11-741/11-441:

Machine Learning with Graphs

Introduction

Yiming Yang

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Outline

- Administrative Stuff
- Course Contents Overview

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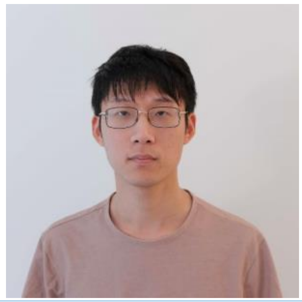
Instructor and Teaching Assistant

- Yiming Yang (LTI & MLD)
- Office hours by appointment (GHC 6717 or via zoom)
- yiming@cs.cmu.edu

- Zhiqing Sun (PhD in LTI)
- Office hours: See piazza
- <zhiqings@andrew.cmu.edu>



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Background

- **Prerequisites**
  - CS courses like data structures, algorithms, programming (e.g., 15-213)
  - Linear algebra (e.g., 21-241 or 21-341), introductory probability (e.g., 21-325)I
- **Preferred but not required**
  - Introductory Machine Learning (e.g., 10-701 or 10-601)
  - Neural network courses
  - This course is mostly self-contained on ML background.

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Sections

- **11-741** (graduate level, 12 units)
  - Previously 11-741 (PhD level) and 11-641 (MS level) are now merged into one without distinction
  - 100% homework (5 HWs) & 100% of the Exam Questions (midterm exam and final exam)
- **11-441** (undergraduate level, 9 units)
  - 80% homework (4 out of the 5HWs) by your own choices; if you do all the 5 HWs, the top-4 scores will be used in grading.
  - 70% of the total exam questions by your own choices; if you choose to do more, only the 70% of the best answered questions will be used in grading.

Grading Policies

	11-741/641 (Grad Level)	11-441 (UG Level)
Midterm Exam	15%	14%
Final Exam	15%	14%
HWs	14% x 5 = 70%	18% x 4 = 72%

Homework

- Programming assignments in Python
- Submission: Due by 11:59pm of the due date.
  - It must be submitted by Gradescope. If Gradescope is down, it must be submitted by email to the TA.
  - A 10% penalty is applied for each day beyond the deadline.

Cheating, Copying, Plagiarism, Etc

- You must be the author of everything that you submit for a grade
- Revising or modifying someone else's work does not make you the author
- It is okay to discuss homework with other students, share ideas, experience, and lessons learned
- Sign the cheating policy form (as the condition to be graded)

Exams

- Open book, with a set of questions (about 10) and a list of possible answers to choose from per question.
- Mid-term exam will cover the 1st half of the lecture contents of the semester, and the final exam will cover the 2nd half.
- The exams will not focus on the contents of the HW assignments.
- No arrangement
  - if you cannot attend the exams, you will just lose the points

Course Materials Online

- **Syllabus** (publicly available)

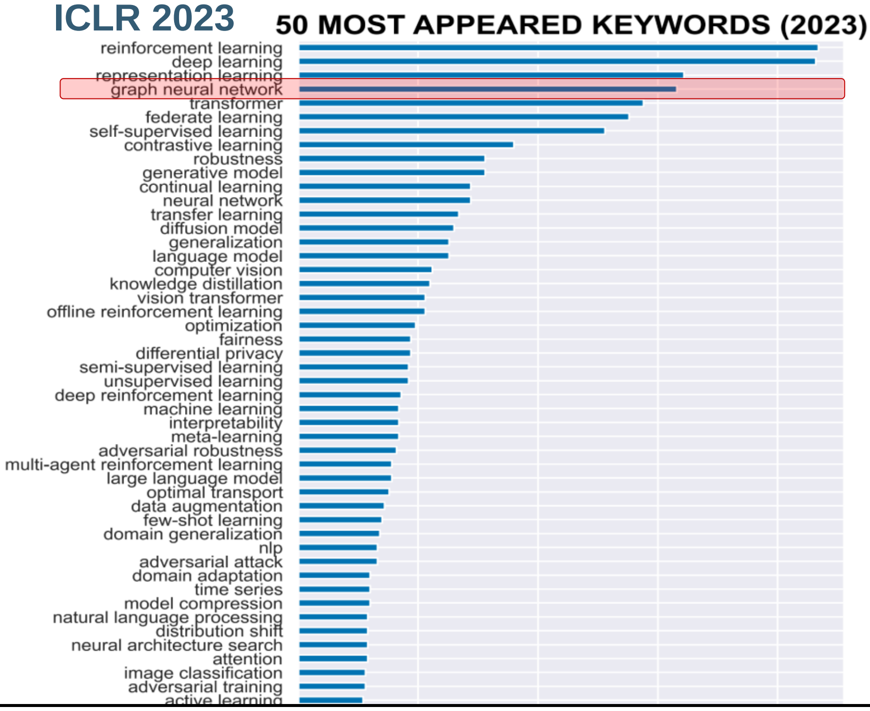
  https://cmu-ml4graph.github.io/s2024/
- **Lecture Slides** (password protected)
  - URLs listed on the schedule of the lectures
  - Login information will be announced via piazza
- **Piazza** (listed at Canvas)
- **Recorded Lectures**
  - Not provided in general, to encourage in-person classes
  - Exceptions (if you catch COVID) can be arranged via the TA

Outline

✓Administrative Stuff

- Course Contents Overview
  - with motivating examples

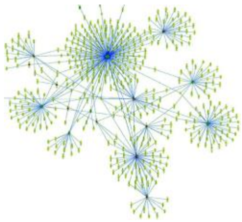
ICLR 2023



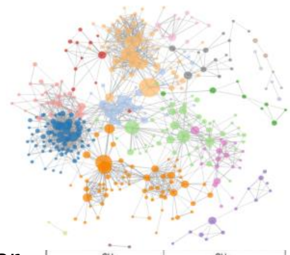
Why graphs?

A common language for representing various types of data

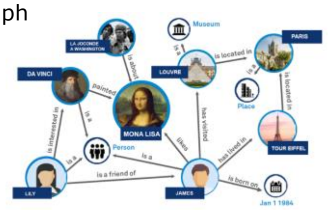
Web Site Hyperlinks



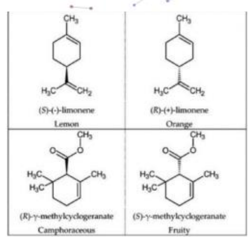
Citation Network



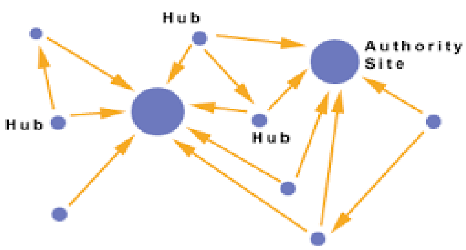
Knowledge Graph



Molecular Structures



Ex 1: Web Page Popularity Analysis

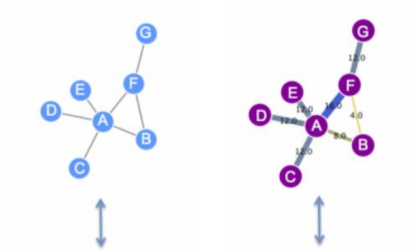


- Which web pages are more trustworthy (good authorities)?
- Which web pages are more resourceful (good hubs)?
- Naïve answer: Count the in/out degrees of each node.
- Better answer
  - A node is authoritive if it is pointed by many good hubs.
  - A node is a good hub if it points to many authoritive nodes
- We end up with a chicken-egg problem!

Representing the Graph Structure

- **Graph** $\boldsymbol{G = (V, E)}$
  - with vertices (V) and edges (E)
- **Adjacency Matrix** $\boldsymbol{A_{n \times n}}$
  - Edge weights, which can be binary (left) or weighted (right)
- **Graph Laplacian** $\boldsymbol{L \overset{\text{def}}{=} D - A}$
  - D is a diagonal matrix with

$$D_{ii} = \sum_{j:j \neq i} A_{ij}.$$



	A	B	C	D	E	F	G
A	0	1	1	1	1	1	0
B	1	0	0	0	0	1	0
C	1	0	0	0	0	0	0
D	1	0	0	0	0	0	0
E	1	0	0	0	0	0	0
F	1	1	0	0	0	0	1
G	0	0	0	0	0	1	0

	A	B	C	D	E	F	G
A	0	8	12	12	12	16	12
B	8	0	0	0	0	4	0
C	12	0	0	0	0	0	0
D	12	0	0	0	0	0	0
E	12	0	0	0	0	0	0
F	16	4	0	0	0	0	12
G	12	0	0	0	0	12	0

Adjacency matrices

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How to deal with the chicken-egg problem?

- HITS (J. Kleinberg, 1998)
  - Calculate $u_1 :=$1st eigenvector of $(A^T A)$
    $v_1 :=$1st eigenvector of (AA^T)
  - u_1 gives the **authority** scores of nodes, and v_1 gives the **hub** scores of nodes.
- PageRank (S. Brin and L. Page, 1998)
  - Define probiotic transition matrix $M_{n \times n}$ with $M[i,j] = P(j|i)$;
  - Calculate $r_1 :=$1st eigenvector of a smoothed version of matrix M, which gives the **PageRank** scores of nodes.
- Both methods utilize the eigendecompostion of those matrices, based on **random walk** over a graph with infinite steps

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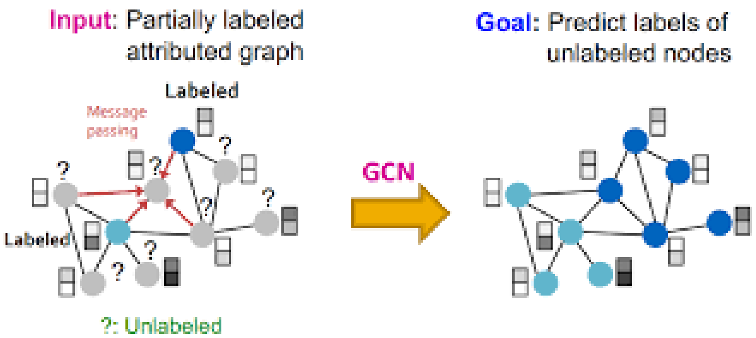
Ex 2. Graph Convolution Network (GCN)
for Semi-supervised Classification [ICLR 2017]



Key Idea: Propagating node features (embeddings) over the graph, yielding the connected nodes with smooth labeling.

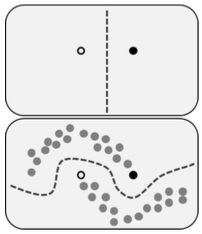
Fundamental Question
(since internet became popular in mid 1990's)

What is a document, anyway?

1. A piece of text (a human point of view)
2. A bag of words (a traditional IR point of view)
3. A sequence of tokens (a neural language model point of view)
4. A bag of links (from the graph connectivity point of view)
5. A bag of linked pages (each link reaching out a web page)
6. A node in a connected graph (each node have its own words).

Key Idea in SSL for Node Classification

Upper: Decision boundary based on labeled data only



Lower: Decision boundary based on labeled + unlabeled data

Key Question: How do we represent the manifold in data?

Controlling the Smoothness of Node Embedding

- Graph Laplacian $L \stackrel{\text{def}}{=} D - A$
  - A is the adjacency matrix
  - D is a diagonal matrix, with $D_{ii} \sum_{j:j \neq i} A_{ij}$
- Using (a subset) the eigenvectors of L we can control the smoothness of node embedding over the graph.

Various Graph Neural Networks

- Graph **Convolution** Network (GCN) [ICLR 2017]
  - node-level classification
- Graph **Attention** Network (GAT) [ICLR 2018)
  - node-level classification by leveraging masked self-attentional layers
- Graph **Isomorphism** Network(GIN) [ICLR 2019]
  - graph-level classification with multi-layer perceptron
- Graphormer [NeurIPS 2021]
  - graph-level classification with **graph-adapted Transformer**
- SignNet [ICLR 2023]
  - graph-level regression with Laplacian Eigenvectors for graph positional encoding

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Part I. Fundamentals & Building Blocks

- Word2vec Embedding Methods (1 lecture)
- Recurrent Neural Networks (RNN) (1 lecture)
- Convolution Neural Networks (CNN) (1 lecture)

  HW1. CNN & RNN classifiers
- Attention Models (1 lecture)
- LM Architectures (1 lecture)
- Classification Fundamentals (4 lectures)

  HW2, Soft-max & SGD

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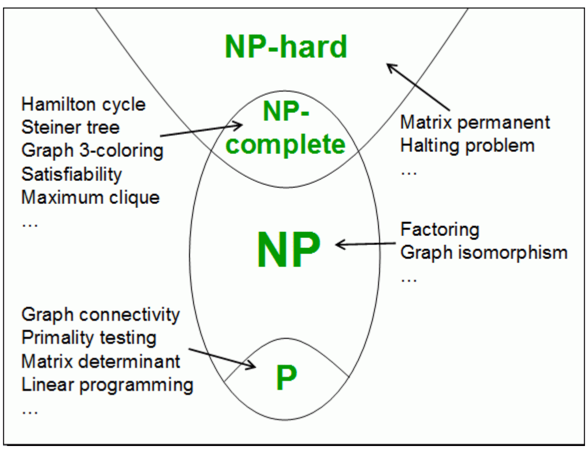
Part II. Graph-based Learning Topics

- ✓ **Social Popularity Analysis (3 lectures)**
  - HW3. PageRank models
- Node Embedding (1 lecture)
- ✓ **Graph Neural Networks for Classification (2 lectures)**
  - HW4. GCN models
- Knowledge Graph Embedding (2 lectures)
  - HW5. Node Embedding with TransE
- Neural Solvers for Combinatorial Optimization (3-4 lectures)
- Reasoning w/ Heterogeneous Graphs (2 lectures)
- Invited Talks (2; industrial applications & insights)

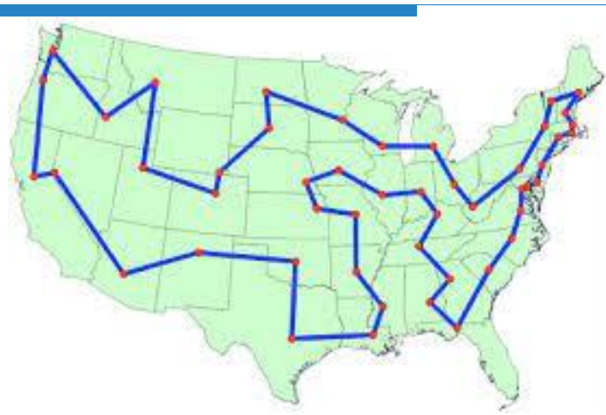
Computational Problems



NP-Completeness (NPC)

- NPC is "the hardest problems in NP"
- If some NPC problem has a polynomial time algorithm, all problems in NP do.
- Our focus is to on recent neutral network solvers
  - For large NPC problems that traditional solvers cannot handle
  - With graph-based learning and approximation techniques

Ex 3. Traveling Salesman Problem (TSP)



Task: Given a graph with n nodes, find the shortest tour where each node is visited once and only once expect the starting node (as the ending node).

Relating TSP to LM

ChatGPT Input

- Prompt: a sequence of words as the instruction

ChatGPT output

- Response: the generated sequence of words per the instruction

TSP Input

- A set of nodes with 2D coordinates in a graph

TSP Output

- The predicted sequence of nodes where each node appears once and only once, and the last node is the starting node.

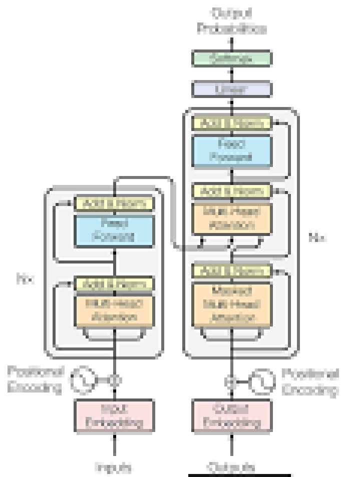
Existing TSP Solvers

- **Exhaustive search is not tractable for large n**
  - $n!$ feasible solutions
  - Dynamic Programming (Held-Karp) takes $O(n^2 2^n)$ time
- **Hand-crafted Heuristic Solvers** (traditional in OR)
  - Not generalizable across problems
- **Deep Reinforcement Learning (DRL,** recent in ML)
  - Not relying on hand-crafted heuristics
  - Learning from a large training-set of graphs for smart search
  - Model applicable to new graphs beyond training examples
  - No need to know the optimal solution(s) for each training graph

Encoder-Decoder Architecture in NLP

BERT

Encoder



GPT

Decoder

1/16/2024 @Yiming Yang, 11-741 S24 Introduction[redacted]

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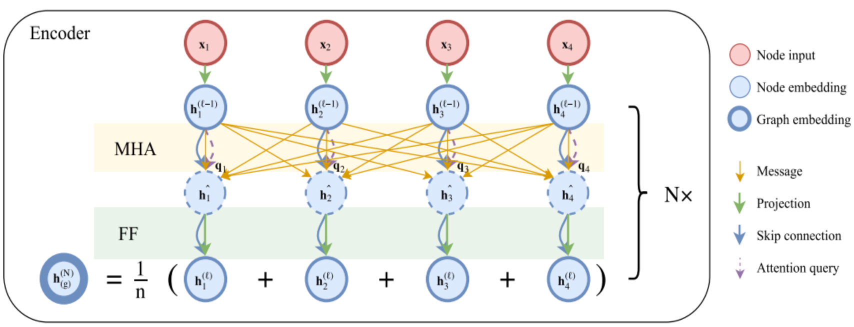
Learn to Solve NPC with DRL

(Kool et al., ICLR 2019 - Transformer Encoder)



Kool, Wouter, Herke van Hoof, and Max Welling. "Attention, Learn to Solve Routing Problems!." International Conference on Learning Representations. 2019.

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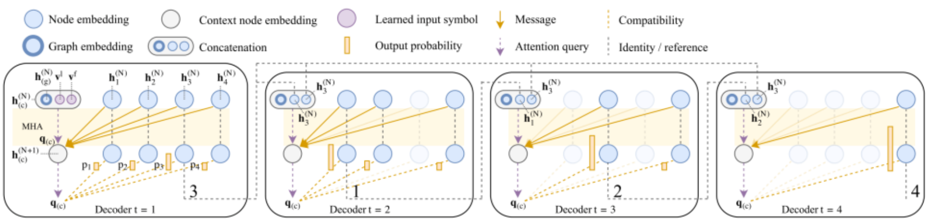

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Recent Developments

- **Good News in 2019**
  - DRL solvers for TSP found near-optimal solutions on evaluation benchmarks
- **Bad News before 2022**
  - Neural-net solvers for TSP **only scale to graphs with $\leq$ 100 nodes**
  - Neural network architectures for TSP may not generalize to other NPC problems (e.g., Maximum Independent Set)
- **Recent Advances**
  - DIMES (Qiu*, Sun*, Yang: NeurIPS 2022): neural DRL solver scale to graphs with 10,000 nodes and improved SOTA results
  - DIFUSCO (Sun, Yang: NeurIPS 2023): neural diffusion model outperforming DIMES in both accuracy and inference time complexity
  - Both offer a generic framework for NPC problems, including TSP, MIS, etc.

High-Level Ideas

- **DIMES (Qiu*, Sun*, Yang, NearIPS 2022)**
  - Removing the decoder part (costly) and modeling with encoder-only
  - Introducing meta learning to make up the (lost) accuracy
- **DIFUSCO (Sun, Yang, NearIPS 2023)**
  - Borrowing the success of “diffusion” from computer vision (Decomposing a tough task into a sequency of easier tasks)
  - Highly efficient due to parallelable training
  - The first graph-based diffusion framework (as apposed to image-based)
  - New SOTA results in TSP and MIS

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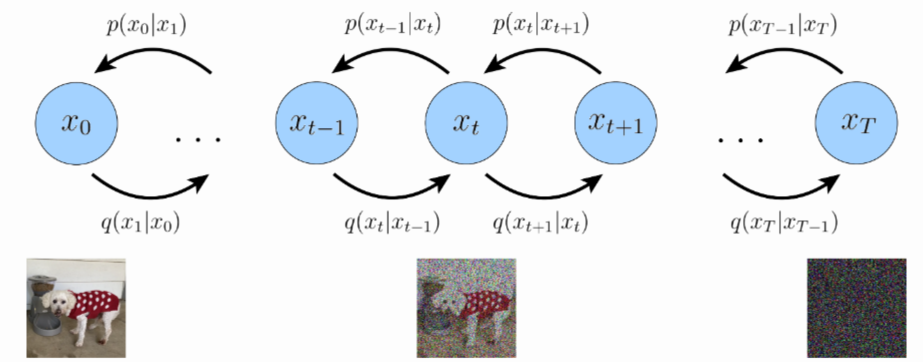
A Diffusion Model in Computer Vision



Visual representation of a Variational Diffusion Model. An input is steadily noised over time until it becomes identical to Gaussian noise; a diffusion model learns to reverse this process.

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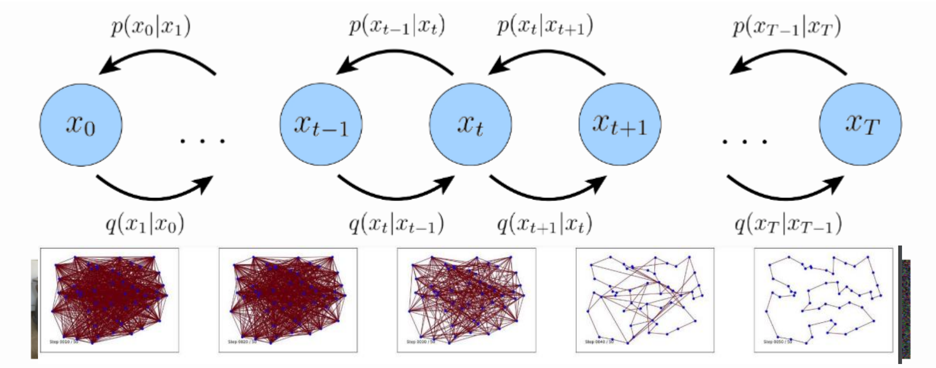
Our Diffusion Model for TSP



Visual representation of a Variational Diffusion Model. An input is steadily noised over time until it becomes identical to Gaussian noise; a diffusion model learns to reverse this process.

Concluding Remarks

- **Why graphs?**
  - A common language for representing many types of entities, relations and human knowledge, supporting graph-based reasoning beyond bag/sequence of tokens
  - Broad applications (social impact analysis, classification/regression tasks, solving NPC problems, and more)
- **Connections to recent deep learning**
  - Novel adaptation/enrichment of popular LLMs, Deep Reinforcement Learning (DRL) and Diffusion Models