

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*

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- 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 Bliggard** (Stanford University)
Utilizing machine learning to accelerate computational catalyst search
- 12:30 *Conclusion*

