Graph Representation Learning

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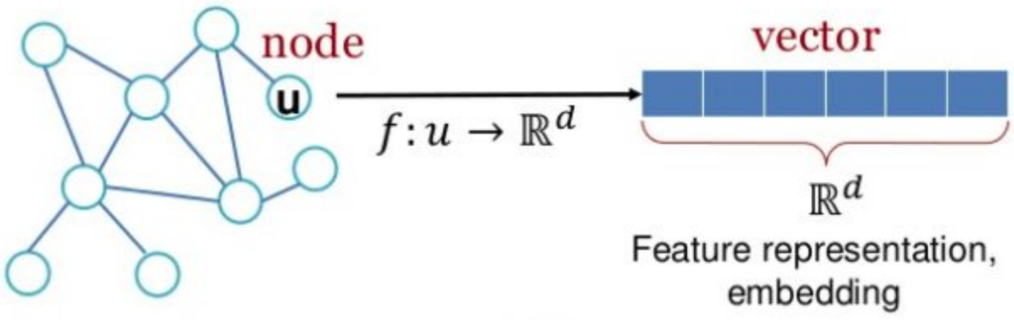
Feature Learning in Graphs

Goal: Map each node into a low dimensional space which encodes network information.

Motivation: Various applications such as clustering, link prediction, label classification, ...



Source: Jure Leskovec, Stanford university

Feature Learning in Networks

- ‘Linearizing’ the graph
  - Create a sentence for each node using random walks
  - Node2vec

- Graph Convolutional Networks
  - Uses Convolutional architecture with deep network.
  - GCN

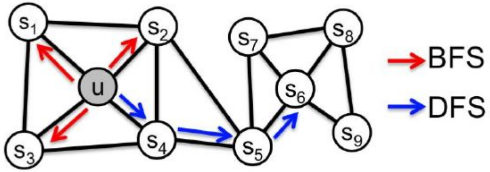
Node2vec: Unsupervised Feature Learning

- Let G = (V, E) be any (un)directed, (un)weighted network. Learn node embeddings $f : V \to R^d$ such that nearby nodes are close together.
- Objective: $$\max_f \sum_{u \in V} \log Pr(N_S(u)|f(u))$$
- Assume Conditional independence: $$Pr(N_S(u)|f(u)) = \prod_{n_i \in N_S(u)} Pr(n_i|f(u))$$
- Then Softmax: $$Pr(n_i|f(u)) = \frac{\exp(f(n_i) \cdot f(u))}{\sum_{v \in V} \exp(f(v) \cdot f(u))}$$

Node2vec: scalable feature learning for networks, A. Grover, J. Leskovec, KDD 2016

How to determine $N_s(u)$?

- Classic strategies to define neighborhood $N_s(u)$ of a node u.
  - BFS captures homophily.
  - DFS captures structural equivalence.

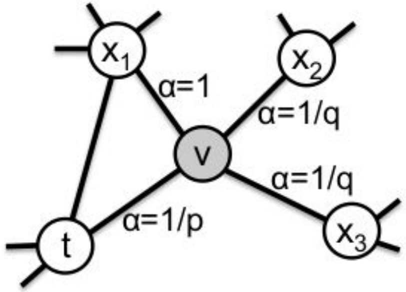


- Interpolating BFS and DFS
  - **Return parameter p**: return back to the previous node.
  - **In-out parameter q:** Moving outward (DFS) vs inwards (BFS)

Random walk procedure

Sampling of nodes uses probability distribution given by

$$P(c_i = x \mid c_{i-1} = v) = \begin{cases} \frac{\pi_{vx}}{Z} & \text{if } (v, x) \in E \\ 0 & \text{otherwise} \end{cases}$$

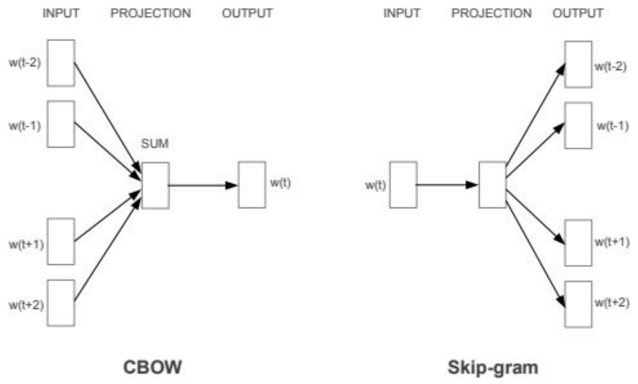


$$\pi_{vx} = \alpha_{pq}(t, x) \cdot w_{vx}$$

$$\alpha_{pq}(t, x) = \begin{cases} \frac{1}{p} & \text{if } d_{tx} = 0 \\ 1 & \text{if } d_{tx} = 1 \\ \frac{1}{q} & \text{if } d_{tx} = 2 \end{cases}$$

Word2vec

The CBOW architecture predicts the current word based on the context, and the Skip-gram predicts surrounding words given the current word

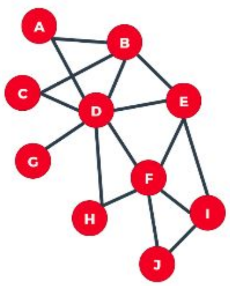


Node2vec extends the skip-gram architecture to networks.

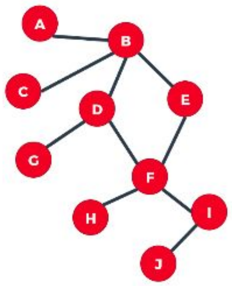
Source: Efficient Estimation of Word Representations in Vector Space, T Mikolov et. al.,

Link Prediction

- It is the task to estimate the probability of links between nodes in a graph.
- Link prediction heuristics scores:
    - Common Neighbors : $|N(u) \cap N(v)|$
    - Jaccard's coefficient : $|N(u) \cap N(v)| \,/\, |N(u) \cup N(v)|$
    - ...
- How we did link prediction using node2vec?



Original graph



Residual graph

+

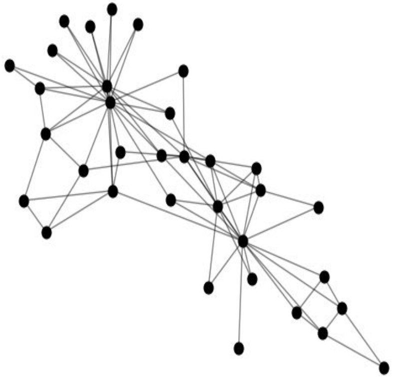
Sampled edges for training/testing

Datasets

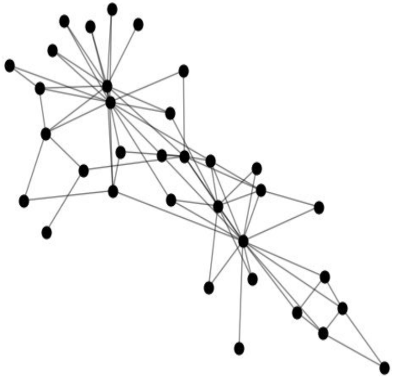
- Zachary’s karate club Network
  - Contains 34 nodes and 78 edges, where each link is between pair who interacted outside the club.
- Facebook dataset
  - Network between facebook friends. It contains 4,039 nodes and 88,234 edges.
- BlogCatalog dataset
  - Network of social relationships of the bloggers listed on the BlogCatalog website. It has 10,312 nodes, 333,983 edges.

Results - Zachary's Karate Club Network

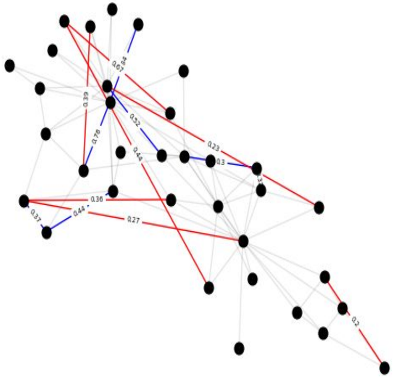
Original Graph



Subgraph



Predictions



Results on Facebook and BlogCatalog Dataset

Table 1 : Mean Auc scores

dataset	Hadamard	Average	L2	L1
Facebook	0.9551	0.6443	0.986	0.9858
BlogCatalog	0.5829	0.6396	0.9032	0.8982

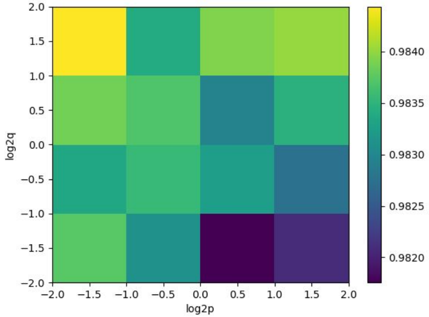


Fig. Grid search over parameters p and q, with Weighted L2

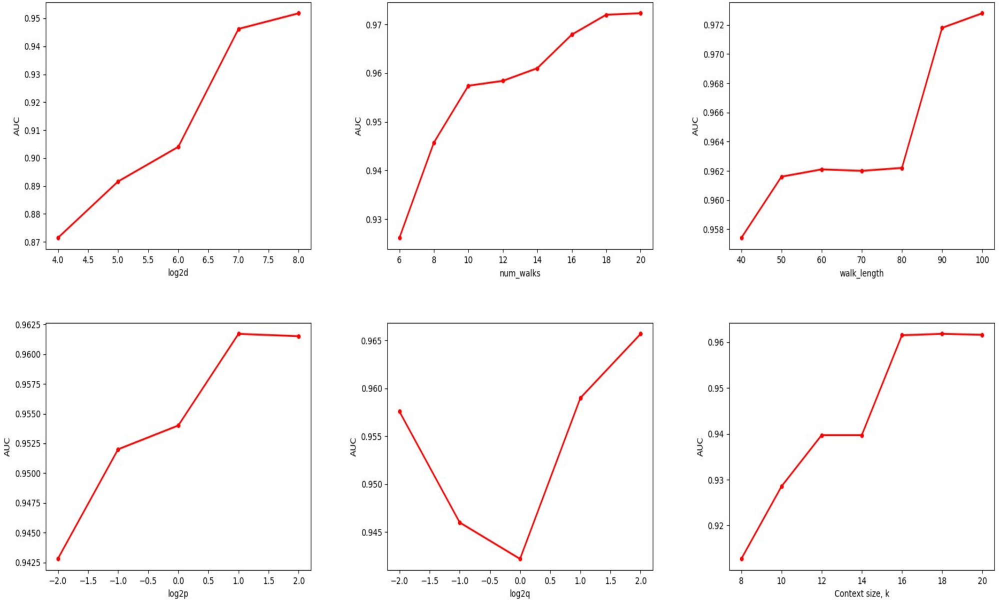


Fig. Parameter Sensitivity plots

Node2vec on weighted signed network

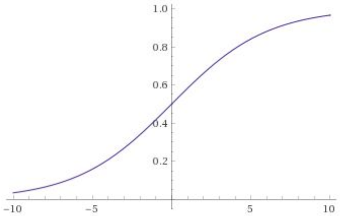
- Future extensions of node2vec:
  - Signed edge networks
  - Heterogeneous information networks
  - …
- We explored ways to extend node2vec for weighted signed network
- Dataset: Bitcoin OTC trust weighted signed network[1]
  - Edge weight range: -10 to 10
  - Contains 5881 nodes and 35592 edges.

1. Bitcoin OTC trust weighted signed network, https://snap.stanford.edu/data/soc-sign-bitcoin-otc.html

Contd.

- Convert edge weight in range 0 to 1.

$$\frac{1}{1+\exp\left(-\frac{x}{3}\right)}$$



- Result of link prediction: 0.88 AUC score with weighted L2 edge function.

OBJECTIVE:

Tuning of hyperparameters

Obtaining GCN embeddings

Unsupervised clustering on the graph using DEC technique

Graph Convolutional Network

Formulation of CNN in context of spectral theory.

Two approaches:

- Spatial - considers local receptive fields upto neighborhoods only.
  - e.g. locality on W, deep locally connected graph
- Spectral - exploiting global structure of graph by graph laplacian to generalize convolutional operator
  - e.g. GCN

Background

- Main aim is faster training and higher accuracy.
- Requirement is learning fast localized spectral filters
- Laplacian L=D-W where D is degree matrix and W is adjacent matrix.
- For easiness we use convolution in fourier domain
- $x *_g y = U((U^T x) \odot (U^T y))$ where is element wise product and U is fourier basis and obtained from eigen decomposition.
- U is some function of eigen value of L which can be well approximated by chebyshev polynomial-

$$g_{\theta'} \star x \approx \sum_{k=0}^{K} \theta'_k T_k(\tilde{L}) x$$

- Taking upto K^{th} order of chebyshev polynomial will give K -localized expression
- If K=1, stacking multiple such layer will give rich class of convolutional filters
- Forward model -

$$Z = f(X, A) = \mathrm{softmax}\left(\hat{A}\ \mathrm{ReLU}\left(\hat{A}XW^{(0)}\right)W^{(1)}\right)$$

where,

$$\hat{A} = \tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}}$$

Experiments

Classification with chebyshev polynomial

Datasets used : Pubmed, Cora, Citeseer

No of layers	Maximum degree	Accuracy
2	3	79.70 %
2	2	80.50 %
3	3	78.70 %
3	2	80.40 %

Table 1: Cora

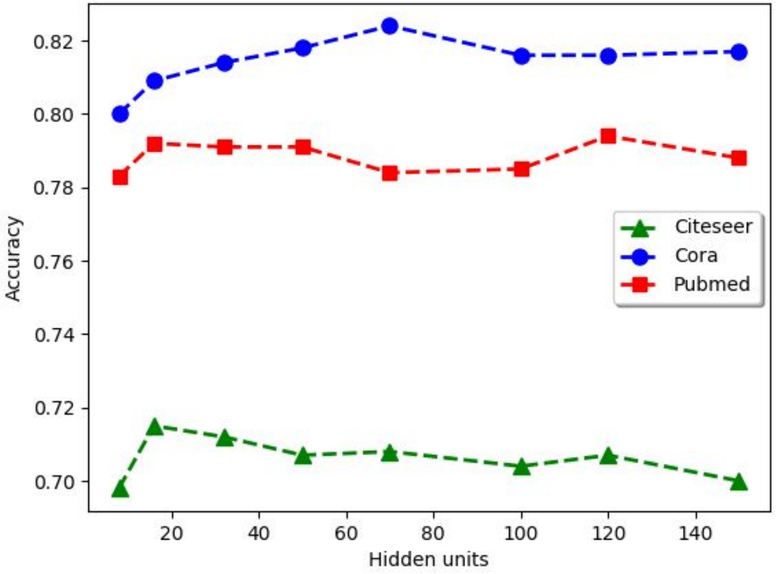
No of layers	Maximum degree	Accuracy
2	3	79.17 %
2	2	79.30 %
3	3	79.30 %

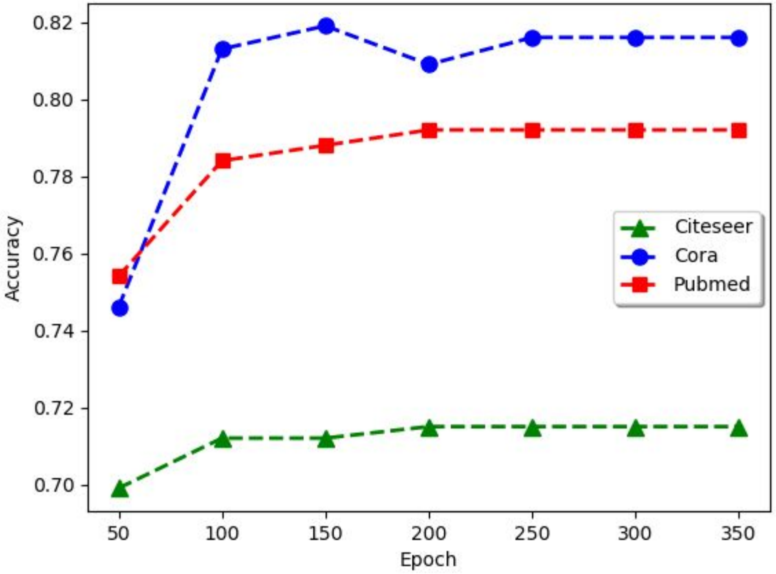
Table 2: Pubmed

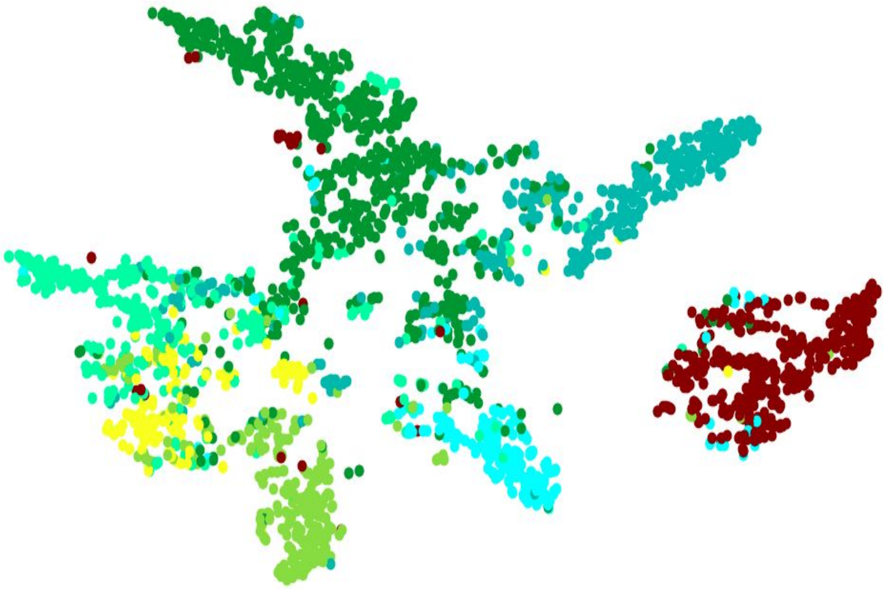
No of layers	Maximum degree	Accuracy
2	2	71.50 %
2	3	71.50 %

Table 3: Citeseer

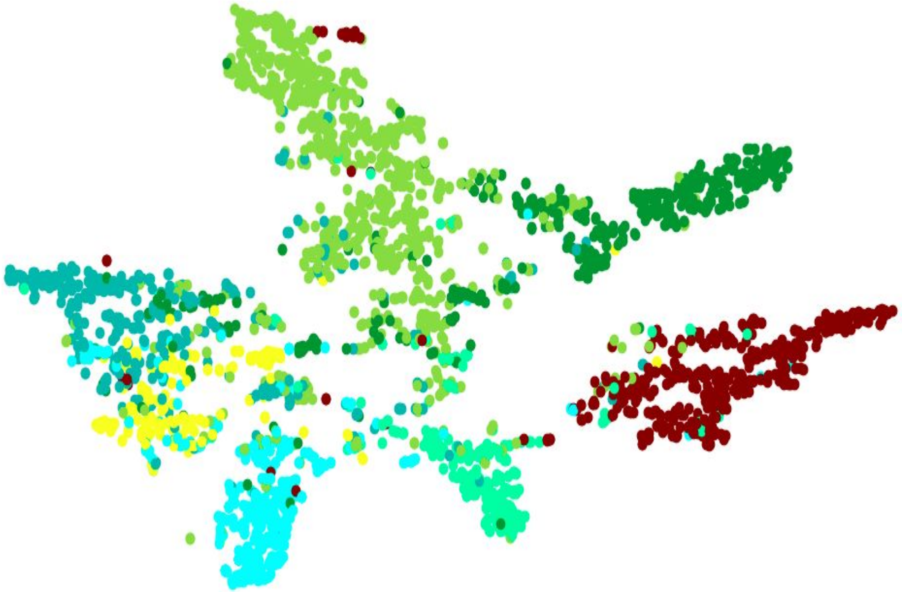
Tuning hyperparameters







200 epoch



400 epoch

Deep embedding Clustering

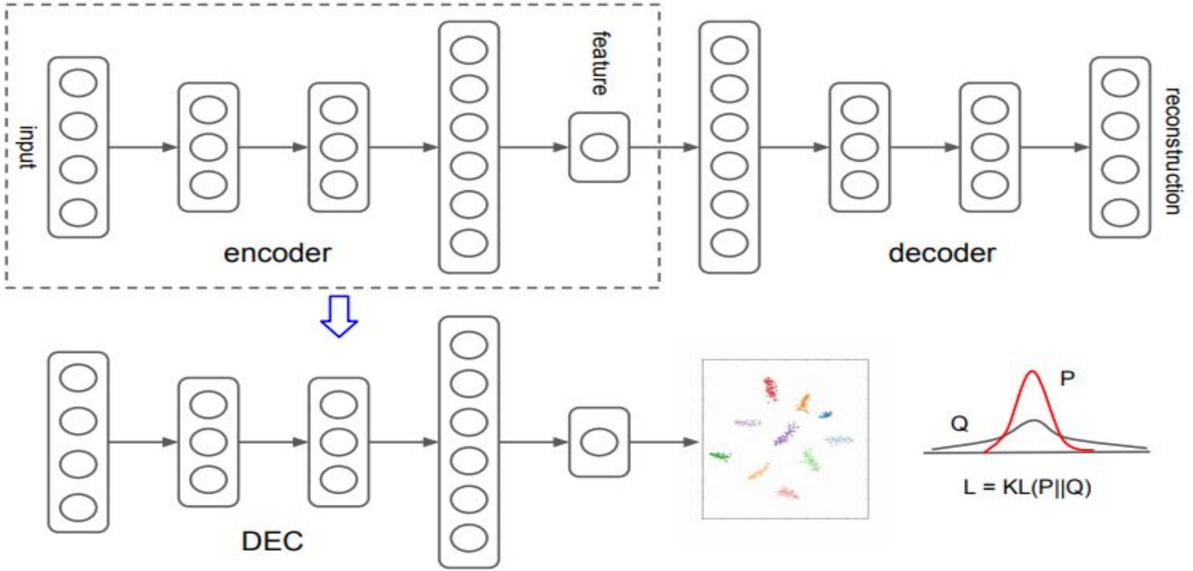
Method which simultaneously learn:

- Unsupervised Clustering using deep neural network
- Non linear mapping high dimension data space to lower dimension data space

Proposed by Xie et. al

DEC has two phases:

- Parameter initialization with deep autoencoders
- Parameter optimization/clustering based on minimizing KL divergence with help of auxiliary target distribution computation.



Implementation

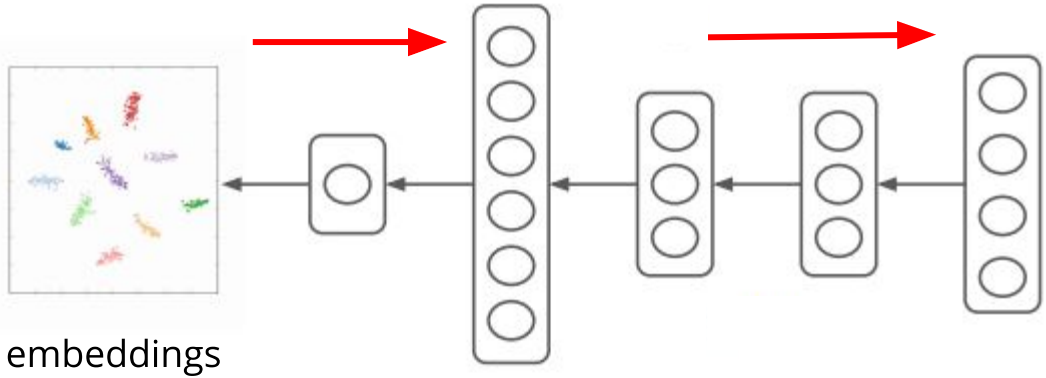
- Determining hyperparameters by cross validation is not an option
- Commonly used parameters are used

Experiments

- Dataset- MNIST
- Clustering Accuracy- 83.42 %
- Number of encoder layers- 3
- Number of decoder layers- 3
- Dropout- 0.2

Finally we tried connecting both these models...

- We obtained graph embeddings from GCN
- Next we used DEC model but instead of encoder we used the embeddings obtained from GCN
- In DEC we used autoencoder where training is done using reconstruction loss
- But, in our model we used original feature vector instead of the gcn embeddings to train on reconstruction loss



embeddings

Dim = Dim of original feature vector

References

[1] node2vec: Scalable Feature Learning for Networks. A. Grover, J. Leskovec. ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD), 2016.

[2] Mikolov, Tomas; et al.. "Efficient Estimation of Word Representations in Vector Space", 2013

[3] William L. Hamilton, Rex Ying, Jure Leskovec, Representation Learning on Graphs: Methods and Applications, IEEE Data Engineering Bulletin, September 2017

[4] Michael Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on ¨ graphs with fast localized spectral filtering (NIPS), 2016

[5] Kipf & Welling, Semi-Supervised Classification with Graph Convolutional Networks, 2016

[6] Junyuan Xie, Ross Girshick, and Ali Farhadi. Unsupervised deep embedding for clustering analysis. ICML 2016.