## Research Experience for Undergraduates

Summer School on Mathematical Foundation of Data Science

June 6, 2022 --- July 15, 2022<br>Join Virtual Zoom Program<br>https://us06web.zoom.us/j/84400970067?pwd=R2Rpb2ZnSldESmJGT2NzMW1XMINpdz09

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UNIVERSITY OF
South Carolina

Organized by
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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 $A x=b ; m$ by $n$ linear system $A x=b ; n$ by $n$ linear system $A x=\lambda x$; and $m$ by $n$ linear system $\mathrm{Av}=\sigma \mathrm{u}$. 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

1. A graph G is k -existentially closed ( k -e.c.) if each k -set of vertices can be extended in all of the possible $2^{k}$ ways. Let $m_{e c}(k)$ be the minimum integer n such that a k-e.c. graph on n vertices exists. It is known that $m_{e c}(1)=4, m_{e c}(2)=9$ and $24 \leq m_{e c}(3) \leq 28$. Improve the bounds of $m_{e c}$ (3).
2. For each integer d , let $\mathrm{F}(\mathrm{d})($ or $\mathrm{f}(\mathrm{d})$ ) be the maximum integer n such that there exists a connected graph on n vertices with positive curvatures and maximum degree d (or dregular graph respectively). It is known that $c_{1}^{d} \leq f(d) \leq F(d) \leq d^{c_{2} d^{2}}$. 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 |
| :---: | :---: | :---: | :---: |
| Monday June 6 | 9:00-10:00 | Welcome and orientation | Lu |
|  | 10:00-12:00 | Linear Algebra | Z. Wang |
|  | 12:00-2:00 | Lunch Break |  |
|  | 2:00-4:00 | Probability Theory and Optimization | Li |
|  | 4:00-5:00 | Recitation | Tom? |
| Tuesday June 7 | 9:00-11:00 | Linear Algebra | Z. Wang |
|  | 11:00-12:00 | Math Programming Lab |  |
|  | 2:00-4:00 | Introduction to Complex Networks | Lu |
|  | 4:00-5:00 | Recitation |  |
| Wednesday June 8 | 9:00-11:00 | Linear Algebra and Deep Learning | Z. Wang |
|  | 11:00-12:00 | Math Programming Lab |  |
|  | 12:00-2:00 | Lunch Break |  |
|  | 2:00-4:00 | Probability Theory and Optimization | Li |
|  | 4:00-5:00 | Recitation | Tom? |
| Thursday June 9 | 9:00-11:00 | Linear Algebra | Z. Wang |
|  | 11:00-12:00 | Math Programming Lab |  |
|  | 12:00-4:00 | Lunch Break |  |
|  | 2:00-4:00 | Introduction to Complex Networks | Lu |
|  | 4:00-5:00 | Recitation | Brooks |
| Friday June 10 | 9:00-11:00 | Linear Algebra | Z. Wang |
|  | 11:00-12:00 | Math Programming Lab | Brooks |
|  | 12:00-2:00 | Lunch Break |  |
|  | 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 |  |  | Instructor/ <br> moderator |
| :---: | :---: | :--- | :--- |
| Monday <br> June 13 | $9: 00-11: 00$ | Deep Learning | Q. Wang |
|  | $11: 00-12: 00$ | Math Programming Lab |  |
|  | $12: 00-2: 00$ | Lunch Break | Lu |
|  | $2: 00-4: 00$ | Introduction to Complex Networks | Thompson |
|  | $4: 00-5: 00$ | Recitation |  |


| Tuesday June 14 | 9:00-11:00 | Deep Learning | Q. Wang |
| :---: | :---: | :---: | :---: |
|  | 11:00-12:00 | Math Programming Lab |  |
|  | 12:00-2:00 | Lunch Break |  |
|  | 2:00-4:00 | Probability Theory and Optimization | Li |
|  | 4:00-5:00 | Recitation | Tom? |
| Wednesday June 15 | 9:00-11:00 | Deep Learning | Q. Wang |
|  | 11:00-12:00 | Math Programming Lab |  |
|  | 12:00-2:00 | Lunch Break |  |
|  | 2:00-4:00 | Introduction to Complex Networks | Lu |
|  | 4:00-5:00 | Recitation | Brooks |
| Thursday June 16 | 9:00-11:00 | Deep Learning | Q. Wang |
|  | 11:00-12:00 | Math Programming Lab |  |
|  | 12:00-2:00 | Lunch Break |  |
|  | 2:00-4:00 | Probability Theory and Optimization | Li |
|  | 4:00-5:00 | Recitation | McKenzie |
| Friday June 17 | 9:00-11:00 | Deep Learning | Q. Wang |
|  | 11:00-12:00 | Math Programming Lab | Brooks |
|  | 12:00-2:00 | Lunch Break |  |
|  | 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 June 20 | 9:00-12:00 | Project introduction | Professors |
|  | 3:00-5:00 | Grouping students into parallel discussions |  |
| Tuesday June 21 | 9:00-10:00 | Parallel research sessions | GAs |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Mentors' Office hours | Professors |
|  | 3:00-5:00 | Self-research time |  |
| Wednesday June 22 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Guest lecture |  |
|  | 3:00-5:00 | Parallel research sessions |  |
| Thursday June 23 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time |  |
|  | 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 |
| :---: | :---: | :---: | :---: |
| Monday June 27 | 9:00-10:00 | Parallel research sessions | GAs |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Guest lecture |  |
|  | 3:00-5:00 | Parallel research sessions | GAs |
| Tuesday June 28 | 9:00-10:00 | Parallel research sessions | GAs |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Mentors' Office hours |  |
|  | 3:00-5:00 | Self-research time |  |
| Wednesday June 29 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time | GAs |
|  | 2:00-3:00 | Guest lecture |  |
|  | 3:00-5:00 | Parallel research sessions |  |
| Thursday June 30 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time | GAs |
|  | 2:00-3:00 | Mentors' Office hours |  |
|  | 3:00-5:00 | Self-research time |  |
| Friday July 1 | 9:00-12:00 | Parallel and joint research sessions | All |
|  | 2:00-4:00 | Social Activity Hour | McKay |
|  |  |  |  |

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

| Day |  | Activity | Instructor/ <br> moderator |
| :---: | :---: | :--- | :--- |
| Monday <br> July 4 | Holiday | No Activity |  |
| Tuesday <br> July 5 | $9: 00-10: 00$ | Parallel research sessions |  |
|  | $10: 00-12: 00$ | Self-research time |  |
|  | $2: 00-3: 00$ | Mentors' Office hours |  |
| Wednesday | 9:00-5:00 | 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 |  |
| Thursday <br> July 7 | $9: 00-10: 00$ | Parallel research sessions |  |
|  | $10: 00-12: 00$ | Self-research time |  |
|  | $2: 00-3: 00$ | Mentors' Office hours |  |
|  | $3: 00-5: 00$ | Parallel research sessions |  |
|  | $9: 00-12: 00$ | Parallel and joint research sessions |  |
|  | $2: 00-4: 00$ | Social Activity Hour | McKay |

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 |
| :---: | :---: | :---: | :---: |
| Monday July 11 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Guest lecture |  |
|  | 3:00-5:00 | Parallel research sessions |  |
| Tuesday <br> July 12 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Mentors' Office hours |  |
|  | 3:00-5:00 | Self-research time |  |
| Wednesday July 13 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Guest lecture |  |
|  | 3:00-5:00 | Parallel research sessions |  |
| Thursday July 14 | 9:00-10:00 | Parallel research sessions |  |
|  | 10:00-12:00 | Self-research time |  |
|  | 2:00-3:00 | Mentors' Office hours |  |
|  | 3:00-5:00 | Self-research time |  |
| Friday July 15 | 10:00-11:00 | Plenary lecture |  |
|  | 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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