MPS I: Matrix product states

1. Overlaps and normalization

Consider overlap of 2-site MPS:

\[
|\psi\rangle = |\sigma_1\rangle |\sigma_2\rangle A^\alpha_{\sigma_1} \otimes B^\beta_{\sigma_2}
\]

\[
\langle \phi | \psi \rangle = \overline{A^\alpha_{\sigma_1} B^\beta_{\sigma_2}} \langle \sigma_1 | \sigma_2 | \sigma_1 | \sigma_2 | \sigma_1 | \sigma_2 | A^\alpha_{\sigma_1} \otimes B^\beta_{\sigma_2}
\]

introduce \( A^t_{\sigma_1} \):

\[
A^t_{\sigma_1} = A^\alpha_{\sigma_1} \otimes B^\beta_{\sigma_2}
\]

reorder \( A^t_{\sigma_1} \):

\[
A^t_{\sigma_1} = A^\alpha_{\sigma_1} \otimes B^\beta_{\sigma_2} = \left( B^\beta_{\sigma_2} A^\alpha_{\sigma_1} \right)^t
\]

Ket:

\[
|\psi\rangle = |\sigma_1\rangle |\sigma_2\rangle A^\alpha_{\sigma_1} \otimes B^\beta_{\sigma_2}
\]

Use diagrammatic rules to keep track of contraction patterns:

Bra:

\[
\langle \phi | = \langle \sigma_1 | \sigma_2 | \sigma_1 | \sigma_2 | \sigma_1 | \sigma_2 | A^\alpha_{\sigma_1} \otimes B^\beta_{\sigma_2}
\]

We accommodated complex conjugation via Hermitian conjugation and index transposition:

\[
A^t_{\sigma_1} = \overline{A^\alpha_{\sigma_1}}
\]

This moves upstairs indices downstairs and vice versa, i.e. invents all arrows in diagram.

Note that in diagram vertex, \( \alpha \) sits left, \( \beta \) right, whereas on \( A^t, \beta \) sits left, \( \alpha \) right.

This convention may seem initially awkward, but it greatly simplifies the structure of diagrams representing overlaps.

Generalization to many-site MPS:

\[
|\psi\rangle = |\sigma_N\rangle \ldots |\sigma_2\rangle |\sigma_1\rangle A^\alpha_{\sigma_N} \otimes \ldots A^\alpha_{\sigma_2} \otimes A^\alpha_{\sigma_1}
\]

Square brackets indicate that each site has a different \( A \) matrix. We will often omit them and use the shorthand, \( A^\alpha_{\sigma} \equiv A^\alpha_{\sigma_2} \), since the \( \ell \) on \( \sigma_2 \) uniquely identifies the site.
Exercise: derive this result algebraically from (7), (9),

If we would perform the matrix multiplication first, for fixed \( \vec{\sigma} \), and then sum over \( \vec{\sigma} \), we would get \( 2^N \) terms, each of which is a product of \( 2^N \) matrices. Exponentially costly!

But calculation becomes tractable if we rearrange summations:

Recipe for ket formula: as chain grows, attach new matrices on the right (in same order as vertices in diagram); resulting in a matrix product structure.

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

Now consider overlap between two MPS:

Exercise: derive this result algebraically from (7), (9),

We expressed all makes via their Hermitian conjugates by transposing indices and inverting arrows. To recover a matrix product structure, we ordered the Hermitian conjugate matrices to appear in the opposite as the vertices in the diagram.
Diagrammatic depiction: 'closing zipper' from left to right.

The set of two-leg tensors $C_{[2]}$ can be computed iteratively:

**Initialization:**

$$C_{[0]} = \mathcal{I}$$

**Iteration step:**

$$C_{[\ell]} = A_{[\ell-1]} C_{[\ell-1]}$$

**Final answer:**

$$<\psi | \phi> = C_{[N]}$$

Cost estimate (if all $A$'s are $D$):

One iteration:

$$\sim D^3 \cdot D \cdot N$$
Remark: A similar iteration scheme can be used to 'close zipper from right to left':

\[ D_{(n+1)}^{y} = D_{(n+1)}^{y} \]

**Initialization:**

\[ D_{1}^{(1)} = \text{(identity)} \]

**Iteration step:**

\[ D_{(i+1)}^{y} = D_{(i+1)}^{y} \]

**Normalization**

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

Use above scheme, with \( \tilde{A} = A \)

**Left-normalization**

A 3-leg tensor \( A_{\alpha}^{\beta} \) is called 'left-normalized' if it satisfies

\[ A^{\dagger} A = 1 \]

Explicitly:

\[ (A^{\dagger} A)^{\beta'}_{\beta} = A^{\dagger} A^{\alpha'}_{\alpha} A_{\alpha}^{\beta} = \delta_{\alpha}^{\beta} \]  

**Graphical notation for left-normalization:** draw 'left-pointing diagonals' at vertices

\[ A, A^{\dagger} \]

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

\[ C_{[\ell]} = C_{[\ell]}', \quad C_{[\ell]}^{\alpha'}_{\alpha} = C_{[\ell]}^{\alpha'}_{\alpha} \]

Hence:

\[ \langle \psi | \psi \rangle = C_{[\ell]}^{\lambda}_{\lambda'} = C_{[\ell]}^{\lambda}_{\lambda'} = C_{[\ell]}^{\lambda}_{\lambda'} = \lambda_{\lambda'} \]

**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:**

\[ | \alpha \rangle = | \sigma_{N} \rangle B_{\alpha}^{\sigma_{N}} \]

\[ \alpha \]

\[ \sigma \]

\[ k \]
Iterating this, we obtain kets and bras of the form

$$|\psi\rangle = |\sigma_n\rangle |\sigma_{n-1}\rangle \ldots |\sigma_1\rangle B_{\sigma}^{\dagger} \ldots B_{\beta}^{\dagger} |\beta_1\rangle |\sigma_{n-1}\rangle |\sigma_n\rangle$$

$$\langle \psi | = B_{\beta}^{\dagger} A_{\sigma}^{\dagger} B_{\alpha} \ldots B_{\beta}^{\dagger} |\beta_1\rangle \ldots |\sigma_{n-1}\rangle |\sigma_n\rangle$$

A three-leg terror \( B_{\beta}^{\dagger} \) \( \sigma_{\beta} \) is called right-normalized if it satisfies

$$B B^{\dagger} = 1.$$  \text{Explanation:}  \( (B B^{\dagger}) = B \sigma_{\beta}^{\dagger} B^{\dagger} \beta_{\beta}^{\dagger} = 1 \beta_{\beta}^{\dagger} \)

Graphical notation for right-normalization: draw 'right-pointing diagonals' at vertices

When all B's are right-normalized, closing the zipper right-to-left is easy:

$$\langle \psi | \psi \rangle = 1$$

Conclusion: MPS built purely from left-normalized \( A \)'s or purely from right-normalized \( B \)'s are automatically normalized to 1.

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2. Various canonical MPS forms

Left-canonical (lc-) MPS:

\[ |\psi\rangle = |\tilde{\sigma}\rangle_N (A^{\sigma_1} \ldots A^{\sigma_N}) \]

\[ A^\dagger A = 1 \]

Right-canonical (rc-) MPS:

\[ |\psi\rangle = |\tilde{\sigma}\rangle_N (B^{\sigma_1} \ldots B^{\sigma_N}) \]

\[ B B^\dagger = 1 \]

Site-canonical (sc-) MPS:

\[ |\psi\rangle = |\tilde{\sigma}\rangle_N (A^{\sigma_1} \ldots A^{\sigma_N}) M^{\sigma_1 \ldots \sigma_N} B^{\sigma_1} \ldots B^{\sigma_N} \]

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

\[ |\psi\rangle = |\tilde{\sigma}\rangle_N (M^{\sigma_1} \ldots M^{\sigma_N}) S^{\sigma_1 \ldots \sigma_N} \]

How can we bring an arbitrary MPS into one of these forms?

Transforming to left-normalized form

Given:

\[ |\psi\rangle = |\tilde{\sigma}\rangle_N (M^{\sigma_1} \ldots M^{\sigma_N}) \]

[or with index: \( |\tilde{s}\rangle_N = \ldots \rightarrow S u \ )]

Goal : left-normalize \( M^{\sigma_1} \) to \( M^{\sigma_1 \ldots \sigma_N} \)

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

\[ M M' = U S V^\dagger M' \equiv \tilde{A} \tilde{M} \]

with \( \tilde{A} = U \), \( \tilde{M} = S V^\dagger M' \)
The properly ensures left-normalization: $\mathbf{U}^\dagger \mathbf{U} = \mathbf{1}$

Truncation, if desired, can be performed by discarding some of the smallest singular values,
$$\sum_{\lambda = 1}^r \lambda < \sum_{\lambda = 1}^N \lambda .$$

(but (10) remains valid!)

Note: instead of SVD, we could also use QR (cheaper!)

By iterating, starting from $M^{\sigma_1}$, $M^{\sigma_2}$, we left-normalize $M^{\sigma_i}$ to $M^{\sigma_{i-1}}$.

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

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

$$\sim M_{\lambda \sigma_N} = U_{\lambda \sigma_N} S_{\lambda \sigma_N} V_{\lambda \sigma_N}^\dagger$$

$$\sim M_{\lambda \sigma_N} x = \lambda \sigma_N \sim M_{\lambda \sigma_N} x = \lambda \sigma_N \sim M_{\lambda \sigma_N} x = \lambda \sigma_N \sim M_{\lambda \sigma_N} x$$

The final singular value, $s_i$, determines normalization:
$$\langle \psi | \psi \rangle = |s_i|^2$$

Transforming to right-normalized form

Given:
$$|\psi\rangle = |\sigma_N \rangle (M^{\sigma_1} \ldots M^{\sigma_N})$$

[or with index:
$$|s_i\rangle = s_i$$]
Strategy: take a pair of adjacent tensors, $M M'$, and use SVD:

$$M M' = M U S V^\dagger \equiv \hat{M} B, \quad \text{with} \quad \hat{M} = M U S, \quad B = V^\dagger. \quad (13)$$

Starting form $M_{\sigma_{N-1}}^{\delta_{N-1}} M_{\delta_{N}}^{\sigma_{N}}$, move leftward up to $M_{\sigma_{1}}^{\delta_{1}} M_{\delta_{1}}^{\sigma_{1}}$.

To right-normalize entire chain, choose $\ell$ and at last site, $\ell = 1$

$$\hat{M}_{1}^{\delta_{1}, \lambda} = U_{1}^{\delta_{1}} S_{1}^{\lambda} V_{1}^{\dagger} \delta_{1}, \quad \lambda \quad \text{determines normalization.} \quad (18)$$

Exercise

(a) Right-normalize a state with right-pointing arrows!

Hint: start at $M_{\sigma_{N-1}}^{\delta_{N-1}} M_{\delta_{N}}^{\sigma_{N}}$ and note the up $\leftrightarrow$ down changes in index placement.

(b) Left-normalize a state with left-pointing arrows!

Hint: start at $M_{\sigma_{1}}^{\delta_{1}} M_{\delta_{1}}^{\sigma_{1}}$.
Transforming to site-canonical form

\[ M = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \]

\[ M' = U^T M U \]

Left-normalize sites \( y \) to \( \ell - 1 \), starting from site \( y \).

Then right-normalize sites \( N \) to \( \ell + 1 \), starting from site \( N \).

Result:

\[ |\psi\rangle = |\sigma_0\rangle \cdots |\sigma_{\ell-1}\rangle (B^\dagger \cdots B^\dagger) |\sigma_0\rangle \cdots |\sigma_{\ell-1}\rangle |\alpha\rangle |\beta\rangle \]

\[ = |\beta\rangle |\sigma_{\ell-1}\rangle |\alpha\rangle |\ell\rangle \]

The states \( |\alpha, \sigma_{\ell-1}, \beta\rangle \) form an orthonormal set:

\[ \langle \alpha' , \sigma_{\ell-1}' , \beta' | \alpha, \sigma_{\ell-1}, \beta \rangle = \delta_{\alpha, \alpha'} \delta_{\sigma_{\ell-1}, \sigma_{\ell-1}'} \delta_{\beta, \beta'} \]

(Exercise: verify this, using \( A^T A = I \) and \( B B^T = I \).)

This is 'local site basis' for site \( \ell \). Its dimension \( D_{\alpha} \cdot D_{\sigma_{\ell-1}} \cdot D_{\beta} \), is usually \( < c c c d^N > \) of full Hilbert space.

Transforming to bond-canonical form

Start from (e.g.) sc-form, use SVD for \( \bar{M} = U S V^T \), combine \( V^T \) with neighboring \( B \), or \( U \) with neighboring \( A \).

\[ \bar{M} = U S V^T \]

or \( \bar{M} = U S V^T \)

\[ A = U \]

\( \bar{B} = V^T B \)

(Exercise: add indices!)
The states \( |\lambda, \lambda'\rangle \) form an orthonormal set.

\[
\langle \lambda, \lambda' \mid \lambda, \lambda' \rangle = \delta_{\lambda}^{\lambda'} \delta_{\lambda}^{\lambda'}
\]  

(29)

This is called the 'local bond basis for bond \( \ell \) ' (from site \( \ell \) to \( \ell+1 \) ). It has dimension \( r \cdot r \) \( (r = \text{dimension of singular matrix } S ) \).

\[
\begin{align*}
A & \tilde{A} \ B \ B \\
\tilde{\mu} & = U S V^\dagger \quad \tilde{A} = \begin{pmatrix} A \\ \lambda \end{pmatrix} U, \ B = V^\dagger \\
& \text{involves sites } \ell \text{ to } N \quad \text{involves sites } 1 \text{ to } \ell-1
\end{align*}
\]

(Exercise: add indices!) (30)