Introduction

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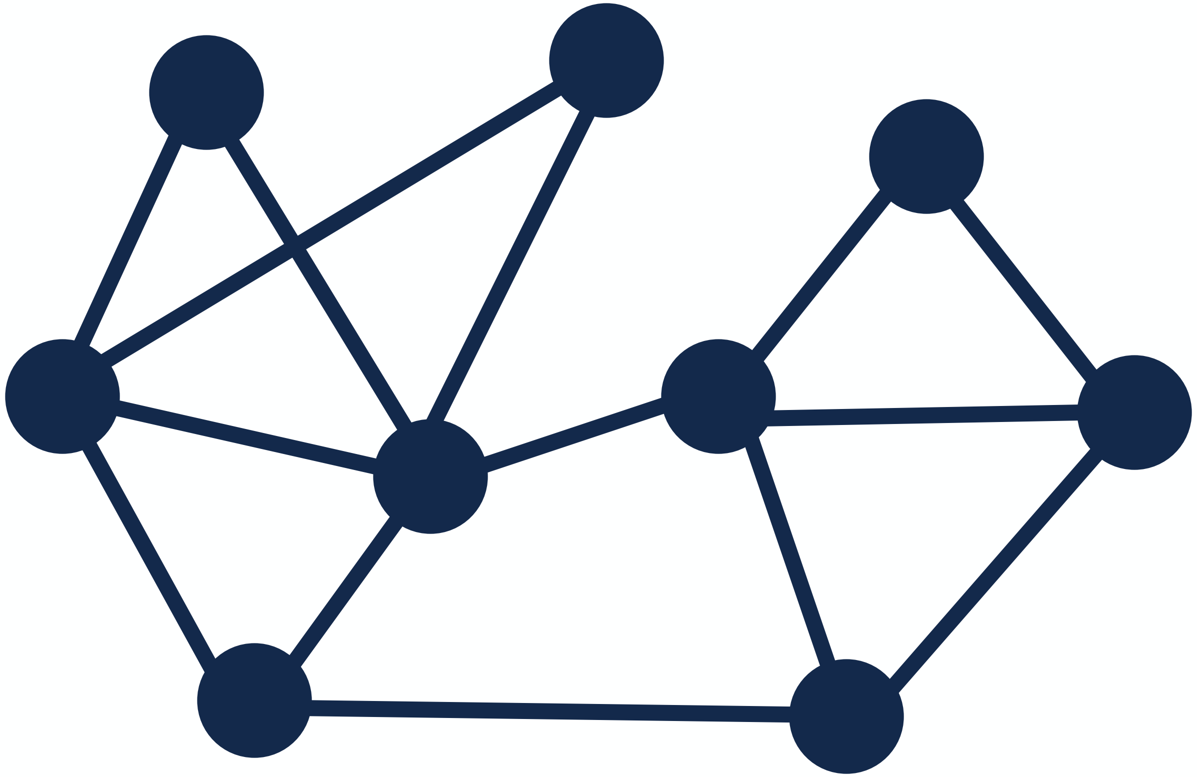
CS598: Deep Learning with Graphs, Fall 2024
University of Illinois at Urbana-Champaign

1

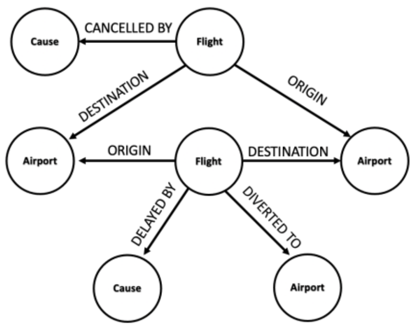
Deep Learning with Graphs

Why Graphs?

- **Graph: *General* language for describing and analyzing entities with relations or interactions.**



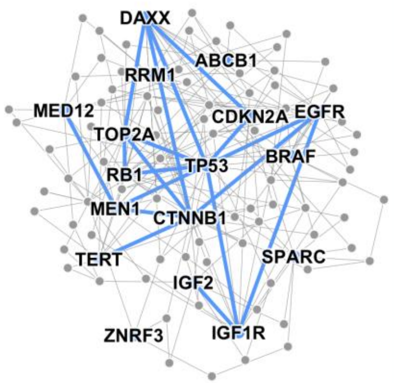
Many Types of Data are Graphs (1)



Event Graphs

Image credit: SalientNetworks

Computer Networks



Disease Pathways

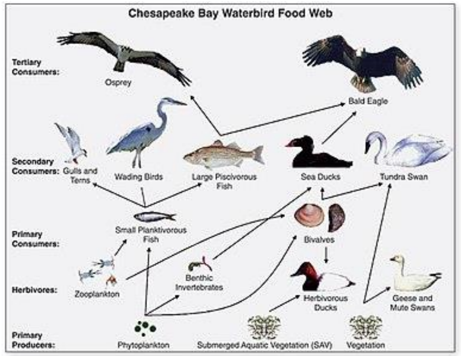


Image credit: Wikipedia

Food Webs

Image credit: Pinterest

Particle Networks

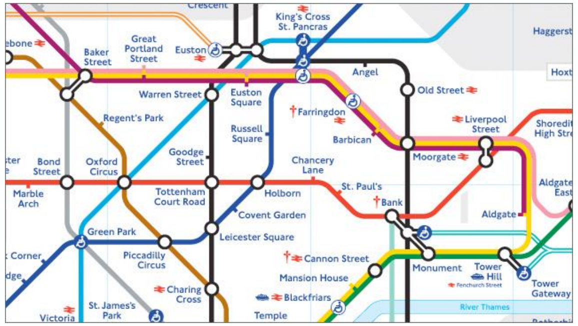


Image credit: visitlondon.com

Underground Networks

Many Types of Data are Graphs (2)

Image credit: Medium

Social Networks

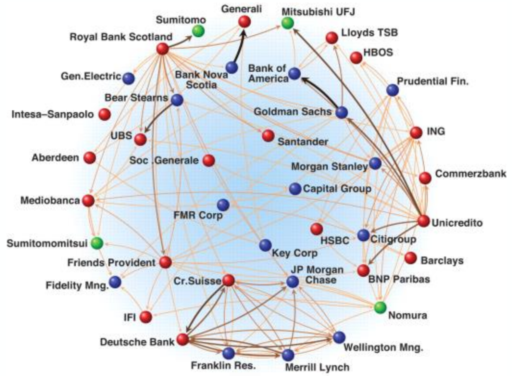
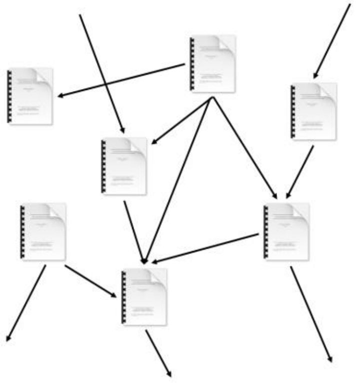


Image credit: Science

Economic Networks

Image credit: Lumen Learning

Communication Networks



Citation Networks

Image credit: Missoula Current News

Internet

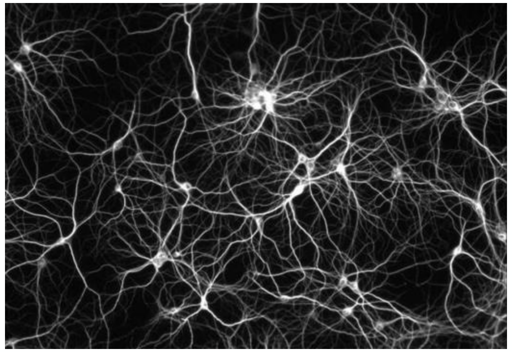


Image credit: The Conversation

Networks of Neurons

Many Types of Data are Graphs (3)

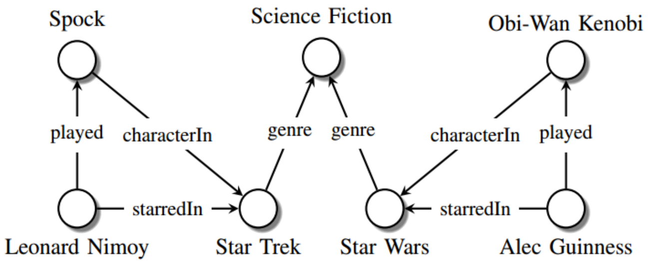


Image credit: Maximilian Nickel et al

Knowledge Graphs

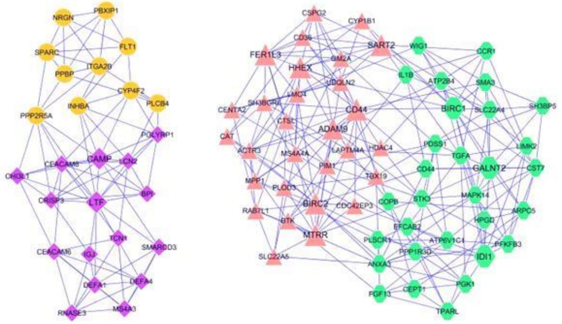


Image credit: ese.wustl.edu

Regulatory Networks

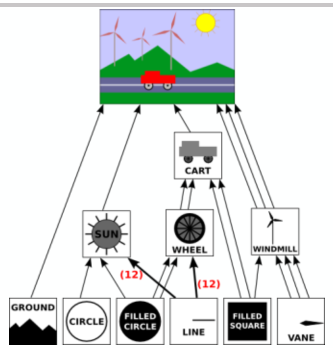


Image credit: math.hws.edu

Scene Graphs

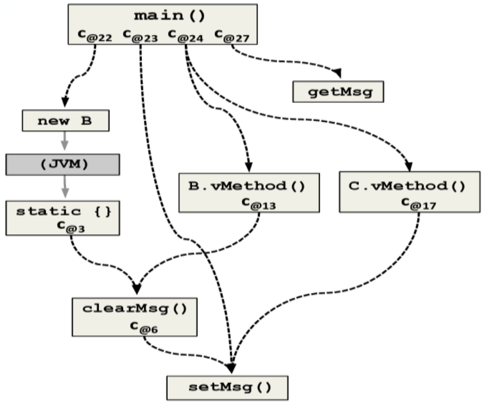


Image credit: ResearchGate

Code Graphs

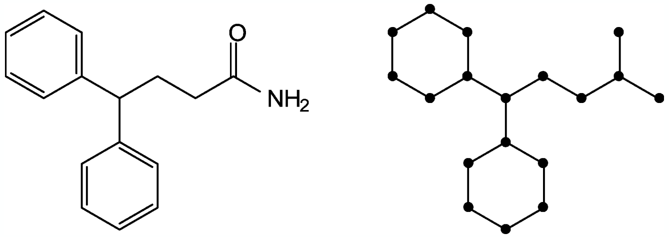


Image credit: MDPI

Molecules

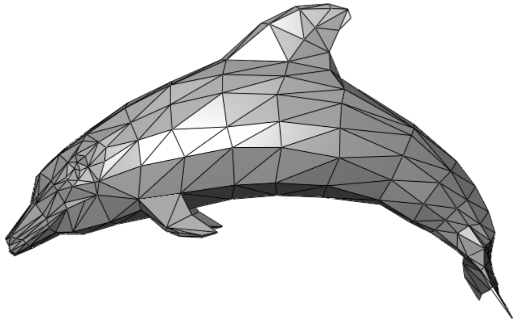


Image credit: Wikipedia

3D Shapes

Graph Machine Learning

Machine learning: predict from data

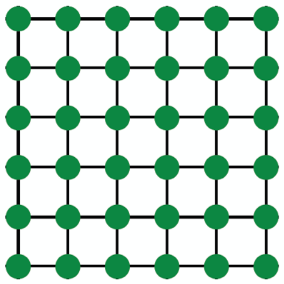
Observation:

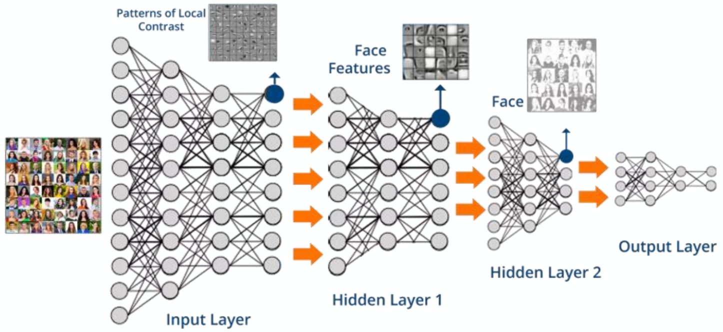
- Relational information – graphs – are ubiquitous
- Standard ML methods do not (explicitly) model relations

Graph machine learning:

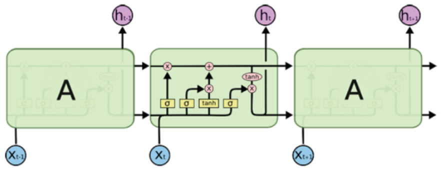
- How do we take advantage of **relational information** for better prediction?

Modern ML Toolbox





Images



Text/Speech

Modern deep learning toolbox is designed for simple sequences & grids.

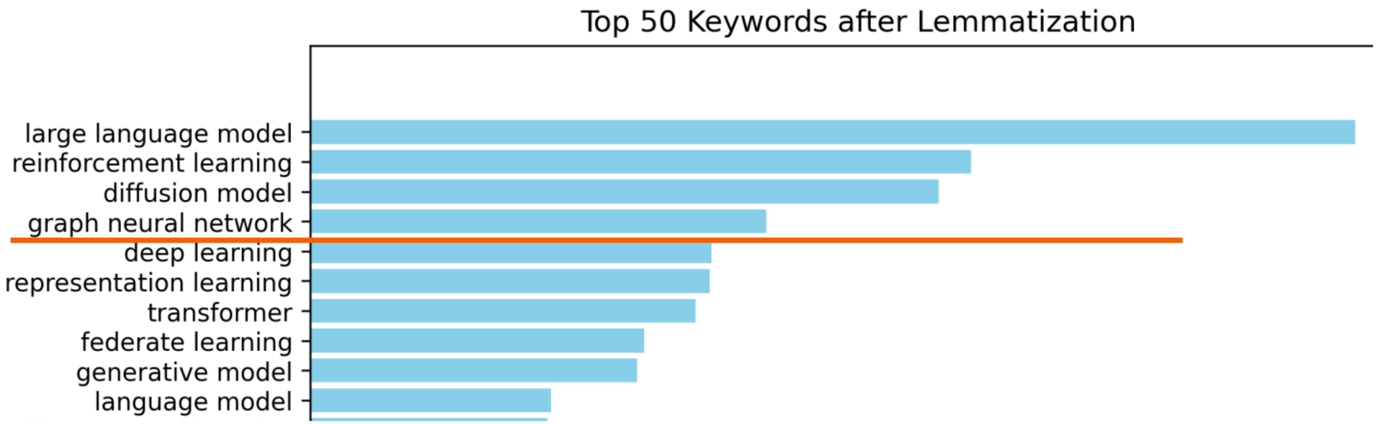
Modern ML Toolbox

- Not everything can be represented as a sequence or a grid.
- How can we develop neural networks that are much more broadly applicable, beyond sequences and images?

- **Graph neural network** is a new class of neural networks, representing a new frontier of deep learning

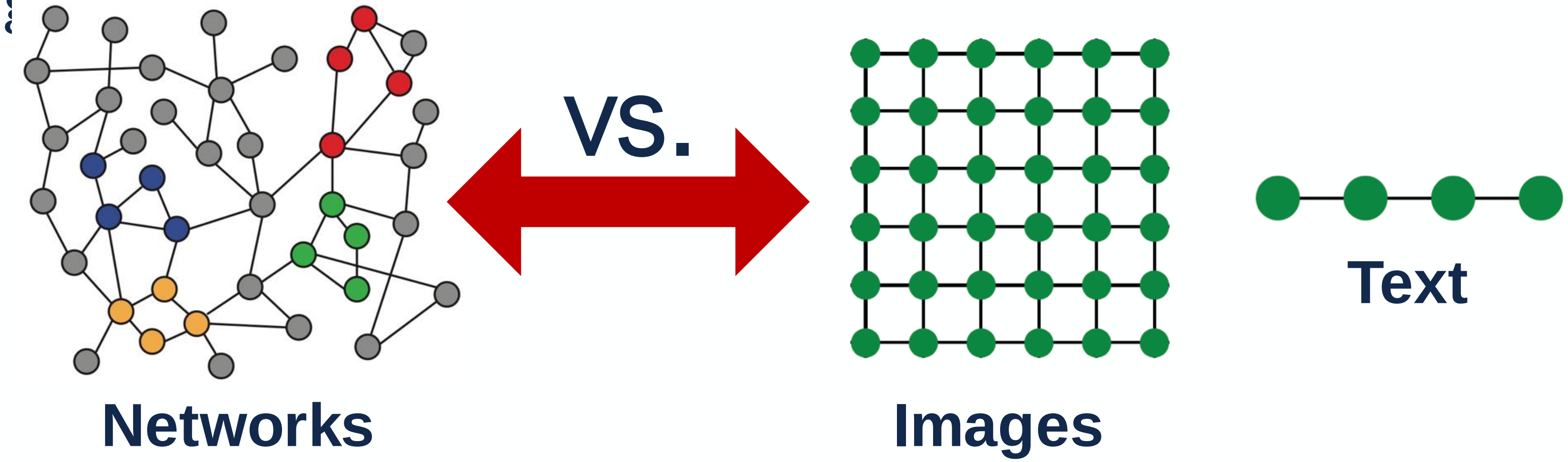
Hot Subfield in AI

ICLR 2024 visualization



Why is Graph Deep Learning Hard?

- **Networks are complex.**
  - Arbitrary size and complex topological structure (i.e., no spatial locality like grids)



  - No fixed node ordering or reference point
  - Often dynamic and have multimodal features

✴️Reminder: Use Graphs Wisely

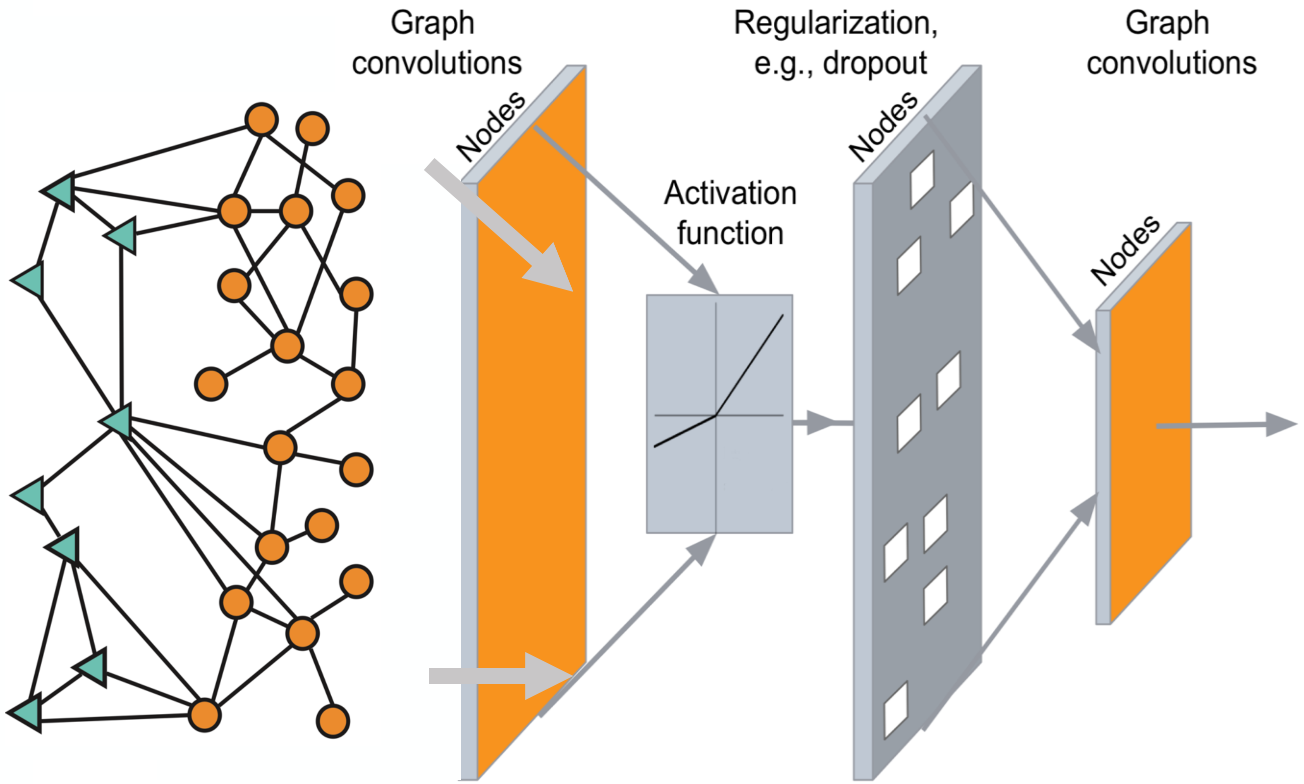
- Graph is a general language, but don't over-use it!
  - E.g., graphs subsumes lattices/sequences
- Suggested checklist
  - Will representing my data as graphs bring more information?
    - If your graph can be fully induced from existing data, think twice
      - E.g., construct K nearest neighbor graph from your embeddings, worth it?
  - Will representing my data as graphs lose information?
    - Graphs are unordered. Graph nodes/edges need features
      - E.g., molecule as graphs -> lose the distance information -> add as edge feature
  - Are there more efficient alternative representations?
    - Understand the trade-off between expressiveness & efficiency. How important is the relational info?
      - E.g., images as grids, text as sequences

This Course

- How can we develop neural networks that are much more broadly applicable?
- **Graphs** are the new frontier of deep learning.

Deep Learning with Graphs

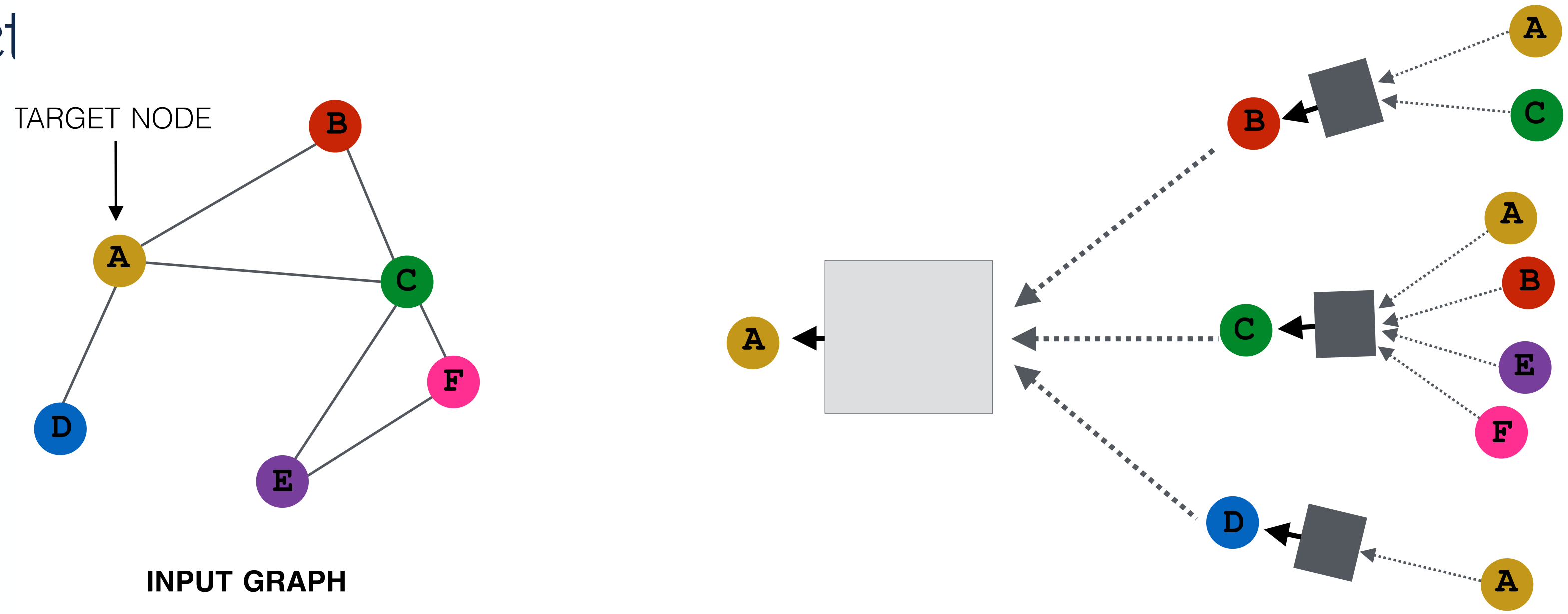
Input:
Network



… **Predictions:**
Node labels,
New links,
Generated
graphs and
subgraphs

Graph Neural Networks

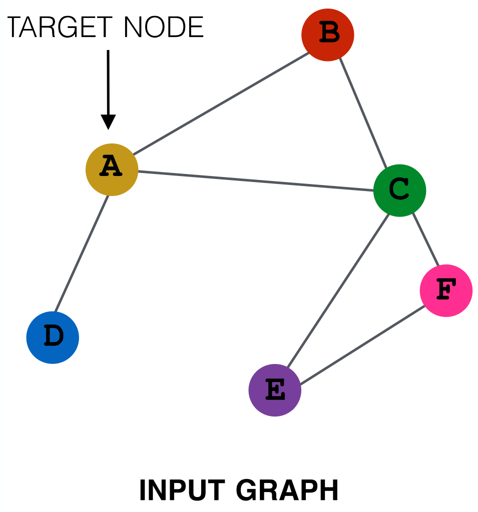
- Each node defines a computation graph.
  - Each edge in this graph is a transformation/aggregation funct

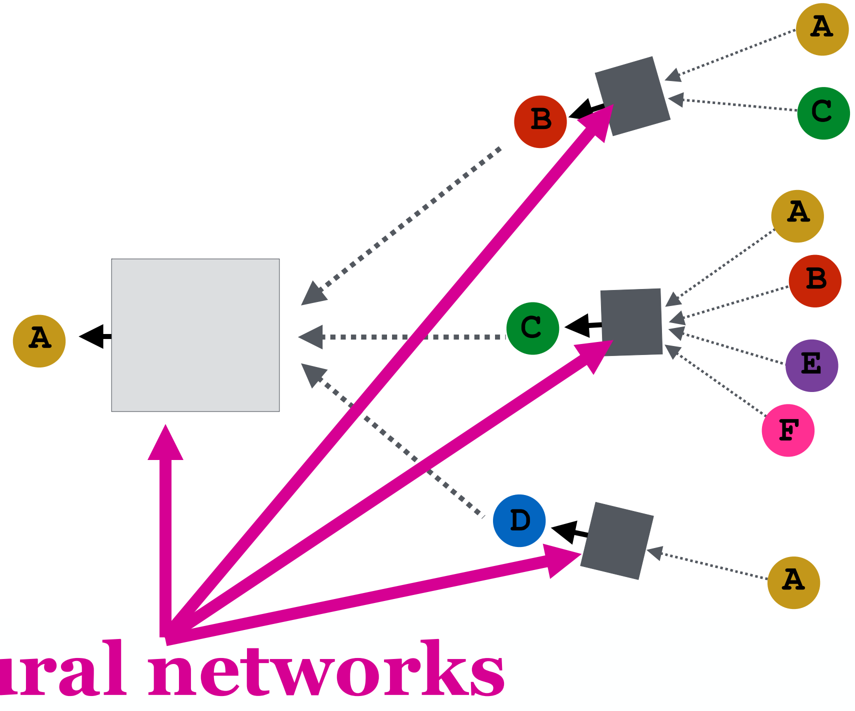


Scarselli et al. 2005. The Graph Neural Network Model. *IEEE Transactions on Neural Networks.*

Graph Neural Networks

- Intuition: Nodes aggregate information from their neighbors using neural networks.

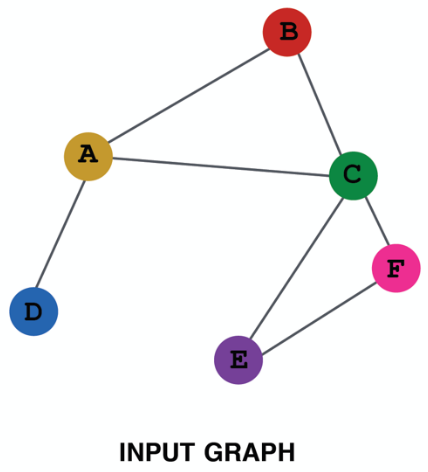




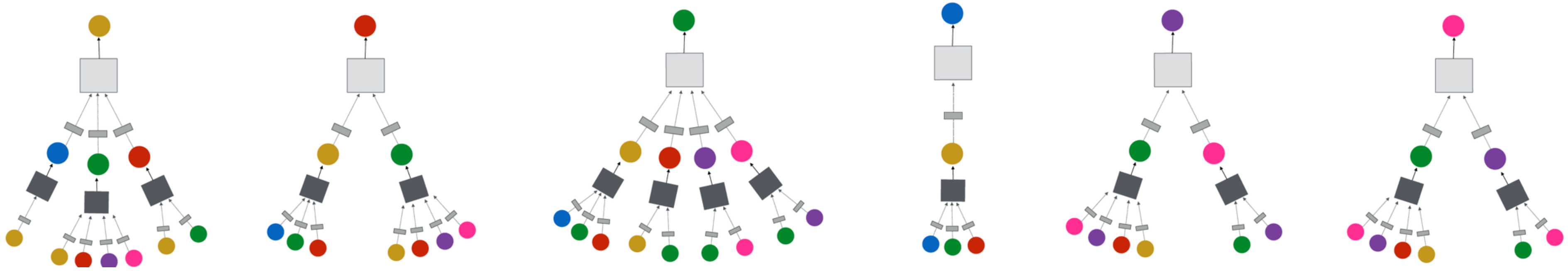
Inductive Representation Learning on Large Graphs. W. Hamilton, R. Ying, J. Leskovec. NIPS, 2017.

Idea: Aggregate Neighbors

- Intuition: Network neighborhood defines a computation graph.

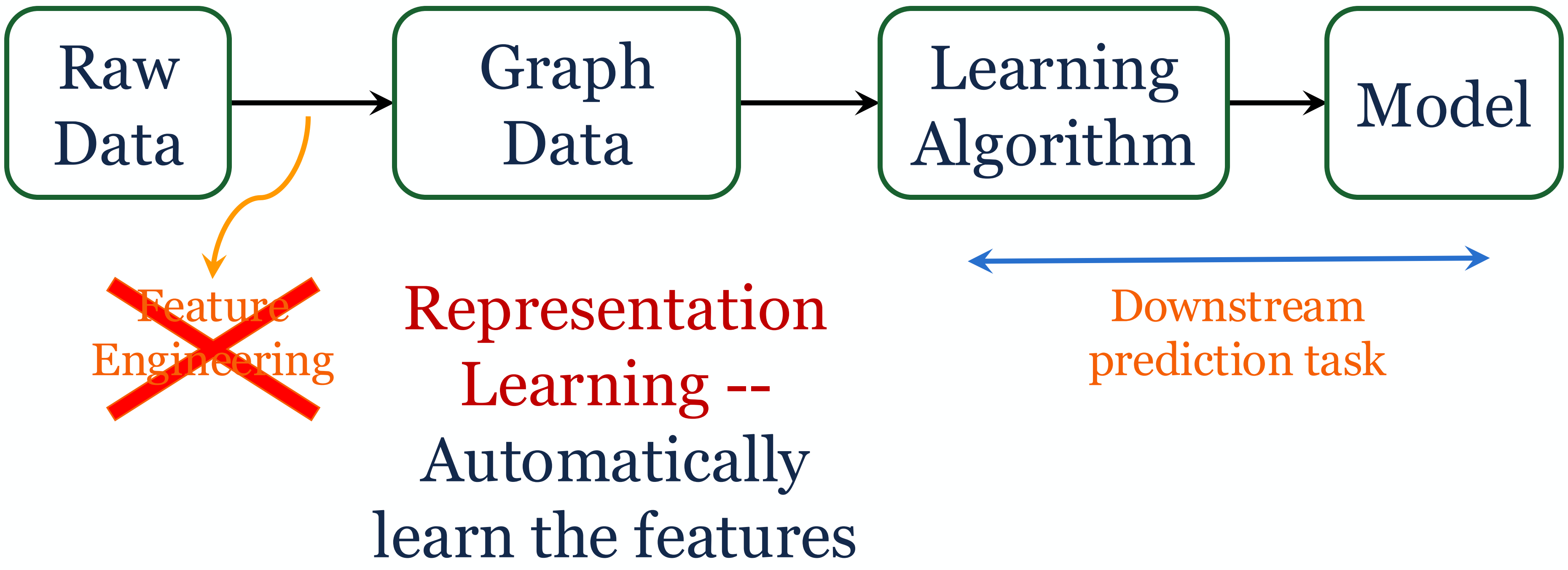


Every node defines a computation graph based on its neighborhood!



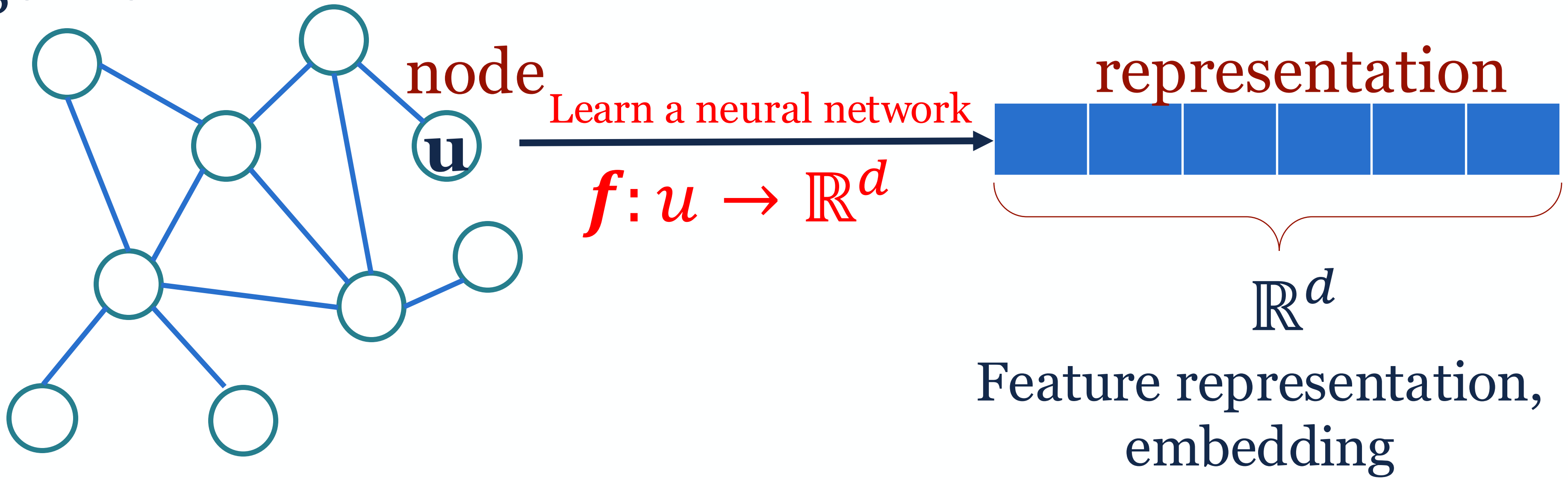
Representation Learning

- (Supervised) Machine Learning Lifecycle: This feature, that feature. Every single time!



Representation Learning

- Map nodes to d-dimensional embeddings such that similar nodes in the network are embedded close together.



Course Outline

- We are going to explore Machine Learning and Representation Learning for graph data:
  - Traditional methods: Graphlets, Graph Kernels
  - Methods for node embeddings: DeepWalk, Node2Vec
  - Graph Neural Networks: GCN, GraphSAGE, GAT, Theory of GNNs
  - Knowledge graphs and reasoning: TransE, BetaE
  - Deep generative models for graphs: GraphRNN, GCPN
  - Applications to Biomedicine, Science, Technology

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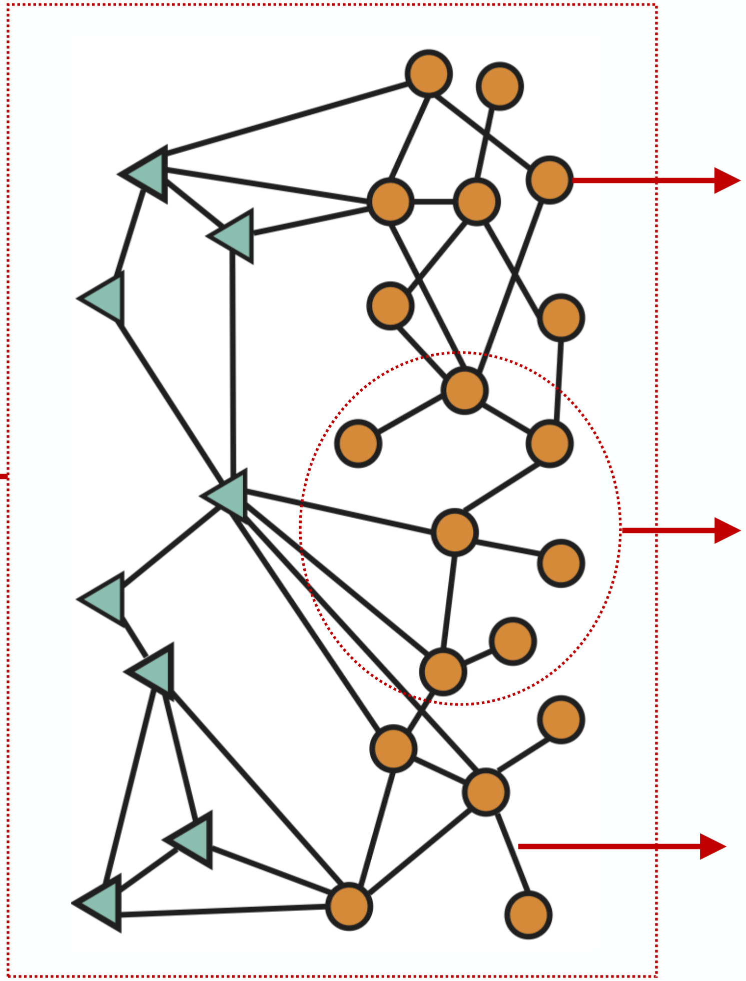
Applications of Graph ML

Different Types of Tasks

Graph-level prediction,
Graph generation



Node level

Community (subgraph) level

Edge-level

Classic Graph ML Tasks

- **Node classification**: Predict a property of a node
  - Example: Categorize online users / items
- **Link prediction**: Predict whether there are missing links between two nodes
  - Example: Knowledge graph completion
- **Graph classification**: Categorize different graphs
  - Example: Molecule property prediction
- **Clustering**: Detect if nodes form a community
  - Example: Social circle detection
- Other tasks:
  - **Graph generation**: Drug discovery
  - **Graph evolution**: Physical simulation

Classic Graph ML Tasks

- **Node classification**: Predict a property of a node
  - Example: C
- **Link predic** ks between two nodes
  - Example: K
- **Graph class**
  - Example: M
- **Clustering**:
  - Example: S
- Other tasks:
  - **Graph generation**: Drug discovery
  - **Graph evolution**: Physical simulation

These Graph ML tasks lead to high-impact applications!

2

Applications of Graph ML

Example of Node-level ML Tasks

Example (1): Protein Folding

- A protein chain acquires its native 3D structure.

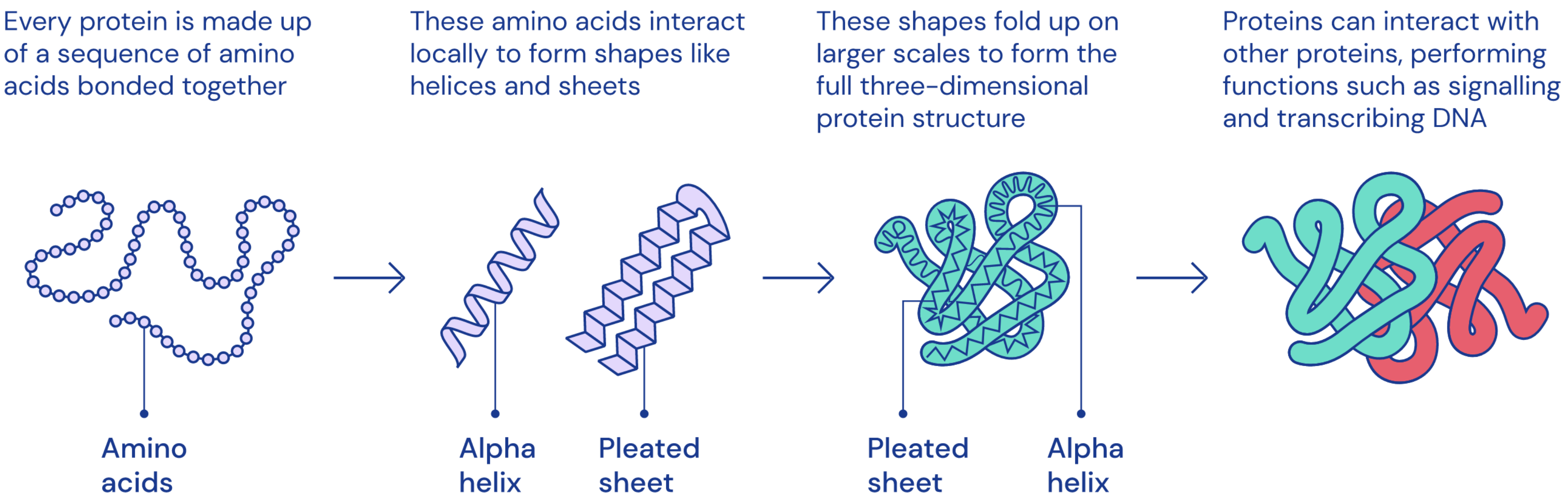


Image credit: DeepMind

Example (1): Protein Folding

- The Protein Folding Problem: Computationally predict a protein’s 3D structure based solely on its amino acid sequence.

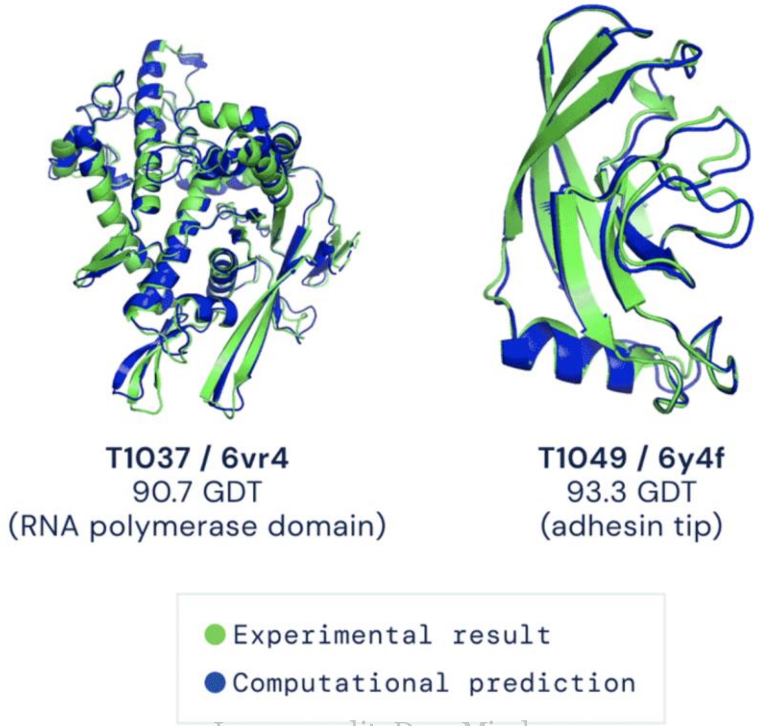


Image credit: DeepMind

AlphaFold: Impact

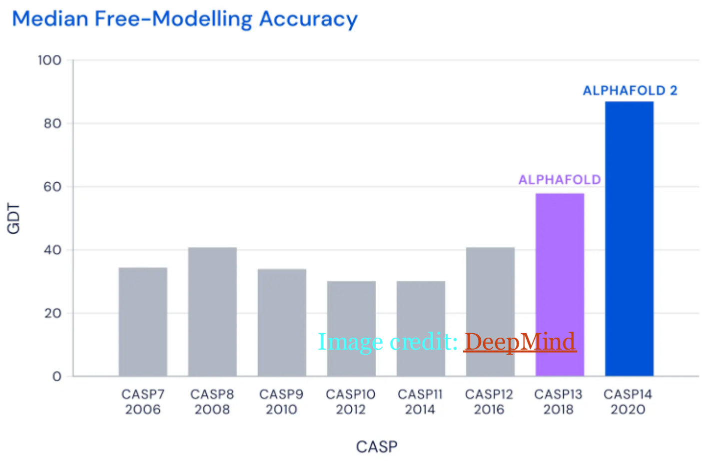


Image credit: DeepMind

Image credit: SingularityHub

DeepMind's latest AI breakthrough can accurately predict the way proteins fold

AlphaFold's AI could change the world of biological science as we know it

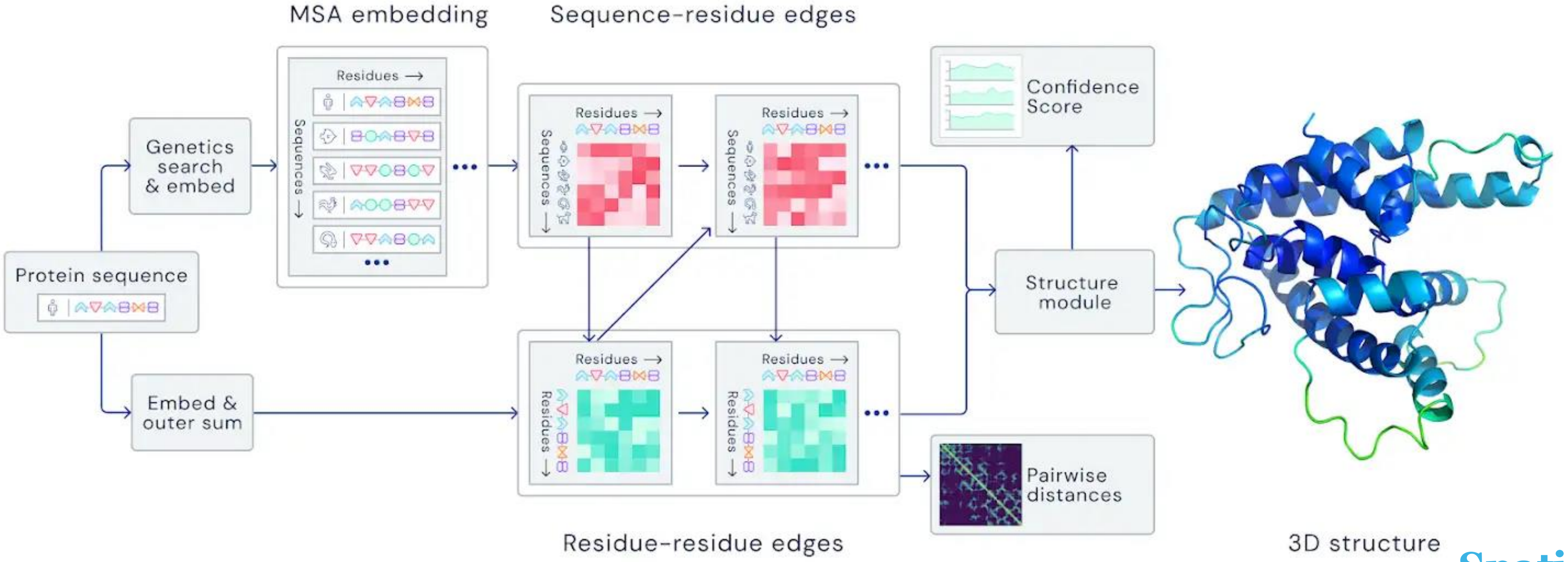
12-14-20

DeepMind's latest AI breakthrough could turbocharge drug discovery

Has Artificial Intelligence 'Solved' Biology's Protein-Folding Problem?

AlphaFold: Solving Protein Folding

- Key idea: "Spatial graph"
  - **Nodes**: Amino acids in a protein sequence
  - **Edges**: Proximity between amino acids (residues)



Spatial graph

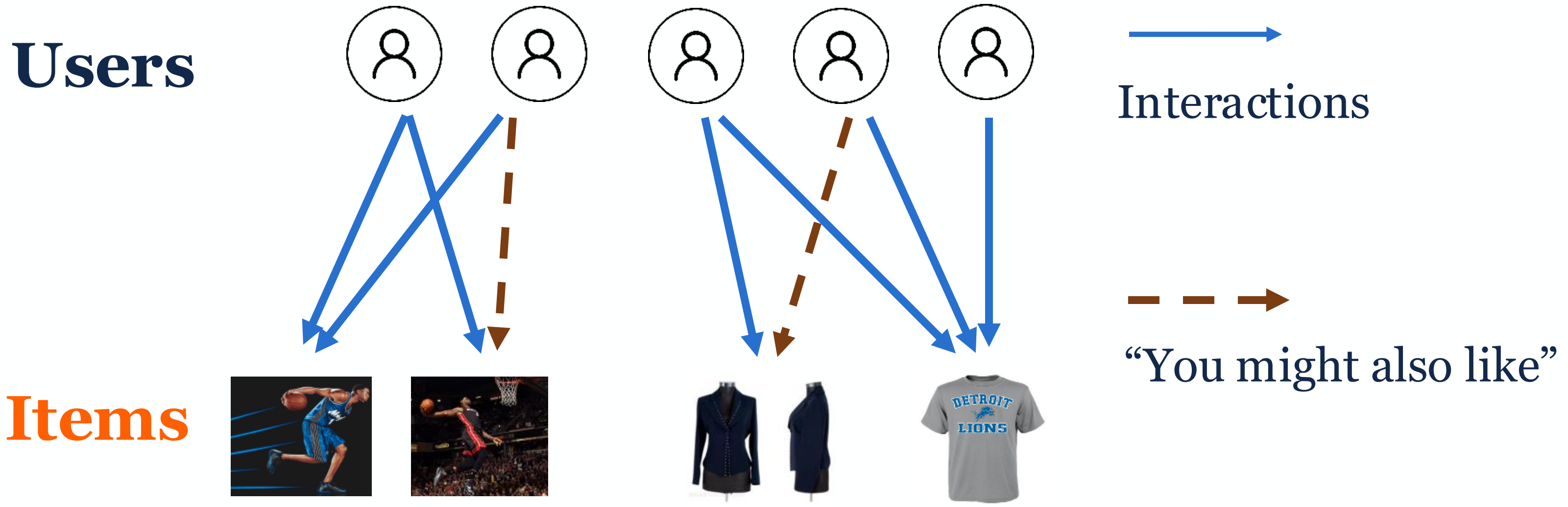
2

Applications of Graph ML

Example of Edge-level ML Tasks

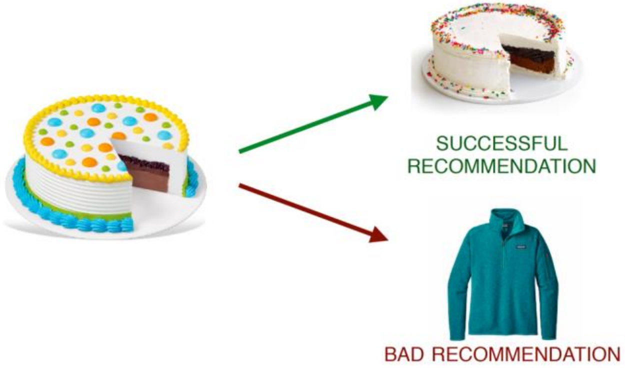
Example (2): Recommender Systems

- **Users interacts with items**
  - Watch movies, buy merchandise, listen to music
  - Nodes: Users and items
  - Edges: User-item interactions
- **Goal: Recommend items users might like**



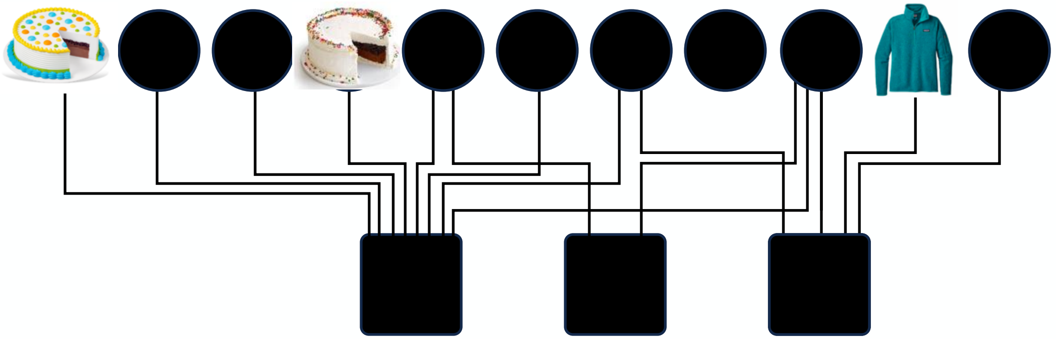
PinSage: Graph-based Recommender

- Task: Recommend related pins to users



Task: Learn node embeddings z_i such that $d(z_{cake1}, z_{cake2}) < d(z_{cake1}, z_{sweater})$

Predict whether two nodes in a graph are related

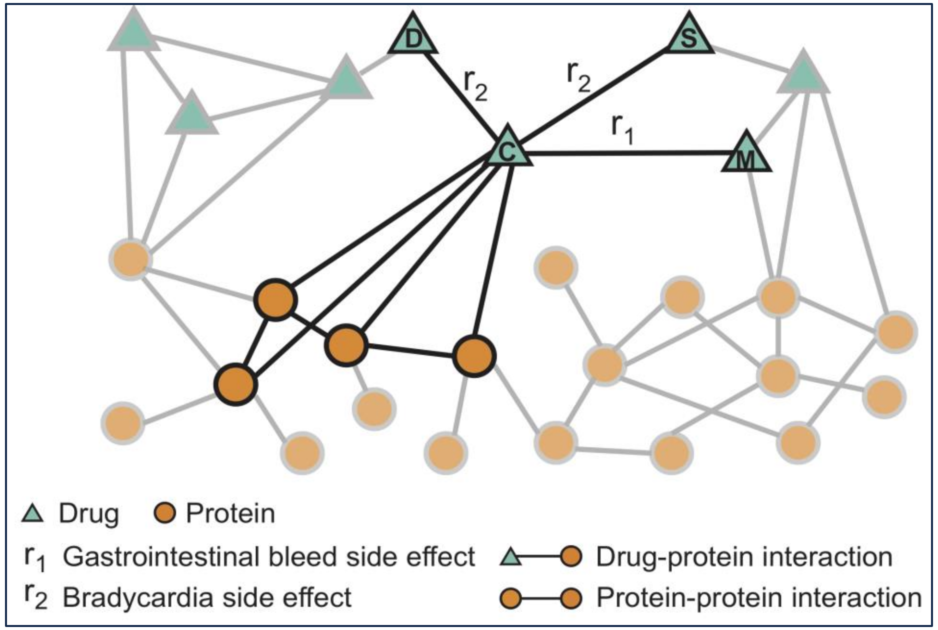


Example (3): Drug Side Effects

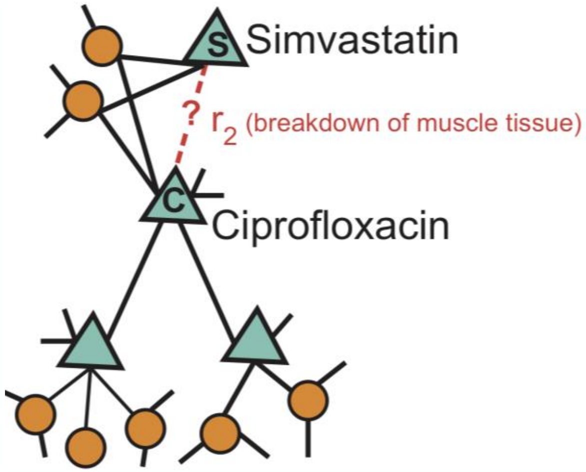
- Many patients take multiple drugs to treat complex or co-existing diseases:
  - 46% of people ages 70-79 take more than 5 drugs
  - Many patients take more than 20 drugs to treat heart disease, depression, insomnia, etc.
- **Task: Given a pair of drugs predict adverse side effects**

Biomedical Graph Link Prediction

- **Nodes**: Drugs & Proteins
- **Edges**: Interactions



- **Query**: How likely will Simvastatin and Ciprofloxacin, when taken together, break down muscle tissue?



Zitnik et al., Modeling Polypharmacy Side Effects with Graph Convolutional Networks, Bioinformatics 2018

Results: *De novo* Predictions

Rank	Drug c	Drug d	Side effect r	Evidence found
1	Pyrimethamine	Aliskiren	Sarcoma	Stage *et al.* 2015
2	Tigecycline	Bimatoprost	Autonomic neuropathy	
3	Omeprazole	Dacarbazine	Telangiectases	
4	Tolcapone	Pyrimethamine	Breast disorder	Bicker *et al.* 2017
5	Minoxidil	Paricalcitol	Cluster headache	
6	Omeprazole	Amoxicillin	Renal tubular acidosis	Russo *et al.* 2016
7	Anagrelide	Azelaic acid	Cerebral thrombosis	
8	Atorvastatin	Amlodipine	Muscle inflammation	Banakh *et al.* 2017
9	Aliskiren	Tioconazole	Breast inflammation	Parving *et al.* 2012
10	Estradiol	Nadolol	Endometriosis	

Case Report

Severe Rhabdomyolysis due to Presumed Drug Interactions between Atorvastatin with Amlodipine and Ticagrelor

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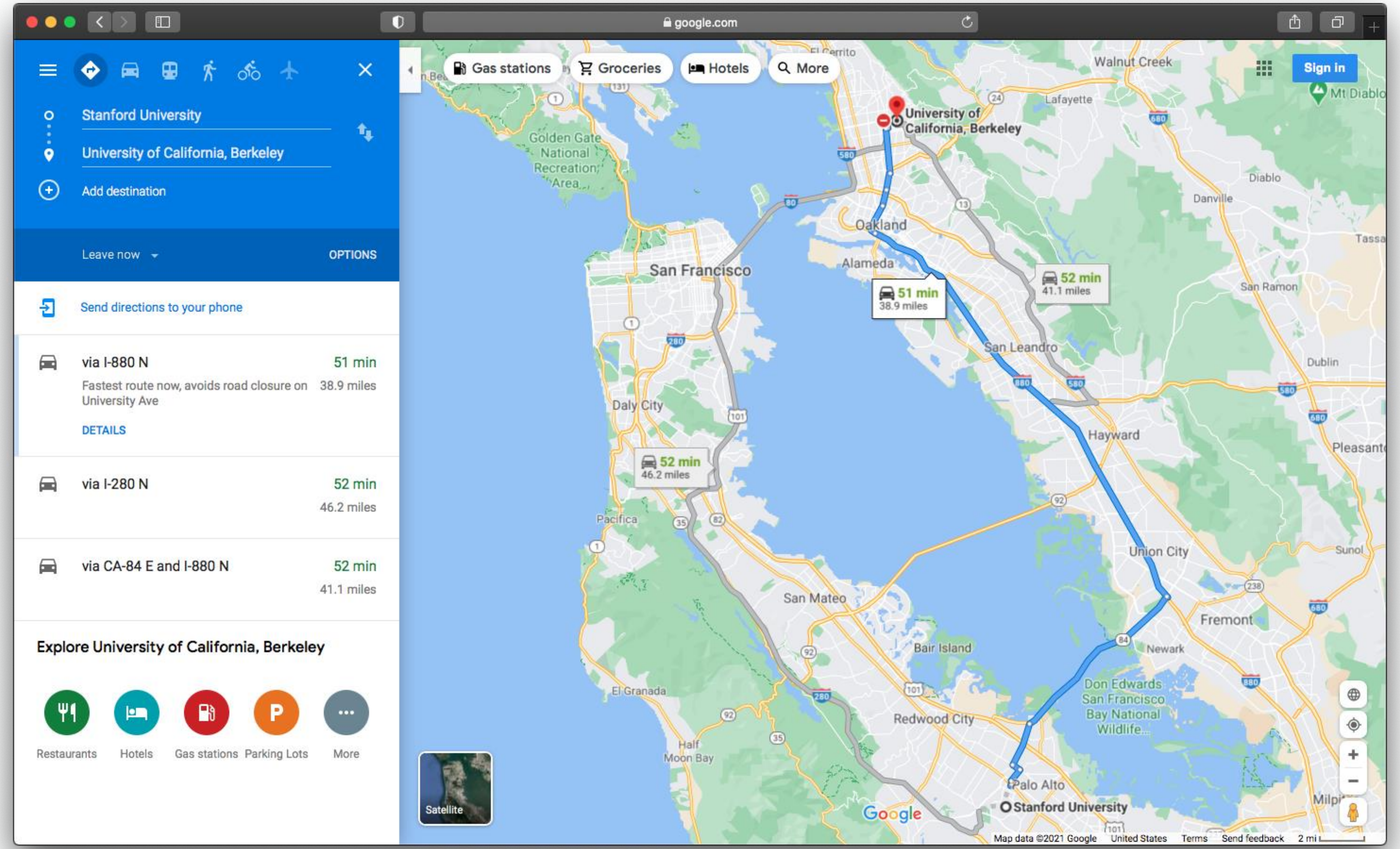
Applications of Graph ML

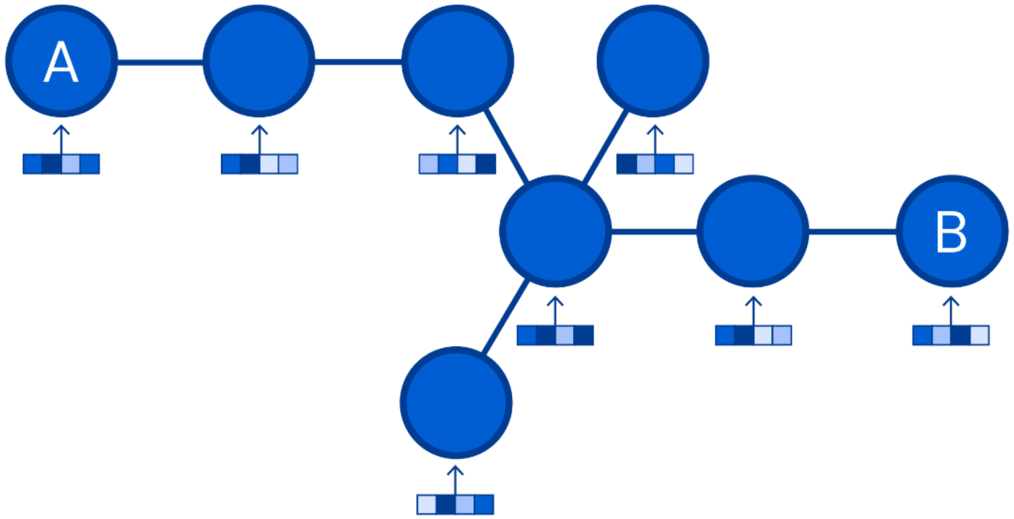
Example of Subgraph-level ML Tasks

Example (4): Traffic Prediction



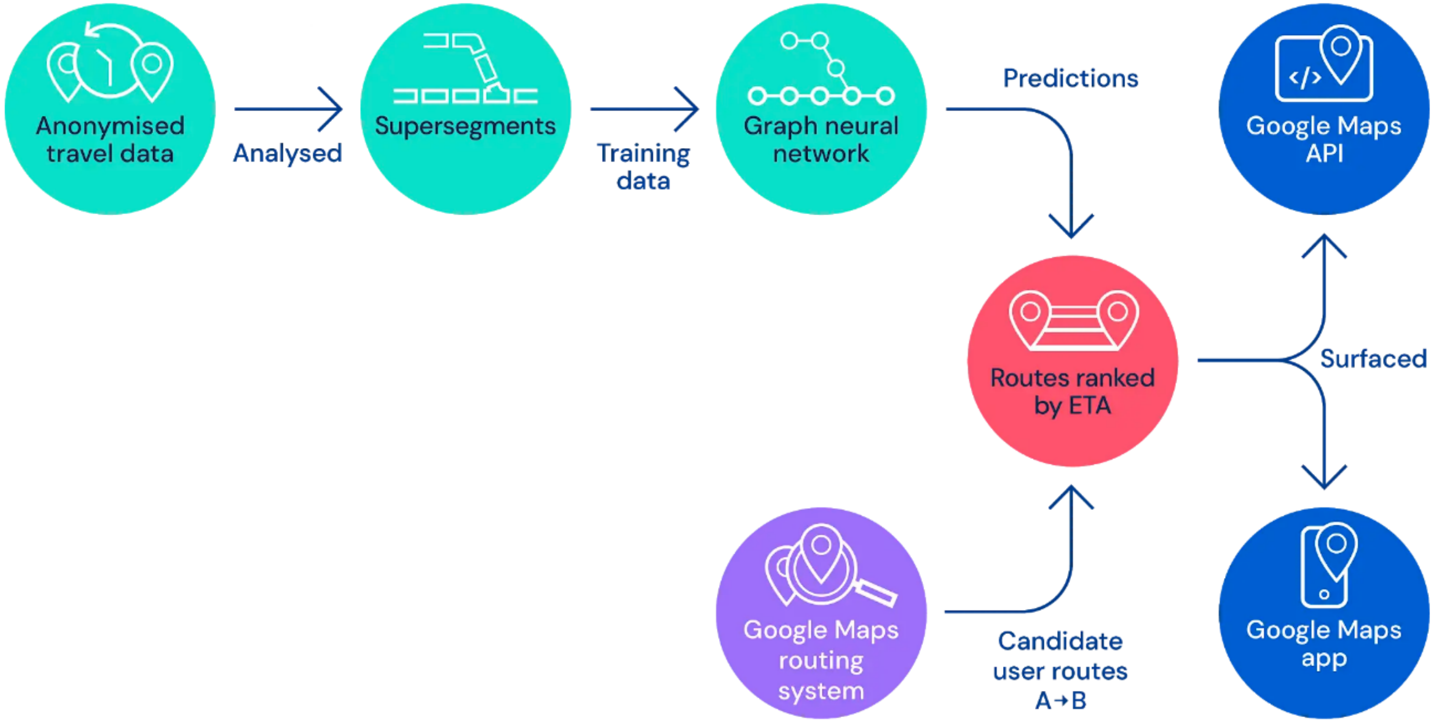
Road Network as a Graph

- **Nodes**: Road segments
- **Edges**: Connectivity between road segments
- **Prediction**: Time of Arrival (ETA)



Traffic Prediction via GNN

- Predicting Time of Arrival with Graph Neural Networks



THE MODEL ARCHITECTURE FOR DETERMINING OPTIMAL ROUTES AND THEIR TRAVEL TIME.

Used in Google Maps

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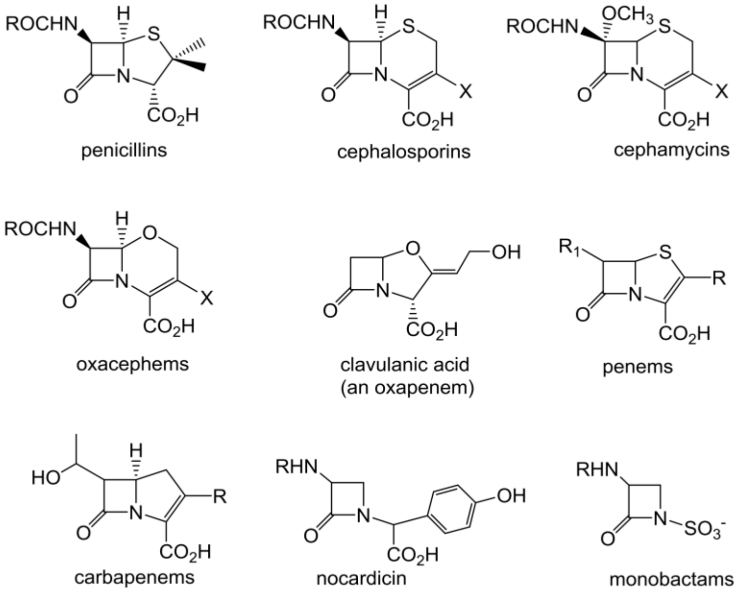
Applications of Graph ML

Example of Graph-level ML Tasks

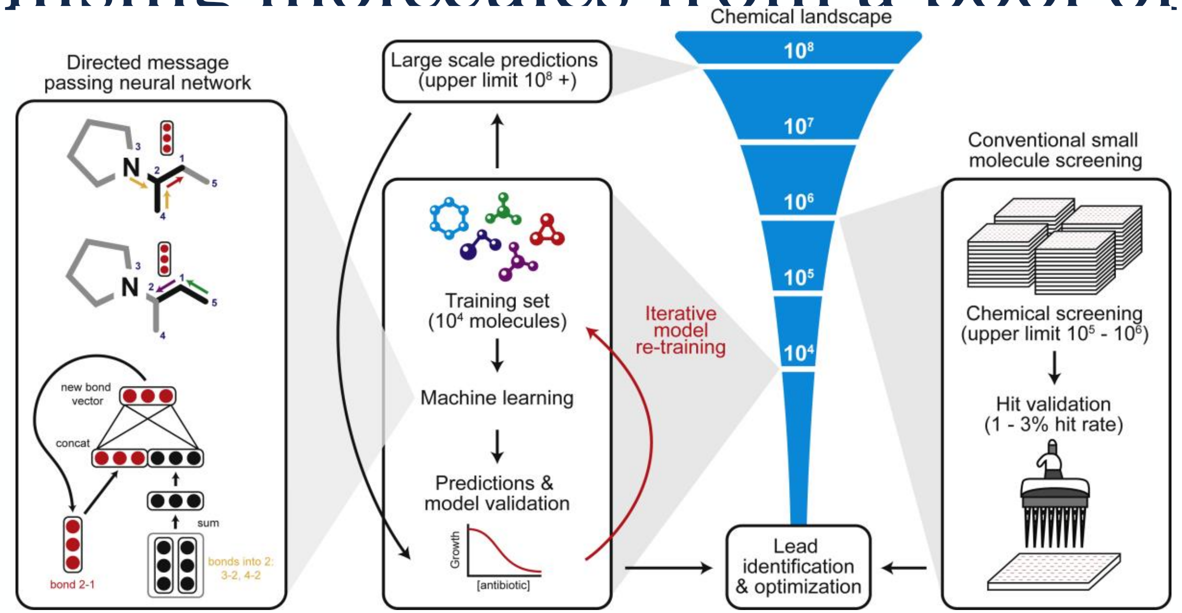
Example (5): Drug Discovery

- Antibiotics are small molecular graphs
  - **Nodes**: Atoms
  - **Edges**: Chemical bonds



Deep Learning for Antibiotic Discovery

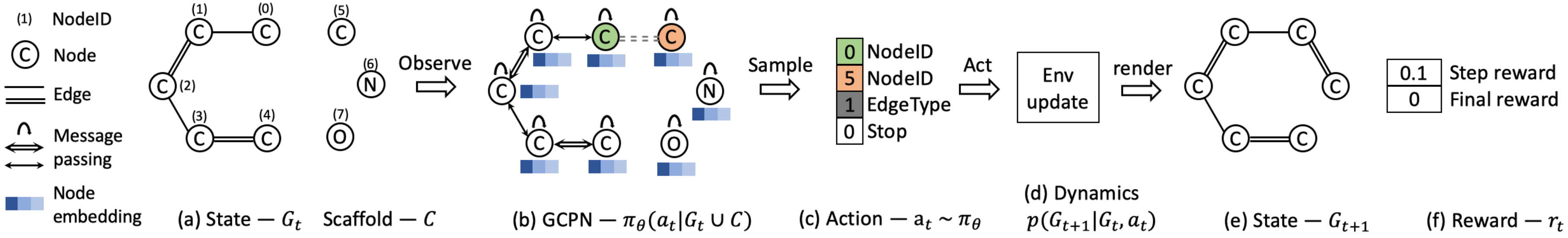
- A Graph Neural Network **graph classification model**
- Predict promising molecules from a pool of candidates



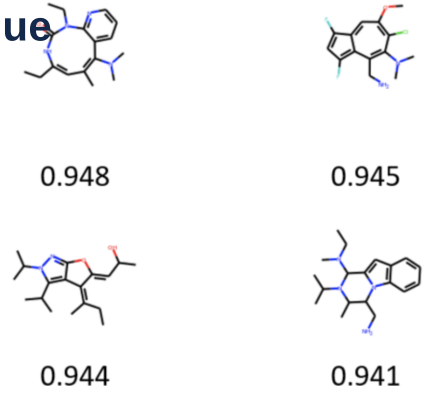
Stokes et al., A Deep Learning Approach to Antibiotic Discovery, Cell 2020

Molecule Generation / Optimization

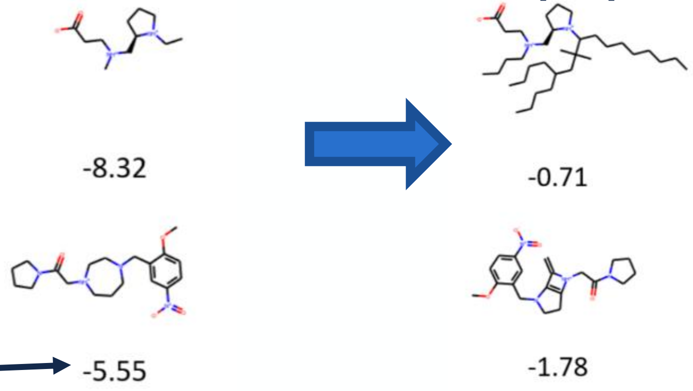
- **Graph generation**: Generating novel molecules



Use case 1: Generate novel molecules with high Drug likeness value



Use case 2: Optimize existing molecules to have desirable properties



Drug likeness

You et al., Graph Convolutional Policy Network for Goal-Directed Molecular Graph Generation, NeurIPS 2018

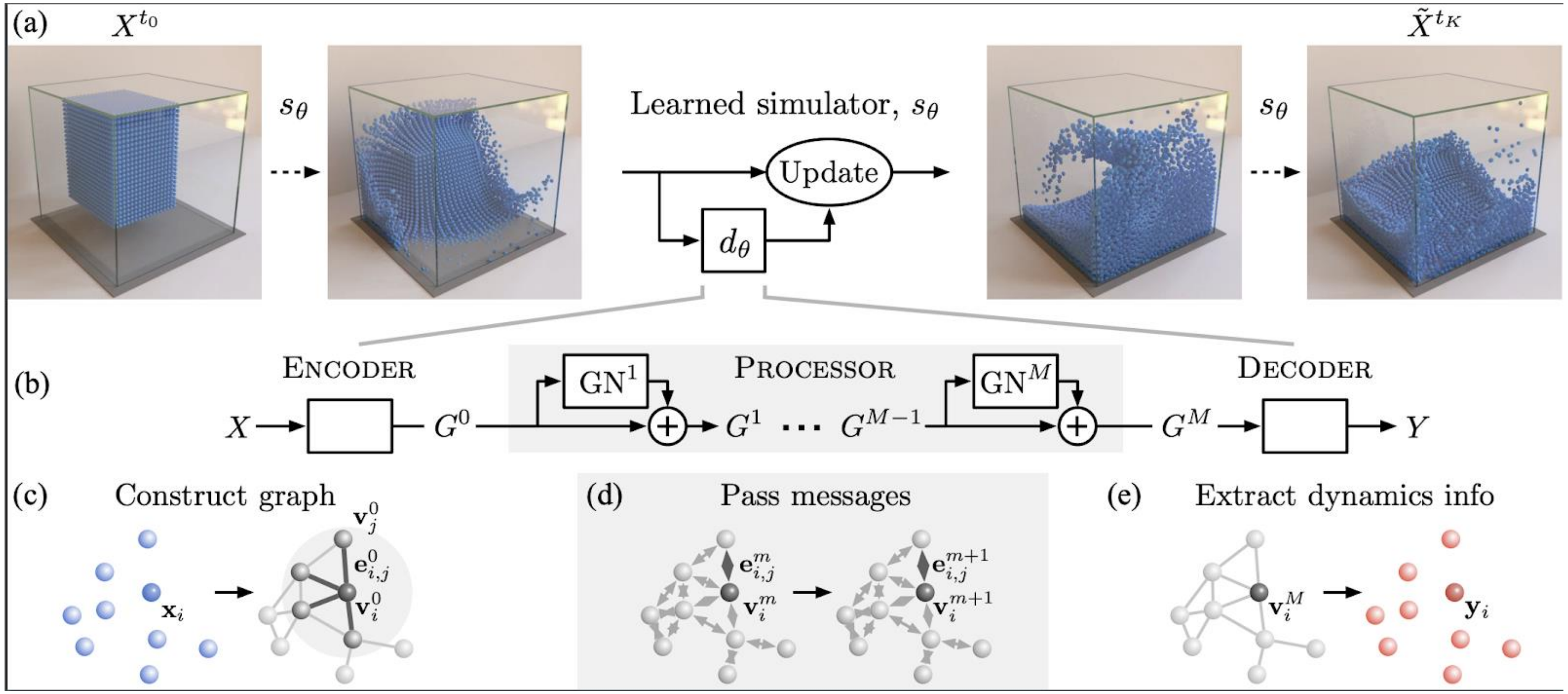
Example (6): Physics Simulation

- Physical simulation as a graph:
  - **Nodes**: Particles
  - **Edges**: Interaction between particles

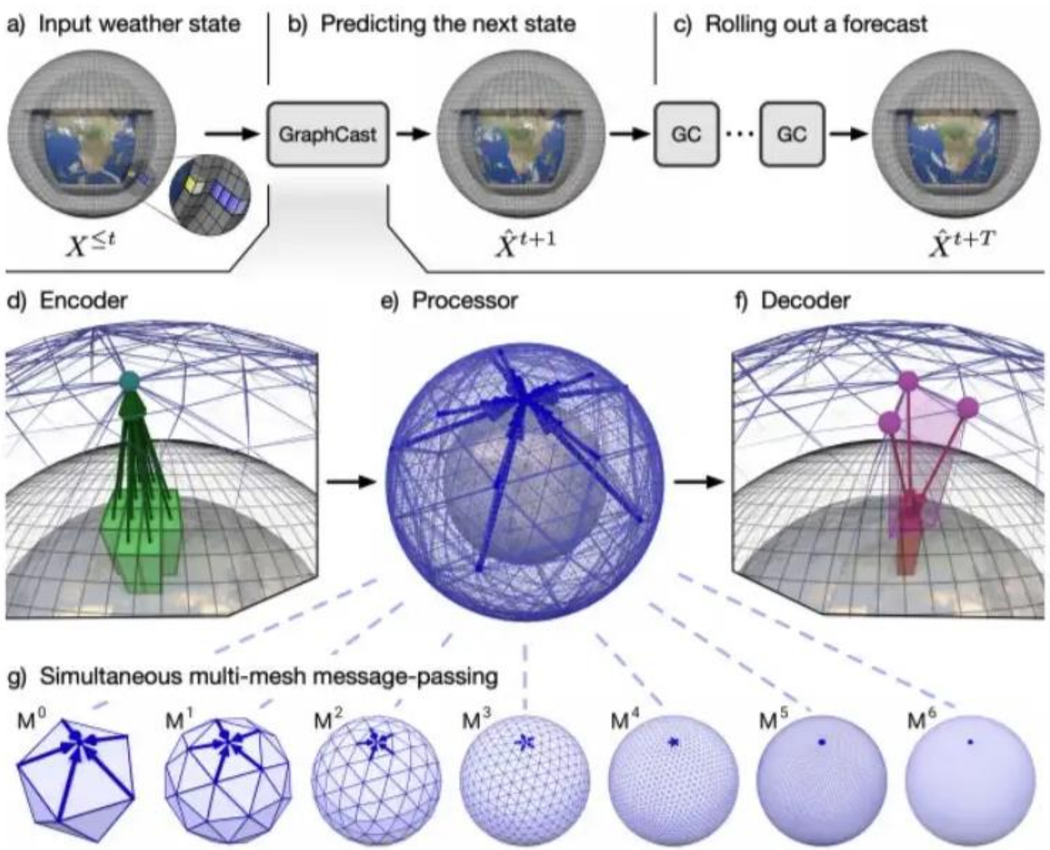
Sanchez-Gonzalez et al., Learning to simulate complex physics with graph networks, ICML 2020

Simulation Learning Framework

- **A graph evolution task:**
  - **Goal**: Predict how a graph will evolve over time



Application: DeepMind weather forecasting



Course Logistics

Course Objective

Takeaways from this course:

- **Knowledge** about graph deep learning
    - Core knowledge: Insights, Coding, Math
    - Latest knowledge: Recent research papers
- **Training** for AI research
    - Experience the full lifecycle as an AI researcher
        - Read, Ideate, Discuss, Code, Write, Review, Present

Prerequisites

- The course is mostly self-contained
- Minimum prerequisites
  - Deep learning: basic concepts
  - Python programming
- Recommended background
  - Deep learning: PyTorch
  - Graph: data structure
  - Machine learning, Probability and statistics
  - Comfortable of using (free) LLM Tools: ChatGPT/Gemini/Copilot/…

We Embrace "ChatGPT Moment"

- Fundamentally changed AI & beyond
- In this course, **we embrace LLMs**
  - **Lectures:** feel free to ask LLMs to help understand lecture materials
  - **Assignments:** feel free to use LLMs to help, but you *must include your prompt*
  - **Projects:** focus on ideas that naively applying LLMs would fail
- But we cherish **non-LLM-able** things
  - **Research training:** asking good questions is always more important than answering given questions

Course Logistics (1)

- Meeting Times:
  - 12:30 PM - 01:45 PM, Wednesday & Friday
  - Urbana-Champaign Campus | Siebel Center for Comp Sci | Room 1304
  - Videos of the lectures will be recorded and posted on Canvas
- Structure of lectures:
  - 70 minutes of a lecture
  - During this time, you can ask questions
  - 10 minutes of a live Q&A/discussion session at the end of the lecture
- Teaching Staff
  - Instruction: Jiaxuan You
  - Course TA: Zirui Cheng

Course Logistics (2)

- Readings:
  - Graph Representation Learning Book by Will Hamilton
  - Research papers
- Optional readings:
  - Papers and pointers to additional literature
  - This will be very useful for course projects
- Communication
- Office Hours

Course Logistics (3)

- Final grade will be composed of:
  - Assignments: 20%
    - 5 coding assignments using Google Colab, each worth 4%
  - Presentation: 20%
    - 5 min lightning presentation
  - Course project: 60%
    - Proposal: 20%; Final report: 70%; Poster: 10%
  - Extra credit: course participation
    - Used if you are on the boundary between grades

ILLINOIS

Thanks!

Deep Learning with Graphs
Jiaxuan You