**COMP90051 Project Report**

**Introduction**

Link prediction is a common technique used in various circumstances, for instance, friend recommendation in social application such as Facebook. However, Facebook link prediction is based on undirected graph, but in this project, we were given a graph with directed edges to recommend potential account the user may be interested in which means some of the techniques used in undirected graph may not work properly or only work with minor amendment. Moreover, the total number of nodes and edges of the given graph are approximately 5 million and 23 million respectively which means, potentially, there are approximately 24 trillion disconnected edges in total. It will consume a very long time to process and learn from the whole graph directly.

**Methods**

1. **Simple Heuristic**

There are many simple heuristics which can be used for link prediction. I selected Katz score and Adamic/Adar score initially. However, I apply minor changes to Katz to precisely describe the local information between two nodes, as address in the followings.

1. Katz

Instead of running Katz on the whole graph for the given nodes, I firstly extract a local subgraph of the original graph (Zhang, & Chen, 2018) to restrict redundant information and reduce computation time. Formally, Katz score is defined as

is a penalty factor for long distance and is the collection of paths between and with length . To approximate this, the upper bound of the path length is set to 3 since the set of paths rarely provide information about link existence from to in the real world. To convert it to a probability, I eventually adopted the following formula

In normal words, if the link from to indeed exists, it will guarantee to generate a probability close to 1 (at least ) and simultaneously heavily penalising longer paths. This is not a bad approach and it yields a ROC-AUC score of about 0.7 (and this is the best I can get with this method by logically augmenting and the upper bound of ).

1. Adamic/Adar

This is a simpler heuristic which only needs to consider the common neighbours. The formula is given as

is the set of neighbours of vertex . Since we are making link prediction on directed graph, there is two types of neighbours, i.e. denotes the predecessors of vertex and denotes the successors of vertex . Apply the transformation, Adamic/Adar score is calculated by

To transform it into a probability, I apply again to the score given by

The reason I bias the number of successors of their common neighbours by 1 is to avoid circumstance when . In this case, which implies

means there is a directed edge from to . This is not logically correct in the real world. This gives a ROC-AUC score of about 0.8, and this is the final approach.

1. **Random Walk Similarity**

In an undirected graph, two nodes are potentially connected if they are similar. To test if this work well on a directed graph, I implement a random walker with Alias Sampling to randomly choose the candidate node from the successors of node where the random walker currently located at (the node2vec embedding of a vertex). Unsurprisingly, the ROC-AUC scores of this pure similarity-based method are all about 0.66.

1. **Classification/Regression**

In this type of undirected graph, all weights of the existing edges are simply 1. Therefore, binary classification or complicated regression can be applied to this problem, I only draw approximately 200 thousand existing edges accompany by the same number of non-existing edges to build the classifier and regressor. However, these generally performed worse than all other methods based on the features I extracted from the graph (around 0.6 ROC-AUC score).

**Analysis**

node2vec embedding for graph is generally the same as word2vec embedding for document. The walk length and number of walks affect the paths. Another factor is the number of adjacent nodes to be taken account into in a path, which is similar to the n-gram choice in word embedding. Hence it works well in an undirected graph since mutual link (such as friendship in Facebook) between two vertices is implied in such type of graph but its performance decreases on directed edge in Twitter link prediction. The method I applied Katz centrality has problem with penalisation of number of paths of a specific length. It simply counts the number of paths, but it ignored the factor of individual nodes on each path. This is also the reason Adamic/Adar method outperforms the Katz method since it rewards the rare feature. I tried to extract various features (including the heuristic scores described previously) for the classifiers and regressors, but it is still worse than the simplest method described before.

I also attempted to build a Deep Graph Convolutional Neural Network with node2vec node embedding, but it fails to run due to the memory limit even though I applied the subgraph extraction.

**Reference List**

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