Tensor DMD Based Control of Multilinear Time Invariant Systems

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Outline

- Motivation from 4D Nucleome
- Tensor algebra
  - Tensors and tensor decompositions
  - Isomorphism and tensor ring
  - Block tensors
  - Tensor SVD
- MLTI system identification
  - Introduce to MLTI systems
  - Higher-Order DMD
    - Higher-Order DMD with control
- 4D Nucleome Example
- Summary/Future work
Motivation from 4D Nucleome

The relationship between genome **Structure** and **Function** over **Time** is referred to as the 4D Nucleome (4DN).

The evolution can be captured via tensors!

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Tensors and tensor decompositions

Tensors are multidimensional arrays generalized from vectors and matrices. An $N$-th order tensor usually is denoted by $X \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}$.

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C. Van Loan, From Matrix to Tensor, Department of Compute Science, Cornell University, 2016.

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Tensors and tensor decompositions

- **Tensor Train Decomposition (TTD)**

  \[
  X = \sum_{r_N=1}^{R_N} \cdots \sum_{r_0=1}^{R_0} X_{r_0:r_1}^{(1)} \circ X_{r_1:r_2}^{(2)} \circ \cdots \circ X_{r_{N-1}:r_N}^{(N)}
  \]

  - *TT-ranks*: \( \mathcal{R} = \{R_0, R_1, \ldots, R_N\} \) with \( R_0 = R_N = 1 \)
  - *Optimal TT-ranks*: for \( n = 1, 2, \ldots, N - 1 \),
    \[
    R_n = \text{rank}(\text{reshape}(X, \prod_{i=1}^{n} J_i, \prod_{i=n+1}^{N} J_i))
    \]

- **Core tensors**: \( X^{(n)} \in \mathbb{R}^{R_{n-1} \times J_n \times R_n} \)
  - *Left-orthonormal*: \( (\bar{X}^{(n)})^\top \bar{X}^{(n)} = I \) where
    \[
    \bar{X}^{(n)} = \text{reshape}(X^{(n)}, R_{n-1}J_n, R_n)
    \]
  - *Right-orthonormal*: \( X^{(n)}(X^{(n)})^\top = I \), where
    \[
    X^{(n)} = \text{reshape}(X^{(n)}, R_{n-1}, J_nR_n)
    \]

- Advantageous in storage consumption and computational robustness

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Higher-Order SVD, CP Decomposition

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Isomorphism and tensor ring

- Even-order paired tensor $A \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$
- Einstein product

\[
(A \ast B)_{j_1i_1\ldots j_Ni_N} = \sum_{k_N=1}^{K_N} \cdots \sum_{k_1=1}^{K_1} A_{j_1k_1\ldots j_Nk_N} B_{k_1i_1\ldots k_Ni_N}
\]

(5)

- When $J_n = I_n$, there exists an isomorphism $\varphi$ from even-order paired tensor space to the general linear group. Moreover, it is a ring!
  - **U-transpose** $T_{i_1j_1\ldots i_Nj_N} = A_{j_1i_1\ldots j_Ni_N}$, denoted by $A^\top \in \mathbb{R}^{I_1 \times J_1 \times \cdots \times I_N \times J_N}$
    - $A = A^\top \Rightarrow$ weakly symmetric
  - **U-diagonal** $D \in \mathbb{R}^{J_1 \times J_1 \times \cdots \times J_N \times J_N}$ if all its entries are zeros except for $D_{j_1j_1\ldots j_Nj_N}$
  - **U-identity** $D_{j_1j_1\ldots j_Nj_N} = 1$ denoted by $I$
  - **U-orthogonal** $A \ast A^\top = A^\top \ast A = I$
  - **U-inverse** $A \ast B = B \ast A = I$ denoted by $A^{-1}$


Block Tensors

- **n-mode row block tensor** $A, B \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$
  \[ |A \quad B|_n \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_n \times 2I_n \times \cdots \times J_N \times I_N} \]

  - $= A$ for only $i_n = 1, \ldots, I_n$, $= B$ for only $i_n = I_n + 1, \ldots, 2I_n$
  - $P \ast |A \quad B|_n = |P \ast A \quad P \ast B|_n$

- **Row block tensor** $A \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$, $B \in \mathbb{R}^{J_1 \times K_1 \times \cdots \times J_N \times K_N}$
  \[ (A \quad B) \in \mathbb{R}^{J_1 \times (I_1 + K_1) \times \cdots \times J_N \times (I_N + K_N)} \]

  - $= A$ for all $i_n = 1, \ldots, I_n$, $= B$ for all $i_n = I_n + 1, \ldots, I_n + K_n$
  - otherwise, $= 0$
  - $(A \quad B) \ast \begin{pmatrix} C \\ D \end{pmatrix} = A \ast B + C \ast D$

---


Block Tensors

Distribute $K$ into every even mode. The factorization of $K$ is arbitrary but a careful choice can facilitate computations

\[
\begin{align*}
Y &= \begin{bmatrix}
X_1 & X_2 & \ldots & X_8
\end{bmatrix} \\
\in & \mathbb{R}^{J_1 \times 2l_1 \times J_2 \times 2l_2 \times J_3 \times 2l_3}
\end{align*}
\]

\[
\begin{bmatrix}
X_1 & X_2 & X_3 & X_4 & X_5 & X_6 & X_7 & X_8 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_1 & X_2 & 1 \\
X_1 & X_2 & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_3 & X_4 & 1 \\
X_3 & X_4 & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_5 & X_6 & 1 \\
X_5 & X_6 & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_7 & X_8 & 1 \\
X_7 & X_8 & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_1^{(1)} & X_2^{(1)} & 1 \\
X_1^{(1)} & X_2^{(1)} & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_3^{(1)} & X_4^{(1)} & 1 \\
X_3^{(1)} & X_4^{(1)} & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_5^{(1)} & X_6^{(1)} & 1 \\
X_5^{(1)} & X_6^{(1)} & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_7^{(1)} & X_8^{(1)} & 1 \\
X_7^{(1)} & X_8^{(1)} & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_1^{(2)} & X_2^{(2)} & 1 \\
X_1^{(2)} & X_2^{(2)} & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_3^{(2)} & X_4^{(2)} & 1 \\
X_3^{(2)} & X_4^{(2)} & 1 \\
\end{bmatrix}
\]

\[
\begin{bmatrix}
X_5^{(2)} & X_6^{(2)} & 1 \\
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\end{bmatrix}
\]

\[
\begin{bmatrix}
X_7^{(2)} & X_8^{(2)} & 1 \\
X_7^{(2)} & X_8^{(2)} & 1 \\
\end{bmatrix}
\]

**Figure 1:** An example of mode row block tensor.
Tensor SVD

The TSVD of an even-order paired tensor $A \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$ is given by

$$A = U \ast S \ast V^\top.$$  \hspace{1cm} (8)

- $U \in \mathbb{R}^{J_1 \times J_1 \times \cdots \times J_N \times J_N}$, $V \in \mathbb{R}^{I_1 \times I_1 \times \cdots \times I_N \times I_N}$ are $U$-orthogonal
- $S \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$ containing singular values $\sigma_r$
- $A = \sum_{r=1}^{R} \sigma_r X_r \ast Y_r^\top$, $R = \text{rank}(\varphi(A))$ is called the unfolding rank
- Tensor Train Decomposition contains information of TSVD
  - $\tilde{A} = \text{permute}(A, [1, 3, \ldots, 2N - 1, 2, 4, \ldots, 2N])$
  - TTD on $\tilde{A}$ with the first $N - 1$ cores are left-orthonormal, and the last $N$ cores are right-orthonormal
  - $\sigma_r$ are the singular values of $\tilde{X}^{(N)} = \text{reshape}(X^{(N)}, R_{N-1}J_N, R_N)$
  - $X_r = \sum_{r_{N-1}=1}^{R_{N-1}} \cdots \sum_{r_0=1}^{R_0} X^{(1)}_{r_0:r_1} \circ X^{(2)}_{r_1:r_2} \circ \cdots \circ X^{(N)}_{r_{N-1}:r}$, similarly for $Y_r$

---

A general representation of MLTI system is given by

\[
\begin{align*}
X_{t+1} &= A \ast X_t + B \ast U_t \\
Y_t &= C \ast X_t
\end{align*}
\]

(9)

\(A \in \mathbb{R}^{J_1 \times J_1 \times \cdots \times J_N \times J_N}\), \(B \in \mathbb{R}^{J_1 \times K_1 \times \cdots \times J_N \times K_N}\) and \(C \in \mathbb{R}^{I_1 \times J_1 \times \cdots \times I_N \times J_N}\) are even-order paired tensors. \(X_t \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}\) and \(U_t \in \mathbb{R}^{K_1 \times K_2 \times \cdots \times K_N}\).

The use of TTD to accelerate DMD computations was first explored by Klus et. al. We discuss a variation of this tensor based DMD procedure to fit our MLTI system representation.

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The fundamental assumption of HODMD: $X_{t+1} = A \ast X_t$, where $X_t \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}$ and $A \in \mathbb{R}^{J_1 \times J_1 \times \cdots \times J_N \times J_N}$.

$$X = \begin{bmatrix} X_1 & X_2 & \ldots & X_M \end{bmatrix},$$

$$X' = \begin{bmatrix} X_2 & X_3 & \ldots & X_{M+1} \end{bmatrix},$$

where $X, X' \in \mathbb{R}^{J_1 \times M_1 \times \cdots \times J_N \times M_N}$. Note that the choice of factors $M_1, M_2, \ldots, M_N$ in the construction of mode row block tensor affects the TT-ranks of $\tilde{X}$, the permuted tensor from $X$.

Then $X' = A \ast X \Rightarrow A = X' \ast X^\dagger$, where $\dagger$ denotes as the Moore-Penrose inverse of an even-order paired tensor.
Algorithm 1 Higher-Order DMD

1: Input: Two data tensors $X, X'$, a TTD threshold $\epsilon_1 > 0$, a matrix SVD threshold $\epsilon_2 > 0$
2: Output: State transition tensor $A$ and DMD U-eigenvalues and DMD tensor modes
3: Apply TSVD for the data tensor $X$ to find the best unfolding rank $R$ approximation to $X$ such that $X \approx U_r \ast S_r \ast V_r^\top$
4: Then $A = X' \ast V_r \ast S_r^{-1} \ast U_r^\top$
5: Let $\tilde{A} = U_r^\top \ast X' \ast V_r \ast S_r^{-1}$ and compute U-eigenvalues and U-eigentensors of $\tilde{A}$, i.e.
\[
\tilde{A} \ast X = \lambda X \quad (10)
\]
6: DMD tensor modes corresponding to the DMD U-eigenvalue $\lambda$ is defined as $W = U_r \ast X$. 

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Using row/column block tensor, one can express

\[ X_{t+1} = (A \quad B) \ast W_t, \]

where, \( W_t = \begin{pmatrix} X_t \\ U_t \end{pmatrix} \). Let

\[ U = \begin{bmatrix} U_1 & U_2 & \ldots & U_M \end{bmatrix}, \]

where, \( U \in \mathbb{R}^{K_1 \times M_1 \times \cdots \times K_N \times M_N} \). Then

\[ X' = G \ast W, \]

where, \( G = (A \quad B) \) and

\[ W = \begin{pmatrix} X \\ U \end{pmatrix} \in \mathbb{R}^{(J_1+K_1) \times M_1 \times \cdots \times (J_N+K_N) \times M_N}. \]

One can compute \( G \) by tensor MP inverse of \( W \), and recover \( A \) and \( B \).
Algorithm 2 Higher-Order DMD with control

1: Input/output data tensors $U$ and $Y$, thresholds $\epsilon_1 > 0$, $\epsilon_2 > 0$ for TSVD
2: Reduced MLTI system $\tilde{A}$, $\tilde{B}$ and $\tilde{C}$
3: Compute TSVD $Y \approx U_{yr} * S_{yr} * V_{yr}^T$
4: Set $X_c = S_{yr} * V_{yr}^T$ and extract $X, X'$
5: Stack the tensors $X$ and $U$ to form column block tensor $W$
6: Compute TSVD $W \approx U_{wr} * S_{wr} * V_{wr}^T$ and split $U_{wr} = \begin{pmatrix} U_A \\ U_B \end{pmatrix}$
7: Compute TSVD $X' \approx U_{xr} * S_{xr} * V_{xr}^T$
8: The reduced MLTI system is given by

\[
\begin{align*}
\tilde{A} &= U_{xr}^T * X' * V_{wr} * S_{wr}^{-1} * U_A^T * U_{xr}, \\
\tilde{B} &= U_{xr}^T * X' * V_{wr} * S_{wr}^{-1} * U_B^T, \\
\tilde{C} &= U_{yr}.
\end{align*}
\]
4D Nucleome Example

In this example, we are given Hi-C measurements of the entire human genome at 1MB resolution and at 12 time points of MyoD-mediated fibroblast reprogramming, resulting in states which are second-order tensors, i.e. matrices, with size $2439 \times 2439$.

**Our goal:** Direct reprogramming

Any cell into any target cell!

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![Diagram showing various cell types connecting to a central 'X' point, representing skin biopsy and any cell for reprogramming.](image)
We use first 10 time points for training and the remaining for testing. Construct the two snapshot tensors

\[ X = [X_1 \ X_2 \ \ldots \ X_9] \in \mathbb{R}^{2439 \times 3 \times 2439 \times 3} \]

\[ X' = [X_2 \ X_3 \ \ldots \ X_{10}] \in \mathbb{R}^{2439 \times 3 \times 2439 \times 3}. \]

Here we choose \( M_1 = 3 \), \( M_2 = 3 \).

\[ U = [u_1 \ u_2 \ \ldots \ u_9] \in \mathbb{R}^{547 \times 3 \times 1 \times 3}, \]

In the all calculations, we assume that the TTD of \( \tilde{X} \) is given
4D Nucleome Example

<table>
<thead>
<tr>
<th></th>
<th>$\epsilon_1 = 0$</th>
<th>$\epsilon_1 = 0.005$</th>
<th>$\epsilon_1 = 0.01$</th>
<th>$\epsilon_1 = 0.05$</th>
</tr>
</thead>
<tbody>
<tr>
<td>TT ranks</td>
<td>[2439,9,3]</td>
<td>[1186,9,3]</td>
<td>[94,9,3]</td>
<td>[16,3,3]</td>
</tr>
<tr>
<td>TSVD (s)</td>
<td>15.7050</td>
<td>3.9635</td>
<td>0.1110</td>
<td>0.0092</td>
</tr>
<tr>
<td>p\text{inv} (s)</td>
<td>(6.8735 + 7.7589 + 10.0421 + 10.7189)/4 = 8.8484</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$e_2$</td>
<td>$1.03e - 13$</td>
<td>$7.57e - 14$</td>
<td>$1.12e - 13$</td>
<td>$0.1818$</td>
</tr>
<tr>
<td>$e_6$</td>
<td>$1.75e - 13$</td>
<td>$1.54e - 13$</td>
<td>$3.80e - 14$</td>
<td>$0.2123$</td>
</tr>
<tr>
<td>$e_{10}$</td>
<td>$5.48e - 13$</td>
<td>$6.94e - 13$</td>
<td>$2.14e - 13$</td>
<td>$0.2027$</td>
</tr>
<tr>
<td>$e_{12}$</td>
<td>0.2606</td>
<td>0.2618</td>
<td>0.2639</td>
<td>0.2193</td>
</tr>
</tbody>
</table>

**Table 1:** Running times of computing the MP inverse and relative errors by HODMD. We omit the first and last TT-ranks.
<table>
<thead>
<tr>
<th></th>
<th>$\epsilon_1 = 0$</th>
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<th>$\epsilon_1 = 0.01$</th>
<th>$\epsilon_1 = 0.05$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>TT ranks</strong></td>
<td>[2986,9,3]</td>
<td>[1186,9,3]</td>
<td>[94,9,3]</td>
<td>[16,3,3]</td>
</tr>
<tr>
<td><strong>TSVD (s)</strong></td>
<td>26.1419</td>
<td>3.9057</td>
<td>0.1018</td>
<td>0.0155</td>
</tr>
<tr>
<td><strong>pinv (s)</strong></td>
<td></td>
<td></td>
<td></td>
<td>$(9.0726 + 13.6808 + 12.0708 + 9.8871)/4 = 11.1778$</td>
</tr>
<tr>
<td>$e_2$</td>
<td>$2.03e-14$</td>
<td>$8.25e-14$</td>
<td>$1.17e-13$</td>
<td>$0.1818$</td>
</tr>
<tr>
<td>$e_6$</td>
<td>$1.57e-13$</td>
<td>$1.24e-13$</td>
<td>$3.33e-14$</td>
<td>$0.2123$</td>
</tr>
<tr>
<td>$e_{10}$</td>
<td>$1.66e-13$</td>
<td>$7.36e-14$</td>
<td>$2.53e-13$</td>
<td>$0.2027$</td>
</tr>
<tr>
<td>$e_{12}$</td>
<td>$0.2606$</td>
<td>$0.2618$</td>
<td>$0.2639$</td>
<td>$0.2193$</td>
</tr>
</tbody>
</table>

**Table 2:** Running times of computing the MP inverse and relative errors by HODMDc
Summary

- Matrix SVD
- Tensor SVD
- Tensor Train Decomposition
  - Left- and right-orthonormalization
  - Tensor MP Inverse
- Multilinear Time Invariant Systems
  - Higher-Order DMD
    - Higher-Order DMD with Control
- Stability, Reachability, Observability
Some Questions about TTD
- First, given the TTD of an even-order paired tensor, can we compute the TTDs of its permuted tensors fast?
- Second, (mode) row/column block tensors in block TT-format?

Develop MLTI systems higher-order balanced truncation and eigenvalue realization algorithm

Develop an observer and feedback control design framework

Applications to cellular reprogramming, tensor data compression, signal processing, etc

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