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### Matt Raymond

ML, Nanochemistry, Computer Science



#### Education

#### University of Michigan

Ph.D. Signal/Image Processing and Machine Learning

GPA: 3.92

- Co-advised by Drs. Angela Violi and Clayton Scott
- President of the student signal processing seminar: websites.umich.edu/~speecsseminar/
- Thesis Topic: Generative Modeling of Nanoparticles Via Transfer Learning

### University of Michigan

M.Sc. Computer Science

GPA: 3.91

- Member of the VioliGroup computational biochemistry lab (3 semesters, 2 summers)
- President of the Machine Learning Theory Reading Group, 1 semester

### Chapman University

B.Sc. Computer Science, Music Minor

GPA: 3.86

• Member of the Provost List, 8 semesters

- Recipient of the Chancellor's Scholarship, 8 semesters
- Tutor and Supplemental Instructor for Computer Science and Math, 4 semesters

#### **Papers**

### Joint Optimization Significantly Improves Gradient Boosting

Ongoing

- Implement GPU-accelerated proximal Nesterov method for joint optimization of piecewise linear ensembles (JOPLEn) with nonsmooth convex losses
- Benchmarked against existing ensemble methods on 65 regression datasets
- JOPLEn significantly improves performance of gradient boosted ensembles  $(p \approx 10^{-8})$
- JOPLEn improves feature sparsity for ensemble feature selection
- In the multitask setting, JOPLEn shares regularization across tasks

## Machine Learning Models for Nanoparticle Growth in Nonthermal Plasma

Ongoing

- Develop surrogate ML models for estimating sticking coefficients of silane nanoparticles in nonthermal plasma
- Supervised undergraduate students
  - Jonathan Lin and Zewei Yu
- Currently cleaning results and preparing paper for publication

### Multitask Learning of Universal Features for Chemistry Datasets

Ongoing

- Develop novel multitask impurity function for gradient boosted trees
- Extend Scikit-Learn to include our method (using Python and Cython)
- Track experiments using Data Version Control and test using PyTest
- Outperform MultiBoost and Dirty LASSO on 7 diverse chemistry datasets, including proteins, nanoparticles, and small molecules
- Show that multiple chemical scales can be represented using a few universal features

### Domain-Agnostic Predictions of Nanoscale Interactions in Proteins and Nanoparticles 04/23 Nature Computational Science (cover Article)

- Developed a Deep Learning framework for predicting generalized nanoscale interactions
- Implemented permutation-invariant Neural Network using Tensorflow (TF)
- Migrated competitors code from TensorFlow (TF) 1 to TF 2 for testing
- Paper DOI: 10.1038/s43588-023-00438-x, Code DOI: 10.24433/CO.8157811.v1

Ann Arbor, MI 08/22 - 04/26

Ann Arbor, MI

08/20-04/22

Orange, CA

08/16 - 05/20

Joint Optimization of Piecewise Linear Ensembles 28/03/24 Conferences Michigan Student Symposium for Interdisciplinary Statistical Sciences Hybrid MD-ML for Efficient Modeling of Particle Growth in Non-Thermal Plasma 2023 APS Annual Gaseous Electronics Meeting 09/23Posters A Taste of Your Own Medicine: Tracing Butyrate Production in The Gut University of Michigan EHAIL Symposium Bacterial butyrate production is associated with improved gut health, but the mechanisms are not well understood Analyzed proprietary gut microbiome data from Michigan Medicine using Python Utilized Fused Graphical LASSO to identify microbial interactions Recovered known interactions and identified novel interactions for in vitro testing 01/21-present Work Directed Study & Research Dr. Scott and Dr. Violi Experience • Perform novel research in sparse structured multitask feature selection Advise computational biochemists on machine learning methodology and literature • Supervise student researchers; Geometric Deep Learning and Deep Gaussian Processes 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 Books Linear Algebra for Data Science, Machine Learning, and Signal Processing Ann Arbor, MI Cambridge University Press 05/23 - 09/23• Proofread and edited textbook draft for Dr. Jeffery Fessler Independently verified proofs and suggested improvements for clarity and correctness • Caught LATEX typesetting errors • Available 2024 from Cambridge University Press **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

- $\bullet\,$  Implemented Needle cast as a plug-and-play header file for NASA core cFE
- Developed a simulated network switch and web interface for straightforward debugging

# AI-Driven Contemporary Archaeology for The International Space Station U-M Course: EECS 587

Orange, CA 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