Stanford CS224W: Machine Learning with Graphs

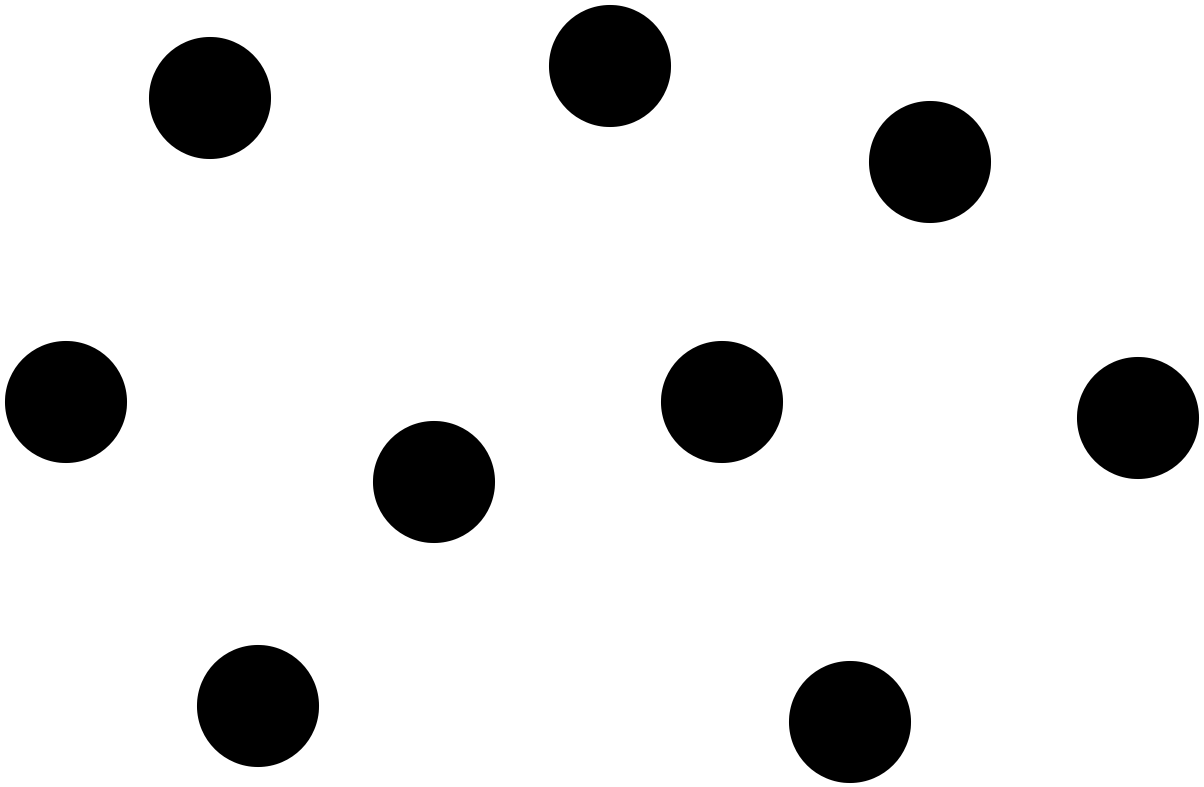
CS224W: Machine Learning with Graphs

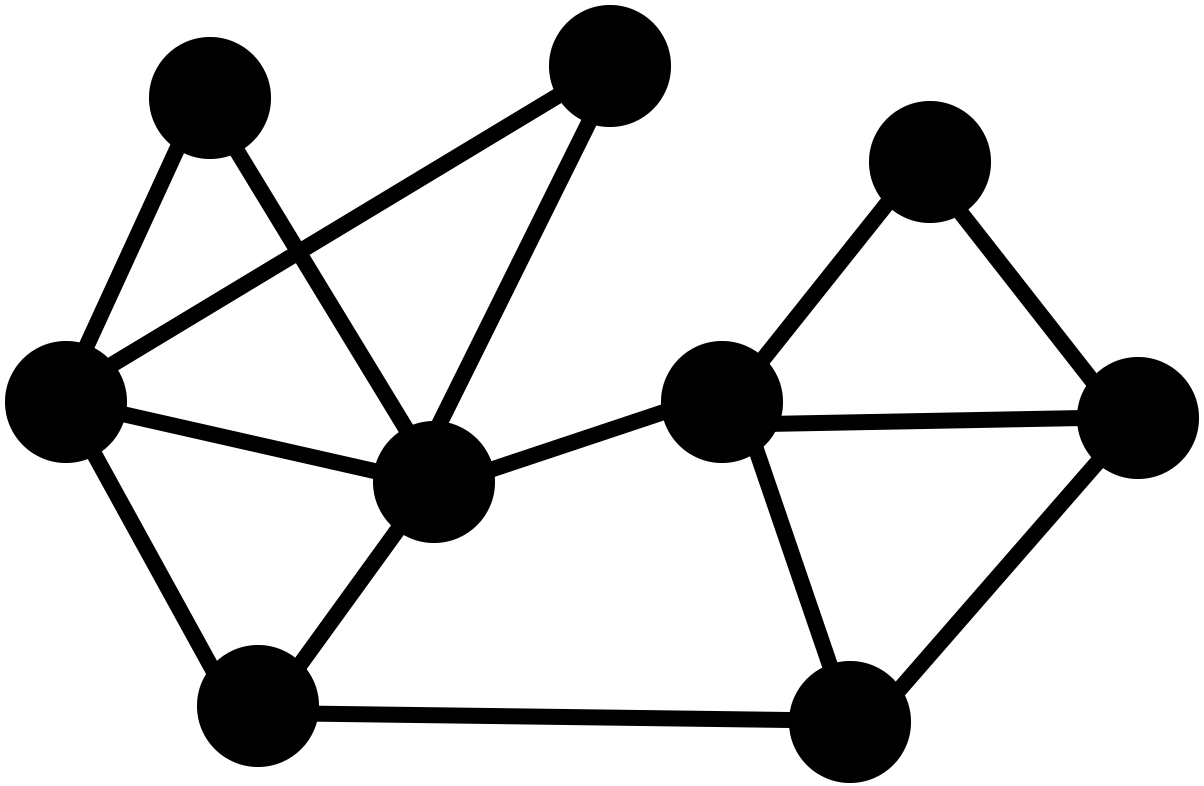
Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Why Graphs?

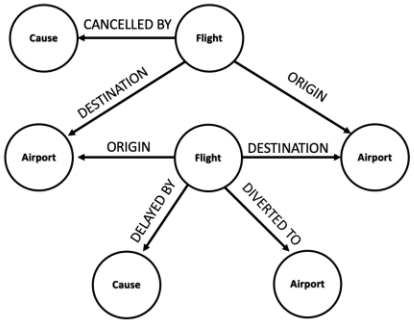
Graphs are a general language for describing and analyzing entities with relations/interactions





Graph

Many Types of Data are Graphs (1)

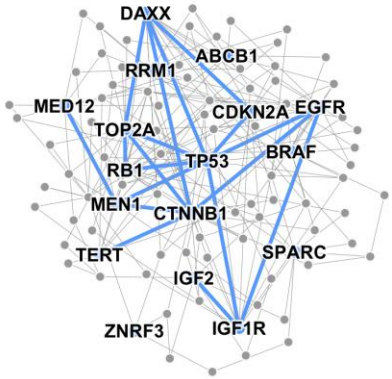


Event Graphs

Image credit: SalientNetworks

Computer Networks

Protein network



Disease Pathways

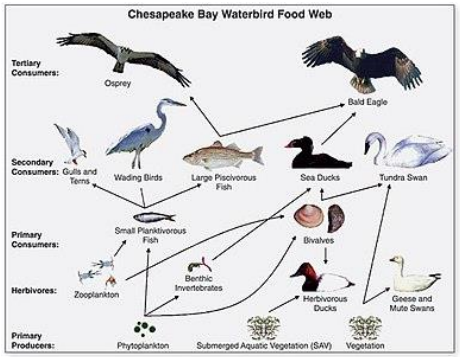


Image credit: Wikipedia

Food Webs

Image credit: Pinterest

Particle Networks

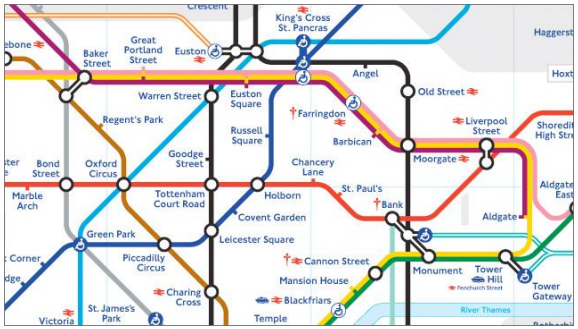


Image credit: visitlondon.com

Underground Networks

Many Types of Data are Graphs (2)

Image credit: Medium

Social Networks

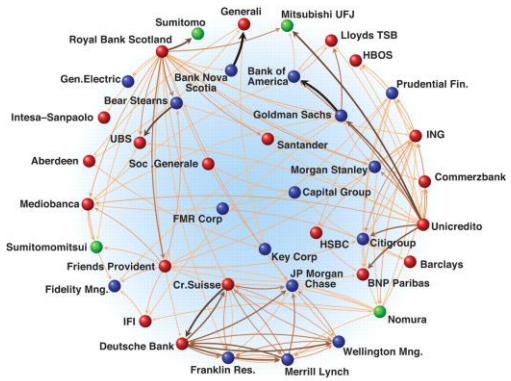
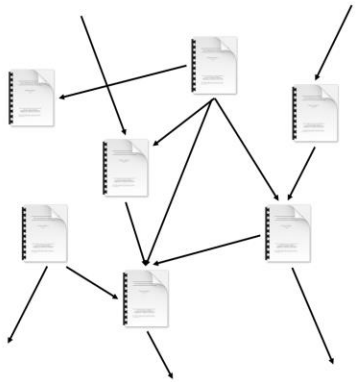


Image credit: Science

Economic Networks

Image credit: Lumen Learning

Communication Networks



Citation Networks

Image credit: Missoula Current News

Internet

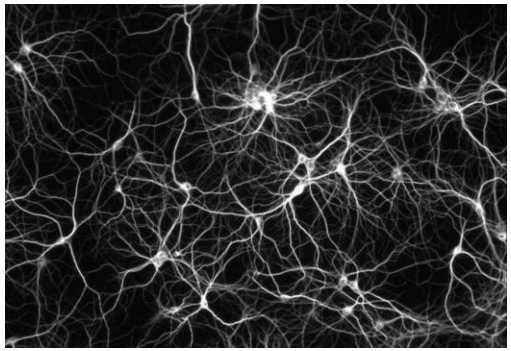


Image credit: The Conversation

Networks of Neurons

Many Types of Data are Graphs (3)

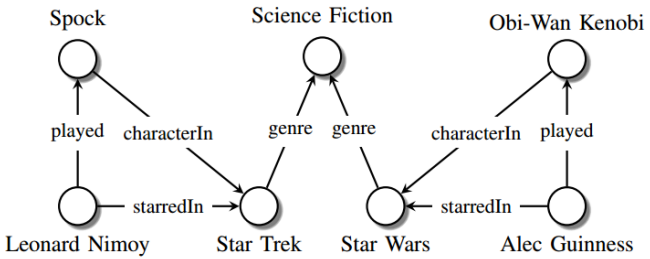


Image credit: Maximilian Nickel et al

Knowledge Graphs

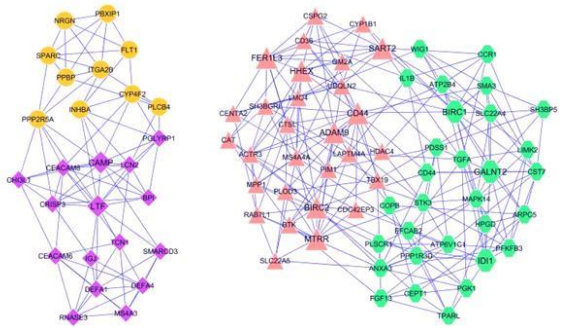


Image credit: ese.wustl.edu

Regulatory Networks

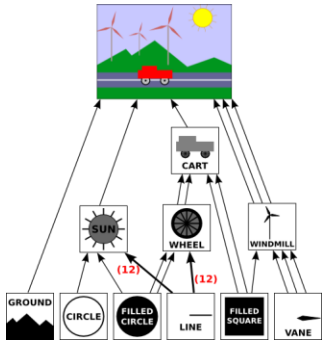


Image credit: math.hws.edu

Scene Graphs

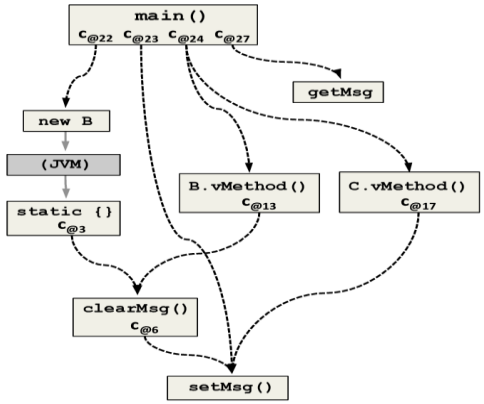


Image credit: ResearchGate

Code Graphs

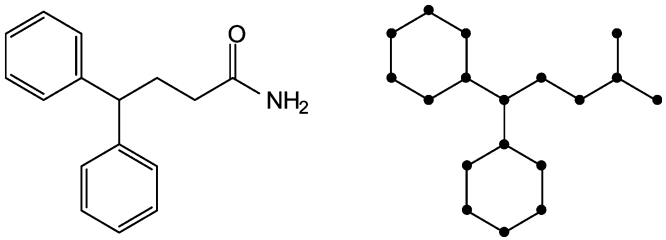


Image credit: MDPI

Molecules

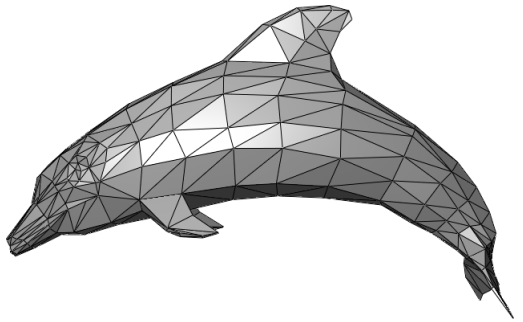
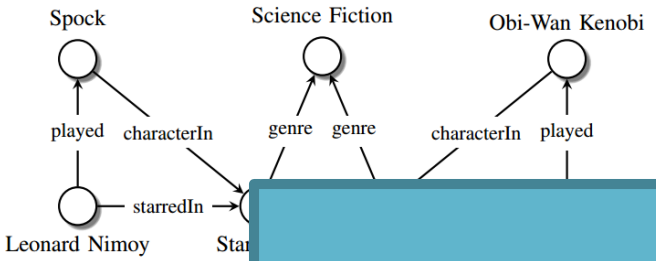
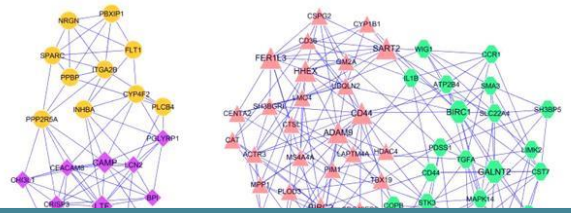


Image credit: Wikipedia

3D Shapes

Graphs and Relational Data





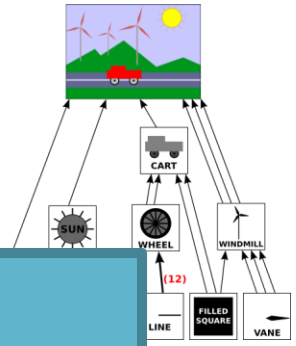


Image cred

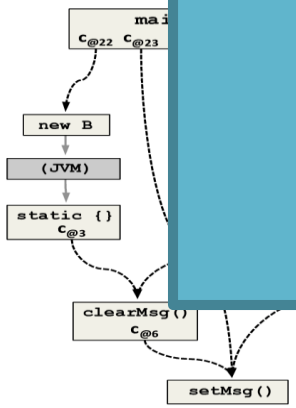
nath.hws.edu

Know

Graphs

Main question:

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



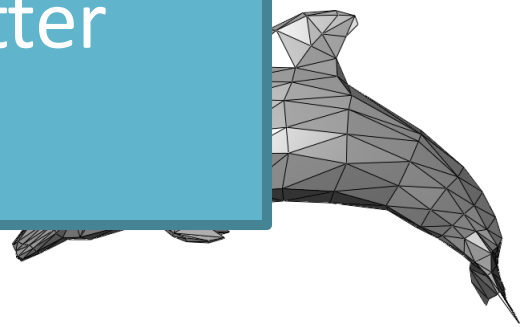


Image credit: ResearchGate

Image credit: MDPI

Image credit: Wikipedia

Code Graphs

Molecules

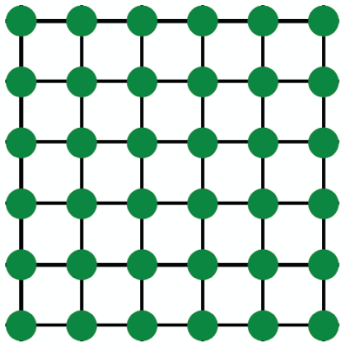
3D Shapes

Graphs: Machine Learning

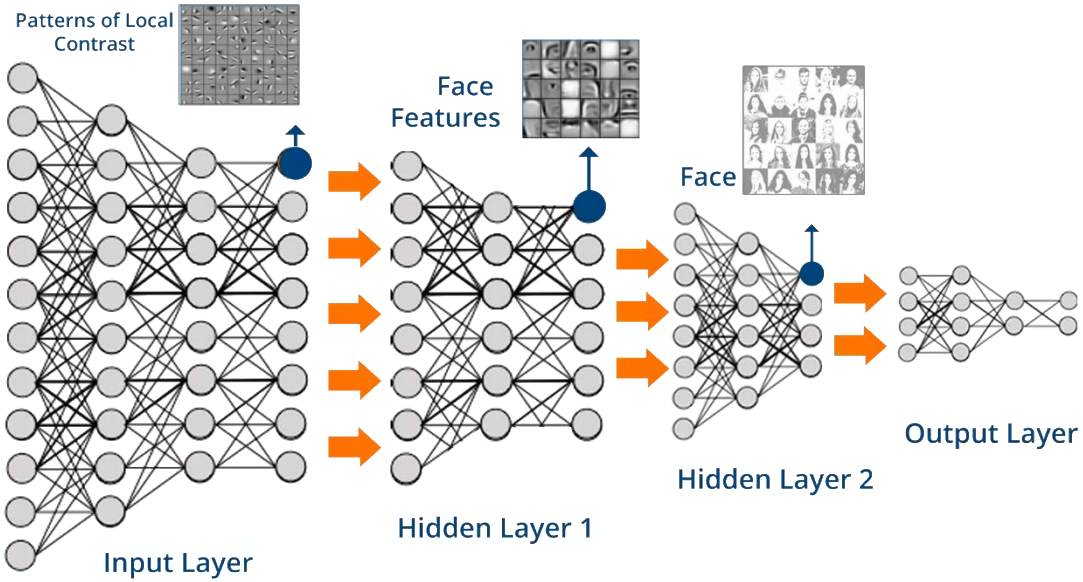
Complex domains have a rich relational structure, which can be represented as a **relational graph**

By explicitly modeling relationships we achieve better performance!

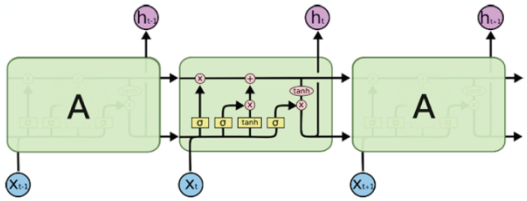
Today: Modern ML Toolbox



Images



Text/Speech



Modern deep learning toolbox is designed for simple sequences & grids

Doubt thou the stars are fire;
Doubt that the sun doth move;
Doubt truth to be a liar;
But never doubt I love...

Text

Audio signals

Images

Modern
deep learning toolbox
is designed for
sequences & grids

Not everything can be represented as a sequence or a grid

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

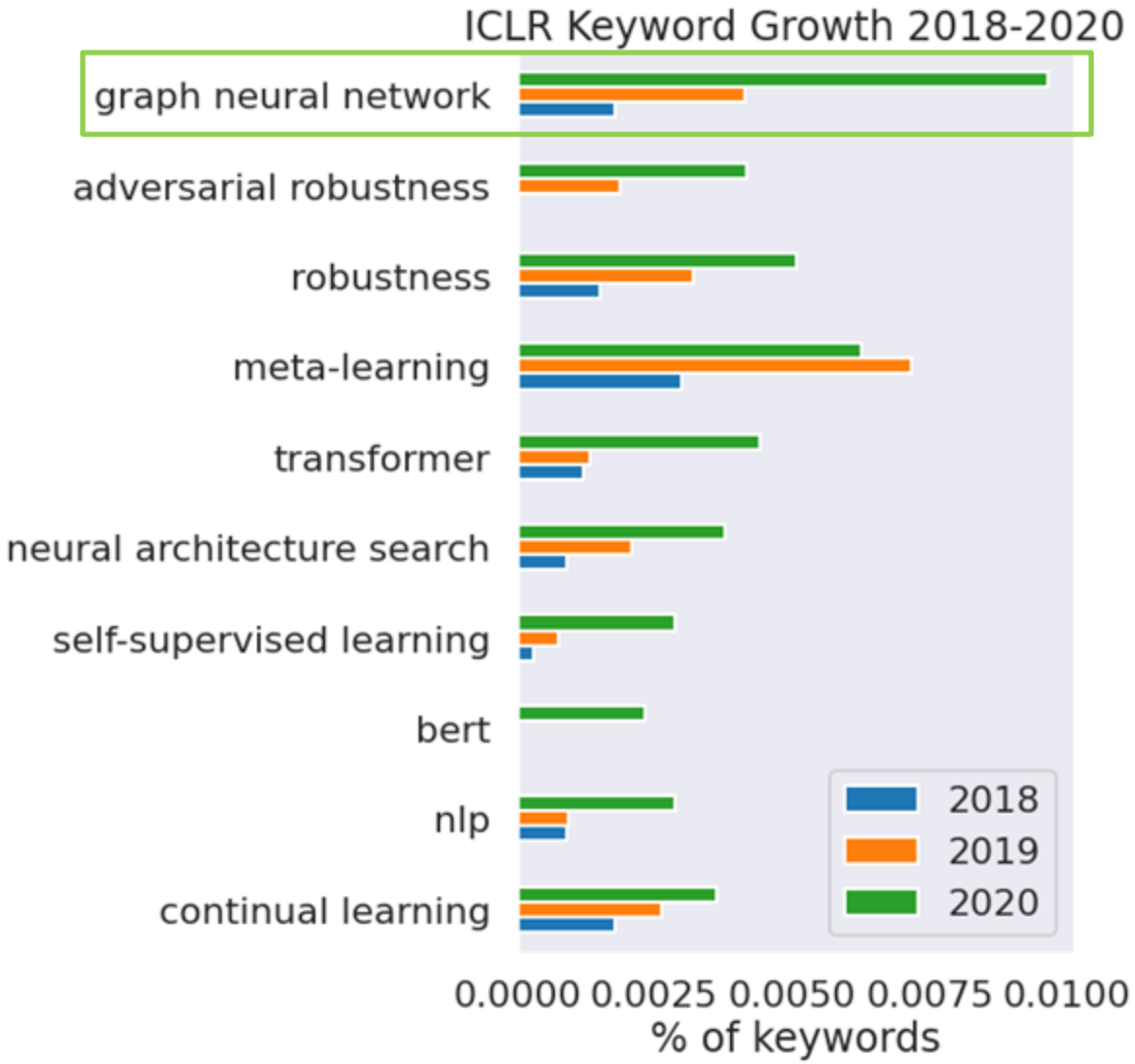
New frontiers beyond classic neural networks that only learn on images and sequences

This Class

Graphs are the new frontier of deep learning

Graphs connect things.

The hottest subfield in ML

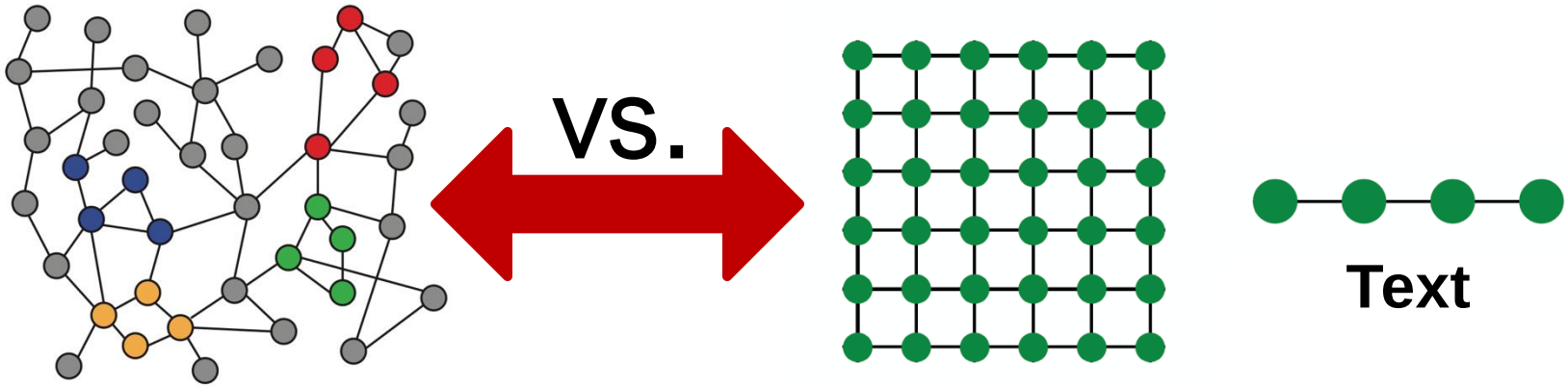


2021 key word ranking:
deep learning
reinforcement learning
representation learning
graph neural network
meta learning
robustness

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

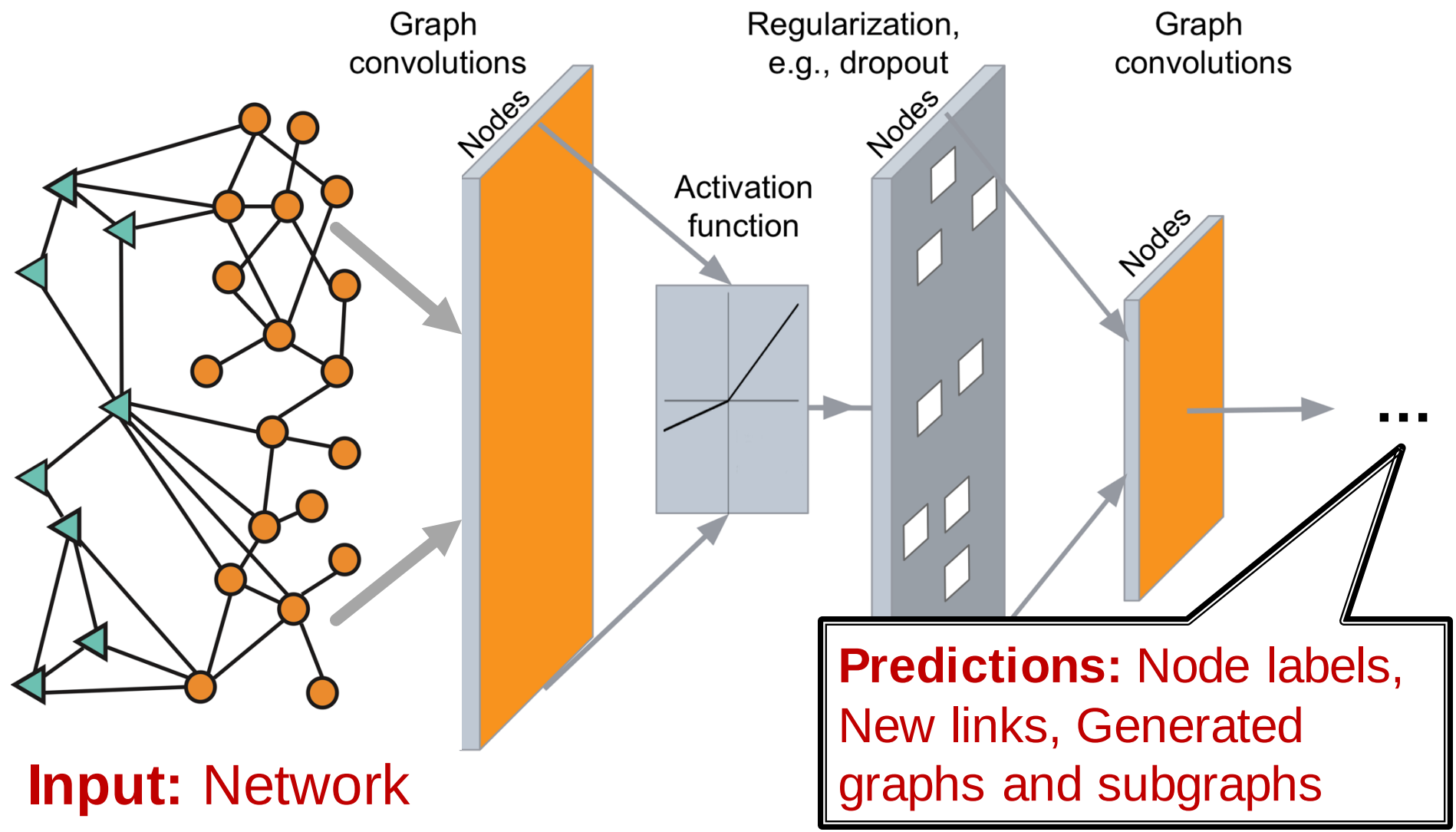
various data types

This Course

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

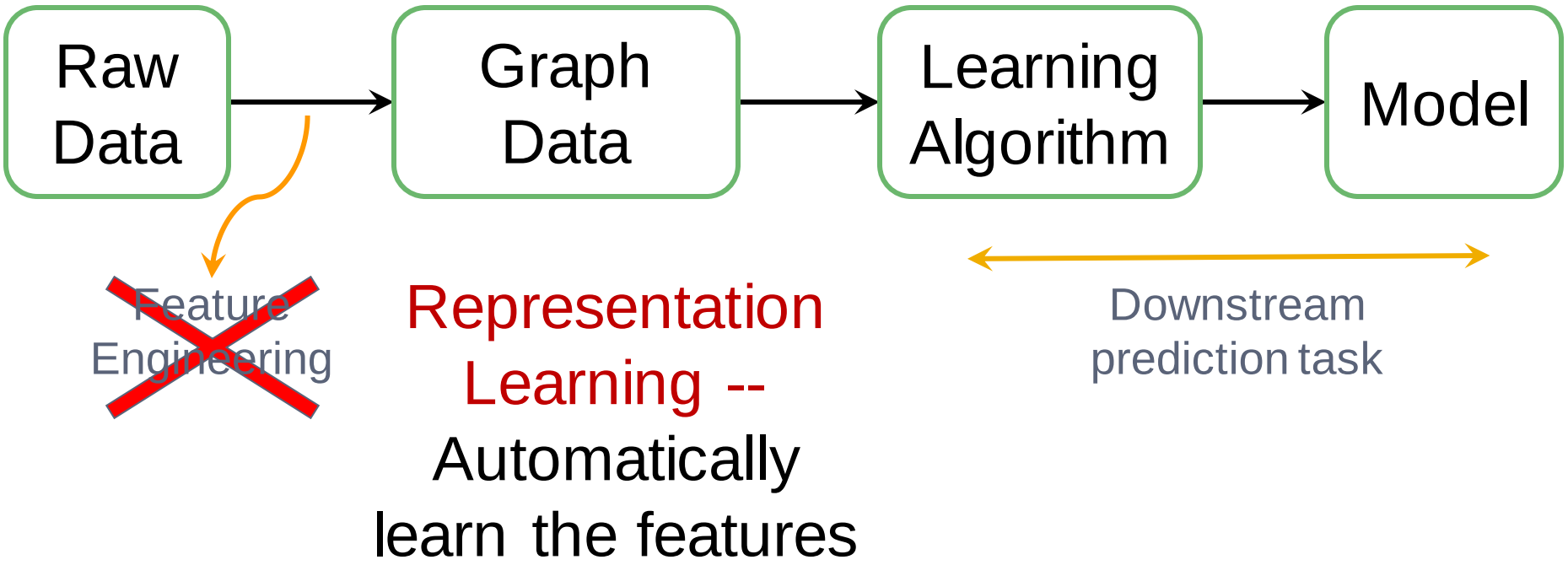
Graphs are the new frontier of deep learning

CS224W: Deep Learning in Graphs



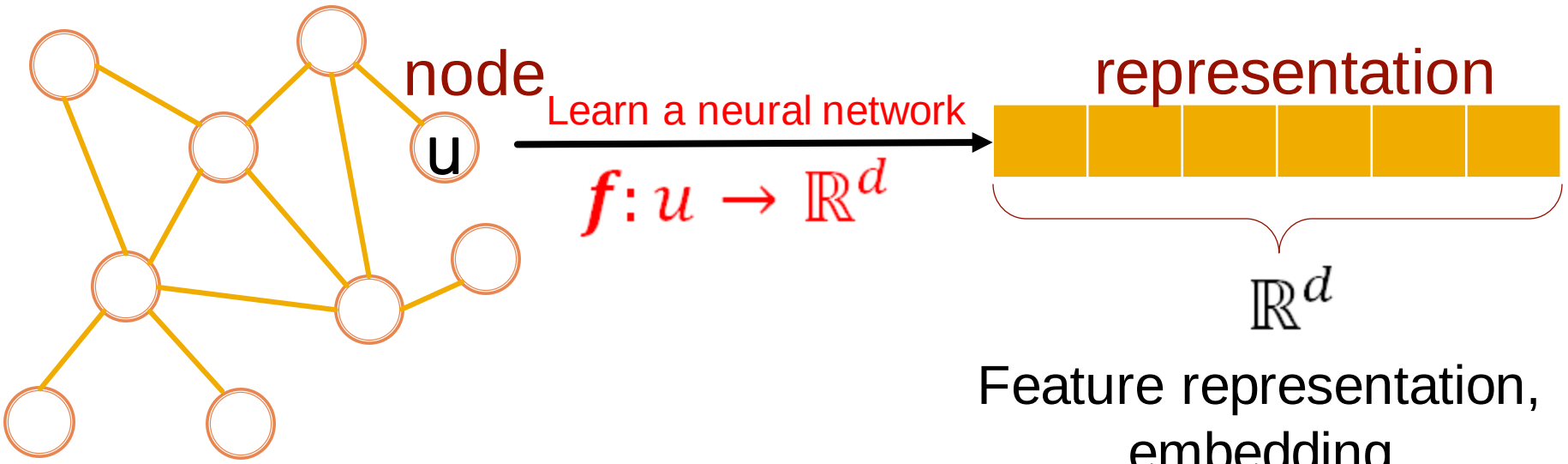
CS224W & Representation Learning

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



CS224W & Representation Learning

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



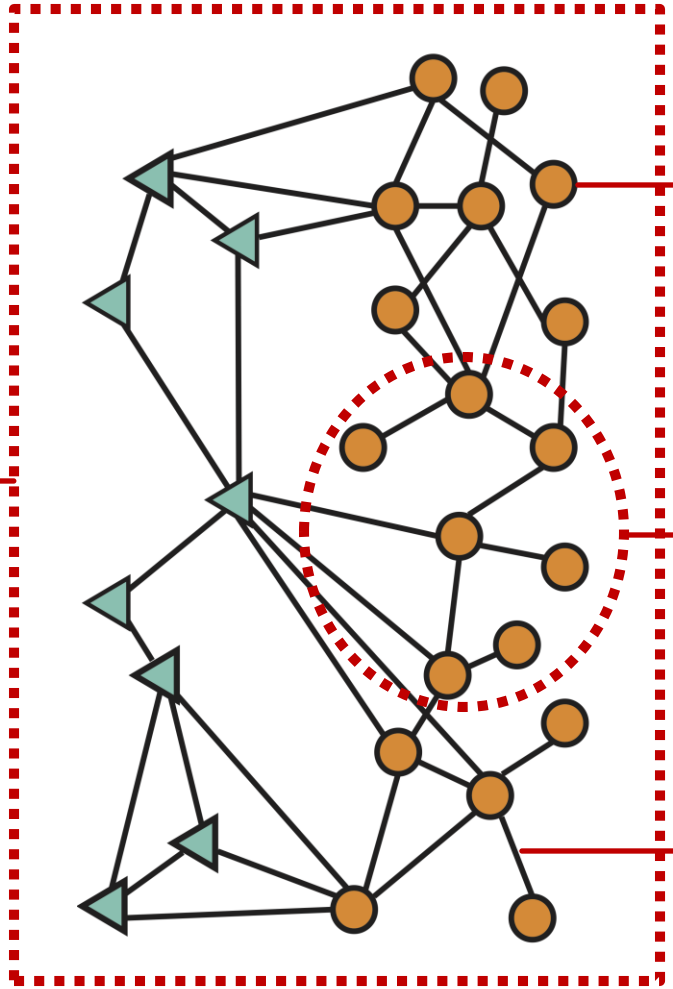
Stanford CS224W: Applications of Graph ML

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Different Types of Tasks



Node level

Community (subgraph) level

Edge-level

Graph-level prediction,

Graph generation

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:** Categorize online users / items
- **Link prediction**: Predict whether there are missing links
  - **Exa**
- **Grap** phs
  - **Exa**
- **Clust** y
  - **Exa**
- **Others**:
  - **Graph generation**: Drug discovery
  - **Graph evolution**: Physical simulation

These Graph ML tasks lead to high-impact applications!

Example of Node-level ML Tasks

Example (1): Protein Folding

A protein chain acquires its native 3D structure

Every protein is made up of a sequence of amino acids bonded together

These amino acids interact locally to form shapes like helices and sheets

These shapes fold up on larger scales to form the full three-dimensional protein structure

Proteins can interact with other proteins, performing functions such as signalling and transcribing DNA

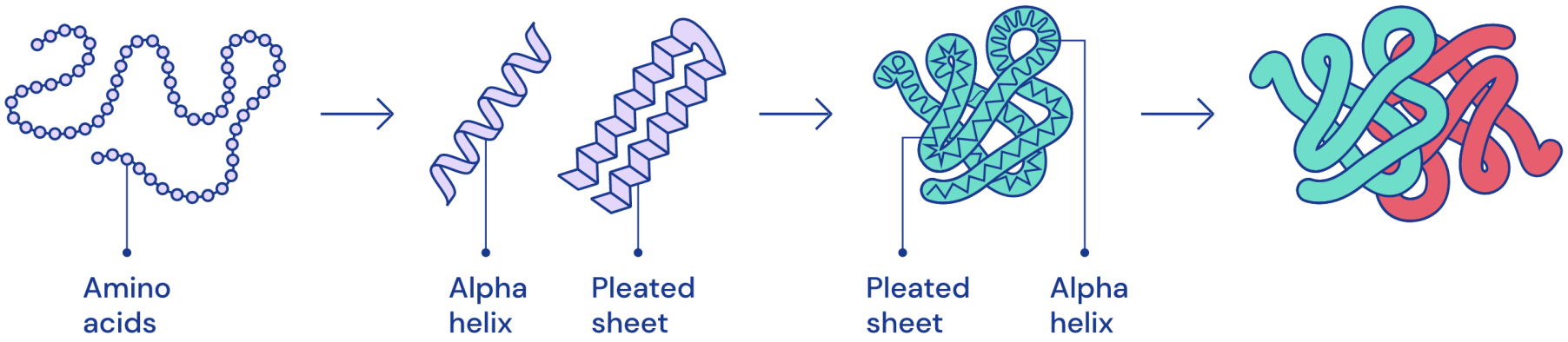
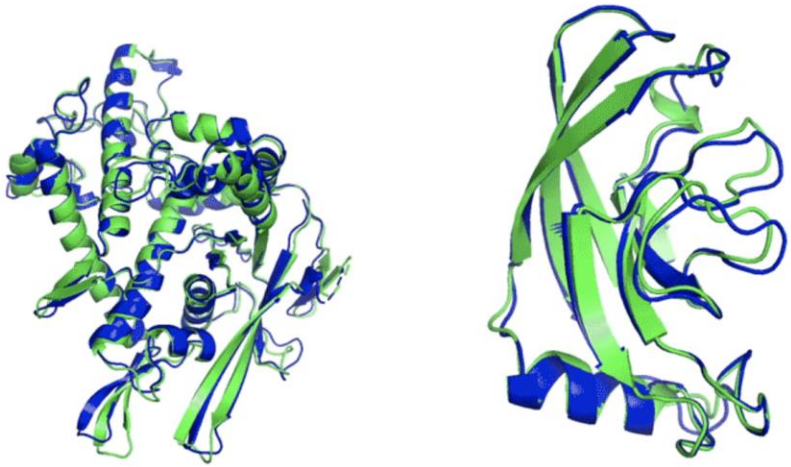


Image credit: DeepMind

The Protein Folding Problem

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



T1037 / 6vr4
90.7 GDT
(RNA polymerase domain)

T1049 / 6y4f
93.3 GDT
(adhesin tip)

Experimental result
Computational prediction

Image credit: DeepMind

AlphaFold: Impact

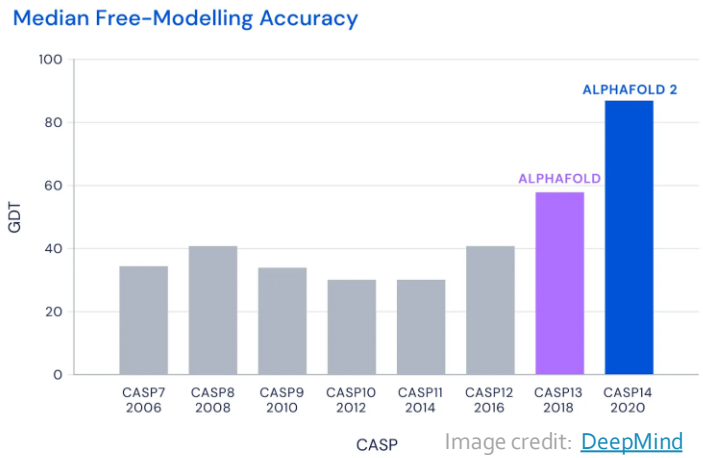


Image credit: DeepMind

Image credit: SingularityHub

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

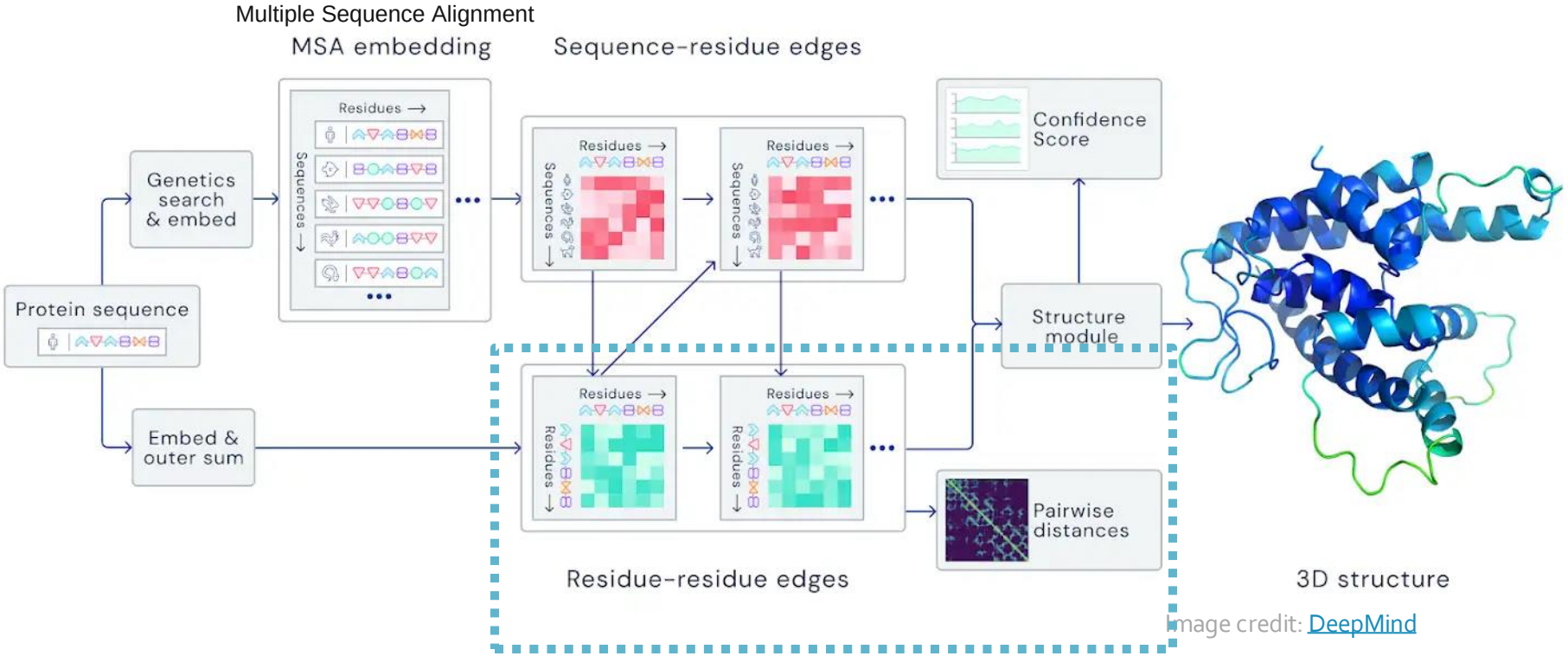
Has Artificial Intelligence 'Solved' Biology's Protein-Folding Problem?

12-14-20

DeepMind's latest AI breakthrough could turbocharge drug discovery

AlphaFold: Solving Protein Folding

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

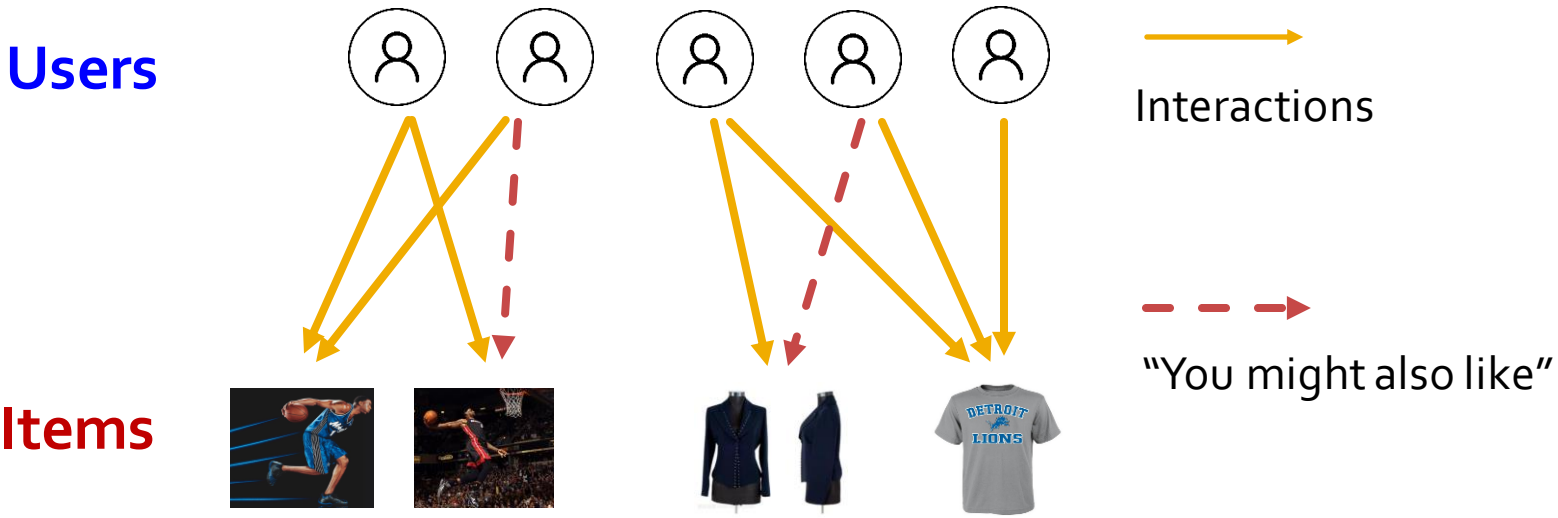


Spatial graph https://www.nature.com/articles/s41586-021-03819-2.pdf

Examples 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**

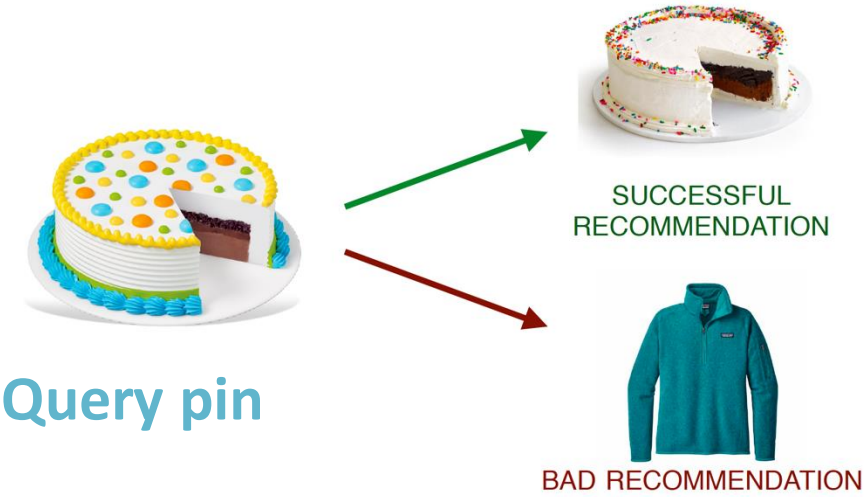


Ying et al., Graph Convolutional Neural Networks for Web-Scale Recommender Systems, KDD 2018

PinSage: Graph-based Recommender

Task: Recommend related pins to users

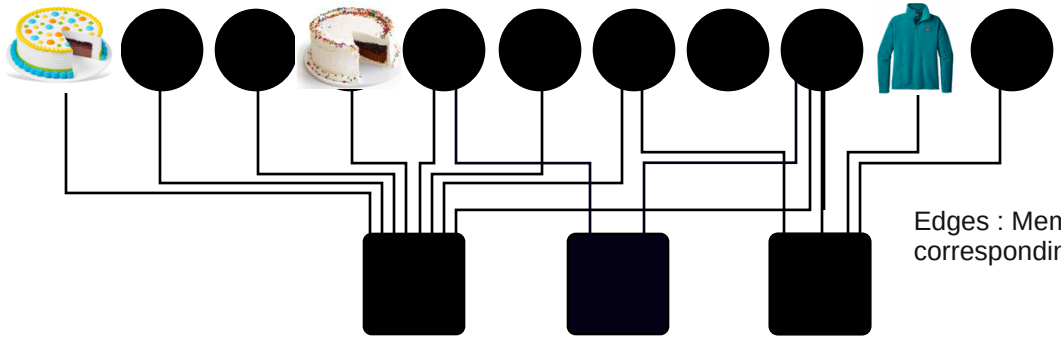
Pinterest



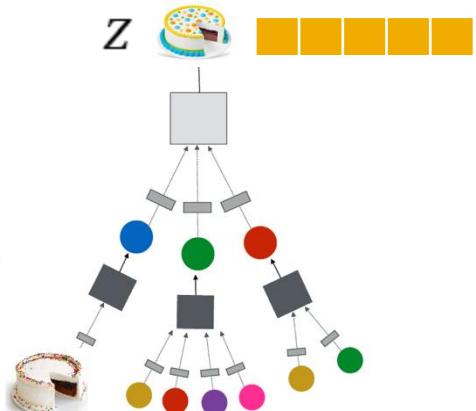
Task: Learn node embeddings z_i such that

$$d(z_{cake1}, z_{cake2}) < d(z_{cake1}, z_{sweater})$$

Predict whether two nodes in a graph are related



Edges : Membership of pins to their corresponding boards

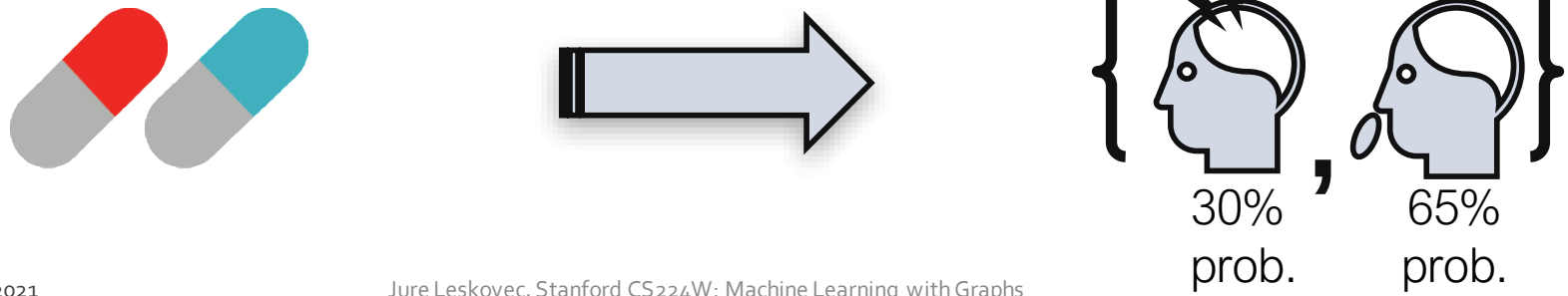


Example (3): Drug Side Effects

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.

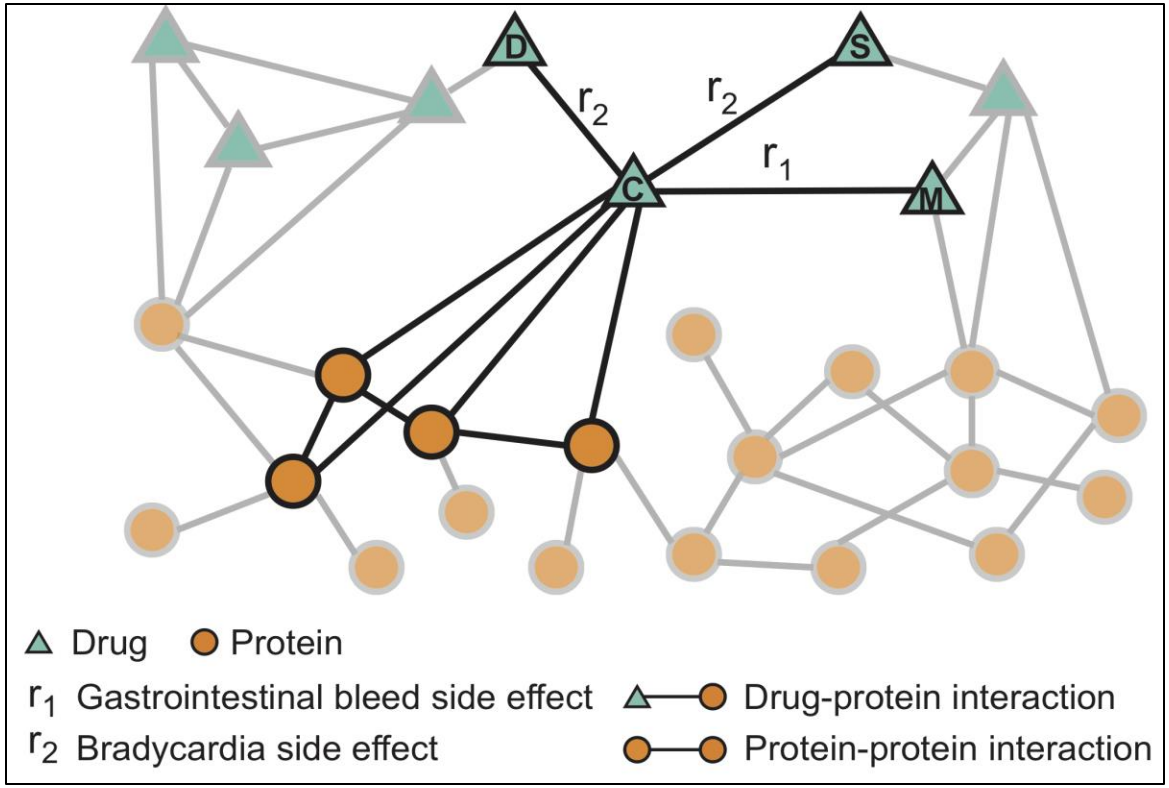
Task: Given a pair of drugs predict adverse side effects



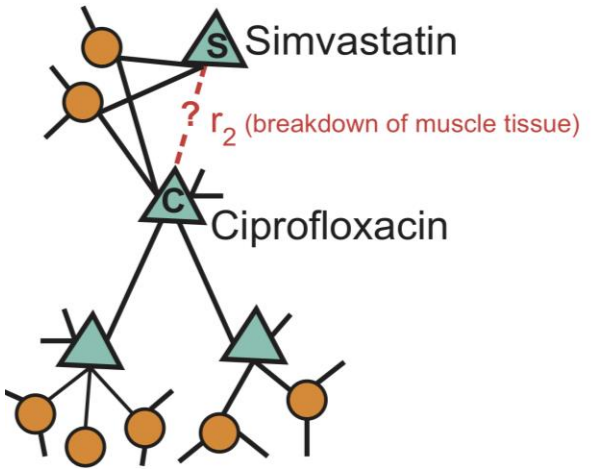
Zitnik et al., Modeling Polypharmacy Side Effects with Graph Convolutional Networks, Bioinformatics 2018

Biomedical Graph Link Prediction

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

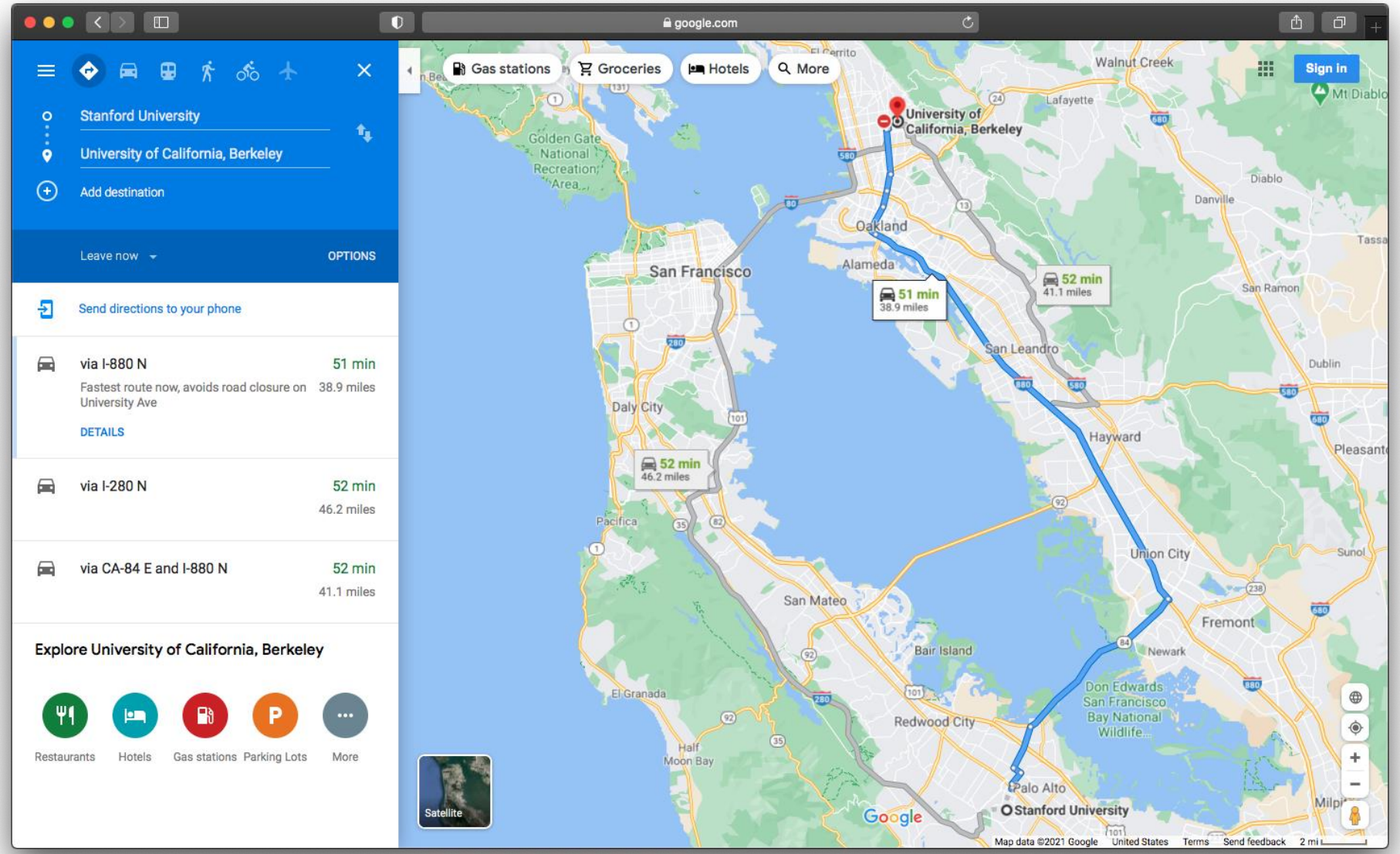


Query: How likely will Simvastatin and Ciprofloxacin, when taken together, break down muscle tissue?



Examples 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)

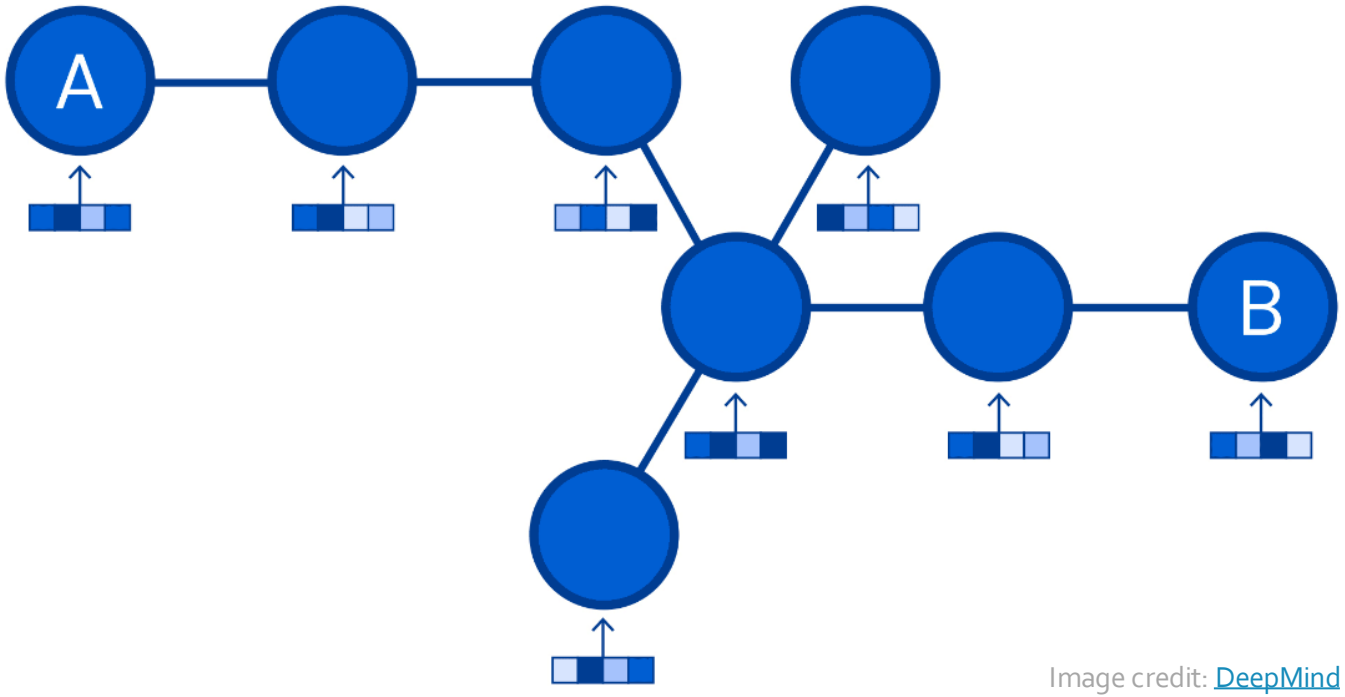
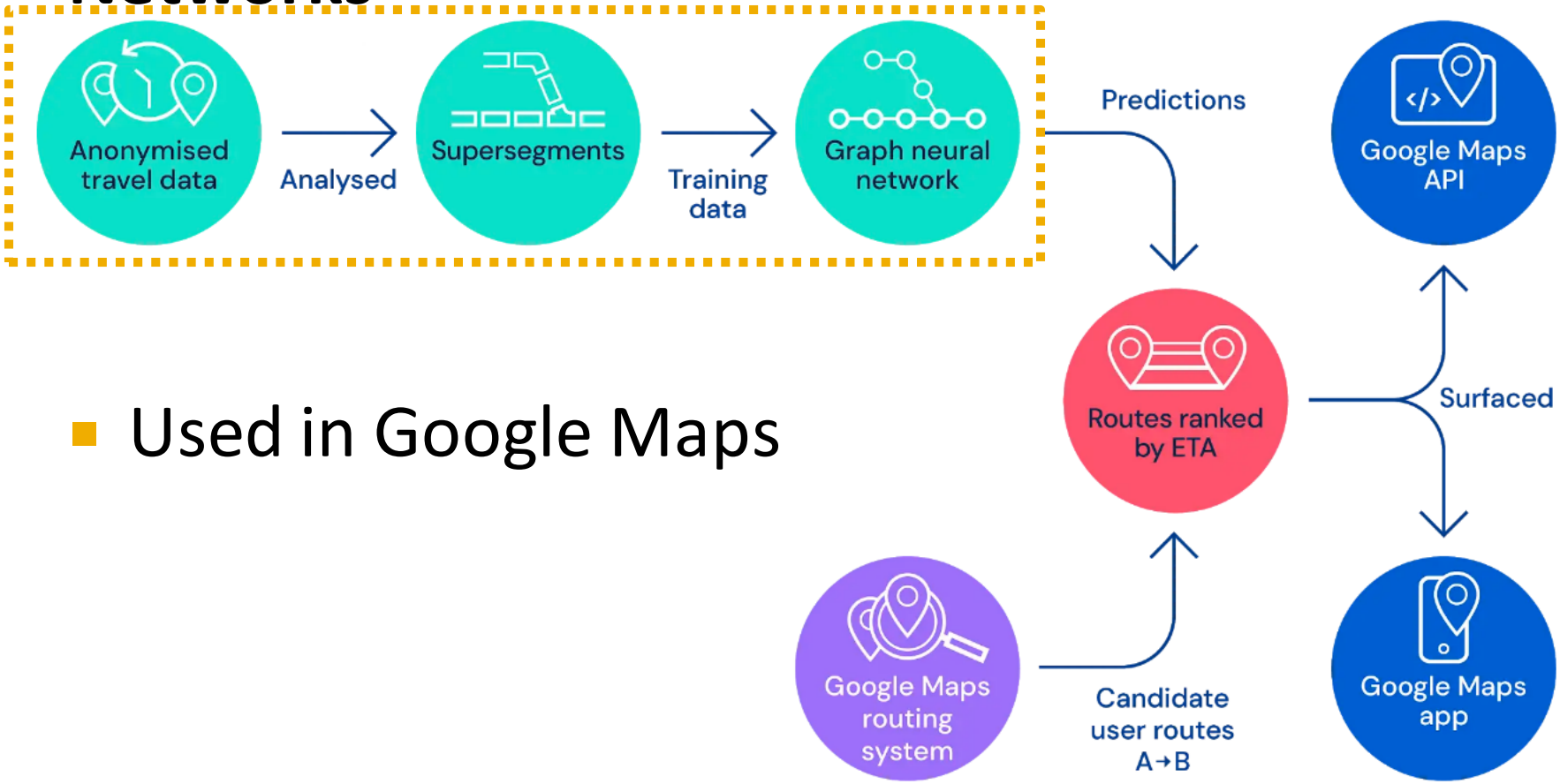


Image credit: DeepMind

Traffic Prediction via GNN

Predicting Time of Arrival with Graph Neural Networks



- Used in Google Maps

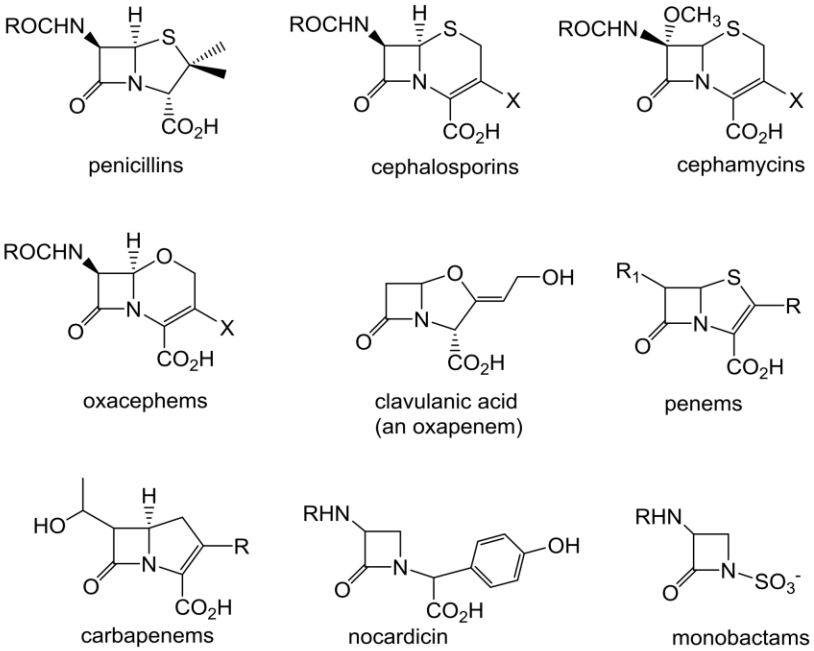
THE MODEL ARCHITECTURE FOR DETERMINING OPTIMAL ROUTES AND THEIR TRAVEL TIME.

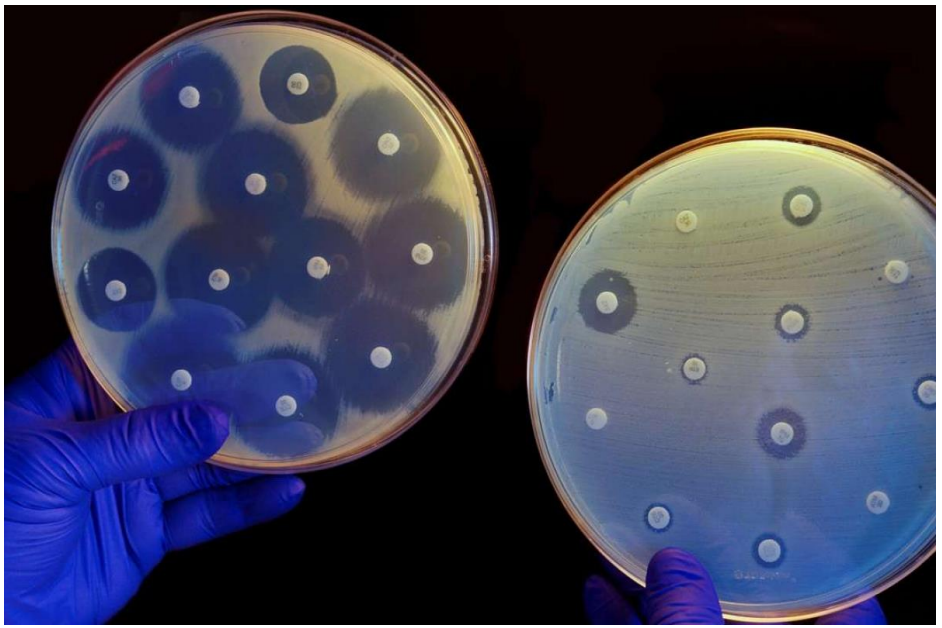
Image credit: DeepMind

Examples of Graph-level ML Tasks

Example (5): Drug Discovery

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



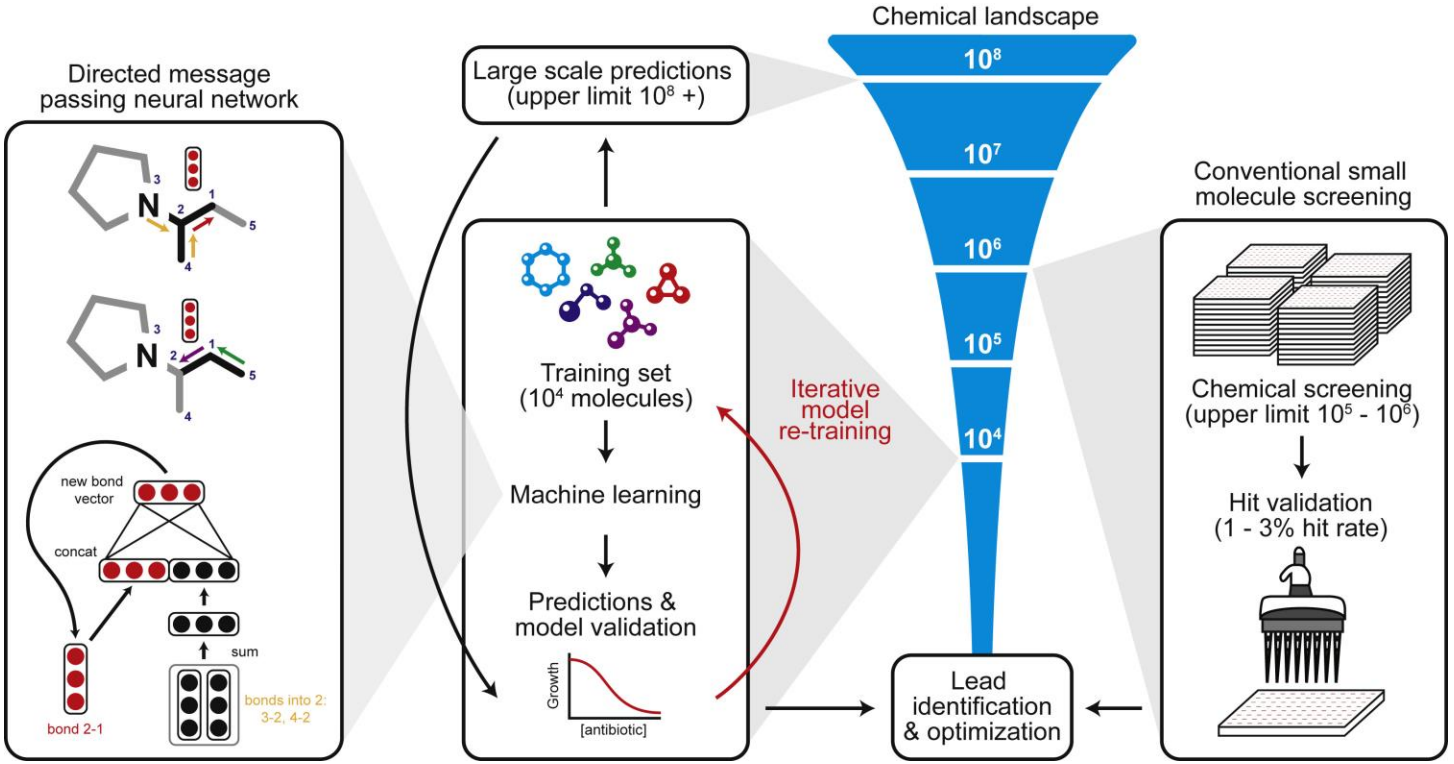


Konaklieva, Monika I. "Molecular targets of β-lactam-based antimicrobials: beyond the usual suspects." Antibiotics 3.2 (2014): 128-142.

Image credit: CNN

Deep Learning for Antibiotic Discovery

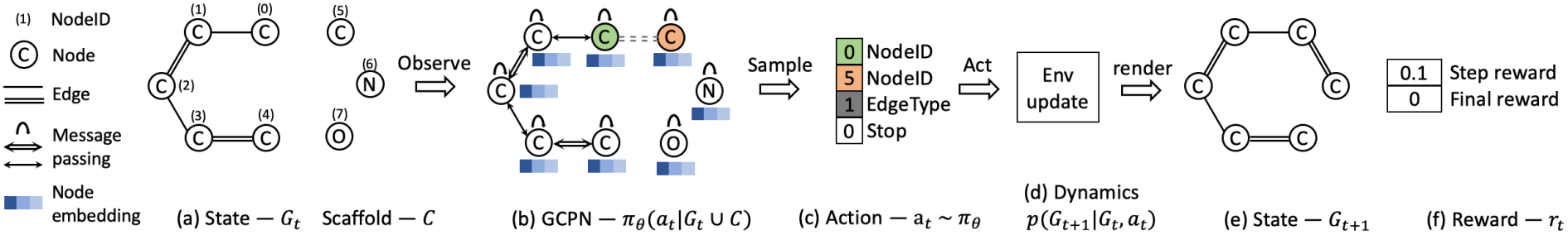
- A Graph Neural Network **graph classification model**
- Predict promising molecules from a pool of candidates



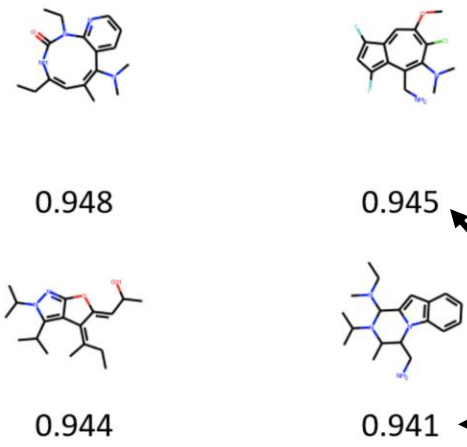
Stokes, Jonathan M., et al. "A deep learning approach to antibiotic discovery." Cell 180.4 (2020): 688-702.

Molecule Generation / Optimization

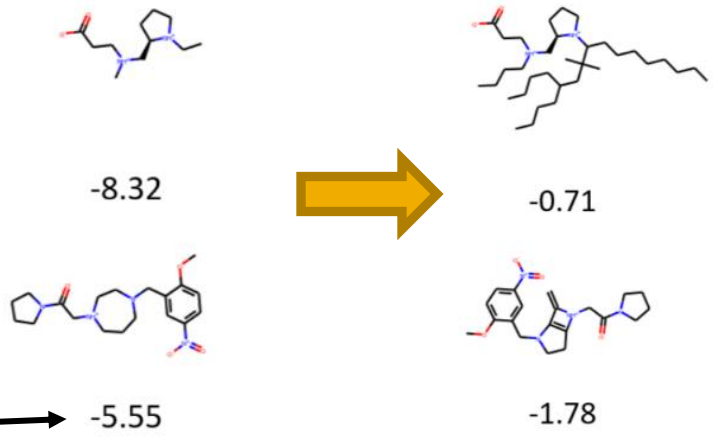
Graph generation: Generating novel molecules



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



Use case 2: Optimize existing molecules to have desirable properties



Drug likeness

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

Example (6): Physics Simulation

Physical simulation as a graph:

- **Nodes**: Particles
- **Edges**: Interaction between particles

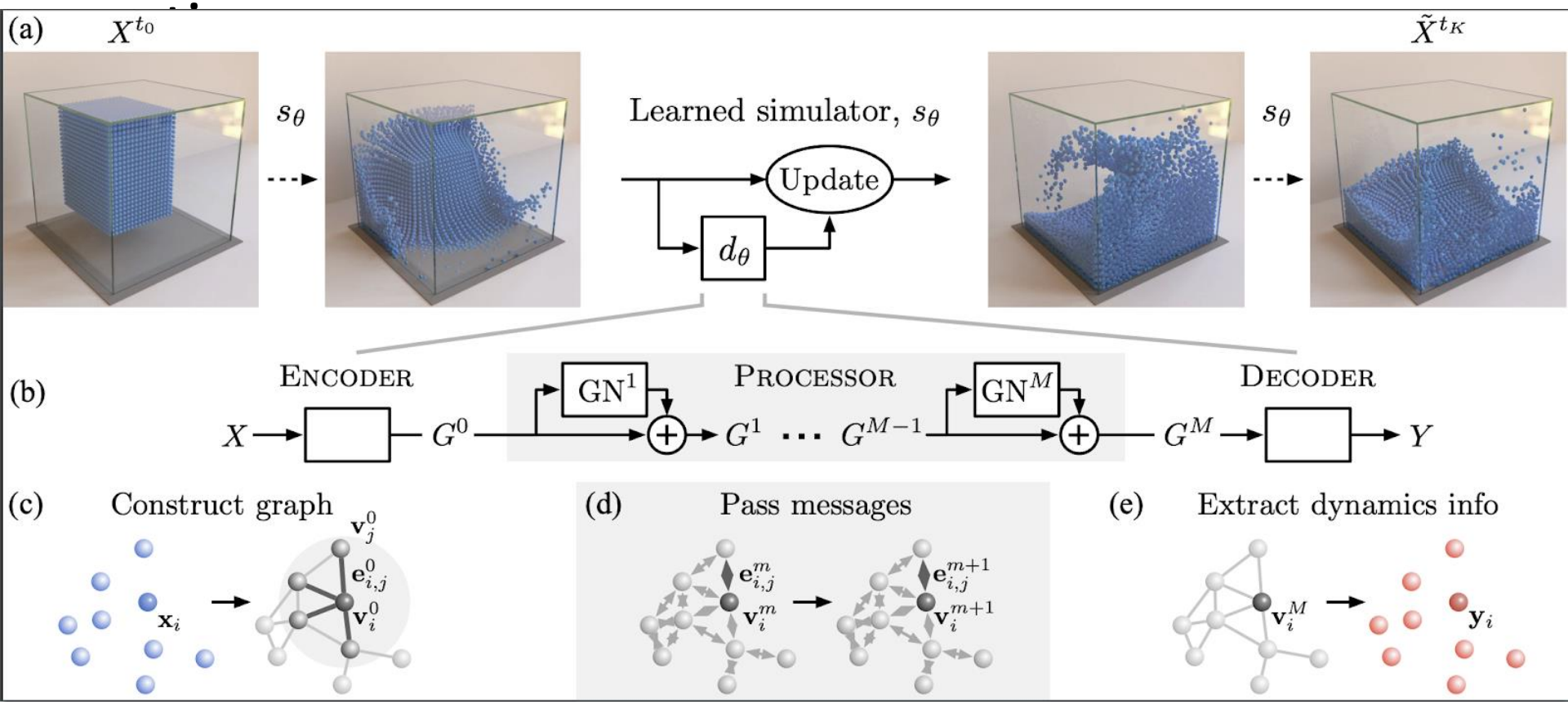
https://www.youtube.com/watch?v=h7h9zF8OO7E

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



Summary

- **Machine learning with Graphs**
  - Applications and use cases
- **Different types of tasks:**
  - Node level
  - Edge level
  - Graph level

Course website: http://web.stanford.edu/class/cs224w/

Course recordings: CS224W: Machine Learning with Graphs | 2021 on Youtube

Past meetup recordings: **YanAITalk** Youtube channel