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MASTER'S DEGREE IN COMPUTER ENGINEERING

APEROL from Networks: Analyzing Pipeline and Embedding Representations for Optimized Learning (from Networks)

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Contents

1 Datasets

Before proceeding to a discussion of the preprocessing of the datasets, it is necessary to inform readers that changes have been made to two of the datasets originally proposed.

The first change refers to the Pennsylvania dataset. The decision was made to replace the original Pennsylvania road network dataset with the corresponding dataset from [1]. The decision to replace the undirected dataset with a directed one was made to ensure greater uniformity among road networks.

The second change refers to the Twitch dataset. Due to concerns regarding the large number of edges in the original dataset during the initial experimental phase, it has been replaced with a smaller Deezer dataset from [2].

Furthermore, the two "Mus Musculus" and "Saccharomyces cerevisiae" datasets are described in greater detail as follows. Both of them have been downloaded from the STRING Database [3], filtered with the following options: a confidence score of > 0.4 for Mus Musculus and > 0.7 for Saccharomyces cerevisiae; and only AB pairs (undirected).

The subsequent table has been revised to reflect the aforementioned modifications. These alterations can be discerned within the table itself, as they are highlighted.

Network	$\|V\|$	$\|E\|$	**Type**
Pennsylvania [4, 1]	1,088,092	3,083,796	Directed
Padua (province) [5]	122,680	304,184	Directed
Hong Kong (city) [6]	43,620	91,542	Directed
Italian Covid-19 Retweet Network [7]	221,574	800,000	Directed
Deezer [8, 2]	143,884	846,915	Undirected
GitHub Developers [9, 10]	37,700	289,003	Undirected
Mus Musculus Protein Interactions [3]	20,969	800,000	Undirected
Saccharomyces cerevisiae Protein Interactions [3]	5,786	100,000	Undirected
Bio-grid-fission-yeast [11]	2,000	25,300	Undirected

Table 1: Datasets used in the project

A preprocessing pipeline is utilized in which all datasets are converted into CSV files and only the useful features are extracted, if present.

Initially, all the datasets were manually converted to CSV files, as some of them were not directly available in this format. Subsequently, a Python script was implemented to automate the following preprocessing of the datasets. Undirected edges (u, v) are represented using a pair of directed edges (u, v) and (v, u). Unweighted datasets are represented as having a uniform weight of 1.0 for all edges. Finally, the node IDs are mapped to numeric consecutive IDs, with the sequence beginning at 0.

2 Experiments

Further information regarding the train-validation-test split in our pipeline is provided below.

Consider graph $G = (V, E)$, where V denotes the set of vertices and E is the set of edges. A first split of the set of edges E is needed for the embedding algorithms, creating E_{embed} and E_{pred}. E_{embed} is used for the subgraph $G_{\text{embed}} = (V, E_{\text{embed}})$ given as input to the embedding methods: the shallow embedding methods will use it to learn a lookup table Z of node embeddings, whereas the deep embedding methods aim to learn a function f that can generalize well. The remaining edges in E_{pred} are instead reserved for the link-prediction task, where the second split occurs: from E_{pred} the sets E_{train}, E_{val}, E_{test} are created for the training, validation and test of the prediction

model.

To train and evaluate the prediction models, labeled *negative* edges are added to each of the three splits. A negative edge in this setting is defined to be an edge $(a, b) \notin E$ with $a, b \in V, a \neq b$ (do not include self-loops). Furthermore, in order to avoid data leakage, the sampled negative edges must be distinct from those used internally by the embedding algorithms during training.

For each edge (u, v) belonging to any of these splits of E_{pred}, its corresponding embedded representation is constructed by combining the embeddings z_u, z_v of its incident nodes, using an operator such as the average, the dot product, or concatenation. These edge embeddings are the ones used as input to the prediction models.

A feasible split for a large graph could be: (from E) 80% for E_{embed} and 20% for E_{pred}; (from E_{pred}) 60% for E_{train}, 20% for E_{val} and 20% for E_{test}.

We revised the implementations that will be adopted for our experiments: [12] for Node2Vec, [13] for LINE, [14] for DVNE, [15] for GraphSage. Depending on specific needs, some of these could be modified or used as an inspiration for different implementations. In particular, DVNE was not evaluated on directed graphs in the original work [16], meaning it may be necessary to explore adaptations for this setting. If no satisfactory solution is found, DVNE will be restricted only for undirected graphs to mantain a fair comparison.

Following some initial experiments, it was decided to use the DEI cluster *"Blade"* as hardware for the computation of the larger graphs. The specifications for the nodes of the cluster are available in the open documentation [17]. More information about the project's memory usage and runtime will be available in the final report.

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Contribution of Authors and AI Usage

The contributions for this project are:

- Datasets: Marco Annunziata (research, writing), Silvia Mondin (search, implementation, writing), Sveva Turola (research, writing);
- Experiments: Marco Annunziata (research, writing), Silvia Mondin (research), Sveva Turola (research);
- Testing of implementations: Marco Annunziata (DVNE), Silvia Mondin (node2vec), Sveva Turola (LINE, GraphSAGE);

The following AI tools were used:

- Copilot was used to suggest code and report snippets.
- DeepL was used to correct the grammar and syntax of the text.