

CS6208 : Advanced Topics in Artificial Intelligence

Graph Machine Learning

Administrative (Week 2)

Semester 2 2022/23

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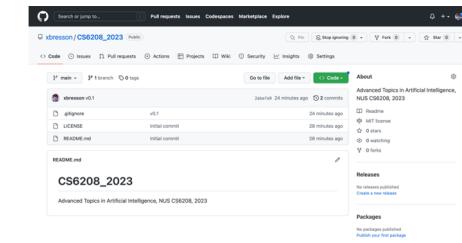
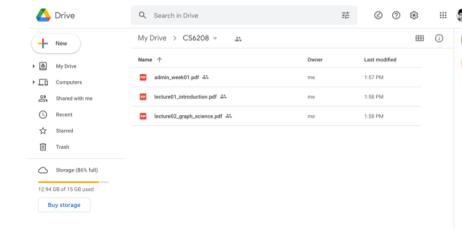
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Material

- Canvas : <https://canvas.nus.edu.sg/courses/38857>
- Slides : <https://drive.google.com/drive/folders/16sqBbQXl8Sq-DL5dfSwvmAmSm69Ae8dI>
Note: I reserve the right to change the slides until the lecture.
- Python notebooks : https://github.com/xbresson/CS6208_2023
Note: You will need to a Gmail account to use Google Colab.



Evaluation

- This module is 100% CA, i.e., there is no final exam.
- There are 2 components:
 - Individual assessment (50%) / 1 paper review : One-page latex report (one or two columns), write a prototype from scratch (no copy-paste with e.g. GitHub) on a dataset not used in the paper and upload on GitHub for reproducibility, identify the paper limitations, innovate and propose improvement(s). Paper is not given – select one GNN paper of interest. Deadline is Week 13.
 - Group assessment (50%) / 1 project : A group size of at most 3 people (1-3). Choose your group wisely (avoid conflict) -- each teammate must contribute equally to the project. Project is not given – select an original project that matches your interest/research. Project must demonstrate understanding, insights and innovation(s). Deliveries are one report (up to 2 latex pages, one or two columns), a GitHub repo to reproduce the results and a short recorded video presentation (each student will present her/his contribution to the project). Deadline is Week 14.
 - More details provided on Week 6 (before recess week).

Class attendance

- Students are expected to attend in-person the lectures

<https://www.comp.nus.edu.sg/covid19>



Update: 16 Aug 2022

University activities to resume

- As Singapore is transitioning to a new normal of living with COVID-19, university activities will resume.
- Students should expect to participate fully in university life and come back for face-to-face classes for all their modules. This excludes the lectures for courses in which instructors are developing Blended Learning as part of the university's plan to create high-quality, integrated e-learning materials to enhance learning flexibility and effectiveness.
- Instructors are also no longer obligated to make video recordings of their classes or to set up hybrid arrangements. The university has discussed and explained the key considerations for this to the NUS Students' Union (NUSSU) previously. Thus, if students are not able to attend classes due to valid reasons including COVID-19, they should discuss with their course instructor on the next steps.
- Students should continue to be responsible for their health and upload their self-administered Antigen Rapid Test (ART) to uNivUS, should they test positive for COVID-19.
 - If the first self-administered ART result is positive, students will be excused from classes (including lectures, tutorials and other academic activities) and assessment(s) from Days 1 to 7 inclusive, where Day 1 refers to the day that students first test positive.
 - If students are still COVID-19 positive from Day 8 onwards, they will need to upload a self-administered ART showing that they are still testing positive, to uNivUS. This will then serve as a valid excuse from classes and assessment(s).
- For the most up-to-date information on COVID-19 Safe Management Measures and related NUS circulars, please visit emergency.nus.edu.sg

Next week

- No lecture for week 3 : Chinese New Year ☺
- If interested in AI+Biology, watch the video talks of the workshop in “Learning and Emergence in Molecular Systems” at UCLA:
<http://www.ipam.ucla.edu/programs/workshops/learning-and-emergence-in-molecular-systems>



The screenshots show the IPAM website's 'Workshops' section for the 'Learning and Emergence in Molecular Systems' event, which took place from January 23 to 27, 2023. The left screenshot shows the 'Overview' page, which includes a brief description of the workshop, a speaker list, and a registration form. The right screenshot shows the 'Speaker List' page, which lists numerous speakers from various institutions.

Workshop Overview:

This workshop will focus on the field of objects or emergent properties. We will study the concrete examples of these systems and how they can be modeled. This is mainly due to the need of formulating and solving many-body quantum mechanics and chaos. On one side, the accurate solution of the Schrödinger equation for large molecular systems is computationally prohibited. One the other side, even if we knew the forces exactly, the dynamical evolution of the system is exponentially sensitive to initial conditions. In addition, it is very difficult to find a model capable to predict future trajectories. Some aspects of these systems remain predictable at a macroscopic scale, but they require completely different variables, such as pressure, temperature and entropy. We call this emergent theory thermodynamics.

In an extremely different direction of machine learning, a fairly simple phenomenon takes place. The reconstructed version of an image will be given by its constituent pixel values. When we analyze the image with a deep neural network (DNN), we will detect edges in the first layer, corners in the next layer, then the object parts and finally, at the top of the neural network, entire objects. We understand the world at the "emergent" level of objects and their relations, without understanding the underlying mechanism. In machine learning DNN, emergence happens automatically through learning and some inductive biases such as symmetry.

A major question we want to address in this workshop is whether we can apply the same learning paradigm to the field of molecular science to learn the correct emergent variables and dynamics.

This workshop will include a poster session; a request for posters will be sent to registered participants in advance of the workshop.

Program Chair:

Xavier Bresson (PoliU)
Klaus-Robert Müller (Technische Universität Berlin)
Petra Tschöpe (Fritz Haber Institute)

Organizing Committee:

Xavier Bresson (PoliU)
Dustin Gabeck (PoliU)
Klaus-Robert Müller (Technische Universität Berlin)
Petra Tschöpe (Fritz Haber Institute)
Max Welling (Microsoft Research)

Speakers:

Mohamed Al-Jarrah (Harvard Medical School)
Xavier Bresson (National University of Singapore)
Steve Bruck (University of Washington)
Sylvia Chon (Technische Universität Berlin)
Kyungwan Cho (New York University)
Cecilia Clement (Free University Berlin)
Bruno Corrêa (Ecole Polytechnique Fédérale de Lausanne (EPFL))
Klaus-Robert Müller (Technische Universität Berlin)
Petar Dots (IBM Research)
Ron Dorfler (Stanford University)
Ran Eliezer (Massachusetts Institute of Technology)
Sergei Kalinin (University of Tennessee)
Peter Kourouklis (Harvard University)
Peter Kralj (University of Ljubljana)
Kris Poon (University of California, Berkeley (UC Berkeley))
Patrick Riley (Riley Therapeutics)
Jutta Rogel (New York University Institute of Technology)
Thomas Schuster (University of Luxembourg)
Mark Tuckerman (New York University)
Anatoli von Lilienfeld (University of Toronto)
Max Welling (Microsoft Research)
Boye Ye (University of California, San Diego (UCSD))

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 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



NUS Course Materials: Ethical Behaviour and Respecting Copyright

All course participants (including permitted guest students) who have access to the course materials on LumiNUS or any approved platforms by NUS for delivery of NUS modules are not allowed to re-distribute the contents in any forms to third parties without the explicit consent from the module instructors or authorized NUS officials



Examples of Disallowed Things

No Posting on any websites (except for the materials explicitly allowed by your lecturer in the respective module)

No selling of material

No sharing of questions/answers which could lead to cheating/plagiarism



Questions?