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Matrix Product States

Preparation of MPS

There are two alternative ways to prepare MPS. The first is by using successive Schmidt decompositions, which as it turns out also produces MPS in *canonical form*. The second is a preparation from maximally entangled pairs, the so called valence bonds states.

Canonical form (from Jens paper)

A general quantum state $|\psi\rangle$ on a chain with N sites can be written in MPS form:

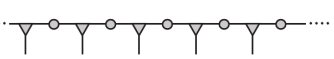
$$|\psi\rangle = \sum_{\sigma_1 \dots \sigma_N} A^{\sigma_1} \dots A^{\sigma_N} |\sigma_1 \dots \sigma_N\rangle,$$

where A^{σ_i} is a $r_{i-1} \times r_i$ matrix, r_i being the rank of the Schmidt decomposition at site i. Note that at the boundary we have $r_0 = r_N = 1$, which means that A^{σ_1} and A^N are vectors, and therefore the matrix product returns a scalar coefficient.

We can rewrite the matrices A^{σ_i} as a product of $r_{i-1} \times r_i$ complex matrices Γ^{σ_i} and positive, real, square diagonal matrices Λ^i

$$|\psi\rangle = \sum_{\sigma_1 \dots \sigma_N} \Gamma^{\sigma_1} \Lambda^1 \Gamma^{\sigma_2} \Lambda^2 \dots \Lambda^{N-1} \Gamma^{\sigma_N} |\sigma_1 \dots \sigma_N\rangle,$$

which diagrammatically looks like

$|\psi\rangle =$ 

This form allows for many possible representations of the same wave function, giving us the opportunity to define a “canonical form” of the MPS.

We can define a set of χ_n wave functions $|\alpha\rangle^n_{L/R}$ to the left/right of a bond, such that

$$|\psi\rangle = \sum_{\alpha=1}^{\chi} \Lambda^n_\alpha |\alpha\rangle^n_L \otimes |\alpha\rangle^n_R, \quad |\alpha\rangle \in H_{L/R}$$

**The MPS representation $\{\Gamma^{\sigma_1} \Lambda^1 \Gamma^{\sigma_2} \Lambda^2 \dots \Lambda^{N-1} \Gamma^{\sigma_N}\}$ is canonical if for every bond, the set of wave functions $|\alpha\rangle^n_{L/R}$ along with Λ^i form a Schmidt decomposition of ψ.
In other words we must have $\langle\hat{\alpha}|\alpha\rangle^n_L = \delta_{\hat{\alpha}\alpha}$, $\langle\hat{\alpha}|\alpha\rangle^n_R = \delta_{\hat{\alpha}\alpha}$ and $\sum(\Lambda^i_\alpha)^2 = 1$ on every bond.**

Schmidt decomposition according to Vidal

Summary from the following papers

Vidal, G. (2003). Efficient Classical Simulation of Slightly Entangled Quantum Computations. Physical Review Letters, 91(14), 147902.

Vidal, G. (2004). Efficient simulation of one-dimensional quantum many-body systems. Physical Review Letters, 93(4), 40502–1.

The local decomposition of the state $|\psi\rangle \in H_2^{\otimes n}$ in terms of n tensors $\{\Gamma^{\sigma_l}\}_{l=1}^{n}$ and $\{\lambda^l\}_{l=1}^{n-1}$ is denoted

$$|\psi\rangle \leftrightarrow \Gamma^{\sigma_1}\lambda^1\Gamma^{\sigma_2}\lambda^2\ldots\lambda^{n-1}\Gamma^{\sigma_n}$$

Here, tensor Γ^{σ_l} has at most three indices $\Gamma^{\sigma_l}_{\alpha\alpha'}$, where $\alpha, \alpha' = 0, \ldots, \chi$ and $\sigma_l = 0, 1$, whereas λ^l is a vector whose components $\lambda^l_{\alpha'}$ store the Schmidt coefficients of the splitting $[1\ldots l] : [(l+1)\ldots n]$. More explicitly we have

$$c_{\sigma_1\ldots\sigma_n} = \sum_{\alpha_1\ldots\alpha_{n-1}} \Gamma^{\sigma_1}_{\alpha_1}\lambda^1_{\alpha_1}\Gamma^{\sigma_2}_{\alpha_1\alpha_2}\lambda^1_{\alpha_2}\ldots\Gamma^{\sigma_n}_{\alpha_{n-1}}$$

so that 2^n coefficients in $c_{\sigma_1\ldots\sigma_n}$ are expressed in terms of about $(2\chi^2+\chi)n$ parameters, a number that grows linearly in n for a fixed value of χ.

Procedure

This decomposition is essentially a concatenation of $n-1$ Schmidt decompositions, and depends on how the qubits have been ordered from 1 to n. We first compute the Schmidt decomposition according to the bipartite splitting of $|\psi\rangle$ into qubit 1 and the $n-1$ remaining qubits.

$$|\psi\rangle = \sum_{\alpha_1}\lambda^1_{\alpha_1}|\Phi^1_{\alpha_1}\rangle|\Phi^{2\ldots n}_{\alpha_1}\rangle = \sum_{\sigma_1,\alpha_1}\Gamma^{\sigma_1}_{\alpha_1}\lambda^1_{\alpha_1}|\sigma_1\rangle|\Phi^{2\ldots n}_{\alpha_1}\rangle$$

We then proceed according to the following three steps:

---

1. Expand each vector $|\Phi^{2\ldots n}_{\alpha_1}\rangle$ in a local basis for qubit 2, $|\Phi^{2\ldots n}_{\alpha_1}\rangle = \sum_{\sigma_2}|\sigma_2\rangle|\tau^{3\ldots n}_{\alpha_1,\sigma_2}\rangle$
2. Write each vector $|\tau^{3\ldots n}_{\alpha_1,\sigma_2}\rangle$ in terms of at most χ Schmidt vectors $\{|\Phi^{3\ldots n}_{\alpha_2}\rangle\}^{\chi}_{\alpha_2}$, i.e. eigenvectors of $\rho^{3\ldots n}$ and the corresponding Schmidt coefficients $\lambda^2_{\alpha_2}$: $|\tau^{3\ldots n}_{\alpha_1,\sigma_2}\rangle = \sum_{\alpha_2}\Gamma^{\sigma_2}_{\alpha_1\alpha_2}\lambda^2_{\alpha_2}|\Phi^{3\ldots n}_{\alpha_2}\rangle$
3. Substitute the equations in (1) and (2) into the first splitting above, i.e.:

$$\begin{aligned}|\Phi^{2\ldots n}_{\alpha_1}\rangle &= \sum_{\sigma_2}|\sigma_2\rangle\sum_{\alpha_2}\Gamma^{\sigma_2}_{\alpha_1\alpha_2}\lambda^2_{\alpha_2}|\Phi^{3\ldots n}_{\alpha_2}\rangle \\ &= \sum_{\sigma_2,\alpha_2}\Gamma^{\sigma_2}_{\alpha_1\alpha_2}\lambda^2_{\alpha_2}|\sigma_2\rangle|\Phi^{3\ldots n}_{\alpha_2}\rangle\end{aligned}$$

followed by

$$\begin{aligned}|\psi\rangle &= \sum_{\sigma_1,\alpha_1}\Gamma^{\sigma_1}_{\alpha_1}\lambda^1_{\alpha_1}|\sigma_1\rangle\sum_{\sigma_2}|\sigma_2\rangle\sum_{\alpha_2}\Gamma^{\sigma_2}_{\alpha_1\alpha_2}\lambda^2_{\alpha_2}|\Phi^{3\ldots n}_{\alpha_2}\rangle \\ &= \sum_{\sigma_1\sigma_2,\alpha_1\alpha_2}\Gamma^{\sigma_1}_{\alpha_1}\lambda^1_{\alpha_1}\Gamma^{\sigma_2}_{\alpha_1\alpha_2}\lambda^2_{\alpha_2}|\sigma_1\rangle|\sigma_2\rangle|\Phi^{3\ldots n}_{\alpha_2}\rangle\end{aligned}$$

Repeating steps 1 to 3 for the Schmidt vectors $|\Phi^{4\ldots n}_{\alpha_3}\rangle, |\Phi^{5\ldots n}_{\alpha_4}\rangle\ldots$ gives us the state $|\psi\rangle$ in terms of tensors Γ^{σ_l} and λ^l.

Tensor decomposition

There are more details on higher-order tensor decomposition (matrix unfolding) here:

De Lathauwer, L., De Moor, B., & Vandewalle, J. (2000). A Multilinear Singular Value Decomposition. - Society for Industrial and Applied Mathematics. Journal on Matrix Analysis and Applications

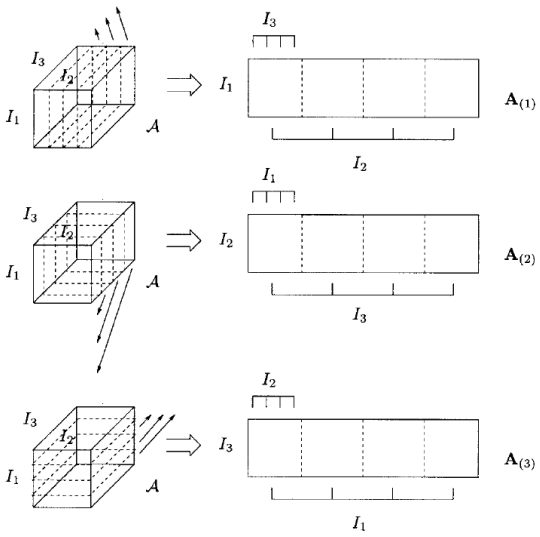


FIG. 1. *Unfolding of the* $(I_1 \times I_2 \times I_3)$*-tensor* $\mathcal{A}$ *to the* $(I_1 \times I_2 I_3)$*-matrix* $\mathbf{A}_{(1)}$*, the* $(I_2 \times I_3 I_1)$*-matrix* $\mathbf{A}_{(2)}$ *and the* $(I_3 \times I_1 I_2)$*-matrix* $\mathbf{A}_{(3)}$ $(I_1 = I_2 = I_3 = 4)$.

And also here:

Bengua, J. a., Phien, H. N., Tuan, H. D., & Do, M. N. (2015). Matrix Product State for Feature Extraction of Higher-Order Tensors, (1944), 10.

A mode-n fiber of a tensor $\boldsymbol{\mathcal{X}} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is defined by fixing all indices but i_n and denoted by $\mathbf{x}_{i_1 \ldots i_{n-1} : i_{n+1} \ldots i_N}$.

Mode-n matricization (also known as mode-n unfolding or flattening) of a tensor $\boldsymbol{\mathcal{X}} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is the process of unfolding or reshaping the tensor into a matrix $\mathbf{X}_{(n)} \in \mathbb{R}^{I_n \times (I_1 \cdots I_{n-1} I_{n+1} \cdots I_N)}$ by rearranging the mode-n fibers to be the columns of the resulting matrix. Tensor element $(i_1, \ldots, i_{n-1}, i_n, i_{n+1}, \ldots, i_N)$ maps to matrix element (i_n, j) such that

$$j = 1 + \sum_{k=1, k \neq n}^{N} (i_k - 1) J_k \quad \text{with} \quad J_k = \prod_{m=1, m \neq n}^{k-1} I_m. \qquad (1)$$

TABLE I: Matrix product state for tensor feature extraction

Input: $\boldsymbol{\mathcal{X}} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times K \cdots \times I_N}$,
ϵ: SVD threshold
Output: $\boldsymbol{\mathcal{G}}^{(n)} \in \mathbb{R}^{\Delta_{n-1} \times \Delta_n \times K}$,
$\mathbf{B}^{(j)}_{i_j}$ $(i_j = 1, \ldots, I_j, j = 1, \ldots, n-1)$
$\mathbf{C}^{(j)}_{i_{(j-1)}}$ $(i_{(j-1)} = 1, \ldots, I_{(j-1)}, j = n+1, \ldots, N+1)$

Set $\mathbf{W} = \mathbf{X}_{(1)}$ % Mode-1 matricization of $\boldsymbol{\mathcal{X}}$
for $j = 1$ **to** $n-1$ % Left-to-right sweep
  $\mathbf{W} = \mathbf{USV}^T$ % SVD of $\mathbf{W}$
  $\mathbf{W} \approx \tilde{\mathbf{U}}\tilde{\mathbf{S}}\tilde{\mathbf{V}}^T$ % Thresholding $\mathbf{S}$ using Eq. (20)
  $\mathbf{B}^{(j)}_{i_j} = \tilde{\mathbf{U}}_{i_j}$ % Set common factors
  $\mathbf{W} = \tilde{\mathbf{S}}\tilde{\mathbf{V}}^T$ % Construct new matrix $\mathbf{W}$
end
Reshape $\mathbf{W} \in \mathbb{R}^{(\Delta_{n-1} K \cdots I_N) \times I_N}$
for $j = N+1$ **down to** $n+1$ % right-to-left sweep
  $\mathbf{W} = \mathbf{USV}^T$ % SVD of $\mathbf{W}$
  $\mathbf{W} \approx \tilde{\mathbf{U}}\tilde{\mathbf{S}}\tilde{\mathbf{V}}^T$ % Thresholding $\mathbf{S}$ using Eq. (20)
  $\mathbf{C}^{(j)}_{i_{(j-1)}} = \tilde{\mathbf{V}}^T_{i_{(j-1)}}$ % Set common factors
  $\mathbf{W} = \tilde{\mathbf{U}}\tilde{\mathbf{S}}$ % Construct new matrix $\mathbf{W}$
end
Set $\boldsymbol{\mathcal{G}}^{(n)} = \boldsymbol{\mathcal{W}}$ % Training core tensor

Texts after symbol "%" are comments.

Local updates

Updating the state $|\psi\rangle$ after a unitary operation U acts on qubit l does only involve transforming Γ^{σ_l}. The computational cost is $\mathcal{O}(\chi^2)$ basic operations.

When a unitary operation V, like a two-qubit gate, is applied to qubits l and $l+1$ only Γ^{σ_l}, λ^l and $\Gamma^{\sigma_{l+1}}$ need to be updated. The

computational cost is $\mathcal{O}(\chi^3)$ basic operations.

Example 1: Three Qubits, following Schollwöck

This example tries to follow the steps in
Schollwoeck, U. (2010). The density-matrix renormalization group in the age of matrix product states. Annals of Physics, 326(1), 96–192.

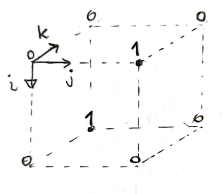
Step 1:

In general, a 3 qubit state can be written as:

$$|\psi\rangle = \sum_{\sigma_1\sigma_2\sigma_3} c_{\sigma_1\sigma_2\sigma_3} |\sigma_1\sigma_2\sigma_3\rangle,$$

where each $\sigma_i \in \{0,1\}$ and the coefficients $c_{\sigma_1\sigma_2\sigma_3}$ are 2^3 complex numbers. These numbers can be visualized as being on the corners of a (hyper)cube, or simply a long list of numbers corresponding to the 8 possible states.

Consider the following state with 3 qubits: $|\psi\rangle = \frac{1}{\sqrt{2}}(|010\rangle + |101\rangle)$. The cube would look as in the figure below.



or simply,

$$\begin{array}{r|l} 0 & |000\rangle \\ 0 & |001\rangle \\ 2^{-1/2} & |010\rangle \\ 0 & |011\rangle \\ 0 & |100\rangle \\ 2^{-1/2} & |101\rangle \\ 0 & |110\rangle \\ 0 & |111\rangle \end{array}$$

The first step in the decomposition is to define a $d \times d^{L-1} = 2 \times 2^2$ matrix that flattens the tensor:

$$\Psi_{\sigma_1,(\sigma_2\sigma_3)} = \begin{array}{r|cccc} & \sigma_1=0,\sigma_3=0 & \sigma_1=0,\sigma_3=1 & \sigma_1=1,\sigma_3=0 & \sigma_1=1,\sigma_3=1 \\ \sigma_2=0 & 0 & 0 & 0 & 2^{-1/2} \\ \sigma_2=1 & 2^{-1/2} & 0 & 0 & 0 \end{array}$$

$$= \begin{pmatrix} 0 & 0 & 0 & 2^{-1/2} \\ 2^{-1/2} & 0 & 0 & 0 \end{pmatrix}$$

Note how the cube has been sliced and concatenated. Basically, the matrix is composed of two (2×2) matrices side by side, one for each value of σ_1.

Now we perform the single value decomposition on $\Psi_{\sigma_1,(\sigma_2\sigma_3)} = USV^\dagger$:

$$\begin{pmatrix} 0 & 0 & 0 & 2^{-1/2} \\ 2^{-1/2} & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 2^{-1/2} & 0 \\ 0 & 2^{-1/2} \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$= \sum_{a_1}^{r_1} U_{\sigma_1,a_1} S_{a_1,a_1} V^\dagger_{a_1,\sigma_2\sigma_3}$$

$$\equiv \sum_{a_1}^{r_1} U_{\sigma_1,a_1} c_{a_1,\sigma_2\sigma_3}$$

where $r_1 \leq d = 2$ is the rank of the decomposition, i.e., the number of nonzero items in S, and $a_1 \in \{0,1\}$. In the last equality S and $V^\dagger$ have been multiplied. It can then be reshaped into a matrix of dimension $(r_1 d \times d) = (4 \times 2)$, called $\Psi_{(a_1\sigma_2),(\sigma_3)}$. This is NOT done by stacking the (2×2) matrices. Instead, note how the σ_2 index selects the upper/lower row, which then become matrices. Pythons numpy.reshape() does this. **Here the label a_1 is the index being summed over (by matrix multiplication), and σ_2, σ_3 serve to select appropriate matrices.**

$$c_{a_1,\sigma_2\sigma_3} = \begin{pmatrix} 0 & 0 & 0 & 2^{-1/2} \\ 2^{-1/2} & 0 & 0 & 0 \end{pmatrix} \to \begin{pmatrix} \begin{pmatrix} \binom{0}{0} & \binom{0}{2^{-1/2}} \end{pmatrix}_{\sigma_3} \\ \begin{pmatrix} \binom{2^{-1/2}}{0} & \binom{0}{0} \end{pmatrix}_{\sigma_3} \end{pmatrix}_{\sigma_2} = \Psi_{(a_1\sigma_2),(\sigma_3)}$$

U is now sliced into $d = 2$ row vectors A^{σ_1}, which we interpret as (1×2) matrices, i.e., $A^{\sigma_1}_{a_1} = U_{\sigma_1,a_1} \to \begin{pmatrix} (1 & 0) \\ (0 & 1) \end{pmatrix}_{\sigma_1}$, where σ_1 labels each row vector.

By now we have achieved the following:

$$c_{\sigma_1\sigma_2\sigma_3} = \sum_{a_1}^{r_1} A^{\sigma_1}_{a_1} \Psi_{(a_1\sigma_2),(\sigma 3)} = \begin{pmatrix} (1 & 0) \\ (0 & 1) \end{pmatrix}_{\sigma_1} \begin{pmatrix} \begin{pmatrix} \binom{0}{0} & \binom{0}{2^{-1/2}} \end{pmatrix}_{\sigma_3} \\ \begin{pmatrix} \binom{2^{-1/2}}{0} & \binom{0}{0} \end{pmatrix}_{\sigma_3} \end{pmatrix}_{\sigma_2}$$

where the labels $\sigma_1, \sigma_2, \sigma_3$ serve to index the inner elements.

So for instance if $|\sigma_1\sigma_2\sigma_3\rangle = |101\rangle$ we get $c_{101} = (0,1)\binom{0}{2^{-1/2}} = 2^{-1/2}$ as expected (check this!).

Step 2:

Next, we apply the SVD decomposition once more

$$\begin{aligned} \Psi_{(a_1\sigma_2),(\sigma_3)} = USV^\dagger &= \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ -1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 2^{-1/2} & 0 \\ 0 & 2^{-1/2} \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \\ &= \sum_{a_2}^{r_2} U_{(a_1\sigma_2),a_2} S_{a_2,a_2} (V^\dagger)_{a_2,(\sigma_3)} \\ &= \sum_{a_2}^{r_2} A^{\sigma_2}_{a_1,a_2} \Psi_{a_2\sigma_3} \end{aligned}$$

where U is replaced by a set of d matrices A^{σ_2} of dimension $r_1 \times r_2 = (2 \times 2)$ with entries $A^{\sigma_2}_{a_1,a_2} = U_{(a_1\sigma_2),a_2}$. As before, $SV^\dagger$ has been reshaped into a matrix Ψ of dimension $r_2 d \times d^{L-3} = (4 \times 1)$.

Explicitly, this reads:

$$\sum_{a_2}^{r_2} A^{\sigma_2}_{a_1,a_2} \Psi_{a_2\sigma_3} = \begin{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \\ \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix} \end{pmatrix}_{\sigma_2} \begin{pmatrix} \binom{-2^{-1/2}}{0} \\ \binom{0}{2^{-1/2}} \end{pmatrix}_{\sigma_3}$$

So far we have achieved the following:

$$c_{\sigma_1\sigma_2\sigma_3} = \sum_{a_1,a_2}^{r_1,r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{a_2\sigma_3}$$

So for instance

$c_{101} = A^{\sigma_1=1} A^{\sigma_2=0} \Psi_{a_2\sigma_3=1} = (0,1) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \binom{0}{2^{-1/2}} = 2^{-1/2}$, as expected.

Step 3:
We perform the SVD decomposition for the last time:

$$\Psi_{(a_1\sigma_2),(\sigma_3)} = USV^\dagger = \begin{pmatrix} -2^{-1/2} \\ 0 \\ 0 \\ 2^{-1/2} \end{pmatrix} \times 1 \times 1$$

where as before we split U into a collection of d vectors with elements $A^{\sigma_3}_{a_2} = U_{(a_2\sigma_3)}$.

Following the previous prescription, we set $A^{\sigma_3} = \begin{pmatrix} \binom{-2^{-1/2}}{0} \\ \binom{0}{2^{-1/2}} \end{pmatrix}_{\sigma_3}$, and we are done.

We now have

```
    $|\psi\rangle = \sum_{\sigma_1\sigma_2\sigma_3}
c_{\sigma_1\sigma_2\sigma_3}|\sigma_1\sigma_2\sigma_3\rangle =
\sum_{a_1,a_2,a_3}^{r_1,r_2,r_3}A^{\sigma_1}_{a_1}A^{\sigma_2}_{a_1,a_2}A^{\sigma_3}_{a_3}
|\sigma_1\sigma_2\sigma_3\rangle$
```

where

```
  $A_{\alpha_1}^{\sigma_1} = \{(1,0) , (0,1)\}$
  $A_{\alpha_1\alpha_2}^{\sigma_2} = \{\begin{pmatrix}0&0\\0&1\end{pmatrix} , \begin{pmatrix}-
1&0\\0&0\end{pmatrix} \}$
  $A_{\alpha_2}^{\sigma_3} = \{\begin{pmatrix}-2^{-1/2}\\0\end{pmatrix} , \begin{pmatrix}0\\2^{-
1/2}\end{pmatrix} \}$
```

Remark on Normalization
It would seem that it is simpler to do the decomposition for unnormalized states using ones everywhere, and then normalize by $1/\sqrt{2}$ perhaps?

Example 2: Four Qubits, following Vidal

Let $|\psi\rangle = \frac{1}{\sqrt{3}}(|1100\rangle + |0011\rangle + |1010\rangle)$

For giggles, disregard the normalization factor for now.
We do a bipartite splitting on the first qubit,

```
           $|\psi\rangle = \sum_{\alpha_1} \lambda_{\alpha_1}^1
|\Phi_{\alpha_1}^1\rangle|\Phi_{\alpha_1}^{2,3,4}\rangle$$\; =
\sum_{\sigma_1,\alpha_1}\Gamma^{\sigma_1}_{\alpha_1}\lambda^{1}_{\alpha_1}|\sigma_1\rangle|\Phi_{\alpha_1}
^{2,3,4}\rangle$
```

where $\Gamma^{\sigma_1}_{\alpha_1}$ comes from the SVD decomposition and $\lambda^1_{\alpha_1}$ are the corresponding singular values, or Schmidt coefficients.

To actually perform the SVD decomposition initially, the tensor $c_{\sigma_1 \ldots \sigma_4}$ needs to be flattened, or "matricized".

We begin by doing a *mode-1* matrix unfolding (or flattening), where we get a matrix$\Psi_{i_1,j} = \Psi_{\sigma_1,(\sigma_2 \ldots \sigma_4}) \in \mathbb{R}^{2 \times (2 \cdot 2 \cdot 2)}$. Note that i_k and j denotes the tensor indices, i.e. $i_k \in 1, 2, \ldots, I_k$, and $j \in 1, 2, \ldots, (\prod_{m \neq k}^{n} I_m)$. An I_k is simply the dimensions of a qubit at k, i.e. 2.

The tensor $c_{\sigma_1 \ldots \sigma_4}$ has nonzero elements c_{1100}, c_{0011} and c_{1010} which, in a mode-1 unfolding, maps to matrix coordinates

$c_{1100} \rightarrow \Psi_{i_1=2,j=2}$
Here $j = 1 + \sum_{k \neq 1}^{4} (i_k - 1) J_k$ with $J_k = \prod_{m \neq 1}^{k-1} I_m$
We can use qubit values directly, by instead rewriting:
$j = 1 + \sum_{k \neq 1}^{4} \sigma_k J_k$

```
    This gives
    $j = 1+ \sigma_2J_2 + \sigma_3J_3 + \sigma_4J_4 = 1 + 1*1 + 0*2 + 0*4 = 2$
```

$c_{0011} \rightarrow \Psi_{i_1=1,j=7}$
Using the same method as above we get
$j = 1 + 0 * 1 + 1 * 2 + 1 * 4 = 7$

$c_{1010} \rightarrow \Psi_{i_1=2,j=3}$
And again,
$j = 1 + 0 * 1 + 1 * 2 + 0 * 4 = 3$

Reinserting the normalization factor we get

```
    $\Psi = \frac{1}{\sqrt{3}}\begin{pmatrix}0&0&0&0&0&0&1&0 \\ 0&1&1&0&0&0&0&0\end{pmatrix}$
```

The SVD decomposition yields:

```
    $U = \begin{pmatrix}0&1 \\ 1&0\end{pmatrix}$


    $S = \frac{1}{\sqrt{3}} \begin{pmatrix}\sqrt{2}&0 \\ 0&1\end{pmatrix}$
```

```
$V^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&1&0&0&0&0&0 \\ 0&0&0&0&0&0&\sqrt{2}&0\end{pmatrix}$
```

where we can identify $\Gamma^{\sigma_1}_{\alpha_1} = U$ (σ_1 labels the row-vectors in U), and $\lambda^1_{\alpha_1} = \{\sqrt{\frac{2}{3}}, \frac{1}{\sqrt{3}}\}$. We also identify $|\Phi^{2,3,4}_{\alpha_1}\rangle$ as

```
       $|\psi\rangle = \sum_{\alpha_1} \lambda_{\alpha_1}^1
|\Phi_{\alpha_1}^1\rangle|\Phi_{\alpha_1}^{2,3,4}\rangle$$\; =
\sum_{\sigma_1,\alpha_1}\Gamma^{\sigma_1}_{\alpha_1}\lambda^{1}_{\alpha_1}|\sigma_1\rangle|\Phi_{\alpha_1}
^{2,3,4}\rangle$
```

Now do step (i)-(iii) in Vidal's approach. Essentially these steps do the decomposition above on $|\sigma_2\sigma_3\sigma_4\rangle$. We have two sets of these vectors depending on the value of σ_1?

```
i.  $|\Phi_{\alpha_1}^{2,3,4}\rangle = \sum_{\sigma_2}
|\sigma_2\rangle|\tau_{\alpha_1,\sigma_2}^{3,4}\rangle$$=|0\rangle|\tau^{3,4}_{\alpha_1,0}\rangle +
|1\rangle|\tau^{3,4}_{\alpha_1,1}\rangle$$=|0\rangle(|10\rangle + |11\rangle) + |1\rangle(|00\rangle)$?
  This means that we should have two different vectors $\tau$. One for each possible $\sigma_2$.



ii. $|\tau_{\alpha_1,\sigma_2}^{3,4}\rangle =
\sum_{\alpha_2}\Gamma_{\alpha_1\alpha_2}^{\sigma_2}\lambda_{\alpha_2}^2|\Phi_{\alpha_2}^{3,4}\rangle$
  This can be accomplished by doing a Schmidt decomposition on each of $|\psi\rangle|_{\sigma_2 = 0}$



>  Expand each vector $|\Phi_{\alpha_1}^{2...n}\rangle$ in a local basis for qubit 2,
$|\Phi_{\alpha_1}^{2...n}\rangle =\sum_{\sigma_2}|\sigma_2\rangle
|\tau_{\alpha_1,\sigma_2}^{3...n}\rangle$
>
>  Write each vector $|\tau_{\alpha_1,\sigma_2}^{3...n}\rangle$ in terms of at most $\chi$ Schmidt vectors
$\{|\Phi_{\alpha_2}^{3...n}\rangle\}_{\alpha_2}^\chi$, i.e. eigenvectors of $\rho^{3...n}$ and the
corresponding Schmidt coefficients $\lambda_{\alpha_2}^2$: $|\tau_{\alpha_1,\sigma_2}^{3...n}\rangle =
\sum_{\alpha_2}\Gamma_{\alpha_1\alpha_2}^{\sigma_2}\lambda_{\alpha_2}^2|\Phi_{\alpha_2}^{3...n}\rangle$
>
> Substitute the equations in (1) and (2) into the first splitting above
```

Example with PBC

Virtual systems: Valence bonds or Maximally entangled pairs

This is a summary of ppt3 and

> Wahl, T. B. (2015). Tensor network states for the description of quantum many-body systems. arXiv Preprint, (August), 156. Retrieved from http://arxiv.org/abs/1509.05984
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> Pérez-García, D., Verstraete, F., Wolf, M. M., & Cirac, J. I. (2007). Matrix Product State Representation. Quantum Inf. Comp., 7, 401. https://doi.org/10.1143/JPSJ.81.074003
>
> Saberi, H. (2008). Matrix-product states for strongly correlated systems and quantum information processing. Dissertation, 141. https://edoc.ub.uni-muenchen.de/9755/1/Saberi_Hamed.pdf

On a spin-S chain of length N, replace each d-dimensional system $|\sigma_i\rangle$ at site i, with two *virtual systems* $|l_i, r_i\rangle$ of dimension $D_i = 1 + 2S'$, called the bond dimension. These are sometimes called *auxiliary* systems. In general D_i can be different for each site but it it needs to be larger than the bond dimension. Note that l and r stand for left and right.


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Let every pair of virtual systems be maximally entangled with the respective neighboring system. This means that $r_i = l_{i+1} = \alpha_i$. The states are

written in the form:

```
      $|I_{i,i+1}\rangle = \sum_{\alpha_i=1}^D |r_i=\alpha_i,l_{i+1}=\alpha_i\rangle$
```

And for the whole chain:

```
      $|I\rangle = \sum_{\alpha_1,\alpha_2,...,\alpha_{N-
1}}|\alpha_0,\alpha_1\rangle|\alpha_1,\alpha_2\rangle...|\alpha_{N-1},\alpha_N\rangle$
```

where each sum denotes an *entangled bond*. **Note that without PBC the leftmost and rightmost sites have only one virtual particle**.

Then, apply a map

```
            $\mathcal{A}^i = \sum_{\sigma_i} \sum_{l_i,r_i} A^{\sigma_i}_{l_i,r_i}|\sigma_i\rangle\langle
l_i,r_i|$
```

to each of the N sites. We then obtain the MPS

```
      $|\psi\rangle = (\bigotimes_i^N \mathcal{A}^i)(\bigotimes_i^{N-1} |I_{i,i+1}\rangle)=
\sum_{\sigma_1...\sigma_N} A^{\sigma_1}...A^{\sigma_N} |\sigma_1...\sigma_N\rangle$
```

Example using valence bonds:

As before, let $|\psi\rangle = \frac{1}{\sqrt{2}}(|010\rangle + |101\rangle)$ be the state of 3 qubits, $d = 2$.

Let each site be replaced by pairs of dimension $D = 2$ in a maximally entangled state, i.e. rewrite it in the (unnormalized) form:

```
        $|I_{1,2} \rangle = \sum_{\alpha_1} |r_1 = \alpha_1, l_2=\alpha_1\rangle = |0,0\rangle_{r_1,l_2} +
|1,1\rangle_{r_1,l_2}$
        $|I_{2,3} \rangle = \sum_{\alpha_2} |r_2 = \alpha_2, l_3=\alpha_2\rangle = |0,0\rangle_{r_2,l_3} +
|1,1\rangle_{r_2,l_3}$
```

where the subscripts r_i, l_i are there to remind us that this is the right and left virtual particles corresponding to site i. Now apply the map $\mathcal{A}$ on each site. :

```
      $\mathcal{A}^1 |I_{1,2}\rangle=\sum_{\sigma_1}\sum_{r_1}A^{\sigma_1}_{r_1}|\sigma_1\rangle\langle
r_1|(\sum_{\alpha_1}|\alpha_1,\alpha_1\rangle)$

            $= \sum_{\sigma_1} A_0^{\sigma_1} |\sigma_1\rangle _{r_1}\langle 0|0,0\rangle_{r_1,l_2} +
A_1^{\sigma_1}|\sigma_1\rangle _{r_1}\langle 1|1,1\rangle_{r_1,l_2}$,


            $= \sum_{\sigma_1} A_0^{\sigma_1} |\sigma_1\rangle |0\rangle_{l_2} +
A_1^{\sigma_1}|\sigma_1\rangle |1\rangle_{l_2}$
```

Similarly,

```
  $\mathcal{A}^2
|I_{1,2}\rangle=\sum_{\sigma_2}\sum_{l_2,r_2}A^{\sigma_2}_{l_2,r_2}|\sigma_2\rangle\langle l_2,r_2|
(\sum_{\alpha_1}|\alpha_1,\alpha_1\rangle)$

      $= \sum_{\sigma_2} (A_{0,0}^{\sigma_2} |\sigma_2\rangle\langle 0,0| +
A_{0,1}^{\sigma_2}|\sigma_2\rangle\langle 0,1| + A_{1,0}^{\sigma_2}|\sigma_2\rangle\langle 1,0| +
A_{1,1}^{\sigma_2}|\sigma_2\rangle\langle 1,1|)_{l_2,r_2} (|0,0\rangle_{r_1,l_2} + |1,1\rangle_{r_1,l_2})$
      $= \sum_{\sigma_2} A_{0,0}^{\sigma_2} |\sigma_2\rangle _{r_2}\langle 0|0\rangle_{r_1} +
A_{0,1}^{\sigma_2} |\sigma_2\rangle _{r_2}\langle 0|1\rangle_{r_1} + A_{1,0}^{\sigma_2} |\sigma_2\rangle
_{r_2}\langle 1|0\rangle_{r_1}+A_{1,1}^{\sigma_2} |\sigma_2\rangle _{r_2}\langle 1|1\rangle_{r_1}$



  $\mathcal{A}^2
|I_{2,3}\rangle=\sum_{\sigma_2}\sum_{l_2,r_2}A^{\sigma_2}_{l_2,r_2}|\sigma_2\rangle\langle l_2,r_2|
(\sum_{\alpha_2}|\alpha_2,\alpha_2\rangle)$
      $= \sum_{\sigma_2} A_{0,0}^{\sigma_2} |\sigma_2\rangle _{l_2}\langle 0|0\rangle_{l_3} +
A_{0,1}^{\sigma_2} |\sigma_2\rangle _{l_2}\langle 0|1\rangle_{l_3} + A_{1,0}^{\sigma_2} |\sigma_2\rangle
```

```
_{l_2}\langle 1|0\rangle_{l_3}+A_{1,1}^{\sigma_2} |\sigma_2\rangle _{l_2}\langle 1|1\rangle_{l_3}$
```

and finally,

```
      $\mathcal{A}^3 |I_{2,3}\rangle=\sum_{\sigma_3}\sum_{l_3}A^{\sigma_3}_{l_3}|\sigma_3\rangle\langle
l_3|(\sum_{\alpha_2}|\alpha_2,\alpha_2\rangle)$

            $= \sum_{\sigma_3} A_0^{\sigma_3} |\sigma_3\rangle _{l_3}\langle 0|0,0\rangle_{r_2,l_3} +
A_1^{\sigma_3}|\sigma_3\rangle _{l_3}\langle 1|1,1\rangle_{r_2,l_3}$


            $= \sum_{\sigma_3} A_0^{\sigma_3} |\sigma_3\rangle |0\rangle_{r_2} +
A_1^{\sigma_3}|\sigma_3\rangle |1\rangle_{r_2}$
```

Above, all cross-terms such as ${}_{r_i}\langle n|m\rangle_{r_i} =_{l_i} \langle n|m\rangle_{l_i} = \delta_{nm}$.

All other combinations are equal to zero, i.e. $\mathcal{A}^1|I_{2,3}\rangle = \mathcal{A}^3|I_{1,2}\rangle = 0$.

Now we multiply

$(\mathcal{A}^1 \otimes \mathcal{A}^2)(|I_{1,2}\rangle \otimes |I_{2,3}\rangle) = \sum_{\sigma_1,\sigma_2} A_0^{\sigma_1} A_{0,0}^{\sigma_2}|0\rangle_{l_3} + A_0^{\sigma_1} A_{0,1}^{\sigma_2}|1\rangle_{l_3}$

```
   $|\psi\rangle=(\bigotimes_i^3 \mathcal{A}^i)(\bigotimes_i^{2} |I_{i,i+1}\rangle)$$=$
```

Hmmm

Bond Dimension

Each $A^{\sigma_i}_{a_i,a_{i+1}}$ above is an $(r_i \times r_{i+1})$ matrix, where r_i is the rank of the Schmidt decomposition at each site i. The *bond dimension* of an MPS is defined by

```
            $D\equiv \max_i r_i$
```

Graphical representation

The following is a summary of the review paper by

> Eisert, J. (2013). Entanglement and tensor network states. Modeling and Simulation, 3(520), 39.

We represent mathematical objects in the following way:

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Scalar

Vector

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Dual vector

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Matrix

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Scalar multiplication

A contracted common index between matrices constitute a matrix multiplication, represented by a shared edge:

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$\sum_{\gamma}^{N} A_{\alpha,\gamma} B_{\gamma,\beta} = C_{\alpha,\beta}.$

A trace is understood as

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and a partial trace as

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Let j_i be a particle with spin-$1/2$ at position i on a chain with n particles. Then the tensor $c_{j_1,j_2,\ldots,j_n}$ is the collection of complex numbers that tells us in what linear combination a state is in, in terms of its basis vectors:

https://d2mxuefqeaa7sj.cloudfront.net/s_72860CA687EA58462BE4EE7EC7675CC2A4C338BF20408382737D46203044AB28_1490006860832_file.png

$|\psi\rangle = \sum_{j_1,j_2\ldots j_n} \; c_{j_1,j_2,\ldots,j_n} \; |j_1, j_2, \ldots, j_n\rangle$

The Schmidt decomposition allows us to rewrite this tensor in terms of matrices. If we use periodic boundary conditions this looks like

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$|\psi\rangle = \sum_{a_1,a_2\ldots,a_n}^{r_1,r_2,\ldots,r_n} \mathrm{Tr}(A^{j_1}_{a_1,a_2} A^{j_2}_{a_2,a_3} \ldots A^{j_n}_{a_n,a_1}) |j_1, j_2, \ldots, j_n\rangle$

where the trace takes care of the periodic boundary.

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Matrix Product Operators