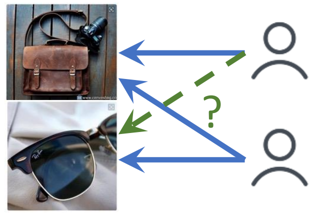
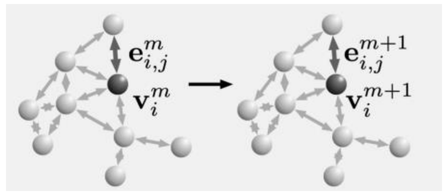
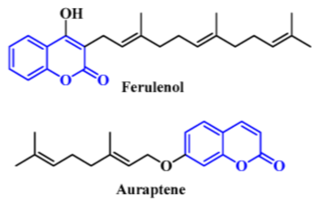
Graph Neural Networks Applications

Rex Ying

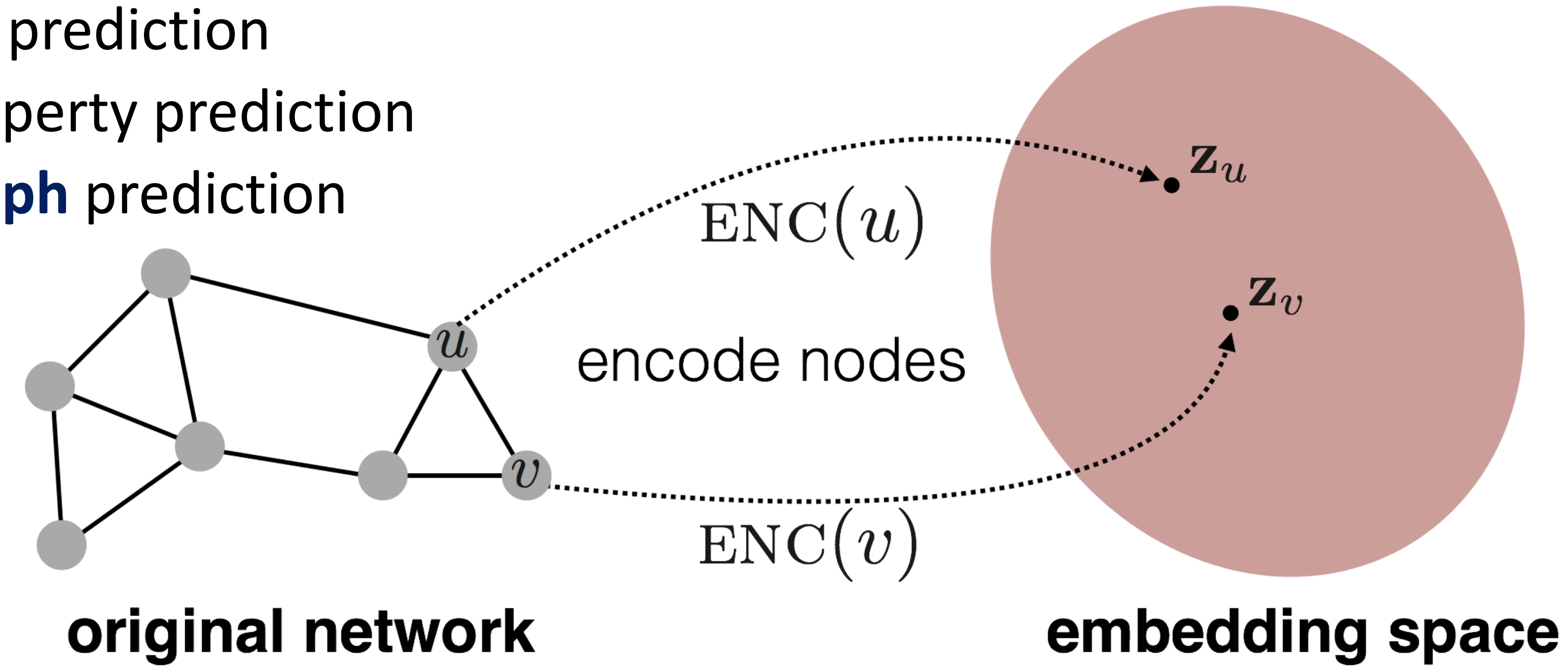




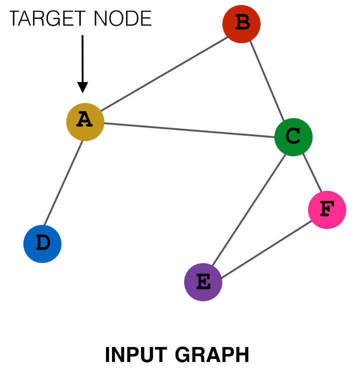


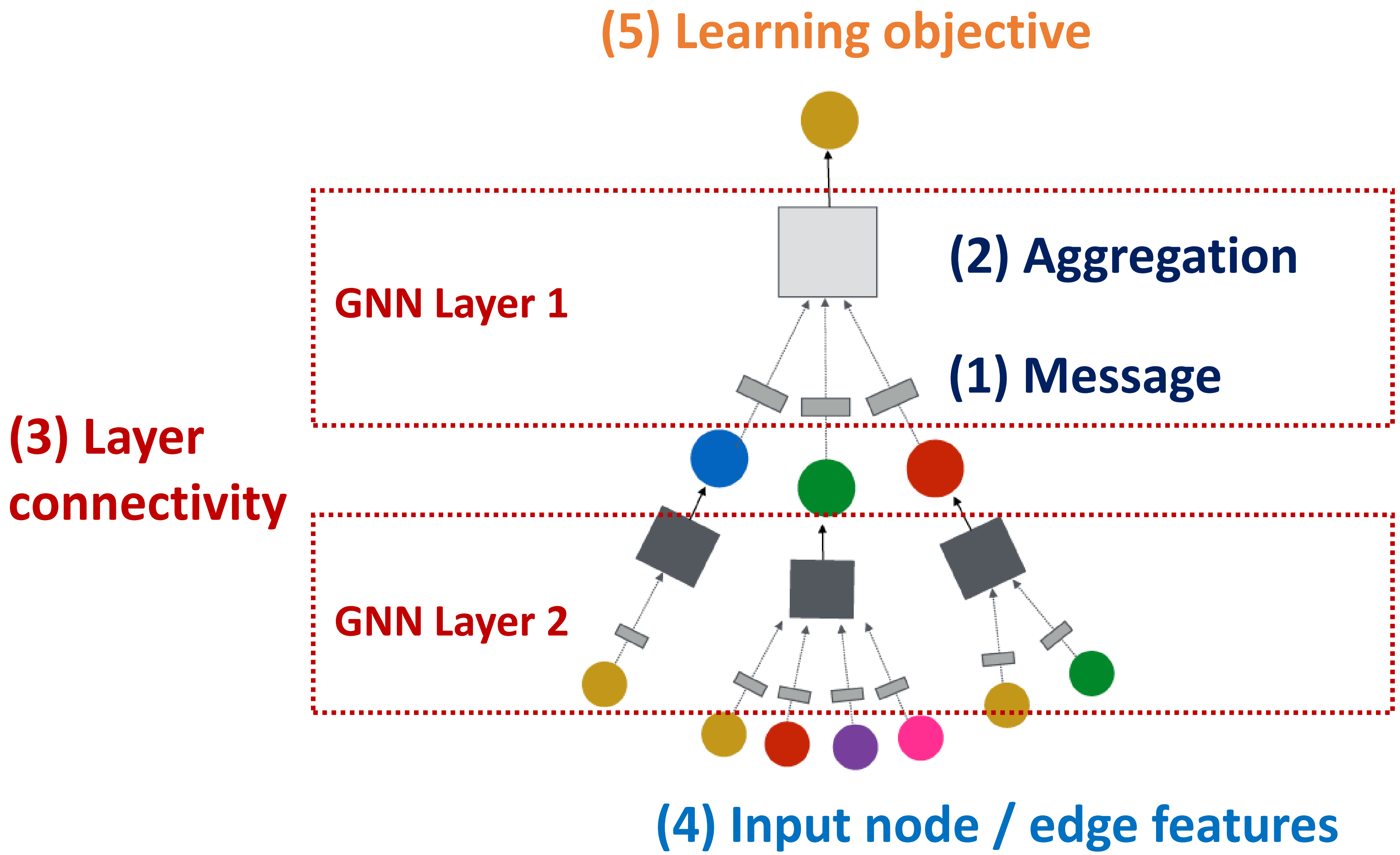
Background: Graph Representation Learning

- Given one or more input graphs, we use a (deep) encoder to map nodes to high-dimensional embedding space
- Objectives
  - **Node** property prediction
  - **Link** / **edge** property prediction
  - **Graph** / **subgraph** prediction



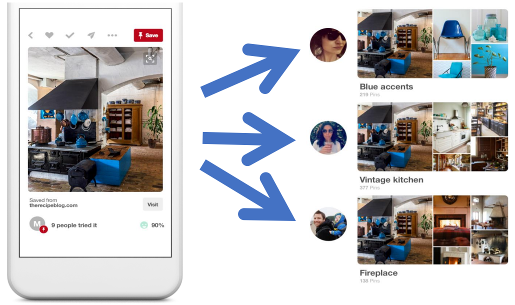
Recap: Graph Neural Networks (GNNs)



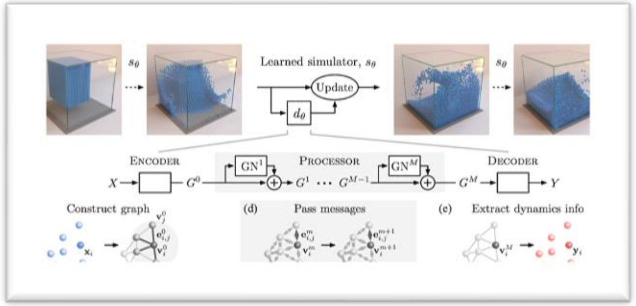


GNN Applications

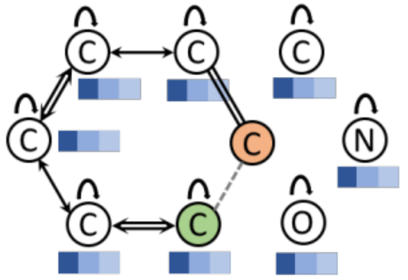
- **Social Networks** → **Recommender System**



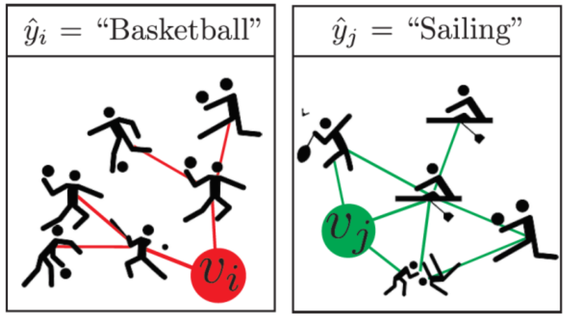
- **Natural Science** → **Physical Simulation**



- **Medicine** → **Drug Side-effects** **Molecule Generation**

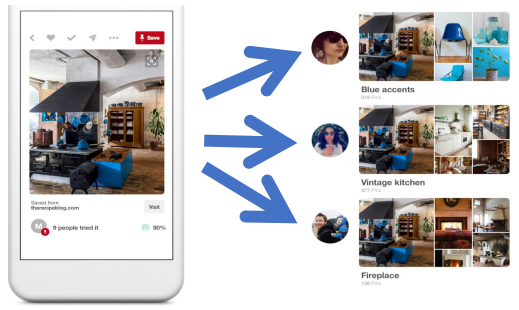


- **Explainability of GNNs**



GNN Applications

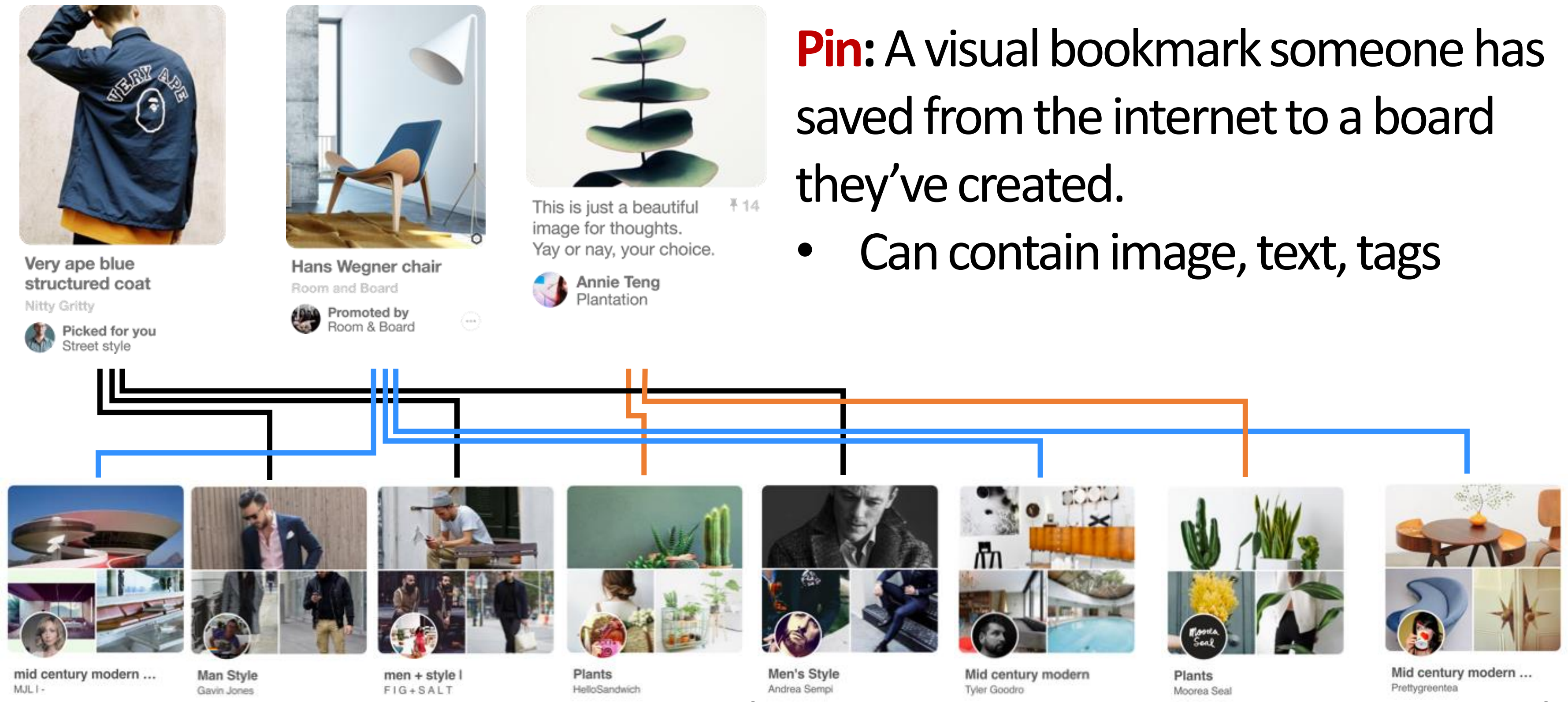
- **Social Networks** $\longrightarrow$ Recommender System



- Natural Science
- Medicine
- Explainability of GNNs

Pinterest Recommender System

Human curated collection of pins



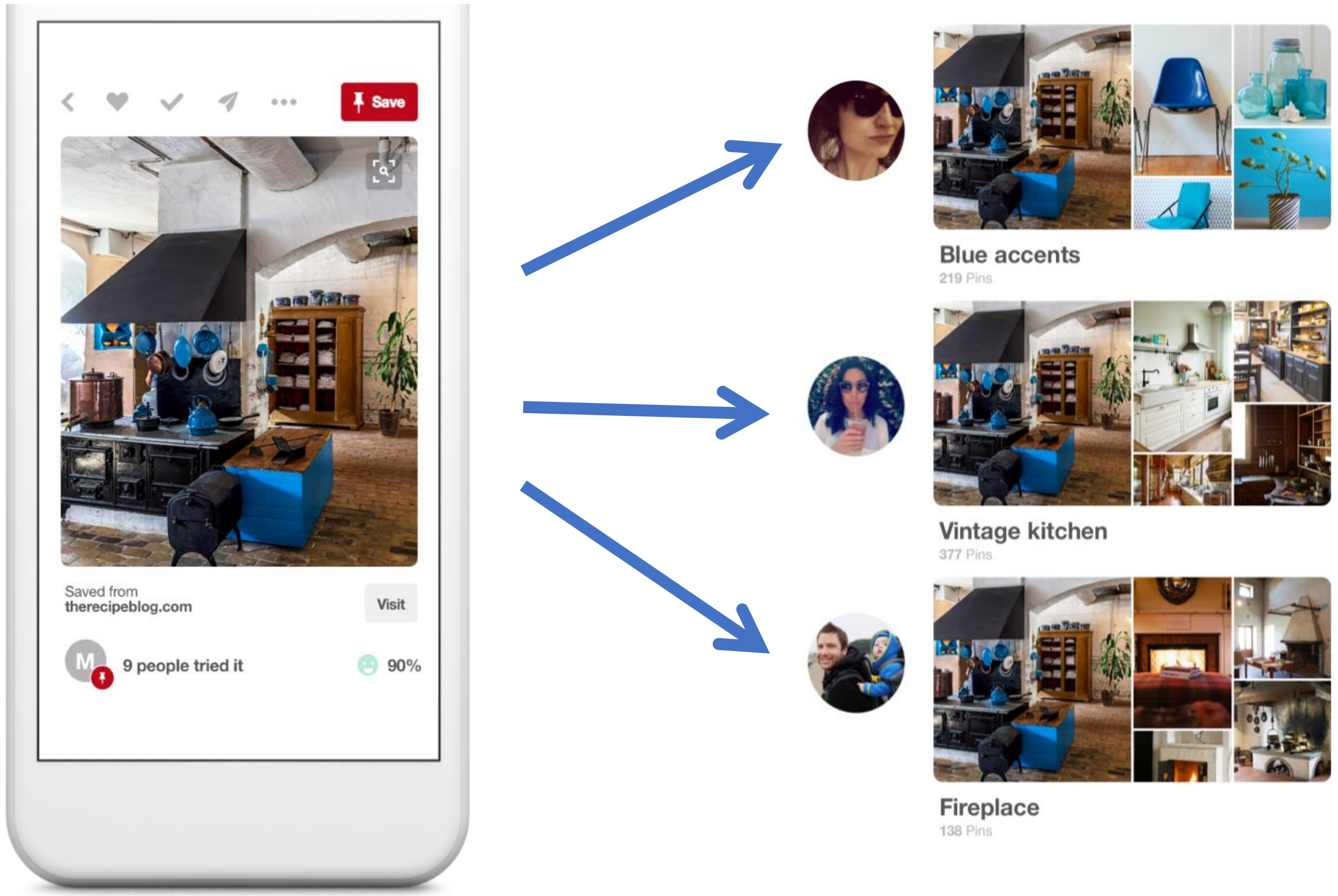
Pin: A visual bookmark someone has saved from the internet to a board they've created.

- Can contain image, text, tags

Board: A collection of ideas (pins having something in common)

Pinterest Recommender System

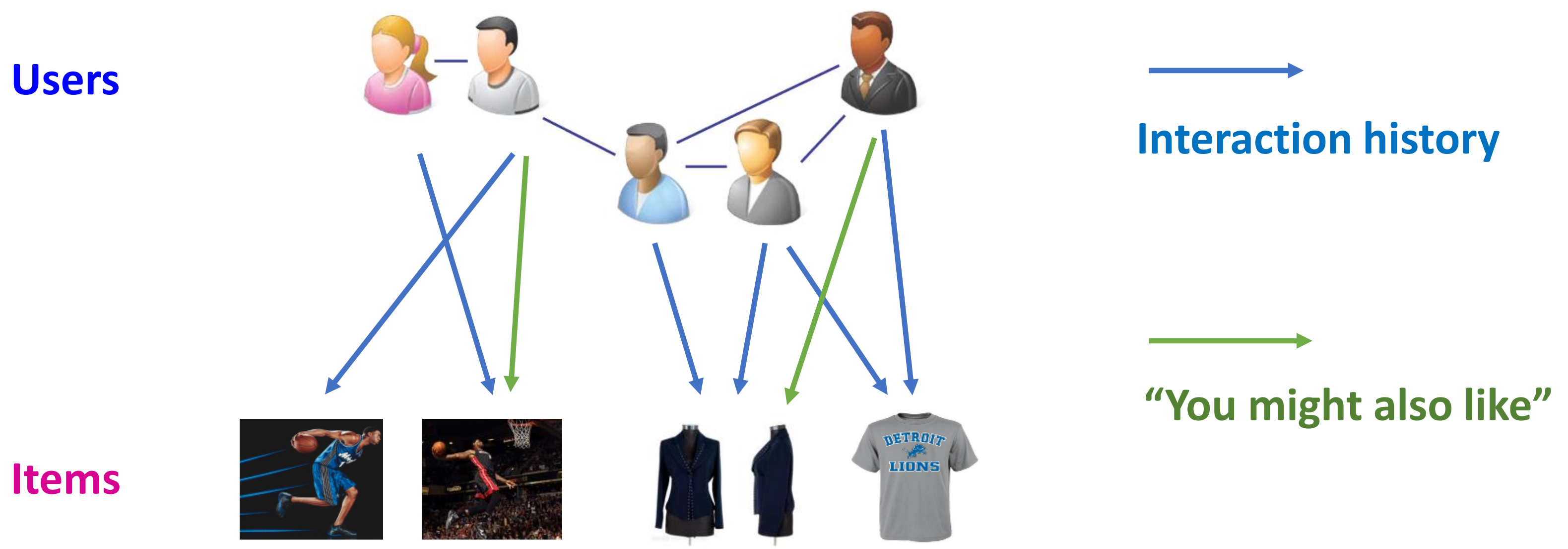
- Social network for idea collections
- 300M users
- 4B+ pins, 2B+ boards



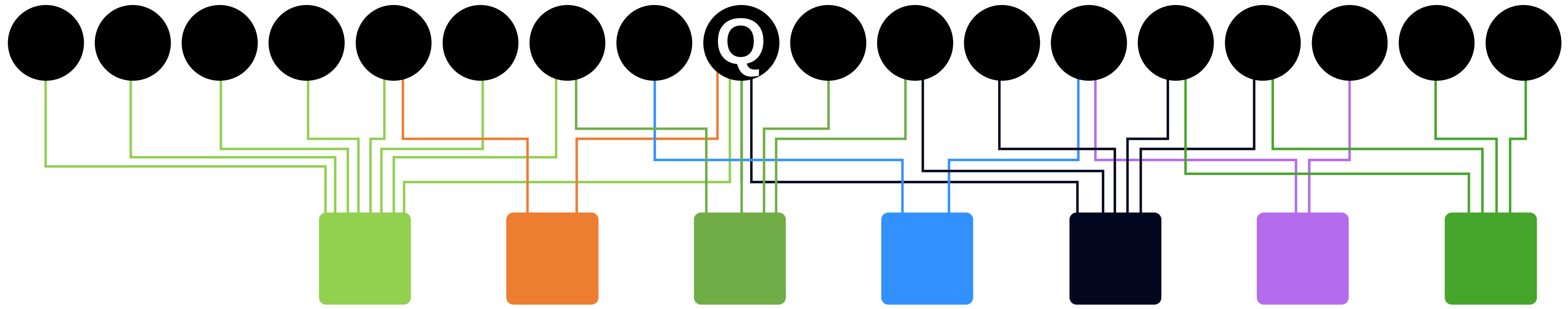
Graph Convolutional Neural Networks for Web-Scale Recommender Systems, KDD 2018

PinSage: Web-scale Recommender System

- Users are related by social network
- Users interact with items (watch movie, buy merchandise, listen to music)
- Predict future interactions from history



Pinterest Graph

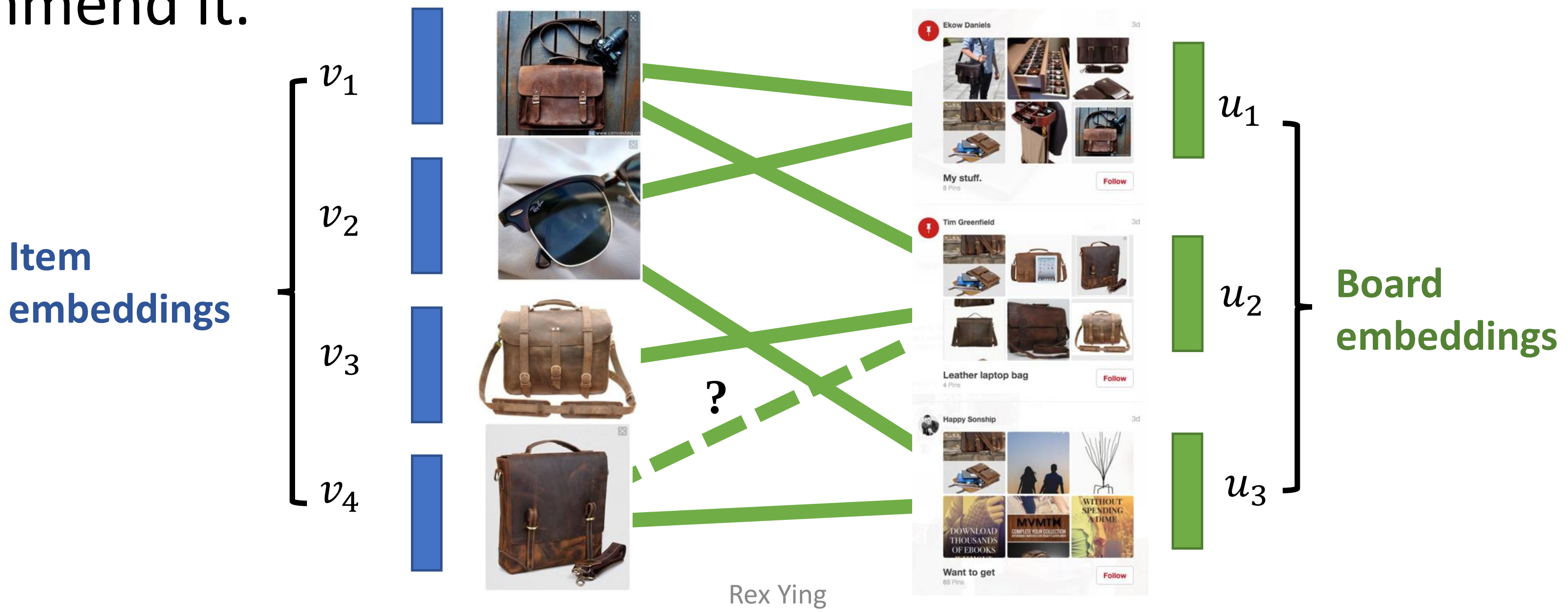


Graph: 2B pins, 1B boards, 20B edges

- **Graph is dynamic:** Need to apply to new nodes without model retraining
- **Rich node features:** Content, images

Recommend by embeddings

- Learn embeddings for **items** and **boards**
- **Query**: which item to recommend to the board with embedding u_2 ?
- **Answer**: find the closest embedding (v_4) by nearest neighbor. Recommend it.



Why is it Hard?

How to scale the training as well as inference of node embeddings to graphs with billions of nodes and tens of billions of edges?

- Scaling up is difficult:
    - Existing collaborative filtering and distributed node embedding methods are inefficient when the underlying graph has billions of nodes and whose structure is constantly evolving

PinSage Overview

- **PinSage** graph convolutional network:
  - **Goal:** Generate embeddings for nodes (e.g., Pins/images) in a web-scale Pinterest graph containing billions of objects
  - **Key Idea:** Borrow information from nearby nodes
    - E.g., bed rail Pin might look like a garden fence, but gates and beds are rarely adjacent in the graph

    - Pin embeddings are essential to various tasks like recommendation of Pins, classification, clustering, ranking
      - Services like “Related Pins”, “Search”, “Shopping”, “Ads”

PinSage Pipeline

1. **Collect** billions of training pairs from logs.
   - **Positive pair**: a pin and a board that contains it
   - **Negative pair**: a random pair of pin and board
     - With high probability the pin is not pinned to the board

2. **Train GNN** to generate similar embeddings for training pairs.
3. **Inference**: generate embeddings for all pins.
4. **Nearest neighbor search** in embedding space to make recommendations.

Neighborhood Sampling

Constructing convolutions via random walks

- Performing convolutions on full neighborhoods is infeasible:
  - How to select the set of neighbors of a node to convolve?
- **Personalized PageRank can help!**
- **Importance pooling:** Define importance-based neighborhoods by simulating random walks and selecting the neighbors with the highest visit counts

Training Objective

- Train so that **pins that are consecutively clicked have similar embeddings.**
- Max-margin loss:

$$\mathcal{L} = \sum_{(u,v)\in \boxed{\mathcal{D}}} \max(0, -\boxed{\mathbf{z}_u^\top \mathbf{z}_v} + \mathbf{z}_u^\top \boxed{\mathbf{z}_n} + \boxed{\Delta})$$

set of training pairs from user logs

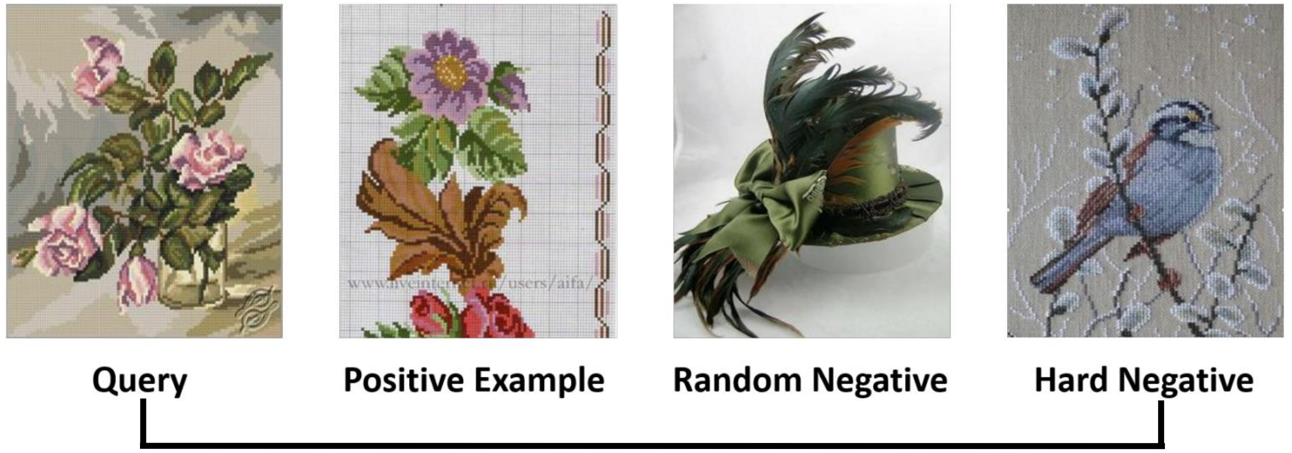
"positive"/true training pair

"negative" example

"margin" (i.e., how much larger positive pair similarity should be compared to negative)

Negative Sampling

- **Hard negative sampling**

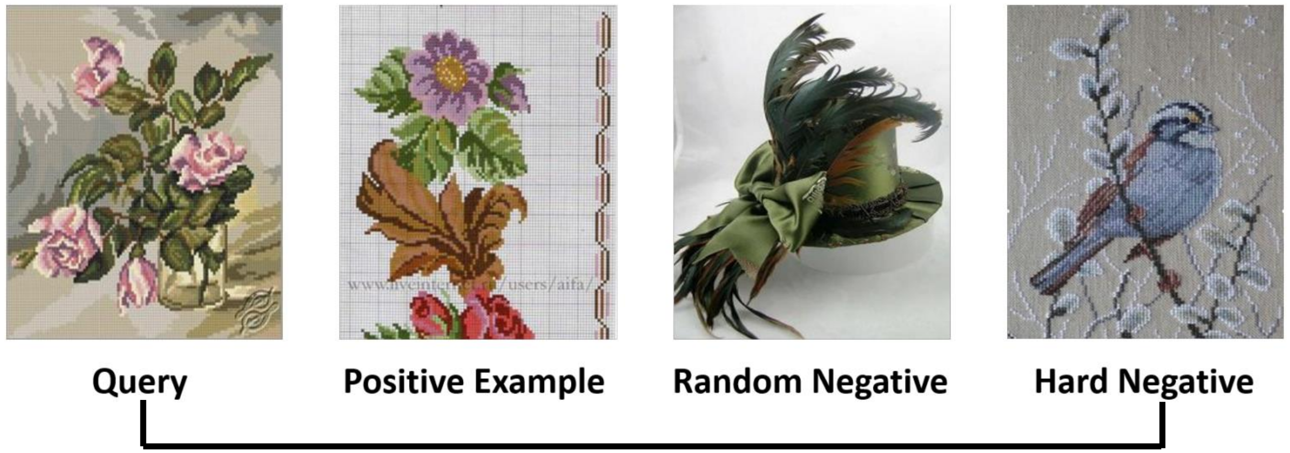


Harder to distinguish from positive

- Use personalized PageRank (PPR)
  - Use nodes that have PPR score ranked at 1000-5000 as hard negatives
  - Have something in common, but not too similar

Negative Sampling

- **Hard negative sampling**



Harder to distinguish from positive

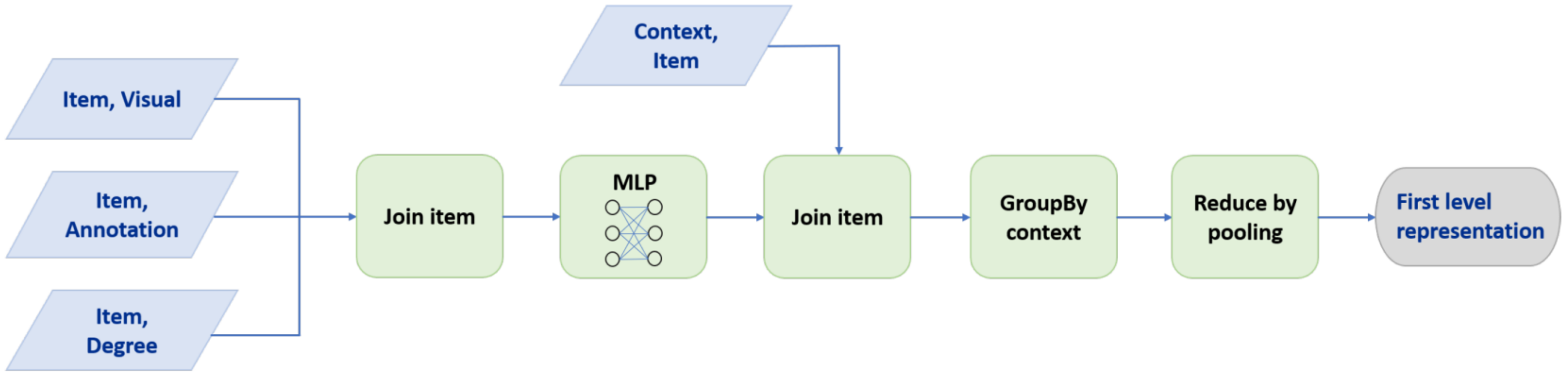
- **Curriculum training** on hard negatives
  - provide harder and harder examples over time

Efficient Inference

Efficient inference via **MapReduce**

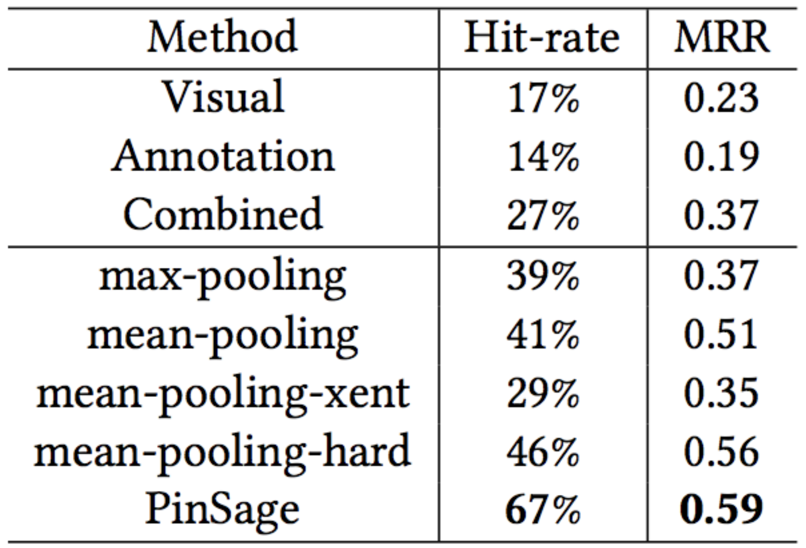
- Bottom-up aggregation of node embeddings lends itself to MapReduce
  - Decompose each aggregation step across all nodes into three operations in MapReduce, i.e., *map*, *join*, and *reduce*
- Avoid repeated computation

For every layer:



Evaluation

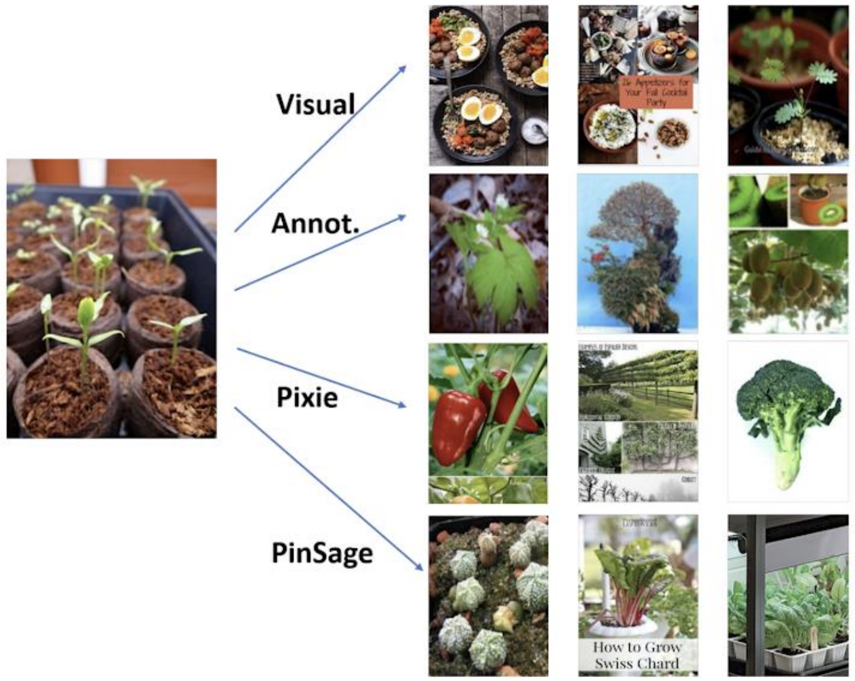
- Baselines:
  - **Visual**: VGG visual embeddings for recommendations
  - **Annotation**: Word2vec embeddings
  - **Combined**: Concatenate embeddings:
    - Uses exact same data and loss function as PinSage



Method	Hit-rate	MRR
Visual	17%	0.23
Annotation	14%	0.19
Combined	27%	0.37
max-pooling	39%	0.37
mean-pooling	41%	0.51
mean-pooling-xent	29%	0.35
mean-pooling-hard	46%	0.56
PinSage	**67%**	**0.59**

PinSage gives 150% improvement in hit rate and 60% improvement in MRR over the best baseline

Evaluation



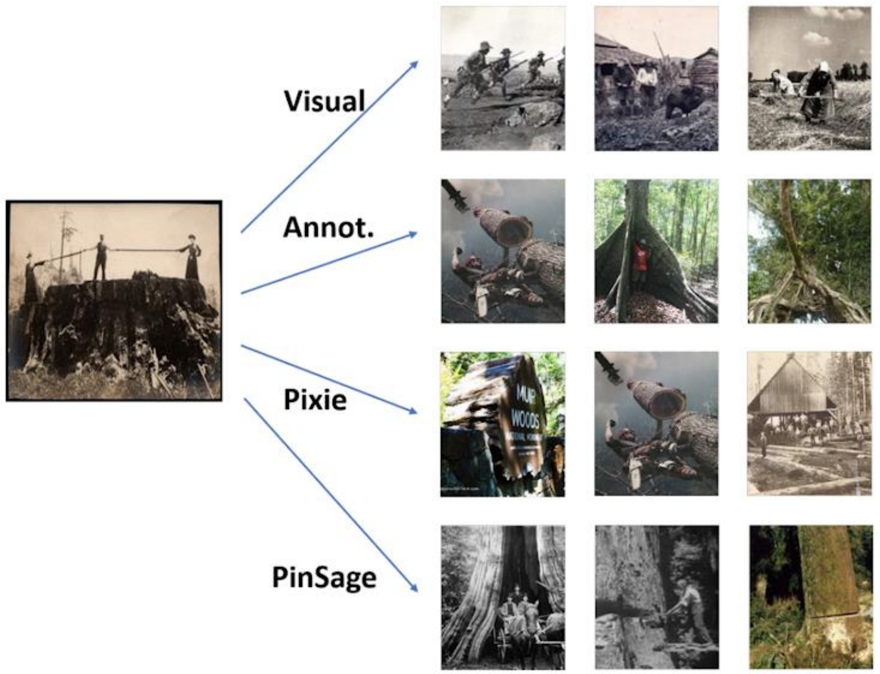


Image information

Text information

Graph information

Combined!

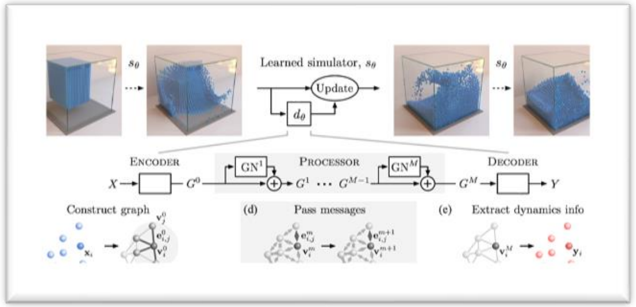
Pixie is a purely graph-based method that uses biased random walks to generate ranking scores by simulating random walks starting at query Pin. Items with top scores are retrieved as recommendations [Eksombatchai et al., 2018]

Summary

- Many online platforms can be modeled as graphs, where nodes are **users**, items and edges represent **interactions**
  - View, purchase, review, follow, likes
- We use **link prediction objective** to train a GNN-based recommender systems
  - Efficient training and inference on a billion-scale graph
- The learned graph embedding captures image/text feature as well as graph structure
- The learned embedding is useful in many downstream tasks beyond recommendation!

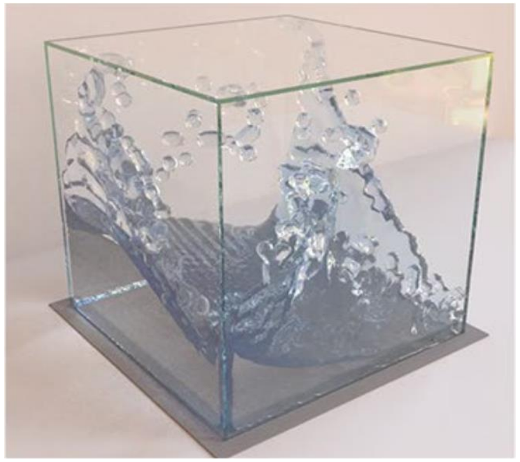
GNN Applications

- Social Networks
- **Natural Science** → Physical Simulation
- Medicine
- Explainability of GNNs

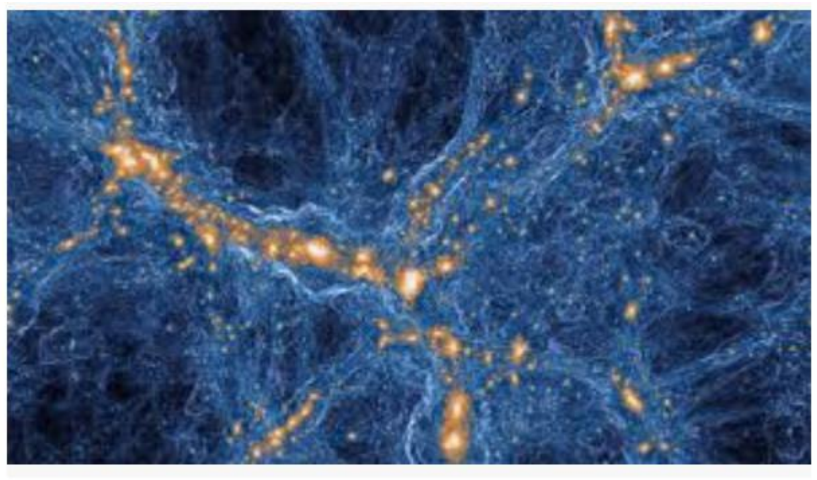


Simulations in Science and Engineering

1. Particle-particle interactions:



Water simulation

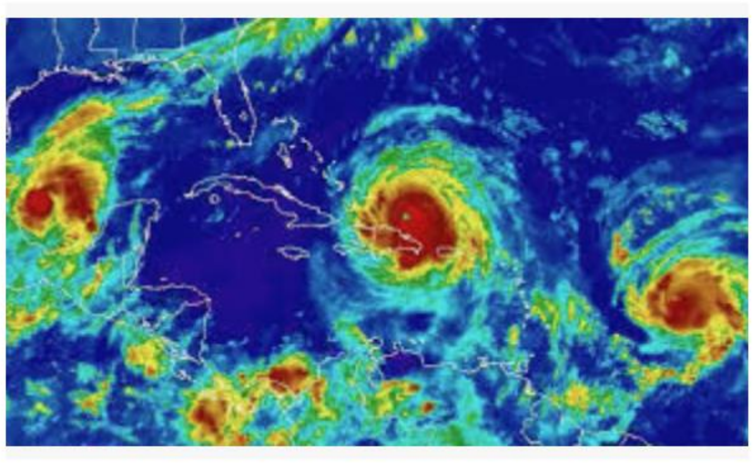


Galaxy formation

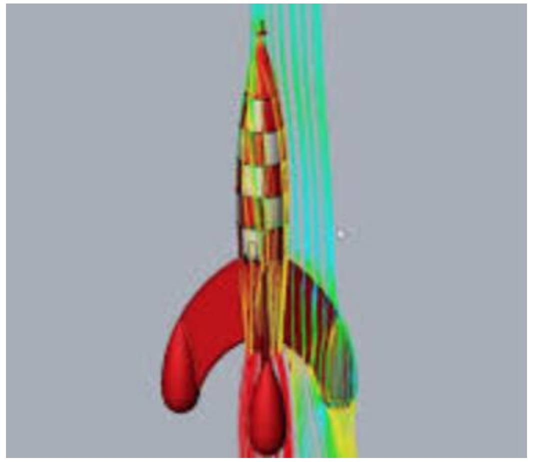
We construct graphs with particles as nodes and interactions as edges

Simulations in Science and Engineering

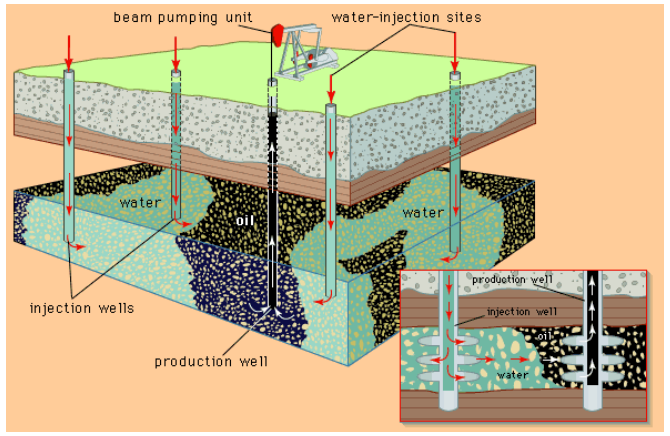
2. PDEs (on grid or mesh)



Weather prediction



Aerodynamics

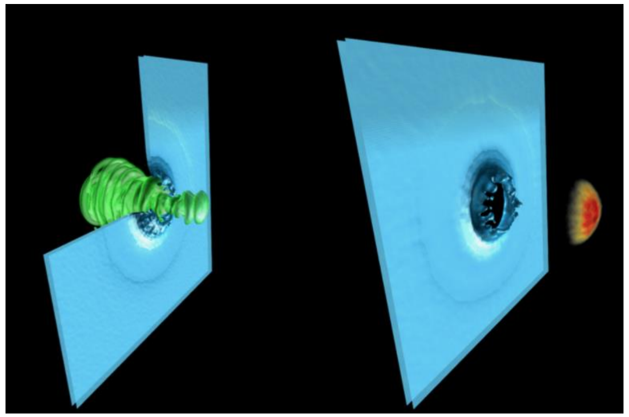


Reservoir simulation

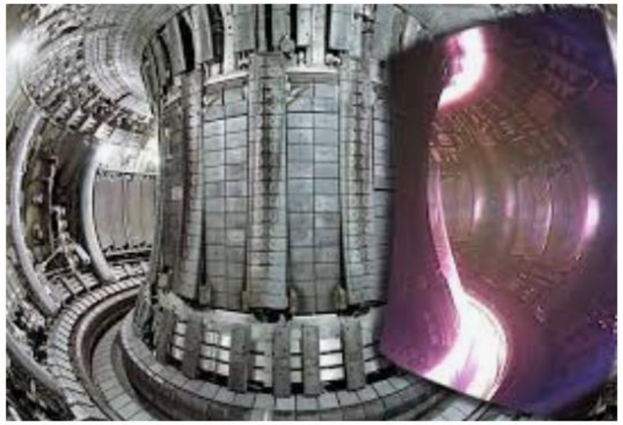
Graph based on grid / mesh structure

Simulations in Science and Engineering

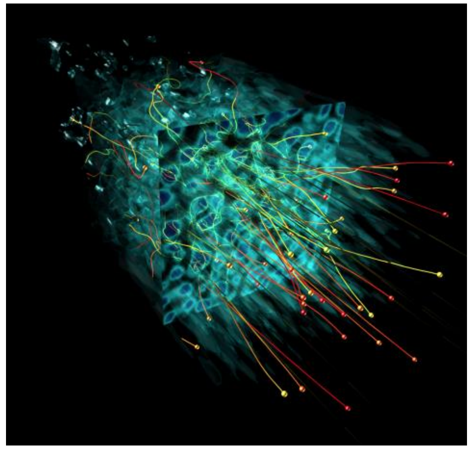
3. Particle-in-Cell (involves both grid and particles)



Laser-plasma particle acceleration



Fusion



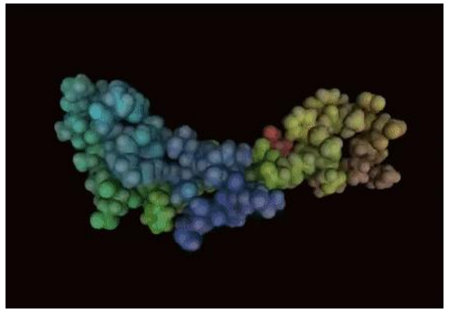
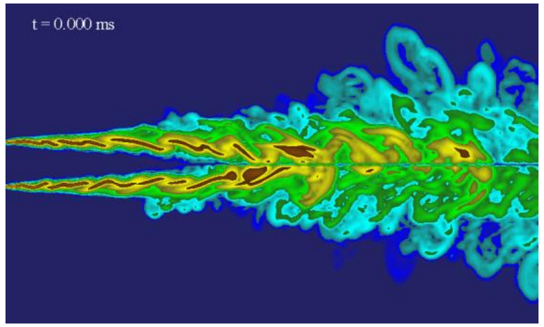
Cosmic-ray acceleration

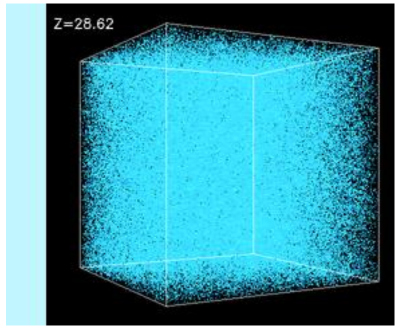
Graph combining grid / mesh with particles!

Why Learning Simulation

Engineered simulators:
1. Substantial effort to build
2. Substantial resources to run
3. Only as accurate as the designer
4. Not always suitable for solving inverse problems

Learned simulators:
1. **Shared** architectures
2. Can be directly optimized for **efficiency**
3. Can be as accurate as the available **data**
4. Gradient-based search for **control**

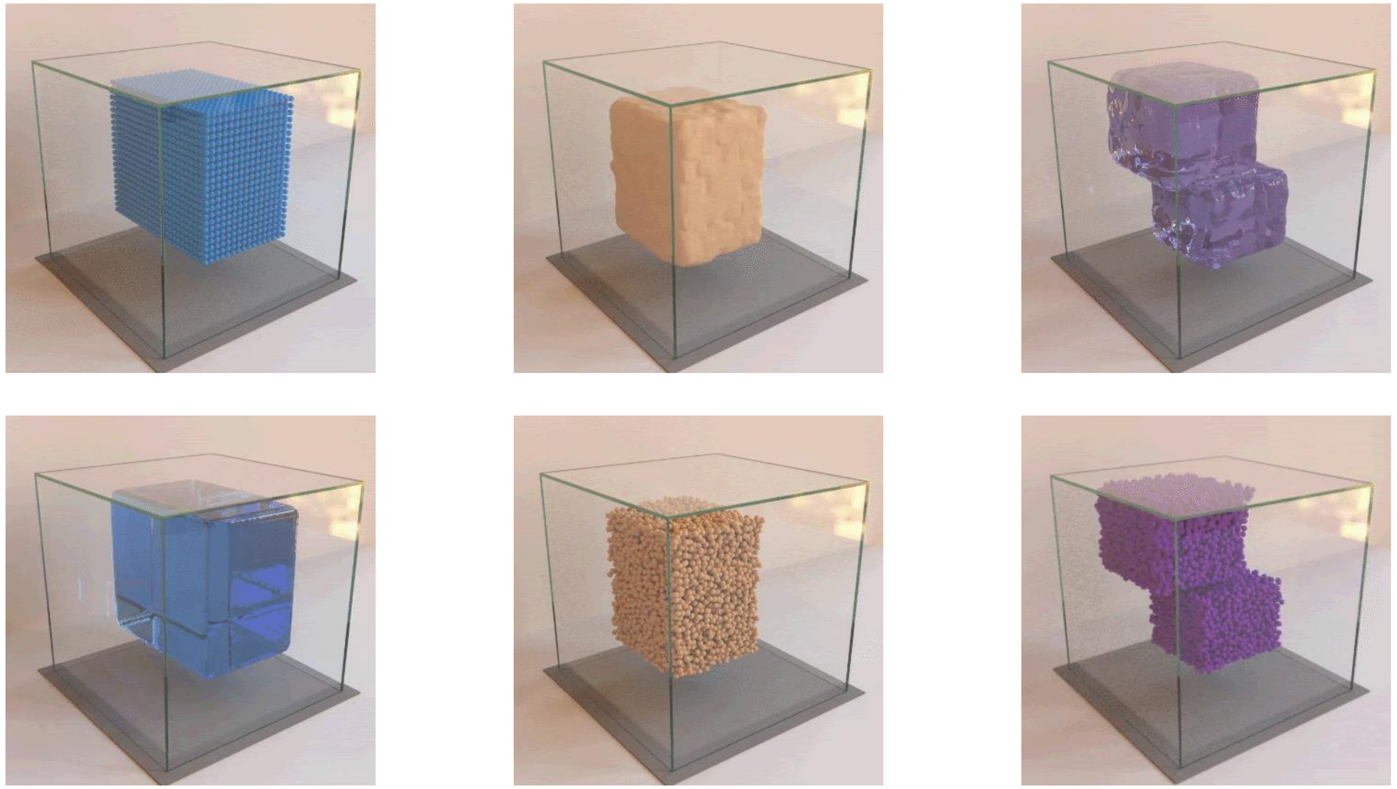





Learning to Simulate Complex Physics with Graph Networks, ICML 2020

Dynamic predictions – Learning Simulation

- Simulating complex fluids and other materials:

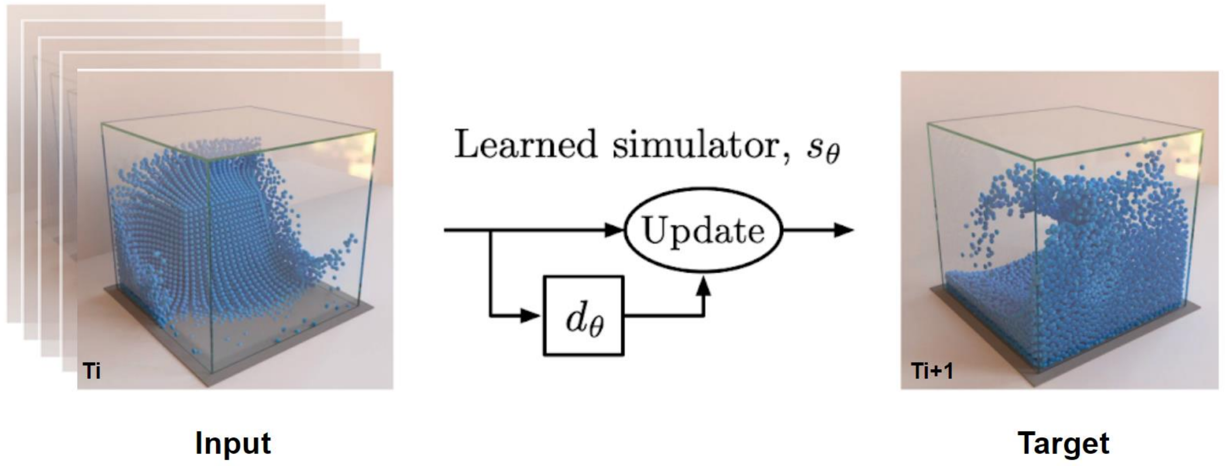


Learning to Simulate Complex Physics with Graph Networks, ICML 2020

Use historical particle information

- During training, we are given **particle properties** (position, velocity …) for a time period $0 - T$
  - Equal and discrete time interval
- We **sample** batches of particle states at consecutive time steps
- Historical particle information

Multiple instances per minibatch



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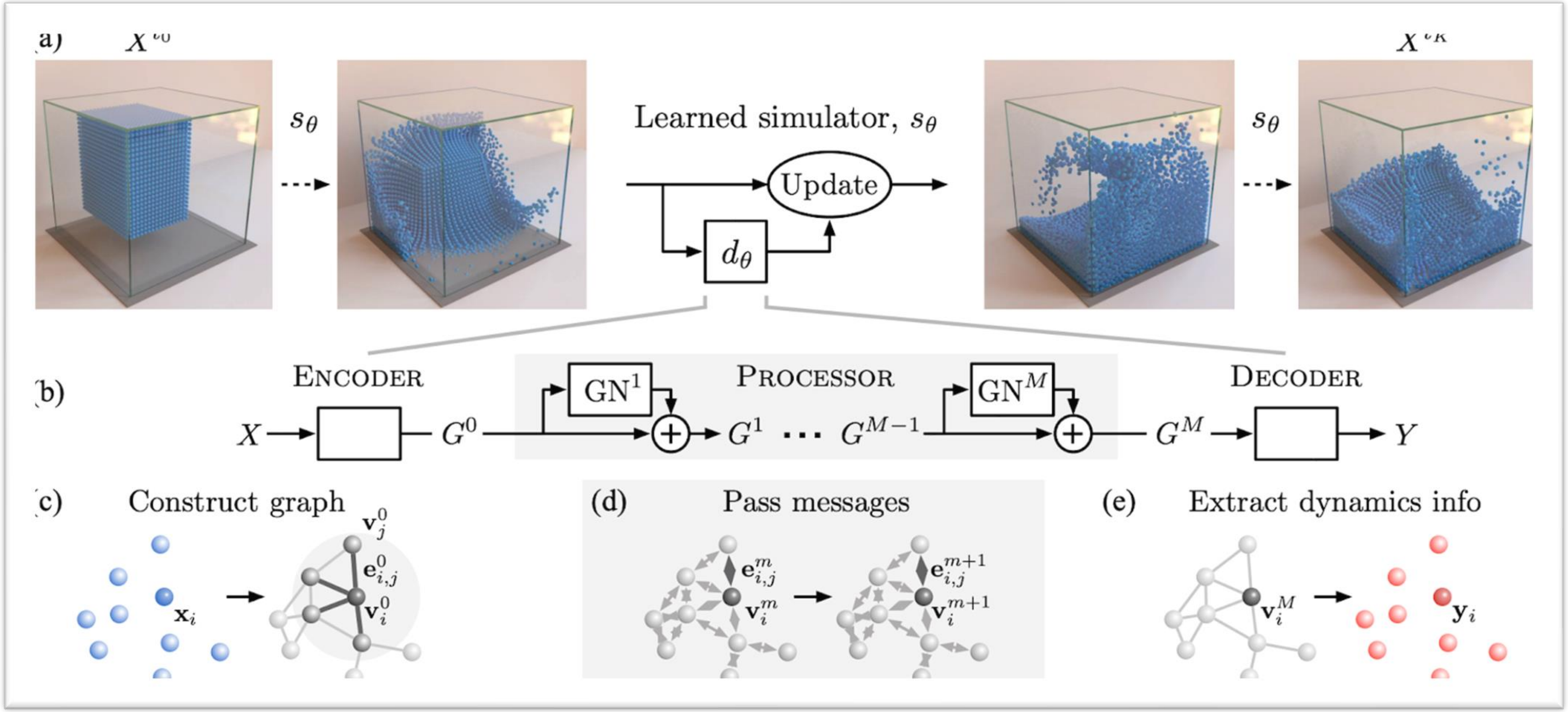
Simulation Architecture



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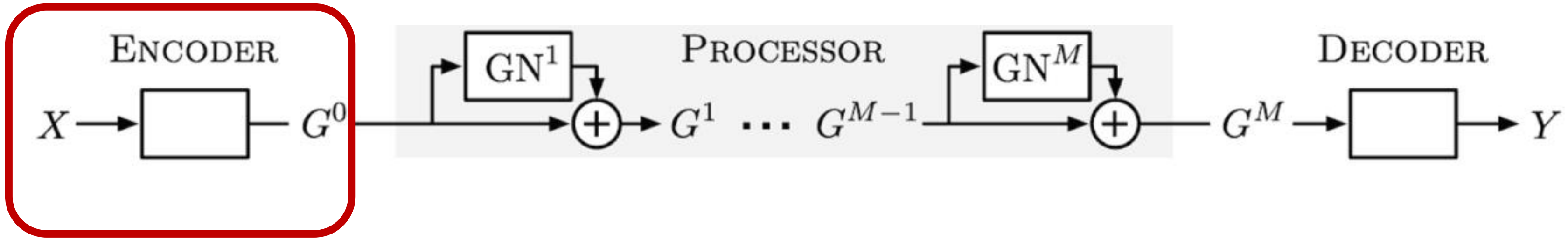
Graph Network Simulator (GNS) Model

Encoder

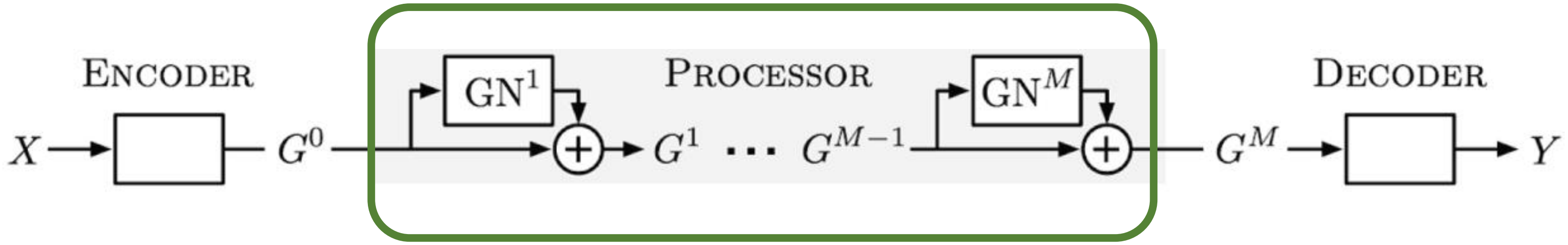


- Node input features:
  - Position, previous 5 velocities, particle type
- Edge input features: displacements
  - Embed features with MLP
- Construct neighbourhood graph
  - K-nearest neighbor (kNN) edges

Learning to Simulate Complex Physics with Graph Networks, ICML 2020

Graph Network Simulator (GNS) Model

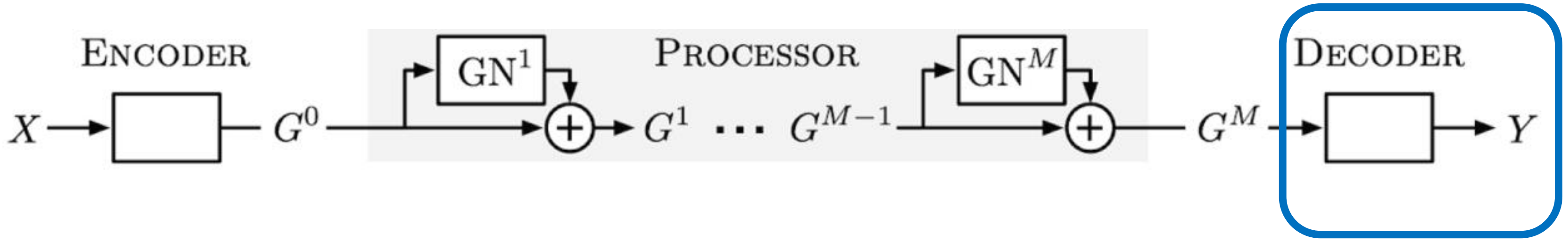
- **Processor**



- Message-passing layers (x10) on the kNN graph
  - Concatenate node and edge features, and compute message function through multi-layer perceptron (MLP)
  - Outputs embeddings for each particle
    - Used to predict next step dynamics

Graph Network Simulator (GNS) Model

Decoder

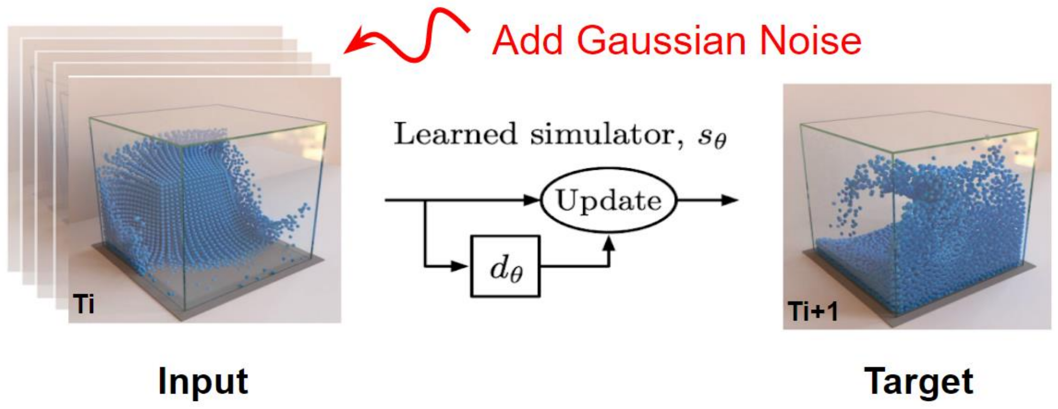


- Decode acceleration
- Feed into Euler integrator to obtain position and velocity
- Sum over L2 Loss for all particles in each pair

Learning to Simulate Complex Physics with Graph Networks, ICML 2020

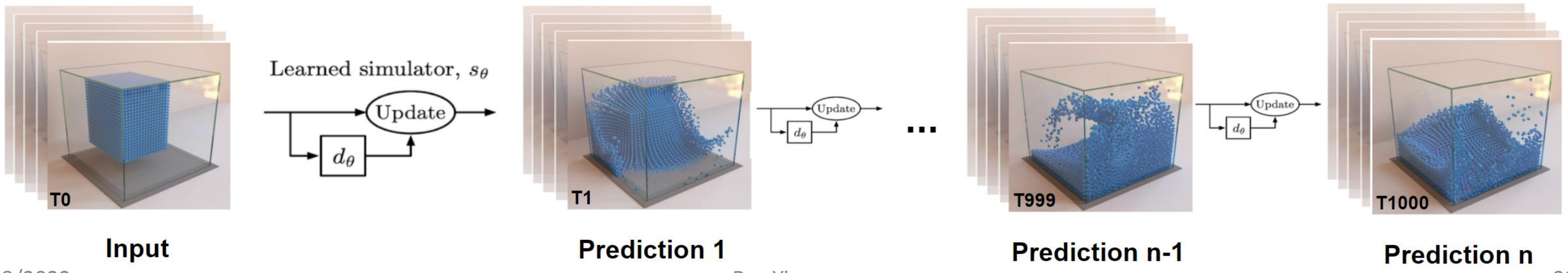
Graph Network Simulator (GNS) Model

- Training time: One-step minibatch training



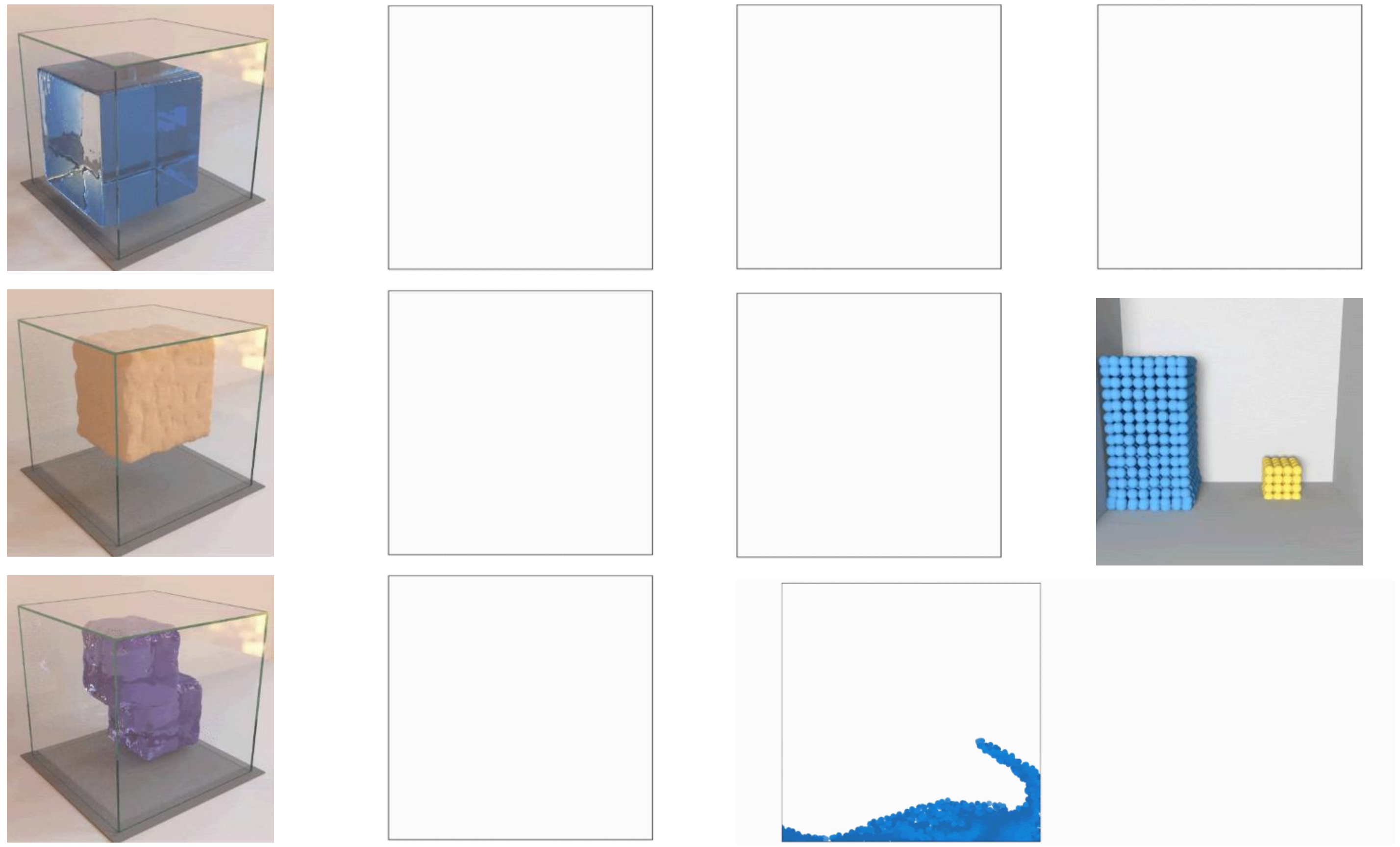
Use noise at training to prevent error accumulation at evaluation

- Test time: 1000s of steps



Generalization

- **Same model and hyperparameters across datasets**



Learning to Simulate Complex Physics with Graph Networks, ICML 2020

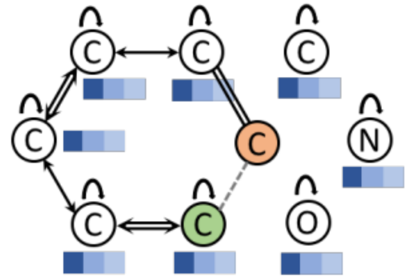
Summary

- In simulation, we are given an initial condition, and use the model to make predictions of the **evolution of the system** over time.
- We model the systems through **particles** (nodes) and **interactions** between particles (edges).
- The model **generalizes** to many different scenarios since the model learns the underlying rules of physical interactions.
- Open question
  - more complex interactions
  - more efficient simulation of large systems

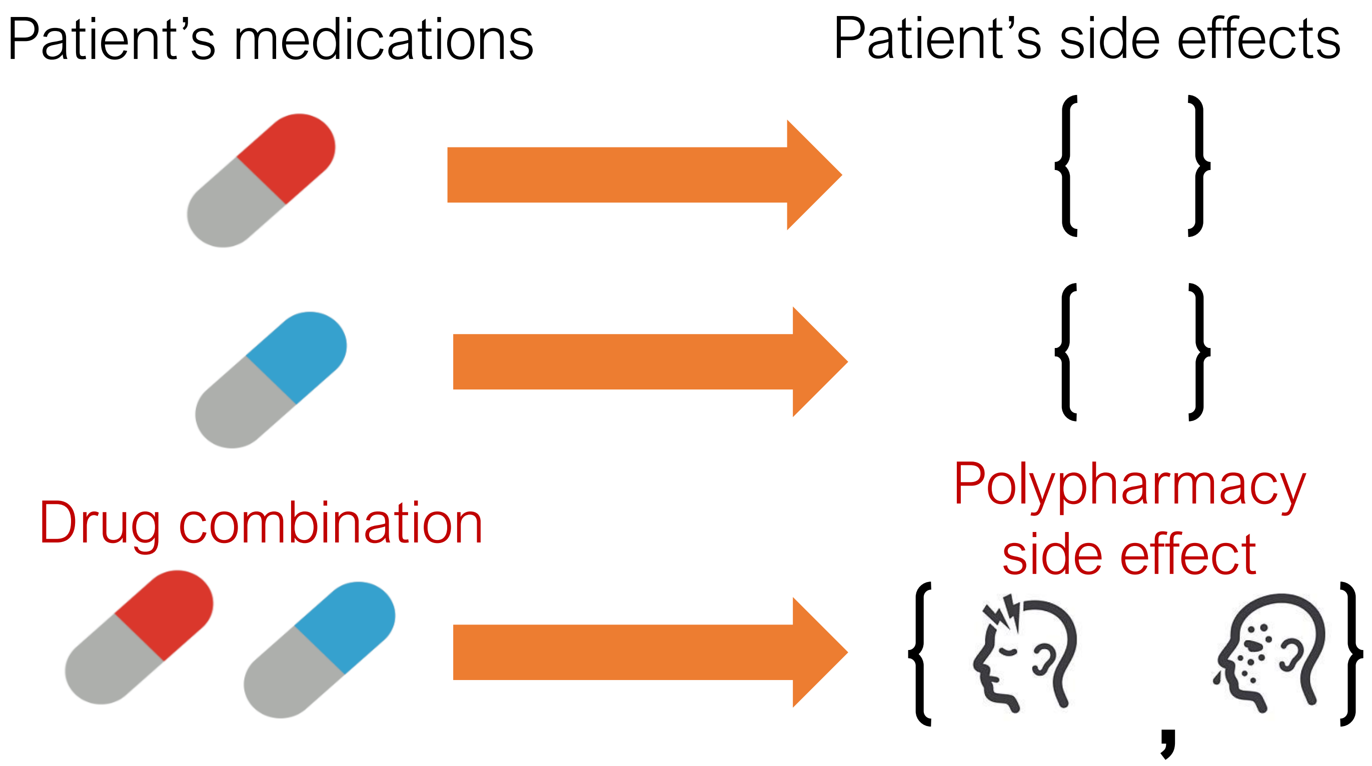
GNN Applications

- **Social Networks**
- **Natural Science**
- **Medicine**
- **Explainability of GNNs**

Drug Side-effects
Molecule Generation



Polypharmacy Side Effects



Polypharmacy: use multiple drugs for a disease

Polypharmacy Side Effects

- Polypharmacy is common to treat complex diseases and co-existing conditions
- High risk of side effects due to interactions
- **15%** of the U.S. population affected
- Annual costs exceed **$177 billion**
- Difficult to identify manually:
    - Rare, occur only in a subset of patients
    - Not observed in clinical testing

Modeling Polypharmacy Side Effects with Graph Convolutional Networks, Bioinformatics 2018

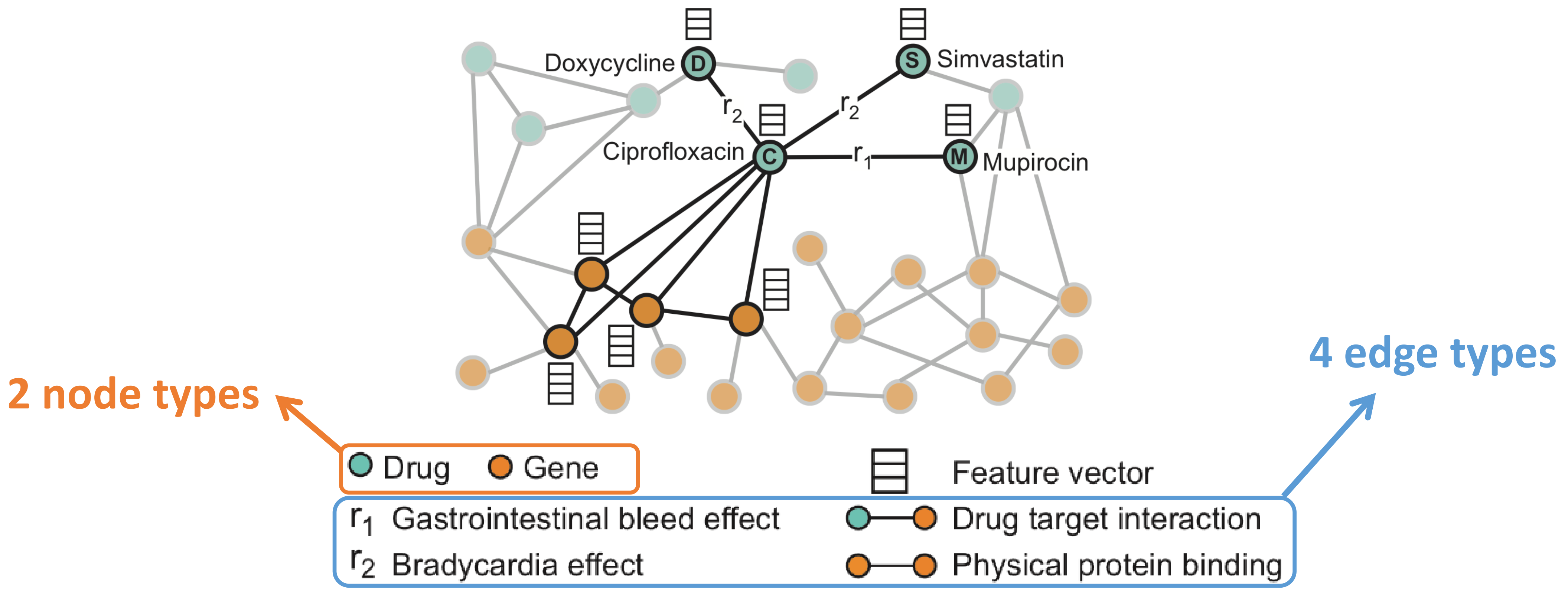
Modeling Polypharmacy

- Systematic experimental screening of drug interactions is challenging
- Idea: Computationally screen/predict polypharmacy side effects
  - Use molecular, pharmacological and patient population data
  - Guide translational strategies for combination treatments in patients

Modeling Polypharmacy Side Effects with Graph Convolutional Networks, Bioinformatics 2018

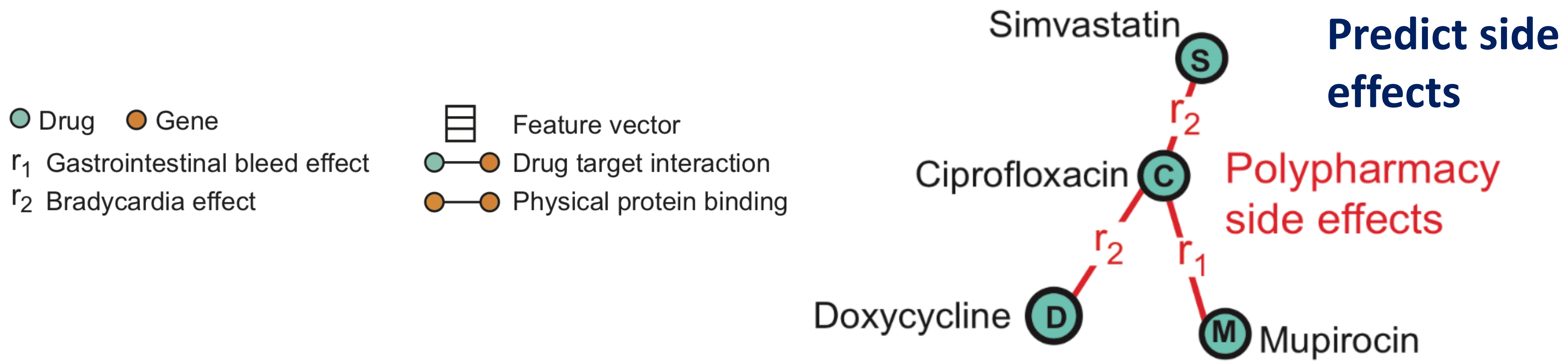
Data: Heterogeneous Graphs

- **Heterogeneous (multimodal) graphs:** graphs with different node types and/or edge types



Task Description

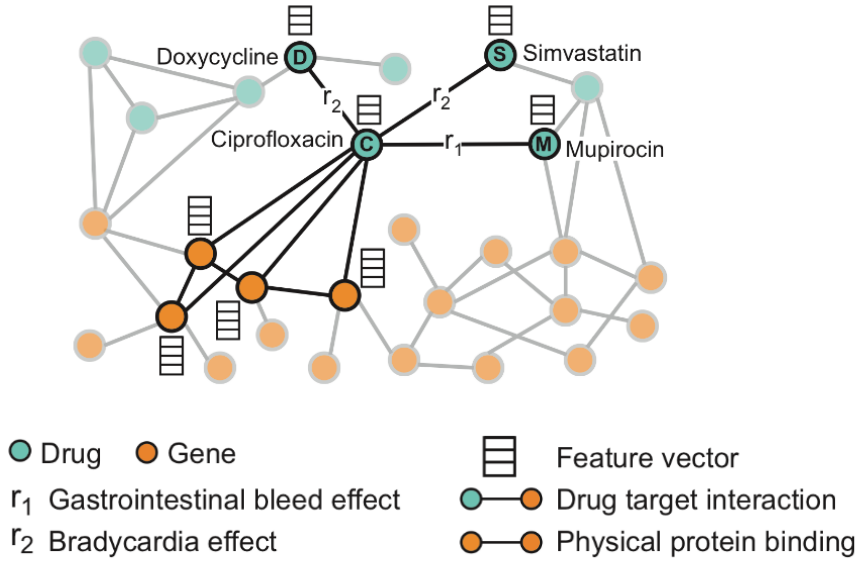
- Predict labeled edges between drugs nodes
  - i.e., predict the likelihood that an edge (c, r_2, s) exists between drug nodes c and s
  - Meaning: Drug combination (c, s) leads to polypharmacy side effect r_2



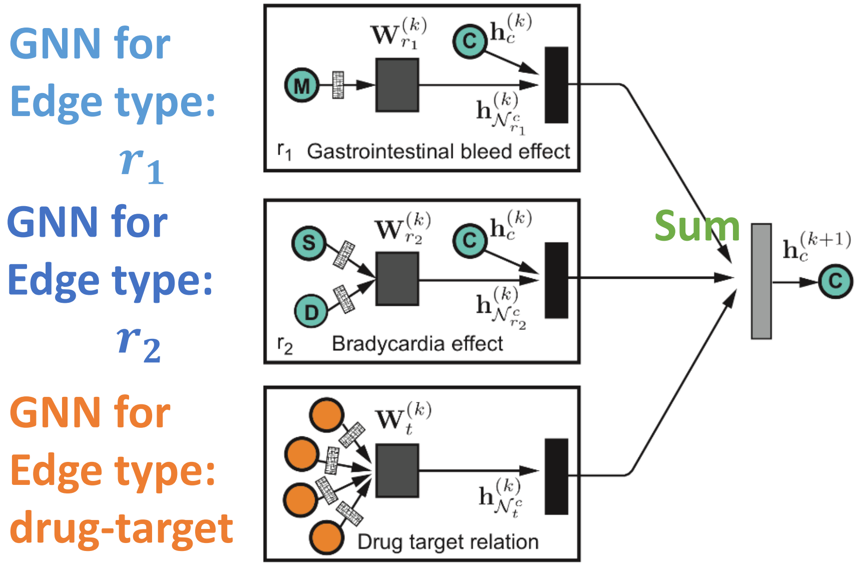
Modeling Polypharmacy Side Effects with Graph Convolutional Networks, Bioinformatics 2018

Model: Heterogenous GNN

- **Key Insight:** Compute GNN messages from each edge type, then aggregate across different edge types
  - **Input:** heterogenous graph
  - **Output:** node embeddings



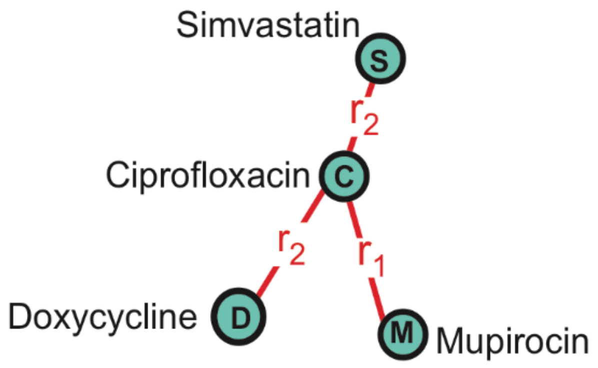
One layer of Heterogeneous GNN



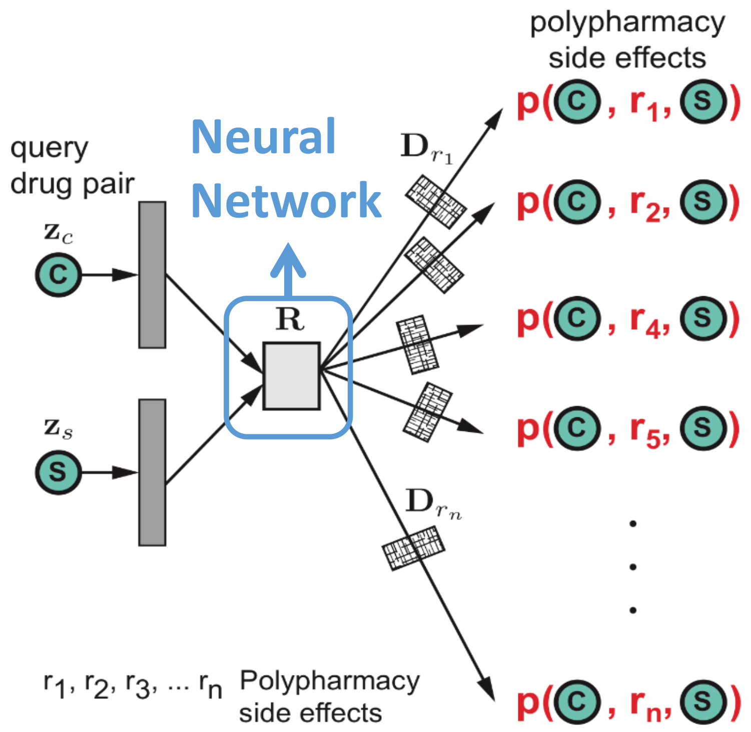
Modeling Polypharmacy Side Effects with Graph Convolutional Networks, Bioinformatics 2018

Making Edge Predictions

- **Inference:** Use pair of computed node embeddings to make edge predictions
  - **Input:** Node embeddings of query drug pairs
  - **Output:** predicted edges



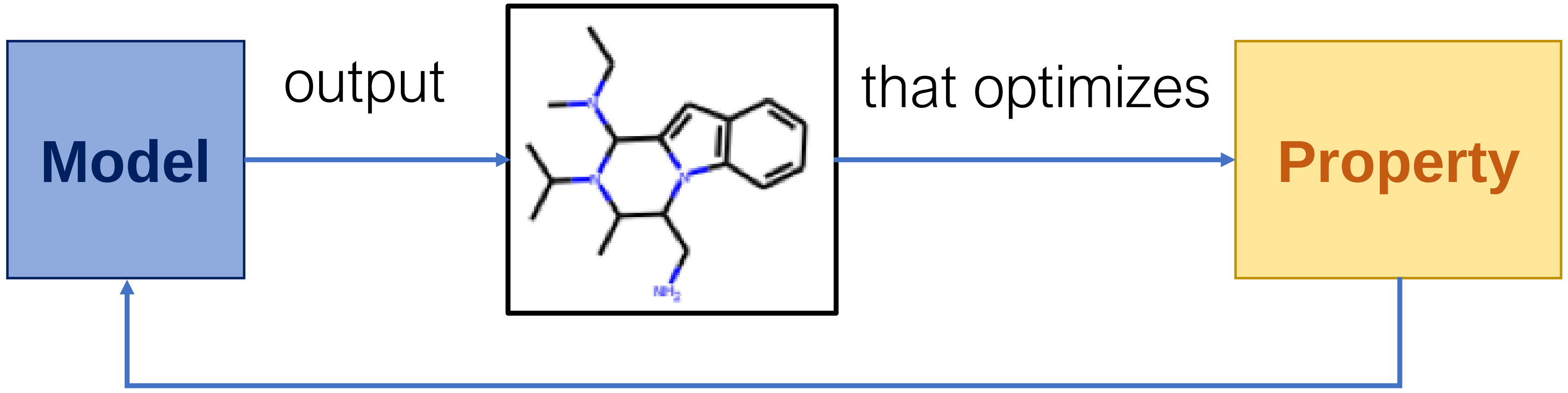
Predict possible edges with NN



Modeling Polypharmacy Side Effects with Graph Convolutional Networks, Bioinformatics 2018

Application: Drug Discovery

Question: Can we learn a model that can generate **valid** and **realistic** molecules with **optimized** property scores?



e.g., `drug_likeness=0.95`

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

Goal-Directed Graph Generation

The goal is to generate graphs that:

- **Optimize a given objective** (High scores)
  - e.g., drug-likeness
- **Obey underlying rules** (Valid)
  - e.g., chemical validity rules
- **Are learned from examples** (Realistic)
  - Imitating a molecule graph dataset

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

The Hard Part:

The goal is to generate graphs that:

- **Optimize a given objective** (High scores)

  Only available at the end of generation

- **Obey underlying rules** (Valid)

  Often not differentiable

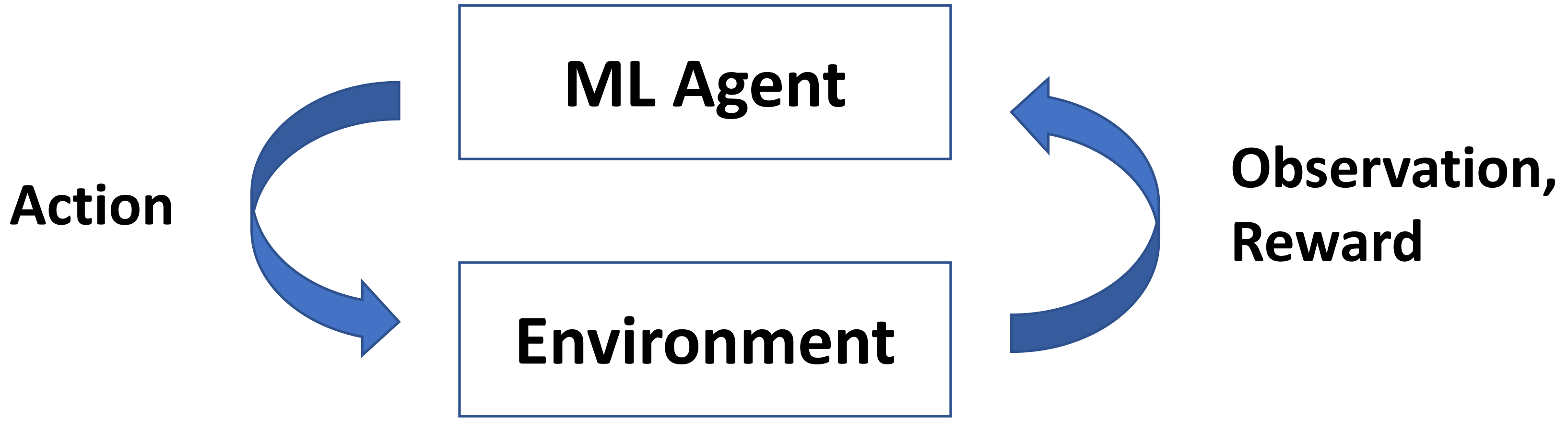
- **Are learned from examples** (Realistic)

  Requires the model to learn the distribution of graph structures

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

Idea: Reinforcement Learning

- An ML agent **observes** the environment, takes an **action** to interact with the environment, and receives positive or negative **reward**
- The agent then **learns from this loop**
- **Key idea**: Agent can directly learn from environment, which is a **blackbox** to the agent



Solution: GCPN

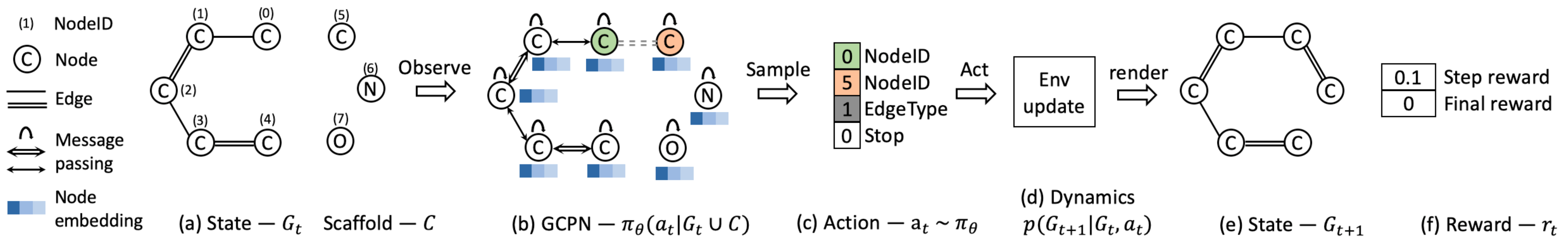
Graph Convolutional Policy Network (GCPN) combines **graph representation** and **reinforcement learning**

Key component of GCPN:

- **Graph Neural Network** captures graph structural information
- **Reinforcement learning** guides the generation towards the desired objectives
  - Generation step-by-step: every step we generate additional edges (bonds) and nodes (atoms) to attach to the generated molecule
  - Delayed reward: we only obtain the final metric (drug-likeness) at the end of the generation process
- **Supervised learning** imitates examples in given datasets

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

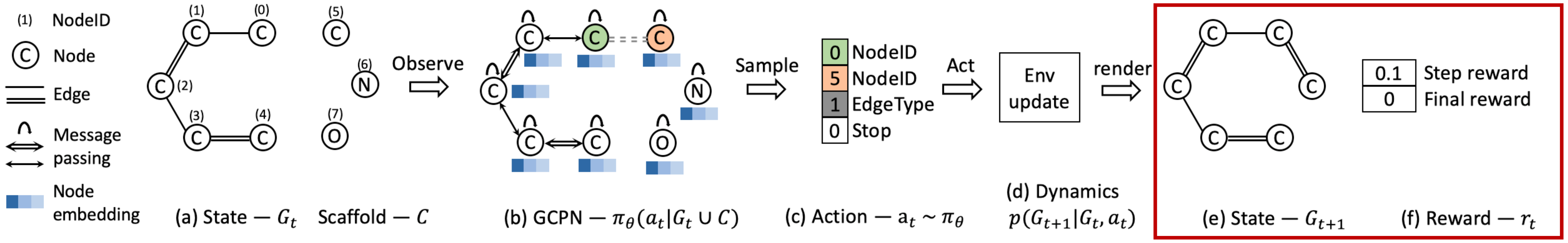
Overview of GCPN



- **(a)** Insert nodes
- **(b,c)** Use GNN to predict which nodes to connect
- **(d)** Take action (check chemical validity)
- **(e, f)** Compute reward

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

How Do We Set the Reward?



- **Step reward:** Learn to take valid action
  - At each step, assign small positive reward for valid action (satisfy valency rules)
- **Final reward:** Optimize desired properties
  - At the end, assign positive reward for high desired property

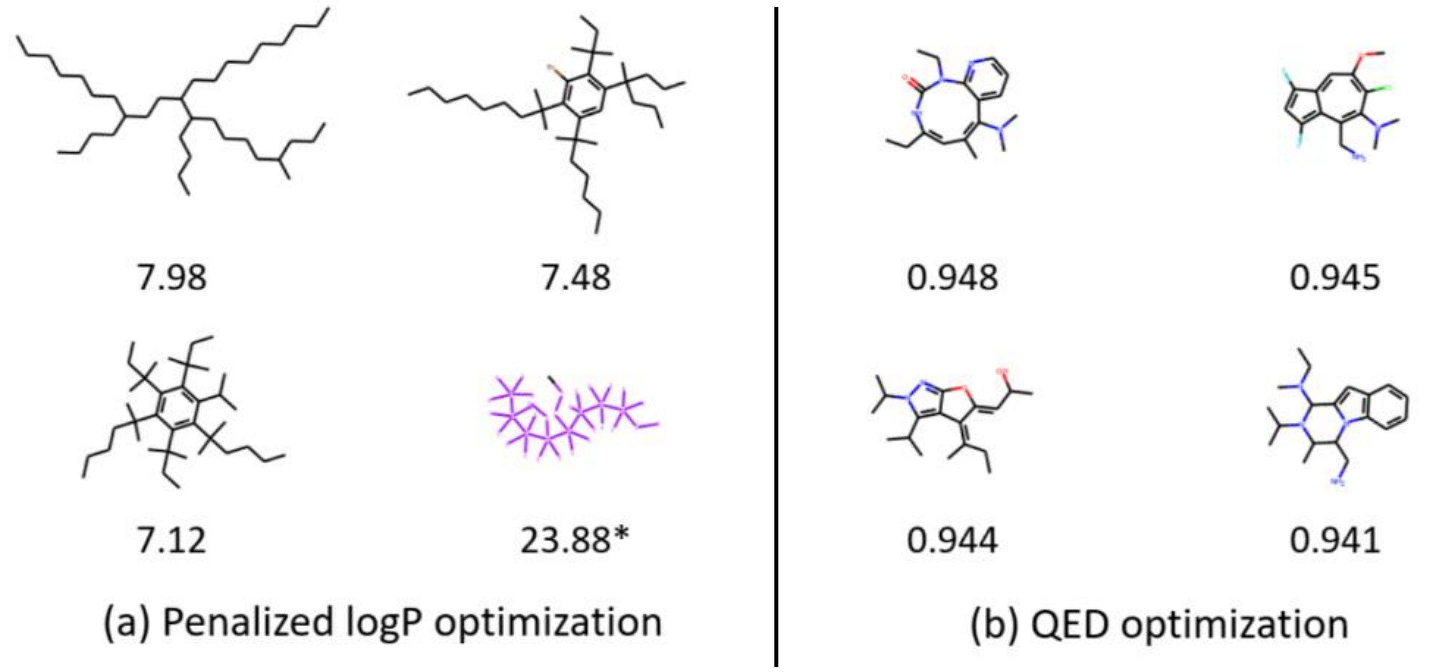
Reward = Final reward + Step reward

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

Qualitative Results

Visualization of GCPN graphs:

- Property optimization Generate molecules with high specified property score

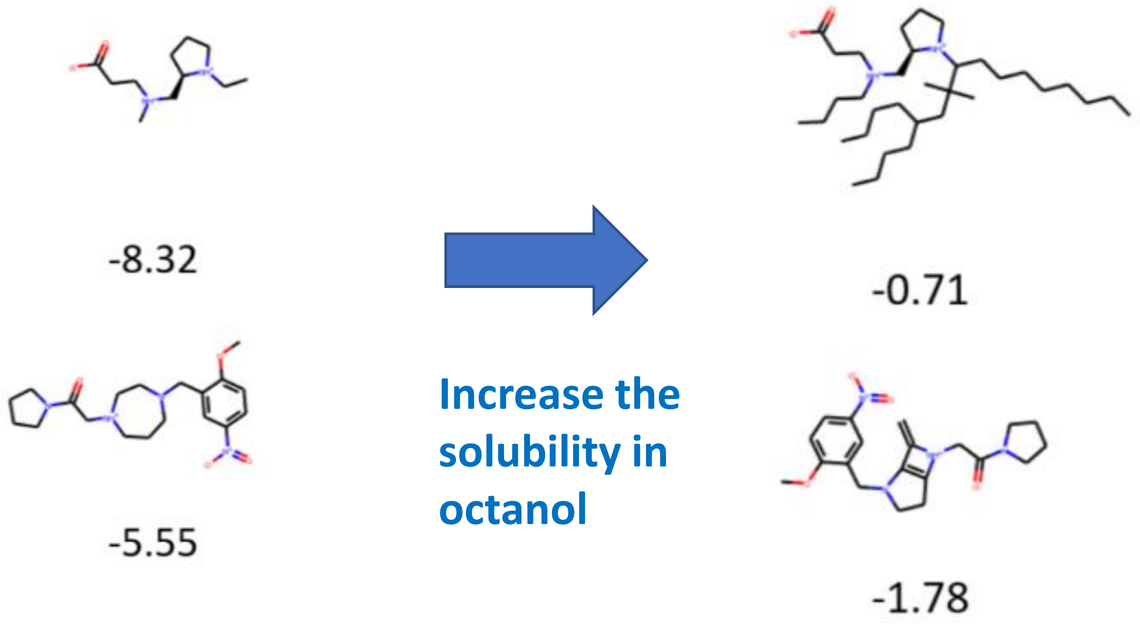


Qualitative Results

Visualization of GCPN graphs:

- Constrained optimization: Edit a given molecule for a few steps to achieve higher property score

Starting structure



Finished structure

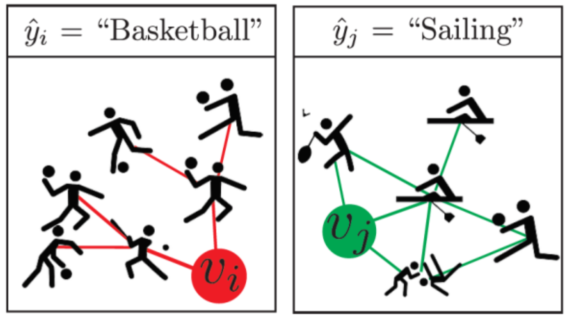
Constrained Optimization of Penalized LogP

Summary

- Many biological applications can be formulated as learning on **heterogeneous** graphs
- An ML algorithm to generate graphs (molecules) is the central problem of drug discovery
  - Imitating a set of given graphs
  - Optimizing graphs towards given goals
  - Other interesting tasks:
    - Retro-synthesis; molecule conformation; drug / molecule property prediction; prediction of the effects of gene knockouts etc.
- Many other interesting tasks!
  - Protein folding, single-cell analysis …

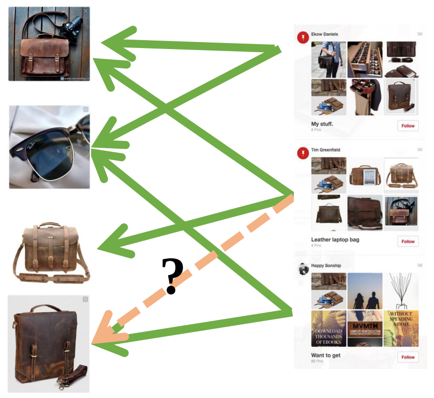
GNN Applications

- **Social Networks**
- **Natural Science**
- **Medicine**
- **Explainability of GNNs**

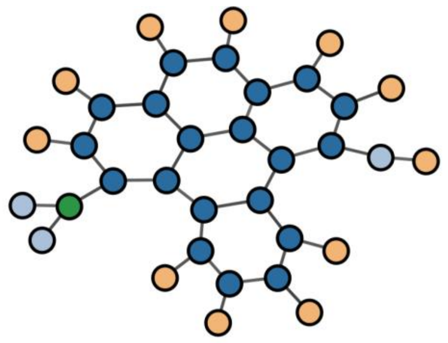


Scalable GNN Explanations

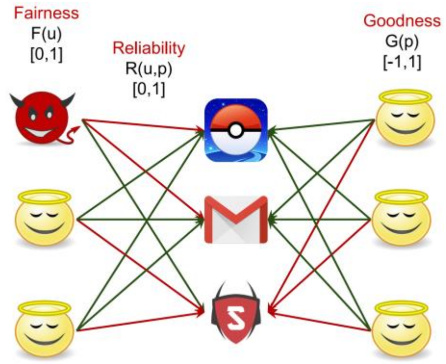
- Many questions after training GNNs:
  - Why is an item recommended to a user? — Explain link prediction
  - Why is the molecule mutagenic? — Explain graph classification
  - Why is the user classified as fraudulent? — Explain node classification
- Being able to answer these questions are important for domain experts



Recommender System



Mutagenic



Anomaly/Abuse Detection

GNNExplainer: Generating Explanations for Graph Neural Networks, NeurIPS 2019

Why is it hard

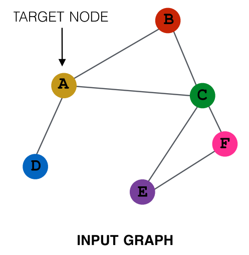
- Explain predictions for multiple tasks
  - Node classification
  - Graph classification
  - Link prediction

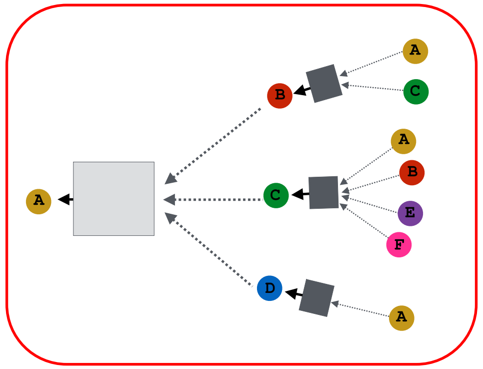
- Model agnostic (*post-hoc*)
  - Can be applied to all models covered in class: GCN, GraphSAGE, GAT etc.

GNNExplainer: Generating Explanations for Graph Neural Networks, NeurIPS 2019

Recap: GNN Framework

- Message Computation
  $m_{ij}^{l} = \mathrm{Msg}(\mathbf{h}_i^{l-1}, \boxed{\mathbf{h}_j^{l-1}}, e_{ij})$ → Previous layer neighbor embedding
- Aggregation
  $M_i^{l} = \mathrm{Agg}\left(\{m_{ij}^{l} | v_j \in \boxed{N_{v_i}}\right)$ →





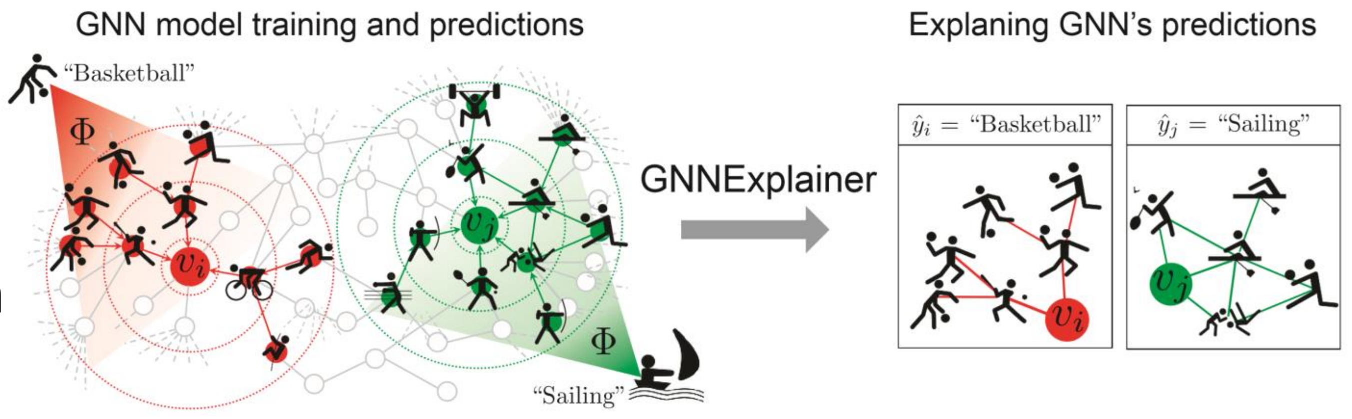
Information used by GNN

- Representation update
  $\mathbf{h}_i^{l} = \mathrm{Update}\left(M_i^{l}, \mathbf{h}_i^{l-1}\right)$
- Stack Multiple layers

GNNExplainer: Generating Explanations for Graph Neural Networks, NeurIPS 2019

Model Explanation

- **Training time:**
  - Optimize GNN on training graphs
  - Save the trained model
- **Test time:**
  - Explain predictions made by th GNN
  - On unseen instances (nodes, edges, graphs)

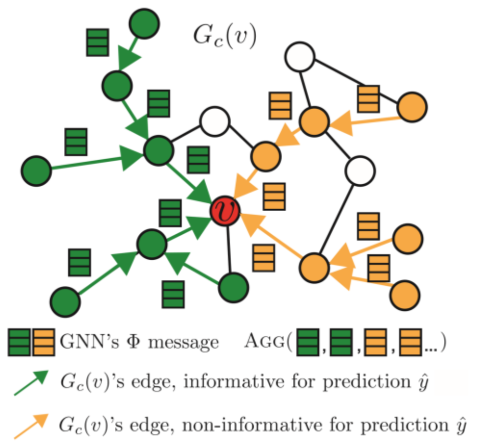


GNNExplainer: Generating Explanations for Graph Neural Networks, NeurIPS 2019

GNNExplainer

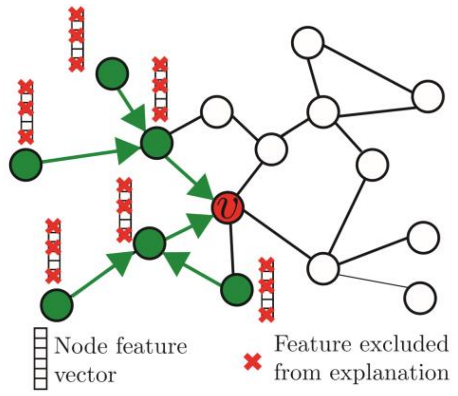
- Message passing structure
- The importance of node features
- Explain both aspects simultaneously

- To explain a given node, learn
  - Important edges in its neighborhood
  - Important node feature dimensions
- Mutual information objective



$G_c(v)$
v
GNN's Φ message
AGG(…)
$G_c(v)$'s edge, informative for prediction $\hat{y}$
$G_c(v)$'s edge, non-informative for prediction $\hat{y}$

Structural explanation



Feature explanation

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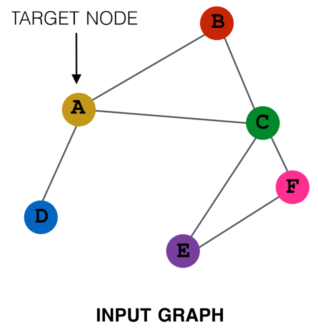
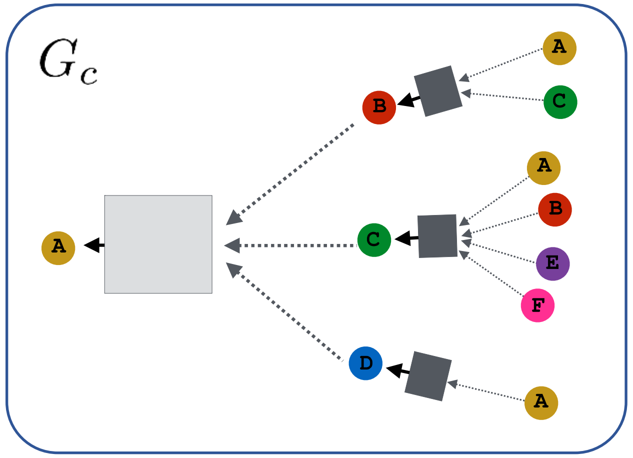
GNN-Explainer Input

- Consider node classification task:





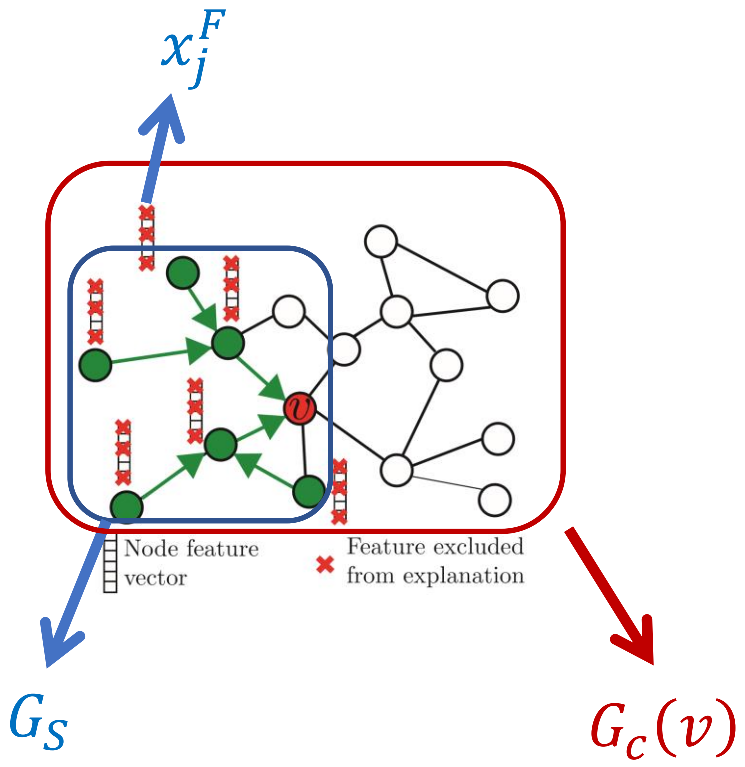
Suppose GNN predicts label $\hat{y}$ for node v

- Input computation graph: $G_c(v)$
- Adjacency matrix: $A_c(v) \in \{0,1\}^{n\times n}$
- Node Feature: $X_c(v) = \{x_j | v_j \in G_c(v)\}$

GNN-Explainer Output

- GNN model ϕ learns $P_\phi(Y \mid G_c(v), X_c(v))$
- Y denotes predicted label of v
- **GNNExplainer** outputs (G_S, X_S^F)

- G_S is a small subgraph of $G_c(v)$ (omit v)
- $X_S^F = \{x_j^F \mid v_j \in G_S\}$ are features for G_S
- Mask F masks out unimportant dimensions



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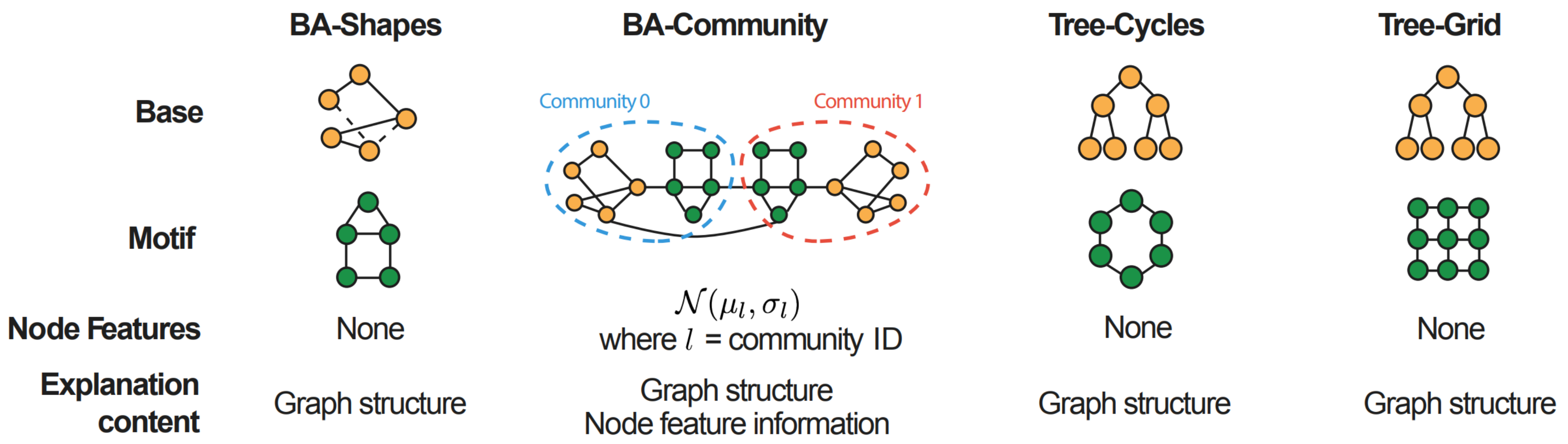
Experiments

- Synthetic task: is a node part of a motif?



	BA-Shapes	BA-Community	Tree-Cycles	Tree-Grid
Node Features	None	$\mathcal{N}(\mu_l, \sigma_l)$ where l = community ID	None	None
Explanation content	Graph structure	Graph structure Node feature information	Graph structure	Graph structure

- Real-world social networks, molecules
    - Graph classification

Explainability Method Comparison

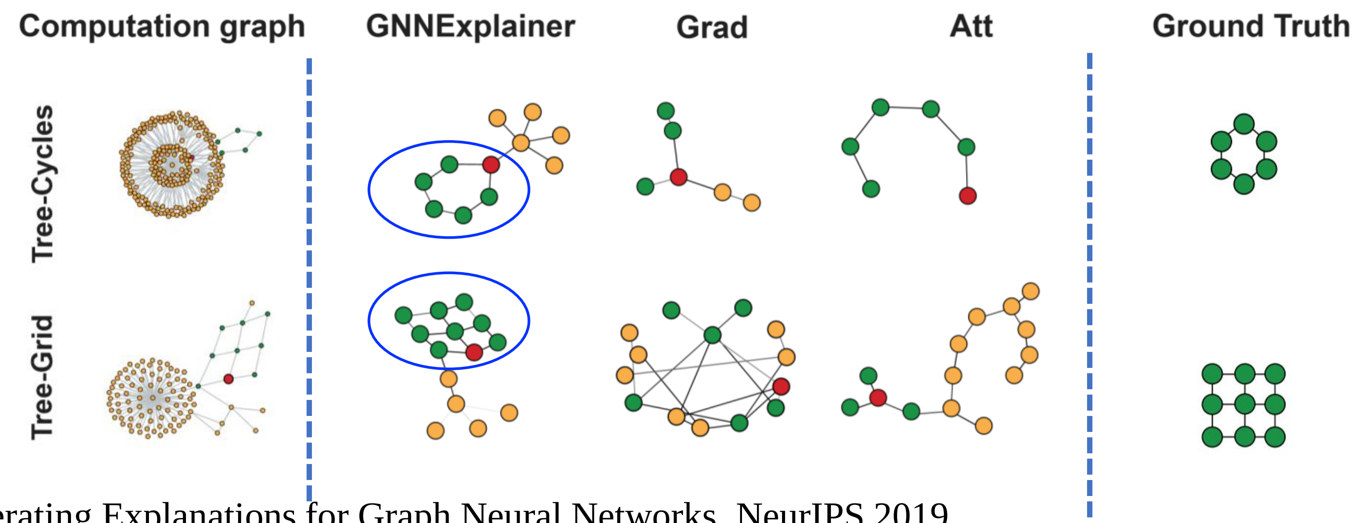
- GNN saliency map based on gradients
  - Large gradient: more important

- Graph Attention Networks (GAT)
  - Edge importance indicated by attention
  - Average attention weights across layers

GNNExplainer: Generating Explanations for Graph Neural Networks, NeurIPS 2019

GNNExplainer

- Explain node classification using GCN
- Base: **Barabasi-Albert Graph**; addon: **Cycle, Grid**



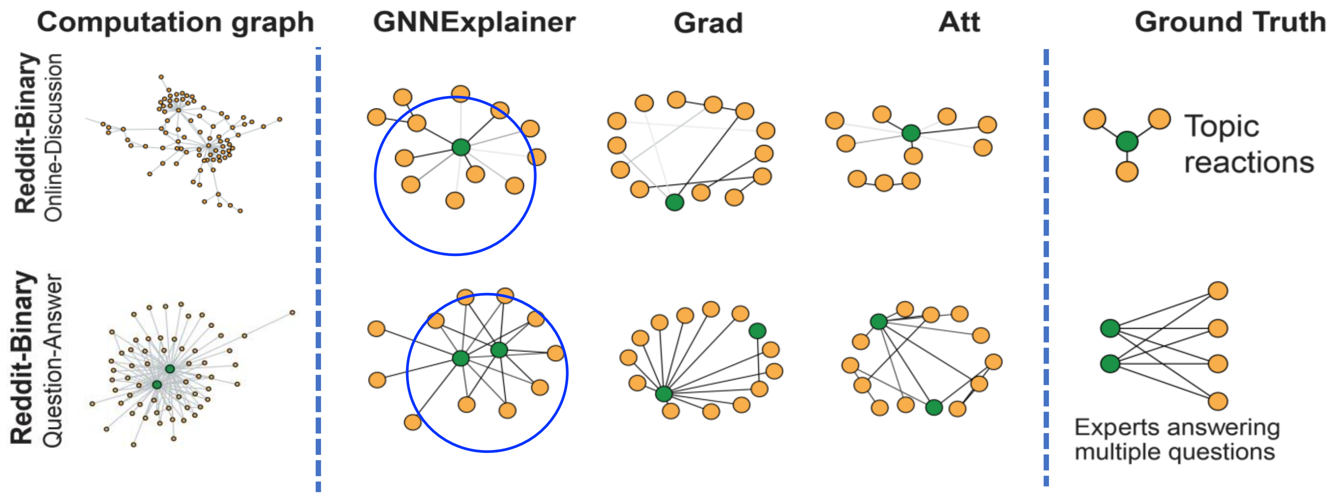
GNNExplainer: Generating Explanations for Graph Neural Networks, NeurIPS 2019

GNNExplainer

Graph Classification

Reddit-Binary: 2000 threads, 2 classes

Discussion community vs. QA community



GNNExplainer: Generating Explanations for Graph Neural Networks, NeurIPS 2019

Conclusion

- We have covered a variety of graph learning applications, in domains including **online social networks**, **natural sciences** and **medicine**.
- Many of the problems were not always formulated as a graph problem!
- Interesting directions to explore
  - Novel ways to **model** problems through the angle of graph learning
  - **Scalable GNN algorithms** for extremely large datasets
  - **AutoML**, **explainability** for GNN applications

Deep Learning on Graph-Structured Data

- New course on **Deep Learning on Graph-structured Data** (Fall 2022)
- The scope will be primarily focused on **theory**, **algorithms** and **applications** related to GNNs and geometric deep learning
    - We also encourage students who primary work on ML for visual, text or other forms of data to explore potential incorporation of graph techniques in their research problems