



Controlling Collective Dynamics of Underactuated Ensembles

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WASHINGTON UNIVERSITY THE

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Final Report

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14. ABSTRACT This project focused on the development of a systematic framework and a set of unifying principles and approaches to advance our understanding of complex ensemble systems and ability to control their collective behavior. The motivation was driven by the applications in rapidly expanding and emerging transdisciplinary domains, such as quantum control, neurostimulation, chronobiology, and robotics, wherein engineers, experimentalists, and clinical practitioners exert exogenous inputs (e.g., electromagnetic pulses, electrical microsimulation, and light protocols) to excite, perturb and, furthermore, optimally control the activity or the spatiotemporal structure of an ensemble system consisting of a large number of dynamical units towards scientific or therapeutic endpoints. The major challenge concerning this class of problems was that one cannot send control signals to individual systems in the ensemble, but only to the ensemble as a whole. This project (1) established new methods for examining fundamental properties, such as ensemble controllability, to understand the theoretical limits of the extent to which ensemble activity and dynamic structures can be perturbed with an exogenous input; and (2) developed effective computational methods for solving optimal control problems involving ensemble systems and networks. The research substantially advanced our understanding of complex ensemble systems and directly contributed to new developments in control and systems theory, which supports the research mission of the AFOSR. It also broadened seminal applications by enabling tractable methods for optimal control designs in brain stimulation, circadian biology, atom cooling, information encoding, and nanoscale chemical cyber-physical computing devices, for which the ability to control the time evolution and dynamic structures, e.g., synchrony, of ensemble systems is fundamen			
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Abstract

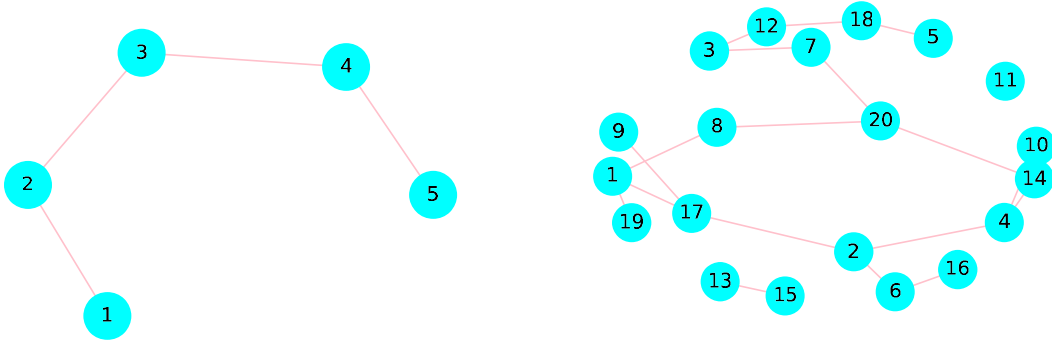
This project focused on the development of a systematic framework and a set of unifying principles and approaches to advance our understanding of complex ensemble systems and ability to control their collective behavior. The motivation was driven by the applications in rapidly expanding and emerging transdisciplinary domains, such as quantum control, neurostimulation, chronobiology, and robotics, wherein engineers, experimentalists, and clinical practitioners exert exogenous inputs (e.g., electromagnetic pulses, electrical microsimulation, and light protocols) to excite, perturb and, furthermore, optimally control the activity or the spatiotemporal structure of an ensemble system consisting of a large number of dynamical units towards scientific or therapeutic endpoints. The major challenge concerning this class of problems was that one cannot send control signals to individual systems in the ensemble, but only to the ensemble as a whole. This project (1) established new methods for examining fundamental properties, such as ensemble controllability, to understand the theoretical limits of the extent to which ensemble activity and dynamic structures can be perturbed with an exogenous input; and (2) developed effective computational methods for solving optimal control problems involving ensemble systems and networks. The research substantially advanced our understanding of complex ensemble systems and directly contributed to new developments in control and systems theory, which supports the research mission of the AFOSR. It also broadened seminal applications by enabling tractable methods for optimal control designs in brain stimulation, circadian biology, atom cooling, information encoding, and nanoscale chemical cyber-physical computing devices, for which the ability to control the time evolution and dynamic structures, e.g., synchrony, of ensemble systems is fundamental.

Accomplishments and New Findings

Through the funding support period, 8 journal and 9 peer-reviewed conference papers have been published or accepted for publications (see Publication List). Owing to the multidisciplinary nature of the research, these papers appeared in leading scientific journals and international conference proceedings across disciplines including control theory and engineering, applied mathematics, physics, and bioengineering. The significant achievements and new findings through the support of this grant award are summarized below.

1 Symmetric Group Methods for Controllability Analysis

We developed a novel and effective algebraic approach to examine controllability of bilinear systems based on the theory of symmetric group. The central idea was to map Lie bracket operations of the vector fields governing the system dynamics to permutation multiplications on a symmetric group, so that controllability and the controllable submanifold can be characterized by permutation orbits [1]. This new finding further enabled a visualization of controllability analysis over an undirected graph and facilitated the design of efficient graph search algorithms to compute controllability [2]. The developed methodology revealed the relationship between controllability of a system and connectivity of the associated graph, which rendered a transparent way to understand controllability over graphs. The method was directly applicable to characterize the degree of controllability and reachability of systems defined on compact Lie groups and on graphs, such as quantum networks, multi-agent systems, and Markov chains.



(a) Graph Representation of Controllability on SO(5) (b) Graph Representation of Controllability on SO(20)

Figure 1: Graph Representation of Controllability.

1.1 Interpreting Controllability over Symmetric Groups

To illustrate the idea, we consider the bilinear system defined on a compact, connected Lie group. Let $\Omega_{ij} \in \mathfrak{so}(n)$ be the matrix whose ij^{th} entry is -1 and ji^{th} entry is 1 for each $i, j = 1, \dots, n$ and $i \neq j$, then the set $\mathcal{B} = \{\Omega_{ij} : 1 \leq i < j \leq n\}$ forms a basis of $\mathfrak{so}(n)$, which is of the dimension $n(n-1)/2$. We call \mathcal{B} the standard basis of $\mathfrak{so}(n)$.

Definition 1 Let $\mathcal{P}(\mathcal{B})$ denote the power set of \mathcal{B} , and define the map $\iota : \mathcal{P}(\mathcal{B}) \rightarrow S_n$ by $\{\Omega_{i_1, j_1}, \Omega_{i_2, j_2}, \dots, \Omega_{i_m, j_m}\} \mapsto (i_m, j_m) \cdots (i_2, j_2) \cdot (i_1, j_1)$, where (i_k, j_k) , $k = 1, \dots, m$, denotes the cyclic notation of permutations.

Theorem 1 The control system defined on $\text{SO}(n)$ of the form

$$\dot{X}(t) = \left[\sum_{k=1}^m u_k(t) \Omega_{i_k j_k} \right] X(t), \quad X(0) = I, \quad (1)$$

where $\Omega_{i_k j_k} \in \mathcal{F} = \{\Omega_{i_1 j_1}, \dots, \Omega_{i_m j_m}\} \subseteq \mathcal{B}$, with $1 \leq i_k < j_k \leq n$ for $k = 1, \dots, m$, are elements of the standard basis of $\mathfrak{so}(n)$, is controllable if and only if there is a subset $\mathcal{S} \subseteq \mathcal{F}$ such that $\iota(\mathcal{S})$ is an n -cycle.

1.2 Computing Controllability of Bilinear Systems over Graphs

The notion of examining controllability through permutation cycles illuminates the interpretation of controllability on graphs. In particular, the Lie algebra structure of $\mathfrak{so}(n)$ allows us to associate each system modeled as in (1) with an undirected, unweighted graph for visualizing “the degree” of controllability of the system on $\text{SO}(n)$ through connectivity of the graph. We create two examples to demonstrate this nontrivial idea.

Example 1 Consider the system on $\text{SO}(5)$, $\frac{d}{dt}X(t) = \sum_{i=1}^4 u_i(t) \Omega_{i, i+1} X(t)$, $X(0) = I$. Let $\mathcal{F} = \{\Omega_{i, i+1} : 1 \leq i \leq 4\}$ denote the set of control vector fields evaluated at the identity matrix I .

The iterated Lie brackets of elements in \mathcal{F} give

$$\begin{aligned} [\Omega_{12}, \Omega_{23}] &= \Omega_{13}, \quad [\Omega_{23}, \Omega_{34}] = \Omega_{24}, \quad [\Omega_{34}, \Omega_{45}] = \Omega_{35}, \\ [\Omega_{12}, \Omega_{24}] &= [\Omega_{12}, [\Omega_{23}, \Omega_{34}]] = \Omega_{14}, \\ [\Omega_{23}, \Omega_{35}] &= [\Omega_{23}, [\Omega_{34}, \Omega_{45}]] = \Omega_{25}, \\ [\Omega_{12}, \Omega_{25}] &= [\Omega_{12}, [\Omega_{13}, [\Omega_{34}, \Omega_{45}]]] = \Omega_{15}, \end{aligned}$$

and thus this system is controllable on $\text{SO}(5)$ by the the Lie algebra rank condition (LARC). Mapping the above Lie brackets to permutations on the symmetric group S_5 of 5 letters under the map ι defined in Definition 1, this controllability result can be visualized on an undirected graph $\Gamma = (V, E)$ through its graph connectivity, where $V = \{1, 2, 3, 4, 5\}$ is the set of vertices and E denotes the set of edges, as shown in Figure 1(a).

Example 2 Consider a system on $\text{SO}(20)$ in the form of (1) governed by the control vector fields,

$$\mathcal{F} = \{\Omega_{1,8}, \Omega_{1,17}, \Omega_{1,19}, \Omega_{2,4}, \Omega_{2,6}, \Omega_{2,17}, \Omega_{3,7}, \Omega_{3,12}, \Omega_{4,10}, \Omega_{4,14}, \Omega_{5,18}, \Omega_{6,16}, \Omega_{7,20}, \Omega_{8,20}, \Omega_{9,17}, \Omega_{12,18}, \Omega_{13,15}, \Omega_{14,20}\}.$$

The graph representation $\Gamma = (V, E)$ of this control system can be constructed and is shown in Figure 1(b), where the set of vertices $V = \{1, \dots, 20\}$ and the edges $E = \{(i, j) : \Omega_{ij} \in \mathcal{F}\}$. The graph Γ consists of three disjoint connected subgraphs $\Gamma_1 = (V_1, E_1)$, $\Gamma_2 = (V_2, E_2)$, and $\Gamma_3 = (V_3, E_3)$, where $V_1 = V \setminus \{11, 13, 15\}$, $E_1 = \{(1, 8), (1, 17), (1, 19), (2, 4), (2, 6), (2, 17), (3, 7), (3, 12), (4, 10), (4, 14), (5, 18), (6, 16), (7, 20), (8, 20), (9, 17), (12, 18), (14, 20)\}$, $V_2 = \{13, 15\}$, $E_2 = \{(13, 15)\}$, $V_3 = \{11\}$, and $E_3 = \emptyset$. Because Γ is not connected, and thus this system is not controllable. The controllable submanifold is identified by the sets of vertices V_1, V_2, V_3 of the connected subgraphs, which is the integral manifold of the involutive distribution $\Delta = \text{span}\{\Omega_{ij}X : i, j \in V_1\} \oplus \text{span}\{\Omega_{ij}X : i, j \in V_2\}$. The connected components $\Gamma_i, i = 1, 2, 3$, can be efficiently computed using graph search algorithms, e.g., the depth first search algorithm [3]. Note that using the LARC to examine controllability of this system of dimension 190 requires generating a large number of Lie brackets, which is computationally expensive. Our new method for computing controllability over graphs using permutations provides an efficient and transparent way to understand the degree of controllability for bilinear systems.

1.3 Controllability of Systems on Euclidean Groups

We extended the symmetric group method to study broader classes of bilinear systems, including systems defined on non-compact Lie groups, e.g., on the special Euclidean group, $\text{SE}(n)$. The main idea for analyzing controllability of systems on $\text{SE}(n)$ was to (1) decompose the system on $\text{SE}(n)$ into the rotational and translational components, and (2) map Lie bracket operations of the vector fields governing the system dynamics to permutation multiplications on a symmetric group, so that controllability and the controllable submanifold can be characterized in terms of the orbits resulting from the symmetric group S_n action on a finite set containing n elements.

Decomposition of the System on $\text{SE}(n)$. Consider the system defined on $\text{SE}(n)$ of the form,

$$\begin{aligned} \frac{d}{dt} \begin{bmatrix} X(t) & x(t) \\ 0 & 1 \end{bmatrix} &= \left(\sum_{s=1}^{m_1} u_s(t) \begin{bmatrix} \Omega_{i_s j_s} & 0 \\ 0 & 0 \end{bmatrix} + \sum_{l=1}^{m_2} v_l(t) \begin{bmatrix} 0 & e_{k_l} \\ 0 & 0 \end{bmatrix} \right) \begin{bmatrix} X(t) & x(t) \\ 0 & 1 \end{bmatrix}, \\ (x(0), X(0)) &= (0, I), \end{aligned} \tag{2}$$

where $\Omega_{i_s j_s} \in \mathcal{B}$ is a basis element of $\mathfrak{so}(n)$, e_{k_l} is the k_l -th standard basis vector of \mathbb{R}^n , and $u_s(t), v_l(t) \in \mathbb{R}$ are piecewise constant control functions for all $s = 1, \dots, m_1$ and $l = 1, \dots, m_2$. Because $\text{SE}(n)$ contains $\text{SO}(n)$ and \mathbb{R}^n as Lie subgroups, the system in (2) can be decomposed into two subsystems on $\text{SO}(n)$ and \mathbb{R}^n , respectively, as

$$\dot{X}(t) = \left[\sum_{s=1}^{m_1} u_s(t) \Omega_{i_s j_s} \right] X(t), \quad X(0) = I, \quad (3)$$

$$\dot{x}(t) = \left[\sum_{s=1}^{m_1} u_s(t) \Omega_{i_s j_s} \right] x(t) + \sum_{l=1}^{m_2} v_l(t) e_{k_l}, \quad x(0) = 0, \quad (4)$$

representing the rotational and translational dynamics of the system in (2), respectively. We then derived the necessary and sufficient controllability condition for the system defined on $\text{SE}(n)$ by analyzing its rotational component on $\text{SO}(n)$ and translational component on \mathbb{R}^n .

Theorem 2 *A system defined on $\text{SE}(n)$ as in (2) is controllable if and only if its rotational component in (3) and translational component in (4) are controllable on $\text{SO}(n)$ and \mathbb{R}^n , respectively.*

Note that controllability of the rotational component modeled in (3), a system defined on $\text{SO}(n)$, was characterized in terms of the length of permutation orbits [1].

2 Computational Optimal Ensemble Control

2.1 Iterative Methods for Optimal Control of Nonlinear Ensemble Systems

Optimal control of bilinear systems has been a well-studied subject in the area of mathematical control. However, due to the lack of principled control strategies, solving emerging optimal control problems involving an ensemble of nearly identical bilinear systems remains a grand challenge. Through this grant support, we developed an iterative method to effectively and systematically solve optimal ensemble control problems. Our main idea was to represent the nonlinear ensemble system as a time-varying linear ensemble system at each iteration and then solve the resulting linear problem in an iterative manner. We examined the convergence of the developed iterative procedure and posed optimality conditions for the convergent solution to converge to the optimal solution of the original nonlinear problem. We also demonstrated the applicability of this method through the design of optimal pulses for broadband excitation of a population of nuclear spins in nuclear magnetic resonance spectroscopy and imaging [2, 4, 5].

Specifically, we considered the quadratic optimal control problem involving a nonlinear ensemble system with a fixed-endpoint or a free-endpoint constraint. We derived the convergence conditions of the iterative algorithm for both cases [4, 5] based on the fixed-point theorem by constructing a contractive iterative procedure. For the optimal control problem with a fixed-endpoint constraint, controllability of the system is required and the eigenvalues of the control weight matrix have to be sufficiently large in order to guarantee the contraction, and thus the convergence. For the case in which a free-endpoint constraint is posed, in addition to the condition on the magnitude of the eigenvalues of the control weight matrix as in the fixed-endpoint problem, special relations between the entries of the contraction matrix are required to guarantee convergence [5]. A practical pulse design problem in magnetic resonance is illustrated below in Example 3.

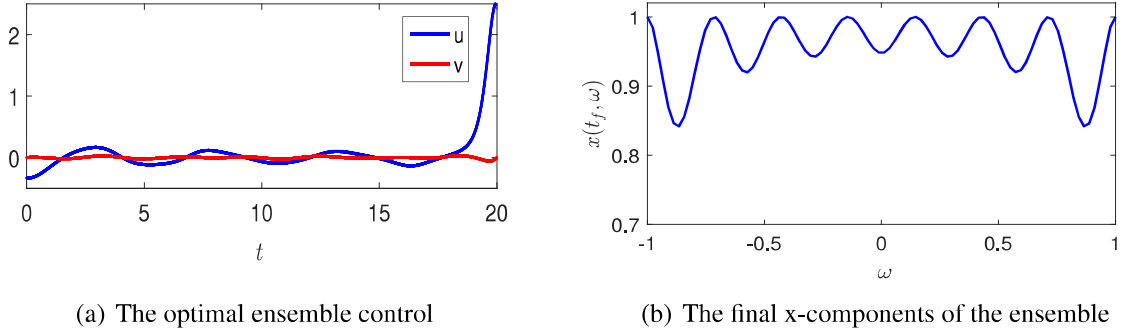


Figure 2: (a) The optimal ensemble control that steers an ensemble of Bloch systems with $\omega \in [-1, 1]$ from $X_0(\omega) = (0, 0, 1)^T$ to a neighborhood of $X_d(\omega) = (1, 0, 0)^T$. The weighted matrix $R = I_3$. (b) The final states $X(20, \omega)$ for 81 spin systems (blue) with their frequencies uniformly spaced within $[-1, 1]$ following the control displayed in (a).

Example 3 (Broadband Excitation of Two-Level Systems) Designing an optimal pulse that excites a collection of two-level systems is an essential control task that enables various applications in quantum science and technology [6, 7]. The dynamics of a two-level system obeys the Bloch equations, which forms a bilinear control system evolving on a sphere, given by

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 & -\omega & u_1 \\ \omega & 0 & -u_2 \\ -u_1 & u_2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad (5)$$

where $X = (x_1, x_2, x_3)^T$ denotes the bulk magnetization of the spins, ω denotes the Larmor frequency of the spins, and u_1 and u_2 are the radio-frequency (RF) fields applied on the y and the x direction, respectively [8]. A typical problem in quantum control is to develop a broadcast control field, the so-called broadband pulse, driving an ensemble of systems as modeled in (5) with $\omega \in [\omega_1, \omega_2]$ from the equilibrium state $X(0, \omega) = X_0(\omega) = (0, 0, 1)^T$ as close as possible to a desired excited state, e.g., $X_d(\omega) = (1, 0, 0)^T$ at a specified time t_f , with minimum energy [6].

We apply the iterative method described above [5] to design a broadband excitation ($\pi/2$) pulse that minimizes the cost functional $J = \frac{1}{2} \int_0^{t_f} u^T(t) R u(t) dt + J_E$, where $u = (u_1, u_2)^T$, the terminal cost $J_E = \int_{-1}^1 [X(t_f, \omega) - X_d(\omega)]^T [X(t_f, \omega) - X_d(\omega)] d\omega$, and $t_f = 20$. Figure 2(a) shows the derived broadband pulse with $R = I_3$, the 3×3 identity matrix. The performance, interpreted by the x -components of the final states, is displayed in Figure 2(b). The iterative algorithm converges in 207 iterations given the stopping criterion $\|X^{(k+1)} - X^{(k)}\| < 10^{-4}$, without requiring any numerical optimization.

3 Exact Broadband Excitation of Two-Level Systems

Designing accurate and high-fidelity broadband pulses is an essential component in conducting quantum experiments across fields from protein spectroscopy to quantum optics. However, constructing exact and analytic broadband pulses remains unsolved due to the nonlinearity and complexity of the underlying spin system dynamics. Through this grant support, we established a nontrivial dynamic connection between nonlinear spin and linear spring systems and show the surprising result that such nonlinear and complex pulse design problems are equivalent to designing

controls to steer linear harmonic oscillators under optimal forcing (see Figure 3). We further derived analytic broadband $\pi/2$ and π pulses that perform exact, or asymptotically exact, excitation and inversion over a defined bandwidth, and also with bounded amplitude [9]. This development opens up avenues for pulse sequence design and lays a foundation for understanding the control of two-level systems.

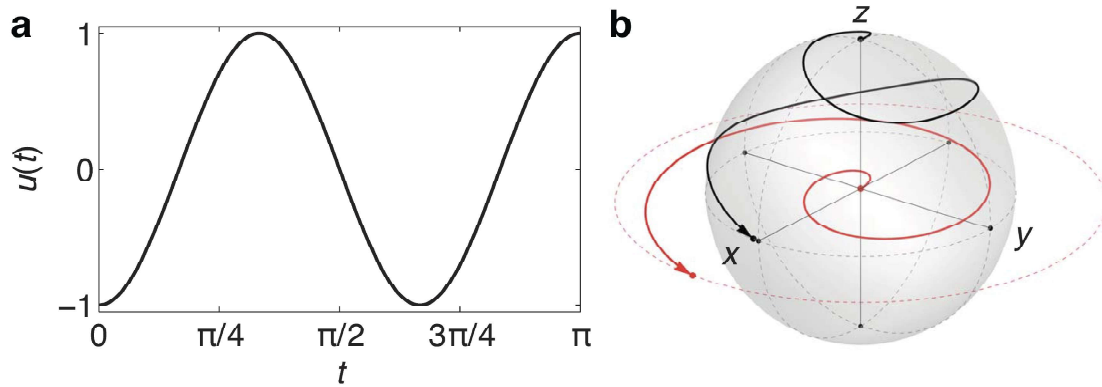


Figure 3: Exact excitation of single spins. (a) The minimum-energy control $u_{\pi/2}^*$ steering the spring from $X_0 = (0, 0)$ to $X_{\pi/2} = (\pi/2, 0)$, with (b) the corresponding trajectories of the spring (red) and spin (black) for $\omega = 3$ and $T = \pi$.

Personnel Supported

Jr-Shin Li, Principal Investigator

Gong Cheng, Postdoctoral Associate

Shuo Wang, Ph.D. Awarded 2018

Wei Zhang, Ph.D. Awarded 2019

Xin Ning, Current Graduate Student

Publications During the Grant Period

(partially or fully supported by this project)

Peer-Reviewed Articles

1. **J.-S. Li**, W. Zhang, and L. Tie, “On Separating Points for Ensemble Controllability,” *SIAM Journal on Control and Optimization* (accepted).
2. W. Miao, V. Narayanan, and **J.-S. Li**, “Parallel Residual Projection: A New Paradigm for Solving Linear Inverse Problems,” *Nature Scientific Reports* (accepted).
3. W. Zhang and **J.-S. Li**, “Analyzing Controllability of Bilinear Systems on Symmetric Groups: Mapping Lie Brackets to Permutations,” *IEEE Transactions on Automatic Control*, doi: 10.1109/TAC.2019.2963164, 2019.
4. S. Wang, E. Herzog, I. Z. Kiss, W. J. Schwartz, G. Bloch, L. Wang, and **J.-S. Li**, “Inferring Dynamic Topology for Decoding Spatiotemporal Structures in Complex Heterogeneous Networks,” *Proceedings of the National Academy of Sciences*, Vol. 115, No. 37, pp. 9300-9305, 2018.
5. W. Zhang and **J.-S. Li**, “On Controllability of Time-Varying Linear Ensemble Systems with Parameters in Unbounded Sets,” *Systems & Control Letters*, Vol. 118, pp. 94-100, 2018.
6. S. Wang and **J.-S. Li**, “Free-Endpoint Optimal Control of Inhomogeneous Bilinear Ensemble Systems,” *Automatica*, Vol. 95, pp. 306-315, 2018.
7. **J.-S. Li**, J. Ruths, and S. Glaser, “Exact Broadband Excitation of Two-Level Systems: Mapping Spins to Springs,” *Nature Communications*, Vol. 8, No. 1, pp. 446, 2017.
8. S. Wang and **J.-S. Li**, “Fixed-Endpoint Optimal Control of Bilinear Ensemble Systems,” *SIAM Journal on Control and Optimization*, Vol. 55, No. 5, pp. 3039-3065, 2017.

Peer-Reviewed Proceedings

1. W. Miao and **J.-S. Li**, “A Geometric Approach to Ensemble Control Analysis and Design,” *The 2020 American Control Conference*, Denver, Colorado, Jul. 2020.
2. X. Ning, W. Bomela, and **J.-S. Li**, “An Iterative Method for Optimal Control of Nonlinear Quadratic Tracking Problems,” *The 2020 American Control Conference*, Denver, Colorado, Jul. 2020.

3. W. Zhang, V. Narayanan, and **J.-S. Li**, “Robust Population Transfer for Coupled Spin Ensembles,” *58th IEEE Conference on Decision and Control*, Nice, France, Dec. 2019.
4. W. Zhang and **J.-S. Li**, “Symmetric Group Methods for Controllability Characterization of Bilinear Systems on Special Euclidean Groups,” *11th IFAC Symposium on Nonlinear Control Systems*, Vienna, Austria, Aug. 2019.
5. S. Wang and **J.-S. Li**, “Optimal Control of Bilinear Ensembles with Free-Endpoint Constraints,” *57th IEEE Conference on Decision and Control*, Miami Beach, Florida, Dec. 2018.
6. S. Zeng, W. Zhang, and **J.-S. Li**, “On the Computation of Control Inputs for Linear Ensembles,” *2018 American Control Conference*, Milwaukee, WI, Jun., 2018.
7. **J.-S. Li**, W. Zhang, and L. Wang, “Computing Controllability of Systems on $SO(n)$ over Graphs,” *56th IEEE Conference on Decision and Control*, Melbourne, Australia, Dec., 2017.
8. L. Tie, W. Zhang, S. Zeng, and **J.-S. Li**, “Explicit Input Signal Design for Stable Linear Ensemble Systems,” *IFAC 2017 World Congress*, Toulouse, France, Jul., 2017.
9. L. Tie, W. Zhang, S. Zeng, and **J.-S. Li**, “Controllability of Linear Ensemble Systems with Constant Drift and Linear Parameter Variation,” *1st IEEE Conference on Control Technology and Applications*, Kohala Coast, Hawaii, Aug., 2017.

Dissertations Supported By Grant

1. S. Wang, “Inference and Control of Dynamic Ensemble and Networked Systems,” PhD Thesis, Washington University in St. Louis, 2018.
2. W. Zhang, “Geometric Control of Ensemble Systems,” PhD Thesis, Washington University in St. Louis, 2019.

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