AFRL-AFOSR-VA-TR-2023-0077

Data Driven Systems and Control Framework for Multiway Dynamical Systems

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10/18/2022
Final Technical Report

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Air Force Research Laboratory
Air Force Office of Scientific Research
Arlington, Virginia 22203
Air Force Materiel Command

REPORT DOCUMENTATION PAGE

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1. REPORT DATE	**2. REPORT TYPE**	**3. DATES COVERED**	
20221018	Final	**START DATE** 20171101	**END DATE** 20221231

4. TITLE AND SUBTITLE
Data Driven Systems and Control Framework for Multiway Dynamical Systems

5a. CONTRACT NUMBER	**5b. GRANT NUMBER**	**5c. PROGRAM ELEMENT NUMBER**
	FA9550-18-1-0028	61102F
5d. PROJECT NUMBER	**5e. TASK NUMBER**	**5f. WORK UNIT NUMBER**

6. AUTHOR(S)
Indika Rajapakse

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)	**8. PERFORMING ORGANIZATION REPORT NUMBER**
REGENTS OF THE UNIVERSITY OF MICHIGAN 503 THOMPSON ST ANN ARBOR, MI 48109 USA	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	**10. SPONSOR/MONITOR'S ACRONYM(S)**	**11. SPONSOR/MONITOR'S REPORT NUMBER(S)**
Air Force Office of Scientific Research 875 N. Randolph St. Room 3112 Arlington, VA 22203	AFRL/AFOSR RTA2	AFRL-AFOSR-VA-TR-2023-0077

12. DISTRIBUTION/AVAILABILITY STATEMENT
A Distribution Unlimited: PB Public Release

13. SUPPLEMENTARY NOTES

14. ABSTRACT
The goal of the proposed research was to explore the use of multiway dynamical systems as a means to rigorously capture the interplay of function, structure and dynamics inherent in many complex systems such as those arising in biology, and to develop a systems and control framework for multiway dynamical systems analogous to classical multivariate control theory which relies on vector based state space representations.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	UU	11
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19a. NAME OF RESPONSIBLE PERSON	**19b. PHONE NUMBER** *(Include area code)*
FREDERICK LEVE	696-9730

Data Driven Systems and Control Framework for Multiway Dynamical Systems

CONTRACT FA9550-18-1-0028

FINAL REPORT

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Objectives

The goal of the proposed research was to explore the use of multiway dynamical systems as a means to rigorously capture the interplay of function, structure and dynamics inherent in many complex systems such as those arising in biology, and to develop a systems and control framework for multiway dynamical systems analogous to classical multivariate control theory which relies on vector based state space representations.

Summary of Accomplishments

We have developed a novel theoretical and computational framework based on tensor algebra and hypergraph representation to study higher order or multiway interactions, see Figure 1. The proposed framework exploits hidden correlations/redundancies that may be present in the higher order interactions to enable compact representation and efficient computations, and is amenable to data-driven model learning, analysis, and control.

In one line of work, we extended classical linear time-invariant (LTI) system notions including stability, reachability, and observability to multilinear time-invariant (MLTI) systems, in which the state, inputs, and outputs are preserved as tensors, and expressed these notions in terms of more standard concepts of tensor ranks/decompositions. We also introduced a tensor decomposition-based model reduction framework which can significantly reduce the number of MLTI system parameters.

In another line of work, we developed the notion of tensor entropy for uniform hypergraphs, which can capture higher order interactions between entities than classical graphs. We showed that this tensor entropy is an extension of von Neumann entropy for graphs and can be used as a measure of regularity for uniform hypergraphs. Moreover, we employed uniform hypergraphs for studying controllability of high-dimensional networked systems. We

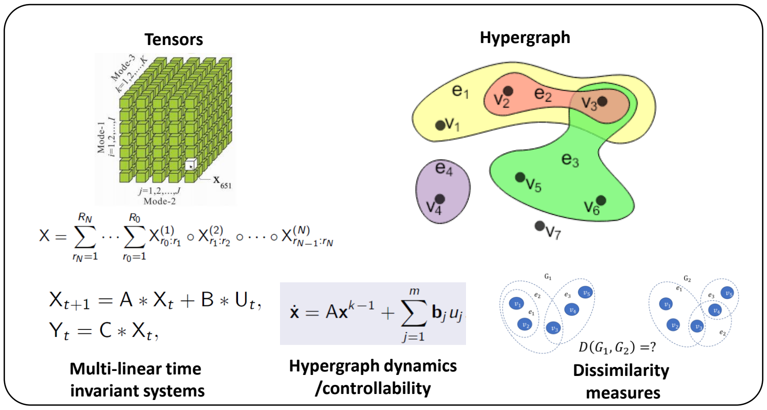

Figure 1: Framework based on tensor algebra and hypergraph representation to study higher order or multiway interactions.

propose another tensor-based multilinear system representation to characterize the multidimensional state dynamics of uniform hypergraphs, and derive a Kalman-rank-like condition to identify the minimum number of control nodes (MCN) needed to achieve full control of the whole hypergraph. We have also developed notions of hypergraph dissimilarity measures to characterize structural differences between two hypergraphs.

We have successfully demonstrated these new tensor/hypegraph-based theoretical and computational developments in a variety of biological and engineering examples.

Outline of Report

In Chapter 1 we describe in more detail the key ideas of our technical approach and some numerical results. Full details can be found in the associated publications. In Chapter 2 we briefly outline how the techniques developed in this program are being transitioned ****. Chapter 3 lists the personnel supported under this program, and finally Chapter 4 lists the publication which resulted from this contract.

Contents

Chapter 1

Summary of Research Results

1.1 Tensor Entropy

This work develops the notion of entropy for uniform hypergraphs via tensor theory. We employed the probability distribution of the generalized singular values, calculated from the higher-order singular value decomposition of the Laplacian tensors, to fit into the Shannon entropy formula. The work showed that this tensor entropy is an extension of von Neumann entropy for graphs. In addition, we established results on the lower and upper bounds of the entropy and demonstrated that it is a measure of regularity for uniform hypergraphs in simulated and experimental data. Tensor train decomposition was exploited in computing the proposed tensor entropy efficiently. Details can be found in the publication [p1].

1.2 Multi Linear Time Invariant Systems Theory

This work proposes new tensor notions for positive definiteness, tensor inversion, and a new way of concatenation of tensors to create block tensors. Further, it develops tensor algebraic conditions for stability, reachability, and observability for the generalized MLTI systems. Finally, the work provides computational and memory complexity analysis for tensor based methods in comparison to unfolding-based matrix methods and demonstrates the framework in four numerical examples. Furthermore, we developed higher-order generalization of balanced proper orthogonal decomposition (BPOD) and its variants for model reduction and identification of MLTI systems from data. Details can be found in the publications [c1,p2,p3].

1.3 Hypergraph Controllability

This work develops a notion of controllability for hypergraphs via tensor algebra and polynomial control theory. A new tensor-based multilinear dynamical system representation is proposed, and a Kalman-rank-like condition is derived to determine the minimum number of control nodes (MCN) needed to achieve controllability of even uniform hypergraphs. This work presents an efficient heuristic to obtain the MCN. Further, it shows that the MCN is related to the hypergraph degree distribution in simulated examples. Finally, MCN is used to examine robustness in real biological networks. Details can be found in the publication [p4].

1.4 Hypergraph Dissimilarity Measures

In this work, we propose two novel approaches for hypergraph comparison. The first approach transforms the hypergraph into a graph representation for use of standard graph dissimilarity measures. The second approach exploits the mathematics of tensors to intrinsically capture multi-way relations. For each approach, we present measures that assess hypergraph dissimilarity at a specific scale or provide a more holistic multi-scale comparison. We test these measures on synthetic hypergraphs and apply them to biological datasets. Details can be found in the publication [p5].

1.5 Applications to Wound Healing

Our internally developed computational algorithm, the Data Guided Control (DGC) algorithm (US10672501B2), has successfully predicted TFs to promote direct conversion of one cell type to another (direct reprogramming). Recently we introduced an extension of the DGC, called hybrid reprogramming, to predict the activation and suppression of TF sets which promotes reprogramming. We have applied this technology to the acceleration of wound healing in an in vitro analog. We developed imaging methods to assess wound healing efficiency with our reprogramming regimes (Figure 1.1). In preliminary experiments, addition of the TF MYOD1 and silencing (siRNA) of TFs PRRX1 or TFAP2C resulted in wound closure that was approximately five times faster than wound closure for controls (Figure 1.2). In ongoing experiments, we anticipate generating additional data that confirm the accelerated wound healing result with hybrid reprogramming. There is lack of mathematical and computational methods for hybrid reprogramming which we plan to address in this proposed project.

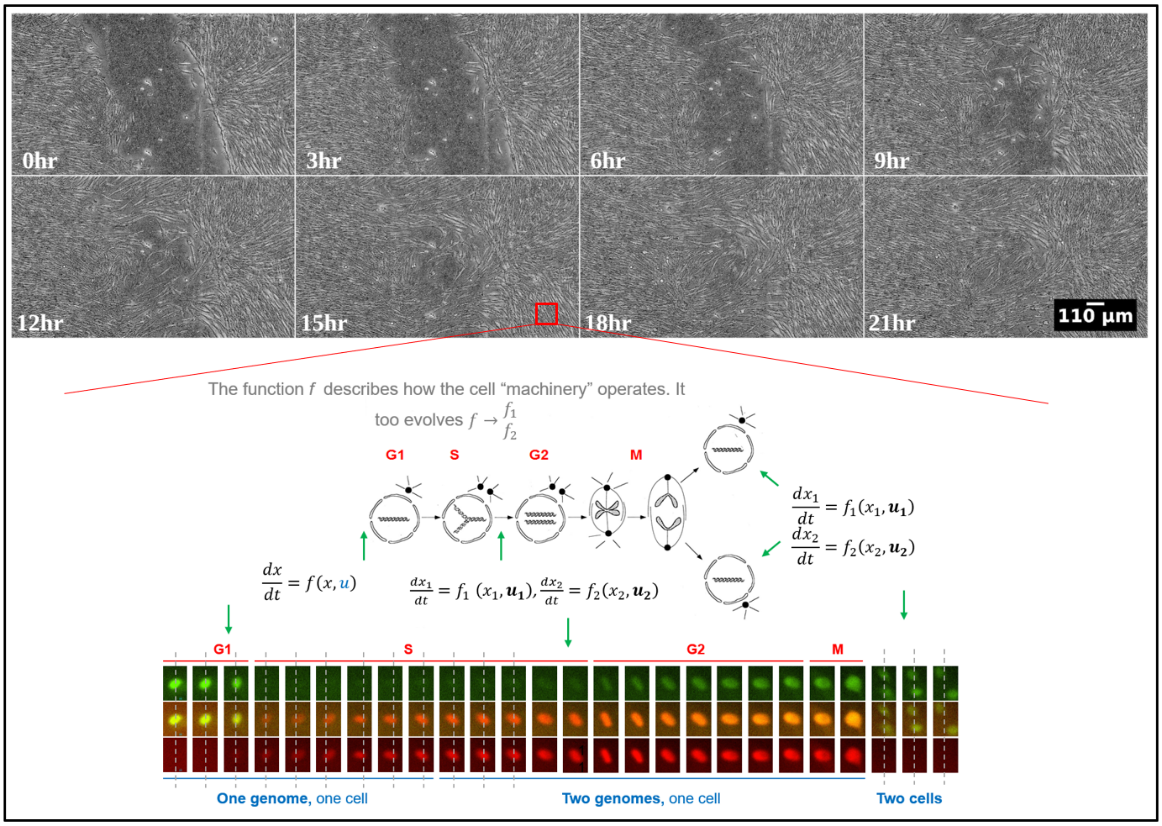

Figure 1.1: **Fibroblast Scratch Assay and Cell Cycle Dynamics.** Top (Greyscale image): Background subtracted transmitted light images for a scratch assay with initial cell density of 8k/well. Images captured every 15 minutes for 48 hours on a Zeiss Celldiscoverer 7. Middle: Mathematics of the cell cycle. Bottom: The PIP-FUCCI reporter system constitutes fluorescent markers for accurate delineation of the G1 to S transition (PIP-mVenus) as well as S and G2 (mCherry-Gem1-110). Vertical dotted lines represent genome-wide biochemical measurements.

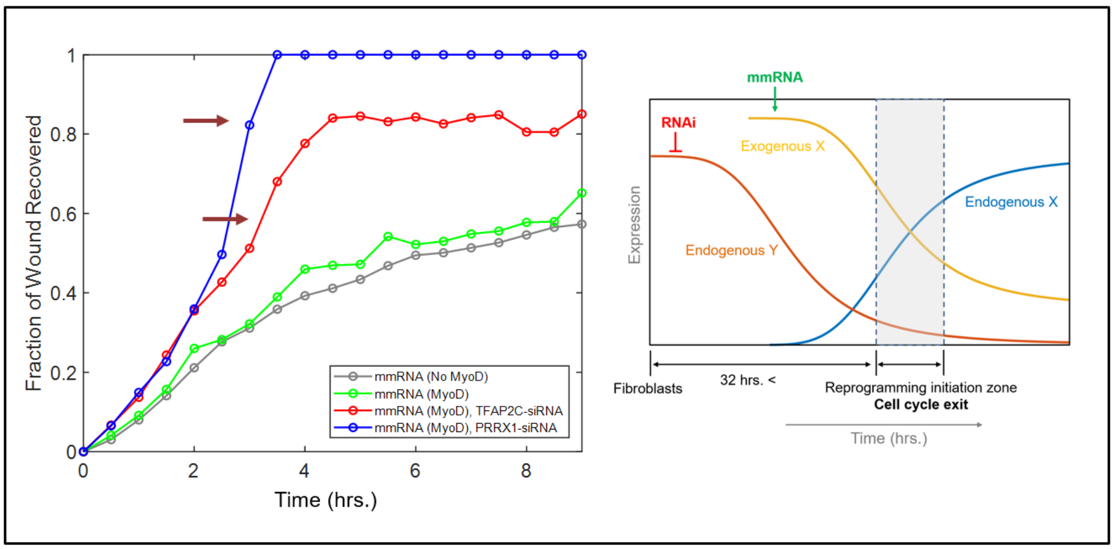

Figure 1.2: **Transcription Factor-mediated Wound Recovery.** Addition of the transcription factor MYOD1 and suppression of the transcription factor TFAP2C or PRRX1 (blue and red data) in primary human fibroblasts improves wound recovery.

Chapter 2

Transitions

We have been using graph based methods for cellular reprogramming in iReprogram, Inc. We plan to use hypergraph methods developed under this program in near future for similar appalications..

Chapter 3

Personnel Supported

University of Michigan personnel: Indika Rajapakse, Anthony Bloch, Can Chen
RTRC personnel: Amit Surana

Chapter 4

Publications

Journal Papers

[p1] Chen, Can, and Indika Rajapakse. “Tensor entropy for uniform hypergraphs.” IEEE Transactions on Network Science and Engineering, vol. 7, no. 4, pp. 2889-2900, 2020.

[p2] C. Chen, A. Surana, A. M. Bloch, and I. Rajapakse, “Multilinear Control Systems Theory”, SIAM Journal on Control and Optimization, vol. 59, no. 1, pp. 749-776, 2021.

[p3] C. Chen, A. Surana, A. Bloch, and I. Rajapakse, “Data-Driven Model Reduction for Multilinear Control Systems via Tensor Trains”, preprint: arXiv:1912.03569.

[p4] C. Chen, A. Surana, A. M. Bloch, and I. Rajapakse, “Controllability of Hypergraphs”, IEEE Transactions on Network Science and Engineering, 10.1109/TNSE.2021.3068203, 2021.

[p5] A. Surana, C. Chen, and I. Rajapakse, “Hypergraph dissimilarity measures”, arXiv preprint arXiv:2106.08206, 2021.

[p6] S. M. Lindsly, C. Chen, S. Dilworth, S. Jeyarajan, C. Stansbury, A. Cicalo, W. Meixner, N. Beckloff, C. Ryan, A. Surana, M. Wicha, “Deciphering Multi-way Interactions in the Human Genome”, bioRxiv. 2021 Jan 1.

Conference Papers

[c1] C. Chen, A. Surana, A. Bloch, I. Rajapakse, Multilinear Time Invariant System Theory, Proc. of SIAM Conference on Control and its Applications, 2019, pp. 118-125.

Invited Sessions

The following invited session was organized with AFOSR support and contain AFOSR-funded papers:

-2020 SIAM Conference on Control and Applications, Data Guided Dynamics and Control of Network Systems; Organizers: I. Rajapakse, and A. Surana.

Talks

[t1] Can Chen, Multilinear Time Invariant System Theory, SIAM Conference on Control and Applications, 2019

[t2] Amit Surana, Beyond pairwise interactions: dynamics and structure, Control, Dynamical-Systems, and Computation Seminar Series, UCSB, 2021.

[t3] Amit Surana, Hypergraph Dissimilarity Measures, SIAM Conference on Control and Applications, 2021.

[t4] Can Chen, Controllability of Hypergraphs, SIAM Conference on Control and Applications, 2021.