This Talk

- 1) Node embeddings ✓
  - Map nodes to low-dimensional embeddings.
- 2) Graph neural networks ✓
  - Deep learning architectures for graph-structured data
- 3) Applications 

Part 3: Applications

Outline for This Section

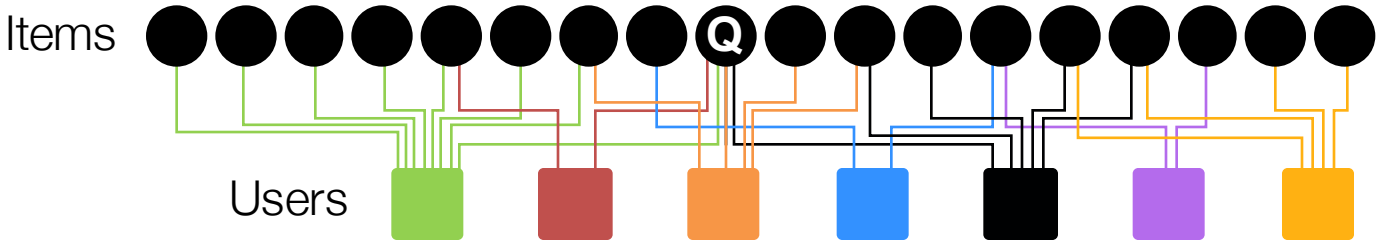
- **Recommender systems**
  - **RW-GCNs**: GraphSAGE-based model to make recommendations to millions of users on Pinterest.
- **Computational biology**
  - **Decagon**: Predicting polypharmacy side-effects with graph neural networks.
- **Practical insights**
  - Code repos, useful frameworks, etc
- **Future directions**

RW-GCNs:
Graph Convolutional Networks for Web-Scale Recommender Systems

Based on material from:

- Ying et al. Graph Convolutional Neural Networks for Web-Scale Recommender Systems. *Under Review.*

Bipartite Graph for RecSys



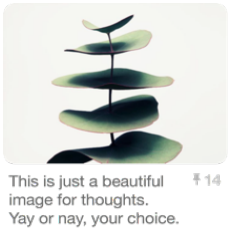
- Graph is dynamic: need to apply to new nodes without model retraining
- Rich node features: content, image

Graph Neural Nets for RecSys

- **Two sources of information in traditional recommender systems:**
  - **Content features:** User and item features, in the form of images, categories *etc.*
  - **Network structure:** User-item interactions, in the form of graph/network structure.
- Graph neural networks naturally incorporate both!!

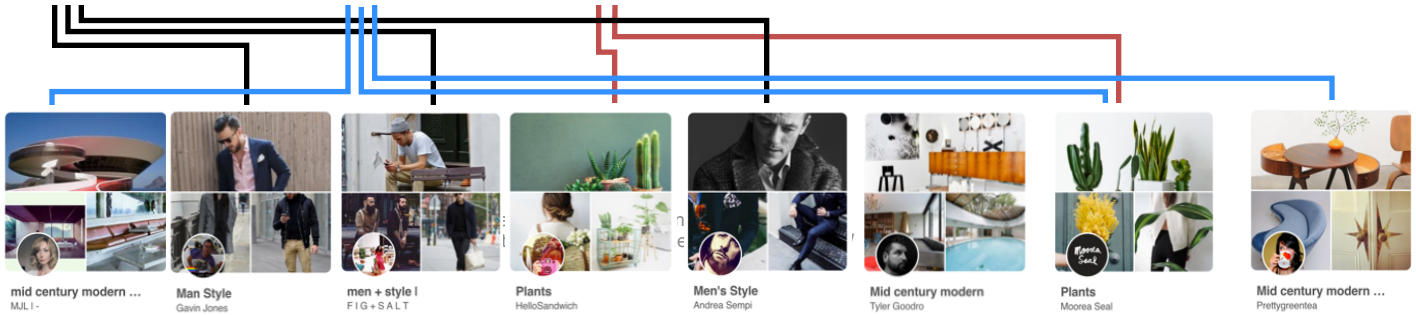
Application: Pinterest

Human curated collection of pins



Pins: Visual bookmarks someone has saved from the internet to a board they've created.

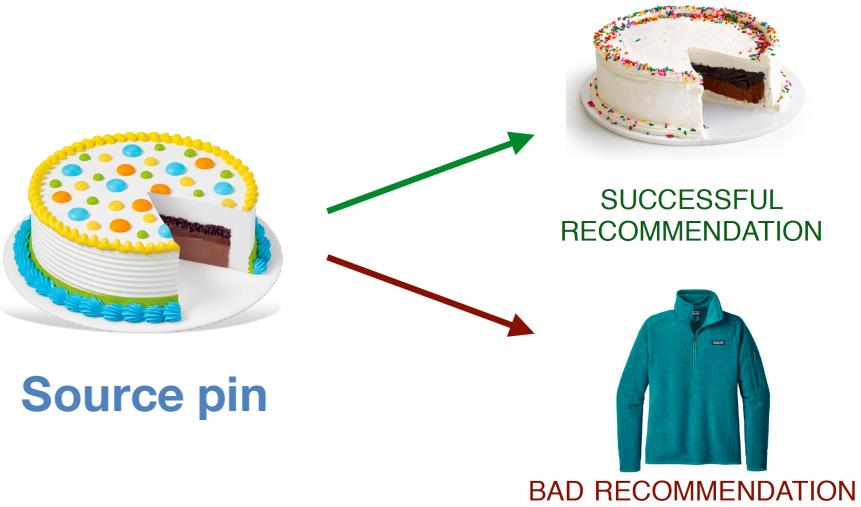
Pin features: Image, text, link



Boards

Application: Pinterest

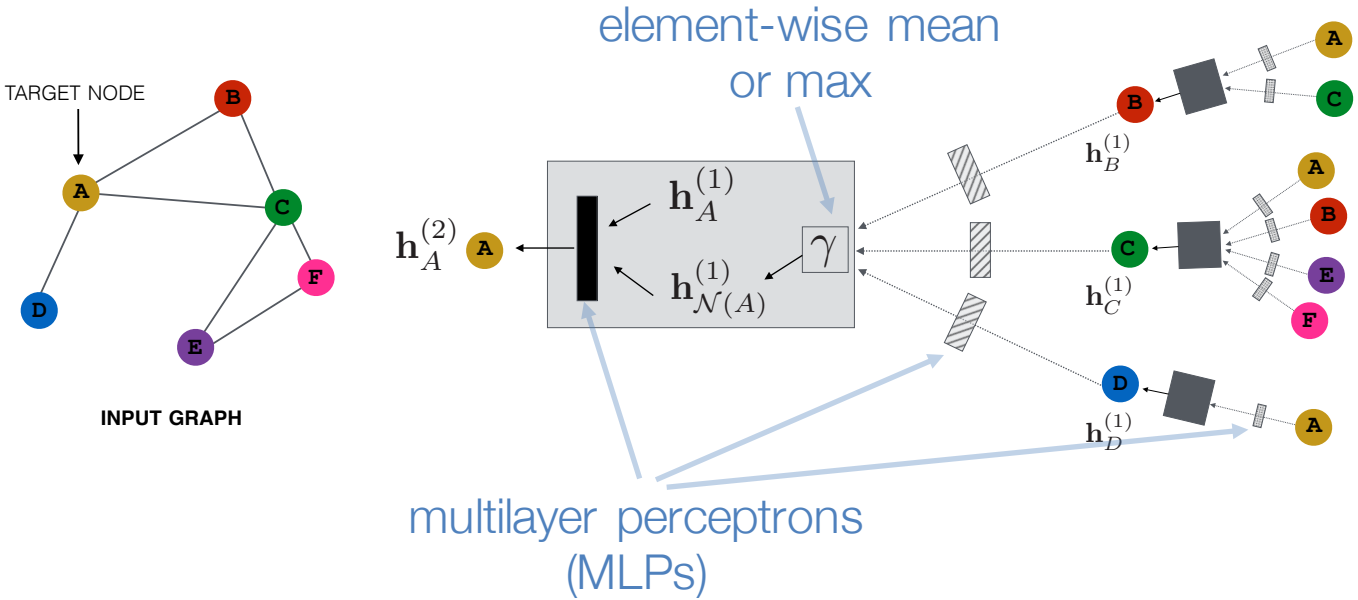
Task: Recommend related pins to users.



- **Challenges:**
  - **Massive size:** 3 billion pins and boards,16 billion interactions
  - **Heterogeneous data:** Rich image and text features

RW-GCN Overview

- Random-Walk GCNs = RW-GCNs
- Architecture is an extension of GraphSAGE:



Overview of RW-GCN Pipeline

1. **Collect** billions of training pairs from user logs.
2. **Train** system to generate similar embeddings for training pairs.
3. **Generate** embeddings for all pins.
4. **Make recommendations** using nearest neighbor search in the embedding space (in real time).

RW-GCN Overview

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

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

set of training pairs from user logs

"positive"/true training pair

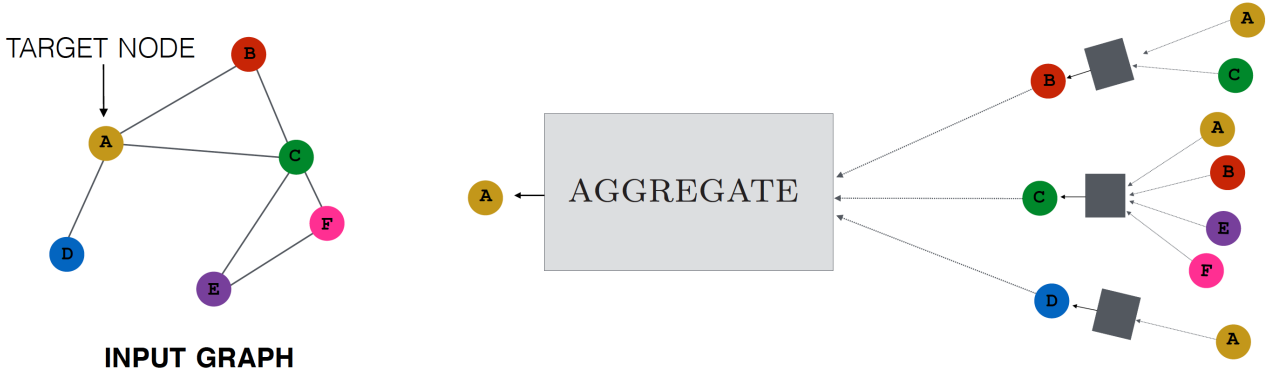
"negative" sample

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

RW-GCN Efficiency

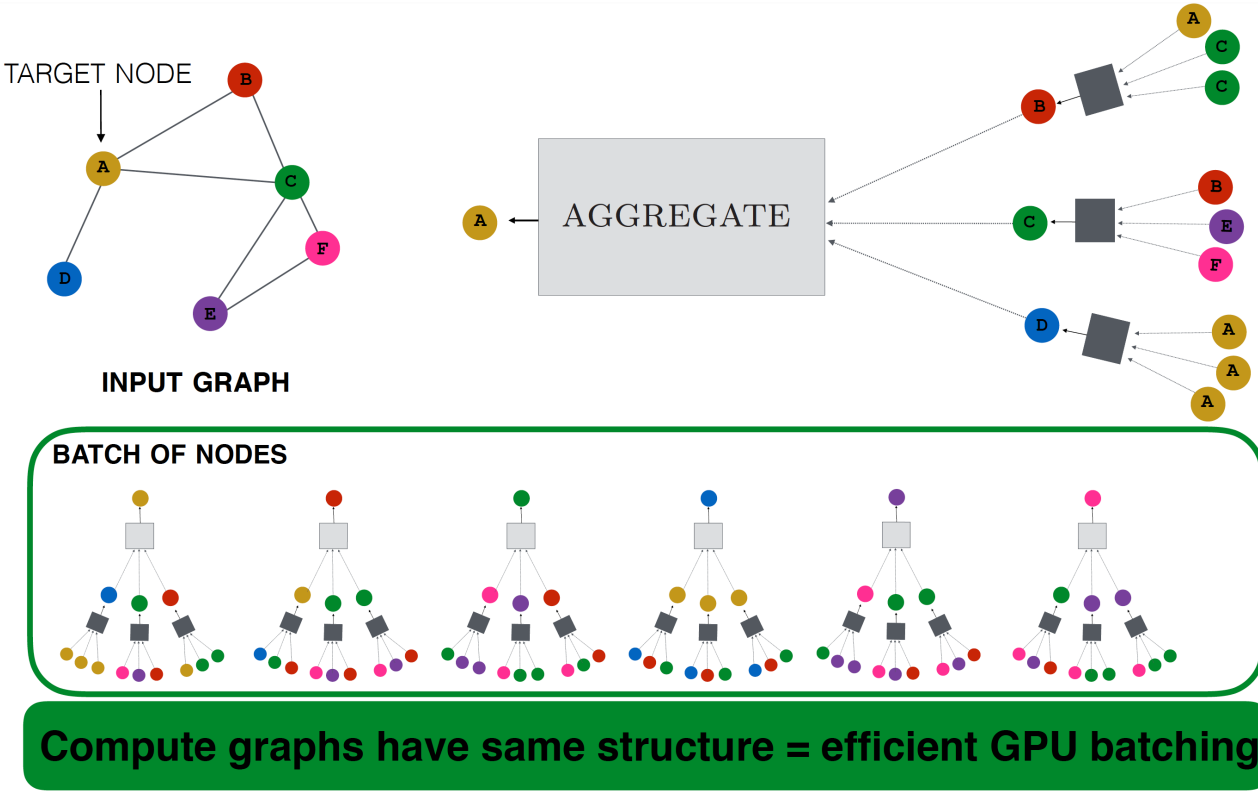
- **10,000X larger than any previous graph neural network application.**
- **Key innovations:**
  1. Sub-sample neighborhoods for efficient GPU batching
  2. Producer-consumer training pipeline
  3. Curriculum learning for negative samples
  4. MapReduce for efficient inference

Neighborhood Subsampling



Every node has unique compute graph. Can't batch on GPU!

Neighborhood Subsampling



Neighborhood Subsampling

- **Random-walk**-based neighborhood
  - Approximates personalized PageRank (PPR) score.
  - Sampled neighborhood for a node is a list of nodes with the top-K PPR score.
- **Advantage:**
  - Algorithm finds the most relevant nodes(item) for high degree nodes

Producer-consumer Pipeline

- Select a batch of pins
- Run random walks
- Construct their computation graphs

CPU (producer)

- Multi-layer aggregations
- Loss computation
- Backprop

GPU (consumer)

Curriculum Learning

- **Idea:** use harder and harder negative samples
- Include more and more hard negative samples for each epoch

Source pin

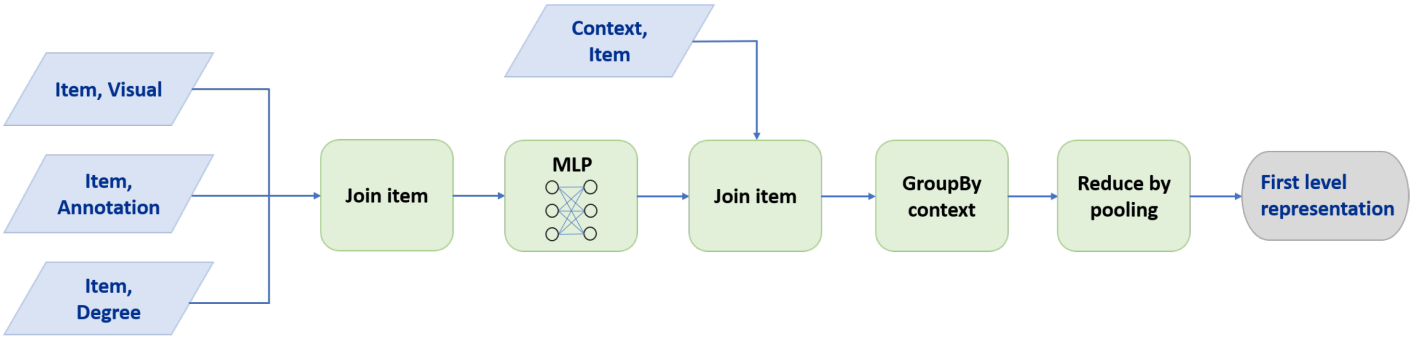
Positive

Easy negative

Hard negative

MapReduce Inference

- How to efficiently infer representations on nodes we have not seen during training time?
- **Key insight**: avoid repeated computation by sharing computation in MapReduce layers!

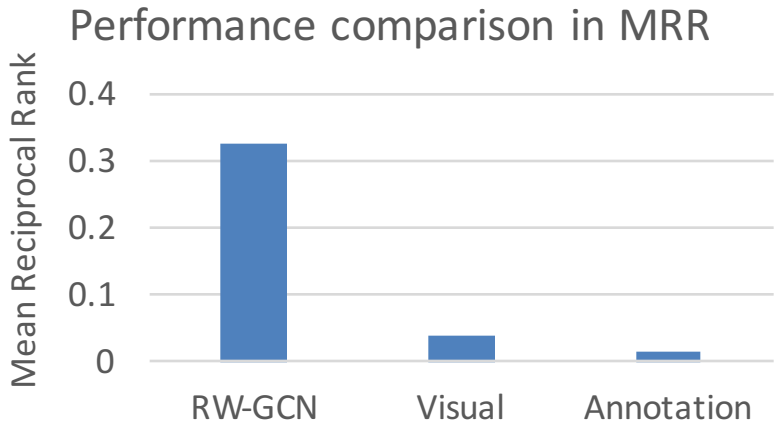


RW-GCN Performance

- **72% better recommendation quality than standard GraphSAGE model.**
- **Key innovations:**
  1. **Weigh importance** of neighbors according to approximate PPR score.
  2. **Use curriculum training** to provide harder and harder training examples over time.

RW-GCN Performance

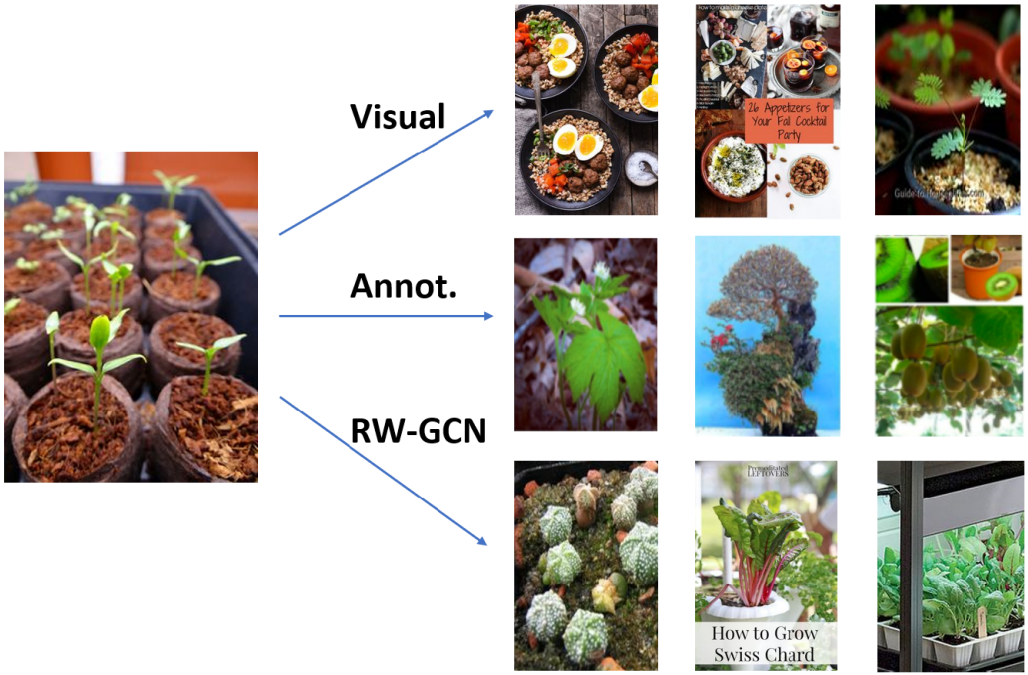
Set-up: Rank true "next-clicked" pin against 10^9 other candidates.



MRR: Mean reciprocal rank of true example.

Baselines: Deep content-based models

Example Recommendations



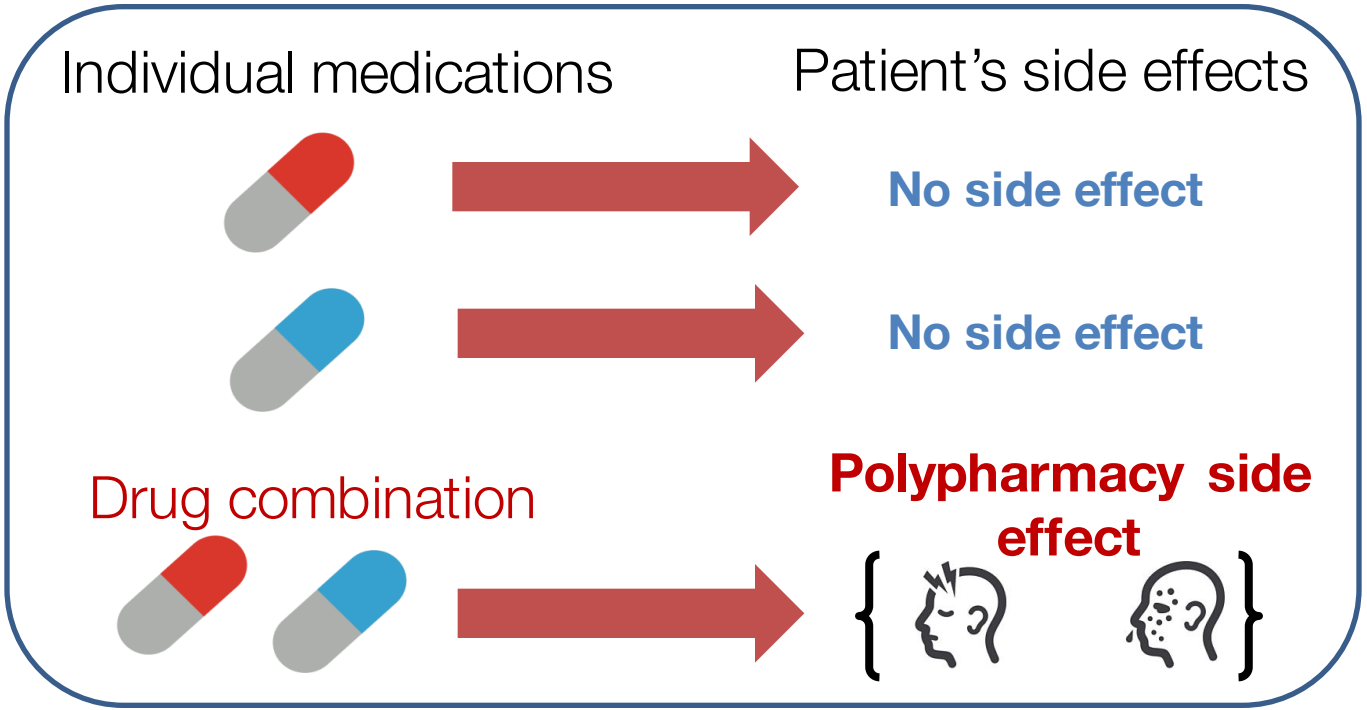
Decagon:
A Graph Convolutional Approach to Polypharmacy Side Effects

Based on material from:

- Zitnik et al. 2018. Modeling polypharmacy side effects with graph convolutional networks. *Bioinformatics & ISMB*.

Polypharmacy Side Effects

Goal: Predict side effects of taking multiple drugs.



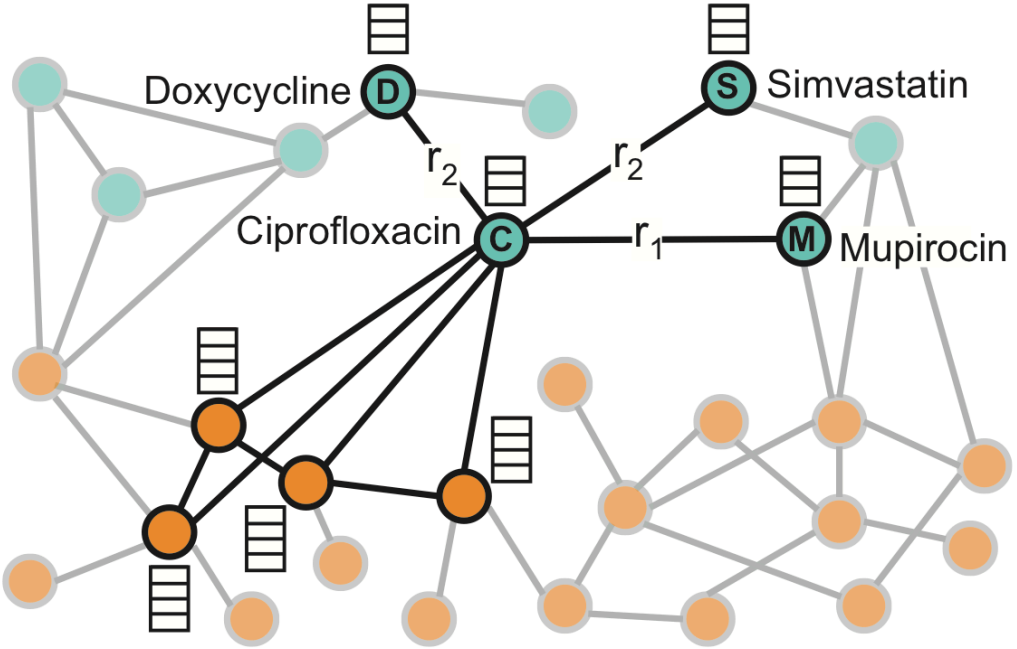
Polypharmacy Side Effects

- 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

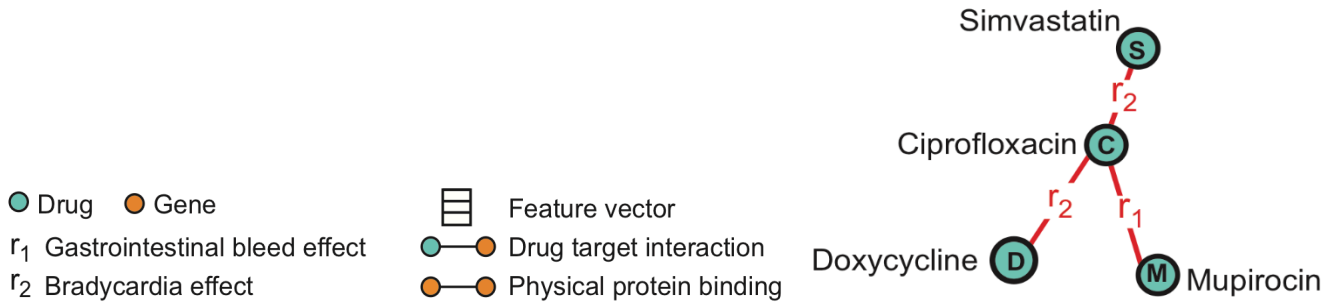
- Systematic experimental screening of drug interactions is challenging
- Idea: Computationally screen/predict polypharmacy side effects
  - Use molecular, pharmacological and patient population data
  - Guide strategies for combination treatments in patients

Data: Heterogeneous Graphs

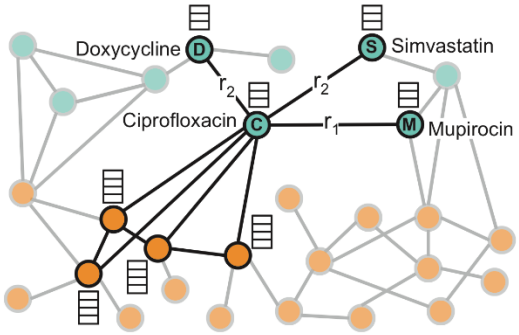


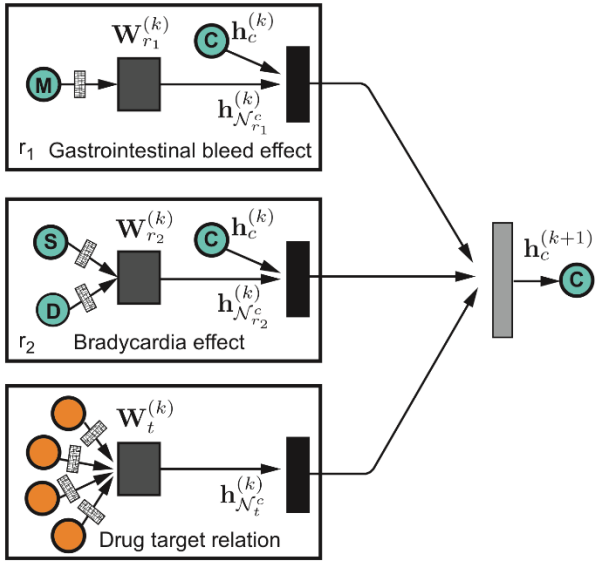
Task Description

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



Neural Architecture: Encoder

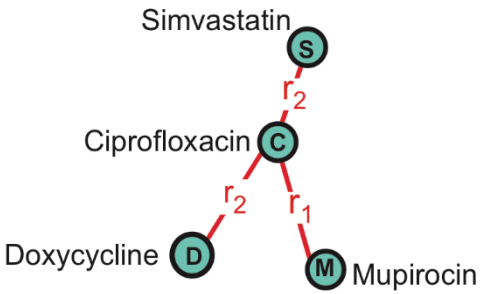


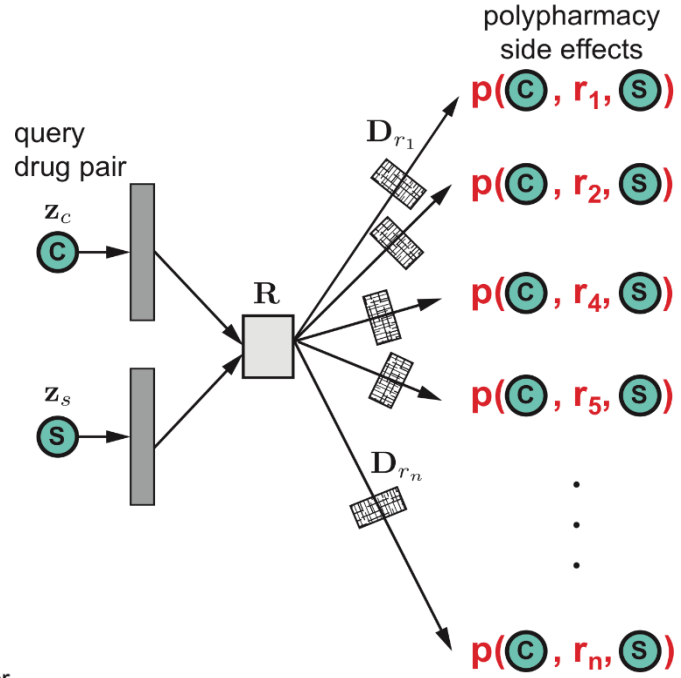


- Input: graph, additional node features
- Output: node embeddings

Drug Gene
r1 Gastrointestinal bleed effect
r2 Bradycardia effect
Feature vector
Drug target interaction
Physical protein binding

Making Edge Predictions





- Input: Query drug pairs and their embeddings
- Output: predicted edges

Drug Gene
r_1 Gastrointestinal bleed effect
r_2 Bradycardia effect

Feature vector
Drug target interaction
Physical protein binding

Experimental Setup

- **Data:**
  - Molecular: protein-protein interactions and drug target relationships
  - Patient data: Side effects of individual drugs, polypharmacy side effects of drug combinations
- **Setup:**
  - Construct a heterogeneous graph of all the data
  - Train: Fit a model to predict known associations of drug pairs and polypharmacy side effects
  - Test: Given a query drug pair, predict candidate polypharmacy side effects

Prediction Performance

	AUROC	AUPRC	AP@50
Decagon (3-layer)	**0.834**	**0.776**	**0.731**
Decagon (2-layer)	0.809	0.762	0.713
RESCAL	0.693	0.613	0.476
Node2vec	0.725	0.708	0.643
Drug features	0.736	0.722	0.679

- Up to 54% improvement over baselines
- First opportunity to computationally flag polypharmacy side effects for follow-up analyses

Practical Insights

GraphSAGE TensorFlow Ex.

- **A quick example:** Using GraphSAGE for a supervised node classification task.
- Key steps:
  1. Preprocess network and training data.
  2. Run GraphSAGE

GraphSAGE TensorFlow Ex.

- Preprocessing

```
from networkx.readwrite import json_graph
import json
import numpy as np

Data = json_graph.node_link_data(G)
with open('data-G.json') as f:
    f.write(json.dumps(data))

class_map = {nodes[i]: labels[i] for i in range(len(nodes))}
with open('data-class_map.json') as f:
    f.write(json.dumps(data))

id_map = {nodes[i]: i for i in range(len(nodes))}
with open('data-id_map.json') as f:
    f.write(json.dumps(data))

np.save(feats, 'data-feats.npy')
```

Save graph

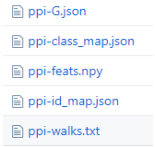
Save labels

Save nodes

Save features

GraphSAGE TensorFlow Ex.

- Example: PPI data (available in GraphSAGE repo)



- Run both training and evaluation (random split of data)

```
python –m graphsage.utils ppi-G.json ppi-walks.txt
python -m graphsage.supervised_train --train_prefix=./ --model=graphsage_mean
```

- Alternative models:
  - gcn, graphsage_seq, graphsage_maxpool
- Easy to customize using Tensorflow

Future Directions

(Sub)graph embedding

- Existing approaches
  - Pool learned node embeddings via element-wise max/mean/sum
  - Add a “virtual” node representing the entire (sub)graph
- Is there better pooling strategy?
  - Handle massive graphs?
  - Learn “coarsened” representations?

Dynamic graphs

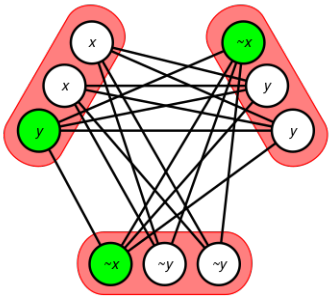
- Many graphs evolve over time:
  - Recommender systems
  - Financial transaction and event graphs
  - Social networks
- Applications:
  - Predict graph evolution
  - Anomaly detection (e.g., fraud)

Dynamic graphs

- Challenges:
  - How to efficiently and incrementally update the learned representations?
  - How to incorporate edge timing?
  - How to “forget” old/irrelevant info?

Combinatorial Applications

- Efficient SAT solvers via graph embeddings (Selsam et al., 2018).
- Learn embeddings of clause and literals (form a bipartite graph
- **Graph embeddings for neural theorem proving?**



Reinforcement Learning

- **Idea:** Allow agents to use node embedding information to make decisions
- **So far**: Used for combinatorial optimization (Dai et al., 2017) and question answering (Das et al., 2018)
- **New directions:**
  - Game playing?
  - Graph representations of dialogue state?

Using Graph Neural Networks

- **Popular Code Bases:**
  - GCN (Tensorflow): https://github.com/tkipf/gcn/
  - GraphSAGE (Tensorflow): https://github.com/williamleif/GraphSAGE
  - GraphSAGE (PyTorch): https://github.com/williamleif/graphsage-simple/

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