Next Waves in Veridical Network Embedding

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Abstract
Embedding nodes of a large network into a metric (e.g., Euclidean) space has become an area of active research in statistical machine learning, which has found applications in natural and social sciences. Generally, a representation of a network object is learned in a Euclidean geometry and is then used for subsequent tasks regarding the nodes and/or edges of the network, such as community detection, node classification and link prediction. Network embedding algorithms have been proposed in multiple disciplines, often with domain-specific notations and details. In addition, different measures and tools have been adopted to evaluate and compare the methods proposed under different settings, often dependent of the downstream tasks. As a result, it is challenging to study these algorithms in the literature systematically. Motivated by the recently proposed PCS framework for Veridical Data Science, we propose a framework for network embedding algorithms and discuss how the principles of predictability, computability and stability (PCS) apply in this context. The utilization of this framework in network embedding holds the potential to motivate and point to new directions for future research.

Keywords:Network Embedding, Representational Learning, Latent Variable Models, Feature Engineering, Veridical Data Science.

1 Introduction

Complex relationships amongst a collection of objects can be encoded in network data. A major challenge with data of this form is that it is difficult to directly use this data structure for certain analysis that provides insight into the properties of the network, such as for clustering nodes, community detection, and predicting future links between nodes. For example, in social networks, there may be interest in identifying whether two users are friends [3, 16], or which product a user would be interested in [38]. In linguistic networks, semantic and syntactic relationships between different words can be of interest [31]. In biological networks, we may wish to identify relationships between a specific gene and certain symptoms or diseases or the existence of interaction between proteins [48, 16], while in chemical networks we may wish to predict certain properties of a molecule [15]. Most methods which aim to address these tasks, including most commonly used machine learning methods, generally require data consisting of features (i.e., vectors) in Euclidean space. This allows the many well developed procedures for statistical learning in Euclidean geometry, such as gradient based optimization, to be applied. Thus, methods which can fully represent this network structure in a well understood geometry are crucial to providing further analysis of network data, and it is an active area of research in both the statistics and machine learning communities.

Many promising methods have been proposed so far, some of which take ideas from language models. For example, Deepwalk [38] and node2vec [16] regard nodes as words and random walks as sentences to learn the low dimensional representations by SkipGram, a Natural Language Processing (NLP) model. Such approaches generate interesting results but may be worrisome in that the way words compose together to make a sentence is not necessarily the same as how nodes connect in a graph. The latter may contain richer graph structural information.

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A defining feature of all network embedding methods is the subsequent analysis which will be performed using the learned representation. This is crucial in analysing the performance of a method. As such, one needs to identify the features of the network which will be required for this analysis, and which should be retained by the embedding process.

In this paper, we summarise the problem of network embeddings for a statistical audience, detailing the key features of any network embedding method. We illustrate and discuss some of the most commonly used algorithms. We then discuss network embedding in the context of the Veridical Data Science principles recently proposed in [55]. Finally, we consider some of the open problems in network embedding for the statistical community, including the use of more general distributions of network features, the opportunities offered by embeddings in non-Euclidean spaces, and the need for more rigorous evaluation and comparison of the embedding methods proposed.

2 Problem Setup

A network is usually represented by $G = (V, E)$, where $V$ is a set of $n$ vertices or nodes, and $E$ is the set of edges between these vertices, together with an adjacency matrix $A$, with $A_{ij}$ indicating the presence or absence of an edge between nodes $i$ and $j$. The edges between nodes can be weighted or unweighted, where, if there is a weight associated with an edge between nodes $i$ and $j$, it is denoted as $W_{ij}$, an element of a weight matrix $W$. It is also possible for these edges to be either directed or undirected. In general, it is assumed that there are no self edges. Similarly, it is possible that there is also some other $m$ covariates associated with each node, which can be expressed as a vector $x_i \in \mathcal{X} \subseteq \mathbb{R}^m$. Edge features are also possible and can be similarly defined.

The goal of network embedding is to map the information present in the network to some representation space, $Z$, which is assumed to be a metric space with associated metric $\rho$. That is, we wish to construct a mapping

$$\Phi : G \times \mathcal{X} \to (Z, \rho).$$  \hfill (1)

When constructing a network embedding, many aspects of the problem need to be considered.

- Which space do we wish to represent the network in?
- What features of the network do we require this embedding to preserve and how do we evaluate whether these features are preserved?
- If we had nodal covariates present in the network, how do we best combine them with the learned representation?
- Given that we have constructed an embedding of our network, what task will this embedding then be used for?

We discuss each of these concerns below.

Representation space

When performing a network embedding, the first question which must be addressed is the space $Z$ which the network will be embedded in. The most popular and practical choice is possibly $Z = \mathbb{R}^d$. It is generally assumed that $d \ll n$, in which case this will also lead to a lower dimensional representation of the network. This dimension reduction may lead to improved computational performance if this representation is then used in further tasks.

While machine learning methods have exclusively used Euclidean geometry for network embedding, in the context of statistical latent space models, other geometries have been considered. Other representation spaces such as the $d$-dimensional unit sphere $S^d$ [28], and the hyperbolic space $\mathbb{H}^d$ are also possible. The hyperbolic space, for example, may capture some tree-like structure of certain networks in real life. See Smith et al [15] for a review of the different latent space geometries used in practice.

Features of network to be preserved

Given that we have chosen a space in which we wish to embed our network, we must then decide what features present in the network we want this embedding to preserve, and how we evaluate the preservation of these features in our embedding space. The structure of the network we wish the embedding to reflect can also be crucial for later tasks using the learned representation. One such example is community detection. An embedding which will be used for community detection should require that if there is a
community structure, based on a quantifiable definition, present in the network, the resulting embeddings of nodes should reflect this. This can be challenging when there are multiple community structures present, such as different subsets of nodes displaying distinct community structure. Nodes in the same community should be embedded closer to each other than nodes in different communities, leading to an effective clustering solution.

Many embeddings seek to preserve a form of “proximity” between nodes to capture similarity between these nodes. Proximity can be captured by both the presence of edges between nodes and also by the weights of these edges (if applicable). The first-order proximity, for example, is commonly used to capture direct similarity between nodes that share an edge. If there is an edge from node $i$ to node $j$ with a large weight $W_{ij}$, then node $i$ and node $j$ are regarded to have high first-order proximity. If the task is clustering, and it is believed that people who communicate frequently tend to belong to the same group, then the first-order proximity may be a good metric to capture this [3, 1, 46, 53].

Some other common features in the literature are second-order proximity [46, 53], $k$-step transition probability [10], homophily [16], structural equivalence [10], and features which capture other additional information associated with nodes such as attributes of nodes [17, 31], text [53], or labels [44]. For example, the second-order proximity measures neighborhood differences. In a social network, it explores the idea that if two people have many friends in common, then they may be friends as well, even without the presence of a direct edge between them. The $k$-step transition probability regards the weight on edge $W_{ij}$ as an unnormalized transition probability in the context of a random walk on nodes of the network. If the current state of a random walk is at node $i$, then the random walk will jump to node $j$ with probability $\frac{W_{ij}}{\sum_k W_{ik}}$ at the next step. A high transition probability from node $i$ to $j$ can be an indication that they are “close” in some sense, which then indicates that they should also be similar in the embedding space. There is also homophily, which requires that people from the same community should be embedded closely to each other, along with structural equivalence, requiring that nodes with alike structural roles (e.g. the center of a community or a hub node) should be embedded similarly [10].

The local neighborhood structure is also explored by some models in a variety of ways. For example, a neural network model can be set up to aggregate information from neighboring nodes at each layer [15, 17, 25].

Another important question is how best to incorporate nodal covariates into either learning the representation or being used with the representation for further tasks. For example, covariates could be used directly to learn the representation [20], as is commonly done in neural network embedding models [17, 23, 51]. It seems natural for embedding methods to also preserve measures of proximity defined on these nodal covariates, of which a detailed review is given in [13].

### 3 Similarity in the representation space

Having chosen an embedding for the network in the representation space we can then consider what similarity is present in this space. Most embeddings are constructed based on the idea that “similarity” in the network should be represented by a “similarity” in the representation space. While there are many choices of network similarity as discussed above, similarity in the representation space has been less explored. In general, where the embedding space is a metric space, then the metric distance between the embedding of nodes provides an automatic similarity. In Euclidean geometry, the related (but not equivalent) dot product is also commonly used, due to computational convenience. Alternative similarity measures include cosine similarity and other variants based on angular separation [19]. These similarities are often used on the unit sphere, where the cosine similarity $s(z_i, z_j) = \frac{z_i^T z_j}{\|z_i\| \|z_j\|}$ coincides with the dot product up to rescaling, and the angular similarity $s(z_i, z_j) = \arccos \left( \frac{z_i^T z_j}{\|z_i\| \|z_j\|} \right)$ coincides with the spherical distance.

### 3.1 Learning the representation

Given a choice of embedding space, the network features we wish to preserve, and the concept of similarity in the embedding space, we must then consider the procedure for learning this embedding. Several procedures have been considered in learning the representation of a network. We first describe some of the most commonly used, before discussing the evaluation of these learning methods.

For unsupervised representation learning, most methods are developed based on the idea of “matching the similarities” of the network and the space. That is, nodes that are “close” in the original network...
should also be “close” in the representation space. One approach is to assume that there is some generating process from the representations to the features of the network or vice versa. The variables to be optimized can be any parameters in the generating process including the representation itself. The generating process can be deterministic, such as using a neural network \[53\] \[17\]. The learning can then be carried out by minimizing the reconstruction error or matching the similarities. For example, SDNE \[53\] uses a deep auto-encoder with the rows of the graph adjacency matrix \(A\) (or the weight matrix for weighted graphs) as inputs. The loss function is

\[
L = L_2 + \alpha L_1 + \nu L_{reg}
\]

\[
= \| (\hat{A} - A) \odot B \|_F^2 + \alpha \sum_{i,j=1}^{n} A_{i,j} \| z_i - z_j \|_2^2 + \frac{\nu}{2} \sum_{k=1}^{K} (\| W^{(k)} \|_F^2 + \| W_r^{(k)} \|_F^2),
\]

where \(z\) is the representation, and \(\hat{A}\) is the reconstruction of input \(A\) based on \(z\). \(\| \cdot \|_F\) is the Frobenius norm of matrix. \(W^{(k)}\) and \(W_r^{(k)}\) are the weights of the encoding and decoding neural networks. \(L_1\) matches the first-order proximity of the two spaces, \(L_{reg}\) is for regularization, and \(L_2\) measures the reconstruction error weighted by \(B\), with \(B_{ij} = 1\) if \(A_{ij} = 0\) and \(B_{ij} = \beta > 1\) if \(A_{ij} > 0\). \(L_2\) seeks to preserve the second-order proximity, i.e. the neighborhood similarity, since the row of the adjacency matrix can be viewed as a characterization of a vertex’s neighbors.

An explicit generating process is not always required. One alternative is to directly consider two similarity measures, \(S(v_i, v_j)\) between nodes in the network, and \(S'(z_i, z_j)\) between their representations in the representation space. We can then define a loss function based on these similarities, with one natural choice being

\[
L(S, S') = \sum_{i,j} S(v_i, v_j) S'(z_i, z_j) + R(z),
\]

for some constraint or regularization term on the embedding, \(R(z)\). For example, in the Laplacian eigenmap method \[4\], \(S(v_i, v_j) = W_{ij}\) is the first-order proximity, \(S'(z_i, z_j) = \| z_i - z_j \|_2^2\), \(R(z)\) is some normalizing constraint on \(z\), and \(L\) is to be minimized. Similarly, in GraRep \[10\], \(S(v_i, v_j) = p_k(v_i | v_j)\) is taken as the \(k\)-step transition probability and \(S'(\Phi(v_i), \Phi(v_j)) = \log \sigma(z_f^T z_i)\), where \(\sigma(x) = \frac{1}{1+\exp(-x)}\), and \(\Phi(v_i) = (z_i, z'_i)\) which is associated with two vectors. \(z'_i\) is the representation when \(v_i\) is viewed as “context” (more details are given in Section \[4\]). In this case \(L\) is then maximized. Most unsupervised methods are of this form, minimizing some reconstruction loss between the network and the representation. We summarize some unsupervised methods, along with their key properties, in Table 1.

### Table 1: Some unsupervised methods, their similarity measures and the corresponding loss function used to learn the representation.

| Methods          | \(S(v_i, v_j)\) | \(S'(z_i, z_j)\) | Loss Function                                                                 |
|------------------|-----------------|------------------|-------------------------------------------------------------------------------|
| Laplacian eigenmap \[4\] | \(W_{ij}\) | \(\| z_i - z_j \|_2^2\) | \(\sum_{i,j} S(v_i, v_j) S'(z_i, z_j), \text{ s.t. } z^T D z = I.\)             |
| Graph factorization \[11\] | \(W_{ij}\) | \(z_i^T z_j\) | \(\frac{1}{2} \sum_{(i,j) \in E} (S(v_i, v_j) - S'(z_i, z_j))^2 + \frac{\lambda}{2} \sum_i \| z_i \|^2\) |
| LINE (1st-Order) \[46\] | \(W_{ij}\) | \(\log \sigma(z_f^T z_j)\) | \(-\sum_{i,j} S(v_i, v_j) S'(z_i, z_j)\)                                    |
| LINE (2nd-Order) \[46\] | \(W_{ij}\) | \(\sum_{\exp(z_f^T z_i)} \) | \(-\sum_{i,j} S(v_i, v_j) S'(z_i, z_j)\)                                    |
| GraRep \[10\]     | \(p_k(v_j | v_i)\) | \(\log \sigma(z_f^T z_j)\) | \(\sum_{i,j} \left[ S(v_i, v_j) S'(z_i, z_j) + \frac{\lambda}{2} \| z_i \|^2 \right] \) |
| Deepwalk \[38\]    | co-occurrence  | \(\log(\sigma(z_f^T z_{v_i})\) | \(\log(\sigma(z_f^T z_{v_i})) + \sum_{i=1}^{K} E_{v_i \sim p_n} \log(1 - \sigma(z_f^T z_{v_i}))\) |
| Node2vec \[10\]    | in RWs          |                  |                                                                               |

If the generating process is probabilistic, parameterized by the representations of the nodes, then the representations can be learnt by maximizing the likelihood function. Deepwalk \[38\] and Node2vec \[10\], for example, maximize the co-occurrence probability of nodes appearing in a random walk across the network. A fully generative probabilistic model is also possible. Smith et al. \[45\] reviewed a number of
parametric models of the form:

\[ P(\text{edge between } (v_i, v_j)) \overset{\text{indep}}{\sim} \text{Bernoulli}(p_{ij}), \quad i \neq j, \]

\[ \logit(p_{ij}) = \alpha + s(z_i, z_j), \]

\[ z_i \overset{i.i.d.}{\sim} P(f|\psi), \]

where \( z_i = \Phi(v_i) \) is the representation of node \( v_i \), and \( s(\cdot, \cdot) \) is some similarity measure such as distance or dot product. We discuss latent space models of this form in more detail below.

For supervised and semi-supervised learning, the learnt representations can be directed towards specific tasks, and are usually able to achieve better performances on prediction than the unsupervised methods. In such cases, a downstream process can immediately take the representations as input to perform certain task of interest, along with a task-specific loss to be optimized. For example, Tu et al. [47] applied support vector machines (SVM) to the representations learnt by Deepwalk for multi-label classification. The version of Deepwalk based on matrix factorization was used. Apart from the matrix factorization loss, the SVM classification loss on those labeled nodes was also added, which results in a mix of supervised and unsupervised loss:

\[
\min_{Z, Y, W, \xi} \mathcal{L} = \min_{Z, Y, W, \xi} \mathcal{L}_{DW} + \frac{1}{2} \|W\|_2^2 + C \sum_{i=1}^T \xi_i,
\]

\[ \text{s.t. } w_i^T z_i - w_j^T z_i \geq 1_{i \neq j} - \xi_i, \forall i, j, \]

where \( \mathcal{L}_{DW} = \|M - Z^T Y\|_2^2 + \frac{1}{2} (\|Z\|_2^2 + \|Y\|_2^2) \).

A purely supervised loss is also possible. There is a rich literature on deep learning on networks (see [56] for a detailed review). Despite the many different architectures that are adopted, many of the neural network models are equipped with a supervised loss. The network takes the graph and the associated node/edge features as input, and produces certain output for the task of interest. The error between the output and the true response is then optimized to learn the network [44, 25, 15, 20]. In the Message Passing Neural Networks [15] framework which unifies a number of earlier methods, the last hidden states (layer) before output can be taken as the representations of the nodes.

The optimization of the loss function, after possible approximations and relaxations, is often carried out by (stochastic) gradient descent [7], and sometimes can be run in parallel if the update is sparse [11, 35, 16]. If the final optimization problem is convex, then techniques in convex optimization can be applied [19]. In some cases, matrix factorization can also be used for optimizing the loss function [10], and recent work has attempted to rephrase common random walk methods under the framework of matrix factorization [29], which could lead to better interpretation of these methods. However, this matrix factorization approach cannot readily scale to large networks, and as such is not of current computational benefit.

Assessing the representation Having constructed our representation we can then assess its performance. Assessment of the representation can be in terms of reconstruction of the original network and also the subsequent inference formed based on the embedding [13]. For downstream inference using the network representation, common tasks include node classification, link prediction and node clustering. These tasks often present further decisions before the final analysis is complete. For example, to perform node clustering using a learned representation, the clustering method to be used and the number of clusters to be considered must also be specified. Similarly, if the goal is link prediction then a sample of the observed links are treated as the test set and removed, with the embedding fit on the remaining edges [27]. As such, when evaluating the overall method on these downstream tasks alone, it is difficult to precisely quantify the effect of the specific embedding chosen. It is thus important to specify which goal is prioritized as part of the network embedding when determining the method to be used. The PCS framework provides a natural workflow to address these concerns.

## 4 Review of representative methods

### Methods from statistics

**Spectral Clustering** One of the most well studied models for the clustering on nodes in a network, in the statistical literature, is spectral clustering. This implicitly constructs an embedding of the network
using a collection of eigenvectors from the spectral decomposition of the graph laplacian. The eigenvectors of the graph laplacian corresponding to the $k$ smallest eigenvalues are then used to construct the matrix $U \in \mathbb{R}^{n \times k}$, where the $i$th row can be thought of as a $k$ dimensional representation of the $i$th node. A distance-based clustering method, such as $k$-means clustering, is then applied to the representation of these nodes in $\mathbb{R}^k$.

Spectral clustering has been widely studied in the statistical literature and as such is one of the few network embedding models for which theoretical properties are known, including consistent recovery of communities in networks [23], and of an underlying latent space [12], along with more general consistency results [52]. However, it has also been shown to not be robust in the presence of outliers [9]. Moreover, spectral clustering is not always computationally feasible for large networks, requiring an expensive singular value decomposition, though it can be accelerated using locally optimal block preconditioned conjugate gradient [21], since only the eigenvectors corresponding to the smallest eigenvalues are needed.

We summarize this and other methods we will discuss further using ideas from model cards [32] in Appendix A.

**Latent Space Models** Another model which is commonly considered to represent networks in the statistical community are latent space models for social networks [19], of which the stochastic block model [55] is a popular special case. Latent space models of this form posit that the true network given by an adjacency matrix can be represented in some lower dimensional latent space and then propose estimation procedures to learn the positions of the nodes in this latent space. These differ somewhat from other network embeddings, which just aim to represent the network in some latent space. This model and extensions, which include clustering in the latent space, learning both the latent space and clusters in that space [15], have been fit using both MCMC and variational inference methods [19, 40]. These inference procedures also inhibit scaling this method to larger networks, due to the expensive likelihood computation required for parametric models of this form, although approximations have been developed [40].

**Methods from machine learning**

**Random-walk based network embedding** Motivated by the advance of natural language processing (NLP), a number of network embedding algorithms have been developed in recent years. Popular models include DeepWalk [38] and Node2vec [16]. The main idea is to view each node in the graph as a word in the corpus. Sentences in NLP correspond to random walks on a graph which are generated according to certain rules. The word embedding methods in NLP can then be applied to learn the network embedding.

Different methods have been used to generate random walks exploring different features of a network. DeepWalk [38] and GraRep [10] do this by directly using the network edge weight. The weights on edge $W_{ij}$ are regarded as unnormalized transition probabilities. If the current state is at node $i$, then the random walk goes to node $j$ with probability $\frac{W_{ij}}{\sum_{k} W_{ik}}$ at the next step, which is basically a finite-state Markov model. Node2vec [16] modified the above transition probability by introducing two additional hyperparameters, which can adjust the random walk between Breadth-first Sampling and Depth-first Sampling, and thus become a second-order Markov chain. After obtaining the random walks, certain objective function is optimized. For example, DeepWalk applies SkipGram [30] with gradient descent steps to minimize $-\log \Pr \left( \{v_{i-w}, \cdots, v_{i-1}, v_{i+1}, \cdots, v_{i+w}\} | \Phi(v_i) \right)$, where $\Phi(v_i)$ is the representation of node $v_i$. For each vertex $v_i$ in the random walk $(v_{i-w}, \cdots, v_{i+w})$ and a pre-specified window size $w$. A natural and common choice for $\Pr (\cdot | \Phi(v_i))$ is to use the softmax function, which assigns independently, for each $v_j$,

$$\Pr(v_j | \Phi(v_i)) = \frac{e^{z_j^T z_{v_i}}}{\sum_{v_k \in V} e^{z_k^T z_{v_i}}}$$

where $\Phi(v_i) = (z_{v_i}, z_{v_i}')$. Each vertex has two roles, either being the “centered node” or the “context node” within the local window of other “centered node”. So two different vectors $z_{v_i}, z_{v_i}'$ are associated respectively. The “centered node” representation $z_{v_i}$ is usually taken as the final representation for output.

However, objectives involving softmax function are not computationally feasible for large networks, since calculating the denominator takes $O(|V|)$ time. One approximation is to use the hierarchical softmax approximation [38, 39]. It builds a binary tree with all the nodes as its leaves. With an input $z_{v_i}$ at the root, the probability $\Pr(v_j | \Phi(v_i))$ is calculated along the path from the root to the leaf of $v_j$, reducing the computational complexity to $O(\log |V|)$. 


Another popular approximation is negative sampling \([29, 16, 10]\). It approximates \(\log \Pr(v_i | \Phi(v_i))\) by
\[
\log(\sigma(z_{v,i}^T z_{v_i})) + \sum_{l=1}^k E_{v_l \sim P_n} \log(\sigma(-z_{v_l}^T z_{v_i})),
\]
where \(\sigma(x) = \frac{1}{1 + \exp(-x)}\) and \(P_n\) is some noise distribution, positing a good model should be able to distinguish data from noise. In practice, \(P_n\) is usually taken as the unigram distribution raised to \(3/4\) power: \(P_n(v_i) \propto [\text{frequency of } v_i]^{3/4}\). Though theoretical guarantees do not exist, it has been found that this choice outperforms several other candidates significantly, such as the unigram and the uniform distributions \([30]\). Corresponding experiments for network embeddings are still absent according to our knowledge. The objective \((2)\) is then maximized by stochastic gradient descent \([7]\). At each iteration, \(v_l, (l = 1, \cdots, k)\) are sampled from \(P_n\), and then a usual gradient ascent step is performed. When the window size is small, each gradient step only updates a small portion of the embedding vectors. Parallel optimization can also be made possible and has been used in practice \([41, 38, 16]\).

**Neural Network Models** There is a rich literature on neural network methods on graphs (see \([56]\) for a detailed review). The graph neural network (GNN) \([44]\) was first proposed in a recursive way:
\[
z_n = f_w(l_n, l_{oo[n]}, z_{oo[n]}, l_{oo[n]}), \quad o_n = g_w(z_n, l_n),
\]
where \(z_n, l_n, l_{oo[n]}, z_{oo[n]}, l_{oo[n]}\), \(o_n\) are the representation of node \(n\), the label of \(n\), the labels of edges with \(n\) being one vertex, the representations of nodes in the neighborhood of \(n\), the labels of nodes in the neighborhood of \(n\), and the output, respectively. \(f_w\) and \(g_w\) are some parametric functions. Each step of the semi-supervised learning process is carried out by first iterating the equation to the unique fixed point, and then performing a gradient descent to minimize the error between the output and the true response of the supervised nodes. One limitation of this model is that in order for the iteration scheme to give a (unique) fixed point, \(f_w\) is essentially required to be a contraction mapping with respect to a complete metric (from which the contraction mapping theorem guarantees the existence and uniqueness of a fixed point). Also, iterating the equation to convergence can be computationally expensive. Many neural network models have been proposed without this recursive definition, but with different convolutional network structures. Some spectral methods use the eigenvectors of the graph Laplacian to construct convolution operators \([8]\). Others may utilize the graph structure to aggregate information from neighbors at each layer to update the representations \([17, 25, 15]\). Message Passing Neural Networks (MPNN) \([15]\) unifies a number of earlier proposed convolutional neural network models. Its update is of the following form at the \((t + 1)\)th layer:
\[
m_v^{t+1} = \sum_{w \in N(v)} M_t(z_w^t, z_{vw}),
\]
\[
z_v^{t+1} = U_t(z_v^t, m_v^{t+1}),
\]
\[
\hat{y} = R(\{z_v^T v \in G\}).
\]
where \(M_t, N(v), z_v^t, e_{vw}, U_t, \hat{y}, R\) are learnable message functions, neighbors of node \(v\), the representation of \(v\) at time \(t\), edge feature, learnable vertex update functions, the output, a learnable readout function, respectively. Some neural network embedding methods, by design, can be generalized to unseen nodes, which is called inductive learning \([17]\). In that case, \(N(v)\) can be taken as a fixed size of neighbors, uniformly sampled from all neighbors of \(v\). The counterpart is transductive learning \([17]\), which requires all nodes to be present during model fitting.

Most of the above mentioned neural network models are supervised or semi-supervised, with a task-specific loss function minimizing the error between the outputs and the targets. There are also unsupervised deep learning methods such as deep autoencoder, GraphSAGE \([17]\), and Deep Graph Infomax \([51]\). Deep autoencoder methods, e.g. SDNE \([53]\), try to minimize the reconstruction error. GraphSAGE \([17]\) uses the following loss function on the final representations \(z_v, v \in V\):
\[
J_G(z_v) = -\log(\sigma(z_v^T z_u)) - QE_{v_u \sim P_n} \log(\sigma(-z_v^T z_{v_u})),
\]
where \(u\) is a node that co-occurs near \(v\) on fixed-length random walk, \(\sigma\) is the sigmoid function, \(P_n\) is a negative sampling distribution, and \(Q\) is the number of negative samples. Deep Graph Infomax \([51]\) is a recently proposed unsupervised method which outperforms previous unsupervised methods, along with some supervised models, on a number of benchmark datasets. It obtains the representations by a
function $\mathcal{E}$, which is usually a learnable neural network, acting on the features $\mathbf{X}$ and the graph adjacency matrix $\mathbf{A}$, with representation $\mathbf{Z} = \mathcal{E}(\mathbf{X}, \mathbf{A}) = (z_1, \ldots, z_N)$. The objective function aims to maximize the mutual information of $z_i$ and $s = \mathcal{R}(\mathbf{Z})$, a graph-level summary statistic, which can be taken as $\mathcal{R}(\mathbf{Z}) = \sigma \left( \frac{1}{N} \sum_{i=1}^{N} z_i \right)$ in practice. The objective function is:

$$
\mathcal{L} = \frac{1}{N + M} \left( \sum_{i=1}^{N} \mathbb{E}(\mathbf{X}, \mathbf{A}) [\log \mathcal{D}(z_i, s)] + \sum_{j=1}^{M} \mathbb{E}(\tilde{\mathbf{X}}, \tilde{\mathbf{A}}) [\log (1 - \mathcal{D}(\tilde{z}_j, s))] \right),
$$

where $(\tilde{\mathbf{X}}, \tilde{\mathbf{A}}) = C(\mathbf{X}, \mathbf{A})$ are the negative samples obtained by the (stochastic) corruption function $C$, and $\mathbf{Z} = (\tilde{z}_1, \ldots, \tilde{z}_M) = \mathcal{E}(\tilde{\mathbf{X}}, \tilde{\mathbf{A}})$ are the representations of negative samples. $\mathcal{D}$ is a discriminator which models the probability of the pairs $(z_i, s)$, and can be taken as $\mathcal{D}(z_i, s) = \sigma(z_i^T W s)$ in practice, with $W$ a learnable matrix.

Having considered this procedure, and the procedures previously discussed, some further questions naturally arise. In particular, for this method, is this algorithm stable under different but reasonable choices of the corruption function $C$ or the encoder $\mathcal{E}(\mathbf{X}, \mathbf{A})$? More generally, will the above methods work well on other networks of different sizes or from different domains? Is the computation required for each of these methods still feasible as the size of the network increases? It is desirable to address questions of this form in a systematic manner. This is a natural motivation to consider a framework for doing this. We will attempt to address these questions using the PCS framework for veridical data science [55].

**An illustrative example** To further illustrate the properties of some of these popular methods, we apply them to a large real network dataset. Here we consider an email network of all students and staff at a US university during one semester in the academic year 2003-2004. This data was first analysed by Kossinets and Watts [22]. We consider here the network of all students at the university, with available nodal information available. We treat this network as unweighted and undirected, with an edge existing between two students if they communicate via email during the semester. By taking the largest connected component, we obtain a graph with 18492 nodes and 260048 edges. We apply spectral embedding (implemented in scikit-learn [37]) and Deepwalk [38] to learn the latent representations, both with default settings. Figure 1 shows the embeddings projected to a plane. The spectral embedding is visualized using the first two eigenvectors, while the Deepwalk is visualized using the first two principal components from a 32-dimensional latent representation. The computational costs (in seconds, run on the same machine with 4 cores in parallel) are given in the right-hand side of Figure 1. The embeddings are then used to perform prediction on the academic fields (12 categories) and the student status (5 categories) for each student. Stratified 5-fold cross-validated accuracies are then computed for random forest classifier and logistic regression. Both classifiers were implemented in scikit-learn in default settings. Figure 2 shows the accuracy of prediction for the two methods on the test set. Since there is randomness in the random-walk as well as the training/test sets splitting, we repeat the whole procedure 100 times, with confidence bands showing the 2.5% and 97.5% sample quantiles.

From this systematic assessment, we can see that: (a) for latent dimension $d = 16, 32$, spectral embedding is better at predicting student status, but worse at predicting academic field compared with Deepwalk; (b) Deepwalk is computationally faster, but spectral embedding is more stable; (c) even for the same predicting task (predicting student status), different machine learning models (random forest and logistic regression) may provide different conclusions about the two methods. When using a random forest classifier, spectral embeddings achieve higher accuracy, while Deepwalk performs better when a logistic regression is used. Even this relatively simple network embedding task illustrates some of the components involved in constructing an embedding of a network and using this representation for further tasks. In the following section, we will discuss these components in the context of [55].

**5 A Veridical Network Embedding?**

The principles of predictability, computability and stability, as introduced in [55], can be used to construct a framework for veridical data science (VDS), and this framework is of clear benefit in the context of network embedding. We will discuss each of these principles in turn and comment on their role in the context of evaluating network embedding models.

*Predictability*, as defined in the PCS framework, seeks to construct a simple metric to evaluate how well a model represents relationships in the original data. This is in terms of some prediction target from
the data, which may be observed or extracted (supervised or unsupervised). Many papers describing network embedding models consider metrics of this form. For example, link prediction on held out edges [16] or classification of nodes with known labels [38]. The held out test set used for this evaluation should not differ from the original data.

We illustrate such a node classification task using the previously described embeddings shown in Figure 1. In Figure 2 we see that the performance of these embeddings varies for the two nodal classifications considered, and that this performance also changes with the downstream classification tool used on these learned embeddings, highlighting the multiple aspects of the embedding process that need to be considering for an eventual prediction task.

One important concern when link prediction is used is the difficulty in sampling edges of a network to remove, and the theoretical properties of network sampling are still somewhat lacking. Recall that in a traditional classification setting where data are assumed to be drawn independently and identically from some distribution, we form training and test splits in order to estimate the generalization error of our classifier (or use multiple training test splits and cross-validation in order to estimate the expected test error). These splits are created via sub-sampling the original data in a way which ‘respects’ the way the observed data are sampled from a hypothetical population distribution. In the case of networks, various candidates for population models of graphs (including [26, 49, 50, 6, 5, 11, 12]) have been proposed, each with their own shortcomings. It is therefore unclear if in practice one should accept a single routine way in which training splits should be chosen, although some work [36] has explored the implications of when a subsampling procedure defined on finite graphs leads to a suitable population limit. These concerns are important when considering tasks that involve sampling a network.

This is closely related to the implementation of validation methods, such as cross validation for network models. While some such methods have recently been proposed [24], they have not yet been applied to evaluate network embedding models, and further work is needed to better understand these procedures on networks.

**Computability**, which in the PCS framework is described as an issue of algorithm efficiency and scalability, is of clear importance in network embedding. Many network embedding procedures seek to embed large networks containing hundreds of thousands of nodes, and the use of simpler low dimensional representations naturally aids computation. However, there is of course a tradeoff between computation and the representation power of the learned embedding; larger embedding dimensions allow for more flexible representations but come at the cost at more expensive computation. Approximations are commonly used to perform this embedding, such as the widely used negative sampling [38, 16] and the hierarchical softmax approximation [38]. These methods induce optimization objectives which are amenable to stochastic gradient descent methods, and allow for the use of minibatches and the possibility of dis-
As these optimization procedures are non-convex, there are also questions as to whether the learned embeddings are global minima of the objectives from which they are learned. Scalability also hinders (more severely) other methods such as spectral clustering and MCMC based methods such as latent space models, limiting the use of these models to networks with at most tens of thousands of vertices.

We see in Figure 1 that, for our illustrative email network, spectral clustering is more computationally expensive than the Deepwalk embedding method for all choices of latent dimension, with both methods becoming more expensive as the latent dimension increases.

Stability seeks to identify how the result of an analysis changes when the data and/or the model are perturbed. As described in [55], this is required across the network embedding procedure, and should take account of all components of the network embedding problem:

- The choice of representation space; for instance, do we use a Euclidean or hyperbolic geometry for the representation space? What embedding dimension do we use?
- The features of the network to be preserved; do we preserve only first order connectivity information, or higher orders?
- Similarity in the representation space; this can be both from the choice of loss function used when training, and also any prescribed similarity measures we use for analysis after training.
- The procedure for learning the representation space; this is on the level of whether we use e.g spectral clustering or Deepwalk, and then also for a particular algorithm the choice of hyperparameters (e.g for Deepwalk, this includes the sampling scheme and any other hyperparameters such as lengths of random walks, window sizes, and the step size/initialization chosen for the gradient descent procedure).
- The subsequent analysis for which the learned embedding is used; for instance, are we interested in link prediction tasks or community detection?
- Changes to the data; what happens if a small number of edges are removed from the network? Does the result of our analysis significantly change if some noise is added to the network (by e.g flipping the labels of a small number of edges?)

We see some aspects of this stability component in Figure 2. For example, as we increase the latent dimension of our embedding space we see that predicted classifications from a spectral embedding are stable, with limited improvement from increased dimension. The embedding learned by Deepwalk, however, appears to vary, sometimes leading to improved classification accuracy and sometimes to worse accuracy as the dimension increases. Similarly, we see that for predicting student status, using the Deepwalk embedding is stable under different classification methods used on the embedding, unlike the spectral embedding. While perturbations of any one component of this procedure can be evaluated, a metric is needed to fully assess the stability of models of this form, which shall be able to capture...
perturbations in the data along with both stages of modeling present in network embedding (learning the representation and the subsequent analysis using this representation)

6 Discussion

Network embedding is an exciting area of active research and new approaches are regularly proposed in the literature. In this paper we have given a brief review of the problem of network embedding, discussed the key components of the task, and reviewed in detail some common procedures from both the statistical and machine learning fields.

We have discussed a framework for the evaluation of network embedding methods, using the principles proposed in [55]. The goal of such a framework is to provide “responsible, reliable, reproducible and transparent results across the data science life cycle” [55], something we believe is crucial, particularly in the context of network embedding. We consider each of the principles of predictability, computability, and stability in this context. We feel that the utilization of a framework such as this can help to direct future work on network embedding and help to better understand the broad existing literature.

There are still many unresolved questions in this literature which provide further opportunities. Embedding richer network features, which may be needed to address domain specific questions [2], is still an open problem. Although applying NLP methods directly to networks has yielded empirical success, a deeper understanding of these models requires further work on the interaction between sampling procedures on networks, and the impact this sampling has on the learning of the embedding. Moreover, there is a question of interpreting which latent structures of the network are being recovered by such schemes, and how they may differ from those produced e.g by spectral clustering. Given the interaction between sampling and censoring, this should also lead to insights for link prediction tasks (which we can think of as a missing data problem). It is hoped that utilization of this framework could help identify empirical evidence to help address these challenges. Another question which has been considered is the geometry of the embedding space used and the result structure this can capture [45]. Further work could explore the relationship between embedding geometries and the PCS framework.

While most existing procedures employ a similar problem setup, many different outcomes are considered in the literature, leading to a wide array of evaluation metrics. As such, a systematic evaluation of competing methods is required to better understand the state of the art and direct further research. The agreement on benchmark datasets and metrics, extending beyond link prediction, would also be required. Extensive simulation studies, based on the principles proposed here for network embedding, would help to identify these benchmarks and metrics, and would undoubtedly identify further directions of interest in the study of network representation. Similarly, while we have exclusively considered the problem of static networks here, there is also much recent research into dynamic networks which can evolve over time [14], [34], [57]. There are many differences when considering how to represent a network with a temporal component, and there are also a wide range of possible evaluation metrics which can be considered for networks of this form. Addressing the concepts of PCS in the development of embedding methods for these networks is an area with many future challenges.
A Model cards

Spectral Clustering of the Graph Laplacian

- **Model Description.**
- **Inputs.** Adjacency matrix $A$ of a graph $G(V,E)$
- **Output.** Cluster assignments of the nodes in the network.
- **Procedure.** Given a Laplacian matrix $L$ of $A$, construct the bottom $k$ eigenvectors of $L$, $u_1, \ldots, u_k$ which give the matrix $U = (u_1, \ldots, u_k) \in \mathbb{R}^{n \times k}$. Perform a distance clustering using the rows of $U$, to cluster each node.
- **Task.** Clustering of the nodes.
- **Source Code.** Implemented in most software packages.

Latent Space Models

- **Model Description.**
- **Inputs.** Adjacency matrix $A$ of a graph $G(V,E)$
- **Output.** Latent position of the nodes in some lower dimensional space.
- **Loss Function.** Posit a latent space. Log likelihood, conditional on that latent space, of the form
  \[ \sum_{i \neq j} \eta_{i,j} A_{i,j} - \log (1 + e^{\eta_{i,j}}), \]
  where $\eta_{i,j}$ is the log odds of the probability of an edge between nodes $i$ and $j$, with $\eta_{i,j} = \alpha + d_{i,j}$, with $d_{i,j}$ some metric distance in the latent space.
- **Task.** Represent nodes in low dimensional Euclidean space.
- **Source Code.** Implemented, for example, in **latentnet** package in R.

DeepWalk [38]

- **Model Description.** Apply SkipGram to learn network embedding with random walks.
- **Inputs.** Graph $G(V,E)$, window size $w$, embedding dimension $d$, number of walks per vertex $\gamma$, walk length $t$.
- **Output.** The vertex representations $\Phi(V) \in \mathbb{R}^{|V| \times d}$.
- **Loss Function.**
  \[ \sum_{W_k} \sum_{v_i \in W_k} -\log \Pr(\{v_{i-w}, \ldots, v_{i-1}, v_{i+1}, \ldots, v_{i+w}\}|\Phi(v_i))). \]
- **Task.** Multi-Label Classification.
  - **Evaluation Data.** BlogCatalog, Flickr, YouTube.
  - **Classification Model.** One-vs-rest logistic regression.
  - **Metrics.** Macro-$F_1$ and Micro-$F_1$ scores.
- **Source Code.** [https://github.com/phanein/deepwalk](https://github.com/phanein/deepwalk)

Deep Graph Infomax [51]

- **Model Description.** An unsupervised embedding method maximizing mutual information.
• **Inputs.** Graph (with features) $A, X$, corruption function $C$, encoder $E(X,A)$, readout function $R(Z)$, discriminator $D$.

• **Output.** The vertex representations $Z = (z_1, \cdots, z_N)$.

• **Loss Function.**

$$
\mathcal{L} = \frac{1}{N+M} \left( \sum_{i=1}^{N} E(X,A) [\log D(z_i, s)] + \sum_{j=1}^{M} E(\tilde{X},\tilde{A}) [\log (1 - D(\tilde{z}_j, s))] \right).
$$

• **Tasks.** Multi-Label Classification, visualization of clustering.
  - **Evaluation Data.**
    - Transductive: Cora, Citeseer, Pubmed;
    - Inductive: Reddit, PPI
  - **Classification Model.** Logistic regression.
  - **Metrics.** Micro-$F_1$ scores on test nodes (unseen nodes for inductive tasks).

• **Source Code.** [https://github.com/PetarV-/DGI](https://github.com/PetarV-/DGI)
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