

CS5284 : Graph Machine Learning

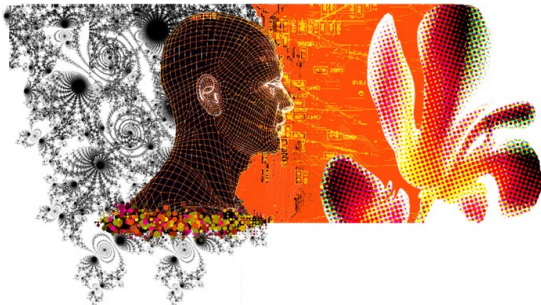
Administrative (Week 1)

Semester 1 2025/26

Xavier Bresson

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National University of Singapore (NUS)



Instructor



Xavier Bresson
xaviercs@nus.edu.sg

- Prof of Computer Science at NUS, Singapore
- Undergraduate in France, PhD at EPFL, Switzerland, Postdoctorate at UCLA, US
- Researcher in Deep Learning and Graphs
- NRF Fellowship
- Speaker at NeurIPS, ICML, ICLR, CVPR, SIAM, KDD
- Teach Bachelor, Master, PhD courses in DS and DL since 2014 at UCLA, EPFL, NYU, NTU
- Consulting & training for companies



Marseille



Paris



Geneva



Los Angeles



Hong Kong



Singapore

<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>

Teaching Assistants



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LIU NIAN

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Kindly show respect to your TAs!

They are experts dedicated to assisting you in succeeding in this module.

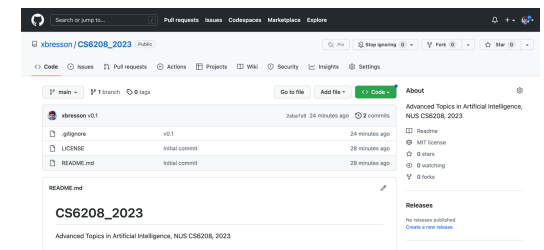
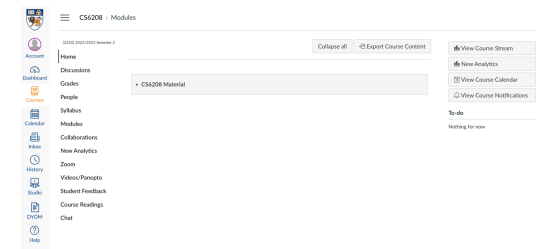
Audience



Which school/dept are you from?

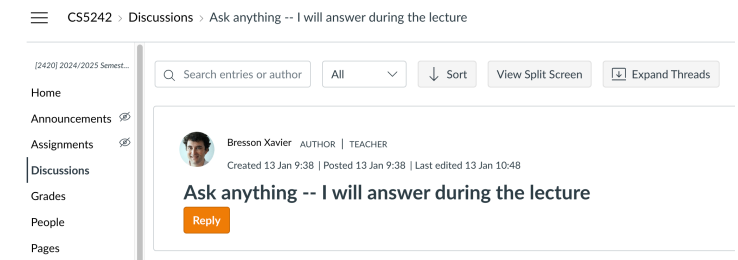
Class Logistics

- Class Schedule
 - Lecture : Wednesdays 6:30pm-8:20pm
 - Venue : LT19
 - Tutorial (starting Week 3) : Wednesdays 8:30pm-9:20pm
 - Venue : <https://nusmods.com/courses/CS5284/graph-machine-learning>
- Material
 - Admin : Canvas <https://canvas.nus.edu.sg/courses/78107>
 - Note: I reserve the right to change the slides until the lecture to fix typos/mistakes, update material.
 - Python notebooks : https://github.com/xbresson/CS5284_2025
Note: You will need to a Gmail account to use Google Colab.



Communication

- Questions
 - Please, ask questions during class 😊
- Canvas
 - Use Home > Discussions > Ask anything
 - I will answer questions during class to benefit everyone 😊
- Email
 - I will answer email questions during class to benefit everyone 😊
- Teaching Assistant
 - Ask questions to your TA during tutorials or via emails



Hierarchical teaching organization



God Lecturer, Xavier Bresson

Busy running his kingdom with course management, research team, university services, etc.
I will mostly communicate with students during the lecture days. I will listen to your prayers and questions, and answer to you and everyone during the lectures.



Divinity TAs, Wang Jiaming, Zeng Yuwei, Ryoji Kubo
Top AI researchers which are here to help you succeeding this course. Please, communicate directly with them, as they have more time and accessibility.

Human Students

Communicate first with your TAs if you have any question about the lectures, tutorials, exams, project, illness, etc. TAs know 95% of responses. They will tell me if there is an important question and I will intervene.



Tentative outline

- This module focuses on the understanding of the foundations of graph machine learning and specifically graph neural networks.
 - Lecture 01 : Introduction to Graph Machine Learning
 - Lecture 02 : Introduction to Graph Science
 - Lecture 03 : Graph SVM
 - Lecture 04 : Recommendation on graphs
 - Lecture 05 : Graph-based visualization
 - Lecture 06 : Shallow graph feature learning
 - Lecture 07 : Graph Convolutional Networks
 - Lecture 08 : Weisfeiler-Lehman GNNs
 - Lecture 09 : Graph Transformers
 - Lecture 10 : Graph generation & molecular science
 - Lecture 11 : Material design
 - Lecture 12 : Integrating GNNs and LLMs
 - Lecture 13 : Deep Learning for Combinatorial optimization

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 DGL).
 - 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 has become part of the toolbox).

Face-to-face class / NO online option will be made available

- NUS policy mandates in-person participation for lectures and tutorials.
- Remote or online attendance is not permissible.
- Attendance at lectures and tutorials requires physical presence.
- In instances where physical attendance poses challenges, students have the option to defer enrolment to the subsequent semester (i.e., Semester 1 AY26/27) for the same course.



QR Attendance

- We will use a QR-based attendance system for lectures.
- Please, scan the QR image I will provide during Wednesday lectures to confirm your attendance.
- Note that a new QR code will be provided for each lecture.



JUST A SAMPLE
NOT ACTIVE

Assessment

- This module is 100% CA, i.e., there is no final exam.
- There are 4 components
 - Assessment 1 (Week 7) : 25%
 - Assessment 2 (Week 13) : 35%
 - Attendance : 5%
 - Group Project (W6-W14) : 35%
 - TOT : 100%
- Assessments 1 & 2 are open-book and composed of Multiple Response Questions (MRQs) and coding questions that follow Tutorials' notebooks (note that LLMs cannot be used during these assessments).
- The primary objective of these assessments is to evaluate your understanding of the module concepts, rather than your ability to use pre-computed solutions from e.g. GitHub, or utilize extensive GPUs.

2024 Student Feedback

- Recommendation: This course may not be suitable for you if
 - You lack confidence in mathematics, particularly in areas like linear algebra, optimization, statistics and graphs.
 - You are not comfortable with coding, as the assessments will require Python, PyTorch and DGL.
 - You are not at ease with self-learning.
 - Your main objective is an easy A-grade.



Agreement

- Please, fill out the agreement :
<https://forms.gle/tt1bxQA4f2CxGEYW9>
- Deadline : End of Week 2, August 24, 2025, 11:59pm.
- Penalty : 5-point deduction from the final grade.

Agreement for CS5284 – Graph Machine Learning

You must sign and submit this agreement by the end of Week 2, i.e., **August 24, 2025, 11:59 PM**.

Failure to submit by the deadline will result in a **5-point deduction** from your final grade.

Date: August 11, 2025

The lecturer of CS5284 – Graph Machine Learning has informed me that:

1. The previous version of this module was rated as **difficult or very difficult** by 98% of students.
2. The module requires **substantial self-learning** in:
 - Mathematics (linear algebra, optimization, statistics, graphs)
 - Coding (Python, PyTorch, DGL)

xavier.bresson@gmail.com [Switch account](#)

Not shared

** Indicates required question*

Full Name *

Date *

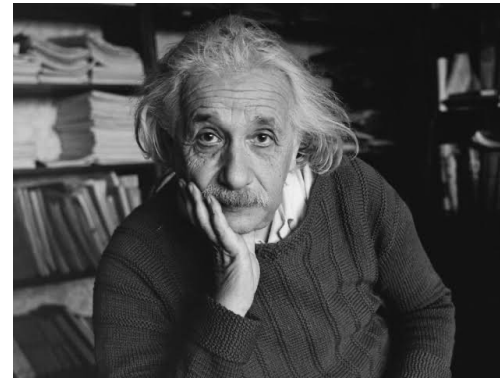
Acknowledgement *
☐ I acknowledge and accept the conditions of this module.

Why is this course challenging?

“The aim of education is to learn how to think, not what to memorize”

“Read more. Reflect deeply. Let your curiosity be your most faithful guide”

-- Albert Einstein's key educational philosophy

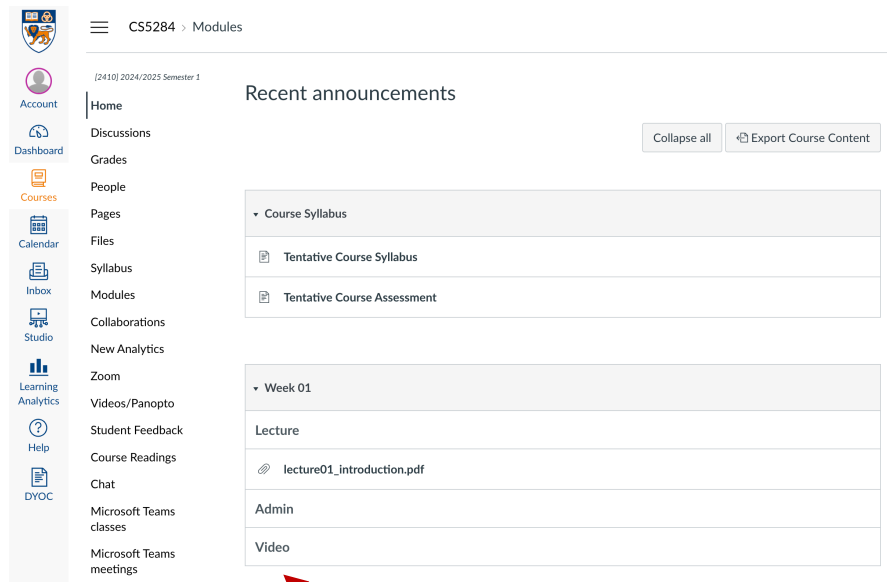


Course philosophy

- The primary focus of the course and assessments is to ensure an understanding of the fundamental concepts behind graph deep learning, i.e. building a first-principles foundation of graph machine learning.
- It is not focused on solely applying pre-built optimized modules in frameworks like PyTorch or TensorFlow, which does not require an academic background.
- Once you grasp how graph machine learning works, you will be equipped to tackle complex projects and quickly address theoretical challenges.
- The depth of understanding required makes the course demanding, which is why 98% of past students have rated it as “difficult” or “very difficult”.
- If you are aiming for an easy A-grade, I strongly recommend considering alternative Level 5 courses that might be more manageable.

Video recording

- Lectures will be recorded and posted on Canvas.



STUDENT CONDUCT AND ACADEMIC INTEGRITY



(1) Student Discipline <https://www.nus.edu.sg/registrar/administrative-policies-procedures/undergraduate/nus-statutes-and-regulations>

Student discipline is governed by the NUS Statutes and Regulations. Any violation, as detailed in Clause 3 of NUS Statute 6, may lead to disciplinary measures, including suspension or expulsion. Please visit the NUS Student Portal for further information on disciplinary matters.

(2) Code of Student Conduct <https://studentconduct.nus.edu.sg/wp-content/uploads/NUS-Code-of-Student-Conduct.pdf>

NUS students are encouraged to familiarise themselves with the NUS Code of Student Conduct, which provides an overview of the behaviour expected of members of the University community.

- **Plagiarism** : The University takes a strong stance against plagiarism and considers it a serious form of academic dishonesty. Any student found to have taken the work or ideas of another person or entity, including through the use of generative Artificial Intelligence (AI), and passed them off as one's own without proper attribution will be subject to disciplinary action. Please refer to the updated NUS Plagiarism Policy. <https://myportal.nus.edu.sg/studentportal/student-discipline/all/docs/NUS-Plagiarism-Policy.pdf>
- **Cheating** : The University prohibits cheating in any form during assessments, tests, quizzes or examinations. Such acts will be considered, at minimum, as “Moderate” offences, resulting in the default sanction of a ‘Fail’ grade for the entire course.



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

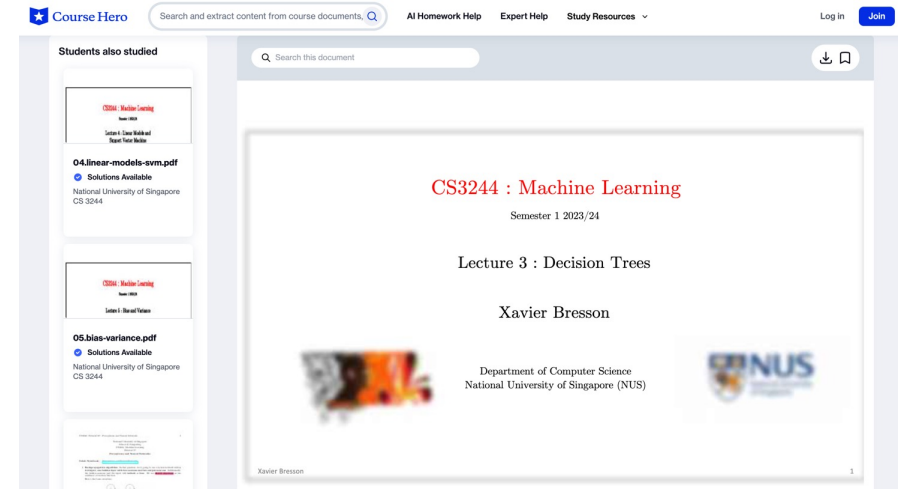


Examples of Disallowed Things

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?