# **Research Experience for Undergraduates**

# Summer School on Mathematical Foundation of Data Science

June 6, 2022 --- July 15, 2022

Join Virtual Zoom Program

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Organized by Prof. Linyuan Lu, Prof. Wuchen Li, Prof. Qi Wang, Prof. Zhu Wang

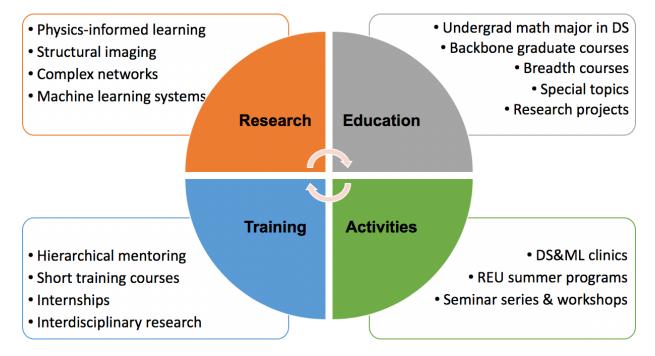


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# Section 1: Program Overview

This REU summer program is part of the NSF RTG project "**RTG: Mathematical Foundation** of Data Science at University of South Carolina", which aims to develop a multi-tier Research Training Program at the University of South Carolina (UofSC) designed to prepare the future workforce in a multidisciplinary paradigm of modern data science. The education and training models will leverage knowledge and experience already existing among the faculty and bring in new talent to foster mathematical data science expertise and research portfolios through a vertical integration of post-doctoral research associates, graduate students, undergraduate students, and advanced high school students. A primary focus of this project is to recruit and train U.S. Citizens, females, and underrepresented minority (URM) among undergraduate and graduate students, and postdocs through research led training in Data Science.



For more information on the NSF RTG project, please visit us at the following URL: https://sc.edu/study/colleges\_schools/artsandsciences/mathematics/my\_mathematics/rtg/index.php

The REU summer program of this year runs virtually from June 6 to July 15. In the first two weeks, we teach four short course modules in Mathematical Foundation of Data Science to prepare undergraduate students for the basic level of research projects. Starting from the third week, students will be divided into four groups to work on research projects. Some guest speakers are invited to give talks on the latest development in the Mathematical Foundation of Data Science. On the last day of the program, students will present their research findings.

# Section 2: Course Modulars

Course module 1: Linear Algebra

Instructor: Zhu Wang

Total hours: 10

Course Contents: Understand fundamental concepts in linear algebra, such as subspaces, projections, least squares, eigenvalue decomposition, and singular value decomposition, etc. Apply these concepts in solving the following central problems in linear algebra: n by n linear system Ax = b; m by n linear system Ax=b; n by n linear system  $Ax=\lambda x$ ; and m by n linear system  $Av=\sigma u$ . The connection of linear algebra with many applications will be discussed as well.

## Course module 2: Probability Theory and Optimization

Instructor: Wuchen Li

Total hours: 10

Course Contents: Study basic concepts in probability, statistics and optimizations: Probability distributions. Cumulative distributions. Moments. Mean. Variance. Covariance. Gaussian distribution. Samples. Fisher information matrix. Optimal conditions. Convexities. Gradient descent. Newton's method. Lagrange multiplier. KKT conditions.

## Course module 3: Introduction to Complex Networks

Instructor: Linyuan Lu

Total hours: 10

Course Contents:

Graphs, trees, subgraphs, graph isomorphisms, paths, walks, cycles, graph product, planar graphs, Euler formula, Kuratowski's theorem, adjacency matrix, spectrum of special graphs, combinatorial Laplacian, matrix tree theorem, normalized Laplacian, Power law graphs, random graphs, Erdos-Renyi random graphs, random graphs for power law graphs, spectrum of random graphs, transportation distance, Ricci curvature of graphs, Concetration of Lipschitz functions over positive curvature graphs.

## Course module 4: Machine Learning

Instructor: Qi Wang

Total hours: 10

Introduce the basic concept in machine learning, especially, to make a distinction between machine learning and optimization of an objective function or loss function. Discuss how to define the loss function using maximum likelihood estimation and Bayesian estimation. Introduce some basic machine learning algorithms such as logistic regression, k-means clustering, k-nearest neighbors, support vector machines, and decision trees. Introduce neural networks and deep learning: machine

learning using deep neural networks, including fully connected convolutional and recurrent neural networks. Discuss some deep learning methods of learning dynamical systems underlying given time-series.

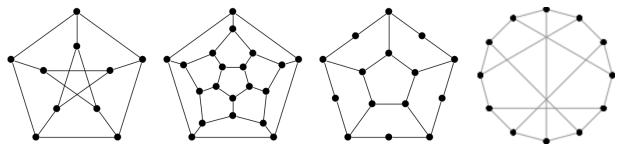
# Section 3: Research Projects

## Research projects in data-driven reduced order modeling

- 1. Dimensionality reduction in the parameter space. Study the classic linear dimensionality reduction approaches such as principal component analysis (PCA) and active subspace (AS), and recently developed deep learning methods for reducing the parameter space such as the nonlinear level-set learning (NLL) method. Compare their performances by considering high-dimensional function approximation problems and the numerical simulations of differential equations.
- 2. Data-driven reduced order modeling. Study the traditional model reduction approaches such as proper orthogonal decomposition (POD) or reduced basis method (RBM), and latest developments on deep learning-based nonlinear model reductions for overcoming the Kolmogorov barrier, such as those based on autoencoders. Compare their performances when simulating convection-dominated phenomena.

#### Research projects in complex graphs

- A graph G is k-existentially closed (k-e.c.) if each k-set of vertices can be extended in all of the possible 2<sup>k</sup> ways. Let m<sub>ec</sub>(k) be the minimum integer n such that a k-e.c. graph on n vertices exists. It is known that m<sub>ec</sub>(1) = 4, m<sub>ec</sub>(2) = 9 and 24 ≤ m<sub>ec</sub>(3) ≤ 28. Improve the bounds of m<sub>ec</sub>(3).
- 2. For each integer d, let F(d) (or f(d)) be the maximum integer n such that there exists a connected graph on n vertices with positive curvatures and maximum degree d (or d-regular graph respectively). It is known that  $c_1^d \le f(d) \le F(d) \le d^{c_2 d^2}$ . Determine the magnitude of F(d) and f(d).
- 3. Classify all planar d-regular graphs with positive curvatures.



Research projects in transport information learning

Study and understand natural gradient methods from information geometry and optimal transport. Implement the natural gradient algorithms for supervised learning problems, and unsupervised learning problems.

1. In one-dimensional space, compute and implement the Fisher and Wasserstein information matrix for Gaussian and exponential distributions. Then, implement the natural gradient methods to learn the parameters.

2. In discrete graphical models, compute and implement the Wasserstein natural gradient methods for learning parameters in Boltzmann machines.

3. In two-layer neural network models, compute and implement the Wasserstein information matrix and its induced natural gradient dynamics.

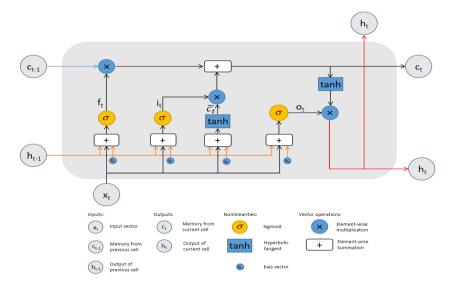
## Research projects in dynamical system learning using time-series data

Physical laws and mechanisms in most real-world systems are formulated as time evolutionary equations known as the dynamical systems, which are either given as a discrete or continuous system. Measurements or outputs of the systems are customarily given in time series. Either solving the dynamical systems for a given initial data or learning the dynamical system with given measured dynamical system data (solutions) are important data science and machine learning problems. Here are some simplified projects related to machine learning of dynamical systems.

1. Survey the machine learning methods for solving dynamical systems and then develop more efficient machine learning algorithms for solving simple dynamical systems exploiting the fundamental structure and property of the underlying dynamical systems.

2. Survey model learning using deep neural networks and develop dynamical system models for given time-series data. Example, 1. learning patient-specific metabolic panel dynamics for lung cancer patients with 10 patient data. 2. Design diagnostic models for septic patients based on patient's time series data, etc.

3. Explore the power of dimension reduction in deep learning of dynamical systems. Using order reduction methods such as encoder/decoder to transform time series data to low dimensional latent space and then develop approximate models in the latent space.



This is an LSTM unit for discrete dynamical systems.

# Section 3: Program Calendar

# Week 1 (Week of June 6-10): Short Courses

Day		Activity	Instructor/ moderator
9:00-10:00		Welcome and orientation	Lu
Mondoy	10:00-12:00	Linear Algebra	Z. Wang
Monday June 6	12:00-2:00	Lunch Break	
June 0	2:00-4:00	Probability Theory and Optimization	Li
	4:00-5:00	Recitation	Tom?
	9:00-11:00	Linear Algebra	Z. Wang
Tuesday	11:00-12:00	Math Programming Lab	
June 7	2:00-4:00	Introduction to Complex Networks	Lu
	4:00-5:00	Recitation	
	9:00-11:00	Linear Algebra and Deep Learning	Z. Wang
Wadnasday	11:00-12:00	Math Programming Lab	
Wednesday June 8	12:00-2:00	Lunch Break	
June 0	2:00-4:00	Probability Theory and Optimization	Li
	4:00-5:00	Recitation	Tom?
	9:00-11:00	Linear Algebra	Z. Wang
Thursday	11:00-12:00	Math Programming Lab	
June 9	12:00-4:00	Lunch Break	
June y	2:00-4:00	Introduction to Complex Networks	Lu
	4:00-5:00	Recitation	Brooks
	9:00-11:00	Linear Algebra	Z. Wang
Friday	11:00-12:00	Math Programming Lab	Brooks
Friday June 10	12:00-2:00	Lunch Break	
June 10	2:00-4:00	Probability Theory and Optimization	Li
	4:00-5:00	Social Activity Hour	Megan

# Week 2 (Week of June 13-17): Short Courses

]	Day	Activity	Instructor/ moderator
	9:00-11:00	Deep Learning	Q. Wang
Monday	11:00-12:00	Math Programming Lab	
June 13	12:00-2:00	Lunch Break	
	2:00-4:00	Introduction to Complex Networks	Lu
	4:00-5:00	Recitation	Thompson

	9:00-11:00	Deep Learning	Q. Wang
T	11:00-12:00	Math Programming Lab	
Tuesday June 14	12:00-2:00	Lunch Break	
Julie 14	2:00-4:00	Probability Theory and Optimization	Li
	4:00-5:00	Recitation	Tom?
	9:00-11:00	Deep Learning	Q. Wang
Wednesday	11:00-12:00	Math Programming Lab	
Wednesday June 15	12:00-2:00	Lunch Break	
Julie 15	2:00-4:00	Introduction to Complex Networks	Lu
	4:00-5:00	Recitation	Brooks
	9:00-11:00	Deep Learning	Q. Wang
Thursday	11:00-12:00	Math Programming Lab	
Thursday June 16	12:00-2:00	Lunch Break	
Julie 10	2:00-4:00	Probability Theory and Optimization	Li
	4:00-5:00	Recitation	McKenzie
	9:00-11:00	Deep Learning	Q. Wang
Estiture	11:00-12:00	Math Programming Lab	Brooks
Friday June 17	12:00-2:00	Lunch Break	
Juie 17	2:00-4:00	Introduction to Complex Networks	Lu
	4:00-5:00	Social Activity Hour	Megan

Week 3 (Week of June 20-24): Introduction of projects,	, group discussions on research projects,
and guest lectures in data sciences	

	Day	Activity	Instructor/ moderator
Monday	9:00-12:00	Project introduction	Professors
June 20	3:00-5:00	Grouping students into parallel discussions	
	9:00-10:00	Parallel research sessions	GAs
Tuesday	10:00-12:00	Self-research time	
June 21	2:00-3:00	Mentors' Office hours	Professors
	3:00-5:00	Self-research time	
	9:00-10:00	Parallel research sessions	
Wednesday	10:00-12:00	Self-research time	
June 22	2:00-3:00	Guest lecture	
	3:00-5:00	Parallel research sessions	
	9:00-10:00	Parallel research sessions	
Thursday	10:00-12:00	Self-research time	
June 23	2:00-3:00	Mentors' Office hours	Professors
	3:00-5:00	Self-research time	
Friday	9:00-12:00	Parallel and joint research sessions	All

June 24	2:00-4:00	Social Activity Hour	McKay

# Week 4 (Week of June 27 - July 1): Introduction of projects, group discussions on research projects, and guest lectures in data sciences

	Day	Activity	Instructor/ moderator
	9:00-10:00	Parallel research sessions	GAs
Monday	10:00-12:00	Self-research time	
June 27	2:00-3:00	Guest lecture	
	3:00-5:00	Parallel research sessions	GAs
	9:00-10:00	Parallel research sessions	GAs
Tuesday	10:00-12:00	Self-research time	
June 28	2:00-3:00	Mentors' Office hours	
	3:00-5:00	Self-research time	
	9:00-10:00	Parallel research sessions	
Wednesday	10:00-12:00	Self-research time	GAs
June 29	2:00-3:00	Guest lecture	
	3:00-5:00	Parallel research sessions	
	9:00-10:00	Parallel research sessions	
Thursday	10:00-12:00	Self-research time	GAs
June 30	2:00-3:00	Mentors' Office hours	
	3:00-5:00	Self-research time	
Eniders	9:00-12:00	Parallel and joint research sessions	All
Friday	2:00-4:00	Social Activity Hour	McKay
July 1			

Week 5 (Week of July 4-8): Introduction of projects, group discussions on research projects, and guest lectures in data sciences

	Day	Activity	Instructor/ moderator
Monday July 4	Holiday	No Activity	
	9:00-10:00	Parallel research sessions	
Tuesday	10:00-12:00	Self-research time	
July 5	2:00-3:00	Mentors' Office hours	
	3:00-5:00	Parallel research sessions	
Wednesday	9:00-10:00	Parallel research sessions	

July 6	10:00-12:00	Self-research time	
	2:00-3:00	Guest lecture	
	3:00-5:00	Parallel research sessions	
	9:00-10:00	Parallel research sessions	
Thursday	10:00-12:00	Self-research time	
July 7	2:00-3:00	Mentors' Office hours	
	3:00-5:00	Parallel research sessions	
E.d.	9:00-12:00	Parallel and joint research sessions	
Friday July 8	2:00-4:00	Social Activity Hour	МсКау
July o			

# Week 6 (Week of July 11-15): Introduction of projects, group discussions on research projects, and guest lectures in data sciences

	Day	Activity	Instructor/ moderator
	9:00-10:00	Parallel research sessions	
Monday	10:00-12:00	Self-research time	
July 11	2:00-3:00	Guest lecture	
	3:00-5:00	Parallel research sessions	
	9:00-10:00	Parallel research sessions	
Tuesday	10:00-12:00	Self-research time	
July 12	2:00-3:00	Mentors' Office hours	
	3:00-5:00	Self-research time	
	9:00-10:00	Parallel research sessions	
Wednesday	10:00-12:00	Self-research time	
July 13	2:00-3:00	Guest lecture	
	3:00-5:00	Parallel research sessions	
	9:00-10:00	Parallel research sessions	
Thursday	10:00-12:00	Self-research time	
July 14	2:00-3:00	Mentors' Office hours	
	3:00-5:00	Self-research time	
Friday	10:00-11:00	Plenary lecture	
July 15	11:00-12:00	Plenary lecture	
	1:00-3:00	Group Reporting and presentation	
	3:00-4:00	Assessment	

Confirmed speakers:

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