Multilinear Time Invariant System Theory

Can Chen, Anthony Bloch, Indika Rajapakse ¹
Amit Surana ²

¹University of Michigan, Ann Arbor
²United Technologies Research Center

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Motivation from 4D Nucleome

Tensor algebra
  - Tensors and tensor decompositions
  - Isomorphism and tensor ring
  - Block tensors

MLTI system theory
  - Stability
  - Reachability
  - Observability

MLTI system identification
  - Higher-order DMD

4D Nucleome example

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

C. Van Loan, From Matrix to Tensor, Department of Computer Science, Cornell University, 2016.
Higher-Order Singular Value Decomposition (HOSVD)

\[ X = S \times_1 U_1 \times_2 U_2 \times_3 \cdots \times_N U_N \]  \hspace{1cm} (1)

- \( \times_n \) are called \( n \)-mode multiplications
- \( U_n \) are unitary matrices
- The tensor Frobenius norm \( \|S_{i_1\ldots j_n \ldots i_N}\| \) are called \( n \)-mode singular values
- \# of nonvanished \( n \)-mode singular values = \( n \)-mode multilinear rank

CANDECOMP/PARAFAC Decomposition (CPD)

\[ X = \sum_{r=1}^{R} X_{r}^{(1)} \odot X_{r}^{(2)} \odot \cdots \odot X_{r}^{(N)} \]  \hspace{1cm} (2)

- \( R \) is called CP rank if it is the smallest integer achieving (2)
- CP rank is greater than or equal to any \( n \)-mode multilinear rank
- Unique under a weak condition: \( \sum_{n=1}^{N} k_{X(n)} \geq 2R + N - 1 \)
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
    \[
    X^{(n)} = \text{reshape}(X^{(n)}, R_{n-1}, J_nR_n)
    \]

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Isomorphism and tensor ring

- Even-order paired tensor $A \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$ introduced by Huang and Qi for elasticity tensors
- Einstein product
  \[
  (A \ast B)_{j_1i_1 \cdots j_Ni_N} = \sum_{k_N=1}^{K_N} \cdots \sum_{k_1=1}^{K_1} A_{j_1k_1 \cdots j_Nk_N} B_{k_1i_1 \cdots k_Ni_N}
  \]  
- 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** $T_{i_1j_1 \cdots i_Nj_N} = A_{j_1i_1 \cdots j_Ni_N}$, 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** All its entries are zeros except for $D_{j_1j_1 \cdots j_Nj_N} = 1$ denoted by $I$
  - **U-identity** $D_{j_1j_1 \cdots j_Nj_N} = 1$
  - **U-orthogonal** $A \ast A^\top = A^\top \ast A = I$
  - **U-inverse** $A \ast B = B \ast A = I$ denoted by $A^{-1}$
  - **U-positive definite** $X \ast A \ast X > 0$ for $X \neq 0$
  - **Unfolding rank** $\text{rank}_U(A) = \text{rank}(\varphi(A))$
Block Tensors

- **n-mode row block tensor** $A, B \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$

$$\begin{vmatrix} A & B \end{vmatrix}_n \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_n \times 2I_n \times \cdots \times J_N \times I_N}$$  \hspace{1cm} (8)

- $= A$ for only $i_n = 1, \ldots, I_n$
- $= B$ for only $i_n = I_n + 1, \ldots, 2I_n$
- $P \ast \begin{vmatrix} A & B \end{vmatrix}_n = \begin{vmatrix} P \ast A & P \ast B \end{vmatrix}_n$
- $\begin{vmatrix} A & B \end{vmatrix}_n \ast \begin{vmatrix} C \end{vmatrix}_n = A \ast C + B \ast D$

- **Mode row block tensor** Distribute $K$ into every even mode. The factorization of $K$ is arbitrary but a careful choice can facilitate computations.

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Figure 1: An example of mode row block tensor.
A general representation of MLTI system is given by

\[
\begin{cases}
X_{t+1} = A \ast X_t + B \ast U_t \\
Y_t = C \ast X_t
\end{cases}
\]  \hspace{1cm} (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 \(U_t \in \mathbb{R}^{K_1 \times K_2 \times \cdots \times K_N}\).

We can write down the explicit solution of (9) which takes an analogous form to the LTI system

\[
X_k = A^k \ast X_0 + \sum_{j=0}^{k-1} A^{k-j-1} \ast B \ast U_j.
\]  \hspace{1cm} (10)
Let $A \in \mathbb{R}^{J_1 \times J_1 \times \cdots \times J_N \times J_N}$ be an even-order square tensor. If $X \in \mathbb{C}^{J_1 \times J_2 \cdots \times J_N}$ is a nonzero $N$-th order tensor, $\lambda \in \mathbb{C}$, and $X$ and $\lambda$ satisfy $A \ast X = \lambda X$, then we call $\lambda$ and $X$ as the U-eigenvalue and U-eigentensor of $A$, respectively.

**Theorem**

Let $\lambda_j$ be the U-eigenvalues of $A$ for $j = \text{ivec}(j, J)$. For an unforced MLTI system, the equilibrium point $X = O$ is:

1. **stable** if and only if $|\lambda_j| \leq 1$ for all $j \in [J]$; for those equal to 1, its algebraic and geometry multiplicities must be equal;
2. **asymptotically stable** if $|\lambda_j| < 1$ for all $j \in [J]$;
3. **unstable** if $|\lambda_j| > 1$ for some $j \in [J]$.

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L. Cui, C. Chen, W. Li, and M. Ng, An eigenvalue problem for even order tensors with its applications, Linear and Multilinear Algebra, (2016).
Stability

Corollary

Suppose that the HOSVD of $A$ is provided with $n$-mode singular values. For an unforced MLTI system, the equilibrium point $X = 0$ is asymptotically stable if the sum of the $n$-mode singular values square is less than one for any $n$.

Corollary

Suppose that the TTD of the permuted $\tilde{A} \in \mathbb{R}^{J_1 \times \cdots \times J_N \times J_1 \times \cdots \times J_N}$ is provided with the first $N - 1$ core tensors left-orthonormal and the last $N$ core tensors right-orthonormal. For an unforced MLTI system, the equilibrium point $X = 0$ is asymptotically stable if the largest singular value of $\bar{A}^{(N)}$ is less than one, where $\bar{A}^{(N)} = \text{reshape}(\tilde{A}, R_{N-1}J_N, R_N)$.

Remark: Truncating the TT-rank $R_N$ of $\tilde{A}$ would not alter the largest singular values of $\bar{A}^{(N)}$. 
Reachability

Definition

The MLTI system (9) is said to be *reachable* on $[t_0, t_1]$ if, given any initial condition $X_0$ and any final state $X_1$, there exists a sequence of inputs $U_t$ that steers the state of the system from $X_{t_0} = X_0$ to $X_{t_1} = X_1$.

Theorem

*The pair $(A, B)$ is reachable on $[t_0, t_1]$ if and only if the reachability Gramian*

$$W_r(t_0, t_1) = \sum_{t=t_0}^{t_1-1} A^{t_1-t-1} \ast B \ast B^\top \ast (A^\top)^{t_1-t-1},$$

(11)

*which is a weakly symmetric even-order square tensor, is $U$-positive definite.*
Reachability

A tensor version of the Kalman rank condition is also provided.

**Theorem**

The pair \((A, B)\) is reachable if and only if the \(J_1 \times J_1 K_1 \times \cdots \times J_N \times J_N K_N\) even-order reachability tensor

\[
\mathcal{R} = |B \ A \ast B \ \ldots \ A^{\lceil J \rceil - 1} \ast B|
\]  

(12)

spans \(\mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}\). In other words, \(\text{rank}_U(\mathcal{R}) = |J|\).

**Remark:** First, any choice of construction for the mode row block tensor works for the reachability tensor. Second, when \(N = 1\), it simplifies to the famous Kalman rank condition for reachability of LTI systems.
**Corollary**

Given the reachability tensor $\mathcal{R}$ in (12), if \( \text{rank}_{2n-1}(\mathcal{R}) \neq J_n \) for some \( n \), the pair \((A, B)\) is not reachable.

**Corollary**

Given the reachability tensor $\mathcal{R}$ in (12), if the CPD of $\mathcal{R}$ satisfies

\[
2N \sum_{n=1:2} k_{A(n)} \geq R + N - 1, \quad 2N \sum_{n=2:2} k_{A(n)} \geq R + N - 1 \tag{13}
\]

with CP rank equal to $|J|$, the pair \((A, B)\) is reachable. Conversely, if the pair \((A, B)\) is reachable, then the CP rank of $\mathcal{R}$ is greater than or equal to $|J|$.
Corollary

Given the reachability tensor \( \mathcal{R} \) in (12), the pair \( (A, B) \) is reachable if and only if the \( N \)-th optimal TT-rank of the permuted tensor \( \tilde{\mathcal{R}} \in \mathbb{R}^{J_1 \times \cdots \times J_N \times K_1 \times \cdots \times K_N} \) is equal to \( |\mathcal{J}| \).

The results of observability can be simply obtained by the duality principle, similarly to LTI systems.

Definition

The MLTI system (9) is said to be observable on \( [t_0, t_1] \) if any initial state \( X_{t_0} = X_0 \) can be uniquely determined by \( Y_t \) on \( [t_0, t_1] \).
Higher-Order DMD

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.

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 TTD for the permuted data tensor $\tilde{X}$ to find the best unfolding rank $R$ approximation to $X$ such that $X \approx U_r S_r V_r^\top$

4: Then $A = X' V_r S_r^{-1} U_r^\top$

5: Let $\tilde{A} = U_r^\top X' V_r S_r^{-1}$ and compute U-eigenvalues and U-eigentensors of $\tilde{A}$, i.e.

\[
\tilde{A} X = \lambda X
\]  \hspace{1cm} (14)

6: DMD tensor modes corresponding to the DMD U-eigenvalue $\lambda$ is defined as $W = U_r X$. 

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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!

Cardiomyocytes  Red blood  Astrocytes  Lymph node  Hepatocytes  Neurons

Skin biopsy  X  Any cell

iReprogram LLC
4D Nucleome Example

We use first 10 time points for training and the remaining for testing. Construct the two snapshot tensors

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

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

Here we choose \( M_1 = 3 \), \( M_2 = 3 \). 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>
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<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>TTD (s)</td>
<td>15.7050</td>
<td>3.9635</td>
<td>0.1110</td>
<td>0.0092</td>
</tr>
<tr>
<td>pinv (s)</td>
<td>$(6.8735 + 7.7589 + 10.0421 + 10.7189)/4 = 8.8484$</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>$e_2$</td>
<td>$1.03e-13$</td>
<td>$7.57e-14$</td>
<td>$1.12e-13$</td>
<td>$0.1818$</td>
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<tr>
<td>$e_6$</td>
<td>$1.75e-13$</td>
<td>$1.54e-13$</td>
<td>$3.80e-14$</td>
<td>$0.2123$</td>
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<tr>
<td>$e_{10}$</td>
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<td>$6.94e-13$</td>
<td>$2.14e-13$</td>
<td>$0.2027$</td>
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<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.
Future Work

- 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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