Multilinear Time Invariant System Theory

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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!

H. Chen, J. Chen, L. Muir, S. Ronquist, W. Meixner, M. Ljungman, T. Ried, S. Smale, and I. Rajapakse, Functional organization of the human 4D Nucleome, National Academy of Sciences, 112(26), pp. 8002–8007, 2015

T. Ried, I. Rajapakse. The 4D Nucleome, Methods, Elsevier, Amsterdam, Netherlands, 2017.
Tensors and tensor decompositions

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

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

- **Higher-Order Singular Value Decomposition (HOSVD)**

  \[
  X = S \times_1 U_1 \times_2 U_2 \times_3 \cdots \times_N U_N
  \]  

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

- **CANDECOMP/PARAFAC Decomposition (CPD)**

  \[
  X = \sum_{r=1}^{R} X^{(1)} \circ X^{(2)} \circ \cdots \circ X^{(N)}
  \]  

  - $R$ 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:** \( \bar{X}^{(n)}(\bar{X}^{(n)})^\top = I \), where

\[
\bar{X}^{(n)} = \text{reshape}(X^{(n)}, R_{n-1}, J_n R_n)
\]  

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I. Oseledets, Tensor-train decomposition, SIAM Journal on Scientific Computing, vol. 33, no. 5, pp. 2295–2317, 2011.

[Online]. Available:https://doi.org/10.1137/090752286.
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
  \[
  (A \ast B)_{j_1 i_1 \ldots j_N i_N} = \sum_{k_N=1}^{K_N} \cdots \sum_{k_1=1}^{K_1} A_{j_1 k_1 \ldots j_N k_N} B_{k_1 i_1 \ldots k_N i_N} \quad (7)
  \]
- 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 \( T_{i_1 j_1 \ldots i_N j_N} = A_{j_1 i_1 \ldots j_N i_N} \), 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 \( D_{j_1 i_1 \ldots j_N i_N} = 1 \) denoted by \( I \)
  - U-identity \( D_{j_1 i_1 \ldots j_N i_N} = 1 \) 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 \( A^{-1} \)
  - 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** $A, B \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_N \times I_N}$

\[
|A \quad B|_n \in \mathbb{R}^{J_1 \times I_1 \times \cdots \times J_n \times 2I_n \times \cdots \times J_N \times I_N}
\]  

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

**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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C. Chen, A. Surana, A. Bloch, and I. Rajapakse, Multilinear time invariant system theory, SIAM Conference on Control and its Applications, accepted to appear, 2019.
Figure 1: An example of mode row block tensor.
A general representation of MLTI system is given by

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

(9)

\[A \in \mathbb{R}^{J_1 \times J_1 \times \cdots \times J_N \times J_N}, \ B \in \mathbb{R}^{J_1 \times K_1 \times \cdots \times J_N \times K_N} \text{ and } C \in \mathbb{R}^{I_1 \times J_1 \times \cdots \times I_N \times J_N}\] 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

\[
X_k = A^k \ast X_0 + \sum_{j=0}^{k-1} A^{k-j-1} \ast B \ast U_j.
\]  

(10)

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Stability

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 $A * X = \lambda X$, then we call $\lambda$ and $X$ as the U-eigenvalue and U-eigentensor of $A$, respectively.

A generalization of Z-eigenvalues and M-eigenvalues proposed by Qi

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 $j \in [J]$.

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

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

which is a weakly symmetric even-order square tensor, is \(U\)-positive definite.
A tensor version of the Kalman rank condition is also provided.

**Theorem**

The pair \((A, B)\) is reachable if and only if the even-order reachability tensor

\[
\mathcal{R} = \begin{vmatrix} B & A \ast B & \ldots & A^{|\mathcal{J}| - 1} \ast B \end{vmatrix}
\]

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

**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

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

with CP rank equal to $|\mathcal{J}|$, 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 $|\mathcal{J}|$. 
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 $\tilde{\mathcal{R}} \in \mathbb{R}^{J_1 \times \cdots \times J_N \times J_1 K_1 \times \cdots \times J_N K_N}$ 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.

$$\tilde{A} * X = \lambda X \quad (14)$$

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

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

**Table 1:** Running times of computing the MP inverse and relative errors by HODMD. We omit the first and last TT-ranks.
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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