GraphNNs Practice

Installation Instructions

FOR ALL:

```
source /opt/anaconda/bin/activate root
conda deactivate
```

CPU/GPU (for cuda 10; adapt the command to your own config):

```
conda create -n graphnn_gpu_env python=3.8 anaconda -y && \
conda activate graphnn_gpu_env && \
conda install pytorch=1.7.1 cudatoolkit=10.2 -c pytorch -y && \
conda install -c dglteam dgl-cuda10.2 -y
```

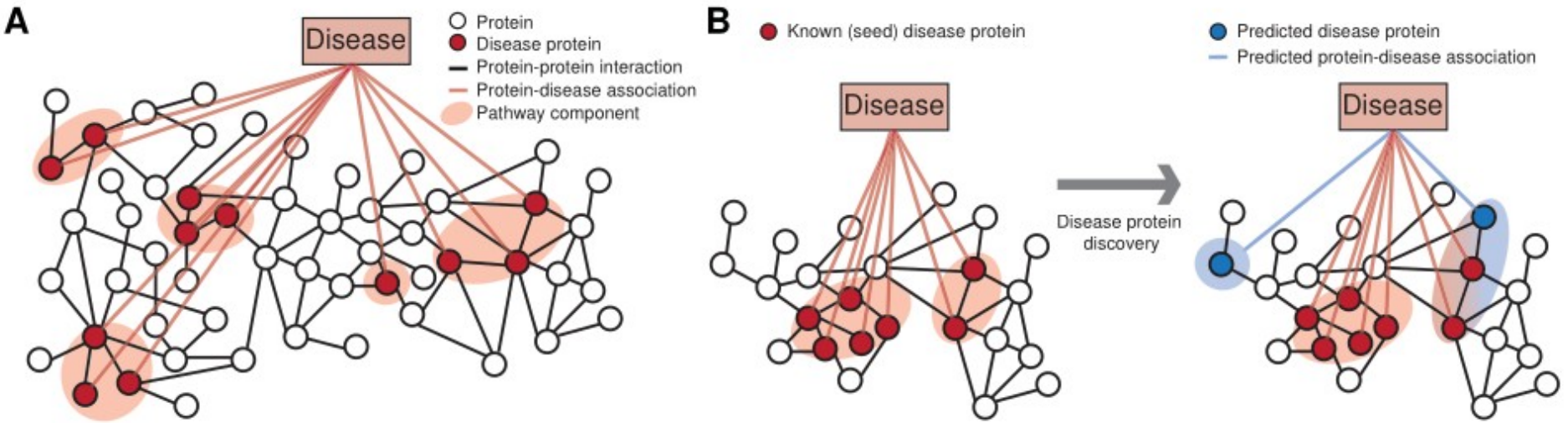
CPU ONLY (should work in all cases):

```
conda create -n graphnn_cpu_env python=3.8 anaconda -y && \
conda activate graphnn_cpu_env && \
conda install -c pytorch pytorch-cpu -y && \
conda install -c dglteam dgl -y
```

Description of the dataset

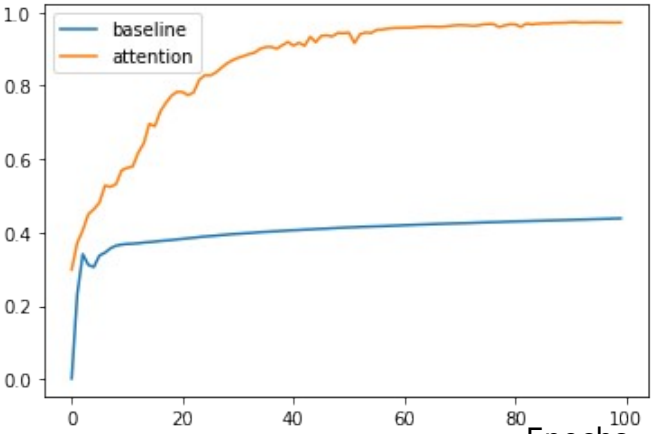
20 graphs for training, 2 graphs for test
2372 nodes on average per graph
Each node has 50 features and 121 labels

https://cs.stanford.edu/~jure/pubs/pathways-psb18.pdf



The task

F1 Score



- Take the code that has been provided and improve it
  (most improvements will come from the architecture)
  (using a Graph Attention Network is highly recommended)
  → This counts for 8/20 points

- Produce a diagram of the architecture that you're using
  (shape information must be included) and explaining the
  difference between :
  * similarity attention (defined in https://arxiv.org/abs/1706.03762 (Vaswani et al.))
  * utility attention (defined in https://arxiv.org/abs/1710.10903 (Veličković et al.))
  Equations and brief mechanism explanation are expected !
  → This counts for 12/20 points

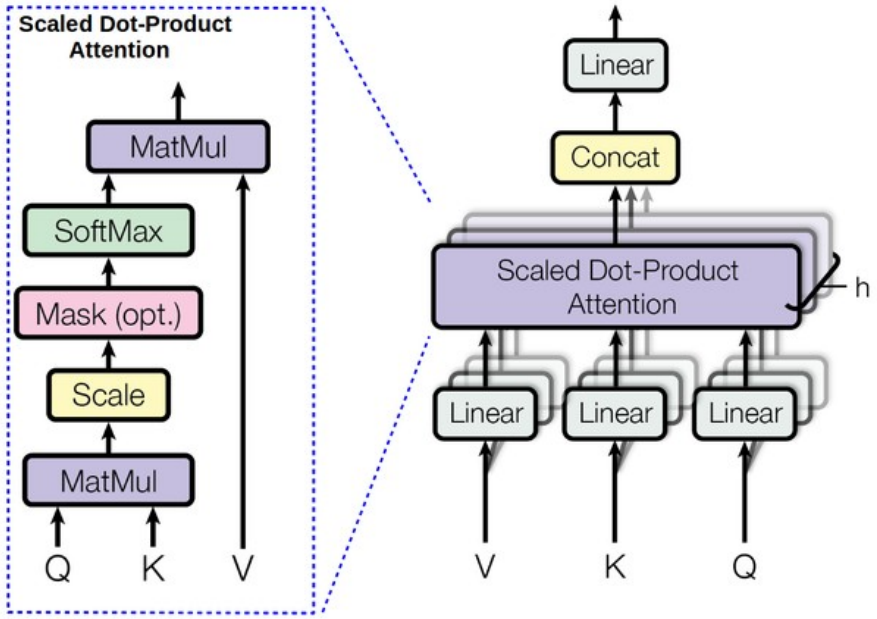
The task

- In summary, you have 4 files to produce:
  → the modified code (`train_ppi.py`)
  → the weights of the model (`model_state.pth`)
  → the diagram of the model (an image) with a summary about difference between utility and similarity attention

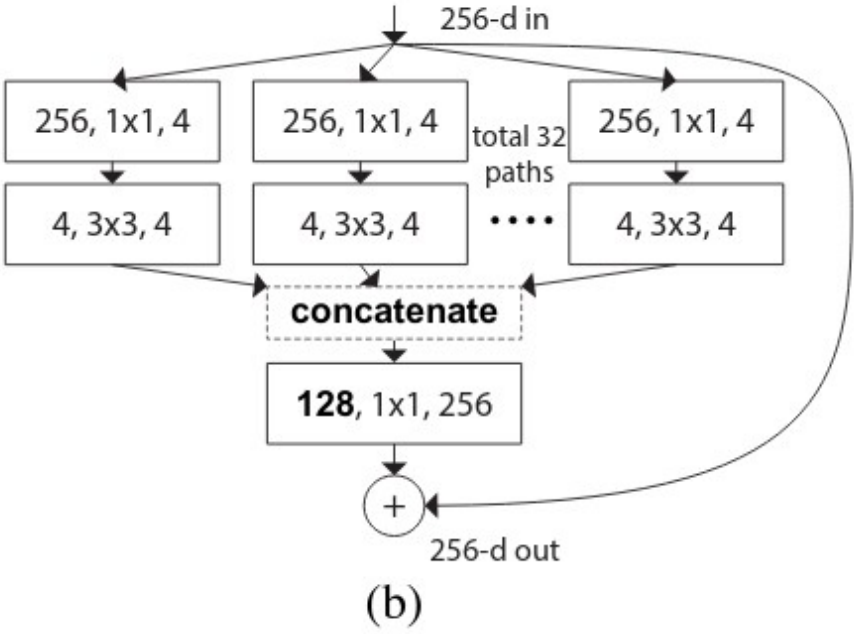
- Do not change the signature the of the `train()` and `test()` functions!

Make sure your submission correctly runs within your conda environnement with:
python3 train_ppi.py --mode test

Diagram (perfectible) examples



Multi-head attention
(shape information is missing)



ResNeXt
(a good legend is missing)

Important Hints

Use a Graph Attention Network (Veličković et al.):
https://arxiv.org/abs/1710.10903

Use the examples from the DGL dependency:
https://github.com/dmlc/dgl
https://www.dgl.ai/

Use inspiration from pytorch geometric (but don’t use it directly):
https://github.com/rusty1s/pytorch_geometric