

# CS6208 : Advanced Topics in Artificial Intelligence

## Graph Machine Learning

Administrative (Week 8)

Semester 2 2022/23

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# Deep learning + discrete optimization

- UCLA/IPAM Workshop “Deep Learning and Discrete Optimization”
  - <http://www.ipam.ucla.edu/programs/workshops/artificial-intelligence-and-discrete-optimization>
- Check out the videos
  - <https://www.youtube.com/playlist?list=PLHyI3FbmV0SfG1vnBcJMn13NsJb7V92ha>

**Artificial Intelligence and Discrete Optimization**  
FEBRUARY 27 - MARCH 3, 2023

OVERVIEW SPEAKER LIST LOGGING APPLICATION & REGISTRATION

### Overview

In recent years, the use of Machine Learning techniques to Operations Research (OR) problems, especially in the Discrete Optimization (DO) a.k.a. Combinatorial Optimization context, opens very interesting scenarios because DO is the “home” of an endless list of decision-making problems that are of fundamental importance in multistage applications.

The workshop will bring together experts in mathematics (optimization, graph theory, sparsity, combinatorics, statistics), operations research (assignment problems, routing, planning, Bayesian search, automation, scheduling), machine learning (deep learning, supervised, self-supervised and reinforcement learning) and artificial intelligence at large (including multi-agent systems, interpretability, fairness, etc.). In addition, the focus will be on:

- Algorithmic challenges and potential of the interaction between AI and OR;
- Data requirements in which such an interaction can be profitable; and
- Application areas that are likely to lead to game-changing results (e.g., transportation, supply chain, public policy, energy).

Program Flyer

**ORGANIZING COMMITTEE**

Xavier Bresson (National University of Singapore)  
Bistra Dilkina (University of Southern California (USC))  
Andrea Lodi (Cornell University)  
Pascal Van Hentenryck (Georgia Institute of Technology)

### Speaker List

Matej Balog (DeepMind)  
Hamsa Bastani (University of Pennsylvania)  
Timo Berthold (Technische Universität Berlin)  
Xavier Bresson (National University of Singapore)  
Bistra Dilkina (University of Southern California (USC))  
Priya Donti (Cornell University)  
Tina Eliassi-Rad (Northeastern University)  
Paul Grigas (University of California, Berkeley (UC Berkeley))  
Tias Guns (KU Leuven)  
Stefanie Jegelka (Massachusetts Institute of Technology)  
Elias Khalil (University of Toronto)  
Thomas Laurent (Loyola Marymount University)  
Andrea Lodi (Cornell University)  
Rahul Mazumder (Massachusetts Institute of Technology)  
Azalia Mirhoseini (Google AI)  
Vinod Nair (Google Brain)  
Louis-Martin Rousseau (École Polytechnique de Montréal)  
Le Song (Georgia Institute of Technology)  
Bartolomeo Stellato (Princeton University)  
Yundong Tian (Artificial Intelligence Center)  
Pascal Van Hentenryck (Georgia Institute of Technology)  
Phebe Vayanos (University of Southern California (USC))  
Petar Velicković (DeepMind Technologies)  
Ellen Vitercik (Stanford University)  
Segev Wasserkrug (IBM Research - Israel)

YouTube

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2023 Artificial Intelligence and Discrete Optimization

Institute for Pure & Applied Mathematics (IPAM)

17 videos 33 views Updated yesterday

Play all Shuffle

In recent years, the use of Machine Learning techniques to Operations Research (OR) problems, especially in the Discrete Optimization (DO) a.k.a. Combinatorial Optimization context, opens very interesting scenarios because DO is the “home” of an endless list of decision-making

- 1 Pascal Van Hentenryck - Fusing Machine Learning and Optimization - IPAM at UCLA  
Institute for Pure & Applied Mathematics (IPAM) • 1K views • 2 days ago
- 2 Bartolomeo Stellato - Learning for Decision-Making Under Uncertainty - IPAM at UCLA  
Institute for Pure & Applied Mathematics (IPAM) • 490 views • 2 days ago
- 3 Phebe Vayanos - Integer optimization for predictive & prescriptive analytics in high stakes domains  
Institute for Pure & Applied Mathematics (IPAM) • 470 views • 2 days ago
- 4 Bistra Dilkina - Machine Learning for MIP Solving - IPAM at UCLA  
Institute for Pure & Applied Mathematics (IPAM) • 522 views • 4 days ago
- 5 Vinod Nair - Restricted Boltzmann Machines for Maximum Satisfiability - IPAM at UCLA  
Institute for Pure & Applied Mathematics (IPAM) • 593 views • 4 days ago
- 6 Andrea Lodi - Continuous cutting plane algorithms in integer programming - IPAM at UCLA  
Institute for Pure & Applied Mathematics (IPAM) • 349 views • 4 days ago

## Group selection

- Group can be composed of 1 or 2 or 3 members, preferably 2-3 but not more than 3.
  - Use Canvas – Discussions – Project group if you need to find groupmate(s).
- Choose your group wisely
  - Each teammate must contribute \*equally\* to the project. Clearly, each member has different skills and it is fine to be weaker in maths, coding, etc. However, it is not fine to let the other teammates to do most of the work.
- Minimize conflict and make a short written “contract” at the beginning of the project regarding the commitment of each team member to the project.
  - Upload the “contract” to Canvas – Assignments – Group project contract with the file name “projectCS6208\_contract\_name1\_name2.pdf”
- • Deadline is Week 8, Tue March 7<sup>th</sup> 2023 11:59pm.
- Penalty : You will lose 25% of the project grade every late day (except medical certificate).
- It is fine that commitments change during the project development but the contributions must remain equally distributed.

## Review paper and group project

- The topics of the review paper and the group project must be different.
  - For example, you cannot review a paper on molecular generation and develop a project on molecular generation. But you can review a paper on graph recommendation and develop a project on molecular generation.
  - There must be significant differences between the review paper and the group project.

# Office hour

- From Week 8, I will offer office hours to discuss lectures, etc
  - When/where?
    - Tue 4:30pm-5:30, my office COM2-04-26
  - How?
    - Appointment : ~~Send me an email for priority,~~ [xavieres@nus.edu.sg](mailto:xavieres@nus.edu.sg)  
Please, use the excel file to make an appointment  
[https://docs.google.com/spreadsheets/d/1ynmNJtMazF7HbKXwot8\\_UY9s-Gm6a9g\\_XuaoA9S1Pv0](https://docs.google.com/spreadsheets/d/1ynmNJtMazF7HbKXwot8_UY9s-Gm6a9g_XuaoA9S1Pv0)
    - Walk-in meeting is fine but priority is by appointment
  - If nobody at 5pm, office hour stops
  - 15min max per student/group (more time if no student is waiting)

# Tentative Lectures

- Introduction to Graph Deep Learning
- Part 1: GML without feature learning (before 2014)
  - Introduction to Graph Science
  - Graph Analysis Techniques without Feature Learning
    - Graph clustering
    - Classification
    - Recommendation
    - Dimensionality reduction
- Part 2 : GML with shallow feature learning (2014-2016)
  - • Shallow graph feature learning
- Part 3 : GML with deep feature learning, a.k.a. GNNs (after 2016)
  - • Graph Convolutional Networks (spectral and spatial)
  - Benchmarking GNNs
  - Graph Transformer
  - Graph ViT/MLP-Mixer
  - Generative GNNs and molecular science
  - Combinatorial optimization
  - GNNs for Recommendation
  - GNNs for knowledge graphs
  - Theory of GNNs



Questions?