



(<http://snap.stanford.edu/>) (<http://stanford.edu/>)



# CS224W: Machine Learning with Graphs

Stanford / Fall 2023

## Logistics

- **Lectures:** are on Tuesday/Thursday 3:00-4:20pm **in person** in the NVIDIA Auditorium (<https://campus-map.stanford.edu/?srch=NVIDIA+Auditorium>).
- **Lecture Videos:** are available on Canvas (<https://canvas.stanford.edu/courses/179477>) for all the enrolled Stanford students.
- **Public resources:** The lecture slides and assignments will be posted online as the course progresses. We are happy for anyone to use these resources, but we cannot grade the work of any students who are not officially enrolled in the class.
- **Contact:** Students should ask all course-related questions on Ed (accessible from Canvas), where you will also find announcements. For external inquiries, personal matters, or in emergencies, you can email us at [cs224w-aut2324-staff@lists.stanford.edu](mailto:cs224w-aut2324-staff@lists.stanford.edu).
- **Academic accommodations:** If you need an academic accommodation based on a disability, you should initiate the request with the Office of Accessible Education (OAE) (<https://oae.stanford.edu/students/accommodations-services/academic-accommodations>). The OAE will evaluate the request, recommend accommodations, and prepare a letter for the teaching staff. Once you receive the letter, send it to our staff email address. Students should contact the OAE as soon as possible since timely notice is needed to coordinate accommodations.

## Instructor



Jure Leskovec

(<https://profiles.stanford.edu/jure-leskovec>)

## Guest Instructor



Joshua Robinson

(<https://joshrobinson.mit.edu/>)

## Course Assistants

(<https://xikunzhang.github.io/>)

Xikun Zhang

(<https://xikunzhang.github.io/>)

Head CA

(<http://hamedn.com/>)

Hamed Nilforoshan

(<http://hamedn.com/>)

Aditya Agrawal

(<https://www.linkedin.com/in/adityaagrawal001>)

Abhinav Garg

(<https://www.linkedin.com/in/abhinavgarg/>)

Matthew Jin

(<https://profiles.stanford.edu/matthewjin>)

Yunqi Li

(<https://www.linkedin.com/in/yunqi-li-716071183/>)

Tolu Oyeniyi

(<https://www.linkedin.com/in/tolu-oyeniyi/>)

Chenshu (Jupiter) Zhu

(<https://www.linkedin.com/in/chenshu-z/>)

Pratham Soni

(<https://stanford.edu/~prathams/>)

Anirudh Sriram

(<https://www.linkedin.com/in/anirudh-sriram-1b136318a>)

## Content

### What is this course about?

Complex data can be represented as a graph of relationships between objects. Such networks are a fundamental tool for modeling social, technological, and biological systems. This course focuses on the computational, algorithmic, and modeling challenges specific to the analysis of massive graphs. By means of studying the underlying graph structure and its features, students are introduced to machine learning techniques and data mining tools apt to reveal insights on a

variety of networks.

**Topics include:** representation learning and Graph Neural Networks; algorithms for the World Wide Web; reasoning over Knowledge Graphs; influence maximization; disease outbreak detection, social network analysis.

## Previous Offerings

You can access slides and project reports of previous versions of the course on our archived websites: CS224W: Winter 2023 (<https://snap.stanford.edu/class/cs224w-2023/>) / CS224W: Fall 2021 (<http://snap.stanford.edu/class/cs224w-2021/>) / CS224W: Winter 2021 (<http://snap.stanford.edu/class/cs224w-2020/>) / CS224W: Fall 2019 (<http://snap.stanford.edu/class/cs224w-2019/>) / CS224W: Fall 2018 (<http://snap.stanford.edu/class/cs224w-2018/>) / CS224W: Fall 2017 (<http://snap.stanford.edu/class/cs224w-2017/>) / CS224W: Fall 2016 (<http://snap.stanford.edu/class/cs224w-2016/>) / CS224W: Fall 2015 (<http://snap.stanford.edu/class/cs224w-2015/>) / CS224W: Fall 2014 (<http://snap.stanford.edu/class/cs224w-2014/>) / CS224W: Fall 2013 (<http://snap.stanford.edu/class/cs224w-2013/>) / CS224W: Fall 2012 (<http://snap.stanford.edu/class/cs224w-2012/>) / CS224W: Fall 2011 (<http://snap.stanford.edu/class/cs224w-2011/>) / CS224W: Fall 2010 (<http://snap.stanford.edu/class/cs224w-2010/>)

## Prerequisites

Students are expected to have the following background:

- Knowledge of basic computer science principles, sufficient to write a reasonably non-trivial computer program (e.g., CS107 or CS145 or equivalent are recommended)
- Familiarity with the basic probability theory (CS109 or Stat116 are sufficient but not necessary)
- Familiarity with the basic linear algebra (any one of Math 51, Math 103, Math 113, or CS 205 would be much more than necessary)

The recitation sessions in the first weeks of the class will give an overview of the expected background.

## Course Materials

Notes and reading assignments will be posted periodically on the course Web site. The following books are recommended as optional reading:

- Graph Representation Learning ([https://www.cs.mcgill.ca/~wlh/grl\\_book/](https://www.cs.mcgill.ca/~wlh/grl_book/)) by William L. Hamilton
- Networks, Crowds, and Markets: Reasoning About a Highly Connected World (<http://www.cs.cornell.edu/home/kleinber/networks-book/>) by David Easley and Jon Kleinberg
- Network Science (<http://networksciencebook.com>) by Albert-László Barabási

## Schedule

Lecture slides will be posted here shortly before each lecture.

This schedule is subject to change. All assignment deadlines are at **11:59pm PT**.

Date: <b>Tue, 9/26</b>
Description: <b>1. Introduction</b> <b>[slides (slides/01-intro.pdf)]</b>
Events:
Deadlines:

Date: <b>Thu, 9/28</b>
Description: <b>2. Node embeddings</b> [slides (slides/02-nodeemb.pdf)]
<ul style="list-style-type: none"> <li>• DeepWalk: Online Learning of Social Representations (<a href="https://arxiv.org/pdf/1403.6652.pdf">https://arxiv.org/pdf/1403.6652.pdf</a>)</li> <li>• node2vec: Scalable Feature Learning for Networks (<a href="https://arxiv.org/pdf/1607.00653.pdf">https://arxiv.org/pdf/1607.00653.pdf</a>)</li> <li>• Network Embedding as Matrix Factorization (<a href="https://arxiv.org/pdf/1710.02971.pdf">https://arxiv.org/pdf/1710.02971.pdf</a>)</li> </ul>
Events: Colab 0 ( <a href="https://colab.research.google.com/drive/10-8W1e_WOX4-YocROm8tHbtm1frUf2S">https://colab.research.google.com/drive/10-8W1e_WOX4-YocROm8tHbtm1frUf2S</a> ), Colab 1 ( <a href="https://colab.research.google.com/drive/1vvloEqxGI1naopTZbh4bmCOLEiCxvcQq">https://colab.research.google.com/drive/1vvloEqxGI1naopTZbh4bmCOLEiCxvcQq</a> ) <b>out</b>
Deadlines:

Date: <b>Tue, 10/3</b>
Description: <b>3. Graph neural networks</b> [slides (slides/03-GNN1.pdf)]
<ul style="list-style-type: none"> <li>• Geometric Deep Learning: the Erlangen Programme of ML (<a href="https://iclr.cc/virtual/2021/invited-talk/3717">https://iclr.cc/virtual/2021/invited-talk/3717</a>)</li> <li>• Semi-Supervised Classification with Graph Convolutional Networks (<a href="https://arxiv.org/pdf/1609.02907.pdf">https://arxiv.org/pdf/1609.02907.pdf</a>)</li> </ul>
Events:
Deadlines:

Date: <b>Thu, 10/5</b>
Description: <b>4. A general perspective on GNNs</b> [slides (slides/04-GNN2.pdf)]
<ul style="list-style-type: none"> <li>• Design Space of Graph Neural Networks (<a href="https://arxiv.org/pdf/2011.08843.pdf">https://arxiv.org/pdf/2011.08843.pdf</a>)</li> <li>• Inductive Representation Learning on Large Graphs (<a href="https://arxiv.org/pdf/1706.02216.pdf">https://arxiv.org/pdf/1706.02216.pdf</a>)</li> <li>• Graph Attention Networks (<a href="https://arxiv.org/pdf/1710.10903.pdf">https://arxiv.org/pdf/1710.10903.pdf</a>)</li> </ul>
Events: Homework 1 (homework/CS_224W_Fall_2023_HW1.pdf) <b>out</b> LaTeX template (homework/CS_224W_Fall_2023_HW1-template.zip)
Deadlines:

Date: <b>Tue, 10/10</b>
Description: <b>5. GNN augmentation and training</b> [slides (slides/05-GNN3.pdf)]
<ul style="list-style-type: none"> <li>• Hierarchical Graph Representation Learning with Differentiable Pooling (<a href="https://arxiv.org/pdf/1806.08804.pdf">https://arxiv.org/pdf/1806.08804.pdf</a>)</li> </ul>
Events:
Deadlines:

Date: <b>Thu, 10/12</b>
Description: <b>6. Theory of GNNs</b> [slides (slides/06-theory.pdf)]
<ul style="list-style-type: none"> <li>How Powerful Are Graph Neural Networks? (<a href="https://arxiv.org/pdf/1810.00826.pdf">https://arxiv.org/pdf/1810.00826.pdf</a>)</li> </ul>
Events: Colab 2 ( <a href="https://colab.research.google.com/drive/1zunZQaGzLr782y3tkq3492rvw9UyY30l">https://colab.research.google.com/drive/1zunZQaGzLr782y3tkq3492rvw9UyY30l</a> ) <b>out</b>
Deadlines:

Date: <b>Tue, 10/17</b>
Description: <b>7. Heterogenous graphs</b> [slides (slides/07-hetero.pdf)]
<ul style="list-style-type: none"> <li>Modeling Relational Data with Graph Convolutional Networks (<a href="https://arxiv.org/pdf/1703.06103.pdf">https://arxiv.org/pdf/1703.06103.pdf</a>)</li> <li>Heterogeneous Graph Transformer (<a href="https://arxiv.org/pdf/2003.01332.pdf">https://arxiv.org/pdf/2003.01332.pdf</a>)</li> </ul>
Events:
Deadlines: Colab 1 <b>due</b>

Date: <b>Thu, 10/19</b>
Description: <b>8. Knowledge graphs</b> [slides (slides/08-kg.pdf)]
<ul style="list-style-type: none"> <li>Translating Embeddings for Modeling Multi-relational Data (<a href="https://papers.nips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf">https://papers.nips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf</a>)</li> <li>Learning Entity and Relation Embeddings for Knowledge Graph Completion (<a href="https://linyankai.github.io/publications/aaai2015_transr.pdf">https://linyankai.github.io/publications/aaai2015_transr.pdf</a>)</li> <li>Embedding Entities and Relations for Learning and Inference in Knowledge Bases (<a href="https://arxiv.org/pdf/1412.6575.pdf">https://arxiv.org/pdf/1412.6575.pdf</a>)</li> <li>Complex Embeddings for Simple Link Prediction (<a href="https://arxiv.org/pdf/1606.06357.pdf">https://arxiv.org/pdf/1606.06357.pdf</a>)</li> <li>RotatE: Knowledge Graph Embedding by Relational Rotation in Complex Space (<a href="https://arxiv.org/pdf/1902.10197.pdf">https://arxiv.org/pdf/1902.10197.pdf</a>)</li> </ul>
Events: Homework 2 (homework/CS_224W_Fall_2023_HW2.pdf) <b>out</b> LaTeX template (homework/CS_224W_Fall_2023_HW2-template.zip)
Deadlines: Homework 1 <b>due</b>

Date: <b>Tue, 10/24</b>
Description: <b>9. Reasoning over knowledge graphs</b> [slides (slides/09-reasoning.pdf)]
<ul style="list-style-type: none"> <li>Embedding Logical Queries on Knowledge Graphs (<a href="https://arxiv.org/pdf/1806.01445.pdf">https://arxiv.org/pdf/1806.01445.pdf</a>)</li> <li>Query2box: Reasoning over Knowledge Graphs in Vector Space Using Box Embeddings (<a href="https://arxiv.org/pdf/2002.05969.pdf">https://arxiv.org/pdf/2002.05969.pdf</a>)</li> <li>Traversing Knowledge Graphs in Vector Space (<a href="https://arxiv.org/pdf/1506.01094.pdf">https://arxiv.org/pdf/1506.01094.pdf</a>)</li> </ul>
Events:
Deadlines: Project Proposal <b>due</b>

Date: <b>Thu, 10/26</b>
Description: <b>10. Fast neural subgraph matching</b> [slides (slides/10-motifs.pdf)]
<ul style="list-style-type: none"> <li>• Network Motifs: Simple Building Blocks of Complex Networks (<a href="https://www.science.org/doi/10.1126/science.298.5594.824">https://www.science.org/doi/10.1126/science.298.5594.824</a>)</li> <li>• Neural Subgraph Matching (<a href="https://arxiv.org/pdf/2007.03092.pdf">https://arxiv.org/pdf/2007.03092.pdf</a>)</li> <li>• SPMiner: Frequent Subgraph Mining by Walking in Order Embedding Space (<a href="http://snap.stanford.edu/frequent-subgraph-mining/">http://snap.stanford.edu/frequent-subgraph-mining/</a>)</li> </ul>
Events: Colab 3 ( <a href="https://colab.research.google.com/drive/18PQ-B2wDmomjPtHroLNg_aH3hFniLNKn">https://colab.research.google.com/drive/18PQ-B2wDmomjPtHroLNg_aH3hFniLNKn</a> ) <b>out</b>
Deadlines: Colab 2 <b>due</b>

Date: <b>Tue, 10/31</b>
Description: <b>11. GNNs for recommenders</b> [slides (slides/11-recsys.pdf)]
<ul style="list-style-type: none"> <li>• Neural Graph Collaborative Filtering (<a href="https://arxiv.org/pdf/1905.08108.pdf">https://arxiv.org/pdf/1905.08108.pdf</a>)</li> <li>• LightGCN: Simplifying and Powering Graph Convolution Network for Recommendation (<a href="https://arxiv.org/pdf/2002.02126.pdf">https://arxiv.org/pdf/2002.02126.pdf</a>)</li> <li>• Graph Convolutional Neural Networks for Web-Scale Recommender Systems (<a href="https://arxiv.org/pdf/1806.01973.pdf">https://arxiv.org/pdf/1806.01973.pdf</a>)</li> </ul>
Events:
Deadlines:

Date: <b>Thu, 11/2</b>
Description: <b>12. Deep generative models for graphs</b> [slides (slides/12-deep-generation.pdf)]
<ul style="list-style-type: none"> <li>• GraphRNN: Generating Realistic Graphs with Deep Auto-regressive Models (<a href="https://arxiv.org/pdf/1802.08773.pdf">https://arxiv.org/pdf/1802.08773.pdf</a>)</li> <li>• Graph Convolutional Policy Network for Goal-Directed Molecular Graph Generation (<a href="https://arxiv.org/pdf/1806.02473.pdf">https://arxiv.org/pdf/1806.02473.pdf</a>)</li> </ul>
Events: Homework 3 (homework/CS_224W_Fall_2023_HW3.pdf) <b>out</b> LaTeX template (homework/CS_224W_Fall_2023_HW3-template.zip)
Deadlines: Homework 2 <b>due</b>

Date: <b>Tue, 11/7</b>
Description: <b>ELECTION DAY - NO CLASS</b>
Events:
Deadlines:

Date: <b>Thu, 11/9</b>
Description: <b>13. Advanced topics in GNNs</b> [slides (slides/13-advanced_gnns.pdf)]
<ul style="list-style-type: none"> <li>Position-aware Graph Neural Networks (<a href="https://arxiv.org/pdf/1906.04817.pdf">https://arxiv.org/pdf/1906.04817.pdf</a>)</li> <li>Identity-aware Graph Neural Networks (<a href="https://arxiv.org/pdf/2101.10320.pdf">https://arxiv.org/pdf/2101.10320.pdf</a>)</li> <li>Adversarial Attacks on Neural Networks for Graph Data (<a href="https://arxiv.org/pdf/1805.07984.pdf">https://arxiv.org/pdf/1805.07984.pdf</a>)</li> </ul>
Events: Colab 4 ( <a href="https://colab.research.google.com/drive/1DkmZD4kvH3aurw5hnxwotOgB7oV33XsN">https://colab.research.google.com/drive/1DkmZD4kvH3aurw5hnxwotOgB7oV33XsN</a> ) <b>out</b>
Deadlines: Colab 3 <b>due</b> Project Milestone <b>due</b>

Date: <b>Tue, 11/14</b>
Description: <b>14. Graph Transformers</b> [slides (slides/14-graph-transformer.pdf)]
<ul style="list-style-type: none"> <li>Do Transformers Really Perform Bad for Graph Representation? (<a href="https://arxiv.org/pdf/2106.05234.pdf">https://arxiv.org/pdf/2106.05234.pdf</a>)</li> <li>Sign and Basis Invariant Networks for Spectral Graph Representation Learning (<a href="https://arxiv.org/pdf/2202.13013.pdf">https://arxiv.org/pdf/2202.13013.pdf</a>)</li> <li>Attending to Graph Transformers (<a href="https://arxiv.org/pdf/2302.04181.pdf">https://arxiv.org/pdf/2302.04181.pdf</a>)</li> </ul>
Events:
Deadlines:

Date: <b>Thu, 11/16</b>
Description: <b>15. Scaling to large graphs</b> [slides (slides/15-scalable.pdf)]
<ul style="list-style-type: none"> <li>Cluster-GCN: An Efficient Algorithm for Training Deep and Large Graph Convolutional Networks (<a href="https://arxiv.org/pdf/1905.07953.pdf">https://arxiv.org/pdf/1905.07953.pdf</a>)</li> <li>Simplifying Graph Convolutional Networks (<a href="https://arxiv.org/pdf/1902.07153.pdf">https://arxiv.org/pdf/1902.07153.pdf</a>)</li> </ul>
Events: Colab 5 ( <a href="https://colab.research.google.com/drive/1iWDTfo8x5vjllmXhizbEKBCGDHgC5YG_">https://colab.research.google.com/drive/1iWDTfo8x5vjllmXhizbEKBCGDHgC5YG_</a> ) <b>out</b>
Deadlines: Homework 3 <b>due</b>

Date: <b>Tue, 11/21</b>
Description: <b>BREAK</b>
Events:
Deadlines:

Date: <b>Tue, 11/23</b>
Description: <b>BREAK</b>
Events:
Deadlines:

Date: <b>Tue, 11/28</b>
Description: <b>16. SNAP Lectures</b> [slides (slides/16-snap.pdf)]
Events:
Deadlines:

Date: <b>Wed, 11/29</b>
Description: <b>Exam</b>
Events:
Deadlines: 11/29 5 PM - 12/1 5 AM

Date: <b>Thu, 11/30</b>
Description: <b>17. Link Prediction and Causality</b> [slides (slides/17-linkpred.pdf)]
<ul style="list-style-type: none"> <li>Intro to Causality for Computer Scientists (notes/Intro_Causality.pdf)</li> </ul>
Events:
Deadlines: Colab 4 <b>due</b>

Date: <b>Tue, 12/5</b>
Description: <b>18. Algorithmic reasoning with GNNs</b> [slides (slides/18-algo-reasoning-gnns.pdf)]
<ul style="list-style-type: none"> <li>What Can Neural Networks Reason About? (<a href="https://arxiv.org/pdf/1905.13211.pdf">https://arxiv.org/pdf/1905.13211.pdf</a>)</li> <li>How Neural Networks Extrapolate: From Feedforward to Graph Neural Networks (<a href="https://arxiv.org/pdf/2009.11848.pdf">https://arxiv.org/pdf/2009.11848.pdf</a>)</li> </ul>
Events:
Deadlines: Colab 5 <b>due</b>

Date: <b>Thu, 12/7</b>
Description: <b>19. Conclusion</b> [slides (slides/19-conclusion.pdf)]
Events:
Deadlines:



Date: <b>Thu, 12/14</b>
Description:
Events:
Deadlines: Project Report <b>due</b>