

Workshop I: From Passive to Active: Generative and Reinforcement Learning with Physics

Monday September 23, 2019

- 8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*
- 8:55–9:00 *Welcome & Opening Remarks: Dean Miguel García-Garibay (Dean of Physical Sciences, UCLA) and Dima Shlyakhtenko (Director, IPAM)*
- 9:00–9:50 **Alexandre Tkatchenko** (University of Luxembourg)
Towards a Unified Machine Learning Model of Molecular Chemical Space
- 10:00–10:15 *Break*
- 10:15–11:05 **Xavier Bresson** (Nanyang Technological University, Singapore)
Graph Convolutional Neural Networks for Molecule Generation
- 11:15–11:30 *Break*
- 11:30–12:20 **Joshua Bloom** (University of California, Berkeley (UC Berkeley))
Physics-Informed (and -informative) Generative Modelling in Astronomy
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Laurent Dinh** (Google)
A primer on normalizing flows
- 3:30–3:45 *Break*
- 3:45–4:35 **Frank Noe** (Freie Universität Berlin)
Deep Generative Learning for Physics Many-Body Systems
- 4:45–5:15 *Lightning Poster Presentations*
- 5:15–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday September 24, 2019

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Philip Kurian** (Howard University)
New horizons in quantum biology: Learning complexity, emergence, and coherence in living matter
- 10:00–10:15 *Break*
- 10:15–11:05 **Olexandr Isayev** (Carnegie Mellon University)
De Novo Drug Design with Deep Reinforcement Learning
- 11:15–11:30 *Break*

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- 11:30–12:20 **Nicola De Cao** (University of Amsterdam)
Deep Generative Models for Molecular Graphs
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Patrick Riley** (Google)
Reinforcement learning for molecular generation
- 3:30–4:00 *Break*
- 4:00–4:50 **Rafael Gomez-Bombarelli** (Massachusetts Institute of Technology)
Coarse graining autoencoders and evolutionary learning of atomistic potentials

Wednesday September 25, 2019

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Alán Aspuru-Guzik** (University of Toronto)
Generative models for molecules.
- 10:00–10:15 *Break*
- 10:15–11:05 **Ross King** (University of Science and Technology in Manchester (UMIST))
Automating Science using Robot Scientists
- 11:15–11:30 *Break*
- 11:30–12:20 **Katya Scheinberg** (Cornell University)
Recent advances in Derivative-Free Optimization and its connection to reinforcement learning.
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Josh Agar** (Lehigh University)
Automatic Feature Extraction from Hyperspectral Imagery using Deep Recurrent Neural Networks
- 3:30–4:00 *Break*
- 4:00–4:50 **Lars Ruthotto** (Emory University)
A Numerical Analysis Perspective on Deep Neural Networks

Thursday September 26, 2019

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Phiala Shanahan** (Massachusetts Institute of Technology)
Generative models for lattice quantum field theory
- 10:00–10:15 *Break*

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- 10:15–11:05 **Richard Hennig** (University of Florida)
Machine-learning for materials and physics discovery through symbolic regression and kernel methods
- 11:15–11:30 *Break*
- 11:30–12:20 **Ankit Patel** (Rice University)
Breaking Bad: Recent Advances from Function Space Characterization of Neural Nets with Implications for Physical Applications
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Jascha Sohl Dickstein** (Google)
Generalizing Hamiltonian Monte Carlo with Neural Networks
- 3:30–4:00 *Break*
- 4:00–4:15 **Joshua Yao-Yu Lin** (University of Illinois at Urbana-Champaign)
Hunting for dark matter substructures in strong lensing with neural networks.
- 4:20–4:35 **Nicholas Charron** (Rice University)
Coarse-graining molecular systems by spectral matching.
- 4:40–4:55 **Ganesh Sivaraman** (Argonne National Laboratory)
A diversified machine learning strategy for predicting and understanding molecular melting points.

Friday September 27, 2019

- 8:00–9:00 *Breakfast (Hosted by IPAM)*
- 9:00–9:50 **Benjamin Nachman** (Lawrence Berkeley National Laboratory)
Likelihood free generative modeling for high energy physics
- 10:00–10:15 *Break*
- 10:15–11:05 **Tess Smidt** (Lawrence Berkeley National Laboratory)
Euclidean Neural Networks for Emulating Ab Initio Calculations and Generating Atomic Geometries*
**also called Tensor Field Networks and 3D Steerable CNNs*
- 11:15–11:30 *Break*
- 11:30–12:20 **Juan Carrasquilla** (Vector Institute)
Simulating quantum circuits with neural machine translation
- 12:30–2:30 *Lunch (on your own)*
- 2:30–3:20 **Giuseppe Carleo** (Flatiron Institute, a Division of the Simons Foundation)
Generative and variational modeling for quantum many-body physics
- 3:30–4:00 *Break*
- 4:00–4:50 **Han Pu** (Rice University)
Solving Quantum Many-Body Problems with Deep Neural Networks

