Large Eigenvalue Problems: Computation of Ground States

Konrad Waldherr

June 2010

Joint work with Thomas Huckle

Overview

1. Problem Setting: Computation of Ground States
2. Efficient Representations of Vectors
    - Alternating Least Squares
    - Matrix Product States
    - Generalizations of Classical Decomposition Schemes
3. Numerical Results
4. Conclusions / Outlook

Problem setting: computation of ground states

Given:

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

Problem setting: computation of ground states

Given:

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

- Interaction within the system (e.g. nearest-neighbour interaction)

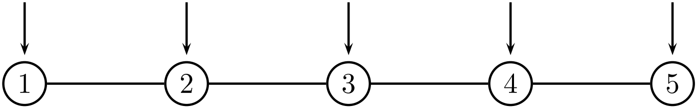
Problem setting: computation of ground states

Given:

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

- Interaction within the system (e.g. nearest-neighbour interaction)

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



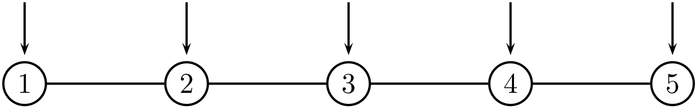
Problem setting: computation of ground states

Given:

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

- Interaction within the system (e.g. nearest-neighbour 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

- Any state of the system is represented by a vector $x \in \mathbb{C}^{2^N}$.
- The physical system can be described by the Hamiltonian $H \in \mathbb{C}^{2^N \times 2^N}$.

Mathematical Model

- Any state of the system is represented by a vector $x \in \mathbb{C}^{2^N}$.
- The physical system can be described by the Hamiltonian $H \in \mathbb{C}^{2^N \times 2^N}$.
- The Hamiltonian may be formulated as a weighted sum of Kronecker products of Pauli and identity matrices.
- Pauli matrices:

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

- Kronecker product:

$$A \otimes B := \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{pmatrix} \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix}$$

Mathematical Model

- Any state of the system is represented by a vector $x \in \mathbb{C}^{2^N}$.
- The physical system can be described by the Hamiltonian $H \in \mathbb{C}^{2^N \times 2^N}$.
- The Hamiltonian may be formulated as a weighted sum of Kronecker products of Pauli and identity matrices.
- Pauli matrices:

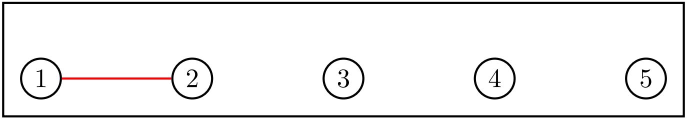
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- Kronecker product:

$$A \otimes B := \begin{pmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{pmatrix} \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \dots & a_{mn}B \end{pmatrix}$$

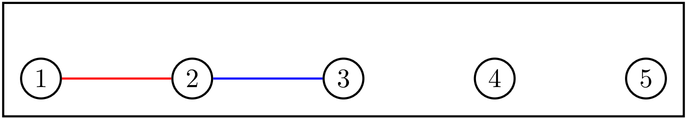
- Then, the ground state corresponds to the **eigenvector related to the smallest eigenvalue**.

Example: Ising-type Hamiltonian



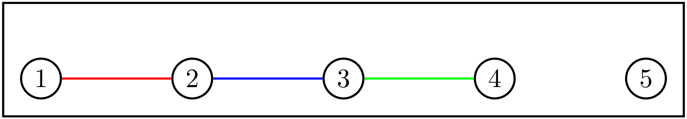
$$H = \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I$$

Example: Ising-type Hamiltonian



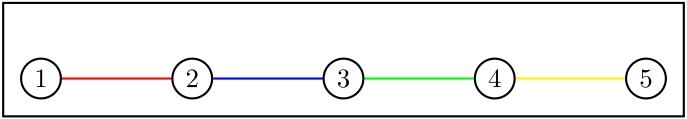
$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I
\end{aligned}
$$

Example: Ising-type Hamiltonian



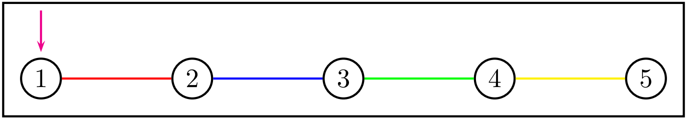
$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I
\end{aligned}
$$

Example: Ising-type Hamiltonian



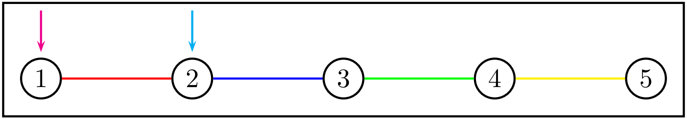
$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z
\end{aligned}
$$

Example: Ising-type Hamiltonian



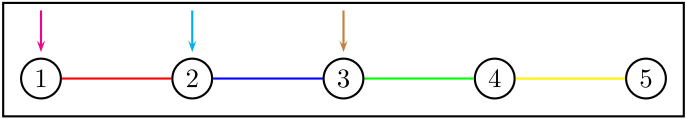
$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I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

Example: Ising-type Hamiltonian



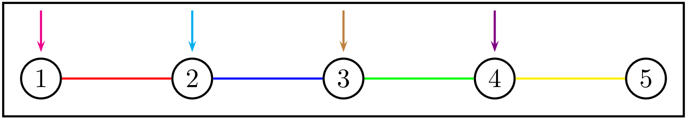
$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I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

Example: Ising-type Hamiltonian



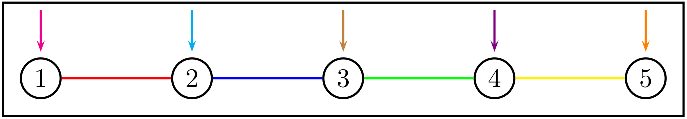
$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I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

Example: Ising-type Hamiltonian



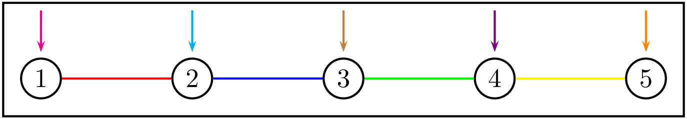
$$
\begin{aligned}
H &= \sigma_z \otimes \sigma_z \otimes I \otimes I \otimes I \\
&+ I \otimes \sigma_z \otimes \sigma_z \otimes I \otimes I \\
&+ I \otimes I \otimes \sigma_z \otimes \sigma_z \otimes I \\
&+ I \otimes I \otimes I \otimes \sigma_z \otimes \sigma_z \\
&+ \sigma_x \otimes I \otimes I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

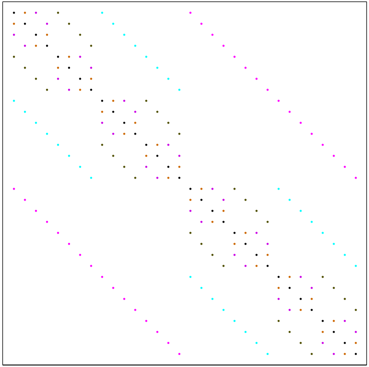
Example: Ising-type Hamiltonian



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

Sparsity Pattern of the Ising-type Hamiltonian





Problem Setting

- General formulation of the Hamiltonian H:

$$H = \sum_{k=1}^{M} \alpha_k Q_1^{(k)} \otimes \cdots \otimes Q_N^{(k)}\ , Q_i^{(k)} \in \{id, \sigma_x, \sigma_y, \sigma_z\} \subset \mathbb{C}^{2\times 2}$$

Problem Setting

- General formulation of the Hamiltonian H:

$$H = \sum_{k=1}^{M} \alpha_k Q_1^{(k)} \otimes \cdots \otimes Q_N^{(k)} \; , Q_i^{(k)} \in \{id, \sigma_x, \sigma_y, \sigma_z\} \subset \mathbb{C}^{2\times 2}$$

- Variational ansatz: Minimization of the Rayleigh quotient:

$$\min_{x \neq 0} \frac{x^\dagger H x}{x^\dagger x}$$

Problem Setting

- General formulation of the Hamiltonian H:

$$H = \sum_{k=1}^{M} \alpha_k Q_1^{(k)} \otimes \cdots \otimes Q_N^{(k)} \;, Q_i^{(k)} \in \{id, \sigma_x, \sigma_y, \sigma_z\} \subset \mathbb{C}^{2\times 2}$$

- Variational ansatz: Minimization of the Rayleigh quotient:

$$\min_{x \neq 0} \frac{x^\dagger H x}{x^\dagger x}$$

- Problem: The vector space $\mathcal{V} = \mathbb{C}^{2^N}$ grows exponentially in N.
- Idea: Choose appropriate subset $\mathcal{U} \subset \mathcal{V}$ and consider

$$\min_{x \in \mathcal{U}} \frac{x^\dagger H x}{x^\dagger x}$$

Tensor decompositions

- Any state x may be considered as a Nth order tensor:

$$x = (x_i)_{i=1,\ldots,2^N} = (x_{i_1,i_2,\ldots,i_N})_{i_j=0,1} \ .$$

- Goal: Find convenient tensor decompositions
- This decomposition should allow
  - polynomial representations,
  - efficient computations of Hx and $y^\dagger x$,
  - good approximations of the eigenvector.

Tensor decompositions

- Any state x may be considered as a Nth order tensor:

$$x = (x_i)_{i=1,\dots,2^N} = (x_{i_1,i_2,\dots,i_N})_{i_j=0,1} \ .$$

- Goal: Find convenient tensor decompositions
- This decomposition should allow
  - polynomial representations,
  - efficient computations of Hx and $y^\dagger x$,
  - good approximations of the eigenvector.
- Decomposition schemes:
  - Tucker decomposition,
  - Canonical decomposition,
  - Matrix Product States (MPS).

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_q$ to be fixed and find optimal x_i:

$$\min_{x_i} \frac{(x_1 \otimes \cdots \otimes x_i \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_i \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots x_i \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_i \otimes \cdots \otimes x_q)}$$

$$= \min_{x_i} \frac{{x_i}^{\mathrm{H}} H_i x_i}{{x_i}^{\mathrm{H}} N_i x_i}$$

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_q$ to be fixed and find optimal x_i:

$$\begin{aligned} & \min_{x_i} \frac{(x_1 \otimes \cdots \otimes x_i \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_i \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots x_i \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_i \otimes \cdots \otimes x_q)} \\ = \quad & \min_{x_i} \frac{x_i^{\mathrm{H}} H_i x_i}{x_i^{\mathrm{H}} N_i x_i} \end{aligned}$$

- Leads to a generalized eigenvalue problem in the size of x_i.

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_2, x_3, \ldots, x_q$ to be fixed and find optimal x_1:

$$\min_{x_1} \frac{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}$$

$$= \min_{x_1} \frac{x_1{}^{\mathrm{H}} H_1 x_1}{x_1{}^{\mathrm{H}} N_1 x_1}$$

- Leads to a generalized eigenvalue problem in the size of x_1.

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^H H x}{x^H x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^H H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^H (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_1, x_3, \ldots, x_q$ to be fixed and find optimal x_2:

$$\min_{x_2} \frac{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^H H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}$$

$$= \min_{x_2} \frac{x_2^H H_2 x_2}{x_2^H N_2 x_2}$$

- Leads to a generalized eigenvalue problem in the size of x_2.

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_1, x_2, x_4, \ldots, x_q$ to be fixed and find optimal x_3:

$$\begin{aligned} & \min_{x_3} \frac{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)} \\ = \quad & \min_{x_3} \frac{x_3{}^{\mathrm{H}} H_3 x_3}{x_3{}^{\mathrm{H}} N_3 x_3} \end{aligned}$$

- Leads to a generalized eigenvalue problem in the size of x_3.

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_1, x_2, \ldots, x_{q-1}$ to be fixed and find optimal x_q:

$$\min_{x_q} \frac{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}$$

$$= \min_{x_q} \frac{x_q{}^{\mathrm{H}} H_q x_q}{x_q{}^{\mathrm{H}} N_q x_q}$$

- Leads to a generalized eigenvalue problem in the size of x_q.

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_2, x_3, \ldots, x_q$ to be fixed and find optimal x_1:

$$\min_{x_1} \frac{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}$$

$$= \min_{x_1} \frac{x_1{}^{\mathrm{H}} H_1 x_1}{x_1{}^{\mathrm{H}} N_1 x_1}$$

- Leads to a generalized eigenvalue problem in the size of x_1.

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1,\ldots,x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_2, x_3, \ldots, x_q$ to be fixed and find optimal x_1:

$$\min_{x_1} \frac{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}$$

$$= \min_{x_1} \frac{x_1{}^{\mathrm{H}} H_1 x_1}{x_1{}^{\mathrm{H}} N_1 x_1}$$

- Leads to a generalized eigenvalue problem in the size of x_1.

Alternating Least Squares

- Suppose $x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$.
- Minimize the Rayleigh quotient

$$\min_x \frac{x^{\mathrm{H}} H x}{x^{\mathrm{H}} x} = \min_{x_1, \ldots, x_q} \frac{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes \cdots \otimes x_q)}{(x_1 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes \cdots \otimes x_q)}$$

- Suppose $x_2, x_3, \ldots, x_q$ to be fixed and find optimal x_1:

$$\min_{x_1} \frac{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} H (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)^{\mathrm{H}} (x_1 \otimes x_2 \otimes x_3 \otimes \cdots \otimes x_q)}$$

$$= \min_{x_1} \frac{x_1^{\mathrm{H}} H_1 x_1}{x_1^{\mathrm{H}} N_1 x_1}$$

- Leads to a generalized eigenvalue problem in the size of x_1.
- Iterate until convergence.

Matrix Product States (MPS)

- In MPS, the vector components are given by

$$x_i = x_{i_1,\dots,i_N} = \text{trace}\left(A_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_N^{(i_N)}\right)$$

with matrices $A_i^{(0)}, A_i^{(1)} \in \mathbb{C}^{D_i \times D_{i+1}}$

- Thus, the vector x may be written as

$$x = \sum_{i=1}^{2^N} x_i e_i = \sum_{i_1,\dots,i_p} \underbrace{\text{trace}\left(A_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_p^{(i_N)}\right)}_{=x_i=x_{i_1,\dots,i_N}} \underbrace{e_{i_1,\dots,i_N}}_{=e_i} .$$

Matrix Product States (MPS)

- In MPS, the vector components are given by

$$x_i = x_{i_1,\dots,i_N} = \text{trace}\left(A_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_N^{(i_N)}\right)$$

with matrices $A_i^{(0)}, A_i^{(1)} \in \mathbb{C}^{D_i \times D_{i+1}}$

- Thus, the vector x may be written as

$$x = \sum_{i=1}^{2^N} x_i e_i = \sum_{i_1,\dots,i_p} \underbrace{\text{trace}\left(A_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_p^{(i_N)}\right)}_{=x_i=x_{i_1,\dots,i_N}} \underbrace{e_{i_1,\dots,i_N}}_{=e_i} .$$

- The MPS formalism leads to

$$x = \sum_{m_1,\dots,m_p} a_{1,m_1 m_2} \otimes \cdots \otimes a_{p,m_p,m_1} .$$

$\Rightarrow$ Efficient computation of $Hx = \left(\sum_{k=1}^{M} \alpha_k Q_1^{(k)} \otimes \cdots \otimes Q_N^{(k)}\right) x.$

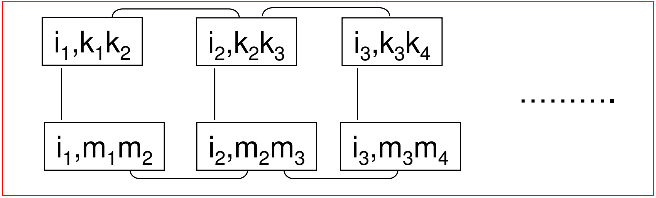
How to compute the inner product efficiently?

$$
\begin{aligned}
x_{MPS}^{H} y_{MPS} &= \sum_{i_1,\ldots,i_N} \overbrace{\left(\operatorname{trace}\left(\bar{A}_1^{(i_1)} \cdots \bar{A}_N^{(i_N)}\right)\right)}^{\bar{x}_{i_1,\ldots,i_N}} \cdot \overbrace{\left(\operatorname{trace}\left(B_1^{(i_1)} \cdots B_p^{(i_p)}\right)\right)}^{y_{i_1,\ldots,i_p}} \\
&= \sum_{i_1,\ldots,i_N} \sum_{k_1,\ldots,k_N} \bar{a}_{1,k_1,k_2}^{(i_1)} \cdots \bar{a}_{N,k_N,k_1}^{(i_N)} \sum_{m_1,\ldots,m_N} b_{1,m_1,m_2}^{(i_1)} \cdots b_{p,m_N,m_1}^{(i_N)}
\end{aligned}
$$

How to compute the inner product efficiently?

$$
\begin{aligned}
x^{H}_{MPS} y_{MPS} &= \sum_{i_1,\ldots,i_N} \overbrace{\left(\text{trace}\left(\bar{A}_1^{(i_1)} \cdots \bar{A}_N^{(i_N)}\right)\right)}^{\bar{x}_{i_1,\ldots,i_N}} \cdot \overbrace{\left(\text{trace}\left(B_1^{(i_1)} \cdots B_p^{(i_p)}\right)\right)}^{y_{i_1,\ldots,i_p}} \\
&= \sum_{i_1,\ldots,i_N} \sum_{k_1,\ldots,k_N} \bar{a}^{(i_1)}_{1,k_1,k_2} \cdots \bar{a}^{(i_N)}_{N,k_N,k_1} \sum_{m_1,\ldots,m_N} b^{(i_1)}_{1,m_1,m_2} \cdots b^{(i_N)}_{p,m_N,m_1}
\end{aligned}
$$

Find an efficient ordering of the summations:

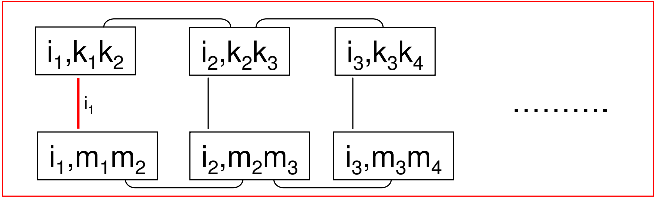


How to compute the inner product efficiently?

$$x^{H}_{MPS} y_{MPS} = \sum_{i_1,\dots,i_N} \overbrace{\left(\mathrm{trace}\left(\bar{A}_1^{(i_1)} \cdots \bar{A}_N^{(i_N)}\right)\right)}^{\bar{x}_{i_1,\dots,i_N}} \cdot \overbrace{\left(\mathrm{trace}\left(B_1^{(i_1)} \cdots B_p^{(i_p)}\right)\right)}^{y_{i_1,\dots,i_p}}$$

$$= \sum_{i_1,\dots,i_N} \sum_{k_1,\dots,k_N} \bar{a}^{(i_1)}_{1,k_1,k_2} \cdots \bar{a}^{(i_N)}_{N,k_N,k_1} \sum_{m_1,\dots,m_N} b^{(i_1)}_{1,m_1,m_2} \cdots b^{(i_N)}_{p,m_N,m_1}$$

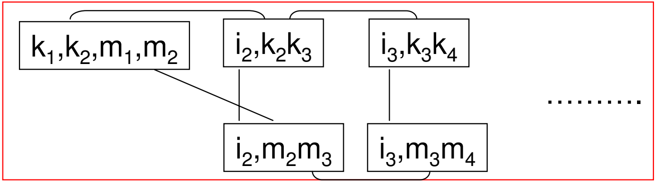
Find an efficient ordering of the summations:



How to compute the inner product efficiently?

$$
\begin{aligned}
x_{MPS}^{H} y_{MPS} &= \sum_{i_1,\ldots,i_N} \overbrace{\left(\mathrm{trace}\left(\bar{A}_1^{(i_1)} \cdots \bar{A}_N^{(i_N)}\right)\right)}^{\bar{x}_{i_1,\ldots,i_N}} \cdot \overbrace{\left(\mathrm{trace}\left(B_1^{(i_1)} \cdots B_p^{(i_p)}\right)\right)}^{y_{i_1,\ldots,i_p}} \\
&= \sum_{i_1,\ldots,i_N} \sum_{k_1,\ldots,k_N} \bar{a}^{(i_1)}_{1,k_1,k_2} \cdots \bar{a}^{(i_N)}_{N,k_N,k_1} \sum_{m_1,\ldots,m_N} b^{(i_1)}_{1,m_1,m_2} \cdots b^{(i_N)}_{p,m_N,m_1}
\end{aligned}
$$

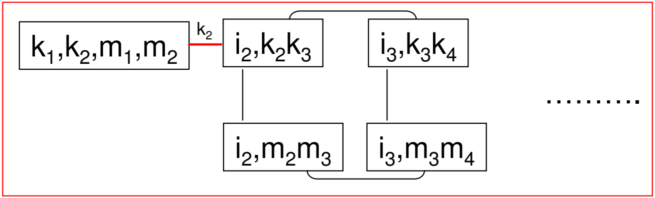
Find an efficient ordering of the summations:



How to compute the inner product efficiently?

$$
\begin{aligned}
x_{MPS}^{H} y_{MPS} &= \sum_{i_1,\ldots,i_N} \overbrace{\left(\operatorname{trace}\left(\bar{A}_1^{(i_1)} \cdots \bar{A}_N^{(i_N)}\right)\right)}^{\bar{x}_{i_1,\ldots,i_N}} \cdot \overbrace{\left(\operatorname{trace}\left(B_1^{(i_1)} \cdots B_p^{(i_p)}\right)\right)}^{y_{i_1,\ldots,i_p}} \\
&= \sum_{i_1,\ldots,i_N} \sum_{k_1,\ldots,k_N} \bar{a}^{(i_1)}_{1,k_1,k_2} \cdots \bar{a}^{(i_N)}_{N,k_N,k_1} \sum_{m_1,\ldots,m_N} b^{(i_1)}_{1,m_1,m_2} \cdots b^{(i_N)}_{p,m_N,m_1}
\end{aligned}
$$

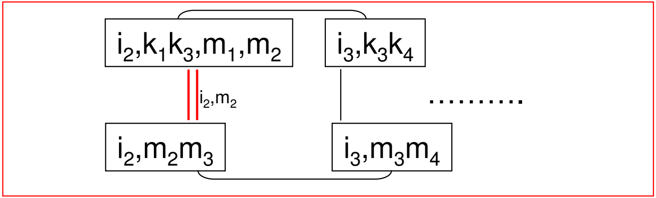
Find an efficient ordering of the summations:



How to compute the inner product efficiently?

$$
\begin{aligned}
x_{MPS}^{\mathrm{H}} y_{MPS} &= \sum_{i_1,\dots,i_N} \overbrace{\left(\mathrm{trace}\left(\bar{A}_1^{(i_1)} \cdots \bar{A}_N^{(i_N)}\right)\right)}^{\bar{x}_{i_1,\dots,i_N}} \cdot \overbrace{\left(\mathrm{trace}\left(B_1^{(i_1)} \cdots B_p^{(i_p)}\right)\right)}^{y_{i_1,\dots,i_p}} \\
&= \sum_{i_1,\dots,i_N} \sum_{k_1,\dots,k_N} \bar{a}_{1,k_1,k_2}^{(i_1)} \cdots \bar{a}_{N,k_N,k_1}^{(i_N)} \sum_{m_1,\dots,m_N} b_{1,m_1,m_2}^{(i_1)} \cdots b_{p,m_N,m_1}^{(i_N)}
\end{aligned}
$$

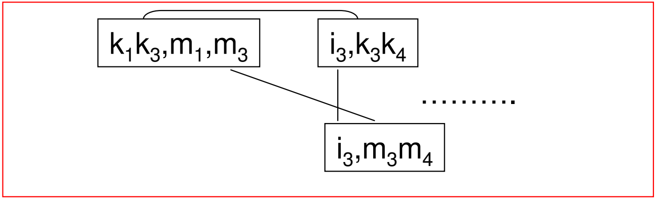
Find an efficient ordering of the summations:



How to compute the inner product efficiently?

$$
\begin{aligned}
x_{MPS}^{H} y_{MPS} &= \sum_{i_1,\ldots,i_N} \overbrace{\left(\mathrm{trace}\left(\bar{A}_1^{(i_1)} \cdots \bar{A}_N^{(i_N)}\right)\right)}^{\bar{x}_{i_1,\ldots,i_N}} \cdot \overbrace{\left(\mathrm{trace}\left(B_1^{(i_1)} \cdots B_p^{(i_p)}\right)\right)}^{y_{i_1,\ldots,i_p}} \\
&= \sum_{i_1,\ldots,i_N} \sum_{k_1,\ldots,k_N} \bar{a}^{(i_1)}_{1,k_1,k_2} \cdots \bar{a}^{(i_N)}_{N,k_N,k_1} \sum_{m_1,\ldots,m_N} b^{(i_1)}_{1,m_1,m_2} \cdots b^{(i_N)}_{p,m_N,m_1}
\end{aligned}
$$

Find an efficient ordering of the summations:



Uniqueness of MPS

- The MPS formalism

$$x = \sum_{i_1,\dots,i_N} \text{trace}\left(A_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_N^{(i_N)}\right) e_{i_1,\dots,i_N}$$

is not unique:

$$A_j^{(i_j)} \longrightarrow M_j^{-1} A_j^{(i_j)} M_{j+1}$$

Uniqueness of MPS

- The MPS formalism

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

is not unique:

$$A_j^{(i_j)} \longrightarrow M_j^{-1} A_j^{(i_j)} M_{j+1}$$

- Replace the matrices $A_j^{(0)}, A_j^{(1)}$ by parts of unitary matrices using the SVD:

$$\begin{pmatrix} A_j^{(0)} \\ A_j^{(1)} \end{pmatrix} = \begin{pmatrix} U_j^{(0)} \\ U_j^{(1)} \end{pmatrix} \Sigma_j V_j \;.$$

Uniqueness of MPS

- The MPS formalism

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

  is not unique:

$$A_j^{(i_j)} \longrightarrow M_j^{-1} A_j^{(i_j)} M_{j+1}$$

- Replace the matrices $A_j^{(0)}, A_j^{(1)}$ by parts of unitary matrices using the SVD:

$$\begin{pmatrix} A_j^{(0)} \\ A_j^{(1)} \end{pmatrix} = \begin{pmatrix} U_j^{(0)} \\ U_j^{(1)} \end{pmatrix} \Sigma_j V_j \ .$$

- Multiply the $\Sigma_j V_j$ parts on the right neighbour.

Uniqueness of MPS

- The MPS formalism

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

  is not unique:

$$A_j^{(i_j)} \longrightarrow M_j^{-1} A_j^{(i_j)} M_{j+1}$$

- Replace the matrices $A_j^{(0)}, A_j^{(1)}$ by parts of unitary matrices using the SVD:

$$\begin{pmatrix} A_j^{(0)} \\ A_j^{(1)} \end{pmatrix} = \begin{pmatrix} U_j^{(0)} \\ U_j^{(1)} \end{pmatrix} \Sigma_j V_j \ .$$

- Multiply the $\Sigma_j V_j$ parts on the right neighbour.
- Replace all A matrices by U matrices, up to one.
- This remaining term will be optimized via ALS.

Minimization Algorithm in terms of MPS

- Start with initial guesses for the $A_j^{(i_j)}$ matrices.
- Replace $A_j^{i_j}$ by $U_j^{(i_j)}$ up to $A_1^{(i_1)}$.
- Consider all U matrices as fixed and optimize $X_1 = A_1$.
- Put this ansatz in the Rayleigh quotient

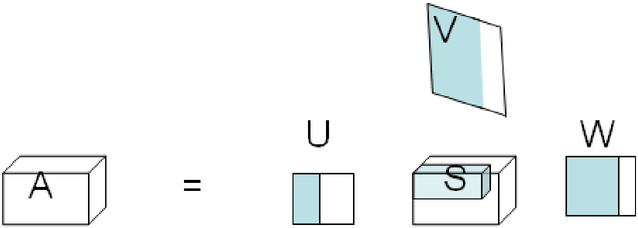
$$\min_{X_1} \frac{\left(\sum_{i_j} \operatorname{trace}\left(X_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_N^{(i_N)}\right) e_{i_1,\ldots,i_N}\right)^\dagger H \left(\sum_{i_j} \operatorname{trace}\left(X_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_N^{(i_N)}\right) e_{i_1,\ldots,i_N}\right)}{\left(\sum_{i_j} \operatorname{trace}\left(X_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_N^{(i_N)}\right) e_{i_1,\ldots,i_N}\right)^\dagger \left(\sum_{i_j} \operatorname{trace}\left(X_1^{(i_1)} \cdot A_2^{(i_2)} \cdots A_N^{(i_N)}\right) e_{i_1,\ldots,i_N}\right)}$$

$$= \min_{X_1} \frac{X_1{}^\dagger R_1 X_1}{X_1{}^\dagger X_1}$$

  with effective Hamiltonian R_1
- Leads to a dense eigenvalue problem for the $(2D^2 \times 2D^2)$ matrix R_1.
- Repeat in the ALS sense.

Decompositions of a tensor

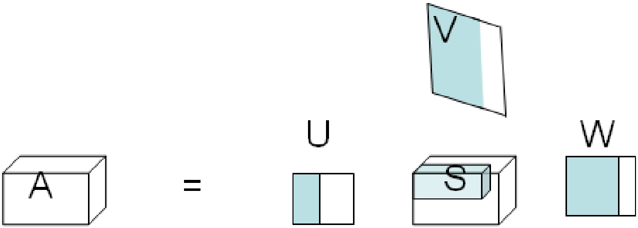
- Tucker decomposition:



Not advantageous in our case ($n_i = 2$)

Decompositions of a tensor

- Tucker decomposition:



Not advantageous in our case ($n_i = 2$)

- **Can**onical **decomp**osition (**Para**llel **Fac**torization):

  - Sum of rank-one tensors
  - The following vector ansatz is based on this canonical decomposition scheme.

Tensor Product Ansatz for the Eigenvector

- The tensor product structure of H, i.e.

$$H = \sum_{k=1}^{M} \alpha_k Q_1^{(k)} \otimes \cdots \otimes Q_N^k$$

suggests some kind of tensor product ansatz for eigenvector x:

$$x = x_1 \otimes x_2 \otimes \cdots \otimes x_q$$

- This ansatz allows easy computation of Hx and $y^\dagger x$
- Use Rayleigh quotient minimization

$$\min_{x_1,\dots,x_q} \frac{(x_1 \otimes x_2 \otimes \cdots \otimes x_q)^\dagger H (x_1 \otimes x_2 \otimes \cdots \otimes x_q)}{(x_1 \otimes x_2 \otimes \cdots \otimes x_q)^\dagger (x_1 \otimes x_2 \otimes \cdots \otimes x_q)} .$$

- Use ALS for finding optimal blocks x_i.

Minimizing the Rayleigh Quotient Using ALS

- Suppose x_L, x_R to be fixed and optimize x_i:

$$\min_{x_i} \frac{(x_L \otimes x_i \otimes x_R)^\dagger \left(\sum_{k=1}^{M} \alpha_k H_L^{(k)} \otimes H_i^{(k)} \otimes H_R^{(k)}\right)(x_L \otimes x_i \otimes x_R)}{(x_L \otimes x_i \otimes x_R)^\dagger (x_L \otimes x_i \otimes x_R)}$$

$$= \min_{x_i} \frac{\sum_{k=1}^{M} \alpha_k \left(\left(x_L^\dagger H_L^{(k)} x_L\right)\left(x_R^\dagger H_R^{(k)} x_R\right) {x_i}^\dagger H_i^{(k)} x_i\right)}{\left(\left(x_L^\dagger x_L\right)\left(x_R^\dagger x_R\right) {x_i}^\dagger x_i\right)}$$

$$= \min_{x_i} \frac{\sum_{k=1}^{M} \alpha_k \left(\beta_k {x_i}^\dagger H_i^{(k)} x_i\right)}{\gamma {x_i}^\dagger x_i} = \min_{x_i} \frac{{x_i}^\dagger \left(\sum_{k=1}^{M} \frac{\alpha_k \beta_k}{\gamma} H_i^{(k)}\right) x_i}{{x_i}^\dagger x_i}.$$

- Leads to a standard eigenvalue problem $\min_{x_i} \frac{{x_i}^\dagger H_i x_i}{{x_i}^\dagger x_i}$.

Tensor Product Ansatz for Eigenvector

- Consider $x = x_1, \ldots, x_q + \sum_{j=1}^{J} y_1^{(j)} \otimes \cdots \otimes y_q^{(j)}$
- Determine optimal $x_1, \ldots, x_q$ (all $y_i^{(j)}$ assumed to be fixed)
- Apply ALS technique:

$$\min_{x_i \neq 0} \frac{\left(x_L \otimes x_i \otimes x_R + \sum_{j=1}^{J} y_L^{(j)} \otimes y_i^{(j)} \otimes y_R^{(j)}\right)^\dagger H \left(x_L \otimes x_i \otimes x_R + \sum_{j=1}^{J} y_L^{(j)} \otimes y_i^{(j)} \otimes y_R^{(j)}\right)}{\left(x_L \otimes x_i \otimes x_R + \sum_{j=1}^{J} y_L^{(j)} \otimes y_i^{(j)} \otimes y_R^{(j)}\right)^\dagger \left(x_L \otimes x_i \otimes x_R + \sum_{j=1}^{J} y_L^{(j)} \otimes y_i^{(j)} \otimes y_R^{(j)}\right)}$$

$$= \min_{x_i \neq 0} \frac{x_i^\dagger H_i x_i + u^\dagger x_i + x_i^\dagger u + \beta}{x_i^\dagger x_i + v^\dagger x_i + x_i^\dagger v + \rho} = \min_{x_i \neq 0} \frac{\begin{pmatrix} x_i^\dagger & 1 \end{pmatrix} \begin{pmatrix} H_i & u \\ u^\dagger & \beta \end{pmatrix} \begin{pmatrix} x_i \\ 1 \end{pmatrix}}{\begin{pmatrix} x_i^\dagger & 1 \end{pmatrix} \begin{pmatrix} I & v \\ v^\dagger & \rho \end{pmatrix} \begin{pmatrix} x_i \\ 1 \end{pmatrix}}$$

- Leads to generalized eigenvalue problem

$$\begin{pmatrix} H_i & u \\ u^\dagger & \beta \end{pmatrix} \begin{pmatrix} x_i \\ 1 \end{pmatrix} = \begin{pmatrix} I & v \\ v^\dagger & \rho \end{pmatrix} \begin{pmatrix} x_i \\ 1 \end{pmatrix}$$

Tensor product ansatz for vectors

- The matrix on the right can be factorized:

$$\begin{pmatrix} I & v \\ v^\dagger & \rho \end{pmatrix} = \begin{pmatrix} I & 0 \\ v^\dagger & \sqrt{\rho - v^\dagger v} \end{pmatrix} \begin{pmatrix} I & v \\ 0 & \sqrt{\rho - v^\dagger v} \end{pmatrix}$$

- Ansatz leads to a standard eigenvalue problem:

$$\begin{pmatrix} I & 0 \\ \frac{-v^\dagger}{\sqrt{\rho - v^\dagger v}} & \frac{1}{\sqrt{\rho - v^\dagger v}} \end{pmatrix} \begin{pmatrix} H_i & u \\ u^\dagger & \beta \end{pmatrix} \begin{pmatrix} I & \frac{-v}{\sqrt{\rho - v^\dagger v}} \\ 0 & \frac{1}{\sqrt{\rho - v^\dagger v}} \end{pmatrix} y = \lambda y \,,$$

$$x = \begin{pmatrix} I & \frac{-v}{\sqrt{\rho - v^\dagger v}} \\ 0 & \frac{1}{\sqrt{\rho - v^\dagger v}} \end{pmatrix} y \,.$$

- u, v, β, ρ are computed explicitly, the matrix H_i is only applied implicitly.

Numerical results: MPS vs. ParaFac

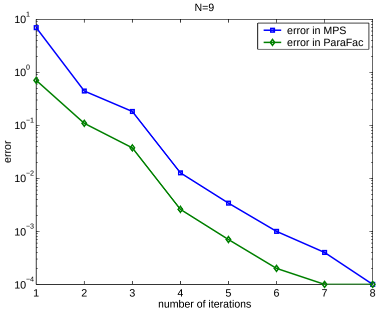


Figure: Approximation error in the computation of the smallest eigenvalue of an Ising-type Hamiltonian of size $2^9 \times 2^9$.

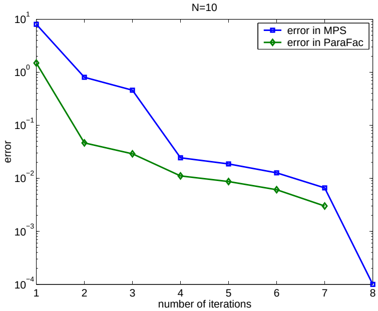
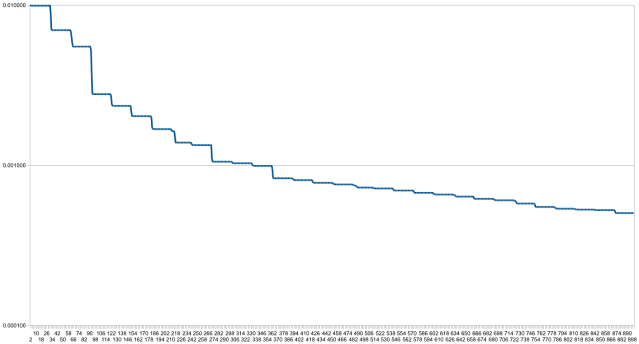


Figure: Approximation error in the computation of the smallest eigenvalue of an Ising-type Hamiltonian of size $2^{10} \times 2^{10}$.

Problems with ALS

- $N = 100$ particles, Ising-type Hamiltonian
- Pattern [15,15,15,15,15,15,10]
- $J = 30$ addends



Problems with ALS

- Problem: Iteration gets stuck into local minima
- Resorts:
  - Better choice for initial guesses
  - Simultaneous optimization

Problems with ALS

- Problem: Iteration gets stuck into local minima
- Resorts:
  - Better choice for initial guesses
  - Simultaneous optimization
- Improvement of the initial guesses
  - Apply optimization routines (e.g. linesearch)
  - Choose orthogonal basis given by Arnoldi vectors of the simplified effective Hamiltonian

$$H_i = \sum_{k=1}^{M} \alpha_k H_i^{(k)} \ .$$

Simultaneous Optimization

- Consider $x = (x_1 \otimes x_2 \otimes \cdots \otimes x_q) + (y_1 \otimes y_2 \otimes \cdots \otimes y_q)$
- Optimize x_i and y_i simultaneously, assume x_L, y_L, x_R, y_R to be fixed

$$\min_{x_i, y_i \neq 0} \frac{(x_L \otimes x_i \otimes x_R + y_L \otimes y_i \otimes y_R)^\dagger H (x_L \otimes x_i \otimes x_R + y_L \otimes y_i \otimes y_R)}{(x_L \otimes x_i \otimes x_R + y_L \otimes y_i \otimes y_R)^\dagger (x_L \otimes x_i \otimes x_R + y_L \otimes y_i \otimes y_R)}$$

$$= \min_{x_i, y_i \neq 0} \frac{x_i{}^\dagger H_i^{xx} x_i + x_i{}^\dagger H_i^{xy} y_i + y_i{}^\dagger H_i^{yx} x_i + y_i{}^\dagger H_i^{yy} y_i}{\beta_{xx} x_i{}^\dagger x_i + \beta_{xy} x_i{}^\dagger y_i + \beta_{yx} y_i{}^\dagger x_i + \beta_{yy} y_i{}^\dagger y_i}$$

$$= \min_{x_i, y_i \neq 0} \frac{\begin{pmatrix} x_i{}^\dagger & y_i{}^\dagger \end{pmatrix} \begin{pmatrix} H_i^{xx} & H_i^{xy} \\ H_i^{yx} & H_i^{yy} \end{pmatrix} \begin{pmatrix} x_i \\ y_i \end{pmatrix}}{\begin{pmatrix} x_i{}^\dagger & y_i{}^\dagger \end{pmatrix} \begin{pmatrix} \beta_{xx} I & \beta_{xy} I \\ \beta_{yx} I & \beta_{yy} I \end{pmatrix} \begin{pmatrix} x_i \\ y_i \end{pmatrix}}$$

- Arnoldi vectors as possible initial guesses

Numerical Results: Parallelization

Test setup:

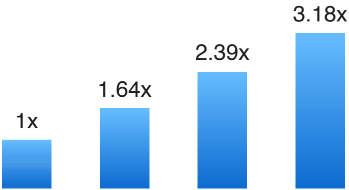
- Shared-memory parallelization
- $N = 60$ particles, Ising-type Hamiltonian
- Pattern: [15 15 15 15]
- $J = 10$ addends, 10 iterations per addend
- Intel Xeon L5520 (8 cores, 2.26 GHz)

Numerical Results: Parallelization

Test setup:

- Shared-memory parallelization
- $N = 60$ particles, Ising-type Hamiltonian
- Pattern: [15 15 15 15]
- $J = 10$ addends, 10 iterations per addend
- Intel Xeon L5520 (8 cores, 2.26 GHz)

Performance result:



Threads	1	2	4	8
Time [min]	83	50	34	26

Conclusions / Outlook

- Conclusions:
  - Computation of ground states corresponds to the solution of eigenvalue problems
  - Several decomposition schemes (MPS, ParaFac)
  - ALS technique leads to eigenvalue problems of smaller size

Conclusions / Outlook

- Conclusions:
  - Computation of ground states corresponds to the solution of eigenvalue problems
  - Several decomposition schemes (MPS, ParaFac)
  - ALS technique leads to eigenvalue problems of smaller size
- Outlook:
  - Improve the ALS (e.g. linesearch methods)
  - Allow different blockings and permutations in the decomposition schemes
  - Parallelization of the simultaneous optimization

Conclusions / Outlook

- Conclusions:
  - Computation of ground states corresponds to the solution of eigenvalue problems
  - Several decomposition schemes (MPS, ParaFac)
  - ALS technique leads to eigenvalue problems of smaller size
- Outlook:
  - Improve the ALS (e.g. linesearch methods)
  - Allow different blockings and permutations in the decomposition schemes
  - Parallelization of the simultaneous optimization

Conclusions / Outlook

- Conclusions:
  - Computation of ground states corresponds to the solution of eigenvalue problems
  - Several decomposition schemes (MPS, ParaFac)
  - ALS technique leads to eigenvalue problems of smaller size
- Outlook:
  - Improve the ALS (e.g. linesearch methods)
  - Allow different blockings and permutations in the decomposition schemes
  - Parallelization of the simultaneous optimization

Thank you very much for your attention.