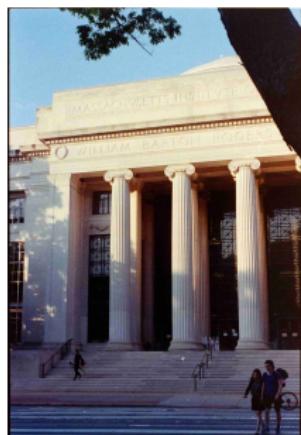
$$\|A\|_{HS} = \sqrt{\sum |A_{ij}|^2} = \sqrt{\text{Tr}(A^\dagger A)} = \sqrt{\sum s_i^2}$$

# Compressing $|\Psi\rangle$ with SVD

Application: image compression

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

The diagram illustrates the Singular Value Decomposition (SVD) of a matrix A. On the left, A is shown as a green rectangle. To its right is an equals sign, followed by the decomposition into three components: U (a maroon rectangle), a diagonal matrix Sigma (a grey rectangle with orange diagonal elements), and V^T (a blue rectangle). An arrow points to the right, indicating the result of approximating A. On the far right, the approximated matrix is shown as a green rectangle (U), followed by a diagonal matrix Sigma (with only the top-left k elements shown in orange), and V^T (a blue rectangle).



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# Compressing $|\Psi\rangle$ with SVD

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

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

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

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

$\lambda_i$ 's = singular values of  $\psi_{lr}$

= eigenvalues of  $\sqrt{\psi^\dagger \psi} = \sqrt{\rho} \implies \lambda_i^2 = \text{eigenvalues of } \rho$

# Compressing $|\Psi\rangle$ with SVD

After SVD:

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

Can simply read off reduced density matrices:

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

Normalization:

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

# 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  $R$ :

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

Eigenvalues of  $\rho_L, \rho_R$  are exactly  $\{\lambda_i\}$ . So,

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

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

# Compressing $|\Psi\rangle$ with SVD

Example:

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

Matrixify and SVD:

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

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

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:



# MPS and DMRG