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Matt Raymond

ML + Computational Chemistry



Ann Arbor, MI

Ann Arbor, MI

08/20-04/22

08/22 - 04/26

Research
Interests

- Generative models for ab initio nanoparticle design
- Transfer learning for small nanochemical datasets
- Machine-learning-based surrogate modeling for computational nanochemistry
- Nonlinear multitask feature selection

Education

University of Michigan

Ph.D. Signal/Image Processing and Machine Learning

GPA: 3.92

- Co-advised by Drs. Angela Violi and Clayton Scott
- Thesis Topic: Generative Nanoparticle Design via Joined Foundation Models

University of Michigan

M.Sc. Computer Science

GPA: 3.91

• Member of the VioliGroup computational biochemistry lab (3 semesters, 2 summers)

Chapman University

B.Sc. Computer Science, Music Minor

GPA: 3.86, Magna Cum Laude

Orange, CA 08/16-05/20

Chicago, IL

04/24

05/24

Honors and

Awards

Top 15 Poster Presentation

Midwest Machine Learning Symposium

• "Joint Optimization Significantly Improves Gradient Boosting" was selected as a "Top 15

Poster" (unranked). [Official Link] [Press Release]

Ann Arbor, MI

Excellence in ECE Honor Roll

University of Michigan

• In recognition for running the SPEECS graduate student seminar during the 2023-2024

academic year. [Press Release]

Music Minor Award

Chapman University

• In recognition of outstanding contributions to the conservatory (i.e., tutoring)

Provost List, 8 semesters

Chapman University

• ≥ 3.800 term GPA while enrolled in ≥ 12 graded credits

Orange, CA 05/20

Orange, CA

08/16-05/20

Fellowships

J. Robert Beyster Computational Innovation Graduate Fellowship

University of Michigan

• Tuition, stipend, and health insurance for a year.

• For performing "cutting-edge research in a variety of fields linking high-performance computing.. to applications of societal importance." [Link]

e-HAIL Summer Student Support Program

University of Michigan

• \$12,000 stipend for summer research.

e-HAIL Summer Student Support Program

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07/24

Ann Arbor, MI

Ann Arbor, MI Summer 2024

Ann Arbor, MI

Summer 2023

Scholarship	Chancellor's Scholarship, 8 semesters Chapman University	Orange, CA 08/16-05/20		
Journal Papers	M. Raymond, P. Elvati, J. C. Saldinger, J. Lin, X. Shi, and A. Violi. "Machine Learning Models for Sticking Probability Prediction of Si Nanoparticles In Non-Thermal Plasma". In: <i>Plasma Sources Science and Technology</i> (2024). In Submission			
	M. Raymond, J. C. Saldinger, P. Elvati, C. Scott, and A. Violi. "Universal Feature Selection for Simultaneous Interpretability of Multitask Datasets". In: <i>Information Fusion</i> (2024). In Submission			
	J. C. Saldinger, M. Raymond, P. Elvati, and A. Violi. "Domain-agnostic predictions of a tions in proteins and nanoparticles". In: <i>Nature Computational Science</i> 3.5 (May 2023), p 2662-8457. DOI: 10.1038/s43588-023-00438-x			
Workshop Papers	M. Raymond , A. Violi, and C. Scott. "Joint Optimization of Piecewise Linear Ensembles". In: <i>IEEE International Workshop on Machine Learning for Signal Processing</i> . Accepted. 2024			
Preprints	M. Raymond, P. Elvati, J. C. Saldinger, J. Lin, X. Shi, and A. Violi. Machine Learning Models for Sticking Probability Prediction of Si Nanoparticles In Non-Thermal Plasma. 2024			
	M. Raymond, A. Violi, and C. Scott. "Joint Optimization of Piecewise Linear Ensem International Workshop on Machine Learning for Signal Processing. Submitted. 2024. arX			
	A. Raymond , J. C. Saldinger, P. Elvati, C. Scott, and A. Violi. <i>Universal Feature Selection for Simulta-</i> tous Interpretability of Multitask Datasets. 2024. arXiv: 2403.14466			
Invited Talks	From Proteins to Nanoparticles: Domain-Agnostic ML for the Nanoscale University of Michigan, Tools and Technology Seminar Series Joined Diffusion Models for Nanoparticle Generation Chapman University, Fowler School of Engineering Seminar Series Machine Learning Models for Nanoparticle Growth in Nonthermal Plasmas University of Minnesota, Dusty Plasma Workshop (DPW)	Ann Arbor, MI 3/25 Orange, CA 11/24 Minneapolis, MN 05/24		
Posters	Joint Optimization of Piecewise Linear Ensembles IEEE Machine Learning for Signal Processing Workshop	London, UK 09/24		
	Machine Learning for Knowledge Transfer in Nanomedicine e-Heath and AI (e-HAIL) Student Symposium	Ann Arbor, MI $09/24$		
	Joint Optimization Significantly Improves Gradient Boosting Dusty Plasma Workshop (DPW)	Minneapolis, MN 05/24		
	ML Boosts Efficiency in Atomic Nonthermal Plasma Simulations Midwest Machine Learning Symposium (MMLS)	Minneapolis, MN 05/24		
	Joint Optimization of Linear Ensembles Michigan Student Symposium for Interdisciplinary Statistical Sciences (MSSISS)	Ann Arbor, MI $03/24$		
	A Taste of Your Own Medicine: Tracing Butyrate Production In The Gut e-Heath and AI (e-HAIL) Student Symposium	Ann Arbor, MI $09/23$		
	Preventative Healthcare via Accessible Data Tools Chapman University Student Scholar Symposium	Orange, CA $05/20$		
Software	 JOPLEn, Global Refinement, and Friedman Refitting Python implementations of "Joint Optimization of Piecewise Linear Ensembles," Global Refinement, and Friedman Refitting [Link] 	09/ 2024		
	 BoUTS and MultiBoost Python implementation of "Boosted Universal and Task-Specific Feature Selection" and MultiBoost. [Link] 	06/24		

NeCLASPython implementation of "Neural Coarse-graining for Location Agnostic Sets" [Link]

08/22

Grant Writing	e-HAIL Summer Student Support Funding University of Michigan • \$12,000 over four months	Ann Arbor, MI 01/24
	e-HAIL Summer Student Support Funding University of Michigan • \$12,000 over four months	Ann Arbor, MI $01/23$
Teaching	Programming Instructor Coding Minds Academy	Irvine, CA 07/20–11/20
	 STEM Tutor Chapman University Group tutoring for Calculus 1-3, Discrete Math, Visual Programming, Assembly Language, Data Structures and Algorithms, Programming Languages, Genetic Biology, and Molecular Genetics 	Orange, CA 09/19-05/20
	Supplemental Instructor for Data Structures and Algorithms Chapman University • Held office hours and supplemental lectures each week	Orange, CA 09/19–12/19
	 Music tutor Chapman University Private tutoring for Music Theory, Music History, Aural Skills, and Music Technology Led group review sessions for music history 	Orange, CA 01/17-05/20
Research Experience	 Directed Study & Research Dr. Scott and Dr. Violi Multitask feature selection, optimization, and protein-nanoparticle interaction prediction Assist in grant writing and student hiring Advise computational biochemists on machine learning methodology and literature Supervised roles: Geometric Deep Learning, Deep Gaussian Processes, Active Learning 	Ann Arbor, MI 01/21–present
	 Directed Study & Research Dr. Meibodi Developed a 3d, web-based collaboration tool for live annotation of architectural designs Utilized Babylon.js, Node.js, React, and Redis 	Ann Arbor, MI 07/20–11/21
	 Directed Study & Research Dr. Linstead Continued work on ISS Archeology project (see "Projects") 	Orange, CA 03/20-05/20
Work Experience	 Data Science Intern Toyoda Gosei Hired, but the internship was canceled because of COVID-19 	Troy, MI 05/20
	Instrument Programmer Lotus Instruments • Developed controls for government-contracted, custom gas chromatography instruments • Analyzed documentation and created custom libraries for serial data transfer	Long Beach, CA 09/19-11/19
	 Software Engineering Intern Toyoda Gosei Saved 2,000 man-hours and \$60,000 per year through automated purchase order tracking Implemented a web-based asset tracking software using full-stack ASP.NET Collaborated with Cost Management to solidify requirements and return on investment 	Troy, MI 05/19-08/19
Service	Coordinater, Signal Processing in EECS (SPEECS) seminar University of Michigan • websites.umich.edu/~speecsseminar/	Ann Arbor, MI 08/23-05/24
	Coordinator, Machine learning theory reading group University of Michigan	Ann Arbor, MI 01/22–02/22

• sites.google.com/umich.edu/mltheory/home

Planning Comittee Member, Engineering Research Symposium

University of Michigan

• Schedule PDF Booklet

Ann Arbor, MI 07/20–02/21

Coordinator, COVID-19 Study Group

Chapman University

Virtual 05/21-07/21

- Study group for students who lost summer internships due to COVID-19
- Used MIT OpenCourseWare for:
 - Operating System Engineering (MIT 6.828)
 - Microeconomic Theory and Public Policy (MIT 14.03)
 - Probabilistic Systems Analysis and Applied Probability (MIT 6.041)

Vice-President, FPV Drone Club

Chapman University

Orange, CA 01/20-05/20

Other Activities

Proofreading Linear Algebra Textbook

 $Cambridge\ University\ Press$

Ann Arbor, MI 05/23-09/23

- Proofread draft of "Linear Algebra for Data Science, Machine Learning, and Signal Processing" for Dr. Jeffery Fessler
- Independently verified proofs and suggested improvements for clarity and correctness
- Caught LATEX typesetting errors
- Available 2024 from Cambridge University Press

Class Projects

The Implicit Bias of Gradient Descent on Separable Multiclass Data $\label{eq:continuous}$

U-M Course: EECS 598, 559

Ann Arbor, MI 12/22, 05/23

- Developed a conjecture and proof sketch for extending *The implicit bias of gradient descent* on separable data to include multiclass PERM losses
- Showed numerically that our conjecture holds for certain well-known loss functions

Real-Time Distributed Learning in Connected & Autonomous Vehicles (CAVs) Ann Arbor, MI U-M Course: EECS 571

- Designed distributed learning protocol for sparse gradient propagation
- Implemented simulated learning environment in Tensorflow
- Demonstrated superior generalization, with fewer assumptions than Federated Learning

Domain Exploration Through Artificial Curiosity

Ann Arbor, MI

12/20

- U-M Course: EECS 545
 Developed simulated Martian terrain for training and evaluation
- Beginning with Shmidhuber's theoretical basis for artificial curiosity, developed an implementation using convolutional auto-encoders
- Defined heuristic "Explorational Value" for evaluating path explored by model
- Performed evaluation against naive models to illustrate effectiveness of artificial curiosity

Needlecast: On-the-Fly Reconfiguration of Spacecraft Flight Software *U-M Course: EECS 587*

Ann Arbor, MI 12/20

• Collaborated with NASA staff to draft specifications for protocols

- Designed a library for booting NASA core Flight System (cFS) applications on-the-fly
- Implemented Needlecast as a plug-and-play header file for NASA core cFE
- Developed a simulated network switch and web interface for straightforward debugging

Preventative Healthcare via Accessible Data Tools

Orange, CA

Chapman Course: CPSC 353

• Developed a web application to rank businesses and other establishments by the number of COVID-19 cases in their area

• Utilized REST APIs and front-end web development to develop a user-friendly interface

AI-Driven Contemporary Archaeology for the International Space Station Chapman Course: CPSC 393

Orange, CA

01/20

05/20

- Analyzed project requirements with Dr. Walsh (co-PI of ISS Archeology)
- Compiled facial training dataset for 240 ISS astronauts
- Utilized convolutional neural networks to label astronauts' faces in NASA photo archives