# MPS notes

## 1) Schmidt decomposition

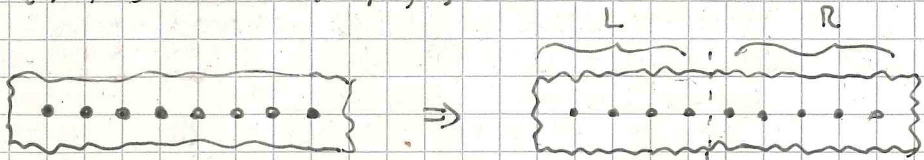
Consider a tensor decomposition of some Hilbert space:

$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$ where we assume (for simplicity) all $\mathcal{H}_i$ have dimension $d$

Given orthonormal basis $\{|a_i\rangle\}_{a_i=1\dots d}$ for the local spaces $\mathcal{H}_i$, we have an orthogonal basis for $\mathcal{H}$ and can write states using it:

$$|\psi\rangle \in \mathcal{H} \Rightarrow |\psi\rangle = \sum_{a_1,\dots,a_N} \psi_{a_1\cdots a_N} |a_1 \cdots a_N\rangle$$

Now let us divide the system described by $\mathcal{H}$ in two parts $L$, $R$ such that $L = \{1,\dots,M\}$ and $R = \{M+1,\dots,N\}$:




$\simeq$ $\mathcal{H}$ $\qquad$ $\simeq$ $\mathcal{H} = \mathcal{H}_L \otimes \mathcal{H}_R$, $\quad \mathcal{H}_L = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_M$, $\mathcal{H}_R = \mathcal{H}_{M+1} \otimes \cdots \otimes \mathcal{H}_N$

The numbers $\psi_{a_1\cdots a_N}$ can be organized into a $d^M \times d^{N-M}$ matrix by separating the indices into two groups:

$$\psi_{a_1\cdots a_N} \Rightarrow \psi_{\underbrace{(a_1\cdots a_M)}_{i_L}\underbrace{(a_{M+1}\cdots a_N)}_{j_R}} \Rightarrow (\psi^{L,R})_{i_L j_R} = \psi_{\underbrace{a_1\cdots a_M}_{i_L}\underbrace{a_{M+1}\cdots a_N}_{j_R}}$$

$(a_1\cdots a_M)$: $d^M$ possible entries $\Downarrow$ order them to get an index running from 1 to $d^M$ $\to i_L$

$(a_{M+1}\cdots a_N)$: $d^{N-M}$ possible entries $\Downarrow$ order them to get an index running from 1 to $d^{N-M}$ $\to j_R$

Let's perform a singular value decomposition of the matrix $\psi^{L,R}$:

$\psi^{L,R} = U S V^\dagger$ where $U$ = unitary $d^M \times d^M$ matrix

$S$ = diagonal $d^M \times d^{N-M}$ matrix with non-negative real eigenvalues

$V$ = unitary $d^{N-M} \times d^{N-M}$ matrix

$$\hookrightarrow (\psi^{L,R})_{i_L j_R} = \sum_{i_L' j_R'} U_{i_L i_L'} S_{i_L' j_R'} (V^\dagger)_{j_R' j_R} = \sum_{r=1}^{\text{rank}} S_r\, U_{i_L r} (V^\dagger)_{r j_R}$$

(rank = # non-zero entries in $S$ assuming descending order in $S$)

We can use this decomposition to rewrite the state $|\psi\rangle$:

$$|\psi\rangle = \sum_{a_1 \cdots a_N} \underbrace{\psi_{a_1 \cdots a_M a_{M+1} \cdots a_N}}_{\psi^{L,R}_{i_L j_R}} |\underbrace{a_1 \cdots a_M}_{i_L} \underbrace{a_{M+1} \cdots a_N}_{j_R}\rangle = \sum_{i_L j_R} \psi^{L,R}_{i_L j_R} |i_L j_R\rangle$$

$$= \sum_{i_L j_R} \sum_r S_r U_{i_L r} (V^\dagger)_{r j_R} |i_L j_R\rangle = \sum_r S_r \underbrace{\left( \sum_{i_L} U_{i_L r} |i_L\rangle \right)}_{|r_L\rangle} \underbrace{\left( \sum_{j_R} (V^\dagger)_{r j_R} |j_R\rangle \right)}_{|r_R\rangle}$$

$$\Rightarrow |\psi\rangle = \sum_{r=1}^{\text{rank}} S_r |r_L r_R\rangle$$

where $\{|r_{L(R)}\rangle\}_{r=1 \cdots \text{rank}}$ are part of an orthonormal basis of $\mathcal{H}_{L(R)}$.

This representation of the state is called a Schmidt decomposition and we can use it to compute partial traces:

$$\rho_L = \mathrm{Tr}_R |\psi\rangle\langle\psi| = \mathrm{Tr}_R \sum_{r r'} S_r S_{r'} |r_L r_R\rangle\langle r'_L r'_R| = \sum_r S_r^2 |r_L\rangle\langle r_L|$$

$$= \sum_r \sum_{i_L i'_L} S_r^2 U_{i_L r} U^*_{i'_L r} |i_L\rangle\langle i'_L| = \sum_{i_L i'_L} \left( \sum_r U_{i_L r} S_r^2 (U^\dagger)_{r i'_L} \right) |i_L\rangle\langle i'_L|$$

$$= U \Lambda U^\dagger$$

where $\Lambda$ is a $d^M \times d^M$ diagonal matrix defined by:

$$(\Lambda)_{ii} = \begin{cases} S_i^2 & ; \ i \in \{1 \cdots \text{rank}\} \\ 0 & , \ \text{otherwise} \end{cases}$$

The entanglement entropy is directly accessible from this

$$\rho_L = \sum_r S_r^2 |r_L\rangle\langle r_L| \Rightarrow S = -\sum_r S_r^2 \log S_r^2$$

and we see that $S \leq \log \text{rank}$.

2) MPS ansatz