1. **Overlaps and normalization**

Consider overlap of 2-site MPS:

\[
\langle \beta' | \beta \rangle = \langle \sigma_1' | \sigma_1 \rangle A^{\sigma_1} A^{\sigma_1'} B^{\sigma_1} B^{\sigma_1'}
\]

Introduce:

\[
A^+ : \langle \beta' | \beta \rangle = A^{\sigma_1} A^{\sigma_1'} B^{\sigma_1} B^{\sigma_1'} < \langle \sigma_1' | \sigma_1 \rangle A^{\sigma_1} A^{\sigma_1'} B^{\sigma_1} B^{\sigma_1'} > \]

Reorder:

\[
B^{\sigma_1} A^{\sigma_1'} A^{\sigma_1} B^{\sigma_1'}
\]

Ket:

\[
| \beta \rangle = \langle \sigma_1' | \sigma_1 \rangle A^{\sigma_1} B^{\sigma_1'}
\]

Use diagrammatic rules to keep track of contraction patterns:

\[
\langle \beta' | \rangle = \langle \sigma_1' | \sigma_1 \rangle A^{\sigma_1} B^{\sigma_1'}
\]
We accommodated complex conjugation via Hermitian conjugation and index transposition:

\[
\begin{align*}
A^{+} & = A^{\alpha \sigma} \\
\text{left} & \quad \text{right}
\end{align*}
\]

This scheme switches upper and lower indices \(\Rightarrow\) inverts all arrows in diagram.

Note that in diagram the vertex \(\alpha\) is left, \(\beta\) right, whereas on \(A^{+}\), \(\beta\) sits left, \(\alpha\) right.

It will simplify the structure of diagrams representing overlaps.

Generalization to many-site MPS:

\[
|\Psi\rangle = |\tilde{\sigma}\rangle_{N} A_{[1]}^{\tilde{\sigma}_{1}} A_{[2]}^{\tilde{\sigma}_{2}} A_{[3]}^{\tilde{\sigma}_{3}} \cdots A_{[N]}^{\tilde{\sigma}_{N}}
\]

Square brackets indicate that each site has a different \(A\) matrix.

We can use shorthand notation and schematic:

\[
A^{\alpha \sigma}_{\beta} \equiv A_{[l]}^{\alpha \sigma_{l}} \quad (l = \text{site #})
\]
Recipe for ket formula: as chain grows, attach new matrices on the right (in the same order as vertices in diagram) resulting in MPS.

\[ \langle \psi | = \langle \bar{\sigma}_1 | A^{i \sigma_1}_{[1]} \bar{A}^{\sigma_2}_{[2]} A^{\sigma_3}_{[3]} \ldots A^{\sigma_N}_{[N]} | 1 \rangle \]

\[ = A^{+}_{[N]} \bar{\sigma}_N \ldots A^{+}_{[3]} \bar{\sigma}_3 A^{+}_{[2]} \bar{\sigma}_2 A^{+}_{[1]} \bar{\sigma}_1 \langle \bar{\sigma}_N | \]

We rewrite using Hermitian conjugates, change schematic by transposing indices and inverting arrows. To recover MPS structure, order Hermitian conjugate matrices to appear in order opposite to vertex order in diagram.

Recipe for bra formula: as chain grows, attach new matrices \( A^+ \) on the left, *opposite to vertex order in diagram.*

Now consider overlap between two MPS:

\[ \langle \psi | 14 \rangle = \]

\[ = \bar{A}^{+}_{[N]} \sigma_N \ldots \bar{A}^{+}_{[1]} \sigma_1 A^{\sigma_1}_{[1]} A^{\sigma_2}_{[2]} \ldots A^{\sigma_N}_{[N]} \]

Fall 2019
**Exercise:** derive result algebraically.

→ Contraction order matters! If we perform matrix multiplication first, for fixed $\overline{\sigma}$, and then sum over $\overline{\sigma}$, we get $\mathcal{O}^N$ terms, each of which is a product of matrices. Exponentially costly!

Calculation is tractable if we rearrange summations:

Diagrammatic depiction: ‘closing zipper’ from left to right

The set of two-leg tensors $C_{\{\sigma\}}$ can be computed iteratively:

**Initialization:**

$$C_{\{\phi\}} = \mathbb{1}$$
Iteration step:

\[
C(e) \lambda \eta = C(e-\eta) \lambda \eta
\]

Final answer:

\[
\lambda^{4} = C_{CNJ}^{1}
\]

Cost estimate (assume all A's are \( D \times 0 \)):

One iteration:

\[
D^{1} \cdot d \cdot D + D^{1} \cdot d \cdot D
\]

Total cost:

\[
D^{3} \cdot d \cdot N \cdot C \cdot d^{N}!
\]

Remark: a similar iteration scheme can be used to ‘close zipper’ from right to left:

\[
\ell l l i \cdot D \cdot D_{CNJ} = \ell l l i \sigma_{i D \cdot D_{CN-1}}
\]
Initialization and iteration step:

\[ \sum_C \mathcal{C}_C = \sum_C \mathcal{C}_C \] (identity)

Normalization: Try above scheme with \[ \langle 4|4 \rangle \]

Left-normalization

A 3-leg tensor \( \tilde{A}_{\alpha \beta} \) is called ‘left-normalized’ if it satisfies

\[
\tilde{A}^T \tilde{A} = \mathcal{I} \quad \Leftrightarrow \quad \left( \tilde{A}^T \tilde{A} \right)^{\alpha \prime \beta} = \tilde{A}^T \tilde{A}^{\beta \prime \alpha} = \mathcal{I}^{\beta \prime \alpha}
\]

Graphical notation:

\[ \begin{array}{c}
\text{left} \quad \begin{array}{c}
\alpha \\
A \\
\beta
\end{array} \quad \begin{array}{c}
\sigma \\
A^T
\end{array} \\
\text{right} \quad \begin{array}{c}
\alpha' \\
\beta'
\end{array}
\end{array} \]

Fall 2019
When all A’s are left-normalized, closing the zipper left-to-right is easy, since all reduce to identity matrices:

\[
C_{(c, e)} \leftarrow C_{(e, e)} \leftarrow \begin{array}{c}
\cdot \\
0
\end{array} = C_{(e, e)} = \leftarrow
\]

Hence:

\[
\langle 4(4) \rangle = \begin{array}{c}
\cdot \\
\cdot
\end{array} = \begin{array}{c}
\cdot \\
\cdot
\end{array} = \cdots = \begin{array}{c}
\cdot
\end{array} = 1
\]

Left-normalized states are automatically normalized to unity.
Right-normalization

So far we have viewed an MPS as being built up from left to right, hence used right-pointing arrows on ket diagram. Sometimes it is useful to build it up from right to left, running left-pointing arrows.

Building blocks:

Iterating, we obtain kets and bras of the form
A 3-leg tensor $B^\sigma_\beta$ is called right-normalized if it satisfies

$$B b^+ = I, \quad (B b^+)_{\beta}^{b'} = B_{\beta}^{\sigma \alpha} b^+ \beta' = I b^{c}.$$ 

Graphical notation for right-normalization:

When all A’s are right-normalized, closing zipper right-to-left is easy

$$\langle 414 \rangle = \begin{array}{c}
\text{Zipper}
\end{array} = \begin{array}{c}
\text{Normalization}
\end{array} = 1$$

Conclusion: MPS built purely from left-normalized $A$ or purely from right-normalized $B$ are automatically normalized to 1.
2. Various canonical MPS forms

Left-canonical (lc-) MPS

\[ |\psi\rangle = (\sigma_1^\alpha \ldots \sigma_N^\alpha) \enspace ; \enspace \sigma_i = 1 \]

Right-canonical (rc-) MPS:

\[ |\psi\rangle = (\sigma_1^\beta \ldots \sigma_N^\beta) \enspace ; \enspace \sigma_i = 1 \]

Site-canonical (sc-) MPS:

\[ |\psi\rangle = (\sigma_1^\alpha \ldots \sigma_1^{\alpha+1} \ldots \sigma_N^\alpha) \enspace ; \enspace \sigma_i = 1 \]

Bond-canonical (bc-) (or mixed) MPS:

\[ |\psi\rangle = (\sigma_1^\alpha \ldots \sigma_N^\alpha) \enspace ; \enspace \sigma_i = 1 \]

Fall 2019
How to bring an arbitrary MPS into one of these forms?

**Transforming to left-normalized form**

Given:

\[ \rho = |\tilde{\sigma}_1 \rangle \langle \tilde{\sigma}_2| \]

Goal: left-normalize

Strategies: take a pair of adjacent tensors, \( M M' \), and use SVD:

\[ M M' = U S V^T M' \equiv A \tilde{M} \]

Here \( A = U \), \( \tilde{M} = S V^T M' \).

Left-Normalization assured by:

\[ U^T U = I \]

Truncation can be performed by discarding some of the smallest singular values (remains left-normalized!)

\[ \Sigma_\lambda \rightarrow \Sigma_\lambda \]

(image)

(F truncation to decrease bond dimension)
Note: if we don’t need to truncate we can use QR (cheaper).

By iterating, starting from $M^\sigma_i M^\sigma_{k}$, we left-normalize $M^\sigma_i \rightarrow M^\sigma_{i-1}$

To left-normalize the entire MPS, choose $l = N$.

As last step, left-normalize last site using SVD on final $\tilde{M}$:

\[ \tilde{M} = U S V^T = \begin{bmatrix} \Sigma \end{bmatrix} \begin{bmatrix} \Lambda \end{bmatrix} \begin{bmatrix} \Omega \end{bmatrix} \]

lc-form:

\[ \sigma_N \lambda_{\sigma_N} \tilde{M} \lambda_{\sigma_N} = U \lambda_{\sigma_N} S_{\sigma_N} V_{\sigma_N}^T = 1 \]

The final singular value, $S_{\sigma_N}$, determines normalization:

\[ \angle \Psi(\Psi) = |S_{\sigma_N}|^2 \]
Transforming to right-normalized form

Given: \[ |\psi\rangle = (\tilde{\sigma})_N (M^{\sigma_1} - M^{\sigma_N}) \]

Goal: right normalize \[ M^{\sigma_N} \rightarrow M^{\sigma_{N+1}} \]

Strategy: take a pair of adjacent tensors, and use SVD:

\[ M^l M^r = M U S V^+ = \tilde{M} \tilde{B}, \quad \tilde{M} = M U S, \quad B = V^+ \]

Starting from \[ M^{\sigma_N-1} M^{\sigma_N} \], move left to \[ M^{\sigma_1} M^{\sigma_{N+1}} \]

Here, right-normalization is assured by: \[ V^+ V = I \quad \Rightarrow \quad B B^+ = I \]
To right-normalize entire chain, choose $\ell = 1$.

\[
\mathbf{M}_1^{\alpha_1 \lambda} = \mathbf{U}_1 \cdot \mathbf{s}_1 \cdot \sqrt{\frac{\sigma_1}{\lambda}}
\]

and as before $s_1$ determines normalization.

\[
\langle q_1 q_1 \rangle = 15 \lambda^2
\]
Transforming to site-canonical form

\[
\begin{align*}
\begin{pmatrix}
\alpha \quad \beta \\
\sigma_1 \
\end{pmatrix}
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\alpha' \\
\sigma_1' 
\end{pmatrix}
\begin{pmatrix}
\sigma_2 \\
\beta 
\end{pmatrix}
= \begin{pmatrix}
\tilde{\alpha} \\
\tilde{\beta} 
\end{pmatrix}
\end{align*}
\]

Left-normalize states \( l \rightarrow l+1 \) starting from site \( l \).

Then right-normalize states \( N \rightarrow l+1 \) starting from site \( N \).

Result:

\[
\begin{align*}
|\psi\rangle &= |\sigma_N\rangle \left( |\sigma_{l+1}\rangle (\tilde{\sigma}_2 \ldots \tilde{\sigma}_N)_{\beta} \right)_{\psi}\tilde{\alpha} \tilde{\beta} \\
&\otimes |\sigma_{l+1}\rangle \ldots |\sigma_l\rangle (A^{\sigma_l} \ldots A^{\sigma_1})_{\alpha} \tilde{\alpha} \tilde{\sigma}_e \tilde{\beta} \\
&= |\beta\rangle_{K} |\sigma_l\rangle |\alpha\rangle_{L} \tilde{\alpha} \tilde{\sigma}_e \tilde{\beta}
\end{align*}
\]

We get an orthonormal set from the states (Exercise in HW):

\[
|\alpha, \sigma_l, \beta\rangle \equiv |\beta\rangle_{K} |\sigma_l\rangle |\alpha\rangle_{L}
\]

\[
\langle \alpha', \sigma_l, \beta' | \alpha, \sigma_l, \beta\rangle = \delta_{\alpha'}^{\alpha} \delta_{\sigma_l}^{\sigma_l} \delta_{\beta'}^{\beta}
\]

This basis is a ‘local site basis’ for site \( l \). Its dimension is usually \( c < d_N \), the dimension of the full Hilbert space.
Transforming to bond-canonical form:

Start from e.g. sc-form, use SVD for \( \tilde{M} \), combine (1)

\[
\begin{align*}
A & \tilde{M} \begin{bmatrix} V_t \\ B \end{bmatrix} = A A \begin{bmatrix} \lambda_1 & \cdots & \lambda_l \\ \vdots & \ddots & \vdots \\ \lambda_1 & \cdots & \lambda_l \end{bmatrix} S B
\end{align*}
\]

We get an orthonormal set of states again:

\[
\langle \tilde{\lambda}_{\alpha}, \tilde{\lambda}_{\beta} | \tilde{\lambda}_{\gamma}, \tilde{\lambda}_{\delta} \rangle = \delta_{\alpha\gamma} \delta_{\beta\delta}
\]

This basis is the ‘local bond basis’ for bond \( \tilde{B} \). It has dimension \( l \times r \).

where \( r \) = dimension of singular matrix \( S \).

Optimization:

\[
\begin{align*}
\tilde{M} &= \begin{bmatrix} V_t \\ B \end{bmatrix} A A \begin{bmatrix} \lambda_1 & \cdots & \lambda_l \\ \vdots & \ddots & \vdots \\ \lambda_1 & \cdots & \lambda_l \end{bmatrix} S B \\
&= \begin{bmatrix} \lambda_1 & \cdots & \lambda_l \end{bmatrix} S^{\dagger} \begin{bmatrix} \lambda_1 & \cdots & \lambda_l \end{bmatrix} \begin{bmatrix} \lambda_1 & \cdots & \lambda_l \end{bmatrix} S^{\dagger}
\end{align*}
\]

\[
\tilde{A} = A U, \quad \tilde{B} = V^T
\]

\[
\langle \tilde{\lambda}_{\alpha}, \tilde{\lambda}_{\beta} | \tilde{\lambda}_{\gamma}, \tilde{\lambda}_{\delta} \rangle = \text{local bond basis for bond } \tilde{B}_{l-1} \text{ (from site } l-1, l)\]
3. Matrix elements and expectation values

One-site operator

\[ \hat{O}_{[\ell]} = \sigma^\ell_+ \sigma^\ell_+ \sigma_i \]

E.g. for spin 1/2:

\[ (S_z)_{\sigma_+} = \frac{1}{\sqrt{2}} (0 1) \quad (S_+ \sigma_+) = (0 0) \]

Consider two states in site-canonical form for site \( \ell \):

\[ \left| \psi \right> = |\overline{o_{\ell}}\rangle \left( A_{\sigma_+}^{\ell} \ldots A_{\sigma_{N\ell}}^{\ell} M_{\sigma_+}^{\ell} \ldots M_{\sigma_{N\ell}}^{\ell} \right) \]

\[ \left| \psi' \right> = |\overline{o_{\ell}'}\rangle \left( A_{\sigma_+}^{\ell'} \ldots A_{\sigma_{N\ell}'}^{\ell'} M_{\sigma_+}^{\ell'} \ldots M_{\sigma_{N\ell}'}^{\ell'} \right) \]

Matrix element:

\[ \left< \psi | \hat{O} | \psi' \right> = C_{(\ell-1)} \]

Close zipper from left and right:

\[ = \overline{M}^{\ell} \bar{\sigma}_+ \sigma_+^{\ell'} C_{(\ell-1)} \bar{M}^{\ell'} \sigma^{\ell}_+ \bar{\sigma}_+^{\ell'} \]

Fall 2019
Consider expectation value: \( \langle \psi | \hat{O} | \psi \rangle \)

Left-normalization means: \( C_{\langle \alpha \rangle} = 1 \)

Right-normalization means: \( D_{\langle \alpha \rangle} = 1 \)

Hence,

\[
\langle \psi | \hat{O} | \psi \rangle = M_\beta \sigma'_x \cdot M^\dagger \sigma_x \cdot \sum \sigma_i \cdot \sum \sigma_i^{+1}
\]

Two-site operator (e.g. for spin chain Hamiltonian term \( \hat{S}_l \cdot \hat{S}_{l+1} \))

Matrix elements:
4. Schmidt decomposition

Consider a quantum system composed of two subsystems \( A, B \) with dimensions \( D, D' \) and orthonormal bases \( \{ |\alpha_A\rangle \}, \{ |\beta_B\rangle \} \).

To be specific, think of physical basis:

\[
|\alpha\rangle_\alpha \equiv |\alpha_A\rangle \quad , \quad |\beta\rangle_\beta \equiv |\beta_B\rangle
\]

General form of pure state on joint set \( A \cup B \):

\[
|\psi\rangle = |\beta\rangle_B |\alpha\rangle_A
\]

Density matrix:

\[
\hat{\rho} = |\psi\rangle \langle \psi| = \sum_{\alpha, \beta} |\alpha\rangle_A \langle \beta|_B |\beta\rangle_B \langle \alpha|_A
\]

Reduced density matrix of subsystem \( A \):

\[
\hat{\rho}_A = \text{Tr}_B (|\psi\rangle \langle \psi|) = \sum_{\alpha, \beta} |\alpha\rangle_A \langle \beta|_B \langle \beta|_B |\beta\rangle_B \langle \alpha|_A
\]

\[
= |\alpha\rangle_A (\hat{\rho}_A)^\dagger_{\alpha, \alpha'} |\alpha'\rangle_A
\]
\[ \begin{align*}
\langle \rho_A \rangle_{\alpha,\beta}^k &= \sum_{\delta} \langle \beta | \rho \rangle \, \chi^{a,\beta} \chi^{f}_{\beta',\alpha'} < \beta'|\beta \rangle \\
\text{with} \\
\phi^{a,\beta} \phi^{f}_{\beta',\alpha'} &= (\phi^{f} \phi^{t})^a_{\beta'}. 
\end{align*} \]

Analogously, RDM of subsystem \( B \):

Diagrammatic derivation:

\[ \hat{\rho}_B = Tr_A \{ \chi \chi^t \} = \langle \beta | \rho_B \rangle \rho_{\beta',\beta} \]

\[ (\rho_B)_{\beta',\beta} = (\phi^t \phi)^{\beta}_{\beta'} \]

Fall 2019
Algebraic derivation:

Singular value decomposition:

Use SVD to find basis for $A + B$ that diagonalizes $Y$

SVD of $Y = USV^\dagger$

With indices:

$Y_{a\beta} = U_{a\lambda} S_{\lambda\mu} V_{\mu\beta}^\dagger

Hence

$Y_{a\beta} = \sum_{\lambda} \lambda_{a\lambda} \lambda_{\lambda\beta} S_{\lambda\lambda}$

where

$\lambda_{a\lambda} = (\alpha)_{\lambda} U_{\lambda\lambda}^a$

$\lambda_{\lambda\beta} = (\beta)_{\lambda} V_{\lambda\beta}^b$
are orthonormal sets of states for $A + B$, and can be extended to yield orthonormal bases if needed.

Orthonormality is guaranteed by

$$u^* u = I, \quad v^* v = I.$$  

Restrict $\sum_\lambda$ to the $r$ non-zero singular values to get a Schmidt decomposition:

$$|\Psi\rangle = \sum_{\lambda} s_\lambda \left| \lambda \right>_A \left| \lambda \right>_B$$

Classical state: $r = 1$

Entangled state: $r > 1$

$r \equiv$ Schmidt number

$$\rho_A = \sum_{\lambda} s_\lambda^2 \left| \lambda \right>_A \left( \lambda \right)$$

$$= \sum_{\lambda} s_\lambda^2 \left| \lambda \right>_A \left( \lambda \right)$$

Fall 2019
In this representation, RDMs are diagonal:

\[ \hat{\rho}_A = \sum_\lambda \langle \lambda | A | \lambda \rangle (| \lambda \rangle \langle \lambda |)_A \quad \text{and} \quad \hat{\rho}_B = \sum_\lambda \langle \lambda | B | \lambda \rangle (| \lambda \rangle \langle \lambda |)_B \]

Entanglement entropy:

\[ S_{AB} = -\sum_\lambda (| \lambda \rangle \langle \lambda |)_A \ln (| \lambda \rangle \langle \lambda |)_B \]

How can one approximate a cheap representation?

\[ \| 14 \| \leq \| 14 \| = \sum_\lambda | \lambda \rangle \langle \lambda | \leq \| 1 \| = \text{Frobenius norm} \]

Define truncated state using singular values:

\[ 14' = \sum_\lambda | \lambda \rangle \langle \lambda | \lambda \]

(If a normalized state is needed, rescale by \( \sum_\lambda \lambda \))

Truncation error: sum of squares of discarded singular values

\[ \| 14 \| - \| 14' \| = \sum_\lambda | \lambda \rangle \langle \lambda | - \sum_\lambda | \lambda \rangle \langle \lambda | = \sum_\lambda (| \lambda \rangle \langle \lambda | - | \lambda \rangle \langle \lambda |) = \sum_\lambda \lambda \]

Useful to obtain ‘cheap’ representation of if singular values decay rapidly.