Graph Neural Networks: An Orientation

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Contents

Goal

- This course is designed to provide an in-depth exploration of Graph Neural Networks (GNNs), one of the most exciting areas of recent developments in machine learning and AI research. Students will gain a comprehensive understanding of GNNs, including their foundations, state-of-the-art models, and practical applications.

- We will start with the basics of graph theory and Graph Convolutional Networks (GCNs), then move into more advanced topics, including Graph Attention Networks (GATs), structure-preserving GNNs, overcoming GCN limitations with models like GCNII, and Graph Transformer Networks. The course will also cover graph pooling techniques, graph autoencoders, and generative models for graphs. Moreover, we will explore handling dynamic graphs and heterogeneous graphs.

- Throughout the course, we will place emphasis on the practical application of these models, focusing on various real-world scenarios and use cases. The course will mix theoretical lectures with practical exercises and coding assignments, giving students a balance between understanding the principles behind GNNs and applying them in practice.

Content

- By the end of the course, students will be able to:
  - Understand the foundational concepts of graph theory and how they apply to machine learning.
  - Understand the architecture, training, and use of various Graph Neural Network models, including GCNs, GATs, and Graph Transformers.
  - Develop and train GNNs to solve real-world problems.
  - Recognize the limitations of current GNNs and understand the solutions offered by state-of-the-art models.
  - Analyze, evaluate, and compare different GNN models based on their performance, applicability, and limitations.
  - Stay up-to-date with the latest research and developments in the field of GNNs.
  - Apply graph neural networks to different fields, such as natural language processing, social network analysis, bioinformatics, and recommendation systems.
- By the end of this course, students should be well-equipped to implement GNNs in their projects or research, as well as understand the current research landscape in the field of Graph Neural Networks.

2. Reference Book

- Students do not need to buy textbooks.
- Most of the lecture materials will be provided in digital format (e.g., PDF files).

Textbooks

- Lingfei Wu, Peng Cui, Jian Pei, Liang Zhao, “Graph Neural Networks: Foundations, Frontiers, and Applications”, Springer, 2022.
- Zhiyuan Liu, Jie Zhou, “Introduction to Graph Neural Networks”, Springer, 2020.

3. Course Schedule

- **Week 1: Introduction to Graph Theory**
  - Overview about graph theory, types of graphs and their applications.
  - Basic graph concepts (nodes, edges, degree, etc.) and graph representation (adjacency and sparse matrix).
  - Centrality measurement: Degree centrality, Betweenness centrality, Closeness centrality, Eigenvector centrality, and PageRank.
  - Graph kernel.

- **Week 2: Fundamentals of Node Embedding and Shallow Models**
  - Overview node embedding, edge embedding, and graph embedding.
  - Shallow models: Random, proximity, and heterogeneous – based models.

- **Week 3: Introduction to Graph Neural Network**
  - GNN overview and motivation.
  - Basic framework of Graph Convolution Networks and convolution operation in GCNs.

3. Course Schedule

- **Week 4: Graph Convolution Network variants (Part 1)**
  - GraphSAGE, ClusterGCN, and GraphSaint.
  - Understanding limitations of GCNs: Over-smoothing, Over-squashing.

- **Week 5: Graph Convolution Network variants (Part 2)**
  - Addressing over-smoothing and scalability.
  - How to train deeper GCN: DeeperGCN.

- **Week 6: Introduction to Graph Attention Networks (GATs)**
  - Basic framework of GATs.
  - Attention mechanism in GATs.
  - Multi-head attention in GATs.

3. Course Schedule

- **Week 7: Structure-Preserving Graph Neural Networks**
  - Motivation for Structure Preservation.
  - Graph Isomorphism Networks (GIN).
- **Week 8: Midterm Exam.**
- **Week 9: Introduction to Graph Transformers**
  - Transformers in NLP.
  - “Attention Is All You Need”.
  - Graph Transformer Network.
- **Week 10: Graph Autoencoders (GAEs) and Variational Graph Autoencoders (VGAEs)**
  - Basic framework of GAEs and Understanding VGAEs.
  - Applications in Graph data generation and anomaly detection.

3. Course Schedule

- **Week 11: Graph Neural Network for Recommendation Systems.**
  - Introduction to Recommendation systems and apply graph into system.
  - Traditional collaborative filtering, Neural graph collab filtering, lightGCN.

- **Week 12: Molecular Structure Analysis**
  - Basic graph for molecular structure.
  - Advanced GNN architectures (e.g., Message Passing Neural Networks, Transformer-based GNNs).
  - Graph task and application.

- **Week 13: Heterogeneous Graph Neural Networks and Knowledge Graph.**
  - Introduction to heterogeneous graph and knowledge graph.
  - Heterogeneous GCN (HGCN), Relational GCN (RGCN), and Graph Attention Networks for Heterogeneous Graphs (HAN)

3. Course Schedule

- **Week 14: Graph Application in Computer Vision and Traffic Management.**
  - Introduction to GNN in computer vision and application: scene graph generation for image classification.
  - Introduction to GNN in traffic management: traffic forecasting and traffic similarity.

- **Week 15: Review Graph Neural Network.**

- **Week 16: Final Exam**

4. Assessment Criteria and Grading Scale

Assessment

- Midterm exam: 30%.
- Final exam: 30%.
- Homework: 30%.
- Attendance: 10%.
- All test questions are made up within lecture slides and assignments.

Tentative Grading Scale

- A: 80 - 100.
- B: 60 - 80.
- C: ~60.
- F: Absence from exams.

Weekly Programming Practice

- Perform practical programming in one class every week.
- Do assignment after practice class every week.

6. Instructor Information

O-Joun Lee (이오준)

- Email: ojlee@catholic.ac.kr.
- Office: T404.
- Office phone number: 5516.

- Office hour: visit office anytime.
- Please feel free to contact me for any class issues

7. Teaching Assistant Information

Van Thuy Hoang

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