Matrix Product States

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1.1: Singular Value Decomposition (SVD) and Schmidt Decomposition

SVD of a matrix M:

$$M = USV^\dagger$$

- U: Orthonormal columns ($U^\dagger U = I$)
- S: Diagonal matrix with non-negative singular values $s_1 \geq s_2 \geq \dots$
- $V^\dagger$: Orthonormal rows ($V^\dagger V = I$)

Schmidt Decomposition of a pure state $|\psi\rangle$:

$$|\psi\rangle = \sum_{a=1}^{r} s_a |a\rangle_A |a\rangle_B$$

- r: Schmidt rank, number of non-zero singular values
- s_a: Singular values, encode entanglement
- Reduced density matrices:

$$\rho_A = \sum s_a^2 |a\rangle\langle a|, \quad \rho_B = \sum s_a^2 |a\rangle\langle a|$$

1.2: QR Decomposition

QR decomposition:

$$M = QR$$

- Q: Orthonormal columns ($Q^\dagger Q = I$), analogous to U in SVD
- R: Upper triangular

Thin QR decomposition (for $N_A > N_B$):

$$M = Q_1 R_1 \quad \text{with} \quad Q_1 \in \mathbb{C}^{N_A \times N_B},\ R_1 \in \mathbb{C}^{N_B \times N_B}$$

Usage in MPS:

- QR is computationally cheaper than SVD
- Used when singular values are not needed explicitly
- Still allows for left-normalized matrices: $\sum_r A_r^\dagger A_r = I$

Note: SVD gives optimal truncations (e.g., best rank-r_0 approximation), while QR is efficient when only orthonormality is required.

1.3: Decomposition into MPS (I)

Any pure state on L sites:

$$|\psi\rangle = \sum_{r_1,\ldots,r_L} c_{r_1\ldots r_L} |r_1 \ldots r_L\rangle$$

SVD-based decomposition:

- Reshape the state into a matrix and apply SVD iteratively.
- Introduce bond indices $a_1, \ldots, a_{L-1}$:

$$c_{r_1\ldots r_L} = A^{[1]}_{1,a_1}{}^{r_1} A^{[2]}_{a_1,a_2}{}^{r_2} \ldots A^{[L]}_{a_{L-1},1}{}^{r_L}$$

- The full state becomes:

$$|\psi\rangle = \sum_{r_1,\ldots,r_L} A^{[1]} \ldots A^{[L]} |r_1 \ldots r_L\rangle$$

Left-canonical form:

$$\sum_r (A^{[\ell],r})^\dagger A^{[\ell],r} = I$$

1.3: Decomposition into MPS (II)

Canonical Forms:

- **Right-canonical:** $\sum_r A^{[\ell],r}(A^{[\ell],r})^\dagger = I$
- **Mixed-canonical:** left-normalized on one side, right-normalized on the other
- Schmidt decomposition appears naturally:

$$|\psi\rangle = \sum_a s_a |a\rangle_A |a\rangle_B$$

Gauge Freedom:

- MPS is invariant under:

$$A^{[\ell]} \to A^{[\ell]}X, \quad A^{[\ell+1]} \to X^{-1}A^{[\ell+1]}$$

- Used to switch canonical forms, impose normalization

QR Decomposition:

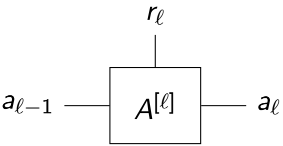
- Faster than SVD, constructs canonical MPS
- Doesn't yield singular values or ranks

1.3: Decomposition into MPS (III)

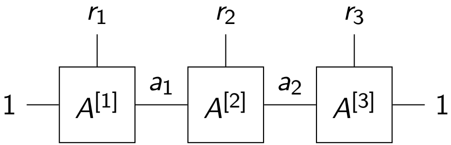
Diagram conventions:

- Box = tensor $A^{[\ell]}$
- Vertical leg = physical index r_ℓ
- Horizontal legs = bond indices $a_{\ell-1}, a_\ell$

Single Tensor



3-site MPS



Canonical normalization:

$$\text{Left: } \sum_r (A^{[\ell],r})^\dagger A^{[\ell],r} = I \quad \text{Right: } \sum_r A^{[\ell],r} (A^{[\ell],r})^\dagger = I$$

Contraction over physical + bond index gives identity.

1.4: MPS and Single-Site Decimation (I)

Iterative block growth:

- Grow system left-to-right by adding sites one at a time
- Truncate block Hilbert space to fixed dimension D

Recursive MPS construction:

$$|a_\ell\rangle = \sum_{a_{\ell-1}, r_\ell} A^{[\ell], r_\ell}_{a_{\ell-1}, a_\ell} |a_{\ell-1}\rangle \otimes |r_\ell\rangle$$

Normalization conditions:

$$\sum_r A^{[\ell], r\dagger} A^{[\ell], r} = I, \quad \sum_r B^{[\ell]} B^{[\ell]\dagger} = I$$

Partial block state representation:

$$|\psi\rangle = \sum_{a_\ell} |a_\ell\rangle_A \otimes |a_\ell\rangle_B$$

(Schmidt-like form, but only one side is orthonormal)

Mixed canonical form:

$$|\psi\rangle = A^{[1]} \cdots A^{[\ell]} S B^{[\ell+1]} \cdots B^{[L]}$$

- Left of bond ℓ: left-normalized tensors
- Right of bond ℓ: right-normalized tensors
- Center: diagonal matrix S contains singular values

Good quantum numbers:

- Magnetization $M = \sum_i M_i$ can be conserved across tensors
- Rule: $M_{\text{left}} + M_r = M_{\text{right}}$
- Enables block structure in tensors

Boundary conditions:

- Open BC: MPS ends in vectors
- Periodic BC: use trace over MPS matrices

$$|\psi\rangle = \sum_r \mathrm{Tr}(M^{[1]} \cdots M^{[L]}) |r_1 \cdots r_L\rangle$$

1.5: The AKLT State as a Matrix Product State

AKLT model (1987):

$$\hat{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2$$

- Spin-1 chain; ground state = AKLT state
- Each spin-1 decomposed into two symmetrized spin-$\frac{1}{2}$ particles
- Neighbouring spin-$\frac{1}{2}$ pairs form singlets

MPS representation:

- Local physical basis $\{|+\rangle, |0\rangle, |-\rangle\}$ from symmetric spin-$\frac{1}{2}$ pairs
- State written using $D = 2$ matrices $\tilde{A}^r$
- Normalization: scale $\tilde{A}^r \to A^r = \sqrt{4/3}\,\tilde{A}^r$

Resulting structure:

$$|\psi_{\mathrm{AKLT}}\rangle = \sum_{\{r\}} \mathrm{Tr}(A^{r_1} A^{r_2} \cdots A^{r_L}) |r_1 \cdots r_L\rangle$$

$\rightarrow$ *One of the simplest exact, non-trivial MPS with entanglement.*

2.1: Efficient Evaluation of Contractions

Problem: Naive contraction of MPS overlaps or expectations costs $\sim d^L$

Key idea:

- Contract site-by-site, avoiding full wavefunction reconstruction
- Reuse intermediate results; sweep from left or right

Overlap contraction:

$$\langle \phi | \psi \rangle = \sum_{r_1 \ldots r_L} \bar{M}^{[1],r_1} \ldots \bar{M}^{[L],r_L} \cdot M^{[1],r_1} \ldots M^{[L],r_L}$$

Cost:

- Naively: $\mathcal{O}(d^L)$
- Efficiently: $\mathcal{O}(LD^3 d)$

Canonical forms:

- Local contractions simplify via orthonormality
- Norm becomes 1 if left- or right-normalized

2.2: Transfer Operator and Correlation Structures

Transfer operator $\mathbb{E}$:

- Propagates operators from site to site in an MPS
- Acts on density matrices: $|a_{\ell-1}\rangle\langle a'_{\ell-1}| \to |a_\ell\rangle\langle a'_\ell|$

Without operator:

$$\mathbb{E} = \sum_r M^{[\ell],r} \otimes \bar{M}^{[\ell],r}$$

With local operator $\hat{O}^{[\ell]}$:

$$\mathbb{E}_O = \sum_{r,r'} O_{rr'} \, M^{[\ell],r} \otimes \bar{M}^{[\ell],r'}$$

Use cases:

- Expectation values and correlation functions
- Correlations decay eigenvalues of $\mathbb{E}$

Insight: MPS encode finite correlation length via exponential decay from the transfer matrix.

Goal: Represent reduced density matrices ρ_ℓ from MPS

Total density operator:

$$|\psi\rangle\langle\psi| = \sum_{r,r'} A^{r_1} \cdots A^{r_L} A^{r'_L\dagger} \cdots A^{r'_1\dagger} |r\rangle\langle r'|$$

Partial trace:

- Tracing out all sites except ℓ gives local density matrix
- Done via sequential contractions using the transfer operator $\mathbb{E}$

Efficient evaluation:

- Use canonical forms: left-normalized left of ℓ, right-normalized right of ℓ
- Then $\rho_\ell = \sum_{r,r'} \mathrm{Tr}\left(A_\ell^{r\dagger} A_\ell^{r'}\right) |r\rangle\langle r'|$

Insight: Reduced density matrices provide entanglement and local observable access directly from MPS.

Goal: Construct $|\psi\rangle + |\phi\rangle$ from two MPS

For PBC (Periodic BC):

- Represent both as: $|\psi\rangle = \sum_r \mathrm{Tr}(M^{[1]} \cdots M^{[L]})|r\rangle$
- Combine tensors: $N^{[i],r} = \begin{bmatrix} M^{[i],r} & 0 \\ 0 & \tilde{M}^{[i],r} \end{bmatrix}$
- Result: trace over block-diagonal structure reproduces original states

For OBC (Open BC):

- Concatenate row vectors on first site and column vectors on last site
- Intermediate tensors: same block-diagonal structure as PBC

Remarks:

- Bond dimension increases: $D_{\text{new}} = D + \tilde{D}$
- Addition is not closed under fixed D; compression may be needed

$\rightarrow$ *Simple but often inefficient; requires recompression for practical use.*

4: Bringing MPS into Canonical Form

4.1: Left-canonical MPS

- Start from arbitrary MPS with OBC
- Apply SVD (or QR) from left to right: $M = USV^\dagger$
- Assign $A = U$: left-normalized tensor
- Multiply $SV^\dagger$ into the next tensor
- Iterate: all tensors become left-normalized

4.2: Right-canonical MPS

- Start SVDs from right: $M = USV^\dagger$
- Assign $B = V^\dagger$: right-normalized tensor
- Multiply US into the previous tensor
- Continue to left: all tensors become right-normalized

$\rightarrow$ *Canonical forms simplify contractions and prepare MPS for efficient manipulation.*

5.1: Compressing an MPS via SVD

Problem: Reduce bond dimension from D_0 to $D < D_0$, preserving the state as best as possible

Approach:

- Use SVD on the MPS in mixed-canonical form
- Retain D largest singular values across each bond
- Truncate tensors A, B, Λ accordingly

Steps:

- At each bond, perform SVD and truncate
- Move boundary left or right, sweep through full chain

Pros and Cons:

- Fast and simple for small compression
- Not globally optimal; truncations depend on direction

$\rightarrow$ *Effective and practical; widely used in TEBD and DMRG sweeps.*

5.2: Variational Compression of an MPS

Goal: Find best approximation $|\tilde{\psi}\rangle$ with reduced bond dimension D

Method:

- Initialize $|\tilde{\psi}\rangle$ using SVD-compressed state
- Sweep through sites, updating tensors $\tilde{M}^{[i]}$
- Minimize distance: $\| |\psi\rangle - |\tilde{\psi}\rangle \|^2$

Properties:

- Nonlinear optimization over MPS tensors
- Converges with repeated sweeps

Efficiency tips:

- Use SVD-compressed state as initial guess
- Two-site optimization improves convergence and stability

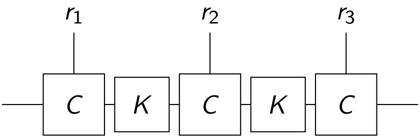
$\rightarrow$ *Slower than SVD, but yields optimal compression in 2-norm.*

CK notation:

$$|\psi\rangle = \sum C^{[1]}K^{[1]}C^{[2]} \dots K^{[L-1]}C^{[L]}|r_1 \dots r_L\rangle$$

Structure:

- $C^{[\ell],r}$: site tensors (isometric)
- $K^{[\ell]}$: diagonal matrices with singular values



→ *CK form exposes Schmidt values via K; orthonormal blocks via C.*

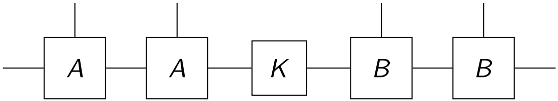
6: Notations and Conversions (II)

Convert CK to canonical forms:

- Left-canonical: $A^{[\ell]} = K^{[\ell-1]} C^{[\ell]}$
- Right-canonical: $B^{[\ell]} = C^{[\ell]} K^{[\ell]}$

Mixed form:

- Left: A-matrices up to site ℓ
- Right: B-matrices from $\ell + 1$ onward
- Middle: uncontracted $K^{[\ell]}$



$\rightarrow$ *Mixed-canonical form is optimal for variational updates and entanglement diagnostics.*

Reference

Ulrich Schollwöck,
"The density-matrix renormalization group in the age of matrix product states,"
Annals of Physics, **326** (2011), 96–192.