

CS6208 : Advanced Topics in Artificial Intelligence

Graph Machine Learning

Administrative (Week 4)

Semester 2 2022/23

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UCLA/IPAM workshop on “Learning and Emergence in Molecular Systems”

- Great workshop on deep learning, physics and chemistry !
- All talks (videos and slides) are available at <http://www.ipam.ucla.edu/programs/workshops/learning-and-emergence-in-molecular-systems>

The screenshot shows the IPAM website with a navigation bar at the top. The main heading is "Workshops". Below it, the specific workshop is "Workshop II: Interpretable Learning in Physical Sciences", part of the Long Program Machine Learning for Physics and the Physics of Learning, held from October 14-18, 2019. The page has tabs for Overview, Speaker List, and Schedule. The Overview section contains an introductory text about the workshop's focus on physical sciences and machine learning, and lists the organizing committee members: Cecilia Clementi, Kyle Cranmer, Nathan Kutz, Francesco Poesani, and Andrew White.

2019

Xavier Bresson

The screenshot shows the IPAM website for the "Workshops" section. The specific workshop is "Learning and Emergence in Molecular Systems", held from January 23-27, 2023. The page has tabs for Overview, Speaker List, Location, and Application & Registration. The Overview section contains an introductory text about the workshop's focus on molecular systems and machine learning, and lists the organizing committee members: Xavier Bresson, Cecilia Clementi, Klaus Robert Müller, Patrick Riley, and Max Welling.

2023

All times in this Schedule are Pacific Time (PT)

Monday, January 23, 2023	
Morning Session	
8:00 - 8:55	Breakfast (hosted by IPAM)
8:55 - 9:00	Welcome & Opening Remarks
9:00	Session Chair: Xavier Bresson (National University of Singapore)
9:00 - 9:50	Frank Noe (Freie Universität Berlin) Advancing molecular simulation with deep learning
10:00 - 10:15	Break
10:15 - 11:05	Patrick Riley (Relay Therapeutics) Symbolic Regression for Discovery of a DFT Functional
11:15 - 11:30	Break
11:30 - 12:20	Mohammed AlQuraishi (Harvard Medical School) OpenFold: Lesson learned and insights gained from rebuilding and retaining AlphaFold2
12:30 - 2:30	Lunch (on your own)
Afternoon Session	
2:30	Session Chair: Alex Tkatchenko (University of Luxembourg)
2:30 - 3:20	Cecilia Clementi (Freie Universität Berlin) Course-graining classical and quantum systems
3:30 - 4:00	Break
4:00 - 4:50	Piyel Das (IBM Research) Design and Evaluation of Foundation Models and Generative AI in Molecular Space

Tentative Outline

- This module focuses on the foundations of graph machine learning.
 - Introduction to Graph Deep Learning
 - Introduction to Graph Science
 - Graph Analysis Techniques without Feature Learning
 - • Graph clustering
 - Classification
 - Recommendation
 - Dimensionality reduction
 - Visualization
 - Shallow graph feature learning
- Graph Convolutional Networks (spectral and spatial)
- Benchmarking GNNs
- Graph Positional Encoding
- Graph ViT/MLP-Mixer
- Generative GNNs and biology
- Combinatorial optimization
- GNNs for Recommendation
- GNNs for knowledge graphs
- Theory of GNNs



Questions?