CS6208 : Advanced Topics in Artificial Intelligence
Graph Machine Learning

Administrative (Week 1)

Semester 2 2022/23

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About Me

Xavier Bresson

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- Prof of Computer Science at NUS, Singapore
- Undergraduate in France (theoretical physics), PhD at EPFL, Switzerland (computer vision), Postdoctorate at UCLA, US (applied mathematics)
- Mostly research on deep learning, graph theory and optimization
- Taught Bachelor, Master, PhD courses in DS and DL since 2014 at UCLA, EPFL, NTU, NYU

https://twitter.com/xbresson
https://scholar.google.com/citations?user=9pSK04MAAAAJ
https://www.youtube.com/channel/UCeONAtqVKCS30Xn6zy1YQ_g
https://github.com/xbresson
https://www.linkedin.com/in/xavier-bresson-738585b
https://www.facebook.com/xavier.bresson.1
https://graphdeeplearning.github.io
https://www.comp.nus.edu.sg/cs/people/xaviercs

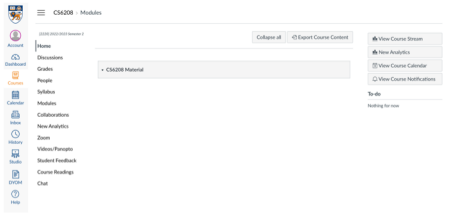
Students

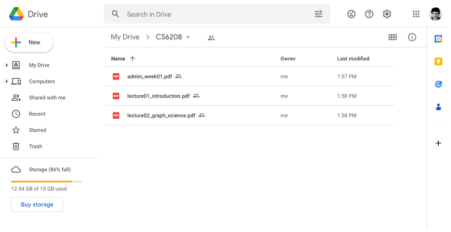
Class Logistics

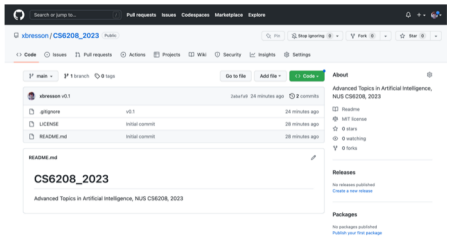
- Class Schedule
  - Lectures : 2 hours on Tuesdays 2-4pm, LT19
- Material
  - Admin : Canvas https://canvas.nus.edu.sg/courses/38857
  - Slides : https://drive.google.com/drive/folders/16sqBbQXl8Sq-DL5dfSwvmAmSm69Ae8dI

    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.







Communication

- Questions
  - Please, ask questions during class ☺
- Emails
  - I do not usually answer individual emails ☹
  - But I will answer email questions during class to benefit everyone ☺
- Teaching assistant
  - No TA (6000-class)

Tentative Outline

- This module focuses on the understanding of the foundations of graph machine learning and specifically graph neural networks.
  - Introduction to Graph Deep Learning
  - Introduction to Graph Science
  - Traditional Graph Machine 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

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).

Learning Outcomes

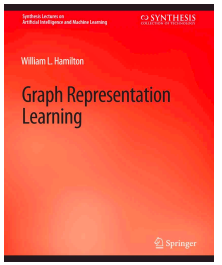
- At the end of this semester, students should be able to
  - Explain the principles different GNN layers and networks.
  - Compare different GNN architectures.
  - Identify and apply GNN techniques to different data problems.
  - Implement popular GNNs (with libraries like DGL, PyG or TensorFlowGNN).
  - Analyze and solve real-world problems using graph networks.

- Short-term goal : Learn the current most powerful graph data analysis tools.

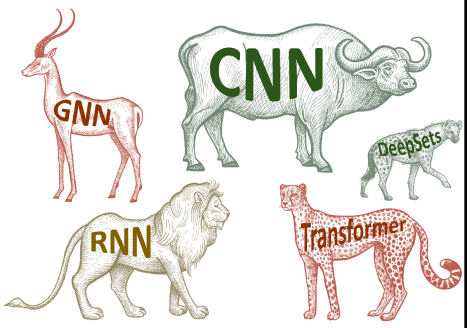
- Long-term goal : Data scientists/deep learning experts have become one of the most-wanted jobs in industry (GNN is part of the toolbox).

Books

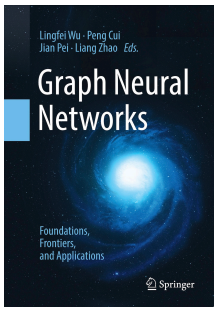
- Graph Representation Learning Book, Springer, 2020
  - William Hamilton, McGill University
  - https://link.springer.com/book/10.1007/978-3-031-01588-5
  - https://github.com/RHxW/CV-DL-Docs/blob/master/GRL_Book.pdf

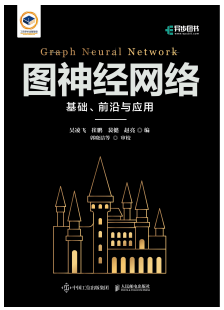


- Geometric Deep Learning: Grids, Groups, Graphs, Geodesics, and Gauges, 2021
  - Michael M. Bronstein (Oxford), Joan Bruna (NYU), Taco Cohen (Qualcomm), Petar Veličković (DeepMind)
  - https://arxiv.org/pdf/2104.13478.pdf



- Graph Neural Networks: Foundations, Frontiers, Applications, Springer, 2022
  - Lingfei Wu (Pinterest), Peng Cui (Tsinghua), Jian Pei, (Duke), Liang Zhao (Emory University)
  - https://graph-neural-networks.github.io (English and Chinese versions)





NUS Course Materials: Ethical Behaviour and Respecting Copyright

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?