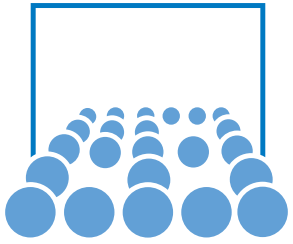
Numerical Linear and Multilinear Algebraic Approaches to Quantum Tensor Networks

Konrad Waldherr

November 8, 2013



Joint work with Thomas Huckle

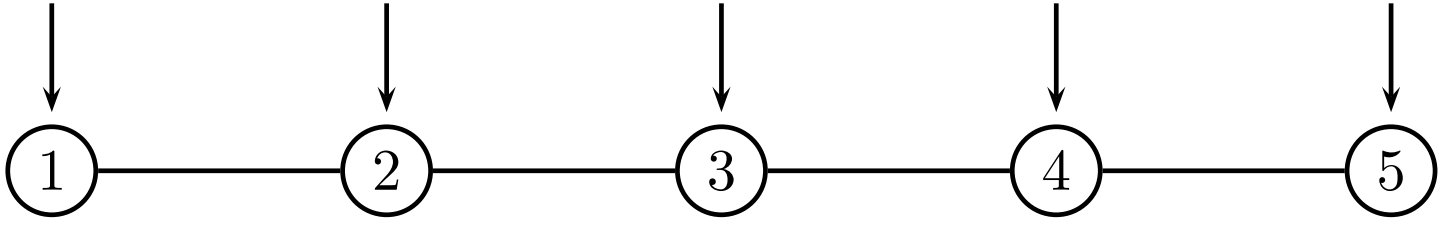
Problem: Computation of Ground States

Given:

- Physical system with N particles (e.g., 1D spin chain)

- Couplings within the system (e.g., nearest-neighbor interaction)

- External interaction (e.g., exterior magnetic field)



Goal:

- Find ground state, i.e., the state related to the smallest energy of the system.

Mathematical Model

- The state of an individual spin is described by a unit vector in $\mathbb{C}^2$.
- The state space of a composed system is the **tensor product** of the state spaces of the constituent subsystems.
- The state of the entire system is represented by a vector in $\mathbb{C}^{2^N}$.

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- The state of the entire system is represented by a vector in $\mathbb{C}^{2^N}$.
- The overall energy of the physical system is described by the Hamiltonian $\boldsymbol{H} \in \mathbb{C}^{2^N \times 2^N}$.
- The Hamiltonian has a representation

$$\boldsymbol{H} = \sum_{k=1}^{M} \alpha_k \boldsymbol{Q}_{\boldsymbol{1}}^{(\boldsymbol{k})} \otimes \cdots \otimes \boldsymbol{Q}_{\boldsymbol{N}}^{(\boldsymbol{k})} \in \mathbb{C}^{2^N \times 2^N} ,$$

where the tensor factors $\boldsymbol{Q}_{\boldsymbol{j}}^{(\boldsymbol{k})}$ are identities or Pauli matrices.

$$\boldsymbol{\sigma_x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \boldsymbol{\sigma_y} = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \boldsymbol{\sigma_z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

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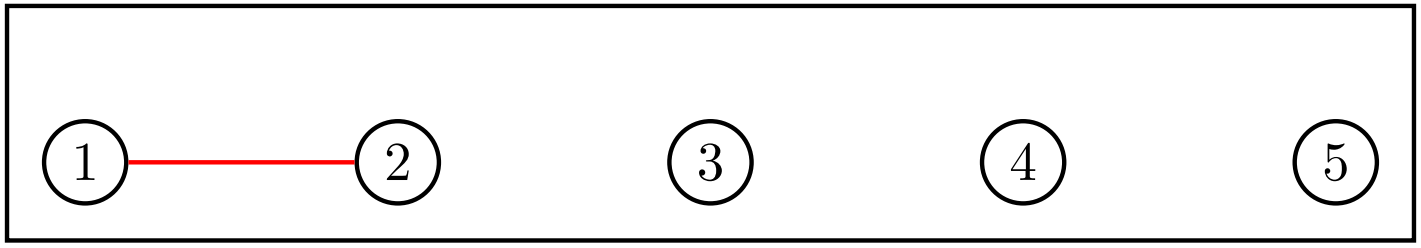
- Then, the ground state corresponds to the **eigenvector related to the smallest eigenvalue**.

Example: Ising-ZZ Hamiltonian



$$H = \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I$$

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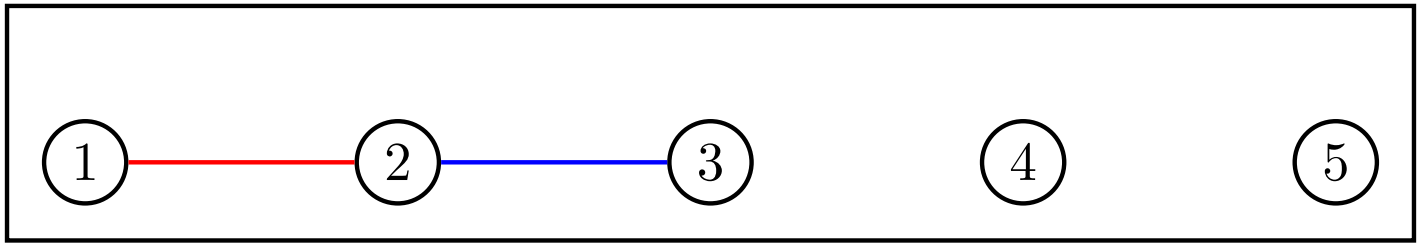

$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I
\end{aligned}
$$

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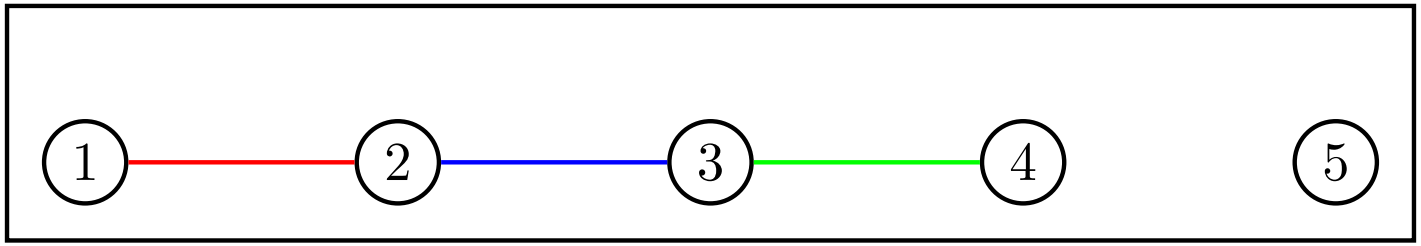

$$
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&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
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$$

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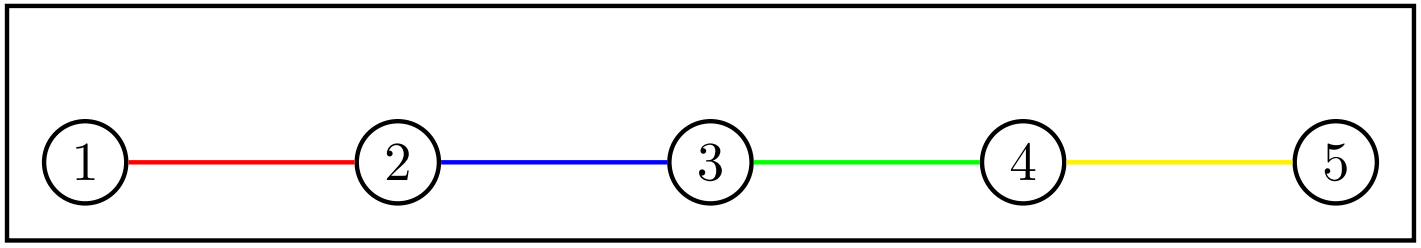

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&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z
\end{aligned}
$$

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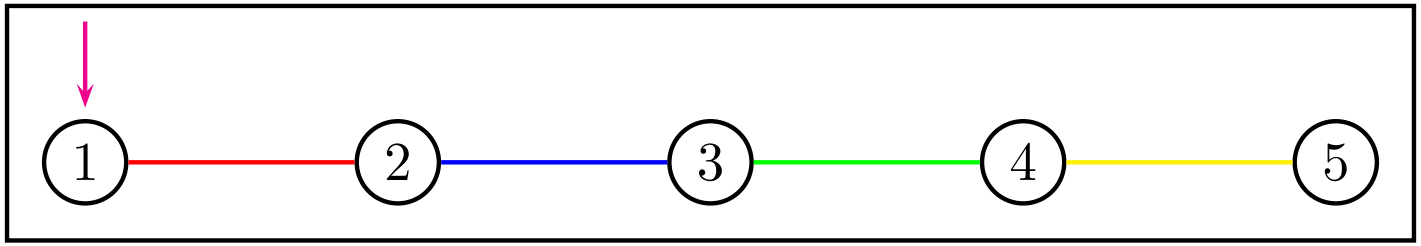

$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I \otimes I \otimes I
\end{aligned}
$$

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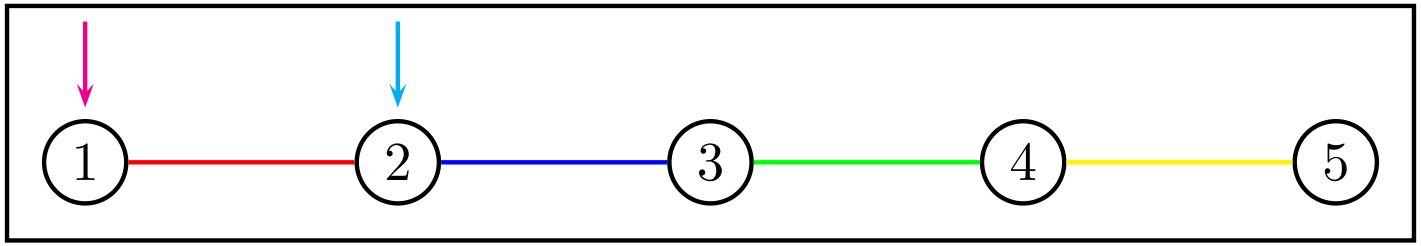

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$$

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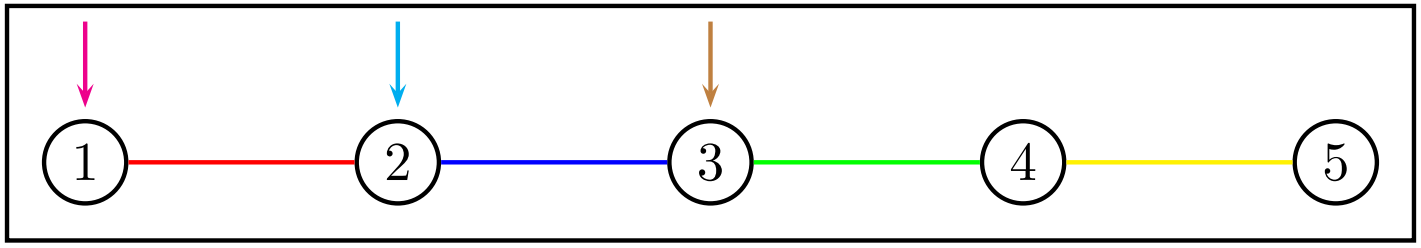

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\begin{aligned}
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&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
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&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I \otimes I \otimes I \\
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\end{aligned}
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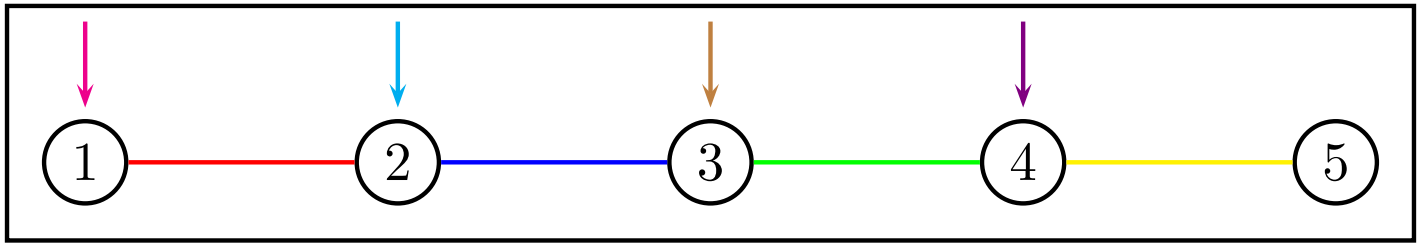

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&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I \otimes I \otimes I \\
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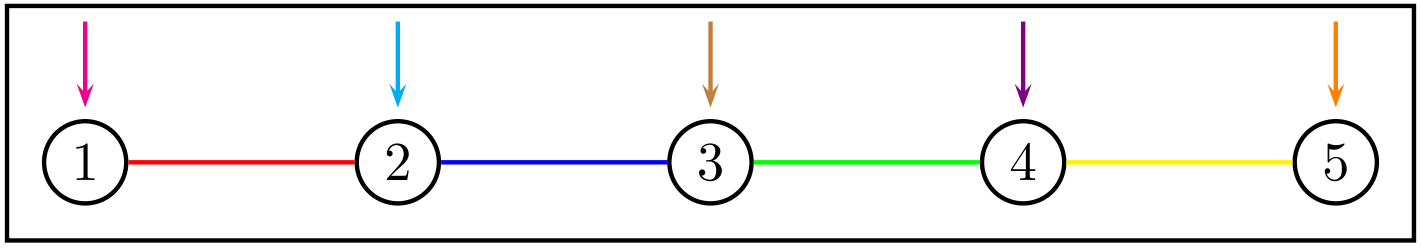

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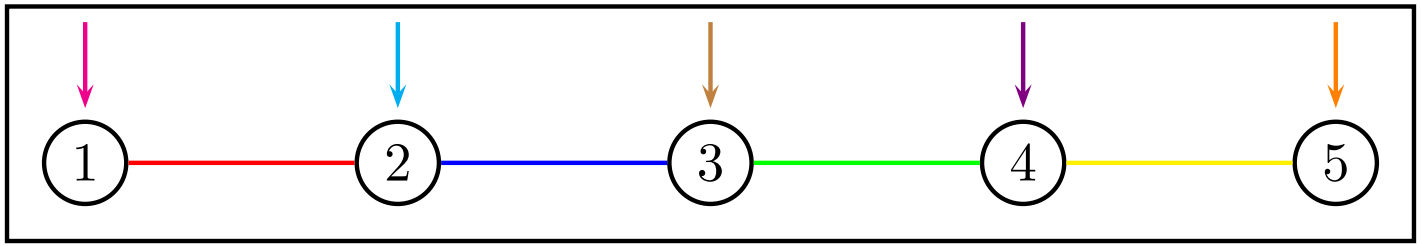
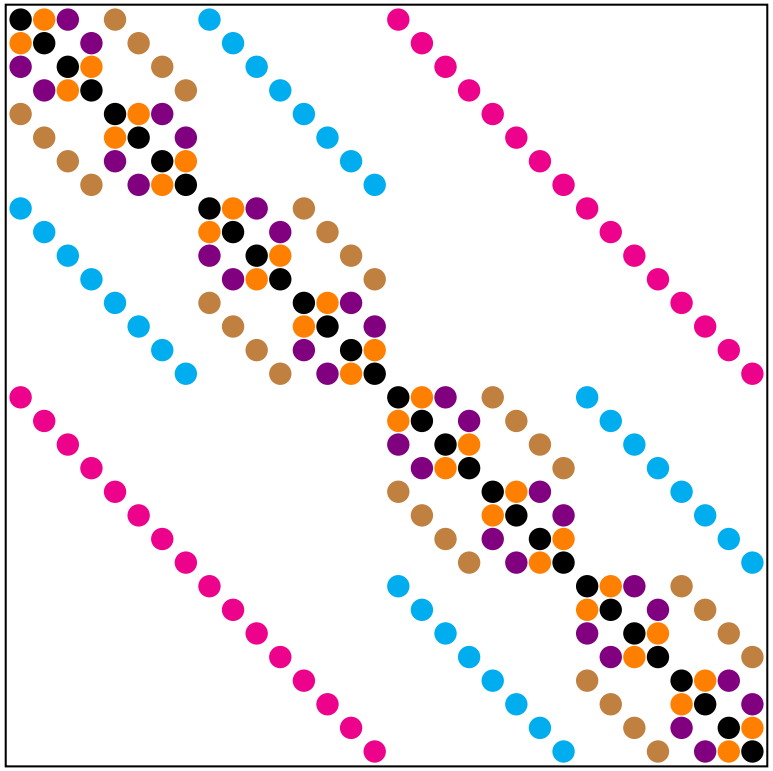
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_x \otimes I \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_x \otimes I \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_x \otimes I \\
&+ I \otimes I \otimes I \otimes I \otimes \sigma_x
\end{aligned}
$$

Sparsity Pattern of the Ising-ZZ Hamiltonian





Problem Setting:

What is the smallest eigenvalue of the huge matrix $H \in \mathbb{C}^{2^N \times 2^N}$?

- Minimization problem:

$$\min_{\boldsymbol{x} \neq \mathbf{0}} \frac{\boldsymbol{x}^{\mathrm{H}} \boldsymbol{H} \boldsymbol{x}}{\boldsymbol{x}^{\mathrm{H}} \boldsymbol{x}} \ .$$

- Challenge: the vector space $\mathbb{C}^{2^N}$ grows **exponentially** in N.

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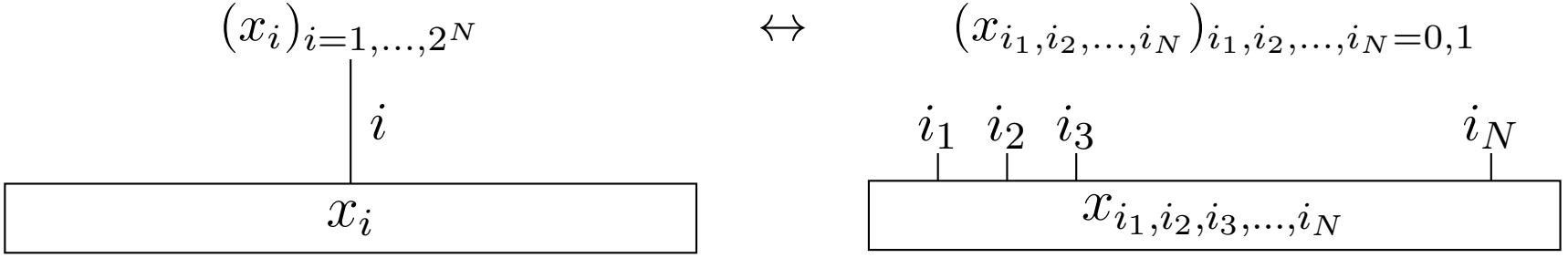
- Challenge: the vector space $\mathbb{C}^{2^N}$ grows **exponentially** in N.
- **Solution: Data-sparse representation format** that
  1. reproduces the underlying physical system,
  2. scales only polynomially in N,
  3. describes the right "corner" $\mathcal{U} \subseteq \mathbb{C}^{2^N}$ of the Hilbert space,
  4. allows for efficient computations of Hx and $x^{\mathrm{H}} y$.

$$\min_{\substack{x \in \mathbb{C}^{2^N} \\ x \neq 0}} \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} \approx \min_{x \in \mathcal{U}} \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{\substack{y \in \mathbb{C}^{\mathrm{poly}(N)} \\ y \neq 0}} \frac{y^{\mathrm{H}} H_{\mathrm{eff}} y}{y^{\mathrm{H}} N_{\mathrm{eff}} y}$$

Tensorization of the Vector

- Consider index i in its binary representation $(i_1, i_2, \ldots, i_N)$.
- Reshape 2^N vector into $2 \times 2 \times \cdots \times 2$ tensor:



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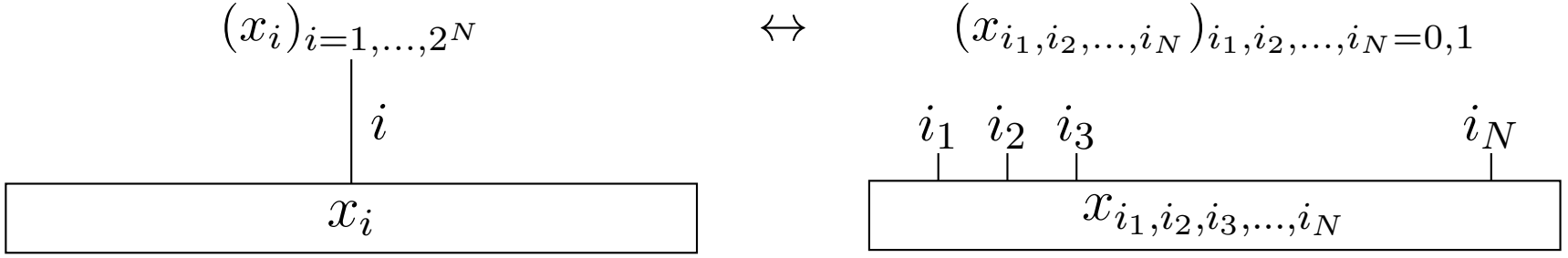

Tensor Decomposition Schemes

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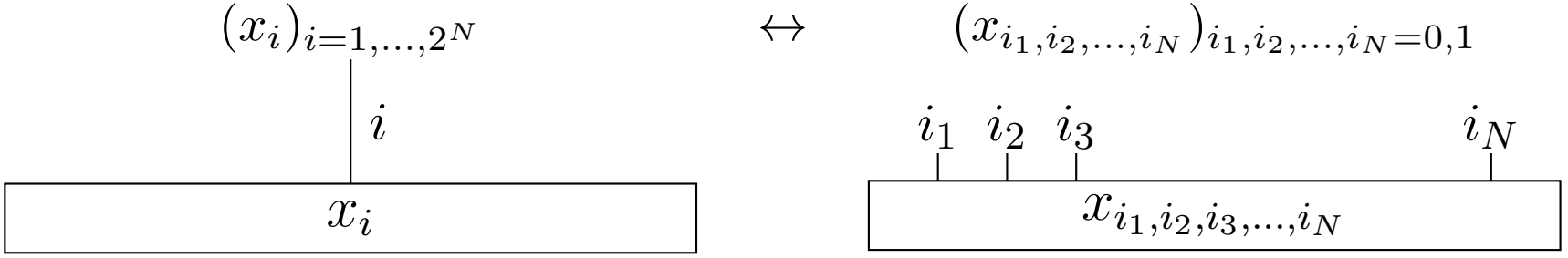
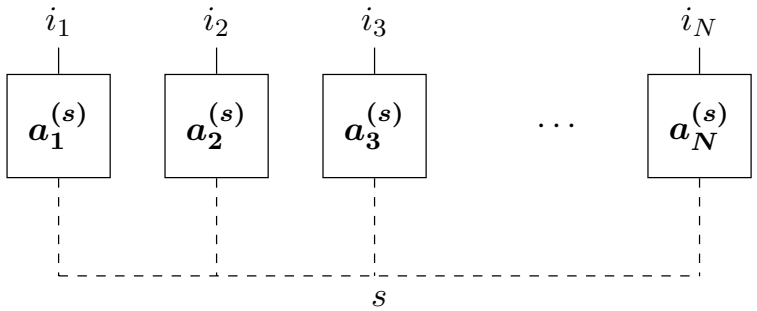


Tensor Decomposition Schemes

$$\boldsymbol{x} = \sum_{s} \boldsymbol{a_1^{(s)}} \otimes \boldsymbol{a_2^{(s)}} \otimes \cdots \otimes \boldsymbol{a_N^{(s)}}$$

Canonical Format:



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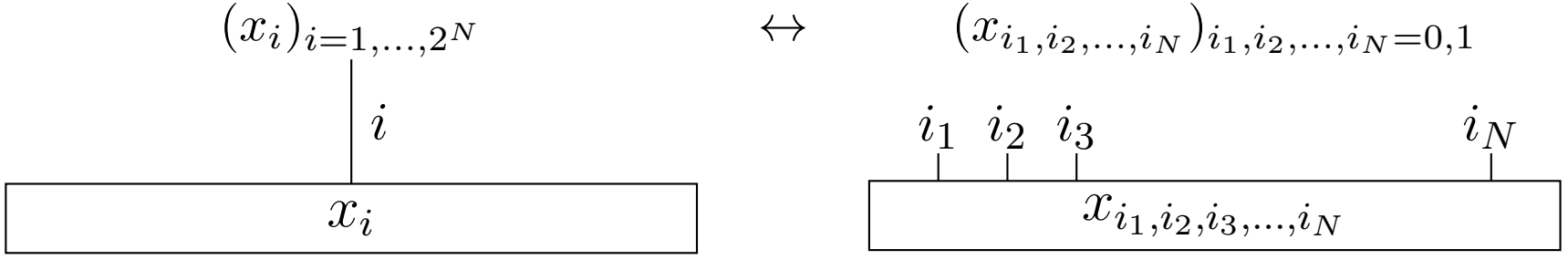
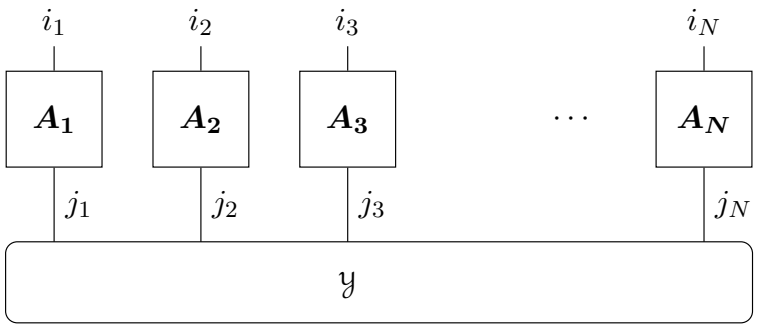


Tensor Decomposition Schemes

$$\boldsymbol{x} = \sum_{j_1,\ldots,j_N} y_{j_1,\ldots,j_N} \boldsymbol{a_{1;j_1}} \otimes \boldsymbol{a_{2;j_2}} \otimes \cdots \otimes \boldsymbol{a_{N;j_N}}$$

Tucker Format:



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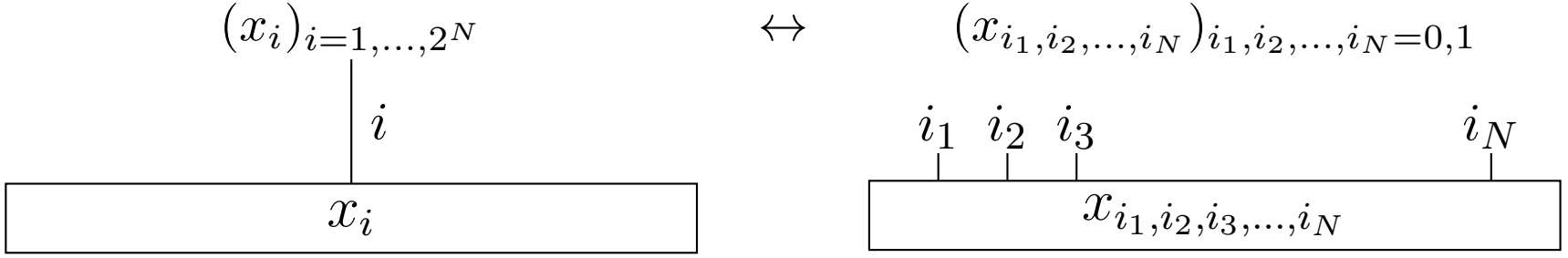
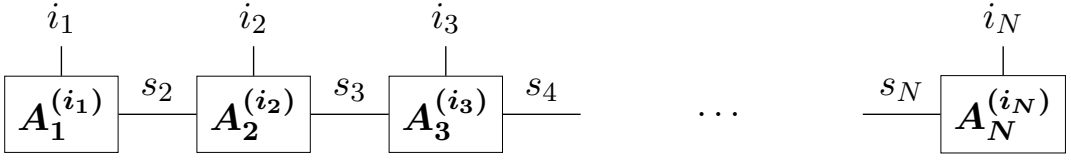


Tensor Decomposition Schemes

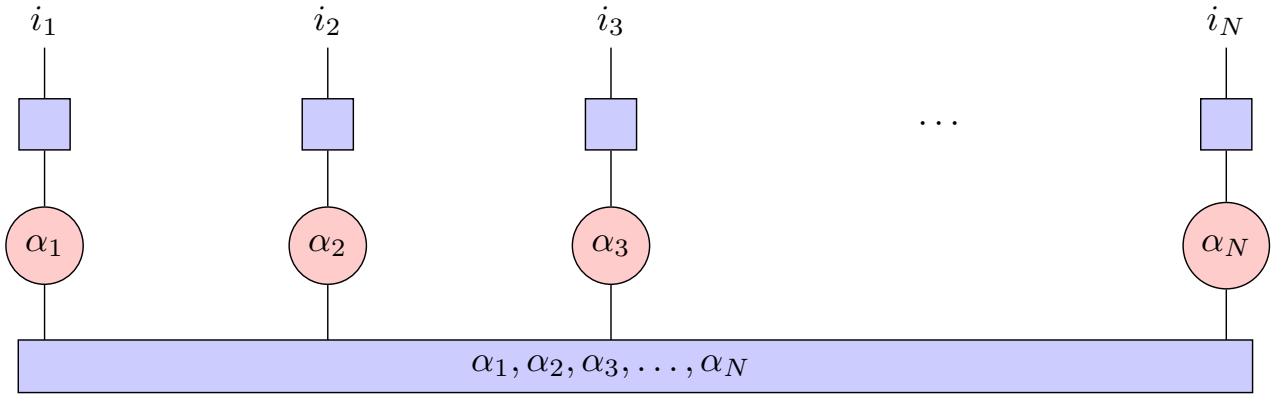
$$\boldsymbol{x} = \sum_{i_1,\ldots,i_N} \left(\boldsymbol{A_1^{(i_1)}} \boldsymbol{A_2^{(i_2)}} \cdots \boldsymbol{A_N^{(i_N)}} \right) \boldsymbol{e_{i_1,\ldots,i_N}}$$

Matrix Product States:

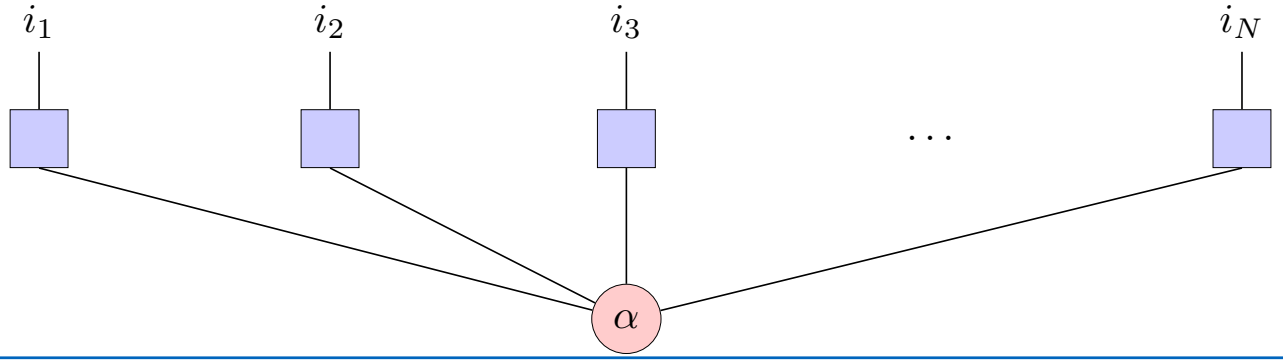


1 ✓

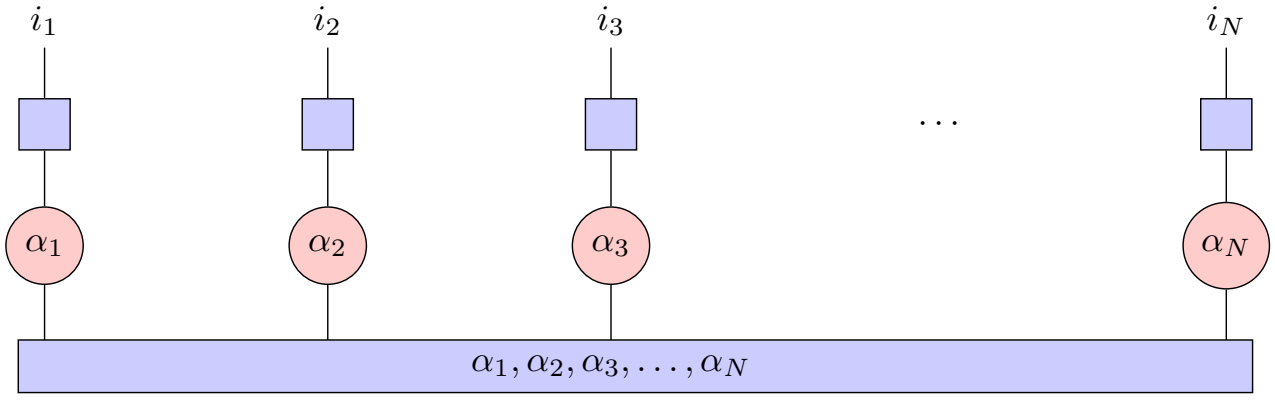
Tucker:


i_1
i_2
i_3
i_N
$\cdots$
α_1
α_2
α_3
α_N
$\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_N$

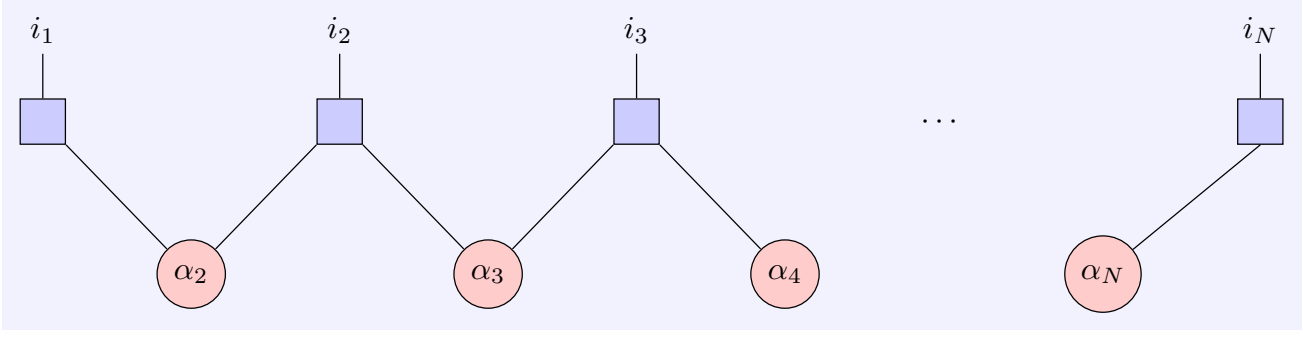
CP:


i_1
i_2
i_3
i_N
$\cdots$
α

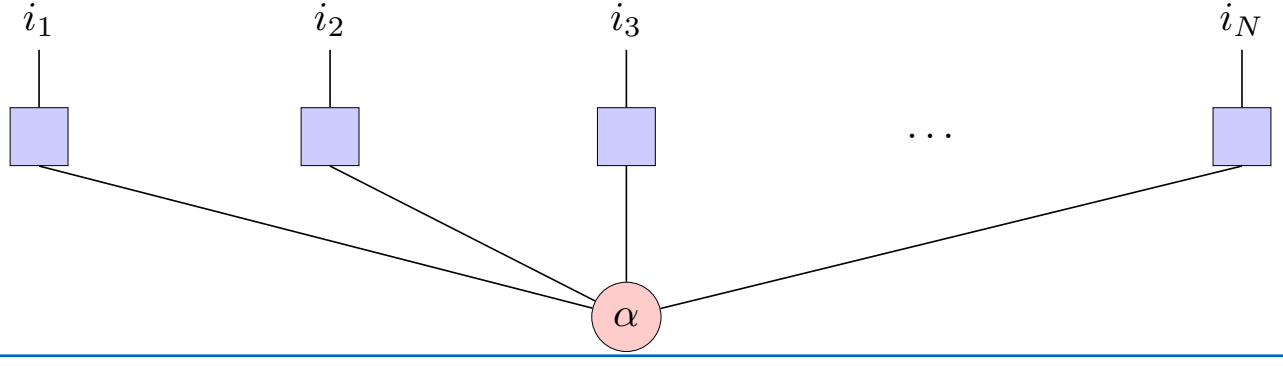
Tucker:



MPS:



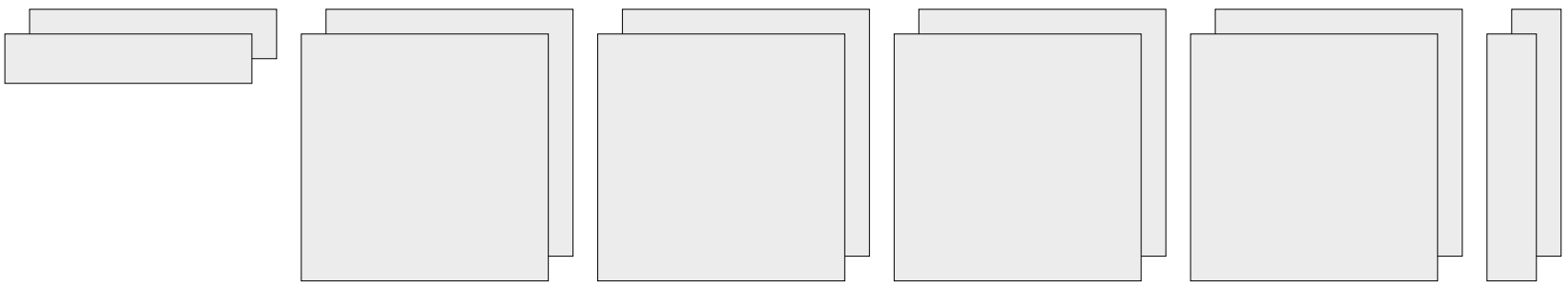
CP:



Matrix Product States: Example

Approximate vector of dimension $2^6 = 64$
by an MPS related to $N = 6$ sites.

$$\boldsymbol{x}_i = \boldsymbol{x}_{i_1,i_2,i_3,i_4,i_5,i_6} = \boldsymbol{A}_1^{(i_1)} \boldsymbol{A}_2^{(i_2)} \boldsymbol{A}_3^{(i_3)} \boldsymbol{A}_4^{(i_4)} \boldsymbol{A}_5^{(i_5)} \boldsymbol{A}_6^{(i_6)}$$



$\boldsymbol{A}_1^{(i_1)}$ $\boldsymbol{A}_2^{(i_2)}$ $\boldsymbol{A}_3^{(i_3)}$ $\boldsymbol{A}_4^{(i_4)}$ $\boldsymbol{A}_5^{(i_5)}$ $\boldsymbol{A}_6^{(i_6)}$

Matrix Product States: Example

Approximate vector of dimension $2^6 = 64$
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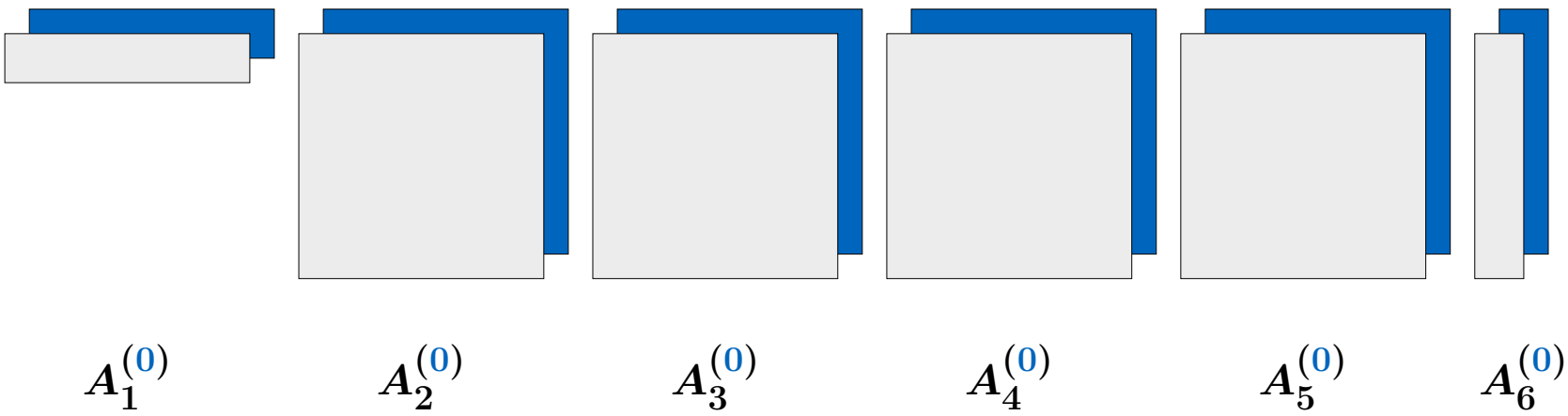
$$\boldsymbol{x}_1 = \boldsymbol{x}_{0,0,0,0,0,0} = \boldsymbol{A}_1^{(0)} \boldsymbol{A}_2^{(0)} \boldsymbol{A}_3^{(0)} \boldsymbol{A}_4^{(0)} \boldsymbol{A}_5^{(0)} \boldsymbol{A}_6^{(0)}$$



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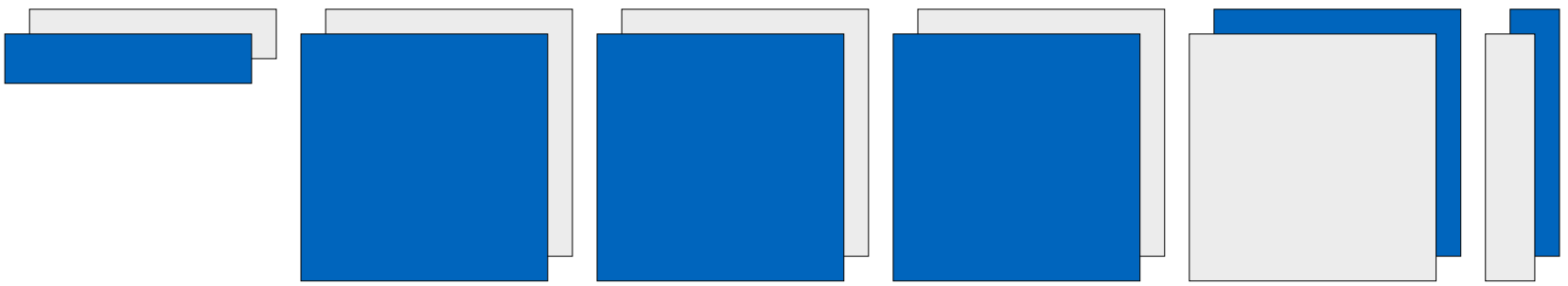
$$\boldsymbol{x}_{60} = \boldsymbol{x}_{1,1,1,1,0,0} = \boldsymbol{A}_{\mathbf{1}}^{(\mathbf{1})} \boldsymbol{A}_{\mathbf{2}}^{(\mathbf{1})} \boldsymbol{A}_{\mathbf{3}}^{(\mathbf{1})} \boldsymbol{A}_{\mathbf{4}}^{(\mathbf{1})} \boldsymbol{A}_{\mathbf{5}}^{(\mathbf{0})} \boldsymbol{A}_{\mathbf{6}}^{(\mathbf{0})}$$



$\boldsymbol{A}_{\mathbf{1}}^{(\mathbf{1})}$ $\boldsymbol{A}_{\mathbf{2}}^{(\mathbf{1})}$ $\boldsymbol{A}_{\mathbf{3}}^{(\mathbf{1})}$ $\boldsymbol{A}_{\mathbf{4}}^{(\mathbf{1})}$ $\boldsymbol{A}_{\mathbf{5}}^{(\mathbf{0})}$ $\boldsymbol{A}_{\mathbf{6}}^{(\mathbf{0})}$

Matrix Product States

$$x = \sum_{i_1,\ldots,i_N} \left(\boldsymbol{A}_{\mathbf{1}}^{(i_1)} \cdot \boldsymbol{A}_{\mathbf{2}}^{(i_2)} \cdots \boldsymbol{A}_{\boldsymbol{N}}^{(i_N)} \right) \boldsymbol{e}_{i_1 i_2 \ldots i_N} \ .$$

- Parameterization uses pair of $D \times D$ matrices along each mode.
- Matrix size D is called bond dimension or rank.
- MPS representation has only $2ND^2$ instead of 2^N entries. [2] ✓

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Ground state of the Ising-ZZ model of $N = 60$ sites:

ϵ	D	DOF
10^{-4}	4	$1,872$
10^{-6}	8	$7,456$
10^{-8}	12	$16,752$
10^{-10}	18	$37,656$
10^{-12}	25	$72,600$

Traditional treatment

$$2^{60} = 1.1529 \times 10^{18}$$

approx. 4.6 Exabyte!!!

Computation of Inner Products

$$
\begin{aligned}
\boldsymbol{x}^{\mathrm{H}}\boldsymbol{y} &= \sum_{i_1,\ldots,i_N} \left(\bar{\boldsymbol{A}}_{\boldsymbol{1}}^{(\boldsymbol{i_1})} \cdots \bar{\boldsymbol{A}}_{\boldsymbol{N}}^{(\boldsymbol{i_N})}\right) \cdot \left(\boldsymbol{B}_{\boldsymbol{1}}^{(\boldsymbol{i_1})} \cdots \boldsymbol{B}_{\boldsymbol{N}}^{(\boldsymbol{i_N})}\right) \\
&= \sum_{i_1,\ldots,i_N} \left(\sum_{k_j} \overline{a_{1;k_1,k_2}^{(i_1)}} \cdots \overline{a_{N;k_N,k_1}^{(i_N)}}\right) \left(\sum_{m_j} b_{1;m_1,m_2}^{(i_1)} \cdots b_{N;m_N,m_1}^{(i_N)}\right)
\end{aligned}
$$

$\Longrightarrow$ Find an efficient ordering of the summations m_j, k_j, i_j.

Requires $\mathcal{O}(ND^3)$ operations.

Computation of the Sum of Two MPS

- Sum of two MPS vectors

$$x = \sum_{i_1,\ldots,i_N} \left(A_1^{(i_1)} A_2^{(i_2)} \ldots A_N^{(i_N)} \right) e_{i_1 \ldots i_N}$$

$$y = \sum_{i_1,\ldots,i_N} \left(B_1^{(i_1)} B_2^{(i_2)} \ldots B_N^{(i_N)} \right) e_{i_1 \ldots i_N}$$

$$x + y =$$

$$= \sum_{i_1,\ldots,i_N} \begin{pmatrix} A_1^{(i_1)} & B_1^{(i_1)} \end{pmatrix} \begin{pmatrix} A_2^{(i_2)} & 0 \\ 0 & B_2^{(i_2)} \end{pmatrix} \cdots \begin{pmatrix} A_N^{(i_N)} \\ B_N^{(i_N)} \end{pmatrix} e_{i_1 \ldots i_N}$$

- Adding MPS leads to an **increase** of the bond dimensions:

$$\boxed{\text{“}MPS_D + MPS_{D'} = MPS_{D+D'}\text{”}}$$

Computation of Matrix-Vector Products

- The MPS concept

$$x_{i_1,i_2,\ldots,i_N} = \left(\boldsymbol{A}_{\boldsymbol{1}}^{(\boldsymbol{i_1})} \boldsymbol{A}_{\boldsymbol{2}}^{(\boldsymbol{i_2})} \cdots \boldsymbol{A}_{\boldsymbol{N}}^{(\boldsymbol{i_N})} \right)$$

can be generalized to operators:

$$O_{\substack{i_1,\ldots,i_N \\ j_1,\ldots,j_N}} = \left(\boldsymbol{W}_{\boldsymbol{1}}^{(\boldsymbol{i_1},\boldsymbol{j_1})} \boldsymbol{W}_{\boldsymbol{2}}^{(\boldsymbol{i_2},\boldsymbol{j_2})} \cdots \boldsymbol{W}_{\boldsymbol{N}}^{(\boldsymbol{i_N},\boldsymbol{j_N})} \right) .$$

- Application of such an MPO to an MPS leads to

$$\left[\left(\sum_{j_1} \boldsymbol{W}_{\boldsymbol{1}}^{(\boldsymbol{i_1},\boldsymbol{j_1})} \otimes \boldsymbol{A}_{\boldsymbol{1}}^{(\boldsymbol{j_1})} \right) \cdots \left(\sum_{j_N} \boldsymbol{W}_{\boldsymbol{N}}^{(\boldsymbol{i_N},\boldsymbol{j_N})} \otimes \boldsymbol{A}_{\boldsymbol{N}}^{(\boldsymbol{j_N})} \right) \right] ,$$

i.e., an MPS of larger bond dimension:

$$\boxed{\text{“}MPO_L \times MPS_D = MPS_{L \cdot D}\text{”}}$$

Variational Ground-State Computations

Variational ansatz:

$$\min_{\boldsymbol{x}\neq\boldsymbol{0}} \frac{\boldsymbol{x}^{\mathrm{H}}\boldsymbol{H}\boldsymbol{x}}{\boldsymbol{x}^{\mathrm{H}}\boldsymbol{x}} \approx \min_{\boldsymbol{x}_{\mathrm{MPS}}} \frac{\boldsymbol{x}_{\mathrm{MPS}}^{\mathrm{H}}\boldsymbol{H}\boldsymbol{x}_{\mathrm{MPS}}}{\boldsymbol{x}_{\mathrm{MPS}}^{\mathrm{H}}\boldsymbol{x}_{\mathrm{MPS}}}$$

Find optimal matrix pairs $\boldsymbol{A}_j^{(i_j)}$ for all sites j:

$$\min_{\boldsymbol{A}_j^{(i_j)}} \frac{\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)^{\mathrm{H}}\boldsymbol{H}\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)}{\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)^{\mathrm{H}}\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)}$$

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Use alternating least squares, variational MPS (vMPS)

$$\min_{\boldsymbol{X}_1^{(i_1)}} \frac{\left(\sum_{i_j}\left(\boldsymbol{X}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)^{\mathrm{H}}\boldsymbol{H}\left(\sum_{i_j}\left(\boldsymbol{X}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)}{\left(\sum_{i_j}\left(\boldsymbol{X}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)^{\mathrm{H}}\left(\sum_{i_j}\left(\boldsymbol{X}_1^{(i_1)}\boldsymbol{A}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)}$$

$$= \min_{\boldsymbol{X}_1} \frac{\boldsymbol{X}_1^{\mathrm{H}}\boldsymbol{H}_1\boldsymbol{X}_1}{\boldsymbol{X}_1^{\mathrm{H}}\boldsymbol{X}_1}$$

Eigenvalue problem of size $(2D^2 \times 2D^2)$.

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Use alternating least squares, variational MPS (vMPS)

$$\min_{\boldsymbol{X}_2^{(i_2)}} \frac{\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{X}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)^{\mathrm{H}}\boldsymbol{H}\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{X}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)}{\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{X}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)^{\mathrm{H}}\left(\sum_{i_j}\left(\boldsymbol{A}_1^{(i_1)}\boldsymbol{X}_2^{(i_2)}\cdots\boldsymbol{A}_N^{(i_N)}\right)\boldsymbol{e}_i\right)}$$

$$= \min_{\boldsymbol{X}_2} \frac{\boldsymbol{X}_2^{\mathrm{H}}\boldsymbol{H}_2\boldsymbol{X}_2}{\boldsymbol{X}_2^{\mathrm{H}}\boldsymbol{X}_2}$$

Eigenvalue problem of size $(2D^2 \times 2D^2)$.

Outline

Matrix product states:

$$x = \sum_{i_1,\ldots,i_N} \left(\boldsymbol{A}_{\mathbf{1}}^{(\boldsymbol{i_1})} \cdot \boldsymbol{A}_{\mathbf{2}}^{(\boldsymbol{i_2})} \cdots \boldsymbol{A}_{\boldsymbol{N}}^{(\boldsymbol{i_N})} \right) \boldsymbol{e}_{\boldsymbol{i_1 i_2 \ldots i_N}} \cdot$$

- MPS as data-sparse representation format to approximate ground states.
- Computations with MPS:
  - inner products,
  - sum of MPS: "$MPS_D + MPS_{D'} = MPS_{D+D'}$"
  - matrix-vector products: "$MPO_L \times MPS_D = MPS_{L \cdot D}$"
- Variational ground-state computations.

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- Variational ground-state computations.
- **Two approaches:**
  - Lanczos method in the MPS format,
  - Connections between symmetries and MPS representations.

The Lanczos Algorithm

Algorithm: Lanczos iteration for Hermitian matrix $\boldsymbol{H}$

Choose initial guess $\boldsymbol{r_0} \neq \boldsymbol{0}$
Define $\beta_0 = \|\boldsymbol{r_0}\|$ and $\boldsymbol{q_0} = \boldsymbol{0}$
for $j = 1, 2, \ldots, m$ **do**

$$\boldsymbol{q_j} = \boldsymbol{r_{j-1}} / \beta_{j-1}$$
$$\boldsymbol{u_j} = \boldsymbol{H q_j}$$
$$\alpha_j = \boldsymbol{q_j^H u_j}$$
$$\boldsymbol{r_j} = \boldsymbol{u_j} - \alpha_j \boldsymbol{q_j} - \beta_{j-1} \boldsymbol{q_{j-1}}$$
$$\beta_j = \|\boldsymbol{r_j}\|$$

$$\boldsymbol{T_m} = \mathrm{tridiag}(\boldsymbol{\beta}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$
$$(\lambda_{\min}, \boldsymbol{y}) = \mathrm{eig}(\boldsymbol{T_m})$$
$$\boldsymbol{v} = \boldsymbol{Q y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m}) \boldsymbol{y}$$

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Computational tasks:

The Lanczos Algorithm

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Computational tasks:

1. Application of the matrix to a vector

The Lanczos Algorithm

Algorithm: Lanczos iteration for Hermitian matrix H

Choose initial guess $r_0 \neq 0$
Define $\beta_0 = \|r_0\|$ and $q_0 = 0$
for $j = 1, 2, \ldots, m$ **do**

$$q_j = r_{j-1}/\beta_{j-1}$$
$$u_j = H q_j$$
$$\alpha_j = q_j^H u_j$$
$$r_j = u_j - \alpha_j q_j - \beta_{j-1} q_{j-1}$$
$$\beta_j = \|r_j\|$$

$$T_m = \text{tridiag}(\beta, \alpha, \beta)$$
$$(\lambda_{\min}, y) = \text{eig}(T_m)$$
$$v = Qy = (q_1, \ldots, q_m)y$$

Computational tasks:

1. Application of the matrix to a vector
2. Computation of inner products

The Lanczos Algorithm

Algorithm: Lanczos iteration for Hermitian matrix H

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Define $\beta_0 = \|r_0\|$ and $q_0 = 0$
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Computational tasks:

1. Application of the matrix to a vector
2. Computation of inner products
3. Sums and linear combinations of vectors

Augmentation of the bond dimensions

- Increase of the bond dimension during the Lanczos algorithm

Lanczos algorithm	Bond dimension
for $j = 1, 2, \ldots, m$	
$\boldsymbol{q_j} = \boldsymbol{r_{j-1}}/\beta_{j-1}$	$D^{(j)}$
$\boldsymbol{u_j} = \boldsymbol{H}\boldsymbol{q_j}$	$LD^{(j)}$
$\alpha_j = \boldsymbol{q_j^{\mathrm{H}}}\boldsymbol{u_j}$	
$\boldsymbol{r_j} = \boldsymbol{H}\boldsymbol{q_j} - \alpha_j\boldsymbol{q_j} - \beta_{j-1}\boldsymbol{q_{j-1}}$	$LD^{(j)} + D^{(j)} + D^{(j-1)} =$
$\beta_j = \lVert\boldsymbol{r_j}\rVert$	$= D^{(j+1)}$
$\boldsymbol{v} = \boldsymbol{Q}\boldsymbol{y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m})\boldsymbol{y}$	$D^{(1)} + D^{(2)} + \cdots + D^{(m)}$

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Lanczos algorithm	Bond dimension
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$\boldsymbol{r_j} = \boldsymbol{H}\boldsymbol{q_j} - \alpha_j \boldsymbol{q_j} - \beta_{j-1}\boldsymbol{q_{j-1}}$	$LD^{(j)} + D^{(j)} + D^{(j-1)} =$
$\beta_j = \lVert \boldsymbol{r_j} \rVert$	$= D^{(j+1)}$
$\boldsymbol{v} = \boldsymbol{Q}\boldsymbol{y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m})\boldsymbol{y}$	$D^{(1)} + D^{(2)} + \cdots + D^{(m)}$

- Solution: keep the ranks $D^{(j)}$ bounded
  $\Longrightarrow$ Projection required

Compression/Projection of MPS

$$\mathcal{P}_D : \boldsymbol{y}_{MPS_{D'}} \mapsto \underset{\boldsymbol{x}_{MPS_D}}{\arg\min} \left\| \boldsymbol{y}_{MPS_{D'}} - \boldsymbol{x}_{MPS_D} \right\|_2^2 =$$

$$\underset{\boldsymbol{A}_j^{(i_j)}}{\arg\min} \left\| \left[\left(\boldsymbol{B}_1^{(i_1)} \cdots \boldsymbol{B}_N^{(i_N)} \right) - \left(\boldsymbol{A}_1^{(i_1)} \cdots \boldsymbol{A}_N^{(i_N)} \right) \right]_{i_1,\ldots,i_N} \right\|_2^2$$

SVD-based truncation:

- Suppose $\boldsymbol{A_1}, \ldots, \boldsymbol{A_{r-1}}$ are already constructed. $\boldsymbol{B_r}$ is $D \times D'$

$$\begin{pmatrix} \boldsymbol{B}_r^{(0)} \\ \boldsymbol{B}_r^{(1)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{U}_r^{(0)} \\ \boldsymbol{U}_r^{(1)} \end{pmatrix} \boldsymbol{\Sigma}_r \boldsymbol{V}_r^{\mathbf{H}} \overset{\text{trunc.}}{\approx} \begin{pmatrix} \tilde{\boldsymbol{U}}_r^{(0)} \\ \tilde{\boldsymbol{U}}_r^{(1)} \end{pmatrix} \tilde{\boldsymbol{\Sigma}}_r \tilde{\boldsymbol{V}}_r^{\mathbf{H}} .$$

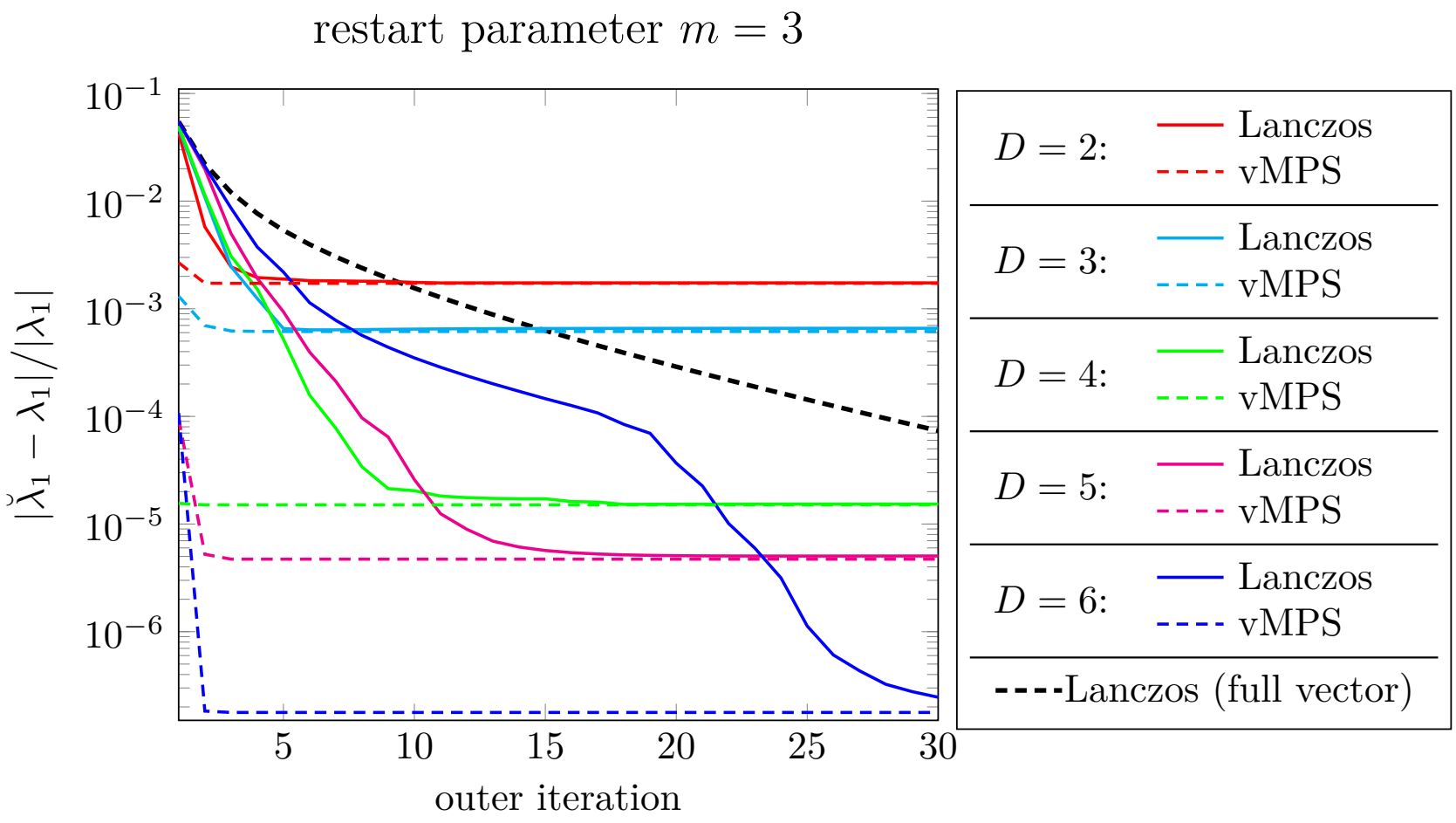
- Define $\boldsymbol{A}_r^{(i_r)} = \tilde{\boldsymbol{U}}_r^{(i_r)}$, a $D \times D$ matrix.
- Proceed with the $D \times D'$ matrix $\tilde{\boldsymbol{\Sigma}}_r \tilde{\boldsymbol{V}}_r^{\mathbf{H}} \boldsymbol{B}_{r+1}^{(i_{r+1})}$.

Restarted Lanczos

Algorithm: Restarted Lanczos iteration

Choose initial guess $\boldsymbol{r_0} \neq \boldsymbol{0}$;
for $iter = 1, 2, \ldots$ **do**
  Define $\beta_0 = \|\boldsymbol{r_0}\|$ and $\boldsymbol{q_0} = \boldsymbol{0}$;
  for $j = 1, 2, \ldots, m$ **do**
    $\boldsymbol{q_j} = \boldsymbol{r_{j-1}} / \beta_{j-1}$;
    $\boldsymbol{u_j} = \boldsymbol{H q_j}$;
    $\alpha_j = \boldsymbol{q_j}^{\mathrm{H}} \boldsymbol{u_j}$;
    $\boldsymbol{r_j} = \boldsymbol{u_j} - \alpha_j \boldsymbol{q_j} - \beta_{j-1} \boldsymbol{q_{j-1}}$;
    $\beta_j = \|\boldsymbol{r_j}\|$;
  $\boldsymbol{T_m} = \mathrm{tridiag}(\boldsymbol{\beta}, \boldsymbol{\alpha}, \boldsymbol{\beta})$;
  $(\lambda_{\min}, \boldsymbol{y}) = \mathrm{eig}(\boldsymbol{T_m})$;
  $\boldsymbol{v} = \boldsymbol{Q y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m}) \boldsymbol{y}$;
  $\boldsymbol{r_0} = \mathcal{P}_D(\boldsymbol{v})$

Numerical Results (Ising Hamiltonian $N = 25$)



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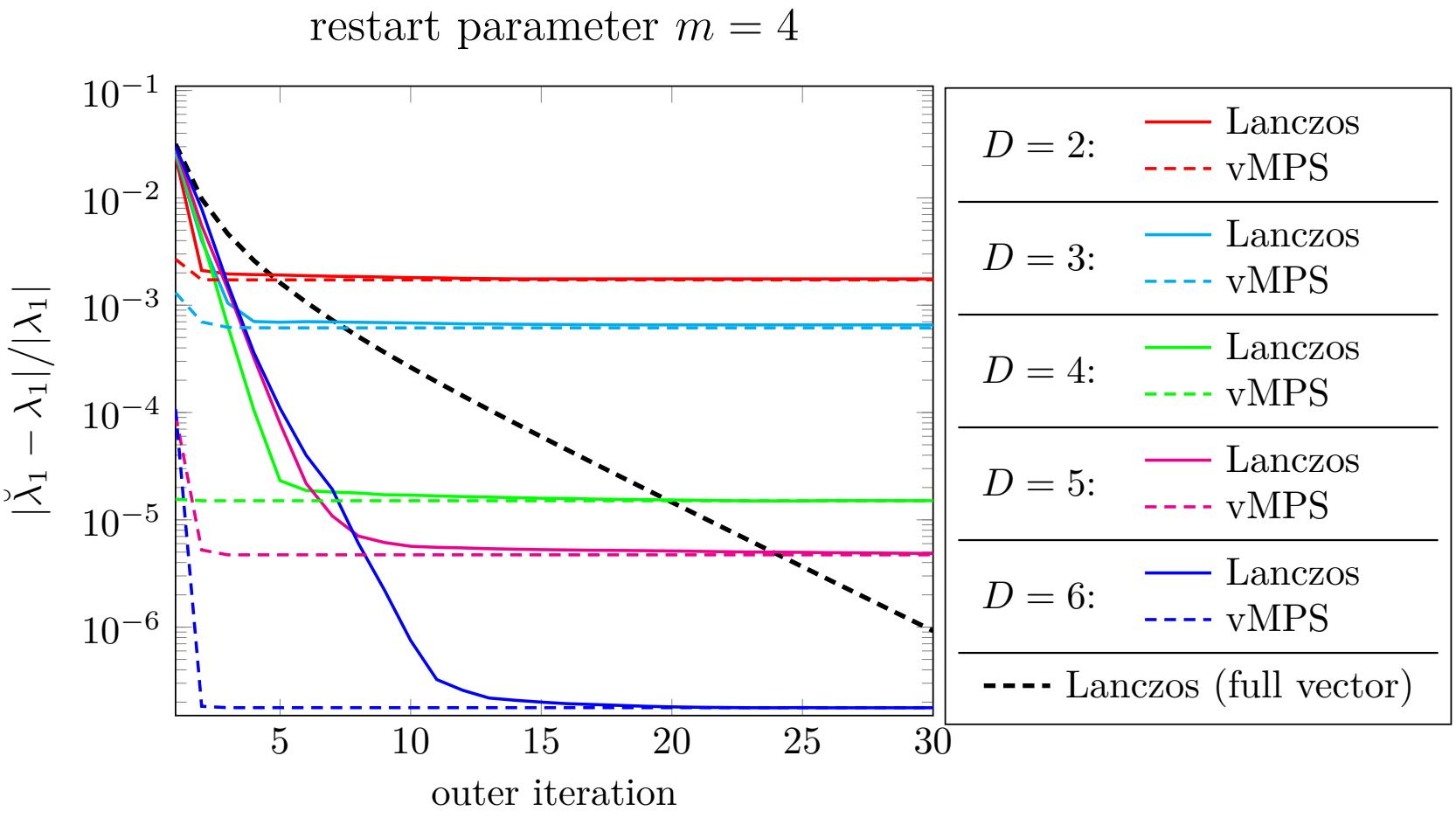

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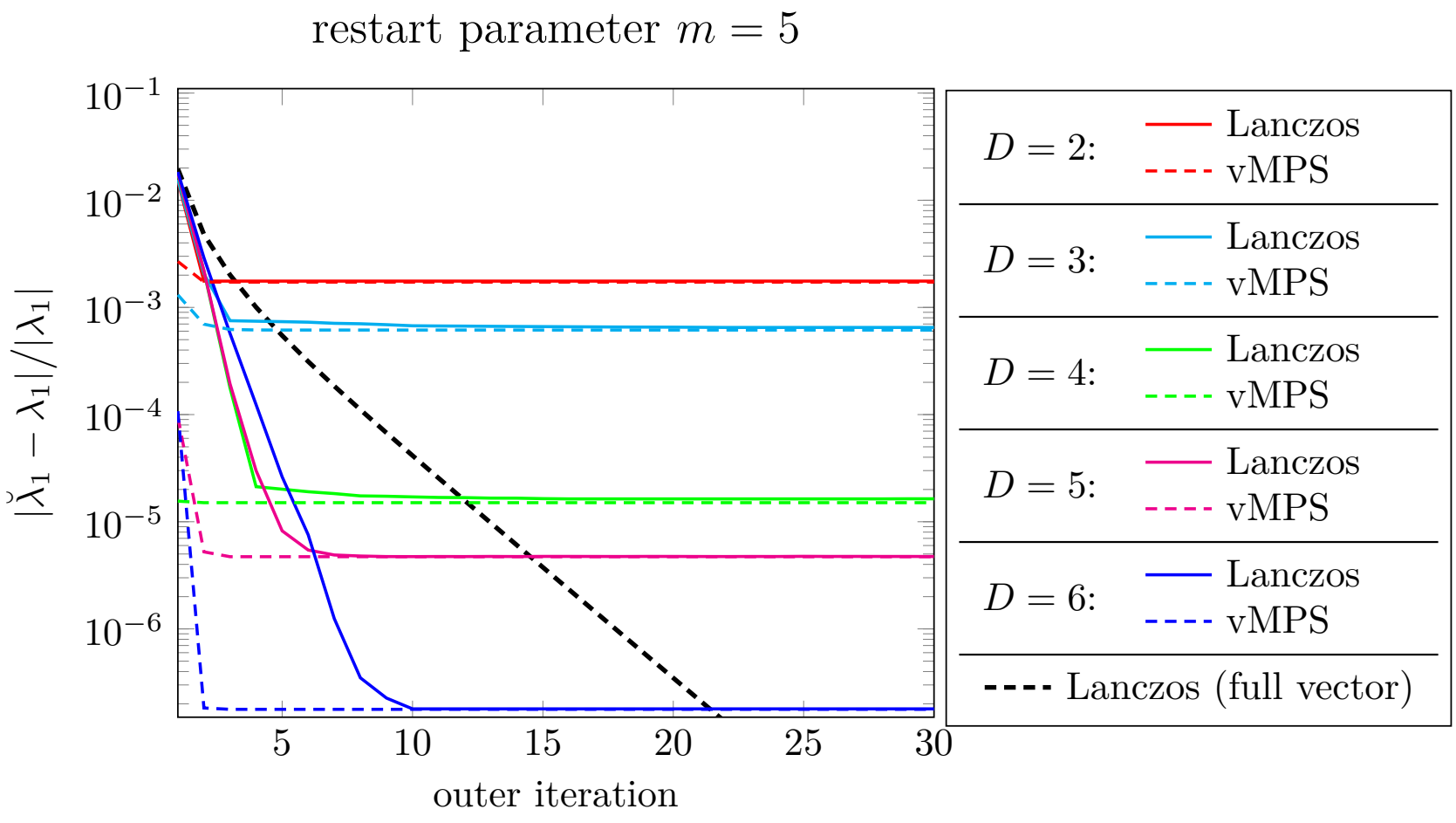
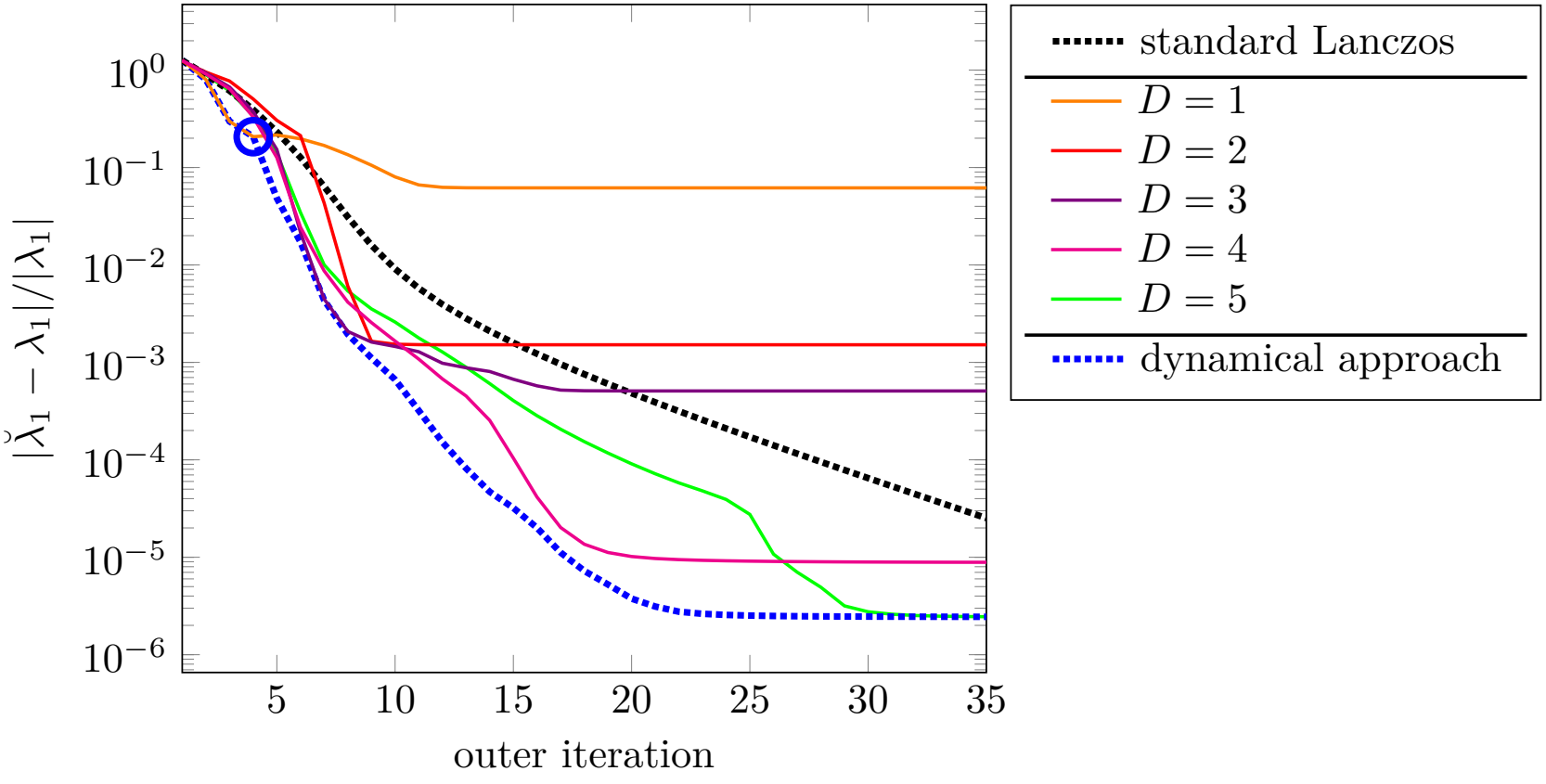


Dynamical Adaptation of the Bond Dimension



Matrix and Vector Symmetries

- $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is persymmetric, if $a_{i,j} = a_{n+1-j,n+1-i}$:

$$\boldsymbol{A} = \boldsymbol{J}\boldsymbol{A}^{\mathrm{T}}\boldsymbol{J} = \begin{pmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{pmatrix} \boldsymbol{A}^{\mathrm{T}} \underbrace{\begin{pmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{pmatrix}}_{=:\boldsymbol{J}}.$$

- $\boldsymbol{A}$ is symmetric persymmetric, if $a_{i,j} = a_{j,i} = a_{n+1-i,n+1-j}$.

Matrix and Vector Symmetries

- $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is persymmetric, if $a_{i,j} = a_{n+1-j,n+1-i}$:

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- $\boldsymbol{A}$ is symmetric persymmetric, if $a_{i,j} = a_{j,i} = a_{n+1-i,n+1-j}$.
- A vector $\boldsymbol{v} \in \mathbb{R}^n$ is called symmetric, if $v_i = v_{n+1-i}$:

$$\boldsymbol{v} = \boldsymbol{J}\boldsymbol{v}$$

- A vector $\boldsymbol{v} \in \mathbb{R}^n$ is called skew-symmetric, if $v_i = -v_{n+1-i}$:

$$\boldsymbol{v} = -\boldsymbol{J}\boldsymbol{v}$$

Symmetries of Spin-$\frac{1}{2}$ Hamiltonians

Symmetry of Spin Hamiltonians

Hamiltonians of typical physical models (Ising-ZZ, various Heisenberg models) are real-valued and symmetric persymmetric.

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Eigenvectors of Symmetric Persymmetric Matrices ([CB76])

The eigenvectors of a symmetric persymmetric matrix are either symmetric or skew-symmetric.

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Eigenvectors of Symmetric Persymmetric Matrices ([CB76])

The eigenvectors of a symmetric persymmetric matrix are either symmetric or skew-symmetric.

Ground States of Spin Hamiltonians

Ground states of typical physical models (Ising-ZZ, various Heisenberg models) are either symmetric or skew-symmetric.

MPS Representation of Symmetric Vectors

$$x_{i_1,i_2,i_3,\ldots,i_{N-1},i_N} = x_{\overline{i_1},\overline{i_2},\overline{i_3},\ldots,\overline{i_{N-1}},\overline{i_N}} \iff \boldsymbol{J}\boldsymbol{x} = \boldsymbol{x} \qquad \text{(BF)}$$

Flip-operator $\bar{i} := 1 - i$.

Example (N=3): $\boldsymbol{x} = \begin{pmatrix} a & b & c & d & d & c & b & a \end{pmatrix}^{\mathrm{T}}$

Theorem: MPS Representation of the Vector Symmetry ([Huckle13])

1. If all MPS matrix pairs $(\boldsymbol{A}_j^{(0)}, \boldsymbol{A}_j^{(1)})$ are connected via

$$\boldsymbol{A}_j^{(i_j)} = \boldsymbol{U}_j \boldsymbol{A}_j^{(\bar{i}_j)} \boldsymbol{U}_{j+1} \ , \ j = 1, \ldots, N \ , \qquad (1)$$

   with involutions $\boldsymbol{U}_j$ ($\boldsymbol{U}_j^2 = \boldsymbol{I}$), the represented vector is symmetric (BF).
2. Any symmetric vector (BF) can be represented by an MPS fulfilling relations (1).

- Reduction factor: ≈ 2

MPS Representation of Symmetric Vectors

Theorem: Uniqueness Result for Symmetric Vectors ([Huckle13])

Assume that the MPS matrices (over $\mathbb{K}$) are related by

$$\boldsymbol{A_j^{(1)}} = \boldsymbol{U_{j-1}} \boldsymbol{A_j^{(0)}} \boldsymbol{V_j} \ ,$$

with square matrices $\boldsymbol{V_j}$ and $\boldsymbol{U_j}$ of appropriate size ($j = 1, \ldots, N$). If any choice of matrices $\boldsymbol{A_j^{(0)}}$ results in the symmetry of the represented vector $\boldsymbol{x}$, i.e.,

$$\boldsymbol{Jx} \ = \ \boldsymbol{x} \ ,$$

then $\boldsymbol{U_j}$ and $\boldsymbol{V_j}$ are—up to a scalar factor—involutions for all j: $\boldsymbol{U_j^2} = u_j \boldsymbol{I}$ and $\boldsymbol{V_j^2} = v_j \boldsymbol{I}$. Furthermore, $\boldsymbol{U_j} = c_j \cdot \boldsymbol{V_j}$, $j = 1, ..., N$ with constants c_j.

- This theorem gives an argument to use involutions as heuristic.
- An involution has as eigenvalues $\pm 1 \Longrightarrow$ choose $\boldsymbol{U_j} = \boldsymbol{J}$.

Exploiting Symmetries in Computations

- Impose symmetry conditions into variational ground-state search
- Suppose that the desired ground-state vector x is symmetric.

$$\boldsymbol{J}\boldsymbol{x} = \boldsymbol{x} \implies \boldsymbol{x}^{\mathrm{H}} \underbrace{(\boldsymbol{x} - \boldsymbol{J}\boldsymbol{x})}_{=\mathbf{0}} = \boldsymbol{x}^{\mathrm{H}} (\boldsymbol{I} - \boldsymbol{J})\, \boldsymbol{x} = 0 \,.$$

- Therefore,

$$\begin{aligned} \lambda_{\min} \leq \frac{\boldsymbol{y}^{\mathrm{H}} \boldsymbol{H} \boldsymbol{y}}{\boldsymbol{y}^{\mathrm{H}} \boldsymbol{y}} &\leq \frac{\boldsymbol{y}^{\mathrm{H}} \boldsymbol{H} \boldsymbol{y}}{\boldsymbol{y}^{\mathrm{H}} \boldsymbol{y}} + \rho \frac{\boldsymbol{y}^{\mathrm{H}} (\boldsymbol{I} - \boldsymbol{J})\, \boldsymbol{y}}{\boldsymbol{y}^{\mathrm{H}} \boldsymbol{y}} \\ &= \frac{\boldsymbol{y}^{\mathrm{H}} (\boldsymbol{H} + \rho(\boldsymbol{I} - \boldsymbol{J}))\, \boldsymbol{y}}{\boldsymbol{y}^{\mathrm{H}} \boldsymbol{y}} \,. \end{aligned}$$

- Apply ground-state algorithm (e.g., vMPS) to the modified Hamiltonian

$$\boldsymbol{H}(\rho) := \boldsymbol{H} + \rho(\boldsymbol{I} - \boldsymbol{J}) \quad \text{for some} \quad \rho > 0 \,.$$

Numerical Results: Number of Iterations

Table : Ising-ZZ model of $N = 60$ spins: Number of ALS sweeps until convergence.

	D								
ρ	2	3	4	5	6	7	8	9	10
0	9	8	6	6	4	4	6	6	3
0.1	7	7	5	6	4	4	6	6	3
0.5	5	6	5	5	4	4	5	6	3
1	5	6	5	5	4	4	5	6	3
2	5	5	5	5	4	4	5	6	3
10	5	4	5	5	4	4	8	5	3
100	5	4	5	5	4	4	9	6	3

Numerical Results: Number of Iterations

Table : Heisenberg-XXX model of $N = 100$ spins: Number of ALS sweeps until convergence.

	D								
ρ	2	3	4	5	6	7	8	9	10
0	66	71	28	13	16	35	13	11	22
0.1	48	24	22	8	12	43	9	8	27
0.5	13	10	14	6	9	31	9	8	17
1	8	10	15	5	8	20	9	8	15
2	6	14	16	5	8	20	9	8	14
10	4	6	46	5	10	9	9	8	9
100	5	5	29	10	9	9	9	9	10

Numerical Studies: Convergence

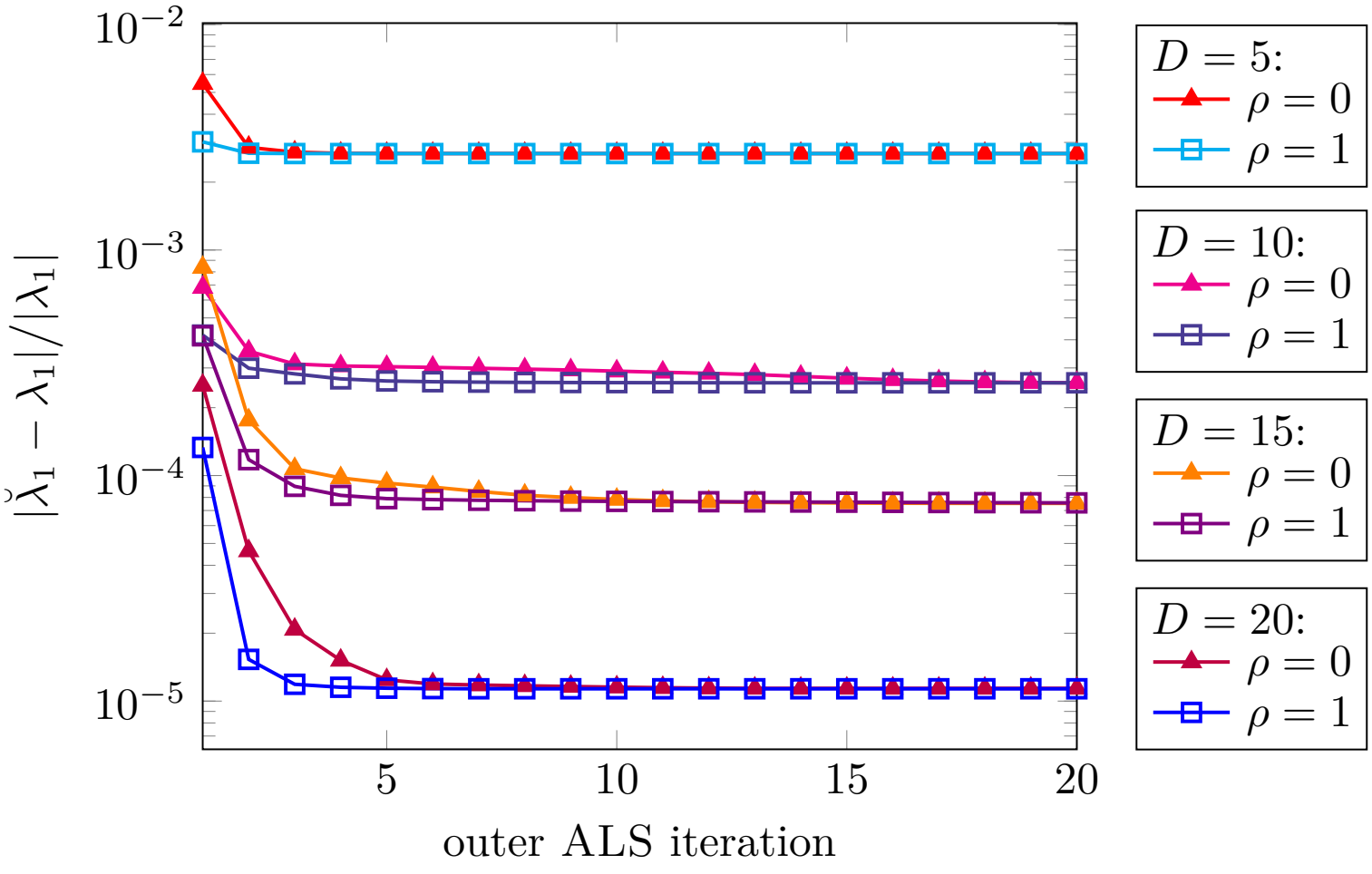

Figure : Heisenberg-XXX model of $N = 100$ spins: Approximation error.

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Thank you for your attention.


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