






# EDISON MUCLLARI

## Curriculum Vitae

### Personal Information

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### Education

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<b>Doctor of Philosophy in Mathematics</b> UNIVERSITY OF KENTUCKY   Lexington, KY DISSERTATION ADVISOR: Qiang Ye, Ph.D. RESEARCH AREA: Deep Learning	MAY 2024
<b>Master of Science in Mathematics</b> UNIVERSITY OF TIRANA   Tirana, Albania ADVISOR: Artur Baxhaku, Ph.D. MASTER THESIS: “ <i>Factorization of numbers and its applications in asymmetric cryptography</i> ” INSTITUTIONAL HONORS: <i>Excellent Student</i>	JULY 2018
<b>Bachelor in Mathematics</b> UNIVERSITY OF TIRANA   Tirana, Albania INSTITUTIONAL HONORS: <i>Excellent Student</i>	JULY 2016

### Research Interest

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Numerical Analysis, Natural Language Processing, Computer Vision, Optimal Transport, Drug Design, Molecular Prediction & Model Predictive Control

### Employment

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<b>Ph.D. Research Intern</b> SRI INTERNATIONAL   Princeton, NJ	MAY 2023 - AUG. 2023
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- Worked under the direct supervision of the Senior Technical Manager at Edge Computing Group and a Distinguished Computer Scientist at SRI International
- Enhanced the Transformer architecture by introducing a new recurrent method, creating a Scalable Transformer that outperformed Transformer XL and Recurrent Memory Transformer, resulting in a more efficient and effective design with a smaller model across various datasets like Word PTB, Wiki-Text 103, enwiki8, text8, and one billion words
- Incorporated the learning ability into the position encoding of Hyperdimensional Computing (HD Computing), opening up numerous opportunities in this field
- Collaborated on optimizing Matrix-Matrix and Matrix-Vector Multiplication by focusing on reducing the number of multiplications and improving computation time

## Research Assistant in Department of Mathematics

MAY 2021 - PRESENT

UNIVERSITY OF KENTUCKY (UKY) | Lexington, KY

- Explored the behaviour of language models, specifically the Gated Recurrent Units (GRU) architecture, and analyzed the gradient impact during the training process
- Proposed the usage of orthogonal matrices to prevent exploding gradient problems and enhance long-term memory, where the employed Neumann series-based Scaled Cayley transformation speed up training and achieve significant improvement over many traditional language models
- Introduced Neumann-Cayley Orthogonal Gated Recurrent Units (NC-GRU) as the cells building the AutoEncoder to enable the creation of neural fingerprints, where the proposed architecture results in a more stable training, reliable molecular fingerprints and extensive numerical experiments show that NC-GRU AutoEncoder is a state-of-the-art framework in many molecular prediction benchmarks
- Successfully integrated the combination of Gated Recurrent Units (GRU) and Generative Adversarial Networks (GAN) to model the extremely complex forward process to generate the observed topside welding image from eight consecutive backside image where the presented results show an improved generator architecture due to the GRU mechanism to discriminate bottom images per timing/order
- Implemented a Machine Learning technique that can predict the best time to extubate a preterm baby that need mechanical ventilation in their early days of life considering that extubation failure happens quite often and the babies are required to be reintubated

## Teaching Assistant and Primary Instructor

AUG. 2019 - PRESENT

UNIVERSITY OF KENTUCKY | Lexington, KY

- Lead interactive discussions about course materials for 60 undergraduate students to encourage collaboration, creating a more inclusive learning environment
- Instructed 15 undergraduate students in an intensive group studying approach to the standard calculus sequence and spent extra time each week with three problem-solving workshops emphasizing collaborative learnings and working closely with a motivated group of students with assistance from an undergraduate assistant
- Supervised the teaching methods of other graduate teaching assistants and provided feedbacks cultivating more effective pedagogy practices
- Designed the curriculum, prepared the lectures for the daily intensive summer class, helped to develop content such as writing or proofreading weekly quizzes, and actively checking in to make sure the students progress is going well
- Provided assistance to undergraduate students in person and/or online based on student need to answer questions or provide time to make up assignments resulting in students showing better understanding of the course material as demonstrated by improved quiz scores each week
- COURSES INCLUDE: Calculus I, II and III; Elementary Calculus and its Applications; Finite Math and Its Applications; Calculus I and II with Life Science Applications; Ordinary Differential Equations

## Doctoral Degree Progress

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### Qualifying Exam

MARCH 2021

TITLE: Cayley Orthogonal Gated Recurrent Units and its application in Bio-molecular data

ABSTRACT: Exploding/vanishing gradients have always been an issue in Gated Recurrent Units (GRU). In our proposed model, NC-GRU, we implement orthogonality using Cayley orthogonal matrices into the GRU gates. Based on the properties of the orthogonal matrices, NC-GRU is able to remember more information from the past. Combining this property with the ability of GRU to forget unnecessary information results in an improved model. Our experiments show that NC-GRU outperforms GRU, LSTM, RNN, scRNN in different tasks. Even after the introduction of Transformers, GRU is still heavily used in Drug Design. We also conducted experiments in Bio-Molecular Data and our numerical results show a state-of-the-art architecture in many benchmarks, including IGC50, LC50, logP and FreeSolv.

Passed Preliminary Exam in Numerical Analysis	Jan. 2021
Passed Preliminary Exam in Modern Algebra	JUNE 2020
Passed Preliminary Exam in Analysis	JUNE 2020

## Summer School and Workshop Experience

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Oxford Machine Learning Summer School, ML x Health | Virtual      AUG. 7 - 10, 2022 / JUNE 27 - 29, 2022

- Organised by AI for Global Goals and in partnership with CIFAR and the University of Oxford's Deep Medicine Program
- Covered 48 hours of lectures of advanced topics in ML theory and its applications in healthcare and medicine
- Accepted to and attended the OxML Health Track ONLINE
- Received the Certificate of Attendance

Workshop on Software and Applications of Numerical Nonlinear Algebra      MAY 31 - JUNE 2, 2022

- Organised by Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany
- Topic of this workshop is solving systems of polynomial equations using numerical algorithms. The participants learned to work with the software HomotopyContinuation.jl, so that they can use it for their own research problems. In addition, the workshop featured a series of lectures on the theory of numerical homotopy continuation, as well as contributed talks by Timothy Duff, Alex Heaton, Julia Lindberg and Maggie Regan
- Accepted to and attended the Virtual event - Videobroadcast

## Service and Outreach

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Graduate Student Congress Representative of the Mathematics Department at UKY	SEPT. 2023 - MAY 2024
Treasurer of the UKY chapter of Society for Industrial and Applied Mathematics (SIAM)	SEPT. 2022 - MAY 2023
Secretary of the SIAM UKY Chapter	SEPT. 2021 - MAY 2022
Graduate Student Colloquium Coordinator at the University of Kentucky (UKY)	SPRING 2021
Co-Coordinator of the UKY Mathematics Department Graduate Student Colloquium	FALL 2021
Peer Mentor of a Graduate Student at the University of Kentucky (UKY)	FALL 2020
University of Kentucky Julia Robinson Math Festival	NOV. 2019
Proctor at the Math Kangaroo Olympiad	MARCH 2018
Contributed to the coordination and execution of the Conference of Natural Sciences and Technology at University of Tirana	NOV. 2017

## Awards and Recognitions

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Fall 2024 Research Assistantship, NSF	Jan. 2024
Spring 2023 Research Assistantship, NSF	Oct. 2023
Research Assistantship, Math Department, UKY	2021 - PRESENT
Graduate Assistantship, Math Department, UKY	2019 - PRESENT
SIAM Certification for outstanding efforts and accomplishments of the UKY SIAM Chapter	AUG. 2023
Best Student, Master of Science of Mathematics, University of Tirana	2018
Outstanding Undergraduate Student, University-wide prize and scholarship, University of Tirana	2014-2016
Excellent Student, Selected by Prime Minister of Albania	2014

**Recurrent Transformer Project** | Princeton, NJ

MAY. 2023 - PRESENT

ADVISORS: Qiang Ye, Ph.D. and David Zhang, Ph.D.

COLLABORATION: Joint work with Zachary Daniels, Ph.D.

TITLE: Beyond Limits: Achieving Scalability with Recurrent Transformers

SUPPORT: Supported by SRI International and NSF under grants DMS-220831

**Improved Techniques for Welding GRU - GAN Training** | Redmond, WA

APR. 2023 - PRESENT

ADVISORS: YuMing Zhang, Ph.D. and Qiang Ye, Ph.D.

COLLABORATION: Joint work with Yue Cao, M.S.

TITLE: Modeling the Dynamics of Weld Pool Behavior using Generative Adversarial Network (GAN)

SUPPORT: Supported in part by NSF under grants No. 2024614 and DMS-2208314, the Institute for Sustainable Manufacturing, Department of Electrical and Computer Engineering, and Department of Mathematics at the University of Kentucky

**Novel Welding GRU - GAN Project** | University of Kentucky

DEC. 2022 - APRIL 2023

ADVISORS: YuMing Zhang, Ph.D. and Qiang Ye, Ph.D.

COLLABORATION: Joint work with Rui Yu, M.S. and Yue Cao, M.S.

TITLE: Do We Need a New Foundation to Use Deep Learning to Monitor Weld Penetration?

ABSTRACT: Deep learning has been successfully used to automate the modeling process that trains a network/model from a given experimental dataset to calculate the output directly using highdimensional complex raw data. However, the trained network is an inverse of the welding process (forward process) that produces the welding phenomena/measured raw data as the output with the penetration as the input of the forward process. Now the question is in addition to the current state of the weld penetration to be estimated if the forward process also has other inputs to determine its output. If it has, then the inverse model has to be constructed accordingly. This will call for a new foundation for deep learning-based monitoring of penetration. This letter proposed a novel innovative generative adversarial network (GAN) with GRU (Gated Recurrent Unit) in the generator, i.e., GRU-GAN, to model the extremely complex forward process to generate the observed topside welding image (output of the forward process) from the backside images (as comprehensive quantification of weld penetration). It is found that the produced topside welding image is not only determined by the current backside image but also by its history. A new foundation thus must be established to guide deep learning-based monitoring of weld penetration. The prediction model/network as an inverse model must be in compliance with the forward process that includes the history of the state of the weld penetration as its input.

SUPPORT: Supported in part by NSF under grants No. 2024614 and DMS-2208314, the Institute for Sustainable Manufacturing, Department of Electrical and Computer Engineering, and Department of Mathematics at the University of Kentucky

**Deep Learning in the Drug Discovery Project** | University of Kentucky

SEPT. 2021 - SEPT. 2022

ADVISORS: Duc Nguyen, Ph.D. and Qiang Ye, Ph.D.

COLLABORATION: Joint work with Vasily Zadorozhnyy, Ph.D.

TITLE: Novel Molecular Representations Using Neumann-Cayley Orthogonal Gated Recurrent Unit

**ABSTRACT:** Advances in Deep Neural Networks (DNNs) have made a very powerful machine learning method available to researchers across many fields of study, including the bio-medical and cheminformatics communities, where DNNs help to improve tasks such as protein performance, molecular design, drug discovery, etc. Many of those tasks rely on molecular descriptors for representing molecular characteristics in cheminformatics. Despite significant efforts and the introduction of numerous methods that derive molecular descriptors, quantitative prediction of molecular properties remains challenging. One widely used method of encoding molecule features into bit strings is molecular fingerprint. In this work, we propose using new Neumann-Cayley Gated Recurrent Units (NC-GRU) inside the Neural Nets encoder (AutoEncoder) to create neural molecular fingerprints, NC-GRU fingerprints. NC-GRU AutoEncoder introduces orthogonal weights into widely used GRU architecture, resulting in faster, more stable training, and more reliable molecular fingerprints. Integrating novel NC-GRU fingerprints and Multi-Task DNN schematics improves the performance of various molecular-related tasks such as toxicity, partition coefficient, lipophilicity, and solvation-free energy, producing state-of-the-art results on several benchmarks.

**SUPPORT:** Supported in part by NSF under grants DMS-1821144, DMS-2053284, and DMS-2151802

**Orthogonality Preserving Recurrent Nets** | University of Kentucky

AUG. 2021 - JULY 2022

**ADVISORS:** Duc Nguyen, Ph.D. and Qiang Ye, Ph.D.

**COLLABORATION:** Joint work with Edison Mucllari, M.S. and Cole Pospisil, M.S.

**TITLE:** Orthogonal Gated Recurrent Unit with Neumann-Cayley Transformation

**ABSTRACT:** In recent years, using orthogonal matrices has been shown to be a promising approach in improving Recurrent Neural Networks (RNNs) with training, stability, and convergence, particularly to control gradients. While Gated Recurrent Unit (GRU) and Long Short Term Memory (LSTM) architectures address the vanishing gradient problem by using a variety of gates and memory cells, they are still prone to the exploding gradient problem. In this work, we analyze the gradients in GRU and propose the usage of orthogonal matrices to prevent exploding gradient problems and enhance long-term memory. We study where to use orthogonal matrices and we propose a Neumann series-based Scaled Cayley transformation for training orthogonal matrices in GRU, which we call Neumann-Cayley Orthogonal GRU, or simply NC-GRU. We present detailed experiments of our model on several synthetic and real-world tasks, which show that NC-GRU significantly outperforms GRU as well as several other RNNs.

**SUPPORT:** Supported in part by NSF under grants DMS-1821144, DMS-2053284 and DMS-21518

## Invited/Conference Talks

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- International Conference on Automation Science and Engineering Aug. 26 - Aug. 30, 2023  
**TITLE:** Do we need a new foundation to use Deep Learning to monitor weld penetration?
- SRI International Intern Presentation Day AUG. 2023  
**TITLE:** Towards Trainable Deep Hyperdimensional Computing
- SRI International (Online) APRIL 2023  
**TITLE:** Novel Welding GRU-GAN architecture and Neumann-Cayley Orthogonal Gated Recurrent Units with Some Applications in Bio-molecular Data
- SIAM Conference on Computational Science and Engineering (CSE23) FEB. 26 - MARCH 3, 2023  
**TITLE:** Neumann-Cayley Orthogonal Gated Recurrent Units with Some Applications in Bio-molecular Data
- University of Kentucky Applied Math Seminar MARCH 2022  
**TITLE:** Cayley Orthogonal Gated Recurrent Units and its application in Bio-molecular data
- University of Kentucky Department of Mathematics Graduate Student Colloquium OCT. 2021  
**TITLE:** Optimal Transport, Monge Problem and Kantorovich Formulation
- University of Kentucky Department of Mathematics Graduate Student Colloquium MAY 2021  
**TITLE:** Convolutional Neural Networks with Applications
- Faculty of Natural Sciences in University of Tirana JULY 2018  
**TITLE:** Factorization of numbers and its applications in asymmetric cryptography

## Publications and Works-in-Progress

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1. **Edison Mucllari**, Zachary Daniels, David Zhang, Qiang Ye. Beyond Limits: Achieving Scalability with Recurrent Transformers. Investigation in progress, 2022.
2. **Edison Mucllari**, Yue Cao, Qiang Ye, YuMing Zhang. Modeling the Dynamics of Weld Pool Behavior using Generative Adversarial Network (GAN). Submitted to IEEE Robotics and Automation Letters
3. **Edison Mucllari**, Rui Yu, Yue Cao, Qiang Ye, YuMing Zhang. Do we need a new foundation to use Deep Learning to monitor weld penetration. IEEE Robotics and Automation Letters, 2023
4. **Edison Mucllari\***, Vasily Zadorozhnyy\*, Duc Nguyen, Qiang Ye. Novel Molecular Representations using Neumann-Cayley Orthogonal Gated Recurrent Unit. Journal of Chemical Information and Modeling, Volume 63, Issue 9, Pages 2603-2894, 2023 (\* - equal contribution)
5. **Edison Mucllari**, Vasily Zadorozhnyy, Cole Pospisil, Duc Nguyen, Qiang Ye. Orthogonal Gated Recurrent Unit with Neumann-Cayley Transformation. [arxiv.org/abs/2208.06496](https://arxiv.org/abs/2208.06496), 2022. Submitted to the Neural Computing and Applications (NCAA) Journal

## Languages and Computer Skills

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Languages:	English(fluent), Albanian(fluent), Italian(basic knowledge)
Programming languages:	PYTHON, BASH, C++, HTML/CSS, PHP, SWIFT, VB, PASCAL
Mathematical and statistical softwares:	Matlab, Mathematica, Maple, SAS, R, LaTeX, Audacity
Machine and Deep learning libraries:	NumPy, SciPy, CuPy, TensorFlow, PyTorch, Theano, Chainer