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mraymond.info

Matt Raymond

ML + Computational Chemistry

Research Interests

- Weakly-supervised diffusion modeling
- Generative models for *ab initio* nanoparticle design
- Transfer learning for small nanochemical datasets
- Machine-learning-based surrogate modeling for computational nanochemistry

Education

University of Michigan — Ann Arbor, MI
Ph.D. Signal/Image Processing and Machine Learning — 08/22–04/26
GPA: 3.92
- Co-advised by Drs. Angela Violi and Clayton Scott
- Thesis Topic: *Generative Nanoparticle Design via Joined Foundation Models*

University of Michigan — Ann Arbor, MI
M.Sc. Computer Science — 08/20–04/22
GPA: 3.91
- Member of the VioliGroup computational biochemistry lab (3 semesters, 2 summers)

Chapman University — Orange, CA
B.Sc. Computer Science, Music Minor — 08/16–05/20
GPA: 3.86, *Magna Cum Laude*

Honors and Awards

Top 15 Poster Presentation — Chicago, IL
Midwest Machine Learning Symposium — 04/24
- "Joint Optimization Significantly Improves Gradient Boosting" was selected as a "Top 15 Poster" (unranked). [Official Link] [Press Release]

Excellence in ECE Honor Roll — Ann Arbor, MI
University of Michigan — 05/24
- In recognition for running the SPEECS graduate student seminar during the 2023-2024 academic year. [Press Release]

Music Minor Award — Orange, CA
Chapman University — 05/20
- In recognition of outstanding contributions to the conservatory (*i.e.*, tutoring)

Provost List, 8 semesters — Orange, CA
Chapman University — 08/16–05/20
- $\geq$3.800 term GPA while enrolled in $\geq$12 graded credits

Fellowships

J. Robert Beyster Computational Innovation Graduate Fellowship — Ann Arbor, MI
University of Michigan — 07/24
- 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 — Ann Arbor, MI
University of Michigan — Summer 2024
- $12,000 stipend for summer research.

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University of Michigan — Summer 2023
- $12,000 stipend for summer research.

Scholarship

Chancellor's Scholarship, 8 semesters — Orange, CA
Chapman University — 08/16–05/20

Journal Papers

M. I. Radaideh, **M. Raymond**, P. Elvati, J. C. Saldinger, M. I. Radaideh, and A. Violi. "Efficient sampling of polycyclic aromatic compounds for free energy predictions through active learning". In: *Energy and AI* 21 (2025), p. 100528. ISSN: 2666-5468. DOI: 10.1016/j.egyai.2025.100528

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: *Plasma Sources Science and Technology* 34.3 (Mar. 2025). DOI: 10.1088/1361-6595/adbae1

M. Raymond, J. C. Saldinger, P. Elvati, C. Scott, and A. Violi. "Universal Feature Selection for Simultaneous Interpretability of Multitask Datasets". In: *Journal of Cheminformatics* (2025). In Submission

J. C. Saldinger, **M. Raymond**, P. Elvati, and A. Violi. "Domain-agnostic predictions of nanoscale interactions in proteins and nanoparticles". In: *Nature Computational Science* 3.5 (May 2023), pp. 393–402. ISSN: 2662-8457. DOI: 10.1038/s43588-023-00438-x

Workshop Papers

M. Raymond, Y. Zhu, J. Zhang, A. Violi, and C. Scott. "Joint Diffusion Sampling via Positive-Unlabeled Guidance for Multi-Modal Data". In: *Proceedings of the ICML 2025 Workshop on Foundation Models for Life Sciences (FM4LS)*. July 2025

M. Raymond, A. Violi, and C. Scott. "Joint Optimization of Piecewise Linear Ensembles". In: *IEEE International Workshop on Machine Learning for Signal Processing*. Accepted. 2024

Preprints

M. Raymond, J. C. Saldinger, P. Elvati, C. Scott, and A. Violi. *Universal Feature Selection for Simultaneous Interpretability of Multitask Datasets*. 2024. arXiv: 2403.14466

Invited Talks

From Proteins to Nanoparticles: Domain-Agnostic ML for the Nanoscale — Ann Arbor, MI
University of Michigan, Tools and Technology Seminar Series — 3/25

Joined Diffusion Models for Nanoparticle Generation — Orange, CA
Chapman University,Fowler School of Engineering Seminar Series — 11/24

Machine Learning Models for Nanoparticle Growth in Nonthermal Plasmas — Minneapolis, MN
University of Minnesota, Dusty Plasma Workshop (DPW) — 05/24

Posters

Joining Diffusion Models for Nanoparticle Design — Chicago, IL
Midwest Machine Learning Symposium (MMLS) — 06/24

Joining Diffusion Models for Nanoparticle Design — Ann Arbor, MI
SciFM25 Conference — 05/30

Accelerating Drug Discovery: Modeling Protein-Nanoparticle Systems — Ann Arbor, MI
DATA Spring 2025 Industry Advisory Board Meeting — 03/25

Machine Learning for Knowledge Transfer in Nanomedicine — Ann Arbor, MI
e-Health and Artificial Intelligence — 09/24

Joint Optimization of Piecewise Linear Ensembles — London, UK
IEEE Machine Learning for Signal Processing Workshop — 09/24

Machine Learning for Knowledge Transfer in Nanomedicine — Ann Arbor, MI
e-Heath and AI (e-HAIL) Student Symposium — 09/24

Joint Optimization Significantly Improves Gradient Boosting — Minneapolis, MN
Dusty Plasma Workshop (DPW) — 05/24

ML Boosts Efficiency in Atomic Nonthermal Plasma Simulations — Minneapolis, MN
Midwest Machine Learning Symposium (MMLS) — 05/24

Joint Optimization of Linear Ensembles — Ann Arbor, MI
Michigan Student Symposium for Interdisciplinary Statistical Sciences (MSSISS) — 03/24

A Taste of Your Own Medicine: Tracing Butyrate Production In The Gut — Ann Arbor, MI
e-Heath and AI (e-HAIL) Student Symposium — 09/23

Preventative Healthcare via Accessible Data Tools — Orange, CA
Chapman University Student Scholar Symposium — 05/20

Software

JOPLEn, Global Refinement, and Friedman Refitting — 09/ 2024
- Python implementations of "Joint Optimization of Piecewise Linear Ensembles," Global Refinement, and Friedman Refitting [Link]

BoUTS and MultiBoost — 06/24
- Python implementation of "Boosted Universal and Task-Specific Feature Selection" and MultiBoost. [Link]

NeCLAS — 08/22
- Python implementation of "Neural Coarse-graining for Location Agnostic Sets" [Link]

Grant Writing

e-HAIL Summer Student Support Funding — Ann Arbor, MI
University of Michigan — 01/24
- $12,000 over four months

e-HAIL Summer Student Support Funding — Ann Arbor, MI
University of Michigan — 01/23
- $12,000 over four months

Teaching

Programming Instructor — Irvine, CA
Coding Minds Academy — 07/20–11/20

STEM Tutor — Orange, CA
Chapman University — 09/19–05/20
- Group tutoring for Calculus 1-3, Discrete Math, Visual Programming, Assembly Language, Data Structures and Algorithms, Programming Languages, Genetic Biology, and Molecular Genetics

Supplemental Instructor for Data Structures and Algorithms — Orange, CA
Chapman University — 09/19–12/19
- Held office hours and supplemental lectures each week

Music tutor — Orange, CA
Chapman University — 01/17–05/20
- Private tutoring for Music Theory, Music History, Aural Skills, and Music Technology
- Led group review sessions for music history

Research Experience

Directed Study & Research — Ann Arbor, MI
Dr. Scott and Dr. Violi — 01/21–present
- 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

Directed Study & Research — Ann Arbor, MI
Dr. Meibodi — 07/20–11/21
- Developed a 3d, web-based collaboration tool for live annotation of architectural designs
- Utilized Babylon.js, Node.js, React, and Redis

Directed Study & Research — Orange, CA
Dr. Linstead — 03/20–05/20
- Continuued work on ISS Archeology project (see "Projects")

Work Experience

Data Science Intern — Troy, MI
Toyoda Gosei — 05/20
- Hired, but the internship was canceled because of COVID-19

Instrument Programmer — Long Beach, CA
Lotus Instruments — 09/19–11/19
- Developed controls for government-contracted, custom gas chromatography instruments
- Analyzed documentation and created custom libraries for serial data transfer

Software Engineering Intern — Troy, MI
Toyoda Gosei — 05/19–08/19
- 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

Service

Coordinater, Signal Processing in EECS (SPEECS) seminar — Ann Arbor, MI
University of Michigan — 08/23–05/24
- `websites.umich.edu/~speecsseminar/`

Coordinator, Machine learning theory reading group — Ann Arbor, MI
University of Michigan — 01/22–02/22
- `sites.google.com/umich.edu/mltheory/home`

Planning Comittee Member, Engineering Research Symposium — Ann Arbor, MI
University of Michigan — 07/20–02/21
- Schedule PDF Booklet

Coordinator, COVID-19 Study Group — Virtual
Chapman University — 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 — Orange, CA
Chapman University — 01/20–05/20

Other Activities

Proofreading Linear Algebra Textbook — Ann Arbor, MI
Cambridge University Press — 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 — Ann Arbor, MI
U-M Course: EECS 598, 559 — 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 — 12/21
- 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
U-M Course: EECS 545 — 12/20
- 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 — Ann Arbor, MI
U-M Course: EECS 587 — 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 05/20

- 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 Orange, CA
Chapman Course: CPSC 393 01/20

- 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