Ouail Kitouni

Ph.D. Candidate

Cambridge, MA 02139, USA
kitouni@mit.edu
okitouni.github.io
okitouni

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

2023 Fall **FAIR**, *Incoming Research Scientist Intern*, Meta AI - Fundamental AI Research, NYC

2023 Summer **MSR**, *Research Intern*, Microsoft Research, Cambridge UK

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

2019–Present **LHCb**, *Ph.D. Researcher*, Large Hadron Collider, European Center for Nuclear Research (CERN)

2018–2019 **DESI**, *Undergraduate Researcher*, Dark Energy Spectroscopic Instrument Collaboration

Selected Publications

[1] *"Expressive Monotonic Networks"*, **ICLR 2023**.

[2] *"Towards Understanding Grokking: An Effective Theory of Representation Learning"*, **NeurIPS 2022 Oral**.

[3] *"NEEMo: Geometric Fitting using a **N**eural **E**stimation of the **E**nergy **Mo**ver's Distance"*, Workshop on Machine Learning and the Physical Sciences **NeurIPS 2022**.

[4] *"Robust and Provably Monotonic Networks"*, Workshop on Machine Learning and the Physical Sciences **NeurIPS 2021**.

[5] *"Controlling Classifier Bias with Moment Decomposition: a method to enhance searches for resonances"*, **Journal of High Energy Physics** 10.1007/JHEP04(2021)07 and the Workshop on Machine Learning and Physical Sciences **NeurIPS 2020**.

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

[7] *'The Benefits of Lipschitz Networks"*, Submitted to Machine Learning: Science and Technology.

[8] *"NuCLR: Nuclear Co-Learned Representations"*, submitted to The Synergy of Scientific and Machine Learning Modeling Workshop **ICML2023**.

Honors and Awards

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

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

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

2018 **U of R Research Presentation Award**, For presenting excellent research at academic conferences.

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).

2014 **Cirta-Science 1st Place**, High school science competition in Algeria.

Languages

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

Research and Projects

Summer 2023 **Knowledge Base Modeling**, *Microsoft Research*

- Developed a neural architecture for joint modeling of properties of entities in a knowledge base with the end goal of augmenting LLMs and making them more interpretable and less prone to hallucination.

Spring 2023 **NuCLR: Nuclear Co-Learned Representations**, *IAIFI/MIT*

- Developed a novel deep learning architecture utilizing multi-task training and shared representations. The model achieved state-of-the-art performance in predicting crucial nuclear physics observables.
- Devised interpretability techniques that revealed the emergence of fundamental aspects of the nuclear shell model within NuCLR's learned representations.

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 ∼**$500k**. Developed:

- a novel physics simulator and used it for design optimization using scalable Bayesian Optimization.
- a Deep Sets neural surrogate for differentiable and lightning-fast fluid dynamics simulation and used it for inverse design of air coolers.
- 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 robust architecture to approximate Lipschitz functions that are monotonic in any subset of its inputs along with a software package that implements it in PyTorch (available on PyPI). The implementation (ported to CUDA) is now used in the High Level Trigger at the LHCb experiment at CERN (collaboration of ∼ 1400 scientists and engineers) and operates at data rates of about 4**TB/s**. The method offered **4× 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 (available on PyPI) 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.
- Developed simulations of physical spectroscopic observations of galaxies and different transients.
- Extended the Dark Energy Spectroscopic Instrument simulation package to simulate Type IIp supernova spectra.
- Implemented an ML pipeline for the classification of spectroscopic observations by the DESI collaboration (**100x faster than the baseline**).

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 **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.

Skills

- Extensive coding experience in Python (multiple packages on PyPI) and some experience in C++.
- 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, Azure ML.

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). Held office hours, graded weekly homework assignments, conducted workshops and proctored exams.

Aug. 2016 – May 2017 **Teaching Assistant and Lab Technician**, *Physics Department*, Brockport
Assisted with experiments, gave lectures, and conducted 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 and Community Service

2023 **Reviewer**, NeurIPS 2023

2023 **Reviewer**, *Synergy of Scientific and Machine Learning Modeling*, ICML 2023

2023 **Reviewer**, *Physics4ML*, ICLR 2023

2020-2021 **Reviewer**, *Physical Sciences Workshop*, NeurIPS 2020 and NeurIPS 2021

Sep 2020 – Present **Mentor**, *Course 8*, MIT
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 – 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. 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

12/08/2022 **NeurIPS2022**, *Towards Understanding Grokking: An Effective Theory of Representation Learning*

11/05/2022 **ML4Jets2022**, *Neural Estimation of Energy Mover's Distance*

10/26/2022 **ACAT 2022**, *Neural Estimation of Energy Mover's Distance*

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 ML 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.*