Edge Latents Guided Graph Attention Networks

STA-695 Final Project

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Outline

1. Introduction to graph and graph learning
2. Introduction to attention mechanism
3. Edge latents guided graph attention networks
4. Results
5. Future dirctions

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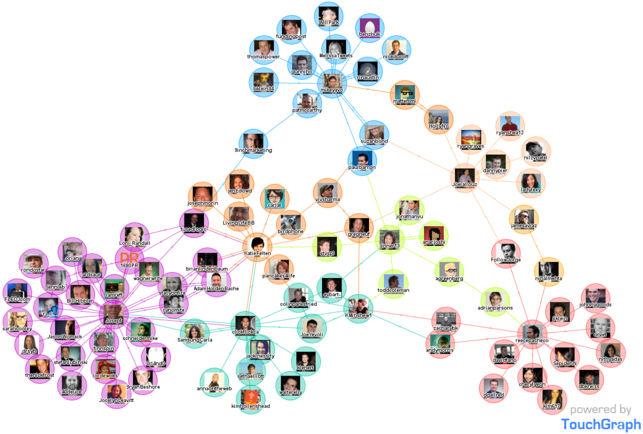
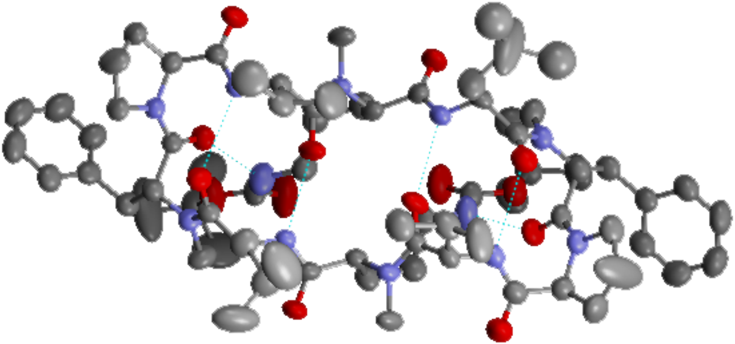
Graph

- A graph is a structure amounting to a set of objects in which some pairs of the objects are in some sense "related".
- Components
  - Nodes (vertices, points)
  - Edges (arcs, lines)
- Graph learning
  - Node classification (regression)
  - Edge classification (regression)
  - Graph classification (regression)
  - Node clustering
  - ...

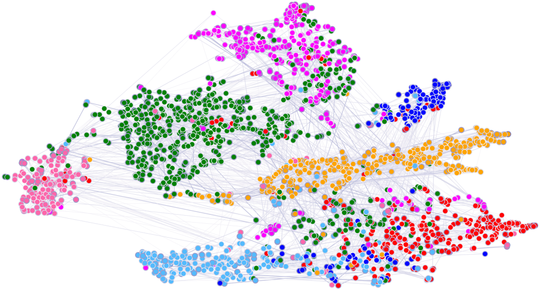
Social network



Protein-protein interaction



Citation graph



- Node: Paper
- Edge: Citation

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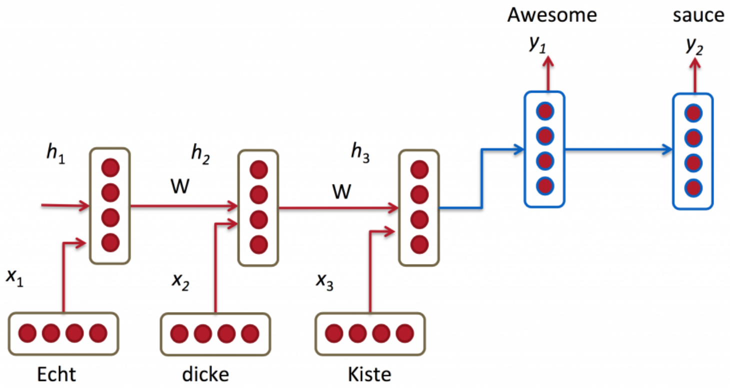
Attention mechanism

- Hot and new topic in deep learning
- Successfully applied to machine translation problem
- A learnable mechanism to aggregate features
- Aggregate by weighted average
- The weights for aggregating is a function of features
- different content of features will have different weights (attention)

RNN based machine translation

- Input sequence are encoded into a single vector by RNN
- Output sequence are generated from this vector by RNN



Why attention mechanism?

- The RNN (LSTM) based method surprisingly works well!
- But, obviously, there is space for improvement

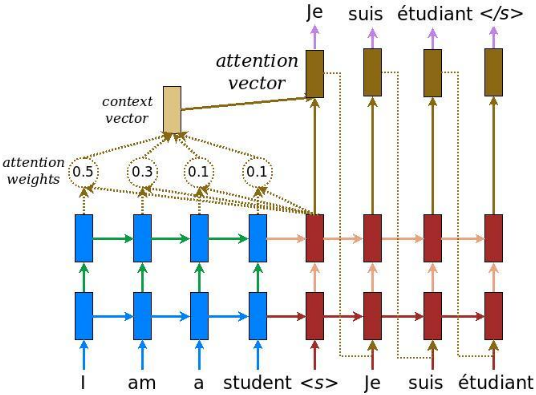
Problem

The dependency between output sequence and input sequence is complex which could not be captured by the encoding RNN

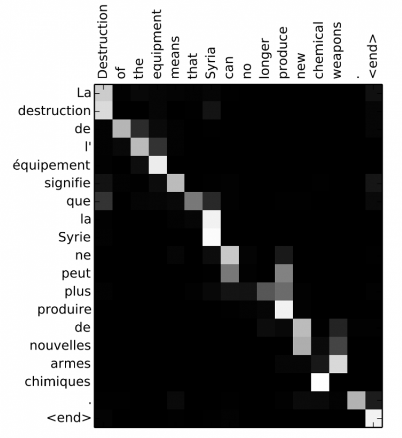
Attention mechanism

- Instead of using the last encoded vector, aggregate a feature vector from all the previous hidden states each time generating an output
- Aggregating could be a weighted average
- Weights are a trainable function of the contents

Machine translation with attention mechanism



Interpreting attention weights



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Graph node classification with attention mechanism

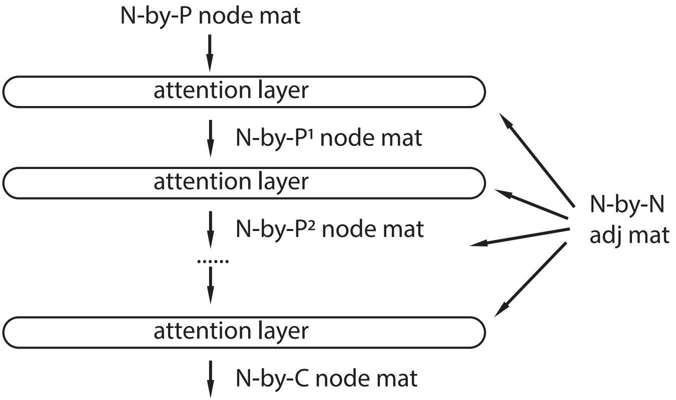
Useful information to classify a node

- features of the node
- features of its neighbor nodes
- label or prediction of its neighbor nodes

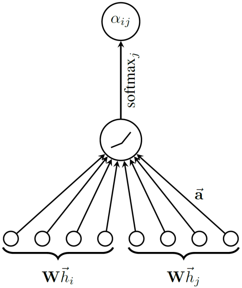
Graph attention network

- aggregate node features using multiple attention layers
- simutaneously classify all nodes of a graph
- neighbor label or prediction are aggregated through back-propagation

Graph attention network

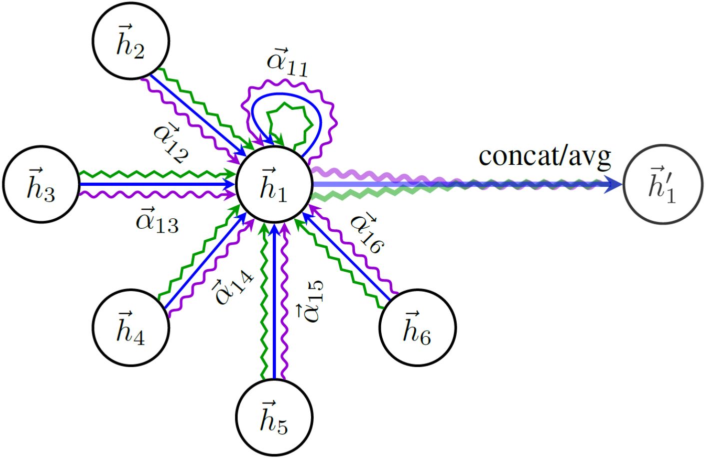


Graph attention mechanism

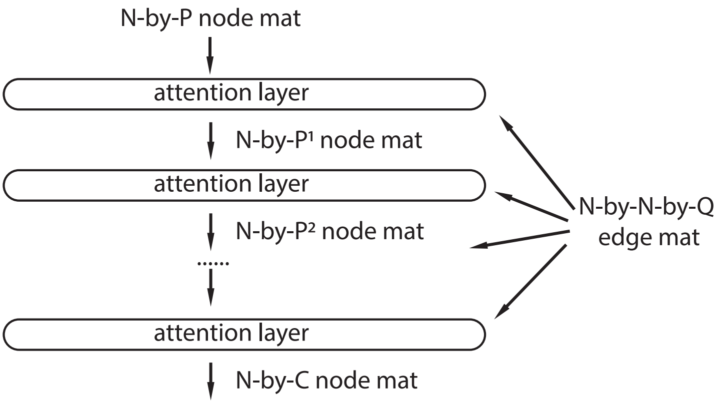


$$\alpha_{ij} = \frac{\exp\left(\mathrm{LeakyReLU}\left(\boldsymbol{a}^T\left[\boldsymbol{W}\boldsymbol{h}_i \,\|\, \boldsymbol{W}\boldsymbol{h}_j\right]\right)\right)}{\sum_{j\in\mathcal{N}_i}\exp\left(\mathrm{LeakyReLU}\left(\boldsymbol{a}^T\left[\boldsymbol{W}\boldsymbol{h}_i \,\|\, \boldsymbol{W}\boldsymbol{h}_j\right]\right)\right)}$$

Multi-head attention



Edge guided graph attention network



Edge latents guided attention

- For different type of edges, attention functions are different
- Edge types are represented by edge latent variables

$$\alpha_{ij} = \frac{\exp\left(\mathrm{LeakyReLU}\left(\sum_l \left(\boldsymbol{a}_l^T \left[\boldsymbol{W}\boldsymbol{h}_i \parallel \boldsymbol{W}\boldsymbol{h}_j\right] + \boldsymbol{v}_l \boldsymbol{g}_{ij}\right)\right)\right)}{\sum_{j \in \mathcal{N}_i} \exp\left(\mathrm{LeakyReLU}\left(\sum_l \left(\boldsymbol{a}_l^T \left[\boldsymbol{W}\boldsymbol{h}_i \parallel \boldsymbol{W}\boldsymbol{h}_j\right] + \boldsymbol{v}_l \boldsymbol{g}_{ij}\right)\right)\right)}$$

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Cora dataset

# Nodes	2708
# Edges	5429
# Features/Node	1433
# Features/Edge	2
# Classes	7
# Training Nodes	140
# Validation Nodes	500
# Test Nodes	1000

Table: Summary of cora dataset

Experimental Results

Method	Accuracy
MLP	55.1%
ManiReg [1]	59.5%
SemiEmb [2]	59.0%
LP [3]	68.0%
DeepWalk [4]	67.2%
ICA [5]	75.1%
Planetoid [6]	75.7%
Chebyshev [7]	81.2%
GCN [8]	81.5%
MoNet [9]	$81.7 \pm 0.5\%$
GAT	$83.0 \pm 0.7\%$
EGAT	$83.4 \pm 0.6\%$

Table: Summary of results

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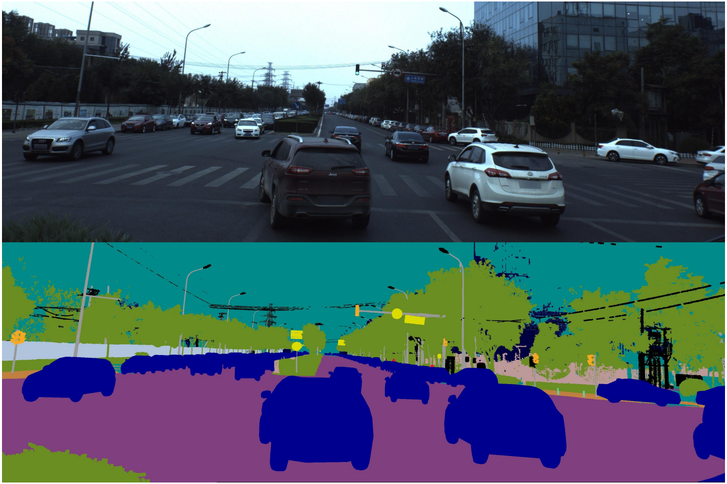
Future directions

- Apply to problems with more edge information
- Address problems with large graphs
- Combine with GCN
- Apply to image semantic segmentation (FCN/MS-D + EGAT)

Semantic segmentation



Semantic segmentation as node classification

Current state-of-the-art method

- Convolution based
- Fully CNN or MS-D (Mixed scale dense CNN)
- Convolution weights are shared by all pixel position

Promising EGAT based method

- Model the problem as a graph node classification
- Fully CNN or MS-D for feature learning
- EGAT for feature aggregation and pixel classification

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