Ouail Kitouni

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Education

2019–Present **Massachusetts Institute of Technology**, *Ph.D. Candidate*, Physics, Statistics, and Data Science joint degree, Nuclear and Particle Experimental Physics Division and The MIT Statistics and Data Science Center

2019 **University of Rochester**, *Bachelor of Science with Highest Distinction*, Physics with Mathematics focus, *GPA: 4.00/4.00* in both

Experience

2022 Summer **FDL**, *ML Researcher Intern*, The NASA/SETI Frontier Development Lab

2021–Present **IAIFI**, *Junior Investigator*, The NSF AI Institute for Artificial Intelligence and Fundamental Interactions

Publications

[1] Ziming Liu*, **Ouail Kitouni***, Eric Michaud, Niklas Nolte, Micheal Williams, Max Tegmark, *"Towards Understanding Grokking: An Effective Theory of Representation Learning"*, 2205.10343. **NeurIPS 2022**.

[2] **Ouail Kitouni***, Niklas Nolte*, Micheal Williams, *"Robust and Provably Monotonic Networks"*, Workshop on Machine Learning and the Physical Sciences **NeurIPS 2021**.

[3] **Ouail Kitouni***, Benjamin Nachman, Constantin Weisser, Micheal Williams, *"Enhancing searches for resonances with machine learning and moment decomposition"*, **Journal of High Energy Physics** 10.1007/JHEP04(2021)07 and the Workshop on Machine Learning and Physical Sciences **NeurIPS 2020**.

[4] Nathan Reff, **Ouail Kitouni**, *"Lower Bounds for the Laplacian Spectral Radius of an Oriented Hypergraph"*, **Australasian Journal of Combinatorics**. 74(3). 408-422.

[5] **Ouail Kitouni***, Niklas Nolte, Micheal Williams, *"NEEMo: Neural Estimation of Energy Mover's Distance"*, Submitted to Workshop on Machine Learning and the Physical Sciences NeurIPS 2022.

[6] **Ouail Kitouni***, Niklas Nolte*, Micheal Williams, *'The Benefits of Lipschitz Networks"*, Submitted to Machine Learning: Science and Technology.

[7] **Ouail Kitouni***, Niklas Nolte*, Micheal Williams, *"Expressive Monotonic Networks"*, Submitted to ICLR 2023.

Honors and Awards

Massachusetts Institute of Technology

2019 **Frank Fellowship**, Awarded to a selection of incoming first-year doctoral students.

University of Rochester

2017-2019 **Dean's List**, Awarded based on GPA

2017-2019 **Whipple Science and Research Scholarship**, Awarded based on academic merit and research excellence.

2018 **Research Presentation Award**, Awarded to students presenting excellent research at academic conferences.

State University of New York – Brockport

2015-2017 **Dean's List**, Awarded based on GPA.

2017 **Bailey Scholarship**, Awarded to one outstanding student across the departments of physics, mathematics, chemistry, and biology.

2017 **Harvard House Award**, Awarded to top student in the Physics department.

2017 **Interdisciplinary Award**, Awarded to top student interested in interdisciplinary research in applied mathematics.

2015-2017 **Honors Scholarship**, Merit scholarship awarded to top incoming first-year students every fall semester.

2016-2017 **Integration Bee Gold Medal**, Competition at SUNY Brockport's Mathematics department (2016/2017).

Constantine, Algeria

2014 **Cirta-Science 1st Place**, Science competition between top high school students across the Constantine region in Algeria, .

Languages

Native Level **Arabic**, **French**, **English**

Coding

- Extensive coding experience in Python and some experience in C++, MATLAB, FORTRAN.
- Extensive experience in developing deep learning software using PyTorch and, occasionally, TensorFlow.
- Experience in various Python libraries NumPy, AstroPy, SciPy, scikit-learn, Pandas, Dask, etc.
- Experience in: UNIX shell scripting and Simple Linux Utility for Resource Management (SLURM), Google Cloud Platform, Nvidia NGC.

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Research and Projects

Summer 2022 **Deep Point Cloud Computational Fluid Dynamics**, *NASA/FDL.*

Worked closely with a team of domain experts in a research/software development sprint on the simulation and optimization of concentrated solar power coolers to increase efficiency and lower cooling costs making them more competitive with traditional energy sources. I developed a pipeline for design optimization of heat exchangers using a hand designed physics simulator which was later replaced by a neural estimator that introduced a large speed-up making large-scale (and physically accurate) design optimization possible.

- Implemented a novel heuristic physics simulator and used it for design optimization using scalable Bayesian Optimization.
- Developed a Deep Sets neural surrogate for differentiable fluid dynamics simulation and inverse design of air coolers.
- Developed an API integrating heat exchanger design and cost optimization showcased at NASA's FDL live showcase.

Spring 2022 **Understanding Grokking: Generalization Beyond Overfitting**, *IAIFI/MIT*

Developed an effective theory to understand transformer architectures' ability to generalize on arithmetic datasets. The theory links generalization to a particular structured representation of the embeddings and predicts a range of phenomena associated with grokking, or delayed generalization. Moreover, we show that grokking is one of four different phases of learning and can be avoided with proper hyper-parameter tuning.

Spring 2022 **Energy Mover's Distance using Lipschitz Networks for Collider Physics**, *IAIFI*

Developed a novel clustering algorithm (leveraging optimal transport and Lipschitz networks) which generalizes previous well-known clustering algorithms in High Energy Physics (anti-kt, Cambridge-Aachen, etc.) to arbitrary geometries and offers new flexibility in dealing with effects such as pile-up and unconventional topologies.

Spring 2021 **Provably Monotonic Lipschitz Networks**, *CERN LHCb*

Developed a novel architecture to approximate Lipschitz functions that are monotone in any subset of its inputs along with a software package that implements it in PyTorch. The implementation (ported to CUDA) is now used in the High Level Trigger at the LHCb experiment at CERN where the monotonicity of certain features is an important inductive bias and where the Lipschitz continuity of the model is critical for robustness against run-time instabilities.

Fall 2020 **Moment Decomposition to Mitigate Bias**, *MIT*

Developed a new form of regularization to make classifiers unbiased in a specified protected attribute. Performance gains of about 12% over state-of-the-art de-biasing techniques were obtained on a particle search benchmark dataset. In addition, the algorithm can be used to control the complexity (number of terms in a polynomial expansion) of the dependence of a model on any feature whether or not it was used directly as input.

Spring 2018 **Deep Learning for Spectroscopic Transient Detection**, *Univeristy of Rochester*

-Investigated various deep learning techniques, specifically long short-term memory and convolutional neural networks, as a basis for an object detection algorithm for spectroscopic observations of supernovae.
-Worked in simulating physical spectroscopic observations of galaxies and different transients.
-Extended the Dark Energy Spectroscopic Instrument simulation package to simulate Type IIp supernova spectra.

Fall 2018 **Search for Type Ia and Other Transients**

Studied supernova spectra and developed a supernova injection algorithm to simulate spectroscopic observations of Type Ia supernovae.

Summer 2016/2017 **Lower Bounds for the Laplacian Spectral Radius of an Oriented Hypergraph**

Studied some properties of oriented hypergraphs and derived new bounds for their Laplacian spectral radius.

Spring 2021 **Multi-scale Long-term Forecasting of Grid Consumption**, *Statistics, Computation and Applications, MIT*

Developed a Temporal Fusion Transformer to forecast consumption patterns amongst different socioeconomic groups in order to understand the effect of dynamic time of day pricing as an intervention technique to mitigate the strain on the power grid in times of irregular demand. Found evidence that suggests the response to the treatment has significant elasticity for less affluent consumers and showed that the London smart-metering trial was largely successful.

Fall 2020 **Learning Symmetries From Scratch**, *Statistical Learning Theory, MIT*

Statistical Learning theory course project supervised by Tomaso Poggio and Lorenso Rosasco. Explored the ability of a Multi-Layer Perceptron to learn symmetries (i.e. learn the weight sharing structure associated with invariance under some group transformation) with a reasonable amount of data and in reasonable time. With an emphasis on machine vision tasks, we validated empirically some previously known results; Locality can account for much of CNNs' superior performance on computer vision tasks and that this property is not easily learned from a standard fully-connected architecture. Locally-connected networks are able to learn the weight sharing structure appropriate to the problem with reasonable data augmentation. Also found evidence that ADAM has an implicit regularization for sparsity.

Teaching Experience

Jan. 2020/2021 **Teaching Assistant**, Massachusetts Institute of Technology
Helped start a new introductory course in Data Science with applications to various physics problems. Developed course material and wrote Jupyter notebooks for hands-on data analysis for students (covering topics such as hypothesis testing, classification, clustering, MCMC methods, etc.). The course is now being ported to MITx and will be an official part of the interdisciplinary degree in statistics.

Aug. 2017 – May 2019 **Teaching Assistant**, *Physics Department*, University of Rochester
Assisted teaching introductory classical mechanics and electromagnetism courses in addition to upper level statistical mechanics (PHY 227, PHY 121, PHY 122). Responsibilities included holding office hours, grading weekly homework assignments, conducting workshops and proctoring exams.

Aug. 2016 – May 2017 **Teaching Assistant and Lab Technician**, *Physics Department*, Brockport
Responsibilities included assisting with experiments, giving lectures, and conducting weekly tutoring sessions for mechanics and electromagnetism courses (PHS 235 and PHS 240).

Aug. 2015 – May 2016 **Tutor**, *Student Learning Center and Modern Languages department*, Brockport
Tutoring Arabic and French.

Leadership Positions

2020/2021 **Reviewer**, *Physical Sciences Workshop*, NeurIPS 2020 and NeurIPS 2021
Reviewed submissions to the physical sciences workshop for NeurIPS 2020 and 2021.

Sep 2020 – Present **Mentor**, *Course 8*, MIT
Mentoring Course 8 (Physics) students. My responsibilities include leading weekly one-on-one meetings, providing guidance to mentees, and helping navigate the major and the field of physics overall. The mentoring program focuses on helping mentees develop problem-solving skills as well as providing them with academic, personal, and career-oriented support.

Sep 2016 – May 2017 **President**, *International Student Organization*, Brockport
Started and ran a weekly cultural exchange program. Organized different activities for international students. Helped organize and manage the annual International Student Festival.

2016 **Peer Mentor**, *Honors College*, Brockport
Mentored first-year students through their transition to college. Provided assistance with course selection, organized workshops on research and academic opportunities, lead weekly meetings, organized various events, and conducted info sessions.

2016 **Leader Volunteer**, *International Orientation*, Brockport
Conducted info sessions, gave tours, etc.

Talks

- Presented my work at Lawrence Berkeley National Lab, July 7th 2022.
- Robust and Monotonic Neural Networks, American Physical Society April Meeting 2022 AI/ML platform, April 12.
- Robust and Monotonic Neural Networks, MIT SDSCon 2022, April 1.
- Provably Robust and Monotonic Networks for Heavy Flavor Selections at LHCb, ACAT 2021, Nov 29.
- Provably Monotnoic Lipschitz Networks, Machine Learning and Physical Sciences Workshop, NeurIPS 2021, Dec 13.
- Robust Deep Learning models in High Energy Physics, Lecture at the MLHEP Summer School 2021.
- Enhancing searches for resonances with robust classifiers using moment decomposition, American Physical Society March Meeting Data Science Platform, March 17, 2021.
- Controlled mass dependence in ML classifiers, PhyStat Workshop, Jan 18, 2021.
- Controlling Classifier Bias with Moment Decomposition, NeurIPS 2020 Physical Sciences Workshop.
- MoDe for Robust and Unbiased Classifiers, CERN's 4th Inter-experimental Machine Learning Workshop, Oct 19-23, 2020.
- Effectiveness of Machine Learning in transient detection, American Astronomical Society (AAS), January 7, 2019.
- Search for Type Ia Supernovae and Other Transients, Rochester Symposium for Physics Students (RSPS), April 7, 2018.
- Lower Bounds for the Laplacian Spectral Radius of an Oriented Hypergraph, Mathematical American Association Seaway Section, 2017.
- Laplacian Eigenvalues of Oriented Hypergraphs, SUNY Undergraduate Research Conference (SURC), April 22, 2017.