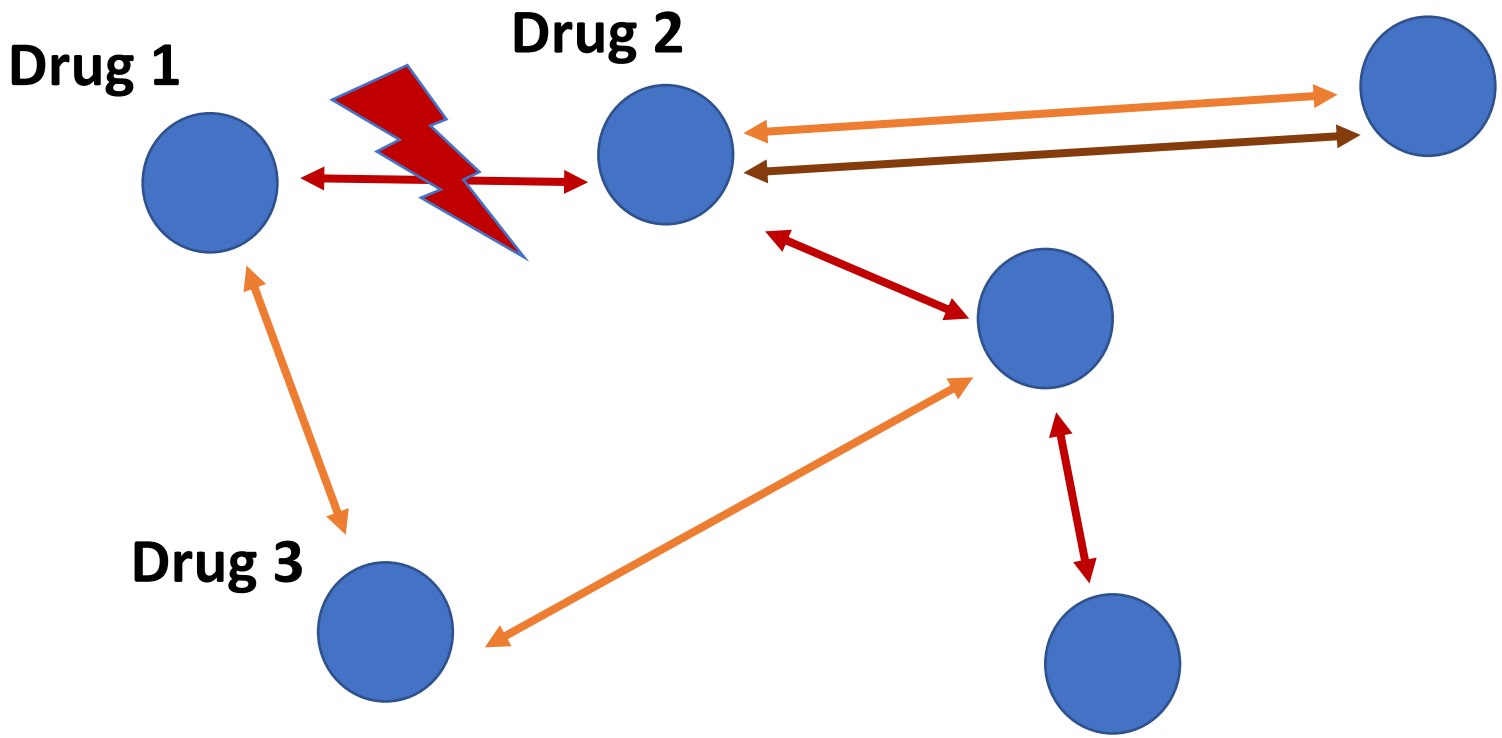
Using Graph Neural Networks for Drug-Drug Interaction Detection

Introduction

- Who are we?
  - Tengfei Ma - IBM Research, Yorktown Heights, NY
  - Veronika Thost – MIT-IBM Watson AI Lab, IBM Research, Cambridge, MA
  - Our Goal: new research/experiment results for later publication
- Who are you?
  - Which year?
  - Why did you select this project? Any specific goals/ideas already?
  - Specific experience with the topic?
  - How much time/week will you approximately spend on the project?

Detecting Drug-Drug Interactions

- Graph of Drugs and potential interactions between them
- Apply graph neural networks to get numerical vector representations of drugs/relations between drugs
- Classify those

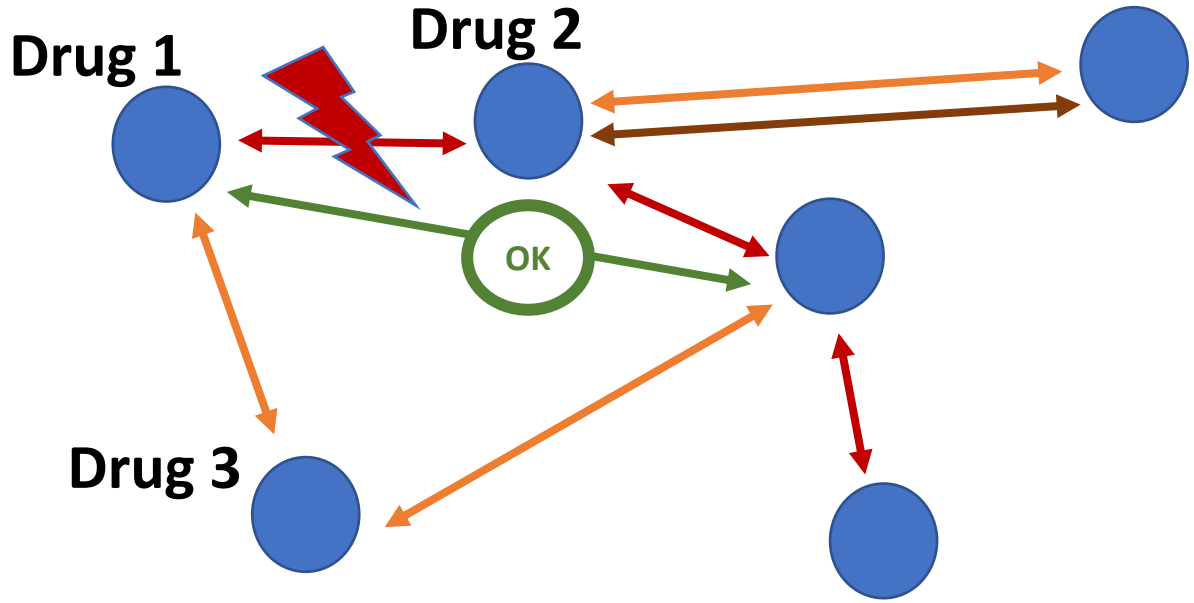


Project Focus: Multiple Evidence

- What if we consider not only DDIs to learn from but other types of information? We will investigate this!

  (Others have done so too but there are enough open questions…)

- Start: "negative" evidence
- How perform existing systems?
- Develop new system or
- Look at other evidence types or
- ??? (if you have ideas)



Literature/Similar Systems (Please read at least first)

- Modeling polypharmacy side effects with graph convolutional networks
  https://academic.oup.com/bioinformatics/article/34/13/i457/5045770
- Deep learning improves prediction of drug-drug and drug-food interactions
  https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5939113/pdf/pnas.201803294.pdf
- MR-GNN: Multi-Resolution and Dual Graph Neural Network for Predicting Structured Entity Interactions
  https://www.ijcai.org/Proceedings/2019/551
- GENN: Predicting Correlated Drug-drug Interactions with Graph Energy Neural Networks
  https://arxiv.org/pdf/1910.02107.pdf
- There are more of course …
- And there will be more literature once we have decided where we go ☺

Outlook: First Steps (Feb 2020 ?)

1. Get familiar with the standard GNN based approach to DDI prediction
   (Literature, maybe also look at their systems/code to get a better idea)
2. Get familiar with my initial code for the project
3. Process the data
4. Implement the baselines
5. Run first experiments

Next Week

- Questions about papers/task?
- Project plan: your milestones presentation deadlines etc.
- Go over Feb 14 presentation
- Tengfei: present ideas we had so far
- Intro to basic code

  Repository: https://github.com/CognitiveHorizons/ddime

Logistics / TBD

- Drugbank Account?
  [DONE]
- Should we meet weekly or bi-weekly?
  [We'll meet weekly for now]
- What are your github IDs?
  [Send per email]
- If useful, we can set up a slack channel
  [Tengfei and Veronika to be added to UMass group slack]
- Feb 14 presentation
  [Send around evaluation criteria, prepare initial version]
- Think more about data/baselines you want to look at (see literature) and model we could propose.
  [Tengfei: prepare presentation of our ideas]

Ideas are always welcome! And thank you for participating!

Any other questions?