The linear span of uniform matrix product states (uMPS)

joint work with Claudia De Lazzari and Tim Seynnaeve

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Overview

1. Tensor Networks

2. Uniform Matrix Product States (uMPS)

3. Results

4. Open Problem

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What are Tensor Networks?

- Vector: $v_j$
- Matrix: $M_{ij}$
- 3-index tensor: $T_{ijk}$
What are Tensor Networks?

\[ i \quad M \quad j \quad N \quad k \quad = \quad \sum_j M_{ij} N_{jkl} \]

**Figure:** Diagrammatic representation of Tensor Contraction
What are Tensor Networks?

- Tensor networks are diagrammatic representation of tensor contraction.

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Figure: Diagrammatic representation of Tensor Contraction

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Matrix Operations via Tensor Networks

- It can be thought of as a generalization of matrix multiplication to higher order tensors.
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\[ i \quad j \quad = \quad \sum_j M_{ij} v_j \]

\[ = \quad A_{ij} B_{jk} \quad = \quad AB \]

\[ = \quad A_{ij} B_{ji} \quad = \quad \text{Tr}[AB] \]

Figure: Matrix operations via Tensor Networks
• Quantum Many-Body system consisting of \( d \) particles, each one with the wave function residing in finite dimensional Hilbert space \( \mathcal{H}_i \), with \( \dim(\mathcal{H}_i) = n \) and the orthonormal basis of \( \mathcal{H}_i \) as \( \{ |e_{h_i}\rangle \}_{h_i=1}^n \).
Motivation from Quantum Physics

- Quantum Many-Body system consisting of $d$ particles, each one with the wave function residing in finite dimensional Hilbert space $\mathcal{H}_i$, with $\dim(\mathcal{H}_i) = n$ and the orthonormal basis of $\mathcal{H}_i$ as $\{|e_{h_i}\rangle\}_{h_i=1}^n$.
- The wave function of many-body system is a tensor product of states $\mathcal{H} = \bigotimes_{i=1}^d \mathcal{H}_i$.

$$\psi = \sum_{h_1,\ldots,h_d=1}^n A_{h_1\ldots h_d} |e_{h_1}\rangle \otimes \cdots \otimes |e_{h_d}\rangle$$
Problem: Curse of Dimensionality!

- We need $d^n$ coordinates, in order to completely describe the wave function.
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Figure: One solution: Quantum Computers!

Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

— Richard P. Feynman —
Another Solution: Tensor Networks!

- Fortunately, most of the physically relevant states occupies exponentially small volume in many-body Hilbert Space [PQSV11].
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- Fortunately, most of the physically relevant states occupies exponentially small volume in many-body Hilbert Space [PQSV11].

**Figure**: Physical Corner of many-body Hilbert Space
Uniform Matrix Product States (uMPS)

Definition

The uniform Matrix Product State parametrization is given by the map

\[ \phi : (\mathbb{C}^{m \times m})^n \rightarrow (\mathbb{C}^n)^{\otimes d} \]

\[ (A_0, \ldots, A_{n-1}) \mapsto \sum_{0 \leq i_1, \ldots, i_d \leq n-1} \text{Tr}(A_{i_1} \cdots A_{i_d}) \, e_{i_1} \otimes \cdots \otimes e_{i_d}. \]

\[ \text{uMPS}(m, n, d) = \text{Im}(\phi) \]

Figure: Graphical representation of uMPS($m, n, d$)
Fundamental Questions

- What is the dimension of $\langle \text{uMPS}(m, n, d) \rangle$?
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• What is the dimension of $\langle \text{uMPS}(m, n, d) \rangle$?

• For which parameters $m, n, d \in \mathbb{N}$ does $\langle \text{uMPS}(m, n, d) \rangle$ fill the ambient space?
Cyc^d(\mathbb{C}^n) := \{ \omega \in (\mathbb{C}^n)^\otimes d \mid \sigma \cdot \omega = \omega \quad \forall \sigma \in C_d \}.
Observations

\[
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\]

Observation 1

The set \( \text{uMPS}(m, n, d) \subseteq \text{Cyc}^d(\mathbb{C}^n) \). Given \( M_1, \ldots, M_d \in \mathbb{C}^{m \times m}, \sigma \in C_d \)

\[
\text{Tr}(M_1 \cdots M_d) = \text{Tr}(M_{\sigma(1)} \cdots M_{\sigma(d)}).
\]
Observations

\[ \text{Dih}^d(\mathbb{C}^n) := \{ \omega \in (\mathbb{C}^n)^\otimes d \mid \sigma \cdot \omega = \omega \quad \forall \sigma \in D_{2d} \}. \]
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\[ \text{Dih}^d(\mathbb{C}^n) := \{ \omega \in (\mathbb{C}^n)^{\otimes d} \mid \sigma \cdot \omega = \omega \quad \forall \sigma \in D_{2d} \}. \]

**Observation 2 ( [Gre14, Theorem 1.1])**

\[ \text{uMPS}(2, 2, d) \subseteq \text{Dih}^d(\mathbb{C}^n). \text{ Given } A_{i_1}, \cdots, A_{i_d} \in \mathbb{C}^{2 \times 2} \]

\[ \text{Tr}(A_{i_1} \cdots A_{i_d}) = \text{Tr}(A_{i_d} \cdots A_{i_1}). \]
Idea 1 - Cayley-Hamilton Technique

Let $c = (c_1, \ldots, c_s) \in \mathbb{C}^s$ be a vector of coefficients and $\{i^j_\ell\}_{1 \leq \ell \leq d, 1 \leq j \leq s}$ be indices; with $i^j_\ell \in [n]$. Assume that for every $n$-tuple $(A_0, \ldots, A_{n-1})$ of $m \times m$ matrices and every $k < m$ the following identity holds:

$$
\sum_{j=1}^{s} c_j \text{Tr}(A_{i^j_1} \cdots A_{i^j_d} A_0^k) = 0.
$$

Then the same identity holds for arbitrary $k \in \mathbb{N}$. 
The following identity holds for any $2 \times 2$ matrices $A_0, A_1, A_2, A_3$ and $k \geq 0$:

$$
\text{Tr}(A_1 A_2 A_0 A_3 A_0^k) + \text{Tr}(A_2 A_3 A_0 A_1 A_0^k) + \text{Tr}(A_3 A_1 A_0 A_2 A_0^k) = \text{Tr}(A_1 A_0 A_2 A_3 A_0^k) + \text{Tr}(A_2 A_0 A_3 A_1 A_0^k) + \text{Tr}(A_3 A_0 A_1 A_2 A_0^k).
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Example - 2 \times 2 matrices

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= \text{Tr}(A_1 A_0 A_2 A_3 A_0^k) + \text{Tr}(A_2 A_0 A_3 A_1 A_0^k) + \text{Tr}(A_3 A_0 A_1 A_2 A_0^k).
\]

By Cayley-Hamilton Technique, enough to show the identity for \( k = 0, 1 \).
Example - $2 \times 2$ matrices

The following identity holds for any $2 \times 2$ matrices $A_0, A_1, A_2, A_3$ and $k \geq 0$:

$$
\text{Tr}(A_1 A_2 A_0 A_3 A^k_0) + \text{Tr}(A_2 A_3 A_0 A_1 A^k_0) + \text{Tr}(A_3 A_1 A_0 A_2 A^k_0)
= \text{Tr}(A_1 A_0 A_2 A_3 A^k_0) + \text{Tr}(A_2 A_0 A_3 A_1 A^k_0) + \text{Tr}(A_3 A_0 A_1 A_2 A^k_0).
$$

By Cayley-Hamilton Technique, enough to show the identity for $k = 0, 1$.

$$
\text{Tr}(A_1 A_2 A_0 A_3) + \text{Tr}(A_2 A_3 A_0 A_1) + \text{Tr}(A_3 A_1 A_0 A_2)
= \text{Tr}(A_1 A_0 A_2 A_3) + \text{Tr}(A_2 A_0 A_3 A_1) + \text{Tr}(A_3 A_0 A_1 A_2).
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Example - 2 × 2 matrices

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= \text{Tr}(A_1 A_0 A_2 A_3 A_0^k) + \text{Tr}(A_2 A_0 A_3 A_1 A_0^k) + \text{Tr}(A_3 A_0 A_1 A_2 A_0^k).
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= \text{Tr}(A_1 A_0 A_2 A_3) + \text{Tr}(A_2 A_0 A_3 A_1) + \text{Tr}(A_3 A_0 A_1 A_2)
$$
Theorem 1

If $n \geq 3$ and $d \geq \frac{(m+1)(m+2)}{2}$, then uMPS($m, n, d$) is contained in a proper linear subspace of the space of cyclically invariant tensors.
**Theorem 1**

If \( n \geq 3 \) and \( d \geq \frac{(m+1)(m+2)}{2} \), then \( u\text{MPS}(m, n, d) \) is contained in a proper linear subspace of the space of cyclically invariant tensors.

**Sketch of Proof:**

- We need to find a non-trivial linear relation between traces of matrices which is not given by cyclic permutation.
Theorem 1

If $n \geq 3$ and $d \geq \frac{(m+1)(m+2)}{2}$, then $u\text{MPS}(m, n, d)$ is contained in a proper linear subspace of the space of cyclically invariant tensors.

Sketch of Proof:

- We need to find a non-trivial linear relation between traces of matrices which is not given by cyclic permutation.
- We proved the following technical identity using Cayley-Hamilton trick

$$\sum_{\sigma \in S_m, \tau \in C_{m+1}} \text{sgn}(\sigma) \text{sgn}(\tau) \text{Tr}(A_{\tau}(0)B^{\sigma(0)} \cdots A_{\tau}(m-1)B^{\sigma(m-1)}A_{\tau}(m)B^\ell) = 0.$$
A bracelet (of length $d$ on the alphabet $[n]$) is an equivalence class of words, where two words are equivalent if they agree up to the action $D_{2d}$. 
Idea 2 - Trace Parametrization

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Technical Lemma

For every bracelet $b = (b_1, \ldots, b_k)$, there is a unique polynomial

$$P_b(T_0, T_1, T_{00}, T_{01}, T_{11}) \in \mathbb{C}[T_0, T_1, T_{00}, T_{01}, T_{11}]$$

such that for every pair $(A_0, A_1)$ of $2 \times 2$ matrices, the following equality holds:

$$\text{Tr}(A_{b_1} \cdots A_{b_k}) = P_b(\text{Tr}(A_0), \text{Tr}(A_1), \text{Tr}(A_0^2), \text{Tr}(A_0A_1), \text{Tr}(A_1^2)).$$
Idea 2 - Trace Parametrization

- $\text{uMPS}(2, 2, d)$ is the image of the polynomial map

$$
\psi : \mathbb{C}^5 \rightarrow \text{Dih}^d(\mathbb{C}^2) \\
(T_0, T_1, T_{00}, T_{01}, T_{11}) \mapsto \sum_b P_b(T_0, T_1, T_{00}, T_{01}, T_{11})e_b,
$$

where $b$ runs over all bracelets of length $d$. 
Idea 2 - Trace Parametrization

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where $b$ runs over all bracelets of length $d$.

- This is the trace parametrization of $uMPS(2, 2, d)$.
Theorem 2

For every $d \in \mathbb{N}$, we have the inequality

$$\dim \langle uMPS(2, 2, d) \rangle \leq \begin{cases} \frac{1}{192} (d + 6)(d + 4)^2(d + 2) & \text{for } d \text{ even}, \\ \frac{1}{192} (d + 7)(d + 5)(d + 3)(d + 1) & \text{for } d \text{ odd.} \end{cases}$$
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Sketch of Proof:

- Using the trace parametrization of $\text{uMPS}(2, 2, d)$, $\dim \langle \text{uMPS}(2, 2, d) \rangle$ is at most the number of degree $d$ monomials in $\mathbb{C}[T_0, T_1, T_{00}, T_{01}, T_{11}]$. 
Open Problem

Conjecture

$$\dim\langle u\text{MPS}(2, 2, d) \rangle = \begin{cases} \frac{1}{192} (d^4 - 4d^2 + 192d + 192) & \text{for } d \text{ even}, \\ \frac{1}{192} (d^4 - 10d^2 + 192d + 201) & \text{for } d \text{ odd}. \end{cases}$$
References

The work presented here is based on:

- De Lazzari C, Motwani HJ, Seynnaeve T. **The linear span of uniform matrix product states.** arXiv preprint arXiv:2204.10363. 2022 Apr 21.

- Code available at: https://github.com/harshitmotwani2015/uMPS/

Pictures of Tensor Networks are taken from https://tensornetwork.org/

Additional Reference

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- Greene J. Traces of matrix products. The Electronic Journal of Linear Algebra. 2014 Jan 1;27:716-34.