Network Science Cheatsheet

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Graph/Node embedding

Disclaimer

Graph/Node embeddings are a recent field of research, with hundreds of publications in the last few years, and scores of new papers published in every machine learning and network science conference. This class is thus only an introduction to the mechanism underlying those approaches.

Embedding of networks

In the context of **graph embedding**, embedding is a shortcut for **embedding in low dimensions**, and can be understood as assigning to some **elements** of the graph a **vector** (i.e., a list of numbers) composed of **d** elements. **d** is the number of dimensions in the embedding space, and **d** should be small.

Types of Network Embedding

According to the type of element which is embedded, we can differentiate:

- Node Embedding (one vector per node)
- Edge Embedding (one vector per edge)
- Substructure Embedding (e.g., one vector per community)
- Whole Graph Embedding (one vector per graph)

In this class, we will introduce only Node Embedding, which is the most popular approach.
Whole graph embedding is also quite popular, for instance to classify types of networks.

Node Embedding

In **node embedding**, the vector assigned to each node should be a proxy, a sort of numeric summary of the position of the node in the graph, in term of topology. Several types of embeddings exist that capture different aspects of the network topology, in particular we will differentiate *locational embedding* from *role embedding*.
Note that node embedding is sometimes called **graph embedding** in the literature.

Embedding distance

Since each node is represented by a vector, it is possible to compute a **distance between nodes** in the embedding. Intuitively, two nodes occupying similar positions in the network (according to what the chosen embedding capture) should have similar embedding vectors. The notion of distance to use (cosine, euclidean, etc.) also depends on the chosen embedding.

Adjacency matrix(A) as an embedding

A naive way to choose an embedding (in n dimensions) could be to consider each row of the adjacency matrix as the vector representation of the node it corresponds to.
This embedding would capture what is called the **structural equivalence**, i.e. the fact that nodes share similar neighborhoods. Two nodes with the same neighborhoods would have the same vectors. If the *Manhattan distance* were used, the distance between nodes in the embedding would correspond to the number of different neighbors.

What is a good embedding?

What is a good embedding depends on the task that we want to achieve. In the perspective of this class, embeddings are mostly used as features for machine learning tasks. As such, they must be 1) In as few dimensions as possible: Machine learning suffers from what is known as the **curse of dimensionality**, and tends to work better with lower dimensions, without talking about computational advantages. 2) As dense as possible. Sparsity –usually associated with high dimensions– makes learning harder.
Furthermore, the embedded properties must be meaningful for the task to achieve. For instance, the notion of distance captured by the adjacency matrix seems in contradiction with the intuition: in graphs, one usually use the number of common neighbors, and/or normalized fraction of neighbors (Jaccard, etc.) rather than a raw count of different neighbors.

Embedding and Dimensionality Reduction

In Machine Learning, when a dataset is composed of too many features, **dimensionality reduction** algorithms can be used to generate a smaller number of synthetic features, defined as combination of the original ones. Common algorithms to do so are for instance **PCA** (Principal Component Analysis) and **T-SNE**[a].
A simple method to generate a better embedding from the adjacency matrix would be to apply Dimensionality Reduction on it to reduce its number of dimension. Its counter-intuitive definition of distance would nevertheless remain a problem.

[a] Maaten and Hinton 2008.

Notations

y	Embedding of the graph
y_i	Vector corresponding to node i in the embedding y
S	Similarity matrix. For each pair of node i, j, S_{ij} represents the graph similarity that we want to preserve.

By default, $S = A$: two nodes have a maximal similarity of 1 if they are connected, and similarity 0 if they are not connected. But one can use a different notion, such as a random walk distance, a neighborhood similarity heuristic, etc.

Node Embedding: LE

Laplacian Eigenmaps (LE)[a] is a method that can be used for node embedding, whose objective function is defined as follows:

$$y = \min \sum_{i \neq j} \|y_i - y_j\|^2 S_{ij}$$

This can be read as follows: to find the embedding y of a graph, we need to assign an embedding y_i to each node i such as the sum (over all node pairs) of the equation $\|y_i - y_j\|^2 S_{ij}$ is minimal. Said differently, its objective is to minimize the product between the **euclidean distance** in the embedding ($\|y_i - y_j\|^2$) and the **similarity** in the graph S_{ij}.
If two nodes are similar/close in the graph (high value), we need to make them as close as possible in the embedding (small value). Nodes dissimilar/distant in the graph can be distant in the embedding with a lesser penalty. To forbid a trivial solution of all nodes being on the same location, the sum of distance between points in the embedding must be equal to a constant.

[a] Belkin2003LaplacianEF

Node Embedding: HOPE

Higher-Order Proximity preserved Embedding (HOPE)[a] objective function is:

$$y = \min \sum_{i,j} |S_{ij} - y_i y_j^T|$$

Said differently, its objective is to minimize the difference between the graph **similarity** S_{ij} and the similarity in the embedding, computed as the product of embedding vectors. Vectors are imposed to be normalized, thus $y_i y_j^T$ corresponds to the *cosine similarity*. Two nodes close (resp. far) in the graph should therefore be close (far) in the embedding. Relative distances should also be conserved.

[a] ou2016asymmetric

LE - HOPE: Complexity

Discovering the solution of LE and HOPE methods can be done efficiently using matrix decomposition approaches. For instance, finding the embedding according to LE in d dimensions for the adjacency matrix can be formalized as finding the d eigenvectors of lowest eigenvalues of $D^{-1/2}LD^{-1/2}$, with D the degree matrix and L the Laplacian matrix.
The computation of the S matrix however, if it is not the adjacency matrix, can be costly since in the general case, it requires n^2 computations.

Random Walk NN based embedding

In recent years, new approaches based on random walks and neural networks have encountered a large success and relaunched a large interest in graph embedding for various applications. They are transpositions of techniques developed for the embedding of words to the graph setting.

Word Embedding

Machine Learning on text suffers from a problem similar to Machine Learning on graphs: words are not numbers and cannot be naturally represented as (meaningful) vectors. Word embedding objective is to assign a (low dimensional) vector to each word such as two words with **similar semantic** have similar vectors.

Matrix decomposition and Eigenvectors

A diagonizable matrix A can be factorized using eigenvectors as follows:

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{-1}$$

where Q is the $n \times n$ matrix whose ith column is the eigenvector q_i of A, and $\mathbf{\Lambda}$ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues, $\mathbf{\Lambda}_{ii} = \lambda_i$. Keeping as embedding the eigenvectors associated with the largest eigenvalues means that we can reconstruct the original matrix with a good precision. This is the same method used by PCA (Principal Component Analysis), on a covariance(or correlation) matrix, which is also a form of similarity matrix.

Word Embedding: word2vec - context

The principle proposed in a famous method called word2vec is to use the context, i.e., the words encountered around a word in sentences of a corpus, to discover the semantic similarity. In summary, the more two words are encountered in a same context, the more they are considered similar. For instance, a corpus might contain sentences such as: *the dog eat dry food*, and *the cat eat dry food*: *cat* and *dog* are found in similar contexts, which should drive them closer in the embeddding. In other sentences, their contexts differs, which should drive them away in the embedding.

Word Embedding: Skipgram/word2vec

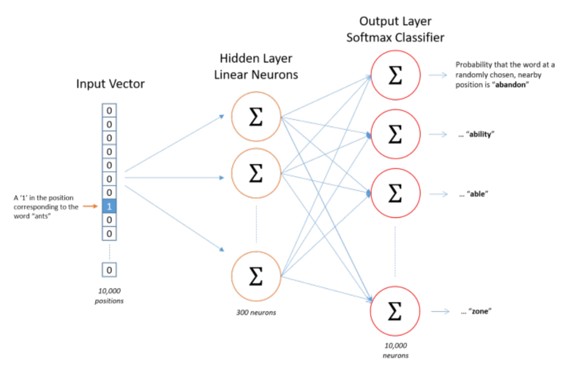
In practice, a word is considered to be in the context of another if it is at a distance less than l in a sentence. From a corpus, one then extracts the probability $p(w_j|w_i)$ for each word w_i, that a word taken at random in its context is w_j.
The objective function of word2vec can be expressed as:

$$y = \min \sum_{(i,j)} p(w_j|w_i) - \sigma(y_i y_j^T)$$

with σ the softmax function defined as $\frac{e^x}{\sum e^x}$, a function commonly used in neural networks to add non-linearity while ensuring that the solution is a probability.

Skipgram: a neural network formulation

The skipgram algorithm is solved, in practice, using tools and methods of neural networks, which make it scalable to large datasets. It can then be represented as follows[a]:



[a] https://towardsdatascience.com/word2vec-skip-gram-model-part-1-intuition-78614e4d6e0b

Word2vec efficacy

Word2Vec (and following word embedding approaches) have encountered an enormous success in the Natural Language Processing domain, and are nowadays used for most practical tasks such as automatic language translation, sentiment analysis, personal assistants, etc.
Various other fields, including network science, have therefore adapted the mechanism to embed other complex elements.

DeepWalk

DeepWalk[a] is the direct transcription of Word2vec to graphs. The principle is to generate random walks in the graph, playing the role of sentences in a corpus. The probability of finding a word in the vicinity of another therefore translates in the probability of encountering a node in a random walk from another.
To sum up, the objective function can now be expressed as:

$$y = \min \sum_{(i,j)} p(n_j|n_i) - \sigma(y_i y_j^T)$$

with $p(n_j|n_i)$ the probability to encounter node n_j in a random walk of a chosen length starting from node n_i. Its objective is therefore to make the distance in the embedding proportional to a random walk based distance in the graph.

[a] Perozzi, Al-Rfou, and Skiena 2014.

DeepWalk complexity

Contrary to matrix decomposition based approaches, DeepWalk do not requires explicitly a similarity matrix S. All pairs (i,j) are obtain by k random walks of length l starting from each of the n nodes. The complexity of obtaining the input data is therefore in $\mathcal{O}(n)$ (l and k being small constants).

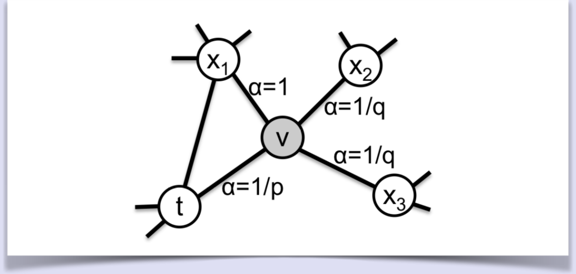
Node2vec

Node2vec[a] is a popular variant of DeepWalk, introducing **biased random walks**. Two parameters guide the random walks: p decreases the probability to revisit the previous node, while q decreases the probability to explore farther nodes, i.e., nodes that were not neighbors of the origin node. It allows to mimic **breadth-first** or **depth-first** like exploration of the graph, capturing more local or more global network structures.

[a] Grover and Leskovec 2016.

Node2vec

Illustration of random walk procedure in node2vec. (Figure from (Grover and Leskovec 2016))



The walk just transitioned from t to v and is now evaluating its next hop. Edge labels indicate the bias as a function of parameters p and q.

Role Embedding

Node2Vec and DeepWalk are **locational** embedding: nodes with similar vectors tend to be close in the graph, in term of graph distance.

Another notion of graph similarity is **role** similarity. Two nodes have similar roles in the graph if their neighborhood is similar, **ignoring node labels**.

Role2Vec — Struc2Vec

Two popular methods for role embedding are Struc2Vec[a] and Role2Vec[b]. They are based on a similar principle: as DeepWalk, they use random walks and SkipGram to generate embedding from contexts. But instead of generating sequences composed of the **labels** of encountered nodes, it generate contexts based on the **attributes/labels/features** of encountered nodes. Nodes with similar vectors thus corresponds to nodes that tend to encounter **nodes with similar properties** in random walks starting from them.

Examples of properties could be node features (age, genre, etc.) or structural properties (degree, clustering coefficient, graphlet belonging, etc).

[a] Ribeiro, Saverese, and Figueiredo 2017.

[b] Ahmed et al. 2019.

Node Classification with embeddings

Machine Learning algorithms such as Logistic Regression or Decision Tree can be trained to predict a property of a node from a vector of features representing the node property. We have seen in a previous class that these features could be manually chosen heuristics such as node centralities.

Vectors yielded by embedding algorithms can naturally be used in the same way. Locational embeddings could be used, for instance to attribute category to objects or political opinions to social media accounts, while role embedding could be used to identify suspicious accounts in social media.

Link Prediction with embeddings: unsupervised

If we consider that the property captured by the embedding is correlated with the probability of being connected by an edge, then the distance in the embedding can be used a heuristic for link prediction.

For instance, with LE and HOPE with $S = A$ or with random walks based approach, the embedding tries to put pairs of nodes connected by an edge closer than unconnected ones. As a consequence, we can assume that the closer two nodes are in the embedding, the more likely it is that they should be connected by an edge.

Link Prediction with embeddings: supervised

In the second approach, we consider each dimension of the embedding as a node feature. For each pair of nodes, we compute a vector by **combining nodes' vectors**.

As with heuristics, a machine learning algorithm is then trained to predict, from the combined vector, how likely it is to have an edge between nodes.

Combining node vectors

There are several methods to combine node vectors. Although it has been observed empirically that the Hadamard product often gives the best results, this choice is often considered a **hyper-parameter**, i.e., all variants are tested and the most efficient is used for the final prediction.

The most used operators are:

Average	(a+b)/2
Concat	$[a_1, a_2, ..., a_d, b_1, b_2, ..., b_d]$
Hadamard	$[a_1 * b_1, a_2 * b_2, ..., a_d * b_d]$
Weighted L1	$[\lvert a_1 - b_1\rvert, \lvert a_2 - b_2\rvert, ..., \lvert a_d - b_d\rvert]$
Weighted L2	$[(a_1 - b_1)^2, (a_2 - b_2)^2, ..., (a_d - b_d)^2]$

with $a = [a_1, a_2, ..., a_d]$ and $b = [b_1, b_2, ..., b_d]$

How many dimensions?

There is no universal method to choose a number of dimensions for the embedding. In the literature, for large graphs, a common value is $d = 128$ dimensions. As a general rule, $d << n$.

Too few dimensions limit the capacity to embed complex information, but too many dimensions limit cross-learning, generalization,(i.e., overfits), and make learning from embeddings harder. More dimensions also require (usually) more computation.

Visualization and embeddings

Network visualization is a domain in itself. Its objective is to assign positions to nodes in a two dimensional space in order to plot the network in a meaningful way.

Algorithms such as HOPE or node2vec are not well adapted to generate visually interpretable 2-dimentional spaces, in part because the distance in the embedding is based on the cosine distance, while humans naturally assume euclidean distance. When embeddings are used for visualization, the first step consists in embedding in a moderate number of dimensions (e.g., 128), and in a second step, a dimensionality reduction algorithm more adapted for visualization such as T-SNE[a] is used to reduce this number to 2 dimensions.

[a] Van der Maaten and Hinton 2008.

Community detection with embeddings

Community detection in graphs is equivalent to the **clustering** task in non-network data. Intuitively, clustering methods try to group elements with similar features, and separate those that are different. Applying a clustering algorithm such as **k-means** on an embedding will therefore yield clusters of nodes, that can be considered as communities. In practice, it has been observed that communities detected by this approach are often similar to those found by modularity maximization.

Note that unlike with modularity, it is often required to provide the desired number of clusters –or a distance scale– to clustering methods.

Going Further

Python Libraries: Karate-club(Rozemberczki, Kiss, and Sarkar 2020)(Goyal and Ferrara 2018a)

Surveys on graph embedding: (Goyal and Ferrara 2018b)(Cai, Zheng, and Chang 2018)(Cui et al. 2018)

Graph Embedding and link prediction (Mara, Lijffijt, and De Bie 2020)

Distances in Graph embedding (Vaudaine, Cazabet, and Largeron 2020)

Comparing heuristics and Graph Embedding for link prediction (Sinha, Cazabet, and Vaudaine 2018)

Stacking embeddings and heuristics models for link prediction: (Ghasemian et al. 2020)

References

[1] Nesreen K Ahmed et al. “role2vec: Role-based network embeddings”. In: *Proc. DLG KDD*. 2019.

[2] Hongyun Cai, Vincent W Zheng, and Kevin Chen-Chuan Chang. “A comprehensive survey of graph embedding: Problems, techniques, and applications”. In: *IEEE Transactions on Knowledge and Data Engineering* 30.9 (2018), pp. 1616–1637.

[3] Peng Cui et al. “A survey on network embedding”. In: *IEEE Transactions on Knowledge and Data Engineering* 31.5 (2018), pp. 833–852.

[4] Amir Ghasemian et al. “Stacking models for nearly optimal link prediction in complex networks”. In: *Proceedings of the National Academy of Sciences* 117.38 (2020), pp. 23393–23400.

[5] Palash Goyal and Emilio Ferrara. “GEM: a Python package for graph embedding methods”. In: *Journal of Open Source Software* 3.29 (2018), p. 876.

[6] Palash Goyal and Emilio Ferrara. “Graph embedding techniques, applications, and performance: A survey”. In: *Knowledge-Based Systems* 151 (2018), pp. 78–94.

[7] Aditya Grover and Jure Leskovec. “node2vec: Scalable feature learning for networks”. In: *Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining*. 2016, pp. 855–864.

[8] Laurens van der Maaten and Geoffrey Hinton. “Visualizing data using t-SNE”. In: *Journal of machine learning research* 9.Nov (2008), pp. 2579–2605.

[9] Alexandru Cristian Mara, Jefrey Lijffijt, and Tijl De Bie. “Benchmarking Network Embedding Models for Link Prediction: Are We Making Progress?” In: *2020 IEEE 7th International Conference on Data Science and Advanced Analytics (DSAA)*. IEEE. 2020, pp. 138–147.

[10] Bryan Perozzi, Rami Al-Rfou, and Steven Skiena. “Deepwalk: Online learning of social representations”. In: *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*. 2014, pp. 701–710.

[11] Leonardo FR Ribeiro, Pedro HP Saverese, and Daniel R Figueiredo. “struc2vec: Learning node representations from structural identity”. In: *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*. 2017, pp. 385–394.

[12] Benedek Rozemberczki, Oliver Kiss, and Rik Sarkar. “Karate Club: An API Oriented Open-source Python Framework for Unsupervised Learning on Graphs”. In: *Proceedings of the 29th ACM International Conference on Information and Knowledge Management (CIKM '20)*. ACM. 2020, pp. 3125–3132.

[13] Aakash Sinha, Rémy Cazabet, and Rémi Vaudaine. “Systematic biases in link prediction: comparing heuristic and graph embedding based methods”. In: *International Conference on Complex Networks and Their Applications*. Springer. 2018, pp. 81–93.

[14] Laurens Van der Maaten and Geoffrey Hinton. “Visualizing data using t-SNE.” In: *Journal of machine learning research* 9.11 (2008).

[15] Rémi Vaudaine, Rémy Cazabet, and Christine Largeron. “Comparing the preservation of network properties by graph embeddings”. In: *International Symposium on Intelligent Data Analysis*. Springer. 2020, pp. 522–534.