Yale

Introduction to Graph Learning

CPSC483: Deep Learning on Graph-Structured Data

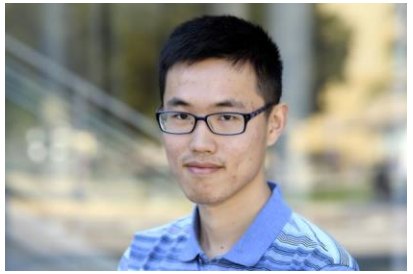
Rex Ying

CPSC483 Course Logistics

- **Welcome to CPSC 483 / 583!**
- **The class meets Monday and Wednesday 11:35 AM-12:50 PM**
  - Most of the lectures will be in-person
  - There will be 2-3 guest lectures, some of which might be held remotely. (including GNN library and applications of graph learning)
- **This is a new course, and feedbacks are especially welcomed!**
  - Many of the content comes from relatively recent research (>2017)
  - Lecture style, homework, projects …

Logistics: Teaching Staff

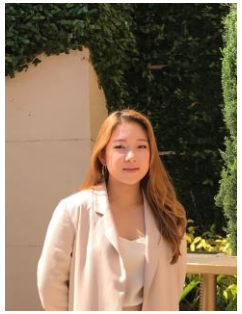
Instructor



Rex Ying

Teaching Assitants

Borui Wang



Hannah Ji

Chen Liu

Guest Lecture

Smita Krishnaswamy

Matthias Fey

Topics

Spectral graph learning, Biology applications

The PyTorch Geometric Library Framework

Course Outline

Lecture	Topic	Lecture	Topic	Lecture	Topic
1	Background: Machine Learning and Graphs as Data Structure	10	GNN Expressive Power	19	GNN AutoML
2	Plethora of Tasks and Features on Graphs	11	PyTorch Geometric Library (virtual)	20	Learning on Dynamic Graphs
3	Graph Neural Networks Models	12	Graph Generative Models	21	Heterogeneous Graphs for Social Networks and Recommender Systems
4	Graph Neural Networks Designs	13	Spectral GNNs	22	Knowledge Graph Reasoning
5	GNN Implementations, Objectives and Loss Functions	14	Self-supervised Learning with GNNs	23	Knowledge Graph Embeddings in Hyperbolic Spaces
6	Graph Attention Networks	15	Explaining GNN Predictions	24	Applications of Graph Learning in Biology and Medicine
7	Scalable GNN Architectures	16	Distributed Node Embeddings	25	Applications in Graphics and Scientific Simulations
8	Multi-hop GNNs and Multi-hop Attentions	17	Geometric Embeddings: Order and Box Embeddings		
9	Theory of Graph Neural Networks	18	Hyperbolic Embeddings and Hyperbolic GNNs		

The syllabus, slides and reading will be available on course website

Logistics: Website

- **Course Website**
  - https://graph-and-geometric-learning.github.io/CPSC483-website/
  - Slides will be posted before or shortly after the class
- **Readings:**
  - Graph Representation Learning Book by Will Hamilton
  - Research papers
- **Optional readings:**
  - Papers and pointers to additional literature
  - **These will be very useful for course projects**
- PyTorch Geometric Readings
  - Python Documentation
  - GitHub Repository (for the latest development)

Logistics: Communication

- **Piazza Q&A website:**
  - Signup at piazza.com/yale/fall2022/cpsc483
    - Register with your @yale.edu email
  - **Please participate and help each other!**
    - Don't post code, annotate your questions, search for answers before you ask
- **Mailing List**
  - Teaching staff: cpsc483_staff@mailman.yale.edu
- We will post course announcements to the course website (make sure you check it regularly)
- Office Hours (also posted and updated on the website
  - Instructor: Wednesday
  - TAs: see course website

Work for the Course & Grading

- **Final grade will be composed of:**
  - **Homework: 30%**
    - Homework 1, 2, 3, 4, each worth 10%
  - **Coding assignment: 20%**
    - 4 (short) coding assignments using Google Colab / Jupyter Notebook
  - **Exam (during the last lecture): 20%**
    - Light-weight **1 hour** exam (closed book).
  - **Course project: 30%**
    - Proposal: 30%
    - Final report: 70%
  - **Extra credit: code contribution (up to 10%)**
    - Opensource contributions: PyG, new library / public benchmarks related to the course
    - Used if you are on the boundary between grades

The assignments will be short. I'm expecting 1-2 hours each (If pre-reqs are met)

Homework, Write-ups

- **Assignments take time. Start early!**
  - A combination of data analysis, algorithm design, and math
  - Generally due on Thursdays 23:59 Pacific Time
- **How to submit?**
  - **Canvas**
  - **Both homework (including code) and project deliverables (pdf)** must be uploaded
    - Code: ipynb file; written assignment: pdf file
  - We prefer LaTeX submissions for written assignments.
  - If you really need to use hand-writing, make sure it's **readable**.
    - TAs have no obligations to use magnifying glasses to figure out what you write
- **Total of 2 Late Periods (LP) per student (up to 5 working days):**
  - Max 1 late period per assignment (no LP for the final report)

Honor Code

- **We strictly enforce the Yale Honor Code**
  - Violations of the Honor Code include:
    - Copying or allowing another to copy from one's own paper
    - Unpermitted collaboration
    - Plagiarism
    - Giving or receiving unpermitted aid on an examination
    - Representing as one's own work the work of another
    - Giving or receiving aid on an assignment under circumstances in which a reasonable person should have known that such aid was not permitted
  - The sanction for even a first offense is severe

Course Projects

- **Course project:**
  - Reproduce, analyze and compare at least 2 methods for the same task (on at least 2 large-scale datasets)
  - Propose new algorithms / architectures and validate on at least 2 datasets
- **Performed in groups of up to 3 students:**
  - Fine to have groups of 1 or 2. The team size will be taken under consideration when evaluating the scope of the project in breadth and depth. But 3 person teams are usually more efficient.
  - Project is the **important work** for the class
  - Can be very beneficial if you aim to work on research in this topic
  - Consult with the teaching staff if you have questions
- **More information will be posted on the course website in 3 weeks**

Course Schedule

Week	Assignment	Due on (11:59pm PT)
1	**Colab 1**	Fri, Sep 16th
2	**Homework 1**	Wed, Sep 21st
	Colab 2	
	Homework 2	
	Project Proposal	
	Colab 3	
	Homework 3	
	Project Milestone	
	Colab 4	
	Project Report	Fri, December 9th **(No Late Period for this)**

Prerequisites

- **The course has relevance to a wide range of topics and background in graph or ML is always helpful!**
- **Minimum Pre-requisites**
  CPSC 201, 223 and one of 365 and 366
  - **Nice-to-have background (have taken a course or have done research)**
    - **Machine Learning (minimum: high familiarity with linear algebra and multi-variable calculus)**
    - Algorithms and graph theory
    - Probability and statistics
  - **Programming:**
    - You should be able to write non-trivial programs (in **Python**)
      - Knowledge about common libraries such as Numpy, Pandas etc. is a plus
    - Ideally you have used **PyTorch** (or equivalent) before. But learning it is not too hard if you have good knowledge in machine learning.

Graph Machine Learning Tools

- **We use PyTorch Geometric (PyG)**
- **We further recommend:**
  - **DeepSNAP**: Library that assists deep learning on graphs.
    - Flexible graph manipulation, standard data split pipeline, …
  - **GraphGym**: Platform for designing Graph Neural Networks.
    - Modularized GNN implementation, simple hyperparameter tuning, flexible user customization
  - Both are helpful for the course project (save your time & provide advanced GNN functionalities)
  - **DGL** is an alternative to PyG
- **Other network analytics tools**: SNAP.PY, NetworkX, Graph-Tool, Graphvis

Yale

Introduction to Graph and Machine Learning on Graphs

CPSC483: Deep Learning on Graph-Structured Data

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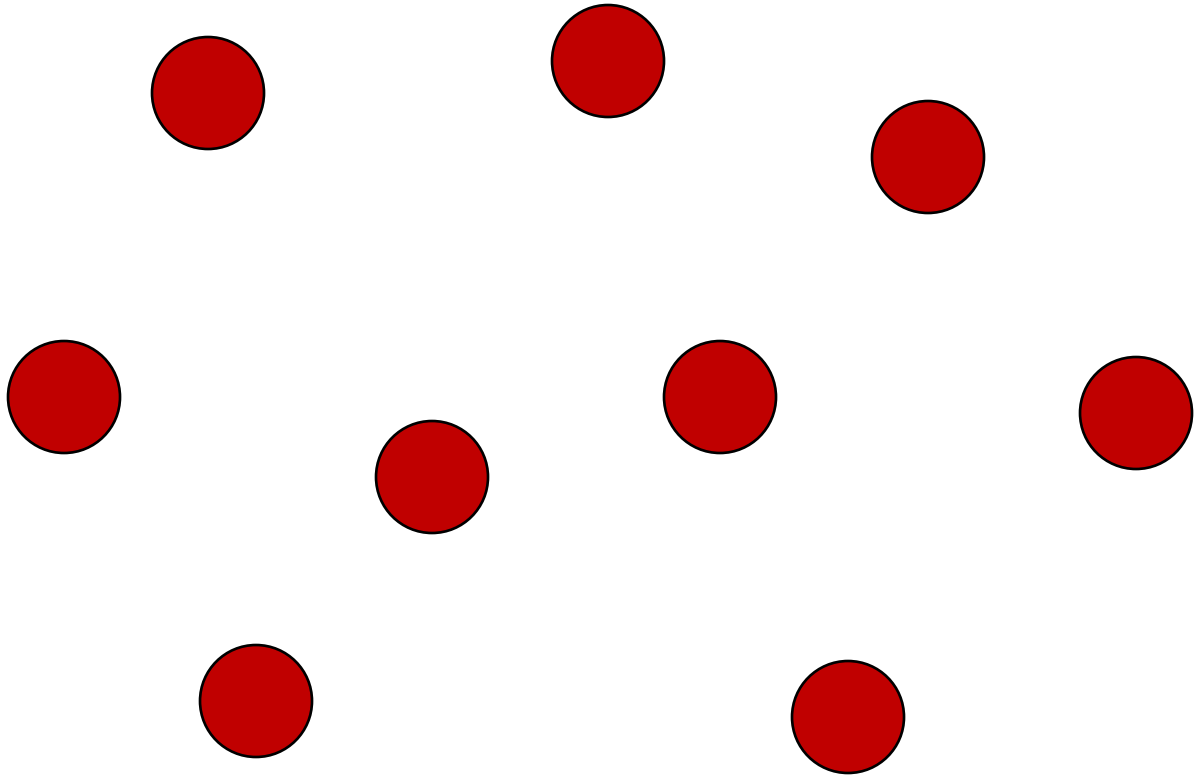
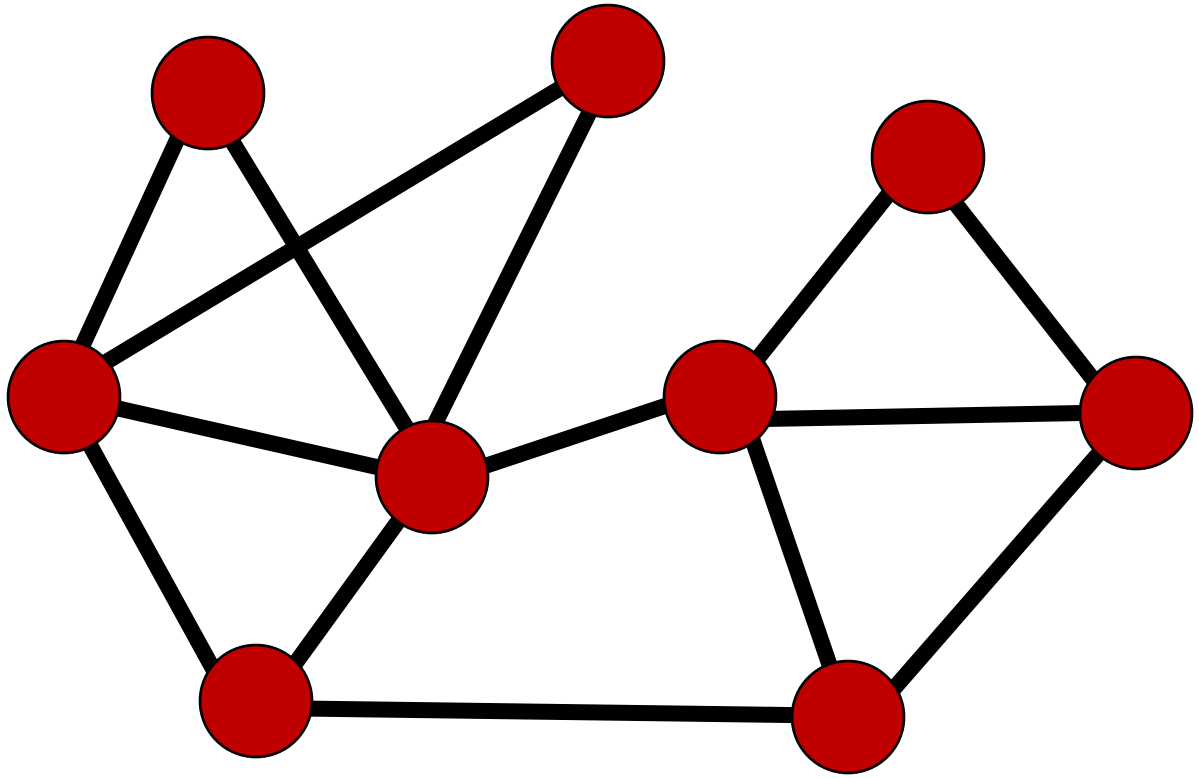
Why Graphs?

Graphs are a general language for describing and analyzing entities with relations/interactions





Graph

Types of Networks and Graphs (1)

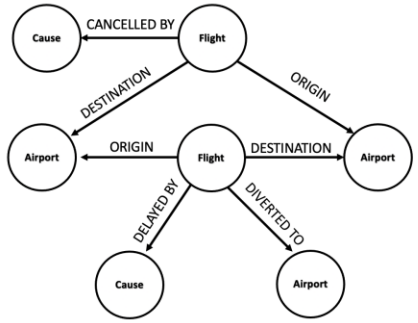
- **Networks (also known as Natural Graphs):**
  - **Social networks:**
    - **Society** is a collection of 7+ billion individuals
  - **Communication and transactions:**
    - Electronic devices, phone calls, financial transactions
  - **Biomedicine:**
    - Interactions between **genes/proteins** regulate life
  - **Brain connections:**
    - Our **thoughts** are hidden in the connections between billions of neurons

Types and Networks and Graphs (2)

- **Graphs (as a representation):**
  - **Information, knowledge** are organized and linked
  - **Software, code** can be represented as a graph
  - **Similarity networks:** Connect similar data points
  - **Relational structures:** Molecules, Scene graphs, 3D shapes, Particle-based physics simulations

Sometimes the distinction between networks & graphs is blurred.

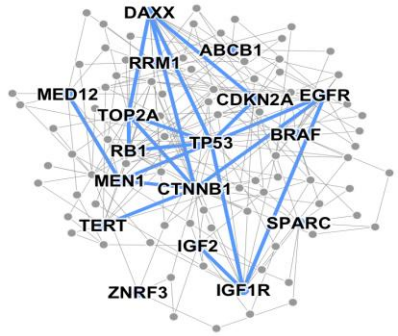
Many Types of Data are Graphs (1)



Event Graphs

Image credit: SalientNetworks

Computer Networks



Disease Pathways

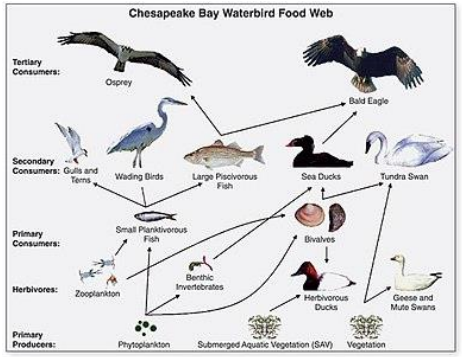


Image credit: Wikipedia

Food Webs

Image credit: Pinterest

Particle Networks

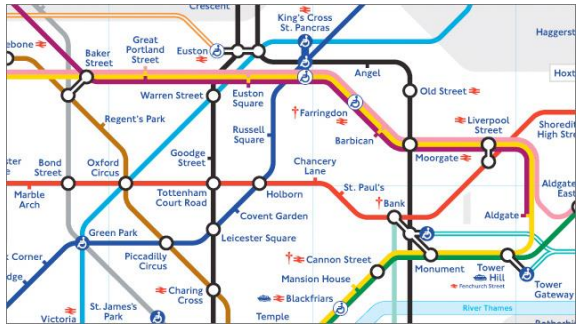


Image credit: visitlondon.com

Underground Networks

Many Types of Data are Graph (2)

Image credit: Medium

Social Networks

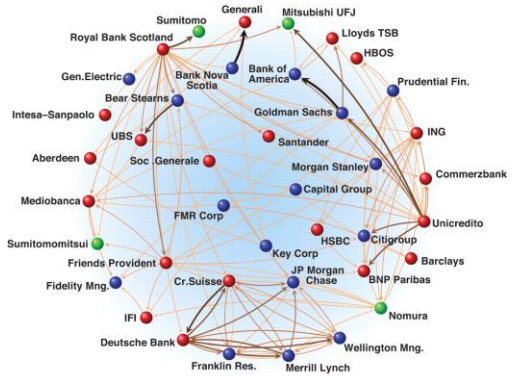
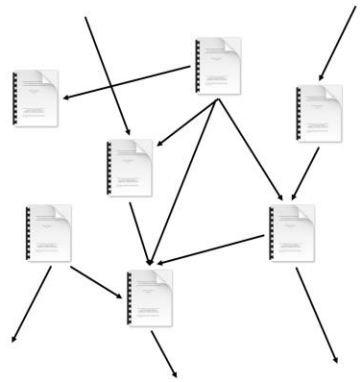


Image credit: Science

Economic Networks

Image credit: Lumen Learning

Communication Networks



Citation Networks

Image credit: Missoula Current News

Internet

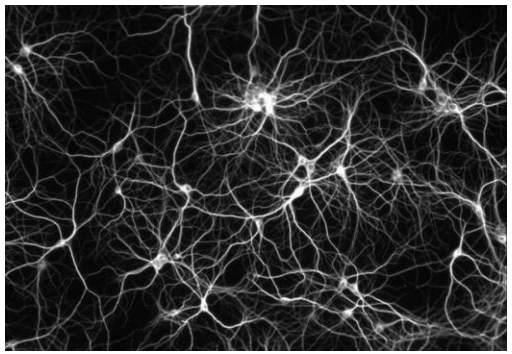


Image credit: The Conversation

Networks of Neurons

Many Types of Data are Graph (3)

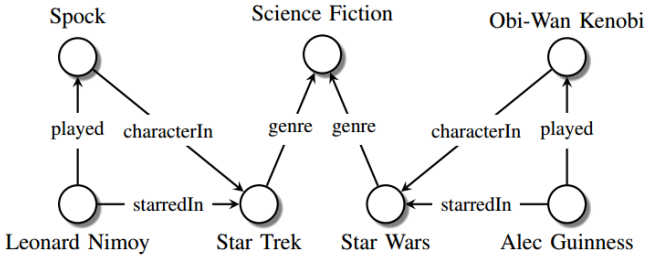


Image credit: Maximilian Nickel et al

Knowledge Graphs

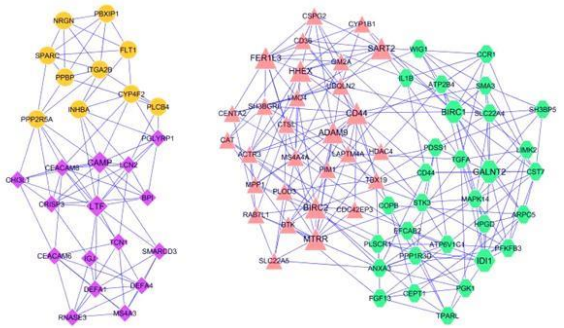


Image credit: ese.wustl.edu

Regulatory Networks

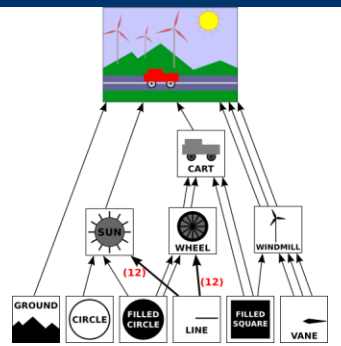


Image credit: math.hws.edu

Scene Graphs

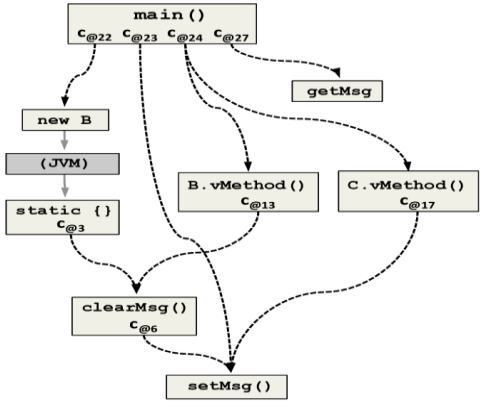


Image credit: ResearchGate

Code Graphs

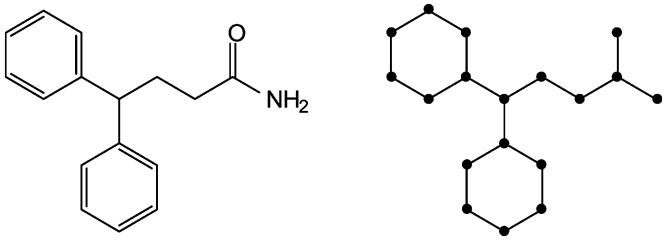


Image credit: MDPI

Molecules

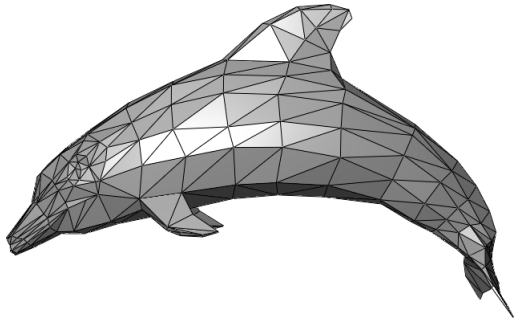
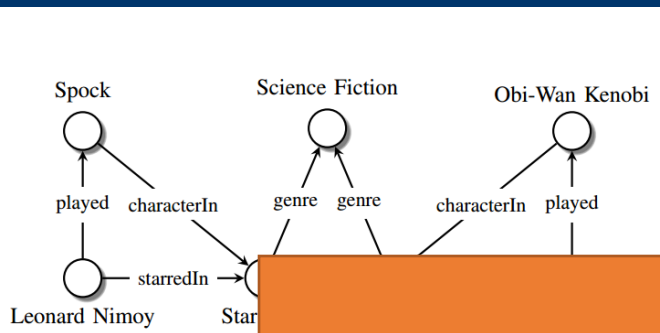
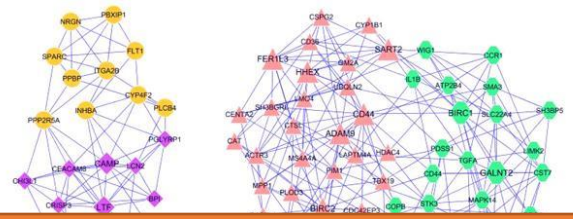


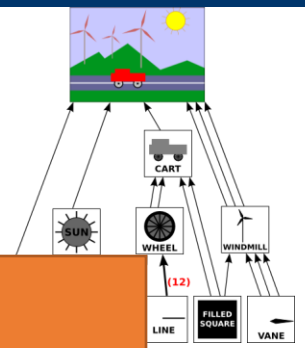
Image credit: Wikipedia

3D Shapes

Graphs and Relational Data







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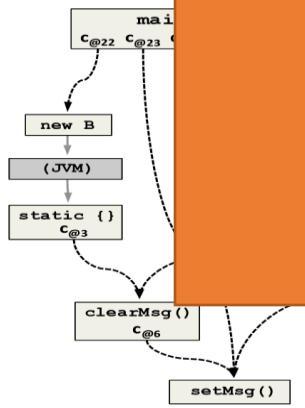
nath.hws.edu

Know

Graphs

Main question:

How do we take advantage of relational structure for better prediction?



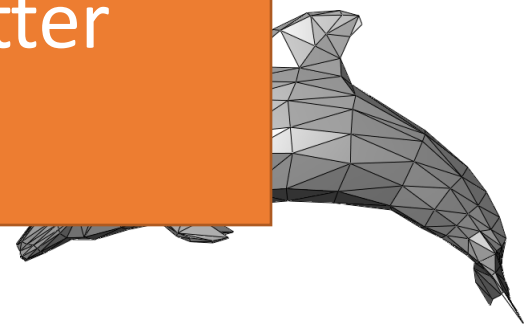


Image credit: ResearchGate

Image credit: MDPI

Image credit: Wikipedia

Code Graphs

Molecules

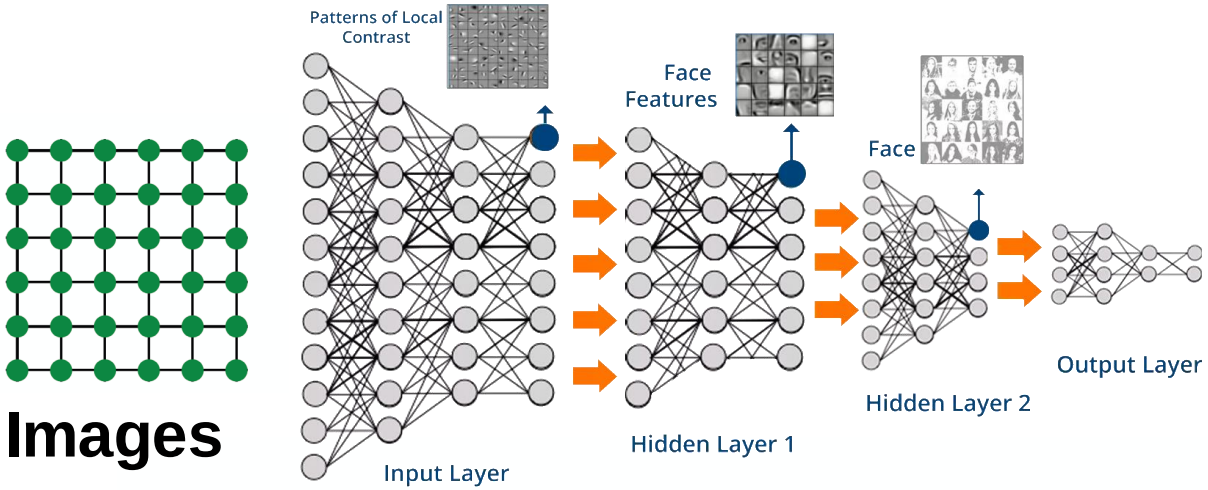
3D Shapes

Graphs: Machine Learning

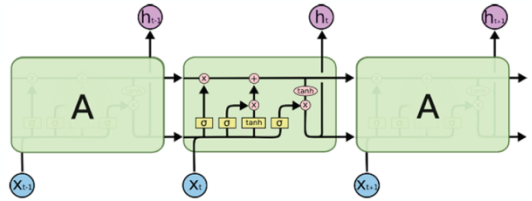
Complex domains have a rich relational structure, which can be represented as a
relational graph

By explicitly modeling relationships we achieve better performance!

Modern ML Toolbox



Text/Speech

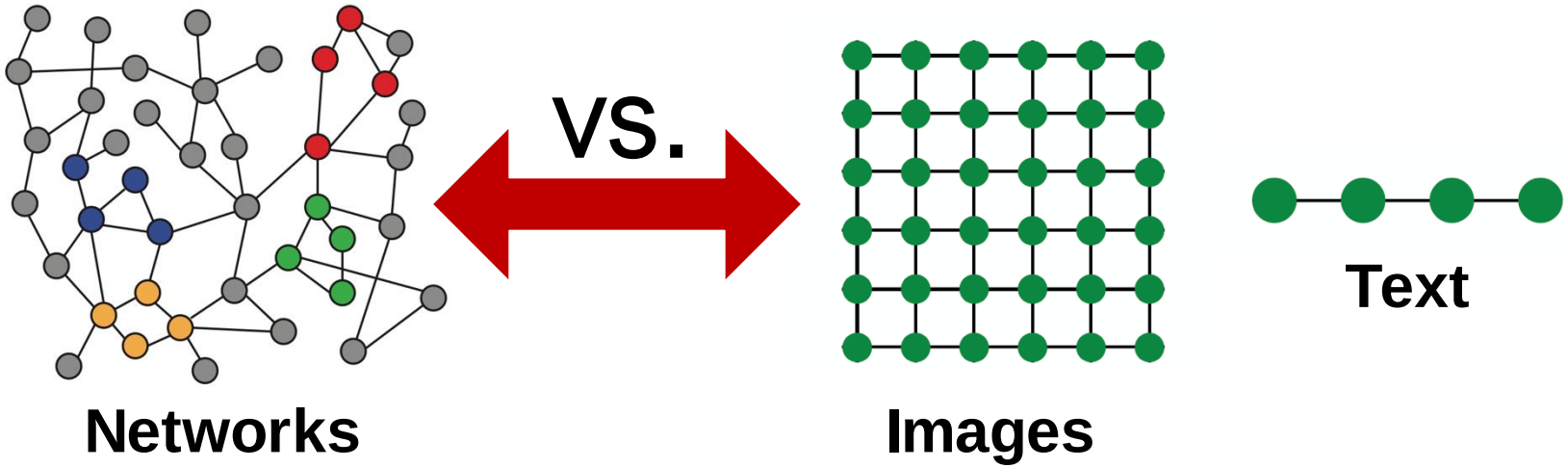


Modern deep learning toolbox is designed for simple sequences & grids

Why is it Hard?

Networks are complex.

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



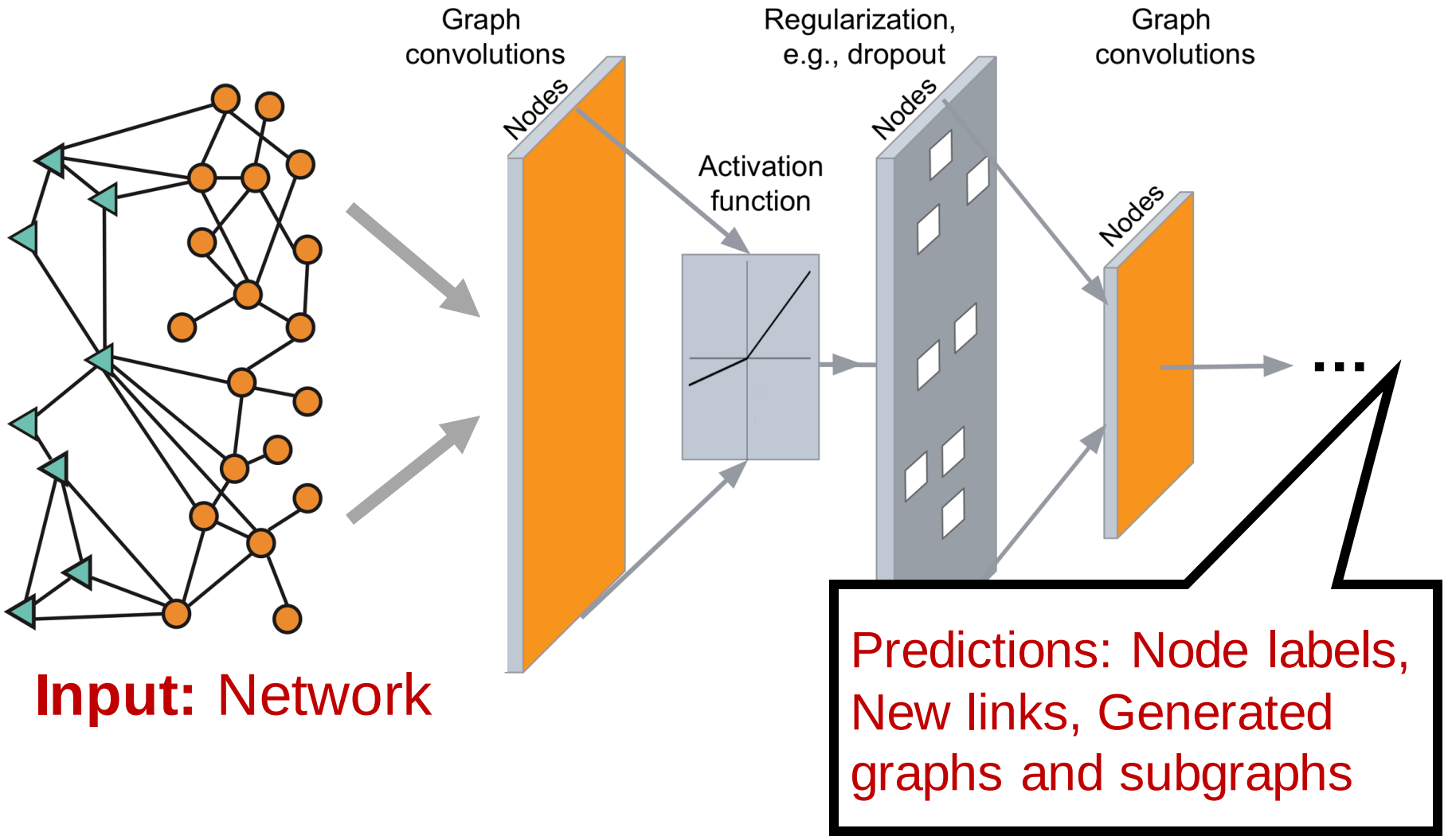
- No fixed node ordering or reference point
- Often dynamic and have multimodal features

This Course

- How can we develop neural networks that are much more broadly applicable?

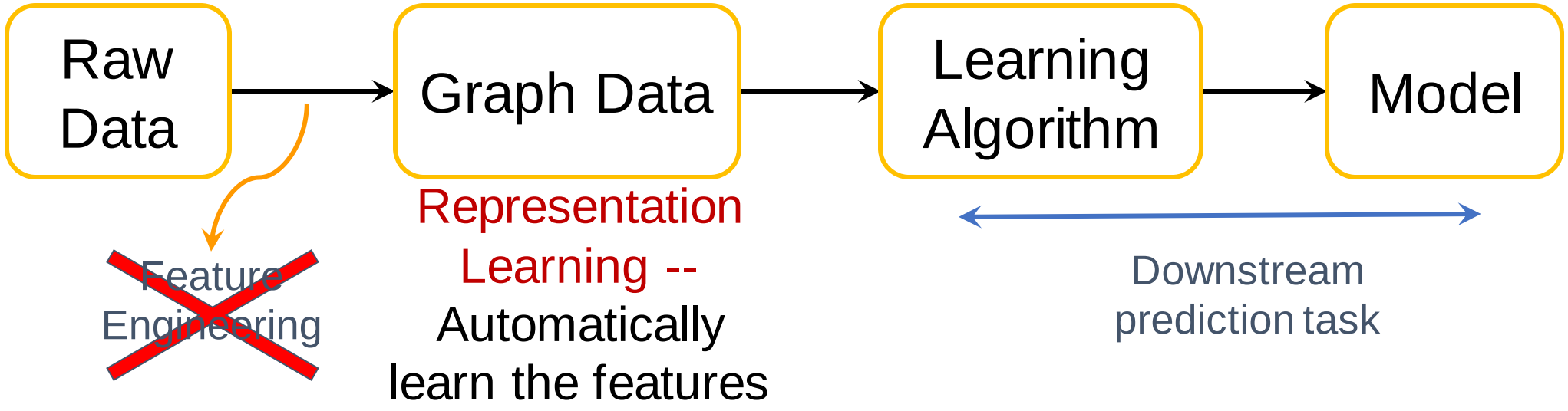
Graphs are currently at the new frontier of deep learning

CPSC483: Deep Learning on Graph-Structured Data



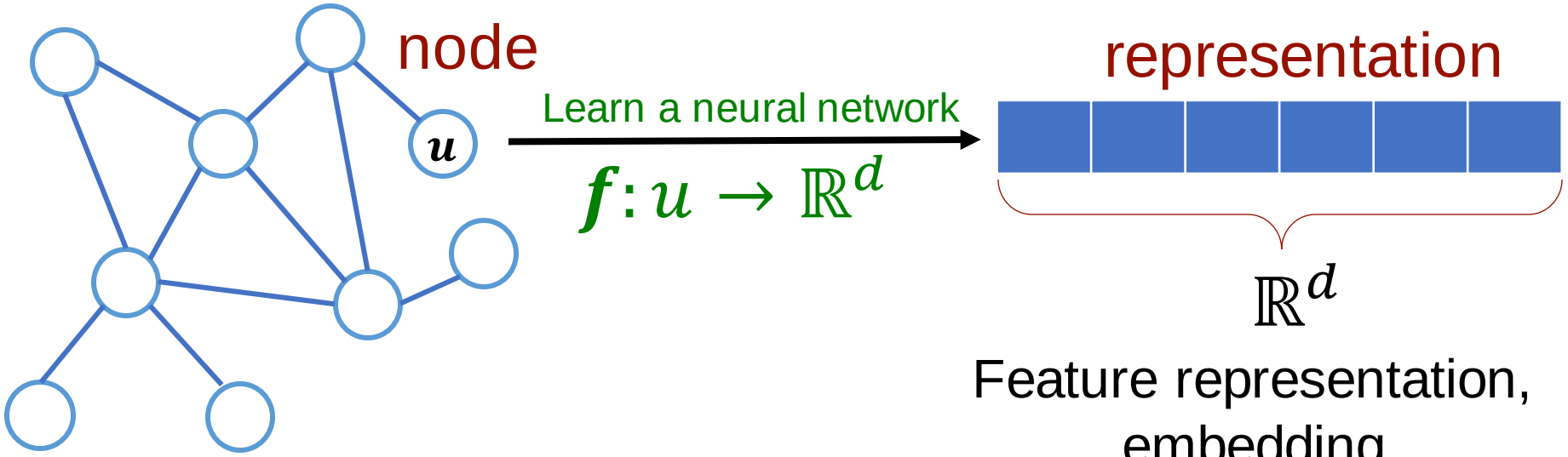
CPSC483 & Representation Learning (1)

- (Supervised) Machine Learning Lifecycle: This feature, that feature. Every Single Time!



CPSC483: Representation Learning (2)

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



CPSC483 Course Outline

We are going to cover various topics in Machine Learning and Representation Learning for graph structured data:

- Traditional methods: Graphlets, Graph Kernels
- Graph Neural Networks: GCN, GraphSAGE, GAT, Design space of GNNs, Theory of GNNs
- Methods for node embeddings: DeepWalk, Node2Vec
- Knowledge graphs and reasoning: TransE, BetaE, ConE
- Different types of inputs: Dynamic Graphs, Heterogeneous Graphs
- Deep generative models for graphs
- Applications to Biomedicine, Science, Industry

Topics Covered in CPSC483/583 (1)

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1	Background: Machine Learning and Graphs as Data Structure	10	GNN Expressive Power	19	GNN AutoML
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Topics Covered in CPSC483/583 (2)

Lecture	Topic	Lecture	Topic	Lecture	Topic
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GNN Fundamentals

Advanced Models

Geometric Embeddings

Real-world, Large-scale Applications

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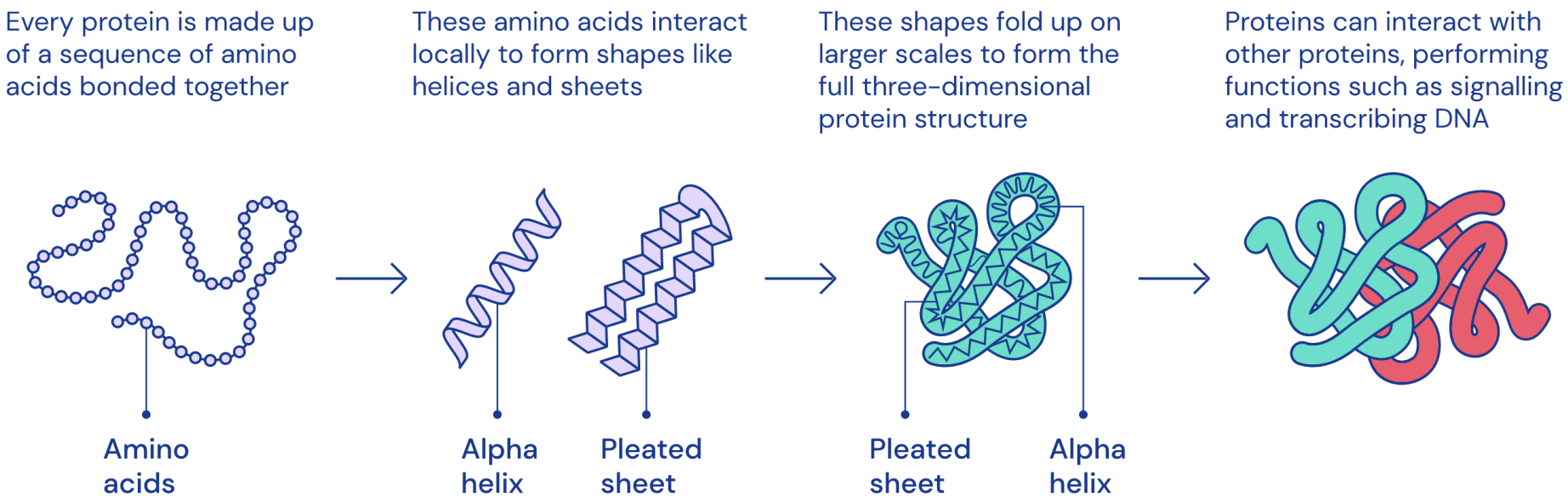
Example of Graph Machine Learning Tasks

Example 1: Protein Folding

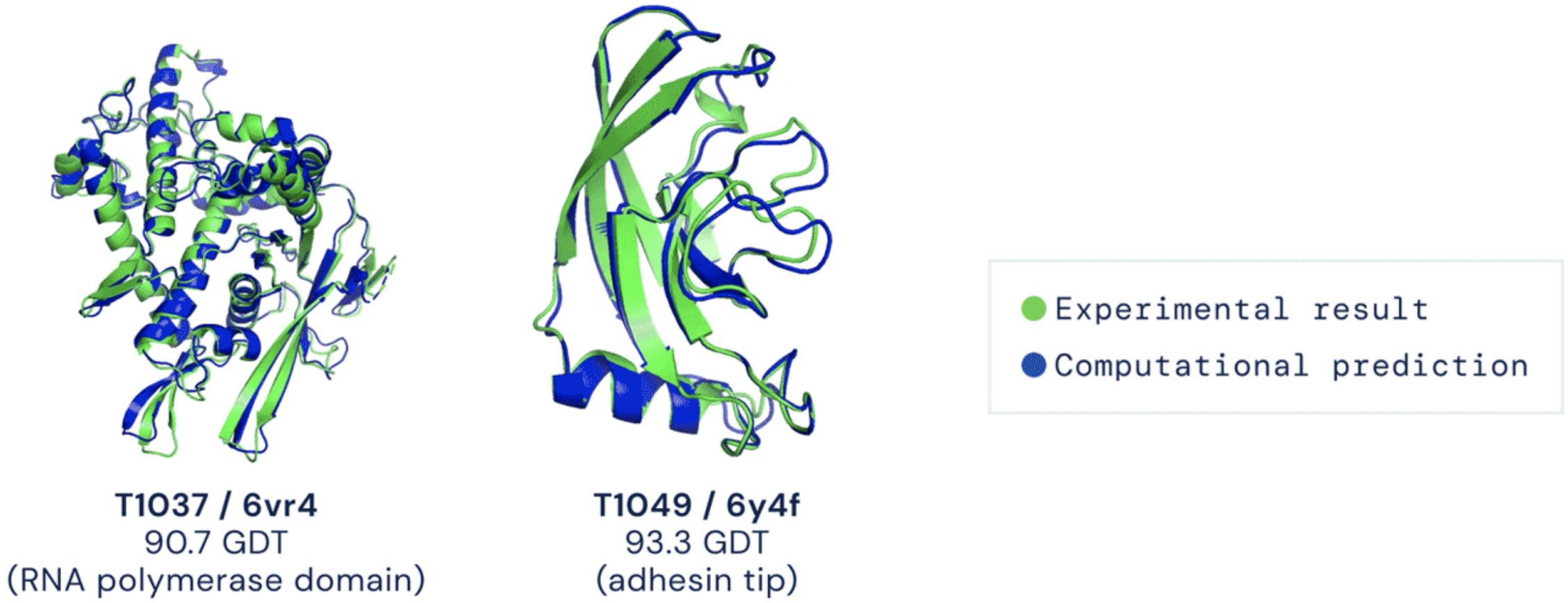
A protein chain acquires its native 3D structure



AW Senior *et al.* Improved protein structure prediction using potentials from deep learning.

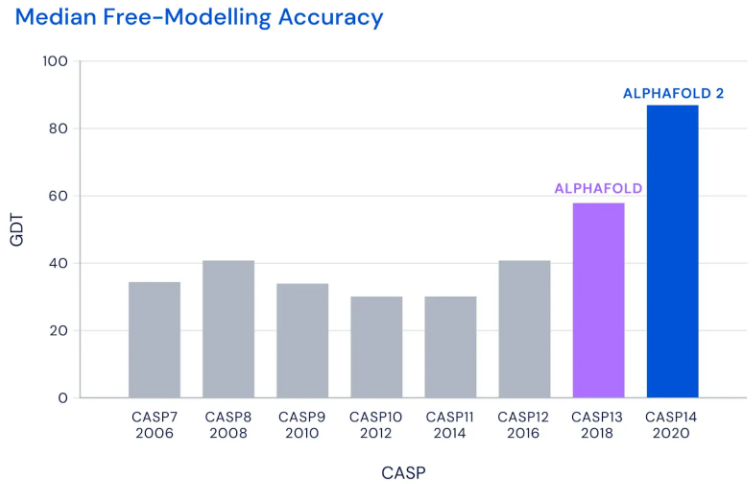
The Protein Folding Problem

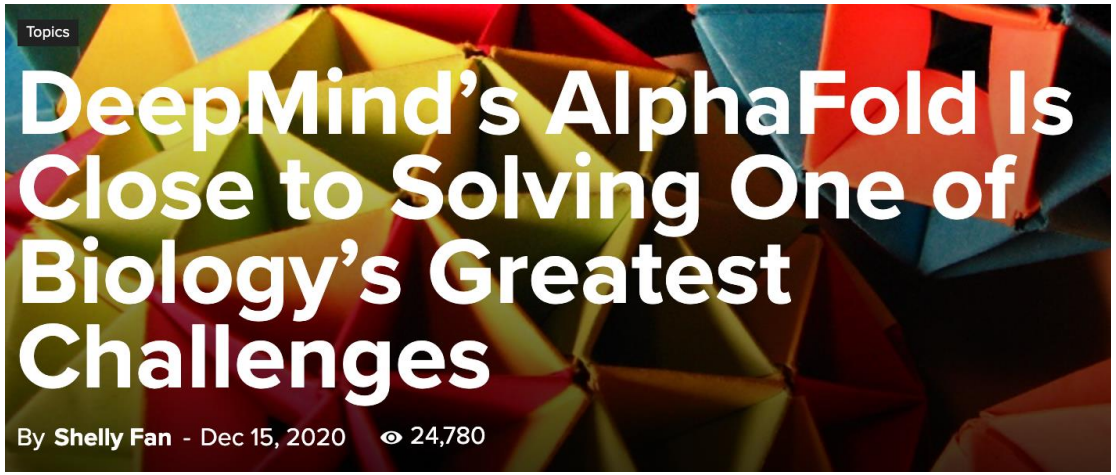
Computationally predict a protein's 3D structure based solely on its amino acid sequence



AW Senior *et al.* Improved protein structure prediction using potentials from deep learning.

AlphaFold: Impact





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

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

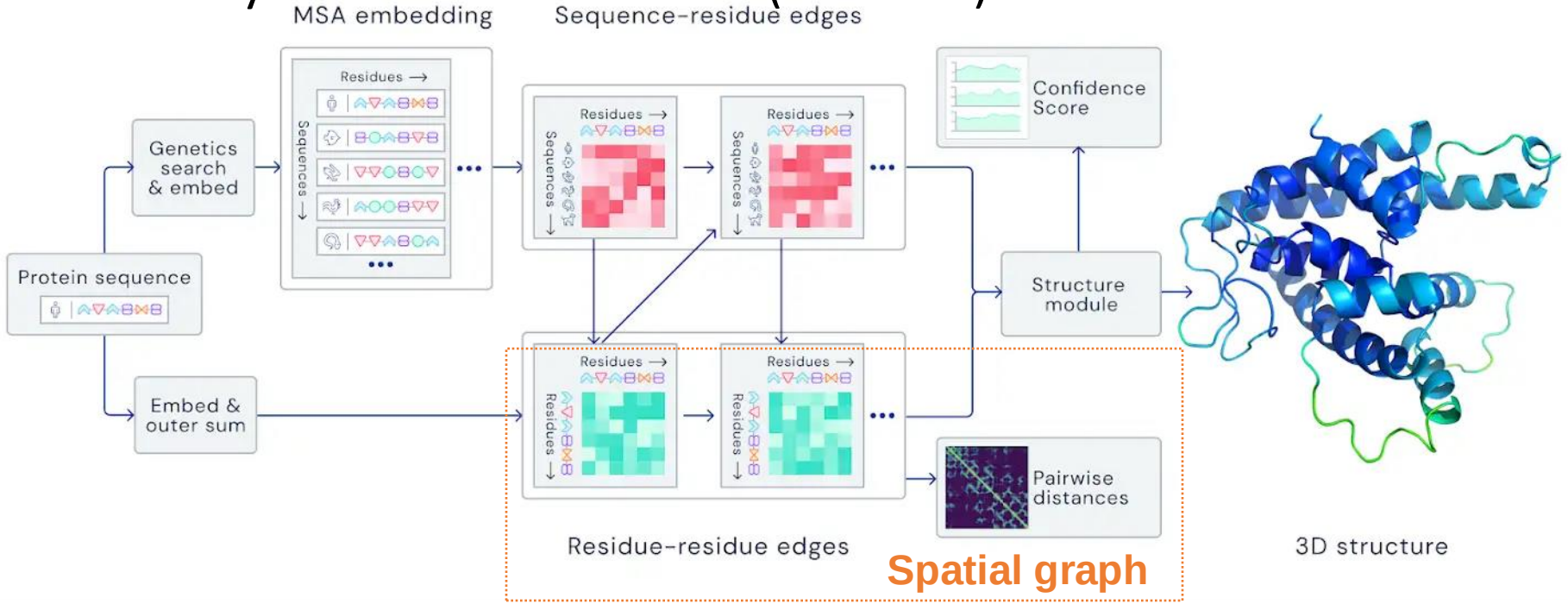
DeepMind's latest AI breakthrough could turbocharge drug discovery

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

AW Senior *et al.* Improved protein structure prediction using potentials from deep learning.

AlphaFold: Solving Protein Folding

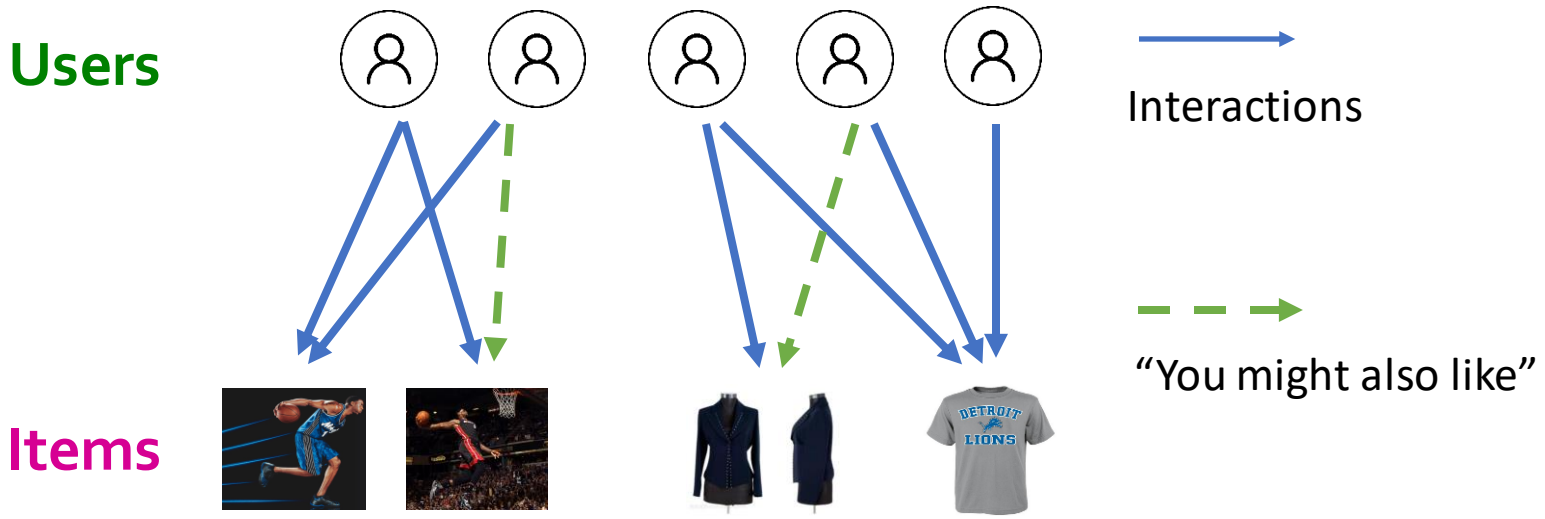
- Key Idea: ***Spatial Graph***
  - **Nodes**: Amino acids in a protein sequence
  - **Edges**: Proximity between amino acids (residues)



AW Senior *et al.* Improved protein structure prediction using potentials from deep learning.

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**



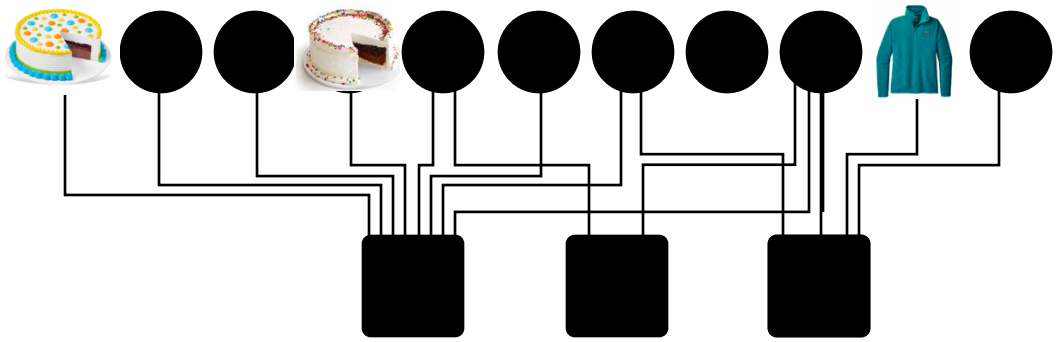
PinSage: Grpah-based Recommender

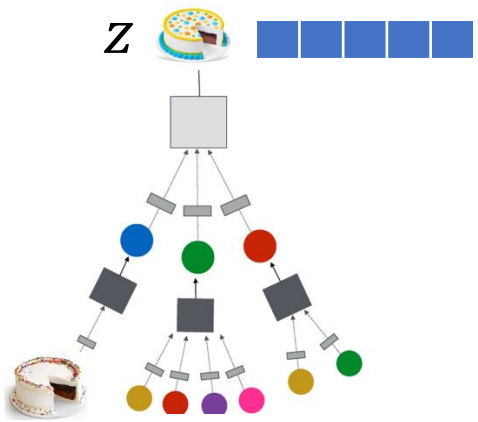
- Task: Recommend related pins to users

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

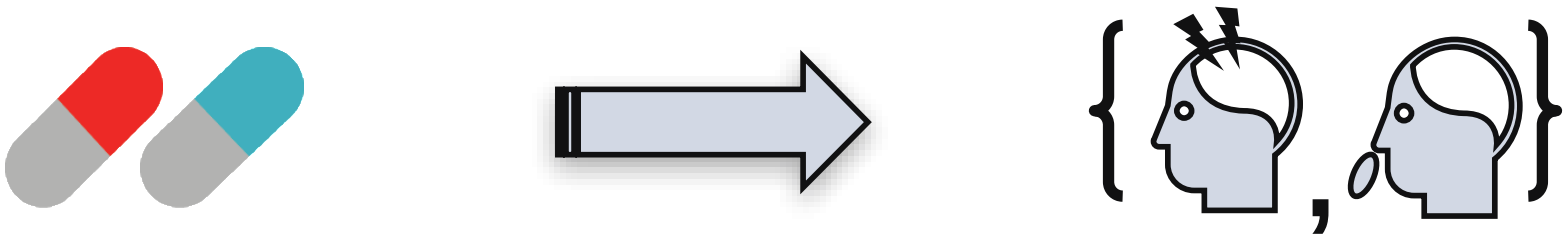




Rex Ying *et al*. Graph convolutional neural networks for web-scale recommender systems.

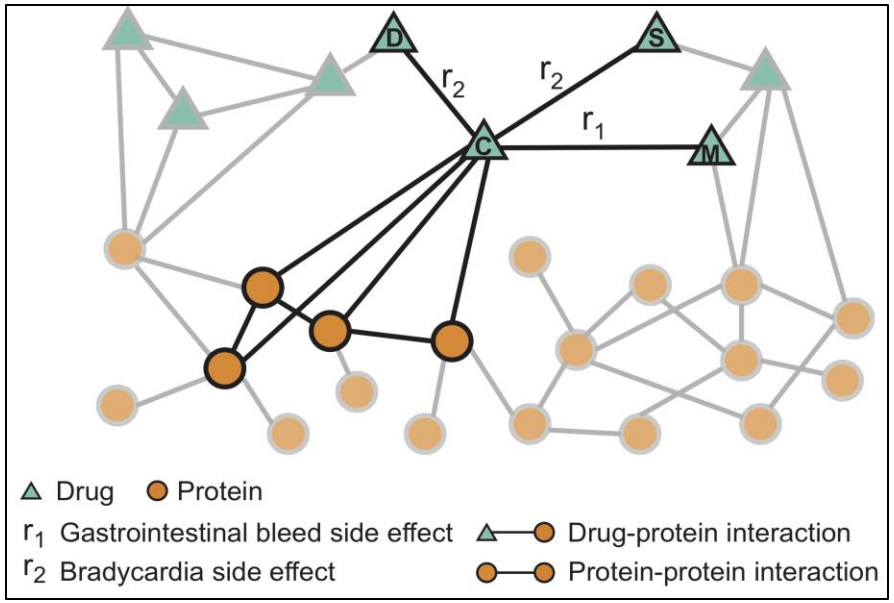
Example 3: Drug Side Effects

- Many patients take multiple drugs to treat complex or co-exsiting 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, tec.
- **Task**: Given a pair of drugs predict adverse side effects

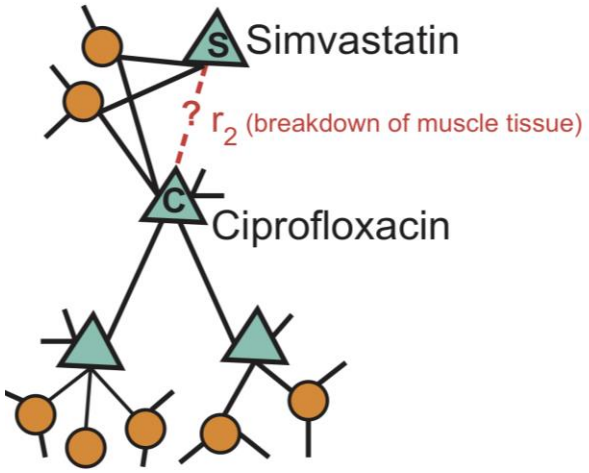


Biomedical Graph Link Prediction

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



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

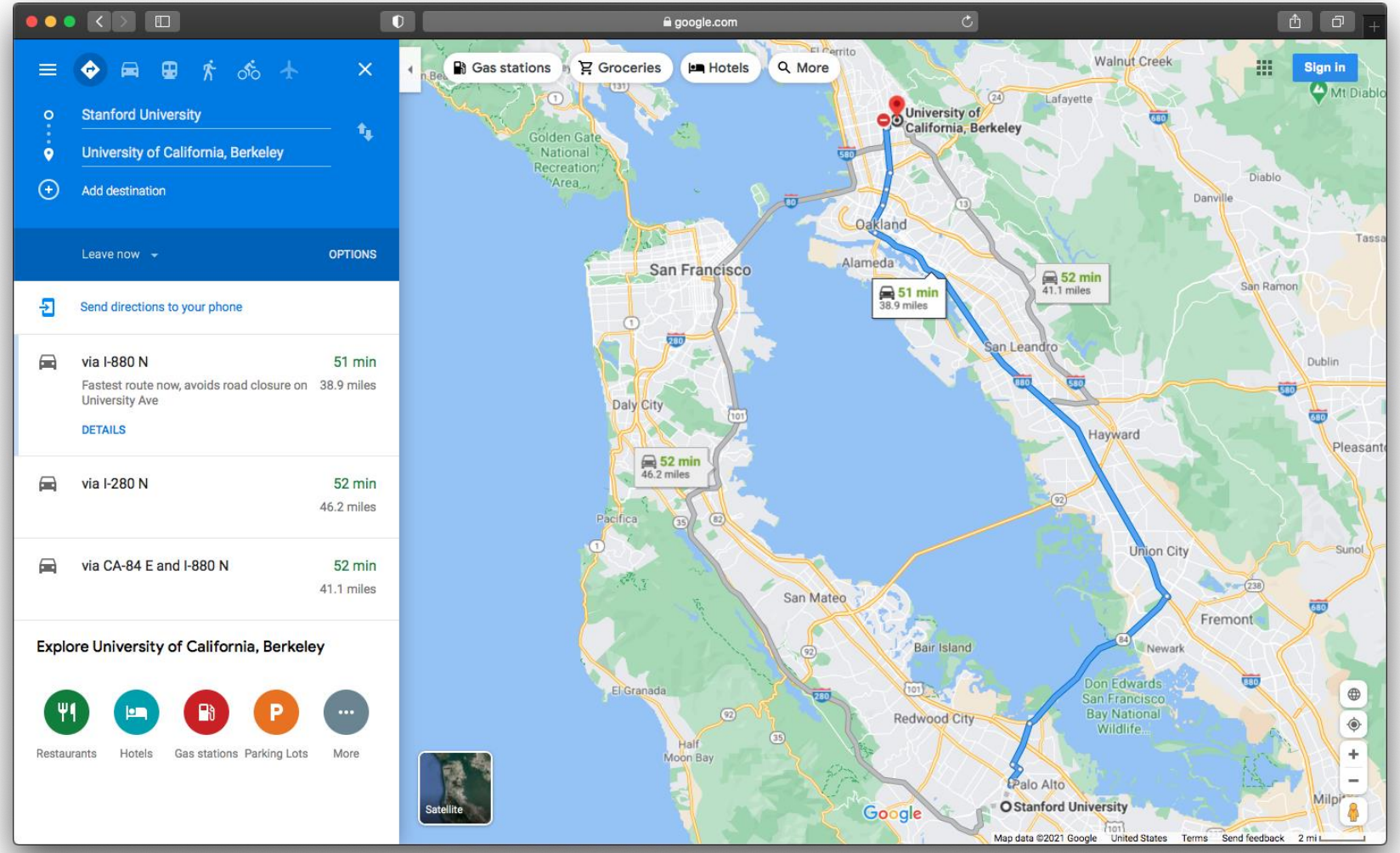


Results: De novo Predictions

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

Example 4: Traffic Prediction



Road Network as a Graph

- **Nodes:** Road segments
- **Edges:** Connectivity between road segments

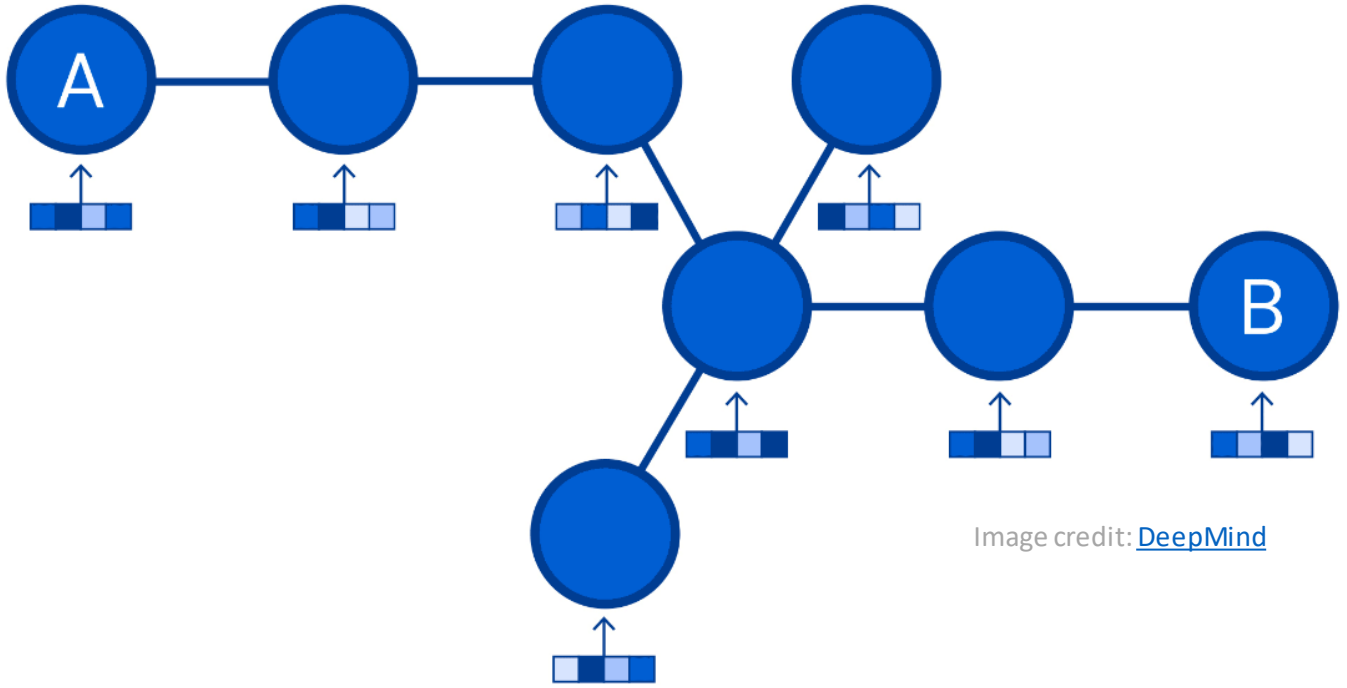
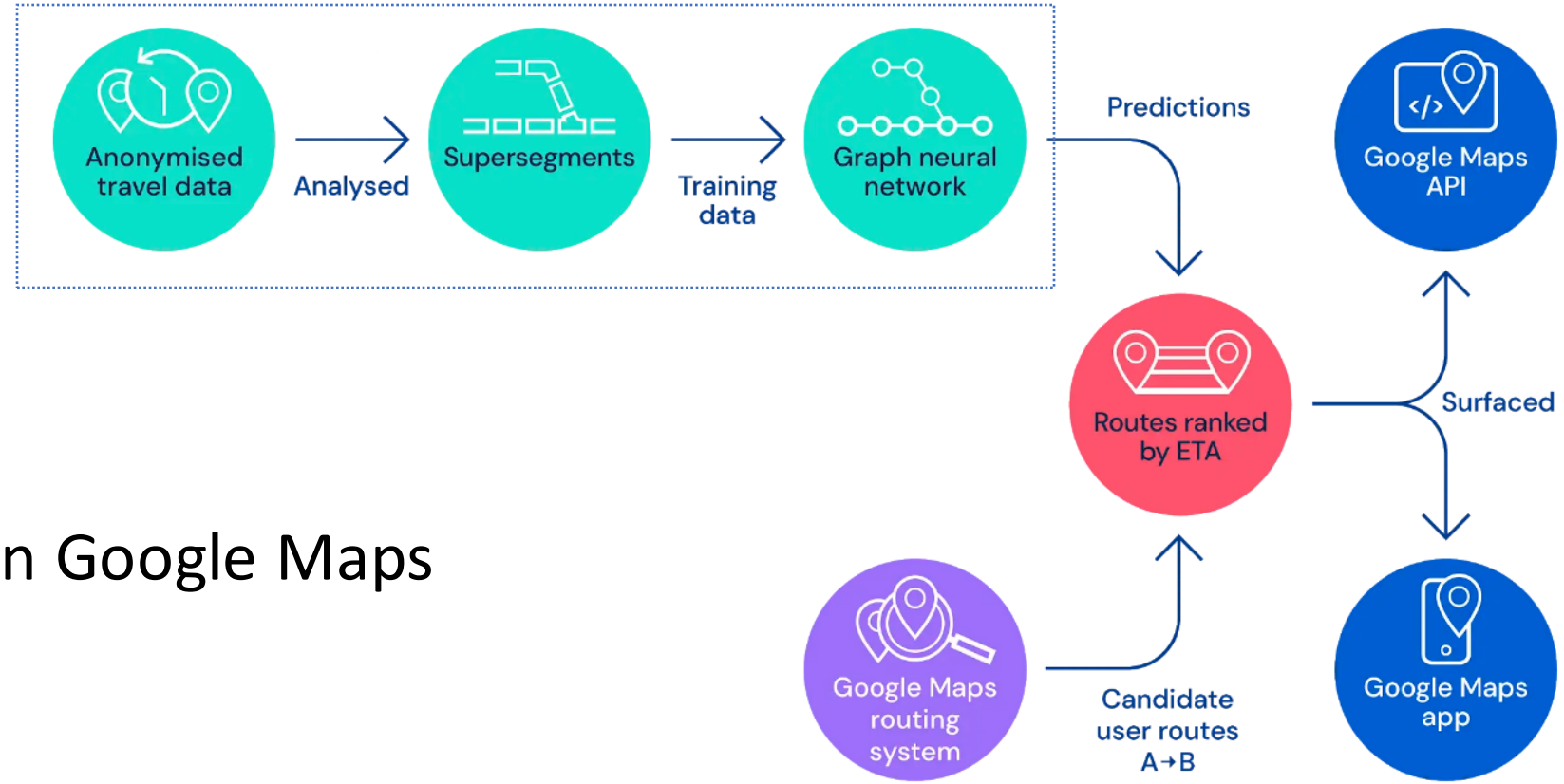


Image credit: DeepMind

Traffic Prediction via GNN

Predict via Graph Neural Networks



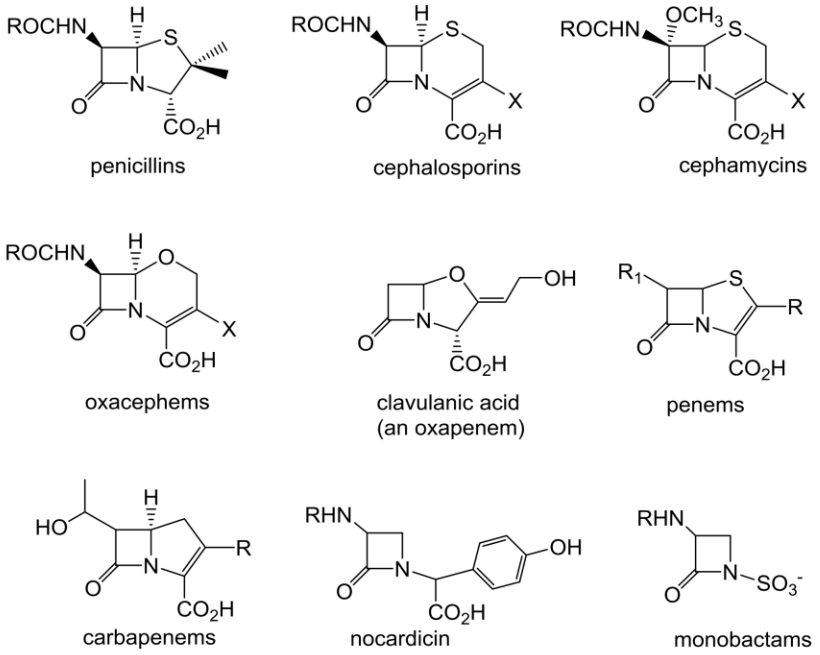
THE MODEL ARCHITECTURE FOR DETERMINING OPTIMAL ROUTES AND THEIR TRAVEL TIME.

Image credit: DeepMind

- Used in Google Maps

Example 5: Drug Discovery

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



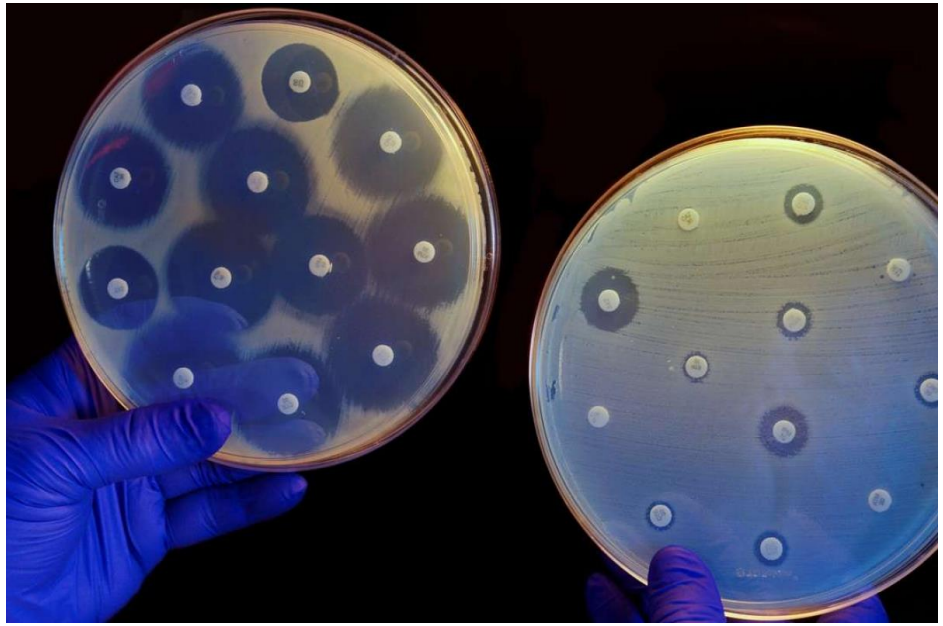
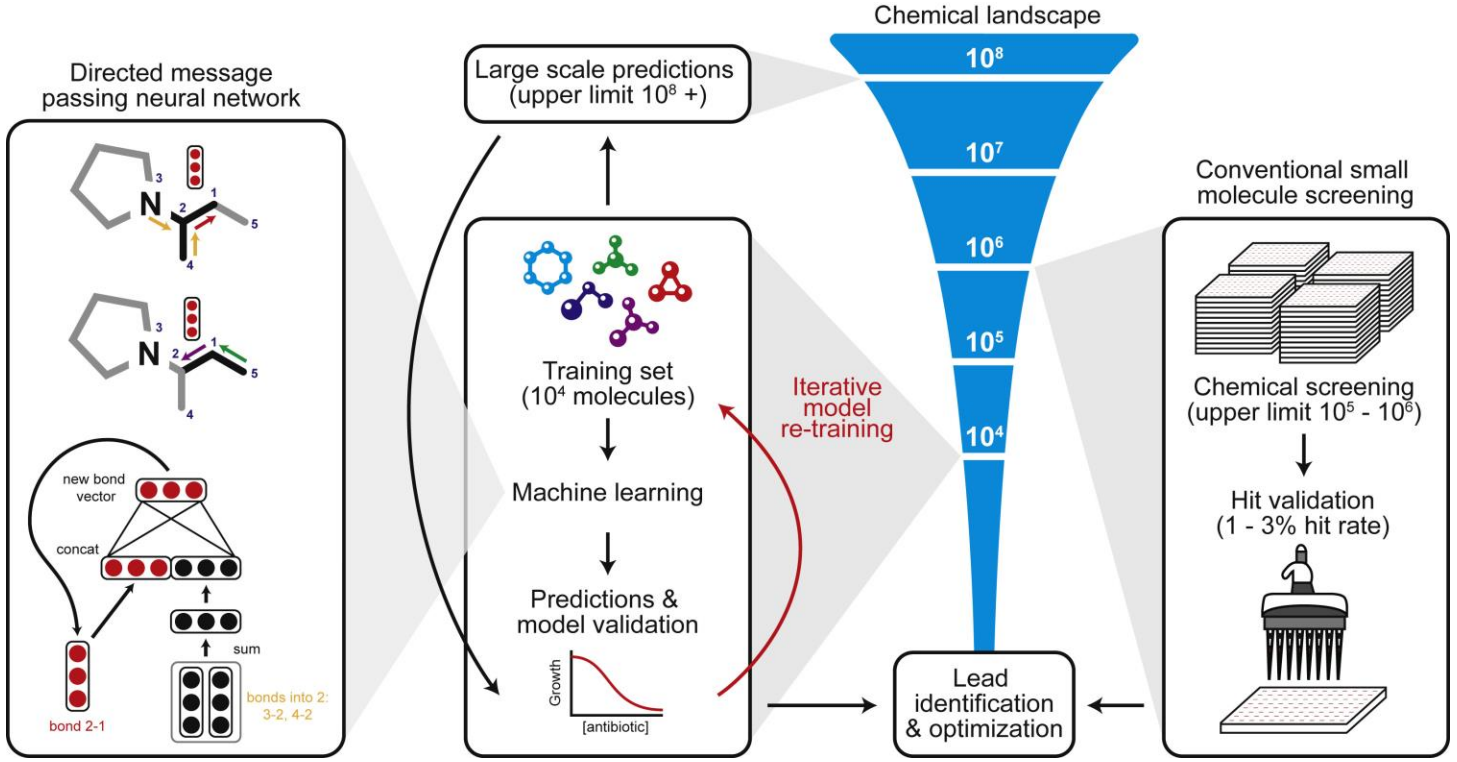


Image credit: CNN

Monika Konaklieva *et al*. Molecular targets of β-lactam-based antimicrobials: beyond the usual suspects.

Deep Learning for Antibiotic Discovery

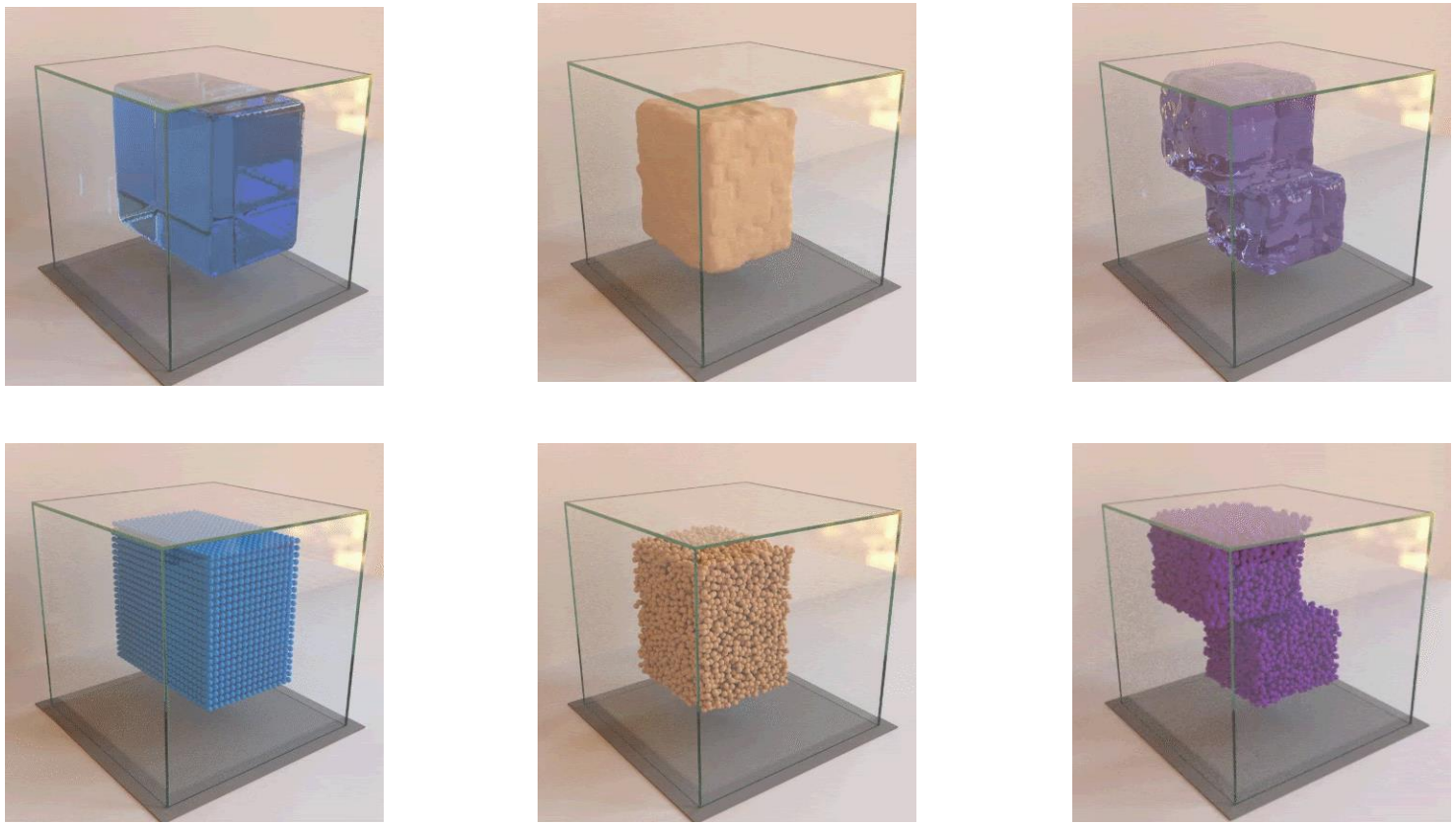
- A Graph Neural Network model
- Predict promising molecules from a pool of candidates



Jonathan M. Stokes *et al*. A deep learning approach to antibiotic discovery.

Example 6: Physics Simulation

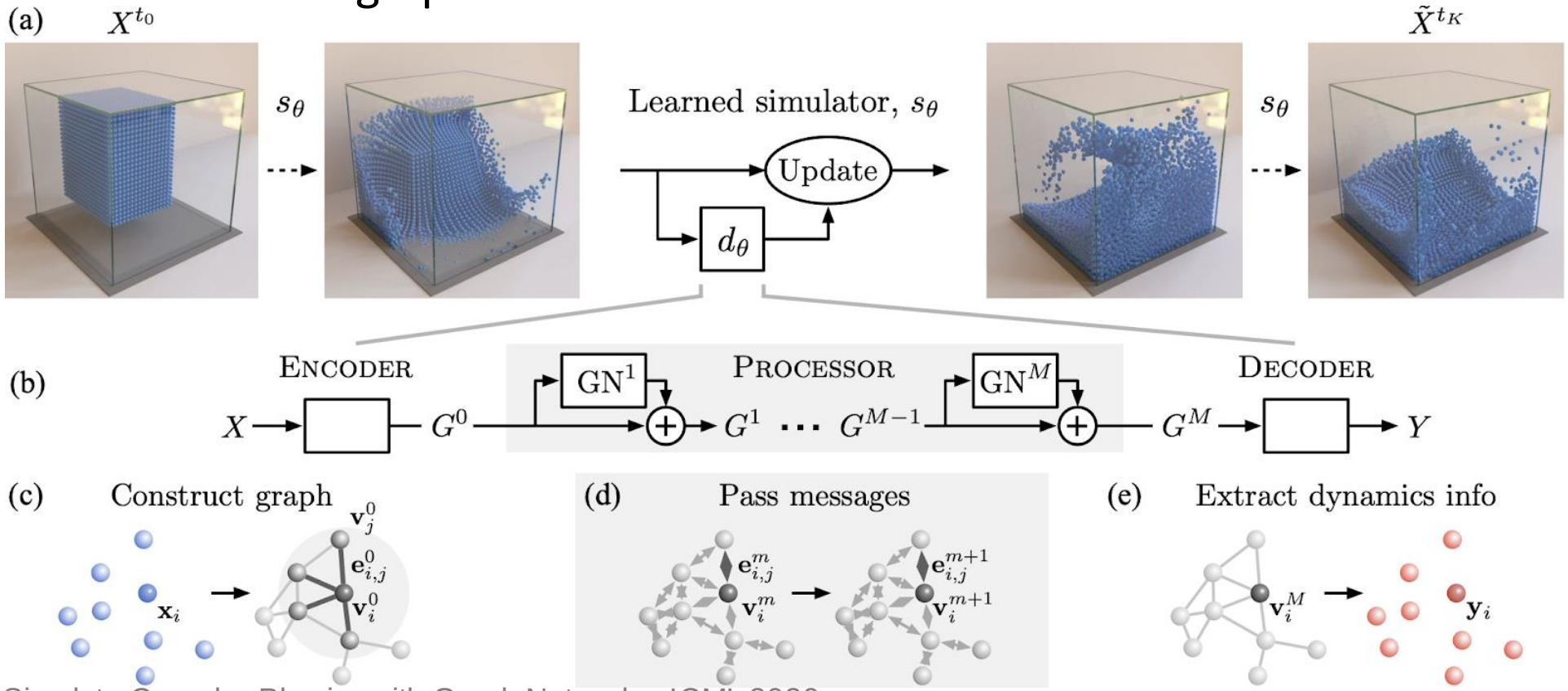
- Physical simulation as a graph
  - **Nodes**: Particles:
  - **Edges**: Interaction between particles



Learning to Simulate Complex Physics with Graph Networks, ICML 2020

Simulation Learning Framework

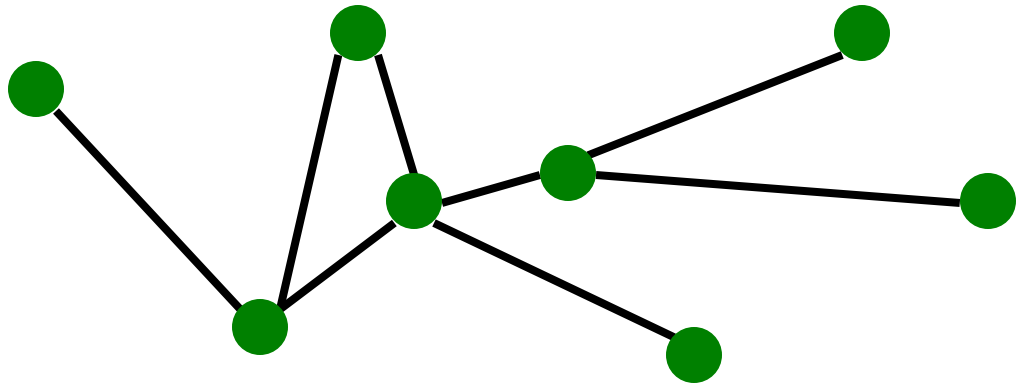
- A graph evolution task
  - Goal: Predict how a graph will evolve over time



Learning to Simulate Complex Physics with Graph Networks, ICML 2020

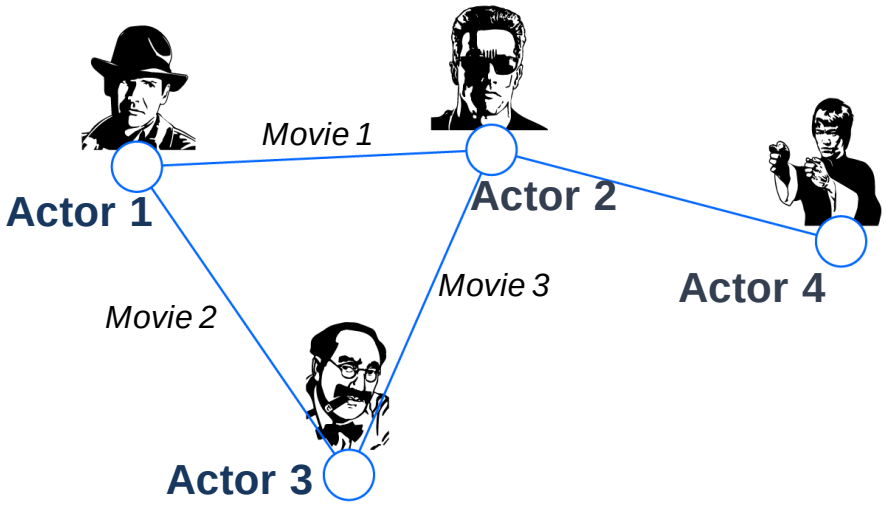
Choices of Graph Representation

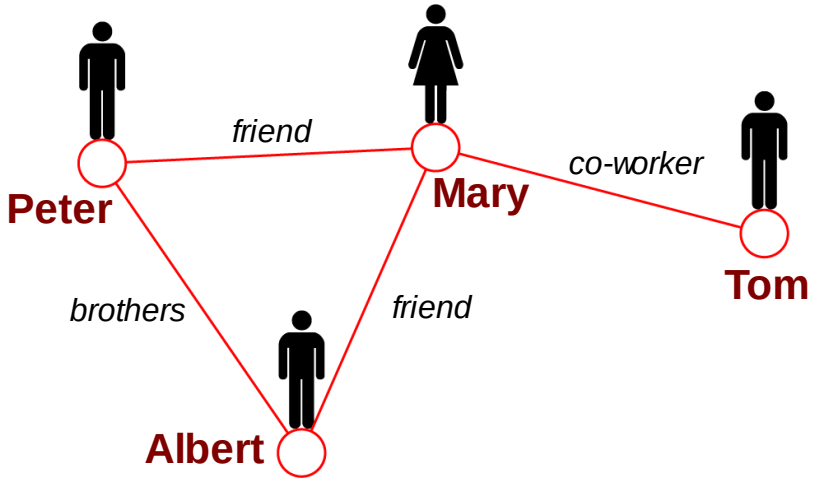
Components of a Network

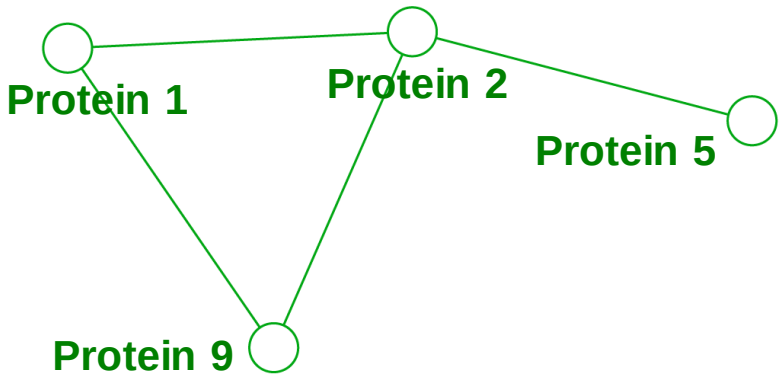


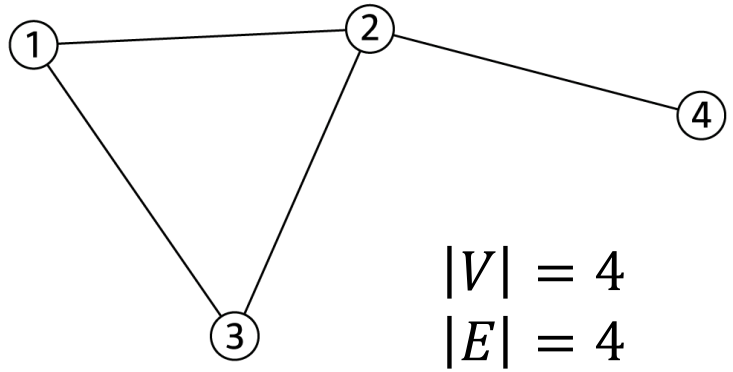
- Objects: nodes, vertices — V
- Interactions: links, edges — E
- System: network, graph — $G(V, E)$

Graphs: A Common Language









$$|V| = 4$$
$$|E| = 4$$

How do you define a graph?

- **How to build a graph:**
  - **What are nodes?**
  - **What are edges?**
- **Choice of the proper network representation of a given domain/problem determines our ability to use networks successfully:**
  - In some cases there is a unique, unambiguous representation
  - In other cases, the representation is by no means unique
  - The way you assign links will determine the nature of the question you can study

Choosing a Proper Representation

- If you connect individuals that work with each other, you will explore a **professional network**
- If you connect scientific papers that cite each other, you will be studying the **citation network**

Image credit: Euro Scientists

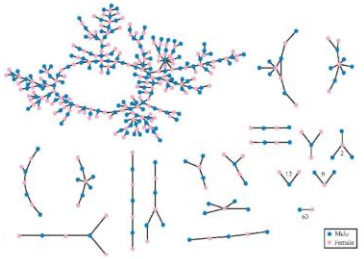


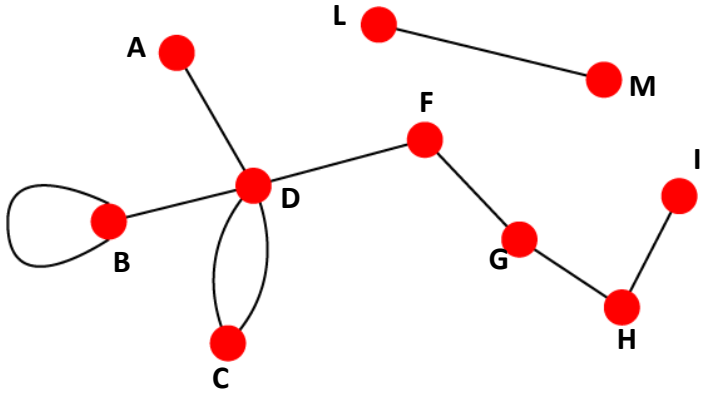
Image credit: ResearchGate

- **If you connect all papers with the same word in the title, what will you be exploring?** It is a network, nevertheless

Directed vs. Undirected Graphs

Undirected

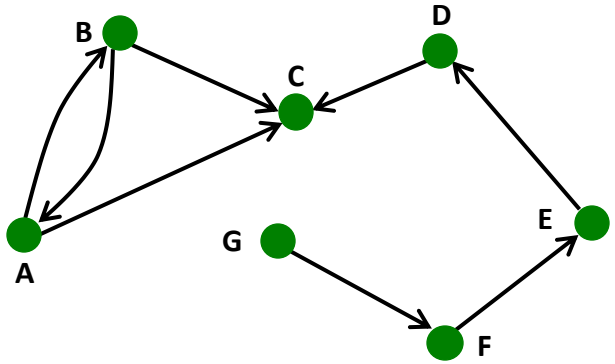
- **Links:** undirected (symmetrical, reciprocal)



- **Examples:**
  - Collaborations
  - Friendship on Facebook

Directed

- **Links:** directed (arcs)



- **Examples:**
  - Phone calls
  - Following on Twitter

Directed vs. Undirected Graphs: Node Degrees

- Node degree d_i: the number of edges adjacent to node i

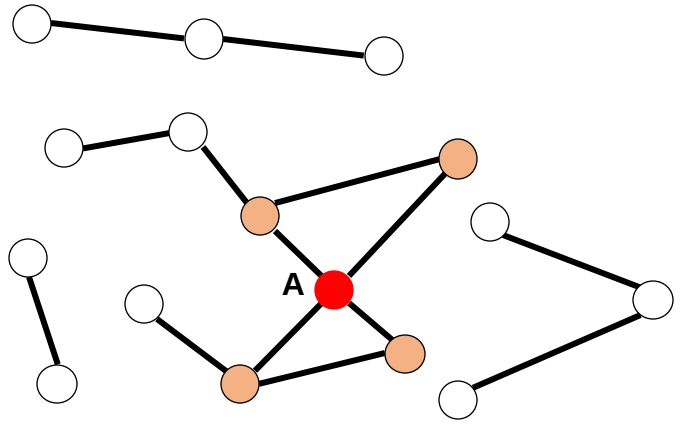
$$d_A = 4$$

- Avg. degree: $\bar{d} = \langle d \rangle = \frac{1}{|V|}\sum_{i=1}^{|V|} d_i = \frac{2|E|}{|V|}$
- In directed networks we define an in-degree and out-degree. The (total) degree of a nodes is the sum of in- and out-degrees.

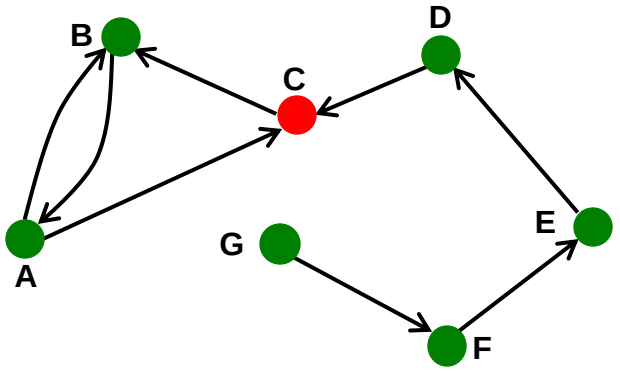
$$d_C^{in} = 2, d_C^{out} = 1, d_c = 3$$

$$\bar{d} = \frac{|E|}{|V|}, \overline{d^{in}} = \overline{d^{out}}$$

Undirected



Directed

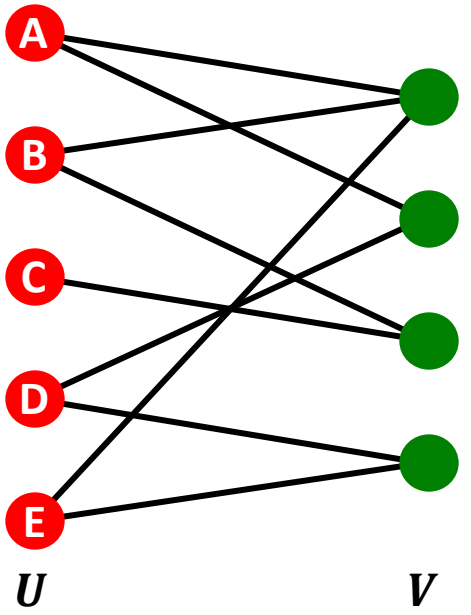


Source: Node with $d^{in} = 0$

Sink: Node with $d^{out} = 0$

Bipartite Graph

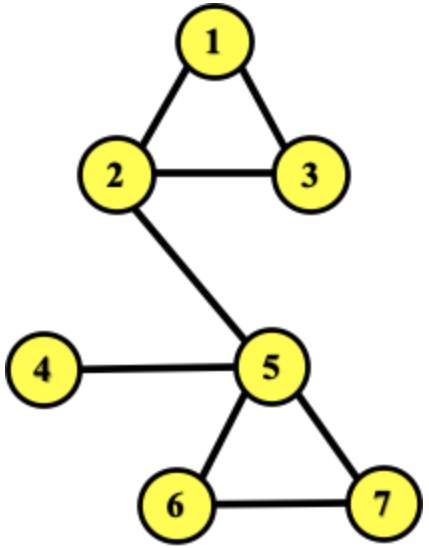
- **Bipartite graph** is a graph whose nodes can be divided into two disjoint sets ***U*** and ***V*** such that every link connects a node in ***U*** to one in ***V***; that is,
  U and ***V*** are **independent sets**



- **Examples:**
  - Authors-to-Papers (they authored)
  - Actors-to-Movies (they appeared in)
  - Users-to-Movies (they rated)
  - Recipes-to-Ingredients (they contain)
- **"Folded" networks:**
  - Author collaboration networks
  - Movie co-rating networks

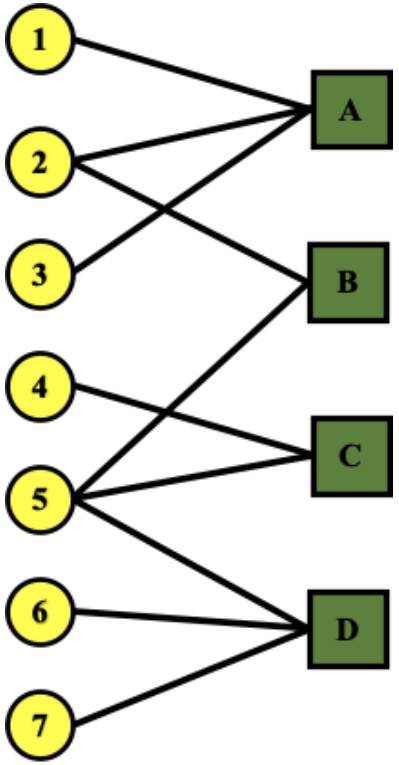
Folded / Projected Bipartite Graphs

Projection U

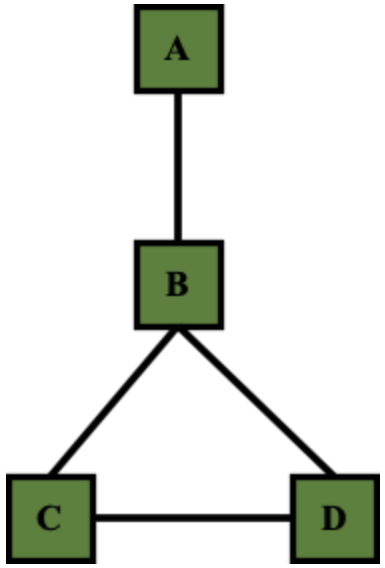


Two nodes are connected if they share the same green neighbor

U **V**



Projection V



Two nodes are connected if they share the same yellow neighbor

Representing Graphs: Adjacency Matrix

$A_{ij} = 1$ if there is a link from node i to node j

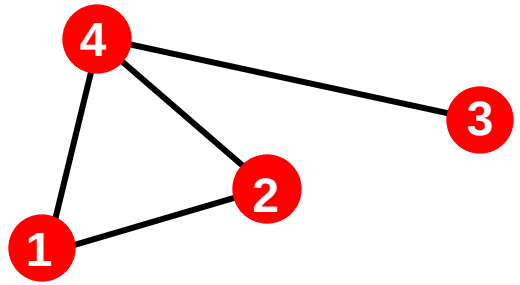
$A_{ij} = 0$ otherwise

$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \qquad A = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Note that for a directed graph (right) the matrix is not symmetric.

Adjacency Matrix

Undirected



$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

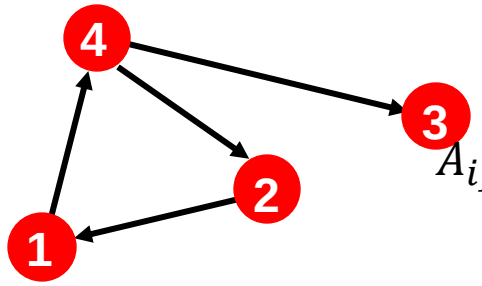
$$A_{ij} = A_{ji}$$

$$A_{ii} = 0$$

$$d_i = \sum_{j=1}^{|V|} A_{ij} \qquad d_j = \sum_{i=1}^{|V|} A_{ij}$$

$$|E| = \frac{1}{2}\sum_{i=1}^{|V|} d_i = \frac{1}{2}\sum_{i,j}^{|V|} A_{ij}$$

Directed



$$A = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

$$A_{ij} = A_{ji}$$

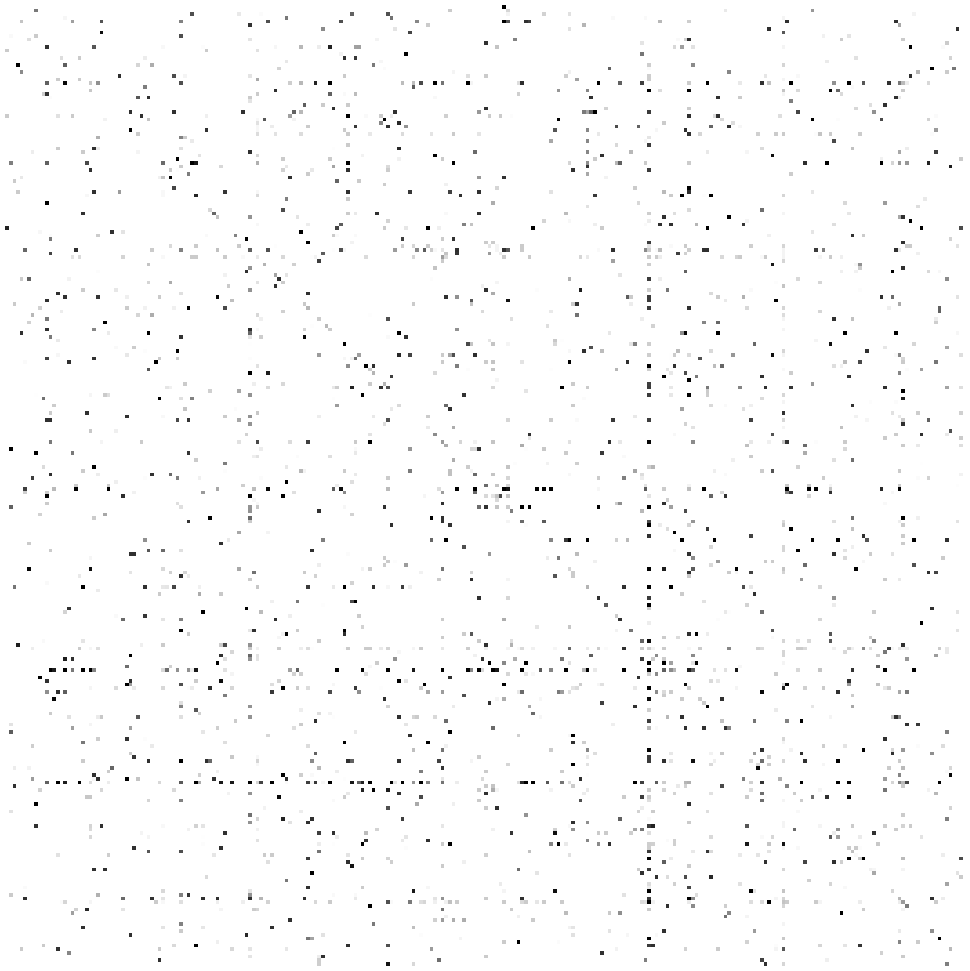
$$A_{ij} \neq A_{ji}$$

$$A_{ii} = 0$$

$$d_i^{out} = \sum_{j=1}^{|V|} A_{ij} \qquad d_j^{in} = \sum_{i=1}^{|V|} A_{ij}$$

$$|E| = \sum_{i=1}^{|V|} d_i^{in} = \sum_{i=1}^{|V|} d_i^{in} = \sum_{i,j}^{|V|} A_{ij}$$

Adjacency Matrics are Sparse



Networks are Sparse Graphs

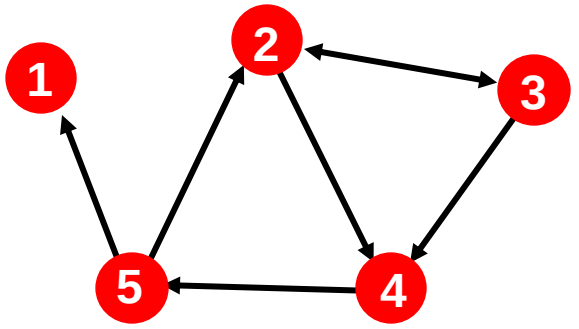
- Most real-world networks are sparse
- $|E| \ll |E|_{\max}$ or $k \ll |V| - 1$

NETWORK	NODES	LINKS	DIRECTED/ UNDIRECTED	|V|	|E|	<k>
Internet	Routers	Internet connections	Undirected	192,244	609,066	6.33
WWW	Webpages	Links	Directed	325,729	1,497,134	4.60
Power Grid	Power plants, transformers	Cables	Undirected	4,941	6,594	2.67
Phone Calls	Subscribers	Calls	Directed	36,595	91,826	2.51
Email	Email Addresses	Emails	Directed	57,194	103,731	1.81
Science Collaboration	Scientists	Co-authorship	Undirected	23,133	93,439	8.08
Actor Network	Actors	Co-acting	Undirected	702,388	29,397,908	83.71
Citation Network	Paper	Citations	Directed	449,673	4,689,479	10.43
E. Coli Metabolism	Metabolites	Chemical reactions	Directed	1,039	5,802	5.58
Protein Interactions	Proteins	Binding interactions	Undirected	2,018	2,930	2.90

- **Consequence: Adjacency matrix is filled with zeros**! (**Density of the matrix ($|E|/|V|^2$):** WWW=1.51×10^{-5}, MSN IM = 2.27×10^{-8})

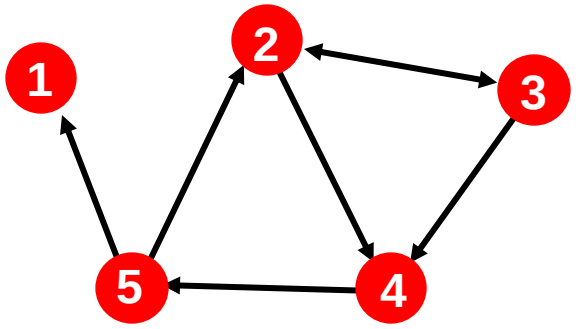
Representing Graphs: Edge List

- **Represent graph as a list of edges:**
  - (2, 3)
  - (2, 4)
  - (3, 2)
  - (3, 4)
  - (4, 5)
  - (5, 2)
  - (5, 1)



Representing Graphs: Adjacency List

- **Adjacency list:**
  - Easier to work with if network is
    - Large
    - Sparse
  - Allows us to quickly retrieve all neighbors of a given node
    - 1:
    - 2: 3, 4
    - 3: 2, 4
    - 4: 5
    - 5: 1, 2



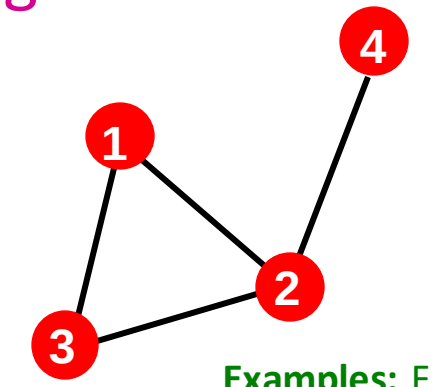
Nodes and Edge Attributes

Possible options:

- Weight (*e.g.*, frequency of communication)
- Ranking (best friend, second best friend…)
- Type (friend, relative, co-worker)
- Sign: Friend vs. Foe, Trust vs. Distrust
- Properties depending on the structure of the rest of the graph: Number of common friends

More Types of Graphs (1)

- Unweighted



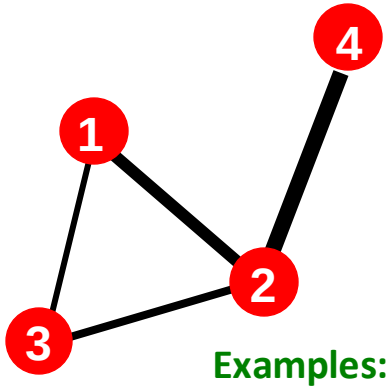
$$A = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$A_{ii} = 0, A_{ij} = A_{ji}$$

$$|E| = \frac{1}{2}\sum_{i,j=1}^{|V|} A_{ij}\,, \bar{d} = \frac{2|E|}{|V|}$$

Examples: Friendship, Hyperlink

- Weighted



$$A = \begin{pmatrix} 0 & 2 & 0.5 & 0 \\ 2 & 0 & 1 & 4 \\ 0.5 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 \end{pmatrix}$$

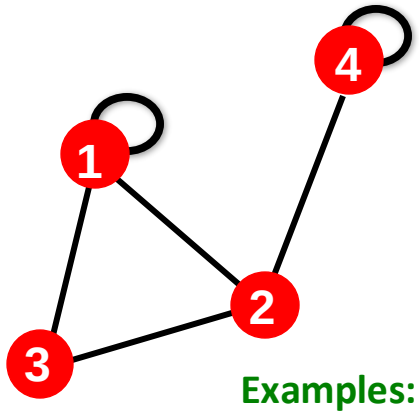
$$A_{ii} = 0, A_{ij} = A_{ji}$$

$$|E| = \frac{1}{2}\sum_{i,j=1}^{|V|} \text{nonzero}(A_{ij})\,, \bar{d} = \frac{2|E|}{|V|}$$

Examples: Collaboration, Internet, Roads

More Types of Graphs (2)

- Self-edges (self-loops) (undirected)



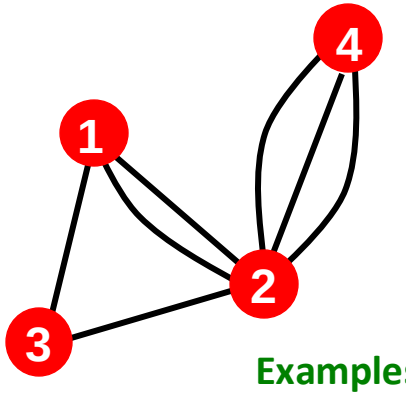
$$A = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 \end{pmatrix}$$

$$A_{ii} \neq 0, A_{ij} = A_{ji}$$

$$|E| = \frac{1}{2}\sum_{i,j=1,i\neq j}^{|V|} A_{ij} + \sum_{i}^{|V|} A_{ii}\,, \bar{d} = \frac{2|E|}{|V|}$$

Examples: Proteins, Hyperlinks

- Multigraph (undirected)



$$A = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 2 & 0 & 1 & 3 \\ 1 & 1 & 0 & 0 \\ 0 & 3 & 0 & 0 \end{pmatrix}$$

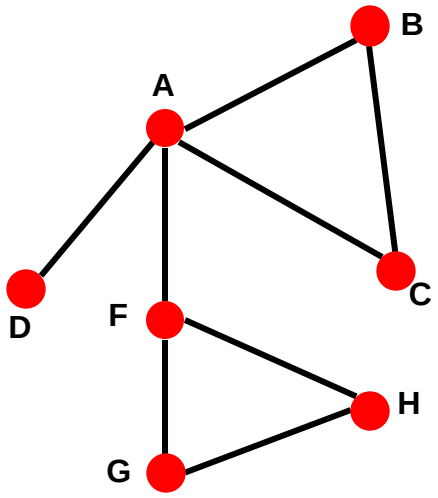
$$A_{ii} = 0, A_{ij} = A_{ji}$$

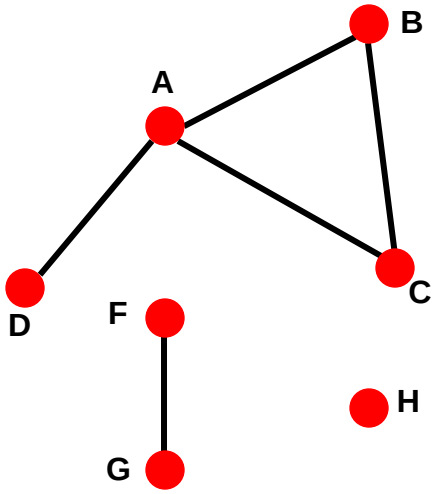
$$|E| = \frac{1}{2}\sum_{i,j=1}^{|V|} \text{nonzero}(A_{ij})\,, \bar{d} = \frac{2|E|}{|V|}$$

Examples: Communication, Collaboration

Connectivity of Undirected Graphs

- **Connected (undirected) graph:**
  - Any two vertices can be joined by a path
- A disconnected graph is made up by two or more connected components





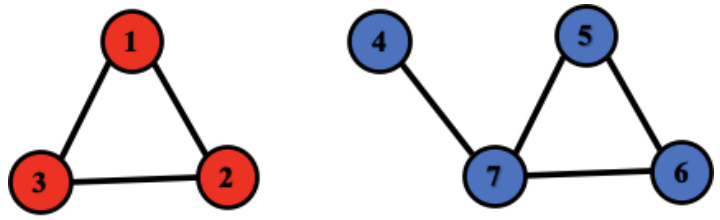
Largest Component:
Giant Component

Isolated node (node H)

Connectivity: Example

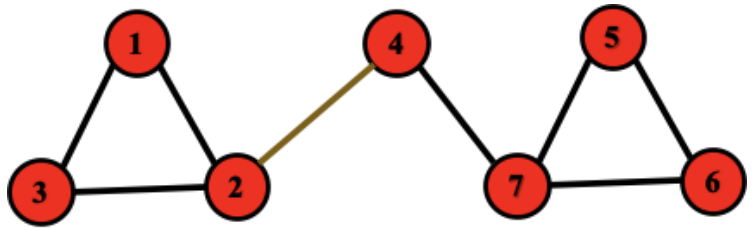
The adjacency matrix of a network with several components can be written in a block- diagonal form, so that nonzero elements are confined to squares, with all other elements being zero:

Disconnected



$$\begin{pmatrix} 0&1&1&0&0&0&0\\ 1&0&1&0&0&0&0\\ 1&1&0&0&0&0&0\\ 0&0&0&0&0&0&1\\ 0&0&0&0&0&1&1\\ 0&0&0&0&1&0&1\\ 0&0&0&1&1&1&0 \end{pmatrix}$$

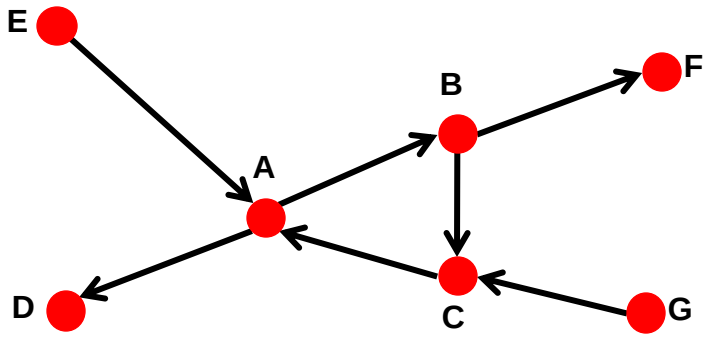
Connected



$$\begin{pmatrix} 0&1&1&0&0&0&0\\ 1&0&1&1&0&0&0\\ 1&1&0&0&0&0&0\\ 0&1&0&0&0&0&1\\ 0&0&0&0&0&1&1\\ 0&0&0&0&1&0&1\\ 0&0&0&1&1&1&0 \end{pmatrix}$$

Connectivity of Directed Graphs (1)

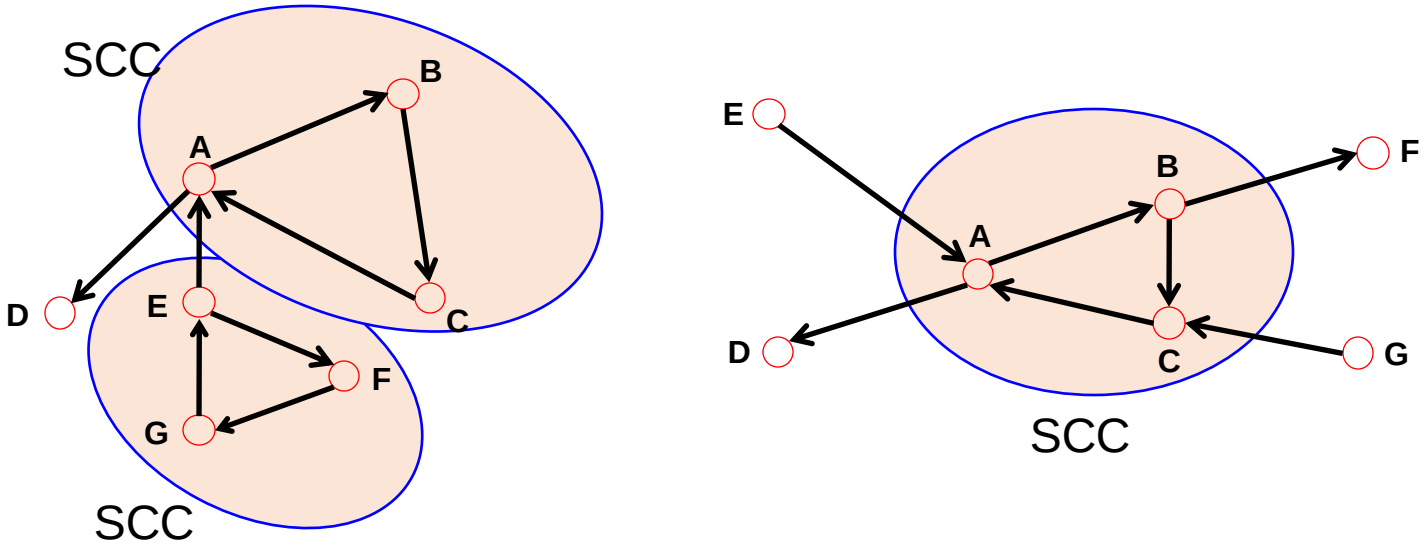
- **Strongly connected directed graph**
  - has a path from each node to every other node and vice versa (e.g., A-B path and B-A path)
- **Weakly connected directed graph**
  - is connected if we disregard the edge directions



Graph on the left is connected but not strongly connected (e.g., there is no way to get from F to G by following the edge directions).

Connectivity of Directed Graphs (2)

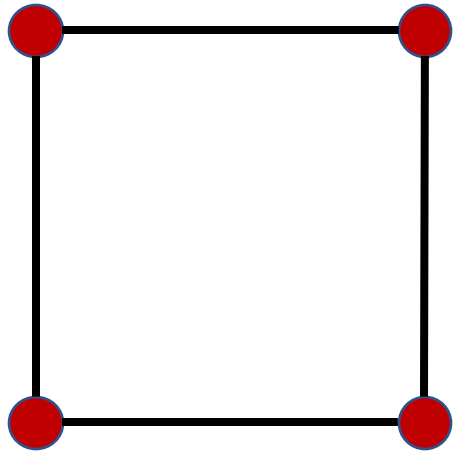
- **Strongly connected components (SCCs)** can be identified, but not every node is part of a nontrivial strongly connected component.

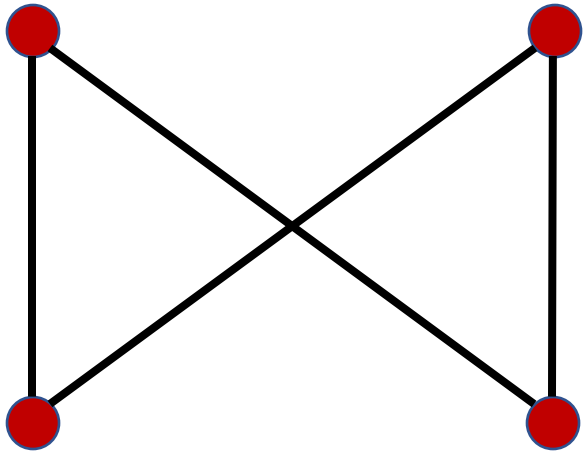


In-component: nodes that can reach the SCC,
Out-component: nodes that can be reached from the SCC.

Isomorphism of Graphs

- Graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are **isomorphic** if there exists a one-to-one and onto map $f: V_1 \mapsto V_2$, with the property that $(a, b) \in E_1$ iff $\big(f(a), f(b)\big) \in E_2, \forall a, b \in V_1$.
- Example:





Summary

- **Machine learning with Graphs**
  - Applications and use cases
- **Different types of tasks:**
  - Biological networks, proteins
  - Recommender systems, social networks
  - Dynamic networks, simulations
- **Choice of a graph representation:**
  - Directed, undirected, bipartite, weighted, adjacency matrix

Readings

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