Matrix Product State

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1D 3-spin chain

Consider a 1D 3-spin linear chain. A generic wave function of this system can be expressed in the S_z basis (product space of the S_z basis on each site). This wave function can be represented with a **state vector** $\vec{c}$, which is merely a vector of expansion coefficients of the state in the given basis

$$|\Psi\rangle = \sum_{i=1}^{2^3} c_{\sigma_1\sigma_2\sigma_3} |\sigma_1\rangle_1 \otimes |\sigma_2\rangle_2 \otimes |\sigma_3\rangle_3 . \tag{1}$$

$\sigma_1, \sigma_2, \sigma_3 = \uparrow, \downarrow$ are often referred to as the **physical degrees of freedom**. Notice once $\sigma_1, \sigma_2, \sigma_3$ are specified, $\langle \sigma_1\sigma_2\sigma_3|\Psi\rangle$ is merely a number.

Consider the following pathological state

$$\sqrt{\sum_{i=1}^{8} i^2} \cdot |\psi\rangle : \begin{array}{cccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ |\uparrow\uparrow\uparrow\rangle & |\uparrow\uparrow\downarrow\rangle & |\uparrow\downarrow\uparrow\rangle & |\uparrow\downarrow\downarrow\rangle & |\downarrow\uparrow\uparrow\rangle & |\downarrow\uparrow\downarrow\rangle & |\downarrow\downarrow\uparrow\rangle & |\downarrow\downarrow\downarrow\rangle \end{array} , \tag{2}$$

which has matrix product state (mps) representation

$$\sqrt{\sum_{i=1}^{8} i^2} \cdot |\psi\rangle :$$

$$\begin{array}{ccc} (-0.376 - 0.926)\, |\uparrow\rangle_1 & \begin{pmatrix} -0.5645 & -0.328 \\ 0.0646 & -0.7547 \end{pmatrix} |\uparrow\rangle_2 & \begin{pmatrix} 9.1525 \\ -0.48 \end{pmatrix} |\uparrow\rangle_3 \\ (-0.9260.376)\, |\downarrow\rangle_1 & \begin{pmatrix} -0.8217 & 0.1947 \\ -0.044 & -0.534 \end{pmatrix} |\downarrow\rangle_2 & \begin{pmatrix} 10.9471 \\ 0.40206 \end{pmatrix} |\downarrow\rangle_3 \end{array} . \tag{3}$$

To generate this mps, start from site 1. First separate $|\uparrow\rangle_1$ from $|\downarrow\rangle_1$

$$c_{\sigma_1(\sigma_2\sigma_3)} : \begin{array}{cccc} |\uparrow\uparrow\uparrow\rangle & |\uparrow\uparrow\downarrow\rangle & |\uparrow\downarrow\uparrow\rangle & |\uparrow\downarrow\downarrow\rangle \\ 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ |\downarrow\uparrow\uparrow\rangle & |\downarrow\uparrow\downarrow\rangle & |\downarrow\downarrow\uparrow\rangle & |\downarrow\downarrow\downarrow\rangle \end{array} . \tag{4}$$

This process can be thought of cutting the system of 3 spins into 2 subsystems, making site 1 subsystem A and sites 2,3 subsystem B. The row space is the Hilbert space for subsystem A and the column space is subsystem B.

$$c_{\sigma_1(\sigma_2\sigma_3)}: \begin{array}{ccccc} & |{\uparrow\uparrow}\rangle_B & |{\uparrow\downarrow}\rangle_B & |{\downarrow\uparrow}\rangle_B & |{\downarrow\downarrow}\rangle_B \\ |{\uparrow}\rangle_A & 1 & 2 & 3 & 4 \\ |{\downarrow}\rangle_A & 5 & 6 & 7 & 8 \end{array} . \tag{5}$$

We can now use our favorite method (QR or SVD) to find a nice (orthonormal) basis for subsystem A. The resultant decomposition

$$c_{\sigma_1(\sigma_2\sigma_3)} = \begin{array}{c} |{\uparrow}\rangle_1 \\ |{\downarrow}\rangle_1 \end{array} \overset{Q}{\begin{pmatrix} q_{1,1} & q_{1,2} \\ q_{2,1} & q_{2,2} \end{pmatrix}} \quad \begin{array}{cccc} & R & & \\ \multicolumn{4}{c}{\begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & r_{1,4} \\ r_{2,1} & r_{2,2} & r_{2,3} & r_{2,4} \end{pmatrix}} \\ |{\uparrow\uparrow}\rangle_{23} & |{\uparrow\downarrow}\rangle_{23} & |{\downarrow\uparrow}\rangle_{23} & |{\downarrow\downarrow}\rangle_{23} \end{array} \tag{6}$$

The remaining matrix can be cut again to separate site 2 from 3

$$\begin{array}{cc} & R \\ \begin{array}{c} b_1 \\ b_2 \end{array} & \begin{pmatrix} r_{1,1} & r_{1,2} & r_{1,3} & r_{1,4} \\ r_{2,1} & r_{2,2} & r_{2,3} & r_{2,4} \end{pmatrix} \\ & |{\uparrow\uparrow}\rangle_{23} \quad |{\uparrow\downarrow}\rangle_{23} \quad |{\downarrow\uparrow}\rangle_{23} \quad |{\downarrow\downarrow}\rangle_{23} \end{array} \rightarrow \begin{array}{cc} & R \\ \begin{array}{c} b_1, |{\uparrow}\rangle_2 \\ b_2, |{\uparrow}\rangle_2 \\ b_1, |{\downarrow}\rangle_2 \\ b_2, |{\downarrow}\rangle_2 \end{array} & \left(\begin{array}{cc} r_{1,1} & r_{1,2} \\ r_{2,1} & r_{2,2} \\ \hdashline r_{1,3} & r_{1,4} \\ r_{2,3} & r_{2,4} \end{array} \right) \\ & |{\uparrow}\rangle_3 \quad |{\downarrow}\rangle_3 \end{array} . \tag{7}$$

Notice how the reshaped matrix naturally has an $\uparrow$ block and a $\downarrow$ block for site 2. This will generalize to any site even if the chain were longer. However, the dimension of the contraction index b (the number of b_1, b_2 etc.) often called **bond dimension** is in general way bigger than 2 for longer chains. Decompose again and we obtain the mps in (3).

Exercise: fill in the numbers $q_{m,n}$ and $r_{m,n}$