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# A Model and Extensive Taxonomy for Machine Learning on Graphs

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## Abstract

Interest in graph representation learning (GRL) has recently skyrocketed. In general, there are three broad types of GRL approaches that have developed in response to the availability of labeled data. The first one is network embedding, which is all about learning relational structure representations without supervision. The second one is called graph regularized neural networks, and it uses graphs to teach semi-supervised learning by adding a regularization goal to neural network losses. Finally, graph neural networks are designed to learn differentiable functions across arbitrary-structured discrete topologies. Interestingly, however, there has been relatively no effort to integrate the three paradigms, even though these fields are somewhat popular. Here, we strive to connect graph neural networks, graph regularization, and network embedding. In an effort to bring together several separate areas of study, we provide a thorough taxonomy of GRL approaches. In particular, we suggest the GRAPHEDM framework, which unifies well-known methods for learning graph representations using semi-supervised (e.g., GraphSage, GCN, GAT) and unsupervised (e.g., DeepWalk, node2vec) means. We fitted more than thirty existing techniques into this framework to demonstrate GRAPHEDM's generalizability. We think this unified perspective does double duty: it lays the groundwork for future study in the field and helps us comprehend the thinking underlying these techniques.

**Keywords:** Learning on Manifolds, Relational Learning, Geometric Deep Learning, and Network Embedding

## 1. Introduction

2. Developing representations for intricate structured data sets is no easy feat. Data defined on a discretized Euclidean domain is one kind of structured data that has seen a plethora of effective models produced in the last ten years. One example is the use of recurrent neural networks for modeling sequential data, like text or movies. These networks are able to collect sequential

information and provide efficient representations, as shown bytheir performance on machine translation and voice recognition tasks. Convolutional neural networks (CNNs) are another example; they have achieved remarkable performance in pattern recognition tasks like image classification and voice recognition by parameterizing neural networks according to structural priors like shift-invariance. These remarkable achievements have only been applicable to certain kinds of data with a straightforward relational structure, such as sequential data or data that follows regular patterns. Data is not always so regular;complex relationship structures often emerge, and comprehending the interplay between objects requires data extraction from such systems. Social networks, computational chemistry, biology, recommendation systems, semi-supervised learning, and other domains make use of graphs, which are universal data structures that can represent complex relational data (made up of nodes and edges) (Gilmer et al., 2017; Stark et al., 2006; Konstas et al., 2009; Garcia and Bruna, 2018). Since graph topologies are not always consistent and may change greatly across graphs and even between nodes in the same graph, it is difficult to construct networks with strong structural priors for graph-structured data. Irregular graph domains are particularly incompatible with operations like convolutions. For example, since all of the pixels in an image have the same neighborhood structure, it is possible to use the same filter weights everywhere in the picture. Nevertheless, given that every node in a network may have a unique neighborhood structure, it is impossible to provide an ordering of nodes (Fig. 1). On top of that, non-Euclidean domains are not applicable to geometric priors (such as shift invariance) used in Euclidean convolutions (for instance, translations may not even be specified on such domains).

3. Research into Geometric Deep Learning (GDL) emerged in response to these difficulties; GDL seeks to apply deeplearning methods to data that is not geometrically normal. A lot of people are very interested in using machine learning techniques on graph-structured data because of how common graphs are in real-world

applications. Learned embeddings are low-dimensional continuous vector representations of graph-structured data; GRL techniques are one such approach. Unsupervised GRL and supervised (or semi-supervised) GRL are the two main categories of GRL learning tasks. The first set of rules is based on the notion of learning low-dimensional Euclidean representations that retain the original graph structure. For a particular downstream prediction job, such node or graph categorization, the second family likewise learns low-dimensional Euclidean representations. In contrast to the unsupervised environment, whereby inputs are often graph structures, the supervised setting typically uses a variety of signals specified on graphs, or node attributes, as inputs. Whereas in the inductive learning scenario, the underlying discrete graph domain may change (for example, when predicting molecular attributes where each molecule is a graph), in the transductive learning context, it can remain stable (for example, when predicting user qualities in a huge social network). Lastly, it should be mentioned that the majority of supervised and unsupervised approaches learn representations in vector spaces that are based on geometry, but there has been a recent uptick in interest in non-Euclidean representation learning. Thiskind of learning attempts to acquire knowledge about embedding spaces that are not based on geometry, such as spherical or hyperbolic spaces. The primary goal of this researchis to use an embedding space that is continuous and similar to the input data's underlying discrete structure (for instance,hyperbolic space is a continuous form of trees; Sarkar, 2011).

We think it is critical to synthesize and explain these techniques in one cohesive and understandable framework since the GRL field is expanding at a remarkable rate. This review aims to provide a comprehensive overview of representation learning techniques for graph-structured data so that readers may have a better understanding of the many ways in which deep learning models use graph structure.

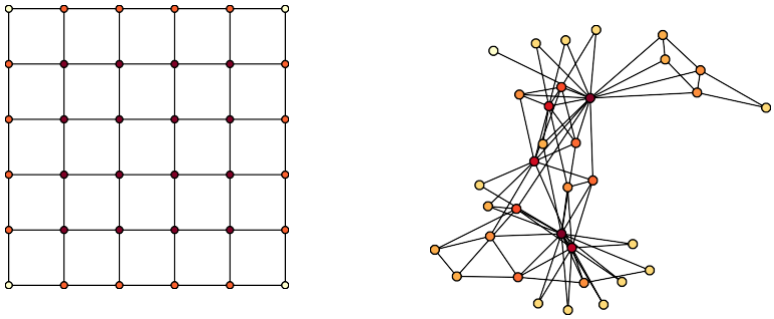
4. There are an assortment of graph representation learning questionnaires available. For a full review of shallow network embedding and auto-encoding approaches, there are various surveys that address the topic.We recommend (Cai et al., 2018;

Chen et al., 2018a; Goyal and Ferrara, 2018b; Hamilton et al., 2017b; Zhang et al., 2018a) for this. Second, for data that is not Euclidean, such manifolds or graphs, Bronstein et al. (2017) provides a comprehensive review of deep learning methods. Thirdly, approaches applying deep learning to graphs, particularly graph neural networks, have been covered in many recent surveys (Battaglia et al., 2018; Wu et al., 2019; Zhang et al., 2018c; Zhou et al., 2018). Rather than establishing links across several areas of graph representation learning, most of these studies focus down on only one.

We develop a general framework called the Graph Encoder Decoder Model (GRAPHEDM) to classify previous work into four main areas: (i) methods for shallow embedding, (ii) methods for auto-encoding, (iii) methods for graph regularization, and (iv) methods for graph neural networks (GNNs). This framework expands upon the encoder-decoder model proposed by Hamilton et al. (2017b).We also provide a Graph Convolution Framework (GCF) for describing convolution-based GNNs, which have shown to be very effective in many different domains. According to Veli˘ckovi'c et al. (2018), we are able to examine and contrast several GNNs, which differ in their design. These GNNs range from those that operate in the Graph Fourier1 domain to those that use self-attention as a neighborhood aggregation function. The goal of this comprehensive synthesis of current research is to provide readers with a better understanding of the many graph-based learning approaches so that they may identify their similarities and differences, as well as their possible expansions and limits. However, there are three ways in which our survey differs from earlier ones:

We introduce a general framework, GRAPHEDM, to describe a broad range of super- vised and unsupervised methods that operate on graph-structured data, namely shal- low embedding methods, graph regularization methods, graph auto-encoding methods and graph neural networks.

Our survey is the first attempt to unify and view these different lines of work from the same perspective, and we provide a general taxonomy (Fig.3) to understand differences and similarities between these methods. In particular, this taxonomy en-



(a) Grid (Euclidean). (b) Arbitrary graph (Non-Euclidean).

Figure 1: An illustration of Euclidean vs. non-Euclidean graphs.

represents more than 30 different GRL algorithms. To better understand the differences between various strategies, it is helpful to describe them within a thorough taxonomy.

• We provide an open-source GRL library that contains cutting-edge GRL methods and crucial graph applications including link prediction and node categorization. You may find our implementation at https://github.com/google/gcnn-survey-paper. It is open to the public.

**Organization of the survey** Section 2 provides a clear statement of the issue setting for GRL and a review of fundamental graph concepts. Section 2.2.1 explains the function of node features in GRL and their relationship to supervised GRL; Section 2.2.2 differentiates between inductive andtransductive learning; Section 2.2.3.1 distinguishes between positional and structural embeddings; and Section 2.2.4distinguishes between supervised and unsupervised embeddings. We also define and discuss the differences between these important concepts in GRL. Section 3 then presents GRAPHEDM, a generic framework that may be used in inductive and transductive learning contexts to define supervised and unsupervised GRL techniques, with or without node characteristics. We provide a comprehensive taxonomy of GRL approaches (Fig. 3) based on GRAPHEDM, which incorporates more than thirty contemporary GRL models. We use this taxonomy to characterize both supervised (Section 5) and unsupervised (Section 4) methods. Section 6 concludes with an overview of graph applications.

## 5. Preliminaries

6. Graph representation learning approaches attempt to address the generalized network embedding issue; for an overview, see Table 1. Here, we offer the notation used throughout the article.

## 6.1 Definitions

| | Notation | Meaning |
|---|---|---|
| Abbreviations | GRL | Graph Representation |
| | GRAPHED | Learning Graph Encoder |
| | M | Decoder Model Graph Neural |
| | GNN | Network |
| | GCF | Graph Convolution Framework |
| Graph notation | $G = (V, E)$ | Graph with vertices (nodes) $V$ and edges $E$ |
| | $v_i \in V$ | Graph vertex |
| | $d_G(\cdot, \cdot)$ | Graph distance (length of shortest path) |
| | $\deg(\cdot)$ | Node degree |
| | $D \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Diagonal degree matrix |
| | $W \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Graph weighted adjacency matrix |
| | $\tilde{W} \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Symmetric normalized adjacency matrix ($\tilde{W} = D^{-1/2}WD^{-1/2}$) |
| | $A \in \{0, 1\}^{\lvert V\rvert \times \lvert V\rvert}$ | Graph unweighted weighted adjacency matrix |
| | $L \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Graph unnormalized Laplacian matrix ($L = D - W$) |
| | $\tilde{L} \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Graph normalized Laplacian matrix ($\tilde{L} = I - D^{-1/2}WD^{-1/2}$) |
| | $L^{\mathrm{rw}} \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Random walk normalized Laplacian ($L^{\mathrm{rw}} = I - D^{-1}W$) |
| GRAPHEDM notation | $d_0$ | Input feature dimension |
| | $X \in \mathrm{R}^{\lvert V\rvert \times d_0}$ | Node feature matrix |
| | $d$ | Final embedding dimension |
| | $Z \in \mathrm{R}^{\lvert V\rvert \times d}$ | Node embedding matrix |
| | $d_l$ | Intermediate hidden embedding dimension at layer $l$ |
| | $H^l \in \mathrm{R}^{\lvert V\rvert \times d_æ}$ | Hidden representation at layer $l$ |
| | Y | Label space |
| | $y^S \in \mathrm{R}^{\lvert V\rvert \times \lvert Y\rvert}$ | Graph ($S = G$) or node ($S = N$) ground truth labels |
| | $\hat{y}^S \in \mathrm{R}^{\lvert V\rvert \times \lvert Y\rvert}$ | Predicted labels |
| | $s(W) \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Target similarity or dissimilarity matrix in graph regularization |
| | $\hat{W} \in \mathrm{R}^{\lvert V\rvert \times \lvert V\rvert}$ | Predicted similarity or dissimilarity matrix |
| | $\mathrm{ENC}(\cdot; \Theta^E)$ | Encoder network with parameters $\Theta^E$ Graph |
| | $\mathrm{DEC}(\cdot; \Theta^D)$ | decoder network with parameters $\Theta^D$ Label |
| | $\mathrm{DEC}(\cdot; \Theta^S)$ | decoder network with parameters $\Theta^S$ |
| | $\mathrm{L}^S_{\mathrm{SUP}}(y^S, \hat{y}^S; \Theta)$ | Supervised loss |
| | $\mathrm{L}_{G,\mathrm{REG}}(W, \hat{W}; \Theta)$ | Graph regularization loss |
| | $\mathrm{L}_{\mathrm{REG}}(\Theta)$ | Parameters' regularization loss |
| | $d_1(\cdot, \cdot)$ | Matrix distance used for to compute the graph regularization loss |
| | $d_2(\cdot, \cdot)$ | Embedding distance for distance-based decoders |
| | $\lVert\cdot\rVert_p$ | $p$–norm |
| | $\lVert\cdot\rVert_F$ | Frobenuis norm |

Table 1: Summary of the notation used in the paper.

**Definition 1** *(Graph). A graph G given as a pair: G = (V, E), comprises a set of vertices (or nodes) V = {$v_1, \ldots, v_{|V|}$} connected by edges E = {$e_1, \ldots, e_{|E|}$}, where each edge $e_k$ is a pair ($v_i$, $v_j$) with $v_i$, $v_j \in V$ . A graph is weighted if there exist a weight function: $w : (v_i, v_j) \rightarrow w_{ij}$ that assigns weight $w_{ij}$ to edge connecting nodes $v_i$, $v_j \in V$ . Otherwise, we say that the graph is unweighted. A graph is undirected if ($v_i$, $v_j$) $\in E$ implies ($v_j$, $v_i$) $\in E$,*
*i.e. the relationships are symmetric, and directed if the existence of edge ($v_i$, $v_j$) $\in E$ does*
*not necessarily imply ($v_j$, $v_i$) $\in E$. Finally, a graph can be homogeneous if nodes refer to one type of entity and edges to one relationship. It can be heterogeneous if it contains different*
*types of nodes and edges.*
For instance, social networks are homogeneous graphs that can be undirected (e.g. to encode symmetric relations like friendship) or directed (e.g. to encode the relation following); weighted (e.g. co-activities) or unweighted.
**Definition 2** *(Path). A path P is a sequence of edges ($u_{i1}$ , $u_{i2}$ ), ($u_{i2}$ , $u_{i3}$ ), . . . , ($u_{ik}$ , $u_{ik+1}$ ) of length k. A path is called simple if all $u_{ij}$ are distinct from each other. Otherwise, if a path visits a node more than once, it is said to contain a cycle.*
**Definition 3** *(Distance). Given two nodes (u, v) in a graph G, we define the distance from u to v, denoted $d_G(u, v)$, to be the length of the shortest path from u to v, or $\infty$ if there exist no path from u to v.*
The graph distance between two nodes is the analog of geodesic lengths on manifolds.
**Definition 4** *(Vertex degree). The degree,* deg($v_i$), *of a vertex $v_i$ in an unweighted graph is the number of edges incident to it. Similarly, the degree of a vertex $v_i$ in a weighted graph is the sum of incident edges weights. The degree matrix D of a graph with vertex set V is the $|V| \times |V|$ diagonal matrix such that $D_{ii}$ =* deg($v_i$).
**Definition 5** *(Adjacency matrix). A finite graph G = (V, E) can be represented as a square $|V| \times |V|$ adjacency matrix, where the elements of the matrix indicate whether pairs of nodes are adjacent or not. The adjacency matrix is binary for unweighted graph, $A \in \{0, 1\}^{|V| \times |V|}$, and non-binary for weighted graphs $W \in \mathrm{R}^{|V| \times |V|}$. Undirected graphs have symmetric adjacency matrices, in which case, $\widetilde{\ }$ denotes symmetrically-normalized adjacency matrix: $W = D^{-1/2}WD^{-1/2}$, where D is the degree matrix.*
**Definition 6** *(Laplacian). The unnormalized Laplacian of an undirected graph is the $|V| \times |V|$ matrix $L = D - W$. The symmetric normalized Laplacian is $L = I - D^{-1/2}WD^{-1/2}$.*
*The random walk normalized Laplacian is the matrix $L^{rw} = I - D^{-1}W$.*
The name random walk comes from the fact that $D^{-1}W$ is a stochastic transition matrix that can be interpreted as the transition probability matrix of a random walk onthe graph. The graph Laplacian is a key operator on graphs and can be interpreted as the analogue of the continuous Laplace-Beltrami operator on manifolds. Itseigenspace capture important properties about a graph (e.g. cut information often used for spectral graph clustering) but can also serve as a basis for smooth functions defined on the graph for semi-supervised learning (Belkin and Niyogi, 2004). The graph Laplacian is also closely related to the heat equation on graphs as it is the generator of diffusion processes on graphs and can be used to derive algorithms for semi- supervised learning on graphs (Zhou et al., 2004).

**Definition 7** *(First order proximity). The first order proximity between two nodes $v_i$ and $v_j$ is a local similarity measure indicated by the edge weight $w_{ij}$. In other words, the first- order proximity captures the strength of an edge between node $v_i$ and node $v_j$ (should it exist).*
**Definition 8** *(Second-order proximity). The second order proximity between two nodes $v_i$ and $v_j$ is measures the similarity of their neighborhood structures. Two nodes in a network will have a high second-order proximity if they tend to share many neighbors.*
Note that there exist higher-order measures of proximity between nodes such as Katz Index, Adamic Adar or Rooted PageRank (Liben-Nowell and Kleinberg, 2007). These notions of node proximity are particularly important in network embedding as many algorithms are optimized to preserve some order of node proximity in the graph.

The generalized network embedding problem
*Network embedding* is the task that aims at learning a mapping function from a discrete graph to a continuous domain. Formally, given a graph $G = (V, E)$ with weighted adjacency matrix $W \in \mathrm{R}^{|V| \times |V|}$, the goal is to learn low-dimensional vector representations $\{Z_i\}_{i \in V}$

(embeddings) for nodes in the graph $\{v_i\}_{i \in V}$ , such that important graph properties (e.g. local or global structure) are preserved in the embedding space. For instance, if two nodes have similar connections in the original graph, their learned vector representations should be close. Let $Z \in \mathrm{R}^{|V| \times d}$ denote the node[2] embedding matrix. In practice, we often want low-dimensional embeddings ($d \ll |V|$) for scalability purposes. That is, network embedding can be viewed as a dimensionality reduction technique for graph structured data, where the input data is defined on a non- Euclidean, high-dimensional, discrete domain.

## NODE FEATURES IN NETWORK EMBEDDING

**Definition 9** *(Vertex and edge fields). A vertex field is a function defined on vertices* $f : V \rightarrow \mathrm{R}$ *and similarly an edge field is a function defined on edges:* $F : E \rightarrow \mathrm{R}$. *Vertex fields and edge fields can be viewedas analogs of scalar fields and tensor fields on manifolds.* Graphs may have node attributes (e.g. gender or age in social networks; article contents for citation networks) which can be represented as multiple vertex fields, commonly referred to as *node features*. In this survey, we denote node features with $X \in \mathrm{R}^{|V| \times d_0}$ , where $d_0$ is theinput feature dimension. Node features might provide useful information about a graph. Some network embedding algorithms leverage this information by learning mappings:

$W, X \rightarrow Z$.

In other scenarios, node features might be unavailableor not useful for a given task: net- work embedding canbe *featureless*. That is, the goal is to learn graph representations via mappings:

$W \rightarrow Z$.

Although we present the model taxonomy via embedding nodes yielding $Z \in \mathrm{R}^{|V| \times d}$, it can also be extended for models that embed an entire graph i.e. with $Z \in \mathrm{R}^d$ as a $d$- dimensional vector for the whole graph (e.g. (Duvenaud et al., 2015; Al-Rfou et al., 2019)), or embed graph edges $Z \in \mathrm{R}^{|V| \times |V| \times d}$ as a (potentially sparse) 3D matrix with $Z_{u,v} \in \mathrm{R}^d$ representing the embedding of edge $(u, v)$. Note that depending on whether node features are used or not in the embedding algorithm, the learned representation could capture different aspects about the graph. If nodes features are being used, embeddings could capture both *structural* and *semantic* graph information. On the other hand, if node features are not being used, embeddings will only preserve structural information of the graph.

Finally, note that edge features are less common than node features in practice, but can also be used by embedding algorithms. For instance, edge features can be used as regularization for node embeddings (Chen et al., 2018c), or to compute messages from neighbors as in message passing networks (Gilmer et al., 2017).

## TRANSDUCTIVE AND INDUCTIVE NETWORK EMBEDDING

Historically, a popular way of categorizing a network embedding method has been by whether the model can generalize to unseen data instances – methods are referred to as operating in either a *transductive* or *inductive* setting (Yang et al., 2016). While we do not use this concept for constructing our taxonomy, we include a briefdiscussion here for completeness.

In transductive settings, it assumed that all nodes in the graph are observed in training (typically the nodes all come from one fixed graph). These methods are used to infer information about or between observed nodes in the graph (e.g. predicting labels for all nodes, given a partial labeling). For instance, if a transductive method is used to embed the nodes of a social network, it can be used to suggest new edges (e.g. friendships) between the nodes of the graph. One major limitation of models learned in transductive settings is that they fail to generalize to new nodes (e.g. evolving graphs) or new graph instances.

On the other hand, in inductive settings, models are expected to generalize to new nodes, edges, or graphs that were not observed during training. Formally, given training graphs ($G_1, \ldots, G_k$), the goal is to learn a mapping to continuous representations that can generalize to unseen test graphs ($G_{k+1}, \ldots, G_{k+l}$). For instance, inductive learning can be used to embed molecular graphs, each representing a molecule structure (Gilmer et al., 2017), generalizing to new graphs and showing error margins within chemical accuracy on many quantum properties. Embedding dynamic or temporally evolving graphs is also another inductive graph embedding problem.

There is a strong connection between inductive graph embedding and *node features* (Sec- tion 2.2.1) as the latter are usually necessary for most inductive graph representation learn- ing algorithms. More concretely, node features can be leveraged to learn embeddings with parametric mappings and instead of directly optimizing the embeddings, one can optimize the mapping's parameters. The learned mapping can then be applied to any node (even those that were not present a training time). On the other hand, when node features are not available, the first mapping from nodes to embeddings is usually a one-hot encoding which fails to generalize

to new graphs where the canonical node ordering is not available.

Finally, we note that this categorization of graph embedding methods is at best an incomplete lens for viewing the landscape. While some models are inherently better suited to different tasks in practice, recent theoretical results (Srinivasan and Ribeiro, 2020) show that models previously assumed to be capable of only one setting (e.g. only transductive) can be used in both.

### POSITIONAL VS STRUCTURAL NETWORK EMBEDDING

An emerging categorization of graph embedding algorithms is about whether the learned embeddings are positional or structural. Position-aware embeddings capture global relative positions of nodes in a graph and it is common to refer to embeddings as positional if they can be used to approximately reconstruct the edges inthe graph, preserving distances such as shortest paths in the original graph (You et al., 2019). Examples of positional embedding algorithms include random walk or matrix factorization methods. On the other hand, structure-aware embeddings capture local structural information about nodes in a graph, i.e. nodes with similar node features or similar structural roles in a network should have similar embeddings, regardless of how far they are in the original graph. For instance, GNNsusually learn embeddings by incorporating information foreach node's neighborhood, and the learned representations are thus structure-aware. In the past, positional embeddings have commonly been used for unsupervised tasks where positional information is valuable (e.g. link prediction or clustering) while structural embeddings have been used for supervised tasks(e.g. node classification or whole graph classification). More recently, there has been attempts to bridge the gap between positional and structural representations, with positional GNNs (You et al., 2019) and theoretical frameworks showing the equivalence between the two classes of embeddings (Srinivasan and Ribeiro, 2020).

### UNSUPERVISED AND SUPERVISED NETWORK EMBEDDING

Depending on whether extra information like node or graph labels is supplied, network embedding may be either supervised or unsupervised. The former case involves using simply the graph structure and, in certain cases, node attributes. Optimization of a reconstruction loss—a measure of the learnt embeddings' ability to mimic the original graph—is often used in unsupervised network embedding with the objective of learning embeddings that retain the graph structure.The objective of supervised network embedding is to improve models for aparticular job, such graph or node classification, and to train embeddings for a specific purpose, like predicting graph or nodeproperties. In Section 3, we go into further depth on the distinctions between supervised and unsupervised approaches, and we utilize the amount of supervision to construct our taxonomy.

## A Taxonomy of Graph Embedding Models

We first describe our proposed framework,GRAPHEDM, a general framework for GRL (Sec- tion 3.1). In particular, GRAPHEDM is general enough that it can be used to succinctly de- scribe over thirty GRL methods (both unsupervised and supervised). We use GRAPHEDM to introduce a comprehensive taxonomy in Section 3.2 and Section 3.3, which summarizes exiting works with shared notations and simple block diagrams, making it easier to under- stand similarities and differences between GRL methods.

### The GraphEDM framework

The GRAPHEDM framework builds on top of the work of Hamilton et al. (2017b), which describes unsupervised network embedding methods from an encoder-decoder perspective.

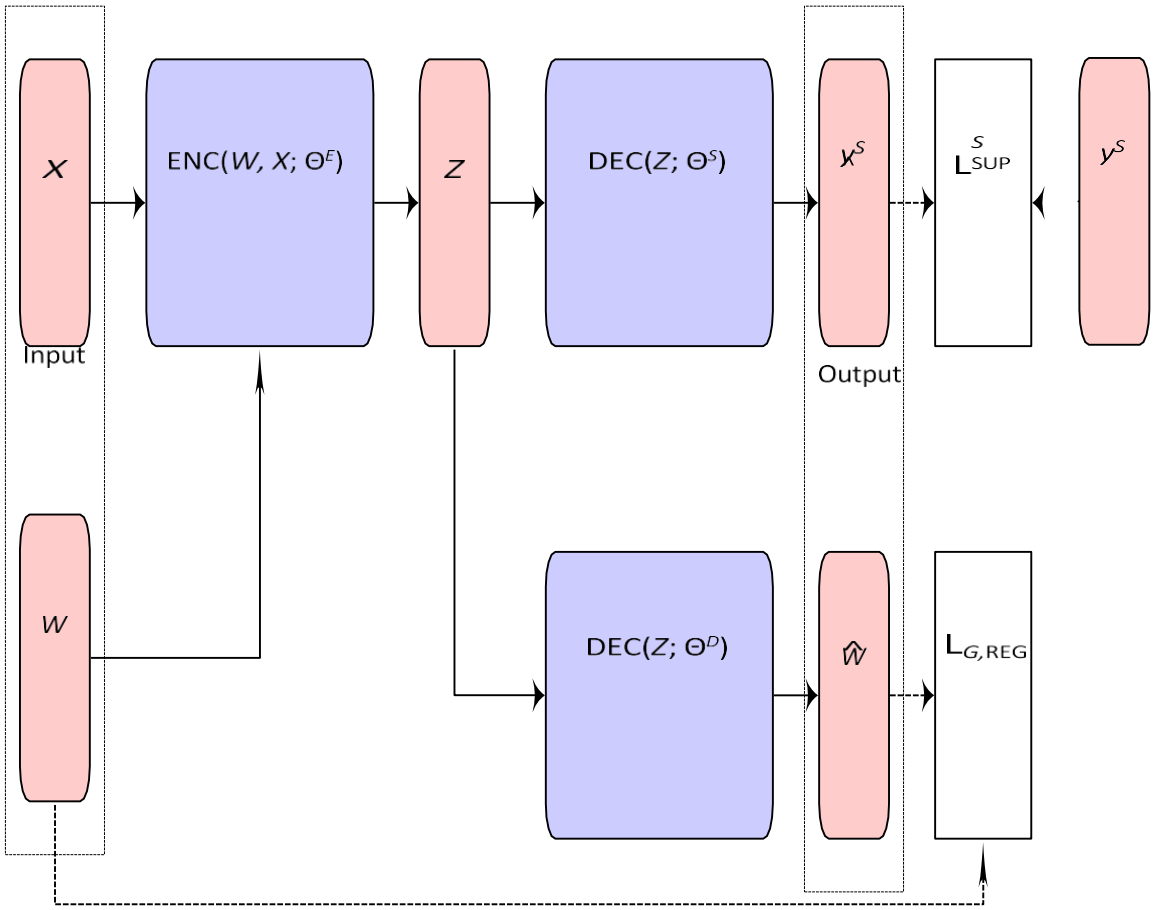



Figure 2: Illustration of the GRAPHEDM framework. Based on the supervision available, methods will use some or all of the branches. In particular, unsupervised methods do not leverage label decoding for training and only optimize the similarity or dissimilarity decoder (lower branch). On the other hand, semi-supervised and supervised methods leverage the additional supervision to learn models' parameters (upper branch).

Cruz et al. (2019) also recently proposed a modular encoder-based framework to describe and compare unsupervised graph embedding methods. Different from these unsupervised frameworks, we provide a more general framework which additionally encapsulates super- vised graph embedding methods, including ones utilizing the graph as a regularizer (e.g. Zhu and Ghahramani (2002)), and graph neural networks such as ones based on message passing (Gilmer et al., 2017; Scarselli et al., 2009) or graph convolutions (Bruna et al., 2014; Kipf and Welling, 2016a).

**Input** The GRAPHEDM framework takes as input an undirected weighted graph $G = (V, E)$, with adjacency matrix $W \in \mathrm{R}^{|V|\times|V|}$, and optional node features $X \in \mathrm{R}^{|V|\times d0}$. In (semi-)supervised settings, we assume that we are given training target labels for nodes (denoted $N$), edges (denoted $E$), and/or for the entire graph (denoted $G$). We denote the supervision signal as $S \in \{N, E, G\}$, as presented below.

**Model** The GRAPHEDM framework can be decomposed as follows:

**Graph encoder network** $\mathrm{ENC}_{\Theta^E} : \mathrm{R}^{|V|\times|V|} \times \mathrm{R}^{|V|\times d0} \rightarrow \mathrm{R}^{|V|\times d}$, parameterized by $\Theta$, which combines the graph structure with node features (or not) to produce node embedding matrix $Z \in \mathrm{R}^{|V|\times d}$ as:

$Z = \mathrm{ENC}(W, X; \Theta^E)$.

As we shall see next, this node embedding matrix might capture different graph prop- erties depending on the supervision used for training.

**Graph decoder network** $\mathrm{DEC}_{\Theta^D} : \mathrm{R}^{|V|\times d} \rightarrow \mathrm{R}^{|V|\times|V|}$, parameterized by $\Theta^D$, which uses the node embeddings $Z$ to compute similarity or dissimilarity scores for all node pairs, producing a matrix $\hat{W} \in \mathrm{R}^{|V|\times|V|}$ as: $\hat{W} = \mathrm{DEC}(Z; \Theta^D)$.

**Classification network** $\mathrm{DEC}_{\Theta^S} : \mathrm{R}^{|V|\times d} \rightarrow \mathrm{R}^{|V|\times|\mathrm{Y}|}$, where Y is the label space. This network is used in (semi-)supervised settings and parameterized by $\Theta$. The output is a distribution over the labels $\hat{y}^S$, using node embeddings, as: $\hat{y}^S = \mathrm{DEC}(Z; \Theta^S)$.

Our GRAPHEDM framework is general (see Fig. 2 for an illustration). Specific choices of the aforementioned $y_G$ (encoder and decoder) networks allows GRAPHEDM to realize specific graph embedding methods. Before presenting the taxonomy and showing realizations of various methods using our framework, we briefly discuss an application perspective.

**Output** The GRAPHEDM model can return a reconstructed graph similarity or dissimilarity matrix $\hat{W}$ (often used to train *unsupervised* embedding algorithms), as well as a output labels $y^S$ for *supervised* applications. The label output space Y varies depending on the supervised application.

**Node-level supervision,** with $y^N \in \mathrm{Y}^{|V|}$, where Y represents the node label space. If Y is categorical, then this is also known as (semi-)supervised node classification (Section 6.2.1), in which case the label decoder network produces labels for each node in the graph. If the embedding dimensions $d$ is such that $d = |\mathrm{Y}|$, then the label decoder network can be just a simple softmax activation across the rows of $Z$, producing a distribution over labels for each node. Additionally, the graph decoder network might also be used in supervised node-classification tasks, as it can be used to regularize embeddings (e.g. neighbor nodes should have nearby embeddings, regardless of node labels).

**Edge-level supervision,** with $\hat{y} \in \mathrm{Y}^{|V|\times|V|}$, where Y represents the edge label space. For example, Y can be multinomial in knowledge graphs (for describing the types of relationships between two entities), setting $\mathrm{Y} = \{0, 1\}^{\#(\text{relation types})}$. It is common to have #(relation types) = 1, and this is is known as *link* nomenclature and position link prediction as an *unsupervised* task (Section 4). Then in lieu of $y^E$ we utilize $W$, the output of the graph decoder network (which is learned to reconstruct a target similarity or dissimilarity matrix) to rank potential edges.

**Graph-level supervision,** with $\hat{y} \in \mathrm{Y}$, where Y is the graph label space. In the graph classification task (Section 6.2.2), the label decoder network converts node embeddings into a single graph labels, using *graph pooling* via the graph edges captured by $W$. More concretely, the graph pooling operation is similar to pooling in standard CNNs, where the goal is to downsample local feature representations to capture higher- level information. However, unlike images, graphs don't have a regular grid structure and it is hard to define a pooling pattern which could be applied to every node in the graph. A possible way of doing so is via graph coarsening, which groups similar nodes into clusters to produce smaller graphs (Defferrard et al., 2016). There exist other pooling methods on graphs such as DiffPool (Ying et al., 2018b) or SortPooling (Zhang et al., 2018b) which creates an ordering of nodesbased on their structural roles in the graph. Details aboutgraph pooling operators is outside the scope of this workand we refer the reader to recent surveys (Wu et al., 2019) for a more in-depth treatment.

## Taxonomy of objective functions

We now focus our attention on the optimization of models that can be described in the GRAPHEDM framework by describing the loss functions used for training. Let $\Theta = \{\Theta^E, \Theta^D, \Theta^S\}$ denote all model parameters.

GRAPHEDM models can be optimized using a combination of the following loss terms:

**Supervised loss** term, $\mathrm{L}^{\mathrm{SUP}}$, which compares the predicted labels $\hat{y}^S$ to the ground truth labels $y^S$. This term depends on the task the model is being trained for. For instance, in semi-supervised node classification tasks ($S = N$), the graph vertices are split into labelled and unlabelled nodes ($V = V_L \cup V_U$), and the supervised loss is computed for each labelled node in the graph:

$$L(y^N, \hat{y}^N; \Theta) = \sum_{n} l(y^N, \hat{y}^N; \Theta),$$

where $l(\cdot)$ is the loss function used for classification (e.g. cross-entropy). Similarly for graph classification tasks ($S = G$), the supervised loss is computed at the graph-level and can be summed across multiple training graphs:

$$L_{sup}(y^S, \hat{y}^S; \Theta) = \sum_{i} l(y_i, \hat{y}_i)$$

$$i|v_i \in V_L$$

**Graph regularization loss** term, $L_{G,REG}$, which leverages the graph structure to impose regularization constraints on the model parameters. This loss term acts as a smoothing term and measures the distance between the decoded similarity or dissim- ilarity matrix $\hat{W}$, and a target similarity or dissimilarity matrix $s(W)$, which might capture higher-order proximities than the adjacency matrix itself:

$$L_{G,REG}(W, \hat{W}; \Theta) = d_1(s(W), \hat{W}), \quad (1)$$

where $d_1(\cdot, \cdot)$ is a distance or dissimilarity function. Examples for such regularization are constraining neighboring nodes to share similar embeddings, in terms of their dis- tance in L2 norm. We will cover more examples of regularization functions in Section 4 and Section 5.

**Weight regularization loss** term, $L_{REG}$, e.g. for representing prior, on trainable model parameters for reducing overfitting. The most commonregularization is L2 regularization (assumes a standard Gaussian prior):

$$L_{REG}(\Theta) = \sum_{\theta \in \Theta} ||\theta||^2.$$

Finally, models realizable by GRAPHEDM framework are trained by minimizing the total loss L defined as:

$$L = \alpha L_{SUP}(y^S, \hat{y}^S; \Theta) + \beta L_{G,REG}^S(W, W^S; \Theta) + \gamma L_{REG}(\Theta), \quad (2)$$

where $\alpha, \beta$ and $\gamma$ are hyper-parameters, that can be tuned or set to zero. Note that graph embedding methods can be trained in a *supervised* ($\alpha \neq 0$) or *unsupervised* ($\alpha = 0$) fashion.

Supervised graph embedding approaches leverage an additional source of information to learn embeddings such as node or graph labels. On the other hand, unsupervised network embedding approaches rely on the graph structure only to learn node embeddings.

A common approach to solve supervised embedding problems is to first learn embeddings with an unsupervised method (Section 4) and then train a supervised model on the learned embeddings. However, as pointed by Weston et al. (2008) and others, using a two-step learning algorithm might lead to sub-optimal performances for the supervised task, and in general, supervised methods (Section 5) outperform two-step approaches.

## Taxonomy of encoders

Having introduced all the building blocks of the GRAPHEDM framework, we now introduce our graph embedding taxonomy. While most methods we describe next fall under the GRAPHEDM framework, they will significantly differ based on the encoder used to produce the node embeddings, and the loss function used to learn model parameters. We divide graph embedding models into four main categories:

**Shallow embedding methods**, where the encoder function is a simple embedding lookup. That is, the parameters of the model $\Theta^E$ are directly used as node embed- dings:

$$Z = \text{ENC}(\Theta^E) = \Theta^E \in \mathrm{R}^{|V| \times d}.$$

Note that shallow embedding methods rely on an embedding lookup and are therefore *transductive*, i.e. they generally cannot be directly applied in *inductive* settings where the graph structure is not fixed.

**Graph regularization methods**, where the encoder network ignores the graph structure and only uses node features as input:

$$Z = \text{ENC}(X; \Theta^E).$$

As its name suggests, graph regularization methods leverage the graph structure through the graph regularization loss term in Eq. (2) ($\beta \neq 0$) to regularize node embeddings.

**Graph auto-encoding methods**, where the encoder is a function of the graph structure only: $Z = \mathrm{ENC}(W ; \Theta^{E})$.

**Neighborhood aggregation methods**, including graph convolutional methods, where both the node features and the graph structure are used in the encoder network. Neighborhood aggregation methods use the graph structure to propagate information across nodes and learn embeddings that encode structural properties about the graph:

$Z = \mathrm{ENC}(W, X; \Theta^E)$.

Historical Context

There is a general two-step process that most machine learning models adhere to. Initially, they forego the need of human feature building in favor of automatically extracting significant patterns from data. According to Bengio et al. (2013), this is the part where representation learning takes place. A second step involves putting these representations to use in supervised (like classification) or unsupervised (like clustering, visualization, and nearest-neighbor search) applications further down the line. This task is referred to as downstream processing.3

To facilitate the downstream process, a good data representation should be both expressive and concise, preserving the original data's significant qualities. Overfitting and other problems induced by the curse of dimensionality may be mitigated, for example, by using low-dimensional representations of high-dimensional datasets. When it comes to GRL, a graph encoder is used for representation learning, while a graph or label decoder is employed for jobs further down the line, such as node classification and link prediction. Graph encoder-decoder networks have traditionally been used for manifold learning. It is usual to presume that input data, even if it exists on a high-dimensional Euclidean space, is inherently contained on a low-dimensional manifold. The classic manifold hypothesis describes this. This inherently low-dimensional manifold is what manifold learning methods aim to retrieve. A discrete approximation of the manifold is often constructed initially, in the form of a graph with edges connecting adjacent points in the ambient Euclidean space. Graph distances are a reasonable surrogate for local and global manifold distances because manifolds are locally Euclidean. Secondly, while keeping graph distances as accurate as feasible, "flatten" this representation of the graph by learning a non-linear mapping from graph nodes to points in low-dimensional Euclidean space. Typically, these representations are more manageable compared to the initial high-dimensional ones, and they may subsequently be used in subsequent applications.

When looking for solutions to the manifold learning issue, non-linear4 dimensionality reduction strategies were all the rage in the early 2000s. For example, spectral approaches are used by Laplacian Eigenmaps (LE) (Belkin and Niyogi, 2002) to calculate embeddings, and IsoMap (Tenenbaum et al., 2000) to maintain global network geodesics by a mix of the Floyd-Warshall algorithm and the conventional Multi-dimensional scaling algorithm. In Section 4.1.1, we outline a few of these techniques that use shallow encoders. Despite their significant influence on machine learning, manifold dimensionality reduction approaches are not scalable to big datasets. Consider the time complexity of IsoMAP: it exceeds quadratic time due to the need to compute all pairs of shortest pathways. Since the mappings from node to embeddings are non-parametric, they cannot generate embeddings for additional datapoints, which is a potentially more significant drawback. The issue of graph embedding has seen several proposals for non-shallow network topologies in recent years. Our GRAPHEDM framework may be used to define graph neural networks and graph regularization networks. When

compared to traditional approaches, GRL models often provide more expressive, scalable, and generalizable embeddings due to their use of deep neural networks' expressiveness.

In the next sections, we review recent methods for supervised and unsupervised graph embedding techniques using GRAPHEDM and summarize the proposed taxonomy in Fig. 3.

## Unsupervised Graph Embedding

Using the taxonomy outlined earlier, we will now provide a summary of current methods for unsupervised graph embedding. Without using task-specific labels for the network or its nodes, these approaches map the graph into a continuous vector space, including its edges and/or nodes. By learning to rebuild matrices that measure the similarity or dissimilarity between nodes, such as the adjacency matrix, some of these approaches aim to learn embeddings that maintain the network structure. There are methods that use a contrastive objective. For example, one could compare nearby node-pairs to faraway ones: nodes that are co-visited in short random walks should have a higher similarity score than distant ones. Another would compare real graphs to fake ones: the mutual information between a graph and all of its nodes should be higher in real graphs than in fake ones.

### Shallow embedding methods

The encoder function in shallow embedding techniques is a basic embedding lookup; these methods are transductive graph embedding methods. The shallow encoder function is simply: for every node vi in V, there is a corresponding low-dimensional learnable embedding vector Zi in Rd.

$$Z = \mathrm{ENC}(\Theta^E) = \Theta^E \in \mathrm{R}^{|V|\times d}.$$

The data structure in the embedding space matches the underlying graph structure, thanks to learnt node embeddings. Generally speaking, it's not dissimilar to principal component analysis (PCA) and other dimensionality reduction techniques;however, the input data may not be linear. Specifically, graph embedding issues may be addressed using techniques for non-linear dimensionality reduction, which often begin with constructing a discrete graph from the data in order to approximate the manifold. Wetake a look at the distance-based and outer product-based approaches to shallow graphembedding.

**Distance-based methods** By using a preset distance function, these approaches maximize embeddings in a way that keeps points that are close together in the graph (as shown by their graph distances, for example) as near together in the embedding space as feasible. In a formal sense, the decoder network may provide either non-Euclidean (Section 4.1.2) or Euclidean (Section 4.1.1) embeddings by computing pairwise distance for a certain distance function d2:

$$W$$

$$\hat{} = \mathrm{DEC}(Z; \Theta^D)$$

with $\hat{W}_{ij} = d_2(Z_i, Z_j)$

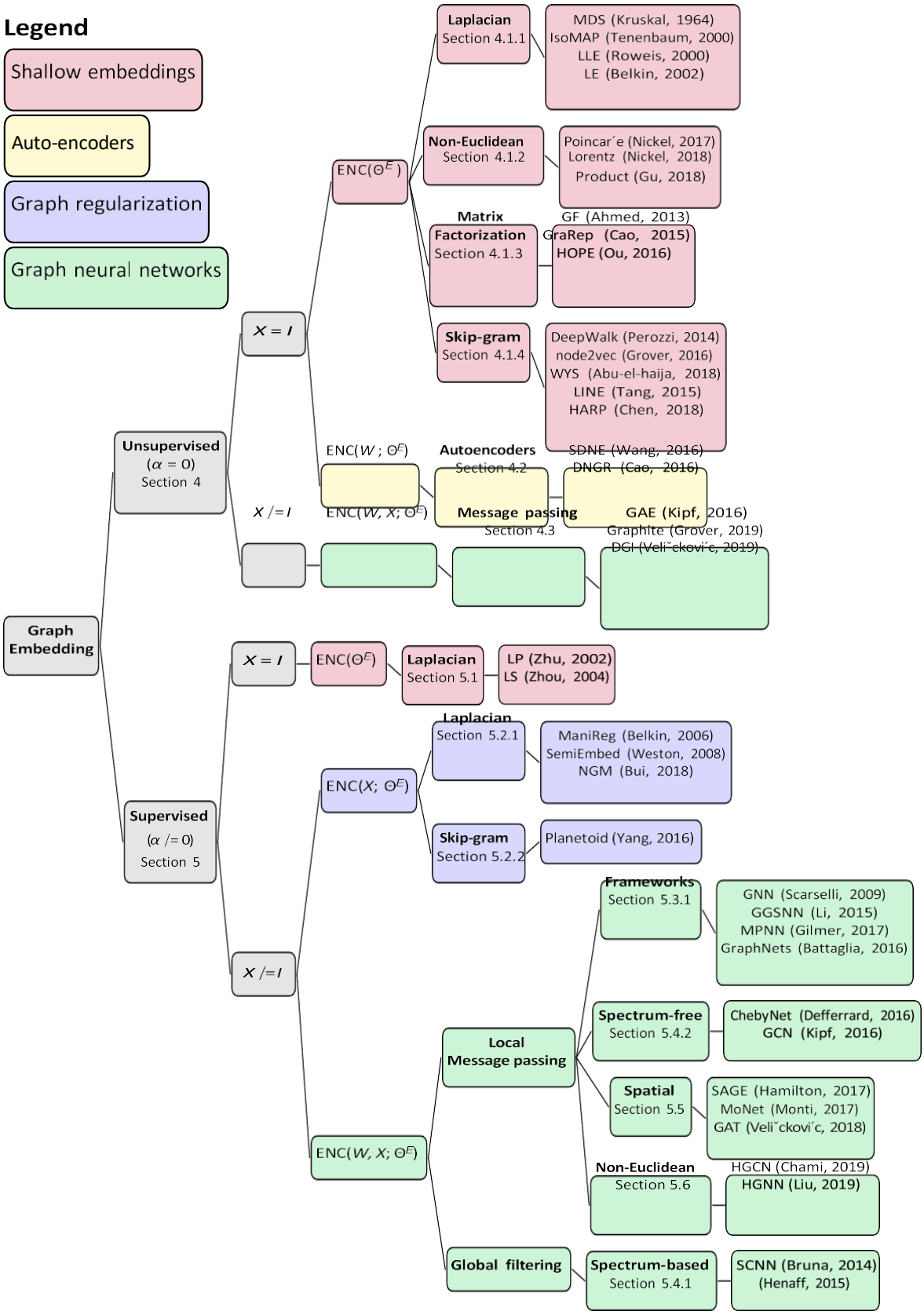



Figure 3: Taxonomy of graph representation learning methods. Based on what

information is used in the encoder network, we categorize graph embedding approaches into four cat- egories: shallow embeddings, graph auto-encoders, graph-based regularization and graph neural networks. Note that message passing methods can also be viewed as spatial convo- lution, since messages are computed over local neighborhood in the graph domain. Recip- rocally, spatial convolutions can also be described using

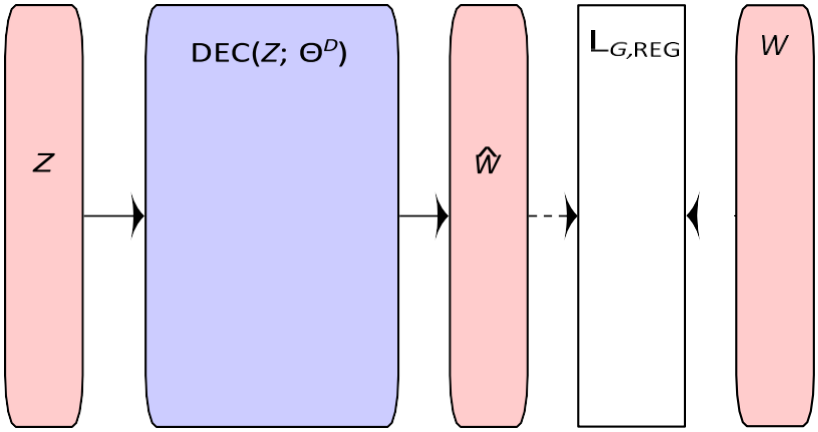



Figure 4: Shallow embedding methods. The encoder is a simple embedding look-up and the graph structure is only used in the loss function.

**Outer product-based methods** These methods on the other hand rely on pairwise dot-products to compute node similarities and the decoder network can be written as:

$$\hat{W} = \mathrm{DEC}(Z; \Theta^D) = ZZ^{\mathrm{T}}.$$

Embeddings are then learned by minimizing the graph regularization loss: $L_{G,\hat{\mathrm{REG}}}(W, \hat{W}; \Theta) = d_1(s(\hat{W}), W)$. Note that for distance-based methods, the function $s(\cdot)$ measures dissimilar- ity or distances between nodes (higher values mean less similar pairs of nodes), while in outer-product methods, it measures some notion of similarity in the graph (higher values mean more similar pairs).

### 4.1.1 Distance-based: Euclidean methods

**Isometric Mapping** As a non-linear dimensionality reduction approach, (IsoMap) (Tenenbaum et al., 2000) assesses the inherent geometry of data residing on a manifold. With the exception of using a different distance matrix, this technique is quite similar to MDS. In contrast to straight-line Euclidean geodesics, IsoMap approximates manifold distances by building a discrete neighborhood graph G and then estimating the manifold geodesic distances using the graph distances (length of shortest paths computed using Dijkstra's algorithm, for example):

$$s(W)_{ij} = d_G(v_i, v_j).$$

To create representations that maintain these graph geodesic distances, IsoMAP use the cMDS method. When data is specified on a Riemannian manifold, for example, IsoMAP may handle distances that do not always originate in a Euclidean metric space, in contrast to cMDS. Unfortunately, computing all pairs of shortest route lengths in the neighborhood graph makes it computationally costly.

**Locally Linear Embedding** Another non-linear dimension reduction approach, sparse matrix operations (LLE) (Roweis and Saul, 2000) improves upon IsoMap's computational complexity and was developed about the same time. The local geometry of manifolds is the basis of LLE, which differs from IsoMAP, which uses geodesics to maintain the global geometry of manifolds. LLE assumes that manifolds are almost linear when examined locally. Linear patch augmentation (LPE) is based on the principle of approximating points using linear combinations of embeddings in their immediate surroundings. The optimal non-linear embedding is then determined by comparing these small neighborhoods on a global scale.

**Laplacian Eigenmaps** Among the non-linear dimensionality reduction strategies, LE (Belkin and Niyogi, 2002) aims to maintain local distances. Important structural information about graphs may be captured by spectral features of the graph Laplacianmatrix. Specifically, the "smoothest" function is the constant eigenvector that corresponds to the eigenvalue zero, and it is defined on the graph vertices. The eigenvectors of the graph Laplacian provide the foundation for these functions. Expanding upon this understanding, LE is a method for reducing dimensions that is not linear. Before representing nodes in the networks using the Laplacian's eigenvectors that correspond to lesser eigenvalues, LE builds a graph from datapoints, such as a k-NN or ε-neighborhood graph. Due to the "smoothness" of Laplacian's eigenvectors with small eigenvalues, nearby points on the manifold (or graph) will have comparable representations. This is the high-level idea for LE. The generalized eigenvector problem is the formal basis for LE learning embeddings:

term using our notations:

$$d_1(W, \hat{W}) = \sum_{ij} W_{ij} \hat{W}_{ij}$$

$$\hat{W}_{ij} = d_2(Z_i, Z_j) = ||Z_i - Z_j||^2.$$

Therefore, LE learns embeddings such that the Euclidean distance in the embedding space is small

$^2$

for points that are close on the manifold.

4.1.2 DISTANCE-BASED:

## NON-EUCLIDEAN METHODS

It was previously supposed that embeddings are learnt in a Euclidean space via the distance-based approaches that were outlined. Since graphs are discrete data structures that do not conform to the standard Euclidean geometry, there have been a number of proposals to study graph embeddings into non-Euclidean spaces rather than traditional geometry. One such space is the hyperbolic one; it is ideal for representing hierarchical data due to its non-Euclidean geometry and continuous negative curvature. For simplicity's sake, imagine hyperbolic space as a continuous tree model, with geodesics (the generalization of shortest routes on manifolds) behaving similarly to shortest paths in discrete tree models. In hyperbolic space, the volume of a ball increases at an exponential rate as its radius does, much as the number of nodes in a tree increases at an exponential rate as their distance from the root does. Hyperbolic space, on the other hand, offers more "room" to accommodate complicated hierarchies and compress representations, as this volume expansion is only polynomial in Euclidean space. Specifically, unlike in Euclidean space, hyperbolic embeddings may embed trees with arbitrarily low distortion in just two dimensions (Sarkar, 2011). Since hyperbolic geometry permits embeddings with far less distortion, it provides an intriguing alternative to Euclidean geometry for graphs exhibiting hierarchical patterns, and hyperbolic space is therefore an obvious choice for embedding data resembling trees. Hyperbolic geometry has a long history of usage in network science research prior to its incorporation into machine learning applications. Using spanning trees, Kleinberg (2007) suggested a greedy technique for geometric roots that does greedy geographic routing after mapping sensor network nodes to hyperbolic plane coordinates. Studying the structural aspects of complex networks—networks having non-trivial topological features used to mimic real-world systems—has also made use of hyperbolic geometry. In 2010, Krioukov et al. established a geometric framework for building scale-free networks, which are a class of complex networks characterized by power-law degree distributions. They also proved that every scale-free graph exhibiting metric structure has, at its core, hyperbolic geometry. A popularity-similarity (PS) framework for modeling the development and expansion of complicated networks was proposed by Papadopoulos et al. (2012). Using their radial coordinates in hyperbolic space and their angular coordinates, popular nodes and similar nodes are likely to be linked in this model. Moreover, this structure has been used to transform graph nodes into hyperbolic coordinates by increasing the probability that the network is generated by the PS model (Papadopoulos et al., 2014). Additional research has improved graph-to-hyperbolic-coordinate mapping efficiency using non-linear dimensionality reduction methods as LLE (Belkin and Niyogi, 2002; Alanis-Lobato et al., 2016; Muscoloni et al., 2017).

More recently, there has been interest in learning hyperbolic representations of hierar- chical graphs or trees, via gradient-based optimization. We review some of these machine learning-based algorithms next.

**Poin ca r é embeddings** Nickel and Kiela (2017) learn embeddings of hierarchical graphs such as lexical databases (e.g. WordNet) in the Poincaré model hyperbolic space.

$$d_2(Z_i, Z_j) = d_{\text{Poincaré}}(Z_i, Z_j)$$

$$= \text{arcosh}\left(1 + 2\frac{\|Z_i - Z_j\|^2}{(1 - \|Z_i\|^2)(1 - \|Z_j\|^2)}\right).$$

Using our notations, this approach learns hyperbolic embeddings via the Poincaré distance function:

Embeddings are thenlearned by minimizing distances between connected nodes while max- imizing distances between disconnected nodes:

$$d_1(W, \hat{W}) = -\sum_{ij}$$

$$W_{ij}\log \frac{e^{-\hat{W}_{ij}}}{\sum_{k|W_{ik}=0} e^{-\hat{W}_{ik}}}$$

$$= - \quad W_{ij} \log \ \text{Softmax}_{k|Wik=0}(-W_{ij}),$$

where the denominator is approximated using negative sampling. Note that since the hyper- bolic space has a manifold structure, embeddings need to be optimized using Riemannian optimization techniques (Bonnabel, 2013) to ensure that they remain on the manifold.

Other variants of these methods have been proposed. In particular, Nickel and Kiela (2018) explore a different model of hyperbolic space, namely the Lorentz model (also known as the hyperboloid model), and show that it provides better numerical stability than the Poincaré model. Another line of work extends non-Euclidean embeddings to mixed- curvature product spaces (Gu et al., 2018), which provide more flexibility for other types of graphs (e.g. ring of trees). Finally, Chamberlain et al. (2017) extend Poincaré embeddings to incorporate skip-gram losses using hyperbolic inner products.

4.1.3 OUTER PRODUCT-BASED:

MATRIX FACTORIZATION METHODS

Matrix factorization approaches learn embeddings that lead to a low rank representation of some similarity matrix $s(W)$, where $s : \mathrm{R}^{|V|\times|V|} \rightarrow \mathrm{R}^{|V|\times|V|}$ is a transformation of the weighted adjacency matrix, and many methods set it to the identity, i.e. $s(W) = W$. Other transformations include the Laplacian matrix or more complex similarities derived from proximity measures such as the Katz Index, Common Neighbours or Adamic Adar. The decoderfunction in matrix factorization methods is a simple outer product:

$$\hat{W} = \mathrm{DEC}(Z; \Theta^D) = ZZ^{\mathrm{T}}. \quad (3)$$

Matrix factorization methods learn embeddings by minimizing the regularization loss in Eq. (1) with:

$$d_1(W, \hat{W}) = \sum_{(v_i,v_j)\in E} (W_{ij} - \hat{W}_{ij})^2.$$

Recall that $A$ is binary adjacency matrix, with $A_{ij} = 1$ *iif* $(v_i, v_j) \in E$. We can express the graph regularization loss in terms of Frobenius norm:

$$\mathrm{L}_{G,\mathrm{REG}}(W, \hat{W}; \Theta) = ||A \cdot (W - \hat{W})||^2_F,$$

where $\cdot$ is the element-wise matrix multiplication operator. Therefore, GF also learns a low- rank factorization of the adjacency matrix $W$ measured in Frobenuis norm. Note that the sum is only over existing edges in the graph, which reduces the computational complexity of this method from $O(|V|^2)$ to $O(|E|)$.

$$\mathrm{L}_{G,\mathrm{REG}}(W, W; \Theta) = ||s(W) - W||^2_F. \quad (4)$$

That is, $d_1(\cdot, \cdot)$ in Eq. (1) is the Frobenius norm between the reconstructed matrix and the target similarity matrix. By minimizing the regularization loss, graph factorization methods learn low-rank representations that preserve structural information as defined by the similarity matrix $s(W)$. We now review important matrix factorization methods.

**Graph factorization** (GF) (Ahmed et al., 2013) learns a low-rank factorization for the adjacency matrix by minimizing graph regularization loss in Eq. (1) using:

**Graph representation with global structure information** (GraRep) (Cao et al., 2015) The methods described so far are all symmetric, that is, the similarity score between two nodes ($v_i$, $v_j$) is the same a the score of ($v_j$, $v_i$). This might be a limiting assumption when working with directed graphs as some nodes can be strongly connected in one direction and disconnected in the otherdirection. GraRep overcomes this limitation by learning two embeddings per node, a source embedding $Z^s$ and a target embedding $Z^t$, which capture asymmetric proximity in directed networks. GraRep learns embeddings that preserve $k$- hop neighborhoods via powers of the adjacency and minimizes the graph regularization loss with:

$$\hat{W}^{(k)} = Z^{(k),s} Z^{(k),t}$$

$$L_{G,\mathrm{REG}}(W, \hat{W}^{(k)}; \Theta) = ||D^{-1}W^k - \hat{W}^{(k)}||^2 ,$$

for each $1 \leq k \leq K$. GraRep concatenates all representations to get source embeddings $Z^s = [Z^{(1),s}| \ldots |Z^{(K),s}]$ and target embeddings $Z^t = [Z^{(1),t}| \ldots |Z^{(K),t}]$. Finally, note that GraRep is not very scalable as the powers of $D^{-1}W$ might be dense matrices.

**HOPE** (Ou et al., 2016) Similar to GraRep, HOPE learns asymmetric embeddings but uses a different similarity measure. The distance function in HOPE is simply the Frobenius norm and the similarity matrix is a high-order proximity matrix (e.g. Adamic-Adar):

$$\hat{W} = Z^s Z^t$$

$$L_{G,\mathrm{REG}}(\hat{W}, W; \Theta) = \|s(W) - W\|_F^2 .$$

The similarity matrix in HOPE is computed with sparse matrices, making this method more efficient and scalable than GraRep.

4.1.4 OUTER PRODUCT-BASED:

## SKIP-GRAM METHODS

Skip-gram graph embedding models were inspired by efficient NLP methods modeling probability distributions over words for learning word embeddings (Mikolov etal., 2013; Pen- nington et al., 2014). Skip-gram word embeddings are optimized to predict context words,

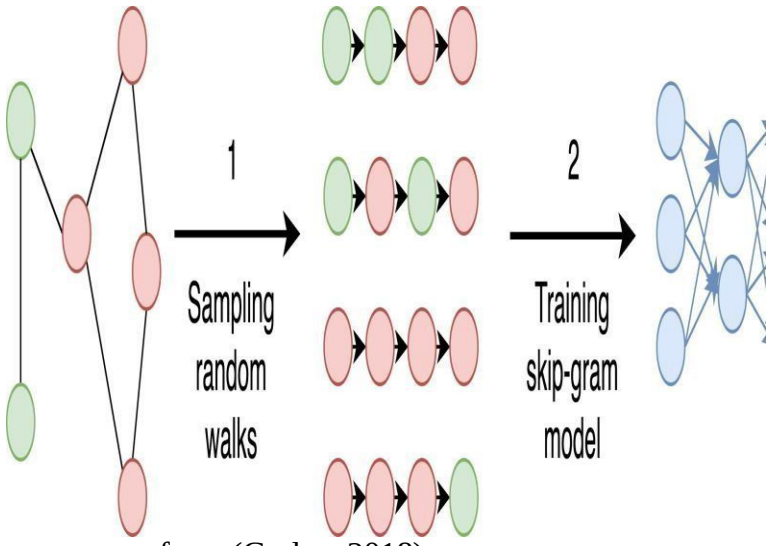



Figure 5: An overview of the pipeline for random-walk graph embedding methods. Reprinted with permission from (Godec, 2018).

or surrounding words, for each target word in a sentence. Given asequence of words ($w_1, \ldots, w_T$), skip-gram will minimize the objective:

$$L = -\sum_{-K \le i \le K, i \neq 0} \log P(w_{k-i} | w_k),$$

for each target words $w_k$. In practice, the conditional trains neural networks by maximizing the probability of probabilities can be estimated using neural networks, and predicting context nodes for each target node in a graph, skip-gram methods can be trained efficiently using negative namely nodes that are close to the target node in terms of sampling. Perozzi et al. (2014) empirically show the hops and graph proximity. For this purpose, node frequency statistics induced by random walks also follow embeddings are decoded into probability distributions over Zipf's law, thus motivating the development of skip-gram nodes using row-normalization of the decoded matrix with graph embedding methods. These methods exploit random softmax.

walks on graphs and produce node sequences that are To train embeddings, DeepWalk generates sequences of similar in positional distribution, as to words in sentences. nodes using truncated unbiased random walks on the In skip-gram graph embedding methods, the decoder graph—which can be compared to sentences in natural function is also an outer product (Eq. (3)) and the graph language models—and then maximize their log-likelihood. regularization term is computed over random walks on the Each random walk starts with a node $v_{i1} \in V$ and graph. repeatedly sample next node at uniform: $v_{ij+1} \in \{v \in V | (v_{ij}, v) \in E\}$. The walk length is a hyperparameter. All generated random-walk can then be passed to an NLP- embedding algorithm e.g. word2vec's Skipgram model. This two-step paradigm introduced by Perozzi et al. (2014) is followed by many subsequent works, such as node2vec (Grover and Leskovec, 2016).

**DeepWalk** (Perozzi et al., 2014) was the first attempt to generalize skip-gram models to graph-structured data. DeepWalk draws analogies between graphs and language. Specif- ically, writing a sentence is analogous to performing a random walk, where the sequence of nodes visited during the walk, is treated as the words of the sentence. DeepWalk

We note that is common for underlying implementations to choice is studied further in (Abu-El-Haija et al., 2017).
use two distinct represen- tations for each node (one for if $s(W) = \mathrm{E}_q \left[ D^{-1}W^q \right]$, then training DeepWalk is
when a node is center of a truncated random walk, and one equivalent to minimizing:
when it is in the context). The implications of this modeling
where $C = \sum_i \sum_j \exp(W_{ij})$ is a normalizing constant.
Notethat computing $C$ requires sum- ming over all
nodes in the graph which is computationally expensive.
DeepWalk overcomes this issue by using a technique
called hierarchical softmax, which computes $C$
efficiently using binary trees. Finally, note that by
computing truncated random walks on the graph,
DeepWalk embeddings capture high-order node
proximity.

**node2vec** (Grover and Leskovec, 2016) is a random-walk based approach for unsuper- vised network embedding, that extends DeepWalk's sampling strategy. The authors in- troduce a technique to generate biased random walks on the graph, by combining graph exploration through breadth first search (BFS) and through depth first search (DFS).Intu- itively, node2vec also preserves high order proximities in the graph but the balance between BFS and DFS allows node2vec embeddings to capture local structures in the graph, as well as global community structures, which can lead to more informative embeddings. Finally, note that negative sampling (Mikolov et al., 2013) is used to approximate the normalization factor $C$ in Eq. (5).

**Watch Your Step** (WYS) (Abu-El-Haija et al., 2018) Random walk methods are very sensitive to the sampling strategy used to generate random walks. For instance, some graphs may require shorter walks if local information is more informative that global graph structure, while in other graphs, global structure might be more important. Both Deep- Walk and node2vec sampling strategies use hyper-parameters to control this, such as the length of the walk or ratio between breadth and depth exploration. Optimizing over these hyper-parameters through grid search can be computationally expensive and can lead to sub-optimal embeddings. WYS learns such random walk hyper-parameters to minimize the overall objective (in analogy: each graph gets to choose its own preferred "context size",such that the probability of predicting random walks is maximized). WYS shows that, when viewed in expectation, these hyperparameters only correspond in the objective to co- efficients to the powers of the adjacency matrix $(W^k)_{1 \le k \le K}$. These coefficients are denoted $q = (q_k)_{1 \le k \le K}$ and are learned through back-propagation. Should $q$'s learn a left-skewed distribution, then the embedding would prioritize local information and right-skewed distri- bution will enhance high-order relationships and graph global structure. This concept has been extended to other forms of attention to the 'graph context', such using a personalized context distributions for each node (Huang et al., 2020).

**Large scale Information Network Embedding** (LINE) (Tang et al., 2015) learns embeddings that preserve first and second order proximity. To learn first order proximity preserving embeddings, LINE minimizes the graph regularization loss:

Intuitively, LINE with second-order proximity decodes embeddings into context conditional distributions for each node $p_2(\cdot|v_i)$. Note that optimizing the second-order objective is computationally expensive as it requires asum over the entire set ofedges. LINE uses negative sampling to sample negative edges according to some noisy distribution over edges. Finally, as in GraRep, LINE combines first and second order embeddings with concatenation $Z = [Z^{(1)}|Z^{(1)}]$.

**Hierarchical representation learning for networks** (HARP) (Chen et al., 2018b) Both node2vec and DeepWalk learn node embeddings by minimizing non-convex functions, which can lead to local minimas. HARP introduces a strategy that computes initial embed- dings, leading to more stable training and convergence. More precisely, HARP hierarchi- cally reduces the number of nodes in the graph via graph coarsening. Nodes are iteratively grouped into super nodes that form a graph with similar properties as the original graph, leading to multiple graphs with decreasing size ($G_1, \ldots, G_T$ ). Node embeddings are then learned for each coarsened graph using existing methods such as LINE or DeepWalk, and at time-step $t$, embeddings learned for $G_t$ are used as initialized embedding for the random walk algorithm on $G_{t-1}$. This process is repeated until each node isembedded in the orig- inal graph. The authors show that this hierarchical embedding strategy produces stable embeddings that capture macroscopic graph information.

**Splitter** (Epasto and Perozzi, 2019) What if a node is not the correct 'base unit' of anal- ysis for a graph? Unlike HARP, which coarsens a graph to preserve high-level topological

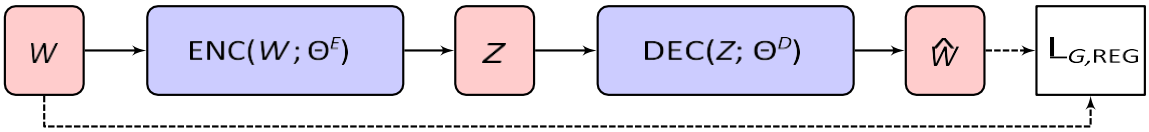



Figure 6: Auto-encoder methods. The graph structure (stored as the graph adjacency ma- trix) is encoded and reconstructed using encoder-decoder networks. Models are trained by optimizing the graph regularization loss computed on the reconstructed

features, Splitter is a graph embedding approach designed to better model nodes which have membership in multiple communities. It uses the Persona decomposition (Epasto et al., 2017), to create a derived graph, $G_P$ which may have multiple *persona* nodes for each original node in $G$ (the edges of each original node are divided among its personas). $G_P$ can then be embedded (with some constraints) using any of the embedding methods discussed so far. The resulting representations allow persona nodes to be separated in the embedding space, and the authors show benefits to this on link prediction tasks.

**Matrix view of Skip-gram methods** As noted by Levy and Goldberg (2014), Skip- grammethods can be viewed as matrix factorization, and the methods discussed hereare related to those of Matrix Factorization (Section 4.1.3). This relationship is discussed in depth by Qiu et al. (2018), who propose a general matrix factorization framework, NetMF, which uses the same underlying graph proximity information as DeepWalk, LINE, and node2vec. Casting the node embedding problem as matrix factorization can offer benefits like easier algorithmic analysis (e.g., convergence guarantees to unique globally-optimal points), and dense matrix undergoing decomposition can be sampled entry-wise (Qiu et al., 2019).

### 6.2 Auto-encoders

Shallow embedding methods hardly capture non-linear complex structures that might arise in graphs. Graph auto-encoders were originally introduced to overcome this issue by us- ing deep neural network encoder and decoder functions, due to their ability model non-linearities. Instead of exploiting the graph structure through the graph regularization term, auto-encoders directly incorporate the graph adjacency matrix in the encoder function. Auto-encoders generally have an encoding and decoding network which are multiple layers of non-linear layers. For graph auto-encoders, the encoder function has the form:

$$Z = \mathrm{ENC}(W; \Theta^E).$$

That is, the encoder is a function of the adjacency matrix $W$ only. These models are trained by minimizing a reconstruction error objective and we review

examples of such objectives next.

**Structural Deep Network Embedding** (SDNE) (Wang et al., 2016) learns auto-encoders that preserve first and second-order node proximity (Section 2.1). The SDNE encoder takes as input a node vector: a row of the adjacency matrix as they explicitly set $s(W) = W$, and produces node embeddings $Z$. The SDNE decoder return a reconstruc- tion $\hat{W}$, which is trained to recover the original graph adjacency matrix (Fig. 7). SDNE

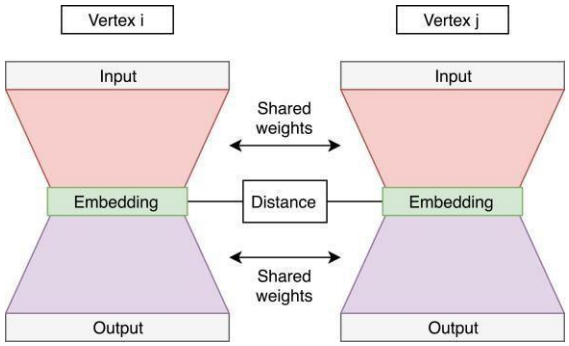



Figure 7: Illustration of the SDNE model. The embedding layer (denoted $Z$) is shown in green. Reprinted with permission from (Godec, 2018).

preserves second order node proximity by minimizing the graph regularization loss:

$$\|(s(W) - \hat{W}) \cdot B\|^2_F + \alpha_{\text{SDNE}} \sum_{ij} s(W)_{ij} \|Z_i - Z_j\|^2_2$$

where $B$ is the indicator matrix for $s(W)$ with $B = 1[s(W) > 0]$. Note that the second term is the regularization loss used by distance-based shallow embedding methods. The first term is similar to the matrix factorization regularization objective, except that $W$ is not computed using outer products. Instead, SDNE computes a unique embedding for each node in the graph using a decoder network.

**Deep neural Networks for learning Graph Representations** (DNGR) (Cao et al., 2016) Similar to SDNE, DNGR uses deep auto-encoders to encode and decode a node similarity matrix, $s(W)$. The similarity matrix is computed using a probabilistic method called random surfing, that returns a probabilistic similarity matrix through graph explo- ration with random walks. Therefore, DNGR captures higher-order dependencies in the graph. The similarity matrix $s(W)$ is then encoded and decoded with stacked denoising auto-encoders (Vincent et al., 2010), which allows to reduce the noise in $s(W)$. DNGR is optimized by minimizing the reconstruction error:

$$L_{G,\text{REG}}(W, \hat{W}; \Theta) = \|s(W) - \hat{W}\|^2_F .$$

### 6.3 Graph neural networks

In graph neural networks, both the graph structure and node features are used in the encoder function to learn structural representations of nodes:

$$Z = \mathrm{ENC}(X, W; \Theta^{E}).$$

We first review unsupervised graph neural networks, and will cover supervised graph neural networks in more details in Section 5.

**Variational Graph Auto-Encoders** (VGAE) (Kipf and Welling, 2016b) use graph convolutions (Kipf and Welling, 2016a) to learn node embeddings $Z = \mathrm{GCN}(W, X; \Theta^{E})$ (see Section 5.3.1 for more details about graph convolutions). The decoder is an outer product: $\mathrm{DEC}(Z; \Theta^{D}) = ZZ^{\mathrm{T}}$. The graph regularization term is the sigmoid cross entropy between the true adjacency and the predicted edge similarity scores:

$$L_{G,\mathrm{REG}}(W, \hat{W}; \Theta) = -\sum_{ij} (1 - W_{ij}) \log(1 - \sigma(\hat{W}_{ij})) + W_{ij} \log \sigma(\hat{W}_{ij}) \quad .$$

Computing the regularization term over all possible nodes pairs is computationally chal- lenging in practice, and the Graph Auto Encoders (GAE) model uses negative sampling to overcome this challenge.

Note that GAE is a deterministic model but the authors also introduce variational graph auto-encoders (VGAE), where they use variational auto-encoders to encode and decode the graph structure. In VGAE, the embedding $Z$ is modelled as a latent variable with a standard multivariate normal prior $p(Z) = \mathrm{N}(Z|0, I)$ and the amortized inference network $q_{\Phi}(Z|W, X)$ is also a graph convolution network. VGAE is optimized by minimizing the corresponding negative evidence lower bound:

$$\begin{aligned}\mathrm{NELBO}(W, X; \Theta) &= -\mathrm{E}_{q_{\Phi}(Z|W,X)}[\log\ p(W|Z)] + \mathrm{KL}(q_{\Phi}(Z|W, X)||p(Z)) \\ &= L_{G,\mathrm{REG}}(W, \hat{W}; \Theta) + \mathrm{KL}(q_{\Phi}(Z|W, X)||p(Z)).\end{aligned}$$

**Iterative generative modelling of graphs** (Graphite) (Grover et al., 2019) extends GAE and VGAE by introducing a more complex decoder, which iterates between pairwise decoding functions and graph convolutions. Formally, the graphite decoder repeats the following iteration:

$$\hat{W}^{(k)} = \frac{Z^{(k)} Z^{(k)\mathrm{T}}}{\|Z^{(k)}\|_2^2} + \frac{11^{\mathrm{T}}}{|V|}$$

$$Z^{(k+1)} = \mathrm{GCN}(\hat{W}^{(k)}, Z^{(k)})$$

where $Z^{(0)}$ are initialized using the output of the encoder network. By using this parametric iterative decoding process, Graphite learns more expressive decoders than other methods based on non-parametric pairwise decoding. Finally, similar to GAE, Graphite can be deterministic or variational.

**Deep Graph Infomax** (DGI) ( Veli̇č kovíć et al., 2019) is an unsupervised graph-level embedding method. Given one or more *real* (positive) graphs, each with its adjacency
matrix $W \in \mathrm{R}^{|V|\times|V|}$ and node features $X \in \mathrm{R}^{|V|\times d_0}$, this method creates *fake* (negative) adjacency matrices $W^{-} \in \mathrm{R}^{|V^{-}|\times|V^{-}|}$ and their features $X^{-} \in \mathrm{R}^{|V^{-}|\times d_0}$. It trains (i) an encoder that processes real and fake samples, respectively giving $Z = \mathrm{ENC}(X, W; \Theta^E) \in \mathrm{R}^{|V|\times d}$ and $Z^{-} = \mathrm{ENC}(X^{-}, W^{-}; \Theta^E) \in \mathrm{R}^{|V|\times d}$, (ii) a (readout) graph pooling function $\mathrm{R} : \mathrm{R}^{|V|\times d} \to \mathrm{R}^d$, and (iii) a descriminator function $\mathrm{D} : \mathrm{R}^d \times \mathrm{R}^d \to [0, 1]$ which is trained to output $\mathrm{D}(Z_i, \mathrm{R}(Z)) \approx 1$ and $\mathrm{D}(Z^{-}, \mathrm{R}(Z^{-})) \approx 0$, respectively, for nodes corresponding to given graph $i \in V$ and fake graph $j \in V^{-}$. Specifically, DGI optimizes:

$$\min_{\Theta} -\mathrm{E}_{X,W}\sum_{i=1}^{|V|}\log \mathrm{D}(Z_i, \mathrm{R}(Z)) - \mathrm{E}_{X^{-},W^{-}}\sum_{j=1}^{|V^{-}|}\log\left(1-\mathrm{D}(Z^{-}_j, \mathrm{R}(Z^{-}))\right), \quad (6)$$

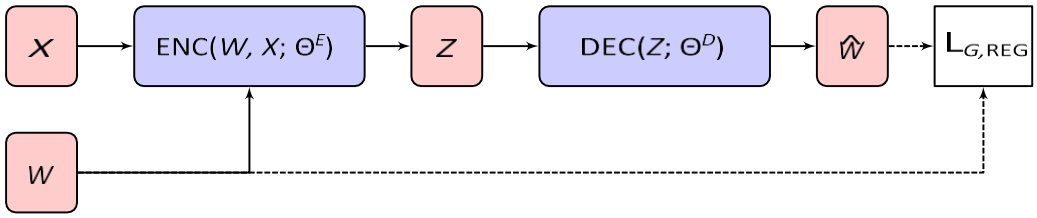



Figure 8: Unsupervised graph neural networks. Graph structure and input features are mapped to low-dimensional embeddings using a graph neural network encoder. Embeddings are then decoded to compute a graph regularization loss (unsupervised).

where $\Theta$ contains $\Theta^E$ and the parameters of R, D. In the first expectation, DGI samples from the real (positive) graphs. If only one graph is given, it could sample some subgraphs from it (e.g. connected components). The second expectation samples fake (negative) graphs. InDGI, fake samples exhibit the real adjacency $W^{-} := W$ but fake features$X^{-}$ are a row-wise random permutation of real $X$, though other negative sampling strategies are plausible. The ENC used in DGI isa graph convolutional network, though any GNN can be used. The readout R summarizes an entire (variable-size) graph to a single (fixed- dimension) vector. Veli̇č kovíć et al. (2019) use R as a row-wise mean, though other graph pooling might be used e.g. ones aware of the adjacency, $\mathrm{R} : \mathrm{R}^{|V|\times d} \times \mathrm{R}^{|V|\times|V|} \to \mathrm{R}^d$.

The optimization (Eq. (6)) is shown by Ve l i ˇc ko víc et al. (2019) to maximize a lower- bound on the Mutual Information (MI) between the outputs of the encoder and the graph

pooling function. In other words, it maximizes the MI between individual node representa- tions and the graph representation.

Graphical Mutual Information (GMI, Peng et al., 2020) presents another MI alternative: rather than maximizing MI of node information and an entire graph, GMI maximizes the MI between the representation of a node and its neighbors.

### 6.4 Summary of unsupervised embedding methods

This section presented a number of unsupervised embedding methods. Specifically, the only supervision signal is the graph itself, but no labels for nodes or the graph are processed by these methods.

Some of these methods (Sec. 4.1) are shallow, and ignore the node features $X$ even if they exist. These shallow methods program the encoder as a "look-up table", parametrizing it by matrix $\in \mathrm{R}^{|V|\times d}$, where each row stores $d$-dimensional embedding vector for a node. These methods are applicable to transductive tasks where is only one graph: it stays fixed between training and inference.

Auto-encoder methods (Sec. 4.2) are deeper, though they still ignore node feature matrix $X$. These are feed-forward neural networks where the network input is the adjacency matrix $W$. These methods are better suited when new nodes are expected atinference test time. Finally, Graph neural networks (Sec. 4.3) are deep methods that process both the adjacency $W$ and node features $X$. These methods are inductive, and are generally empericially outperform the above two classes, for node-classification tasks, especially when nodes have features. For all these unsupervised methods, the model output on the entire graph is $\in \mathrm{R}^{|V|\times|V|}$ that the objective function encourages to well-predict the adjacency $W$ or its transformation $s(W)$. As such, these models can compute latent representations of nodes that trained to reconstruct the graph structure. This latent representation can subsequently be used for tasks at hand, including, link prediction, node classification, or graph classification.

## 7. Supervised Graph Embedding

A common approach for supervised network embedding is to use an unsupervised network embedding method, like the

ones described in Section 4 to first map nodes to an embedding vector space, and then use the learned embeddings as input for another neural network. However, an important limitation with this two-step approach is that the unsupervised node embeddings might not preserve important properties of graphs (e.g. node labels or attributes), that could have been useful for a downstream supervised task.

Recently, methods combining these two steps, namely learning embeddings and predict- ing node or graph labels, have been proposed. We describe these methods next.

### 7.1 Shallow embedding methods

Similar to unsupervised shallow embedding methods, supervised shallow embedding meth-ods use embedding look-ups to map nodes to embeddings. However, while the goal in unsupervised shallow embeddings is to learn a good graph representation, supervised shal- low embedding methods aim at doing well on some downstream prediction task such as node or graph classification.

**Label propagation** (LP) (Zhu and Ghahramani, 2002) is a very popular algorithm for graph-based semi-supervised node classification. It directly learns embeddings in the label space, i.e. the supervised decoder function in LP is simply the identity function:

$$\hat{y}^N = \mathrm{DEC}(Z; \Theta^C) = Z.$$

In particular, LP uses the graph structure to smooth the label distribution over the graph by adding a regularization term to the loss function, where the underlying assumption is that neighbor nodes should have similar labels (i.e. there exist some label consistency between connected nodes). The regularization in LP is computed with Laplacian eigenmaps:

$$\mathrm{L}_{G,\mathrm{REG}}(W, \hat{W}; \Theta) = \sum_{ij} W_{ij} \hat{W}_{ij} \quad (7)$$

where

$$\hat{W}_{ij} = \|\hat{y}_i^N - \hat{y}_j^N\|^2. \quad (8)$$

LP minimizes this energy function over the space of functions that take fixed values on

labelled nodes (i.e. $y\hat{}^N = y^N \ \forall i|v_i \in V_L$) using an iterative algorithm that updates a unlabelled node's label distribution via the weighted average of its neighbors' labels.

There exists variants of this algorithm such as Label Spreading (LS) (Zhou et al.,

## SPECTRUM-FREE METHODS

We now cover spectrum-free methods, which approximate convolutions in the spectral do- main overcoming computational limitations of SCNNs by avoiding explicit computation of the Laplacian's eigendecomposition.

SCNNs filters are neither localized nor paramet- ric, in the sense that the parameters in $F_{ij}^l$ in Eq. (17) are all free. To overcome this issue, sprectrum-free methods use polynomial expansions to approximate spectral filters in Eq. (16) via:

$$F_{i,j}^{l,ij} = P^l(\Lambda)$$

where $P_{ij}^l(\cdot)$ is a finite degree polynomial.

Therefore, the total number of free parameters per filter depends on the polynomial's degree, which is independent of the graph size. Assuming all eigenvectors are kept in Eq. (16), it can be rewritten as:

Attention mechanisms (Vaswani et al., 2017) have been successfully used in language mod- els, and are particularly useful when operating on long sequence inputs, they allow models to identify relevant parts of the inputs. Similar ideas have been applied to graph convolution networks. Graph attention-based models learn to pay attention to important neighbors dur- ing the message passing step. This provides more flexibility in inductive settings, compared to methods that rely on fixed weights such as GCNs.

Broadly speaking, attention methods learn neighbors' importance using parametric func- tions whose inputs are node features at the previous layer. Using GCF, we can abstract patch functions in attention-based methods as functions of the form:

$$f_k(W, H^l) = \alpha(W \cdot g_k(H^l)),$$

where $\cdot$ indicates element-wise multiplication and $\alpha(\cdot)$ is an activation function such as softmax or ReLU.

**Graph Attention Networks** (GAT) (Velič kovi ć et al., 2018) is an attention-based ver- sion of GCNs, which incorporate self-attention mechanisms when computing patches. At every layer, GAT attends over the neighborhood of T ea/ch node and learns to selectively pick nodes which lead to the best performance for some downstream task. Thehigh-level intuition is similar to SAGE (Hamilton et al., 2017a) and makes GAT suitable for induc- tive and transductive problems. However, instead of limiting the convolution step to fixed size-neighborhoods as in SAGE, GAT allows each node to attend over the entirety of its neighbors and uses attention to assign different weights to different nodes in a neighborhood. The attention parameters are trained through backpropagation, and the GAT self-attention mechanism is:

$$g_k(H^l) = \text{LeakyReLU}(H^l B^T b_0 \oplus b_1 B H^T)$$

where $\oplus$ indicates summation of row and column vectors with broadcasting, and $(b_0, b_1)$and $B$ are trainable attention weight vectors and weight matrix respectively. Theedge scores are then row normalized with softmax. In practice, the authors propose to use multi-headed attention and combine the propagated

signals with a concatenation of the average operator followed by some activation function. GAT can be implemented efficiently by computing the self-attention scores in parallel across edges, as well as computing the output representations in parallel across nodes.

**Mixture Model Networks** (MoNet) Monti et al. (2017) provide a general framework that works particularly well when the node features lie in multiple domains such as 3D point clouds or meshes. MoNet can be interpreted as an attention method as itlearns patches using parametric functions in a pre-defined spatial domain (e.g. spatial coordinates), and then applies convolution filters in the graph domain.

Note that MoNet is a generalization of previous spatial approaches such as Geodesic CNN (GCNN) (Masci et al., 2015) and Anisotropic CNN (ACNN) (Boscaini et al., 2016), which both introduced constructions for convolution layers on manifolds. However, both GCNN and ACNN use fixed patches that are defined on a specific coordinate system and therefore cannot generalize to graph-structured data. The MoNet framework is more gen- eral; any pseudo-coordinates such as local graph features (e.g. vertex degree) or manifold features (e.g. 3D spatial coordinates) can be used to compute the patches. More specifi- cally, if $U^s$ are pseudo-coordinates and $H^l$ are features from another domain, then using GCF, the MoNet layer can be expressed as:

$$H^{l+1} = \sigma$$

$$\kappa$$

$$k=1$$

$(W \cdot g_k(U^s))H^l\Theta^l$ , $k$ (23)

where $\cdot$ is element-wise multiplication and $g_k(U^s)$ are the learned parametric patches, which are $|V| \times |V|$ matrices. In practice, MoNet uses Gaussian kernels to learn patches, such that:

$$g_k(U^s) = \exp\left(-\frac{1}{2}(U^s - \mu_k)^T \Sigma_k^{-1} (U^s - \mu_k)\right),$$

where $\mu_k$ and $\Sigma_k$ are learned parameters, and Monti et al. (2017) restrict $\Sigma_k$ to be a diagonal matrix.

(a) GCN layers. (b) HGCN layers.

Figure 13: Euclidean (left) and hyperbolic (right) embeddings of a tree graph. Hyperbolic embeddings learn natural hierarchies in the embedding space (depth indicated by color). Reprinted with permission from (Chami et al., 2019).

### 7.2 Non-Euclidean Graph Convolutions

Hyperbolic shallow embeddings enable embeddings of hierarchical graphs with smaller distortion than Euclidean embeddings. However, one major downside of shallow embeddings is that they are inherently transductive and cannot generalize to new graphs. On the other hand, Graph Neural Networks, which leverage node features, have achievedstate-of-the-art performance on inductive graph embedding tasks.

Recently, there has been interest in extending Graph Neural Networks to learn non- Euclidean embeddings and thus benefit from both the expressiveness of Graph Neural Networks and hyperbolic geometry. One major challenge in doing so is how to perform convolutions in a non-Euclidean space, where standard operations such as inner products and matrix multiplications are not defined.

**Hyperbolic Graph Convolutional Neural Networks** (HGCN) (Chami et al., 2019) and Hyperbolic Graph Neural Networks (HGNN) (Liu et al., 2019) apply graph convolutions in hyperbolic space by leveraging the Euclidean tangent space, which provides a first-order approximation of the hyperbolic manifold at a point. For every graph convolution step, node embeddings are mapped to the Euclidean tangent space at the origin, where convolutions are applied, and then mapped back to the hyperbolic space. These approaches yield significant improvements on graphs that exhibit hierarchical structure (Fig. 13).

### 7.3 Summary of supervized graph embedding

This section presented a number of methods that process task labels (e.g., node or graph labels) at training time. As such,model parameters are directly optimized on the upstream task.

Shallow methods use neither node features *X* nor adjacency *W* in the encoder (Section 5.1), but utilize the adjacency to ensure consistency. Such methods are useful in transductive settings, if only one graph is given, without node features, a fraction of nodes are labeled, and the goal is to recover labels for unlabeled nodes.

## 8. Applications

9. Many different kinds of applications, both supervised and unsupervised, may benefit from graph representation learning techniques. When learning embeddings in an unsupervised setting, task-specific labels are not processed. Instead, the graph serves as a tool for self-monitoring. Using unsupervised embedding techniques (Section4, top branch of the Taxonomy in Fig. 3), one may learn embeddings that preserve the network (i.e. neighborhoods) or the structural equivalence of nodes (for distinction, see Section 2.2.3). Alternatively, in supervised applications, such as graph or node classification, the optimization of node embeddings is done directly for a particular job. Section 5, the bottom branch of the Taxonomy in Figure 3, describes supervised embedding approaches that may be used in this context. Here are a few of the most common GRL jobs and the methods used to do them, as shown in Table 5. What follows is a rundown of typical

supervised and unsupervised graph uses.

### 9.1 Unsupervised applications

#### 9.1.1 Graph reconstruction

10. Graph reconstruction is the gold standard for unsupervised graph applications. The objective here is to train mapping functions (parametric or not) that retain graph features like node similarity while mapping nodes to dense distributed representations. By reducing a reconstruction error—the error in retrieving the original graph from learnt embeddings—models may be trained, and graph reconstruction doesn't need any supervision. For some instances of reconstruction aims, see Section 4, and to learn about the techniques used for this purpose, see Section 5. Similar to dimensionality reduction, the overarching objective of graph reconstruction is to combine incoming data into a low-dimensional representation. Graph reconstruction models aim to compress data specified on graphs into low-dimensional vectors, rather than the usual way of reducing dimensionality (e.g., principal component analysis) which involves converting high-dimensional vectors into low-dimensional ones.

#### 10.1.1 Link prediction

11. The goal of link prediction is to forecast which edges in a graph will eventually take a certain path. To rephrase, link prediction tasks aim to anticipate the appearance of linkages that have not yet been detected, such as links that might emerge in the future for networks that are both dynamic and temporal. Furthermore, malicious linksmay be located and eliminated with the use of link prediction. Common examples of this kind of application are recommendation systems that utilize graph learning models to forecast the interactions between users and products and social networks that use these models to forecast the friendships between users.

12.

| | Method | Training complexity | | Training input |
|---|---|---|---|---|
| | | Memory | Computation | |
| **(a)** | DeepWalk (Perozzi, 2014) | $O(\|V\|d)$ | $O(c^2 d\|V\|\log_2\|V\|)$ | $W$ |
| **(b)** | node2vec (Grover, 2016) | $O(\|V\|d)$ | $O(c^2 d\|V\|)$ | |
| **(c)** | LINE (Tang, 2015) HOPE (Ou, 2016) GF (Ahmed, 2013) | $O(\|V\|d)$ | $O(\|E\|d)$ | |
| **(d)** | SDNE (Wang, 2016) DNGR (Cao, 2016) | $O(\|V\|b\mathrm{D})$ | $O(\|V\|b\mathrm{M})$ | |
| **(e)** | GraRep (Cao, 2015) WYS (Abu-el-haija, 2018) | $O(\|V\|^2)$ | $O(\|V\|^3 c + \|V\|^2 d)$ | |
| **(f)** | HARP (Chen, 2018) | *inherits* | | $W$ |
| **(g)** | Splitter (Epasto, 2019) | *inherits* | | $W$ |
| **(h)** | MDS (Kruskal, 1964) | $O(\|V\|^2)$ | $O(\|V\|^3)$ | $X$ induces $W$ |
| **(i)** | LP (Zhu, 2002) LLE (Roweis, 2000) | $O(\|V\|)$ | $O(\|E\| \times \text{iters})$ | |
| **(j)** | GNN Methods | $O(\|V\|\mathrm{D})$ | $O(\|E\|\mathrm{D} + \|V\|\mathrm{M})$ | $X$, $W$ |
| **(k)** | SAGE (Hamilton, 2017) | $O(bF^H\mathrm{D})$ | $O(bF^{H-1}\mathrm{D} + bF^H\mathrm{M})$ | $X$, $W$ |
| **(l)** | GTTF (Markowitz, 2021) | $O(bF^H\mathrm{D})$ | $O(bF^{H-1}\mathrm{D} + bF^H\mathrm{M})$ | $X$, $W$ |

Summarization and real-world applications of GRL techniques (Table 5). The columns running from right to left show the following: method classes, the hardware cost to train the method, and real cases where the methods have been useful: inputs to the methods, which may be either an adjacency matrix (W) or node characteristics (X), or both. This is how we get the Training Complexity. In the method classes (a-h), "c" represents the size of the context (such as the length of a random walk) and "d" the size of the embedding dictionary; both are parameters of node embedding techniques. The embedding dictionary isstored in (a) DeepWalk and (b) node2vec, with(V d) floating-point entries. During training, a predetermined number of walks with a defined duration are simulated from every node V. Along these walks, the dot products of all node-pairs within a window of size c are computed. Both the hierarchical softmax (a) and the negative sampling (b) are applied to every pair. To see the complexity per batch, just replace the two V terms on the left with batch size b. But to keep things simple, we look at it per period. (c) All edges are cycled through by LINE (Tang, 2015), HOPE (Ou, 2016), and GF (Ahmed, 2013). (d) The adjacency matrix is used to train auto-encoders via SDNE and DNGR, with batch-size b, and the total dimensions of all layers denoted by A dA. To handle floating-point

operations in matrix multiplications, the formula = A dAdA+1 is used. With full-batch, b equals V. (e) GraRep and WYS store a dense square matrix with (V 2) non-zero elements, and they elevate the transition matrix to the power of c. Their complexity is algorithm-specific since (f) HARP (Chen, 2018) and (g) Splitter can execute any algorithm, for example, (a-e). In this case, we assume that both the average number of persons per node for Splitter and the number of times HARP is activated (the graph's scales) are minimal (V). (h) While LE necessitates the entire eigendecomposition of the graph laplacian matrix (to get the eigenvectors corresponding to the fewest eigenvalues), MDS calculates all-pairs similarity. If the number of label classes is small, (i) LP and LLE will loop over edges up to "iters" iterations. (j) include GCN, GAT, MixHop, GIN, GGNN, MPNN, ChebNet, and MoNet graph convolution algorithms (Kipf, 2016; Defferrard, 2016; Abu-el-haija, 2019; Xu, 2018; Li, 2015; Gilmer, 2017; Xu, 2018; Xu, 2018; Monti, 2017). The creators of those techniques gave a full-batch implementation, which we presume is naïve. After adding up all of the floating-point operations performed by its neighbors (a total of E floats), each node in a given layer multiplies that total by the layer filter (a total of V floats). Lastly, sampling approaches such as (k-l) enable learning to scale to bigger networks by reducing the hardware required of the training algorithm and separating memory complexity from graph size. (k) For each node in the batch (with a size of b), (l) GTTF samples F nodes, and for each node's neighbors, F as well. This continues until the tree height reaches H. We disregard the runtime complexity of data pre-processing for (k) and (l) since it has to be calculated only once per graph, independent of the number of (hyperparameter) sweep computations. A common approach for training link prediction models is to mask some edges in the graph (positive and negative edges), train a model with the remaining edges and then test it on the masked set of edges. Note that link prediction is different from graph reconstruction. In link prediction, we aim at predicting links that are not observed in the original graph while in graph reconstruction, we only want to compute embeddings that preserve the graph structure through reconstruction errorminimization.

Finally, while link prediction has similarities with supervised tasks in the sense that we have labels for edges (positive, negative, unobserved), we group it under the unsupervised class of applications since edge labels are usually not used during training, but only used to measure the predictive quality of embeddings. That is, models described in Section 4 can be applied to the link prediction problem.

### 12.1.1 CLUSTERING

**13.** The discovery of communities is one of the numerous real-world applications of clustering. For example, clusters may be seen in biological networks (as collections of proteins with shared characteristics) or social networks (as associations of individuals with same interests).

Keep in mind that clustering issues may be solved using the unsupervised approaches discussed in this review. For example, one might apply a clustering algorithm, such as k-means, to embeddings that are produced by an encoder. Another option is to include clustering into the learning process while using a shallow or Graph Convolution embedding model (Rozemberczki et al., 2019; Chiang et al., 2019; Chen et al., 2019a).

#### 13.1.1 VISUALIZATION

**14.** For visualizing graphs, there are several ready-made tools that map nodes onto two-dimensional manifolds. Network scientists are able to get a qualitative understanding of graph characteristics, node interactions, and node clusters via the use of visualizations. Force-Directed Layouts-based approaches with different web-app Javascript implementations are among the popular tools. To achieve this visualization, onecan use an unsupervised graph embedding method such as t-distributed stochastic neighbor embeddings (t-SNE) or principal component analysis (PCA) after training an encoder-decoder model (which is equivalent to a shallow embedding or graph convolution network) (Maaten and Hinton, 2008; Jolliffe, 2011). Graph learning techniques are often evaluated qualitatively using this approach (embedding → dimensionality reduction). To color the nodes in 2D visualization plots, one may utilize their characteristics if the nodes have any. As seen in visual representations of different approaches, good embedding algorithms place nodes in the embedding space that have comparable properties close together (Perozzi et al., 2014; Kipf and Welling, 2016a; Abu-El-Haija et al., 2018). To conclude, approaches that map every graph to a representation may also be projected into two dimensions to display and qualitatively assess graph-level features, in addition to mapping every node to a 2D coordinate (Al-Rfou et al., 2019).

### 14.1 Supervised applications

#### 14.1.1 NODE CLASSIFICATION

**15.** An essential supervised graph application is node classification, which aims to develop representations of nodes that can reliably predict their labels. In citation networks, node labels may represent scientific

subjects; in social networks, they might represent gender and other characteristics. One typical use case is semi-supervised node classification due to the high cost and time commitment associated with labeling huge graphs. The objective in semi-supervised situations is to use node linkages to predict characteristics of unlabeled nodes, with just asmall percentage of nodes being tagged. Since there is a single partly labeled fixed graph in this context, it is considered transductive. Inductive node classification is another option; this is the process of determining how to categorize nodes in different networks. Keep in mind that if the node attributes are descriptive of the goal label, they may greatly improve performance on classified nodes jobs. In fact, by integrating structural data with semantic information derived from features, state-of-the-art performance on multiple node classification benchmarks has been attained by more recent approaches as GCN (Kipf and Welling, 2016a) or GraphSAGE (Hamilton et al., 2017a). However, other approaches, such random walks on graphs, do not take use of feature information and so perform worse on these tasks.

### 15.1.1 GRAPH CLASSIFICATION

**16.** One example of a supervised application is graph classification, the goal of which is to use an input graph to predict labels at the graph level. Due to the constant introduction of novel graphs during testing, graph classification problems are fundamentally inductive. Biochemical activities and online social networks are also common choices. Graphs representing molecules are often used in the biological field. A feature vector that is a 1-hot encoding of an atom's number may serve as a node in these graphs, and a bond can be represented by an edge between two nodes, with the kind of the bond being indicated by the feature vector. One example of a task-dependent graph-level label is MUTANG, which indicates the mutagenicity of a medicine against bacteria (Debnath et al., 1991). Typically, people are represented as nodes in online social networks, while connections or interactions are symbolized by edges. As an example, there are a lot of graphs in the Reddit graph classification jobs (Yanardag and Vishwanathan, 2015). An edge will link two nodes in a graph that represents a conversation thread, such as when one person comments on another's remark.

Given a comment graph, the objective is to identify the community (sub-reddit) where the conversation occurred.While tasks such as nodeclassification and edge prediction include pooling at the node and edge levels, respectively, graph classification tasks need a different kind of pooling to aggregate data at the node and graph levels. As said before, expanding this concept ofpooling to any kind of graph is a challenging and ongoing topic of study. Node order shouldn't affect the pooling function. For example, several approaches use basic pooling, including taking the mean or total of all latent vectors at the node level in the network (Xu et al., 2018). Ying et al., 2018b; Cangea et al., 2018; Gao and Ji, 2019; Lee et al., 2019 are among the approaches that employ differentiable pooling. Tsitsulin et al. (2018a), Al-Rfou et al. (2019), and Tsitsulin et al. (2020a) all provide supervised approaches for learning graph-level representations, but there are also many unsupervised methods. Some unsupervised graph-level models that stand out include reviewed by Viswanathan et al. (2010) and Kriege et al. (2020) as graph kernels (GKs).

Although GKs are not our primary concern, we do touch on their links to GRAPHEDM here. Graph-level tasks, such graph categorization, are suitable for GKs. In order to convert any two graphs into a scalar, GK may automatically apply a similarity function. Counting the number of walks (or pathways) that two graphs have in common is one way that traditional GKs calculate graph similarity. For example, each walk may be stored as a series of node labels. Common practice dictates using node degrees as labels in the absence of explicit labels. The capacity ofGKs to identify (sub-)graph isomorphism is a common metric for analysis. When ordering of nodes is ignored, two (sub-)graphs are considered isomorphic if they are identical. According to the 1-dimensional Weisfeiler-Leman (1-WL) heuristic, two sub-graphs are considered isomorphic since sub-graph isomorphism is NP-hard. In each graph, histograms are used to tally the statistics of the nodes (e.g., how many nodes with the label "A" have an edge to nodes with the label "B"). If two graphs' histograms, obtained from the same 1-hop neighborhood, are equal, then the graphs are considered isomorphic according to the 1-WL heuristic. An example of a GNN that has been shown to achieve the 1-WL heuristic is the Graph Isomorphism Network (GIN; Xu et al., 2018). This means that GIN can only map two graphs to the same latent vector if they are considered isomorphic according to the 1-WL heuristic. In some newer studies, GKs and GNNs are used together. Using the similarity of the "tangent space" of the goal with respect to the Gaussian-initialized GNN parameters, Du et al. (2019) models the similarity of two graphs, and Chen et al.

(2020) extracts walk patterns. There isn't any GNN training in either (Du et al., 2019; Chen et al., 2020). Instead, kernel support vector machines and other kernelized algorithms are used to the pairwise Gram matrix during training. Therefore, our GCF and GRAPHEDM frameworks are not well-suited to include these methodologies. However, there are other approaches that don't rely on indirectly computing graph-to-graph similarity scalar scores but instead directly map graphs to high-dimensional latent spaces. One example is Morris et al.'s (2019) k-GNN network, which is deliberately coded as a GNN but can actually implement the k-WL heuristic (which is identical to 1-WL but where histograms are produced up-to k-hop neighbors). Therefore, our GCF and GRAPHEDM frameworks can define the k-GNN model classes.

Conclusion and Open Research Directions

We presented a standard method for comparing ML models trained on graph-structured data in this survey. Deep graph embedding techniques, graph auto-encoders, graph regularization techniques, and graph neural networks are all included in our expanded GRAPHEDM framework, which was before used for unsupervised network embedding. Additionally, we presented a graph convolution framework (GCF) for describing and comparing graph neural networks that rely on convolution, such as spatial and spectral graph convolutions in particular. We included more than 30 supervised and unsupervised techniques for graph embedding in our exhaustive taxonomy of GRL methods, which we presented using this framework.

With any luck, the results of this poll will inspire further GRL research, which should lead to solutions for the problems these models are experiencing right now. The taxonomy is very useful for practitioners since it helps them understand the many tools and applications available and makes it easy to choose the right technique for each situation. Furthermore, academics who have just published Researchers may use the taxonomy to organize their inquiries, locate relevant literature, establish reliable baselines for comparison, and choose suitable methods for data analysis.

Although GRL approaches have shown to be very effective in node classification and link prediction, there are still several issues that need to be addressed. We then go on to talk about the difficulties and future prospects of graph embedding models in terms of research.

**Evaluation and benchmarks**

Standard benchmarks for node classification or link prediction are usually used to evaluate the approaches presented in this review. To illustrate the point, graph embedding techniques are often evaluated against citation networks. The findings may differ greatly depending on the datasets' splits or training processes (such as early halting), which is a problem with these tiny citation benchmarks, as shown in recent research (Shchur et al., 2018).

Using strong and consistent evaluation methodologies, as well as expanding the scope of assessment beyond small node categorization and link prediction benchmarks, is crucial for the improvement of GRL approaches. New graph benchmarks with leaderboards (Hu et al., 2020; Dwivedi et al., 2020) and graph embedding libraries (Fey and Lenssen, 2019; Wang et al., 2019; Goyal and Ferrara, 2018a) are examples of recent development in this approach. Similarly, in order to test GNNs' reasoning skills, Sinha et al. (2020) suggested a series of exercises based on first-order logic.

**Fairness in Graph Learning** To prevent models from correlating'sensitive' characteristics with the model's predicted output, a new area called Fairness in Machine Learning is developing (Mehrabi et al., 2019). Considering the association of the graph

structure (the edges) and the feature vectors of the nodes with the final output, these considerations might be particularly significant for graph learning challenges.

Bose and Hamilton (2019) state that adversarial learning is the most prevalent method for implementing fairness requirements in models. This method may be used to GRL in order to debias the model's predictions with respect to the sensitive feature(s). But there are no certain assurances on the precise amount of bias eliminated using adversarial approaches. The debiasing job itself may be difficult to accomplish with several debiasing strategies(Gonen and Goldberg, 2019). Provable guarantees for debiasing GRL have been the focus of recent work in the field (Palowitch and Perozzi, 2019).

## Application to large and realistic graphs

Graph learning techniques are typically reserved for datasets of tens of thousands to hundreds of thousands of nodes. Still, there are far bigger graphs in the actual world, with billions of nodes. A Distributed Systems configuration with several computers, like MapReduce, is necessary for methods that scale for big graphs (Lerer et al., 2019; Ying et al., 2018a) (Dean and Ghemawat, 2008). Is there a way for a researcher to use a home computer to apply a learning approach to a very big graph that fits on a single hard drive (e.g., with a one terabyte size) but does not fit on RAM? See how this stacks up against a computer vision challenge using a large picture collection (Deng et al., 2009; Kuznetsova et al., 2020). Any model that can fit on RAM can be trained on personal computers, regardless of the size of the dataset. Graph embedding models, in particular those whose parameters grow in size as the graph's nodes do, may find this issue very difficult to solve.

Even picking the right graph to utilize as input might be challenging at times in business. The Google system Grale, which learns the right graph from several characteristics, is described by Halcrow et al. (2020). For graph learning on massive datasets, Grale uses similarity search methods (such as locality sensitive hashing). A recent study by Rozemberczki et al. (2021) adds an attention network to the Grale model, enabling end-to-end learning.

We anticipate that learning algorithms for big graphs that are still executable on a single computer will present new mathematical and practical problems. We are hopeful that scholars would prioritize this area so that non-expert practitioners, like a neurology researcher, may access and use these learning methods to evaluate the human brain's sub-graph, which is comprised of neurons and synapses represented as nodes and edges.

**Molecule generation** Learning on graphs has a great potential for helping molecular scientists to reduce cost and time in the laboratory. Researchers proposed methods for predicting quantumproperties of molecules (Gilmer et al., 2017; Duvenaud et al., 2015) and for generating molecules with some desired properties (Liu et al., 2018; De Cao and Kipf, 2018; Li et al., 2018; Simonovsky and Komodakis, 2018; You et al., 2018). A review of recent methods can be found in (Elton et al., 2019). Many of these methodsare concerned with manufacturing materials with certain properties (e.g. conductance and malleability), and others are concerned drug design (Jin et al., 2018; Ragoza et al., 2017; Feng et al., 2018).

**Combinatorial optimization**

Numerous fields encounter computationally challenging challenges, such as routing science, cryptography, decision-making, and planning. Computationally hard problems are those for which the techniques used to find the best solution have poor scalability. We cite (Bengio et al., 2018) for a summary of the ways that have recently attracted attention in

solving combinatorial optimization issues by using machine learning approaches, such as reinforcement learning. Recently, there has been interest in using graph embeddings to approximate solutions to NP-hard problems (Khalil et al., 2017; Nowak et al., 2017; Selsam et al., 2018; Prates et al., 2019). Graphs are a natural representation for many hard issues, such as SAT and vertex cover; in fact, many problems may be described in terms of graphs. These techniques use a data-driven approach to solving computationally difficult issues, such as determining whether a specific instance (e.g., node) is part of the best solution from among many instances of the problem. Find assignments that strive to accomplish a goal (e.g., the minimal conductance cut) in other works that optimize graph partitions (Bianchi et al., 2020; Tsitsulin et al., 2020b). All of these methods use GNNs as their starting point since GNNs, thanks to their relational inductive biases, can better depict graphs than regular neural networks (e.g. permutation invariance). Current solutions still outperform these data-driven approaches,but GNNs have shown promise in generalizing to bigger problem cases (Nowak et al., 2017; Prates et al., 2019). Lamb et al. (2020) provides a comprehensive overview of GNN- based approaches to combinatorial optimization in their latest study on neural symbolic learning.

**Non-Euclidean embeddings** The underlying space geometry is an important part of graph embeddings, as we saw in Sections 4.1.2 and 5.6. All graphs are discrete complex, non-Euclidean structures with high dimensions; however, there is currently no simple method for encoding such data into embeddings with low dimensions that maintain the graph topology (Bronstein et al., 2017). Hyperbolic and mixed-product space embeddings are two examples of non-Euclidean embeddings that have recently attracted attention and made strides in the field of learning (Gu et al., 2018; Nickel and Kiela, 2017). In comparison to their Euclidean counterparts, these non-Euclidean embeddings have the potential for embeddings that are more expressive. For example, compared to Euclidean embeddings, hyperbolic embeddings exhibit significantly less distortion when representing hierarchical data (Sarkar, 2011). This has led to state-of-the-art outcomes in numerous contemporary applications, including linguistics tasks (Tifrea et al., 2018; Le et al., 2019) and knowledge graph link prediction (Balazevic et al., 2019; Chami et al., 2020).

Non-Euclidean embeddings often bring two difficulties: first, hyperbolic space precision problems (e.g., at the Poincar'e ball boundary) (Sala et al., 2018; Yu and De Sa, 2019), and second, difficult Riemannian optimization (Bonnabel, 2013; Becigneul and Ganea, 2018). Furthermore, it is not apparent how to choose the appropriate shape for an input graph. An intriguing area for future research is the process of selecting or learning the appropriate geometry for a specific discrete graph, even though there are already discrete measures for the graphs' tree-likeliness, such as Gromov's four-point condition (Jonckheere et al., 2008; Abu-Ata and Dragan, 2016; Chen et al., 2013; Adcock et al., 2013).

Assurances based on theory Recent developments in graph embedding model design have outperformed state-of-the-art methods in several domains. Nevertheless, our knowledge of the theoretical promises and constraints of graph embedding models is currently restricted. Xu et al. (2018), Verma and Zhang (2019), Morris et al. (2019), and Garg et al. (2020) all apply current findings from learning theory to the issue of GRL, which is a new field of study on GNN representational power. If we want to know what the theoretical benefits and drawbacks of graph embedding techniques are, we need to build theoretical frameworks.

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