Workshop IV: Synergies between Machine Learning and Physical Models

Monday December 5, 2016

8:00–8:55 *Check-In/Light Breakfast (Hosted by IPAM)*

8:55–9:00 *Welcome and Opening Remarks*

9:00–9:50 **Efthimios (Tim) Kaxiras** (Harvard University)
Machine Learning for the Materials World

10:00–10:15 *Break*

10:15–11:05 **Yuval Peres** (Microsoft Research)
Using random walks to analyze Prediction with Expert Advice

11:15–11:30 *Break*

11:30–12:20 **Ralf Banisch** (Freie Universität Berlin)
Learning dynamics with dynamical distances: From diffusion maps to commute maps and coherence

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Soumik Pal** (University of Washington)
Markov chains on partitions and their diffusion analogs

3:30–4:00 *Break*

4:00–4:50 **Marina Meila** (University of Washington)
Geometric manifold learning methods and collective variables

5:00–6:30 *Poster Session & Reception (Hosted by IPAM)*

Tuesday December 6, 2016

8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Alán Aspuru-Guzik** (Harvard University)
Machine learning for organic materials design

10:00–10:15 *Break*

10:15–11:05 **Geoffrey Hutchison** (University of Pittsburgh)
Learning from Conjugated Polymers: Statistical Data Mining from 50 Million and Counting

11:15–11:30 *Break*

(Tuesday schedule continued on next page)

(Tuesday schedule continued from previous page)

11:30–12:20 **Kyle Michel** (Citrine Informatics)
The study of materials systems through machine learning and physical models

12:30–2:30 *Lunch (on your own)*

2:30–3:20 **Eric Stahlberg** (National Cancer Institute)
Accelerating Cancer Research Using Advanced Computing Solutions

3:30–4:00 *Break*

4:00–4:50 **Aram Harrow** (Massachusetts Institute of Technology)
Quantum Monte Carlo vs Tunneling in Adiabatic Optimization

Wednesday December 7, 2016

8:15–9:00 *Check-In/Breakfast (Hosted by IPAM)*

9:00–9:50 **Matthew Spellings** (University of Michigan)
Navigating colloidal design space with machine learning

10:00–10:15 *Break*

10:15–11:05 **Ioana Dumitriu** (University of Washington)
Two Clustering Problems for the Stochastic Block Model

11:15–11:30 *Break*

11:30–12:20 **David Beratan** (Duke University)
Molecular discovery in silico and in cranio

12:30–2:00 *Lunch (on your own)*

2:00–2:50 **Sadasivan Shankar** (Harvard University)
Machine Learning for Materials Design: Combination of Theoretical methods, Heuristics, and Hybrid Techniques

3:00–3:15 *Break*

3:15–4:05 **Rebecca Willett** (University of Wisconsin-Madison)
Sparsity and Scarcity in Discrete Event Data Analysis

4:15–4:30 *Break*

4:30–5:20 **Alvaro Vazquez-Mayagoitia** (Argonne National Laboratory)
Large Data production and workflows for materials discovery using parallel computing

Thursday December 8, 2016

8:15–9:00	*Check-In/Breakfast (Hosted by IPAM)*
9:00–9:50	**Johannes Hachmann** (SUNY Buffalo) *A Software Ecosystem for the Data-Driven Design of Chemical Systems and the Exploration of Chemical Space*
10:00–10:15	*Break*
10:15–11:05	**John Parkhill** (University of Notre Dame) *TensorMol 0.0 a Package for Statistical Models of Molecular Structure*
11:15–11:30	*Break*
11:30–12:20	**Thomas Bligaard** (Stanford University) *Utilizing machine learning to accelerate computational catalyst search*
12:30	*Conclusion*

IPAM strives to provide an inclusive environment free of harassment. IPAM does not tolerate sexual harassment, other forms of harassment, or sexual assault. Please familiarize yourself with our community agreement which includes instructions on reporting incidents by using the QR code to the right.