Workshop II: Interpretable Learning in Physical Sciences

Monday October 14, 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 **Cecilia Clementi** (Rice University)
Learning molecular model from simulation and experimental data

10:00–10:15 *Break*

10:15–11:05 **Yannis Kevrekides** (Princeton University)
No equations, no variables, no space and no time: data driven models and gauge-invariant data mining

11:15–11:30 *Break*

11:30–12:20 **Michael Mahoney** (University of California, Berkeley (UC Berkeley))
Why Deep Learning Works: Heavy-Tailed Random Matrix Theory as an Example of Physics Informed Machine Learning

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Shirley Ho** (Flatiron Institute/Princeton University)
Simulating the Universe with Deep Learning

3:30–3:45 *Break*

3:45–4:35 **Julia Ling** (Citrine Informatics)
Model Interpretability for Building Confidence and Sparking Insight in Scientific Applications

4:45–5:15 *Lightning Poster Presentations*

5:15–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday October 15, 2019

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Weinan E** (Princeton University)
Machine learning based multi-scale modeling

10:00–10:15 *Break*

10:15–11:05 **Andrew White** (University of Rochester)
Maximum Entropy Methods for Combining Physics-Based Simulation with Empirical Data

11:15–11:30 *Break*

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11:30–12:20 **Heather Kulik** (Massachusetts Institute of Technology)
Molecular design blueprints: materials and catalysts from new simulation and machine learning tools

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Atilim Gunes Baydin** (University of Oxford)
Universal Probabilistic Programming in Simulators

3:30–4:00 *Break*

4:00–4:50 **Mark Waller** (Wallerlab)
Planning Chemical Syntheses with Deep Neural Networks and Discipline Scale Data

Wednesday October 16, 2019

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **J. Nathan Kutz** (University of Washington)
Coordinates, governing equations and limits of model discovery

10:00–10:15 *Break*

10:15–11:05 **Peter Frazier** (Cornell University)
Accelerating Scientific Discovery through Interpretable Machine Learning and Intelligent Experimentation

11:15–11:30 *Break*

11:30–12:20 **Peter Battaglia** (DeepMind Technologies)
Learning structured models of physics

12:30–2:00 *Lunch (on your own)*

2:00–2:50 **Judea Pearl** (University of California, Los Angeles (UCLA))
Interpretability and explainability from a causal lens

3:00–3:15 *Break*

3:15–4:05 **Adji Bousso Dieng** (Columbia University)
Structured Deep Generative Models

4:15–4:30 *Break*

4:30–5:20 **Gianni De Fabritiis** (Universitat Pompeu Fabra)
Can we machine learn drug discovery?

Thursday October 17, 2019

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Sergei Kalinin** (Oak Ridge National Laboratory)
Deep Learning Dive into the Scanning Transmission Electron Microscopy: Materials Design, Learning Physics, and Atomic Manipulation

10:00–10:15 *Break*

10:15–11:05 **Anatole von Lilienfeld** (University of Basel)
Quantum Machine Learning

11:15–11:30 *Break*

11:30–12:20 **Kieron Burke** (University of California, Irvine (UCI))
Density functionals from machine learning

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Kyle Cranmer** (New York University)
Simulation-based inference, interpretability, and experimental design

3:30–4:00 *Break*

4:00–4:50 **Zachary Lipton** (Carnegie Mellon University)
Interpretability: of what, for whom, why, and how?

Friday October 18, 2019

8:00–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Stephan Hoyer** (Google Inc.)
Improving PDE solvers and PDE-constrained optimization with deep learning and differentiable programming

10:00–10:15 *Break*

10:15–11:05 **Pratyush Tiwary** (University of Maryland)
Learning to learn, learning to forget

11:15–11:30 *Break*

11:30–12:20 **Andrew Ferguson** (University of Chicago)
Machine learning of protein folding funnels from experimental data and construction of latent space molecular simulators

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Francesco Paesani** (University of California, San Diego (UCSD))
Data-driven models for predictive molecular simulations

3:30–4:00 *Break*

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4:00–4:50 **Tristan Bereau** (Max Planck Institute for Polymer Research)
Physics in and out of machine learning for molecular simulations: priors and predictive constraints