Research Experience for Undergraduates
Summer School on Mathematical Foundation of Data Science

June 3, 2024 --- July 12, 2024

LeConte 101
Department of Mathematics
University of South Carolina
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Organized by:

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Prof. Peter Binev,
Prof. Xinfeng Liu,
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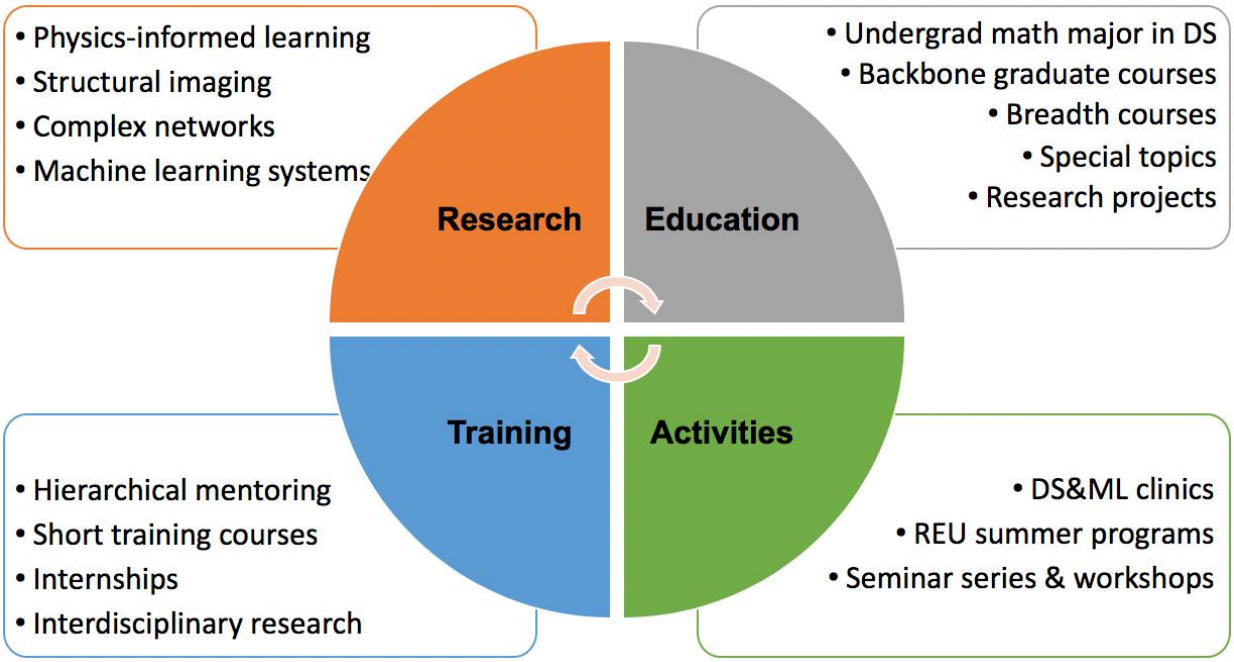
Section 1: Program Overview

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 in-person and virtually from June 6 to July 15. Starting from the first week, students will be divided into several 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: Research Projects

2.1 - Developing AI tools for Scanning Tunneling Microscopy (STM)
(Advisor: Peter Binev)

Scanning Tunneling Microscopy (STM) is used to observe the atomic structure of the surface of the materials. Data acquisition tasks in STM usually require a human-in-the-loop component to constantly evaluate the structural phenomena on the surface and navigate towards the ones of interests. Using AI to take care of most of these evaluations would allow a rapid increase in materials research. The first step in achieving this is the development of data processing tools and deep learning routines to recognize the usual structures and classify them. The research project involves investigating and training deep learning autoencoders to extract pattern information from artificial and real data, as well as using this information to advance different image processing tasks.

2.2 - Neural network projected schemes for Wasserstein gradient flows
(Advisor: Wuchen Li)

We develop a numerical analysis and computation of neural network projected schemes for approximating Wasserstein type gradient flows. We approximate the Lagrangian mapping functions of gradient flows by the class of two-layer neural network functions with ReLU (rectified linear unit) activation functions or tanh activation functions. The numerical scheme is based on a projected gradient method, namely the Wasserstein natural gradient, where the projection is constructed from the mapping spaces onto the neural network parameterized mapping space. We establish theoretical guarantees for the performance of the neural projected dynamics. Numerical examples, including gradient drift Fokker-Planck equations, porous medium equations, and Keller-Segel models, will be used to test the accuracy of neural network projected dynamics.

2.3 - Computational studies for Her2 signaling pathway on cancer cell stemness
(Advisor: Xinfeng Liu)

Solid tumors exhibit significant heterogeneity in composition. Among the diverse cell types present, cancer stem cells (CSCs) stand out as highly tumorigenic and are often resistant to conventional chemotherapeutic agents, contributing to tumor recurrence. Therefore, gaining insights into tumor growth kinetics is crucial for devising effective cancer treatment strategies. In this project, we will employ mathematical modeling coupled with computational analysis to investigate Her2 signaling dynamics, focusing on the interplay between CSCs and non-stem cancer cells. Specifically, we will explore how the overexpression of the oncogene HER2, regulated by MAP kinase signaling pathways and interleukin-1 (IL1) regulations, influences tumor progression. The utilization of mathematical modeling and computational simulations holds significant promise for advancing drug development efforts aimed at efficiently targeting cancer tumors.

2.4 - Data-Driven Reduced-Order Modeling
(Advisor Zhu Wang)

Modern model-based optimization and control problems in computational science and engineering often involve numerical simulations of parameterized governing systems. For such problems, high-fidelity models, although precise, are usually computationally too expensive to meet the practical requirement on sufficient efficiency. Therefore, model order reduction has been developed to construct from data low-

dimensional models to replace the high-fidelity, high-dimensional models for fast simulations. In this project, we will investigate reduced order models built on different subspaces from linear, quadratic to nonlinear ones.

2.5 - Research projects in Graph Theory (Advisor: Linyuan Lu)

Project a: Deep Learning

In the realm of graph theory, the quest often revolves around identifying extremal objects while adhering to specific constraints. These elusive objects exist within an expansive search space, rendering traditional heuristic methods ineffective. However, recent successes lie in the application of Deep Learning techniques to address such challenges. Notably, these techniques have been instrumental in constructing some large Ramsey Graphs and extremal graphs based on specific graph parameters. This project aims to explore and tackle graph-theoretic problems using deep learning methodologies.

Project b: Spectral graph theory

Spectral graph theory is an elegant subfield of graph theory that leverages the eigenvalues and eigenvectors of matrices naturally associated with graphs for their study. Over the past few decades, spectral graph theory has produced a wealth of results and found applications across diverse mathematical domains. In this project, we will delve into specific problems and conjectures within this fascinating field.

Section 3: Program Calendar

Week 1

Day		Activity	Moderator
Monday June 3	9:00-12:00	Introduction to the REU program	
	12:00-2:00	Lunch break	
	2:00-5:00	Group assignments	
Tuesday June 4	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Wednesday June 5	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Thursday June 6	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Friday June 7	9:00-10:30	Parallel research sessions	
	10:30-12:00	Group presentation	
	12:00-2:00	Lunch break	
	2:00-5:00	Social/free time	

Week 2

Day		Activity	Moderator
Monday June 10	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Tuesday June 11	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Wednesday June 12	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Thursday June 13	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Friday June 14	9:00-10:30	Parallel research sessions	
	10:30-12:00	Group presentation	
	12:00-2:00	Lunch break	
	2:00-5:00	Social/free time	

Week 3

Day		Activity	Moderator
Monday June 17	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Tuesday June 18	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Wednesday June 19	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Thursday June 20	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Friday June 21	9:00-10:30	Parallel research sessions	
	10:30-12:00	Group presentation	
	12:00-2:00	Lunch break	
	2:00-5:00	Social/free time	

Week 4

Day		Activity	Moderator
Monday June 24	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Tuesday June 25	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Wednesday June 26	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Thursday June 27	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Friday June 28	9:00-10:30	Parallel research sessions	
	10:30-12:00	Group presentation	
	12:00-2:00	Lunch break	
	2:00-5:00	Social/free time	

Week 5

Day		Activity	Moderator
Monday July 1	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Tuesday July 2	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Wednesday July 3	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Thursday July 4	Holiday	No activities	
Friday July 5	Holiday	No activities	

Week 6

Day		Activity	Moderator
Monday July 8	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Tuesday July 9	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Wednesday July 10	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Thursday July 11	9:00-12:00	Parallel research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Parallel research sessions	
Friday July 12	9:00-10:30	Parallel research sessions	
	10:30-12:00	Joint research sessions	
	12:00-2:00	Lunch break	
	2:00-5:00	Final presentations and group photo	

Section 4: Contact Information

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