Ouail Kitouni

Ph.D. Candidate

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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] "Towards Understanding Grokking: An Effective Theory of Representation Learning", 2205.10343. NeurIPS 2022.
- [2] "Robust and Provably Monotonic Networks", Workshop on Machine Learning and the Physical Sciences NeurIPS 2021.
- [3] "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] "Lower Bounds for the Laplacian Spectral Radius of an Oriented Hypergraph", Australasian Journal of Combinatorics. 74(3). 408-422.
- [5] "NEEMo: Neural Estimation of Energy Mover's Distance", Submitted to Workshop on Machine Learning and the Physical Sciences NeurIPS 2022.
- [6] 'The Benefits of Lipschitz Networks", Submitted to Machine Learning: Science and Technology.
- [7] "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 and research excellence.
 - 2018 Research Presentation Award, For 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

Research and Projects

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

I developed a pipeline for design optimization of heat exchangers using a hand designed physics simulator and improved on it with a neural surrogate that introduced a large speed-up making large-scale (and physically accurate) design optimization possible. The optimized design lowered the cooler cost by 70% and saved \sim \$500k. Developed:

- o a novel physics simulator and used it for design optimization using scalable Bayesian Optimization.
- o a Deep Sets neural surrogate for differentiable and lightning-fast fluid dynamics simulation and used it for inverse design of air coolers.
- o 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 monotonic 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 (collaboration of ~ 1400 scientists and engineers) at CERN. The method offered $4\times$ speed-up over the competing alternatives and offers unique robustness and OOD guarantees.

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, University 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.
- Developed simulations of physical spectroscopic observations of galaxies and different transients.
- $\ \, \odot \ \, \text{Extended the Dark Energy Spectroscopic Instrument simulation package to simulate Type IIp supernova spectra. }$
- o Implemented an ML pipeline for the classification of spectroscopic observations by the DESI collaboration.

Summer Lower Bounds for the Laplacian Spectral Radius of an Oriented Hypergraph

2016/2017 Studied some properties of oriented hypergraphs and derived new bounds for their Laplacian spectral radius.

Spring 2021 **Grid Consumption Multi-scale Long-term Forecasting**, Stats, 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 for significant elasticity of the response to the treatment among less affluent consumers and showed that the London smart-metering trial was 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.

Coding

- o Extensive coding experience in Python and some experience in C++, MATLAB, FORTRAN.
- o Extensive experience in developing deep learning software using PyTorch and, occasionally, TensorFlow.
- \odot 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.

Teaching Experience

- Jan. Teaching Assistant, Massachusetts Institute of Technology
- 2020/2021 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 Teaching Assistant, Physics Department, University of Rochester
 - May 2019 Assisted teaching introductory classical mechanics and electromagnetism courses in addition to upper level statistical mechanics (PHY 227, PHY 121, PHY 122). Held office hours, graded weekly homework assignments, conducted workshops and proctored exams.
- Aug. 2016 Teaching Assistant and Lab Technician, Physics Department, Brockport
 - May 2017 Assisted with experiments, gave lectures, and conducted weekly tutoring sessions for mechanics and electromagnetism courses (PHS 235 and PHS 240).
- Aug. 2015 Tutor, Student Learning Center and Modern Languages department, Brockport
 - May 2016 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 **Mentor**, Course 8, MIT
 - Present Mentoring Course 8 (Physics) students. Lead weekly one-on-one and group meetings, provided guidance to mentees, and helped them navigate the major and the field of physics overall. Helped mentees develop problem-solving skills as well as provided them with academic, personal, and career-oriented support.
- Sep 2016 President, International Student Organization, Brockport
- May 2017 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. 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

- 07/07/2022 Lawrence Berkeley National Lab, Lipschitz Networks
- 04/12/2022 American Physical Society April Meeting 2022 AI/ML platform, Robust and Monotonic Neural Networks
- 04/01/2022 MIT SDSCon 2022, Robust and Monotonic Neural Networks
- 12/13/2021 NeurIPS ML and Physical Sciences Workshop, Provably Robust and Monotonic Networks
- 11/29/2021 ACAT 2021, Provably Robust and Monotonic Networks for Heavy Flavor Selections at LHCb
- summer 2021 ML-HEP Summer School, Robust Deep Learning models in High Energy Physics
- 03/17/2021 American Physical Society March Meeting Data Science Platform, Enhancing searches for resonances with robust classifiers using moment decomposition.
- 01/18/2021 PhyStat Workshop, Controlled mass dependence in ML classifiers.
- 01/18/2021 NeurIPS ML and Physical Sciences Workshop, Controlling Classifier Bias with Moment Decomposition.
- 10/19/2020 CERN's 4th Inter-experimental Machine Learning Workshop, MoDe for Robust and Unbiased Classifiers.
- 01/07/2019 American Astronomical Society (AAS), Effectiveness of Machine Learning in transient detection
- 04/07/2018 Rochester Symposium for Physics Students (RSPS), Search for Type Ia Supernovae and Other Transients
 - 2017 Mathematical American Association Seaway Section, Lower Bounds for the Laplacian Spectral Radius of an Oriented Hypergraph
- 04/22/2017 SUNY Undergraduate Research Conference (SURC), Laplacian Eigenvalues of Oriented Hypergraphs.