Learning distributed representations of graphs with Geo2DR

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Abstract

We present Geo2DR, a Python library for unsupervised learning on graph-structured data using discrete substructure patterns and neural language models. It contains efficient implementations of popular graph decomposition algorithms and neural language models in PyTorch which are combined to learn representations using the distributive hypothesis. Furthermore, Geo2DR comes with general data processing and loading methods which can bring substantial speed-up in the training of the neural language models. Through this we provide a unified set of tools and design methodology to quickly construct systems capable of learning distributed representations of graphs. This is useful for replication of existing methods, modification, or even creation of novel systems. This work serves to present the Geo2DR library and perform a comprehensive comparative analysis of existing methods re-implemented using Geo2DR across several widely used graph classification benchmarks. We show a high reproducibility of results in published methods and interoperability with other libraries useful for distributive language modelling.

1 Introduction

Many real world phenomena such as molecules, protein structures [1], application process calls [2], and social networks [3] can be naturally represented using graphs. For example, in chemistry the graph makes an intuitive model for a molecule where nodes represent atoms and edges the bonds between them. Here the graph is an appropriate representation as it captures not only the presence of the atoms in the molecule, but the edges also capture the specific bonding patterns between the atoms which is important for distinguishing isomers that a classical chemical formula cannot describe. In other words, the resulting graph topology created by the relationships between the nodes in a graph reveal a structural complexity that can be analysed as a source of information in pattern recognition tasks.

An operational assumption made in learning on graph-structured data is that similar graphs will also exhibit similar topological properties. Hence the ability to quantify the similarity of different graph topologies is central to the development of graph learning algorithms. Various approaches have been proposed interpreting, and translating, this assumption for machine learning tasks. Early approaches focused predominantly on defining kernel functions which approximate the comparability of graphs using invariants or substructures such as nodes, subgraphs or random walks [4]. Whilst powerful and intuitive in nature, such kernels are dependent and often tied to kernel methods such as support vector machines (SVM) to perform learning tasks [3].

More recently deep learning approaches for graph representation learning have gained significant research activity with the successful interpretation of graph convolutional operators for learning representations of nodes [5, 6, 7, 8]. Representations at the graph level are then constructed through the successive application of different pooling operations which aggregate node representations towards a single fixed size vector representation for the entire graph [9, 10, 11].
Yet another approach focuses on self-supervised learning of vector embeddings through the distributive modelling of discrete higher order substructure patterns across the graphs in a dataset. This approach makes use of the distributive hypothesis [12] originally used in statistical language modelling to create vector space models of graphs and its substructure patterns [3, 2, 13]. Herein, the vector positions of the distributed vector representations are contextualised by the substructure patterns within graphs with respect to the patterns within other graphs across the dataset.

The difficulty of reliably constructing graph learning methods has driven the need for toolkits and libraries to facilitate their development for replication, extension or even creation of new models. Several such libraries have been made for graph kernels [14, 15] and for graph neural networks [16, 17, 18, 19]. However, as far as the authors are aware, no such toolkit exists specifically for learning distributed representations of graphs. This project, Geo2DR (Geometric to Distributed Representations), aims to fill this gap.

Geo2DR is a Python library to support the construction of systems capable of learning distributed representations of graphs. This framework for self-supervised learning of substructures and entire graphs is based around a simple two stage design methodology. The first stage consists of inducing discrete substructure patterns such as graphlets, rooted subgraphs, or anonymous walks within and across the graphs in a dataset to construct a vocabulary and corpus dataset contextualizing the patterns and graphs. The second stage consists of utilising neural language embedding methods to learn distributed representations of graphs contextualised by the induced substructure patterns.

Geo2DR contains multiple modules to facilitate this process. It includes efficient decomposition algorithms for inducing substructure patterns such as graphlets, shortest paths, anonymous walks across datasets of graphs and recording metadata to support the first stage. It then provides PyTorch [20] implementations of common neural embedding methods based on the distributive hypothesis to achieve the second stage. This includes models such as Skipgram and CBOW for learning substructure pattern embeddings [21, 3] and PV-DBOW and PV-DM for directly learning representations of arbitrary sized graphs [22, 2, 13]. Reference data processing and formatting tools are included for transforming publicly available datasets such as Kersting et al. for Geo2DR. Additionally, we include options in corpus construction and loading methods which load datasets from disk to memory for substantial speed up in the training of the neural embeddings models. Notably, through the use of PyTorch all implemented neural language models support both CPU and GPU processing.

Geo2DR is released under the MIT License and is available on GitHub [1]. It is a growing project with reference re-implementations of existing systems and simple implementations of novel models that may be used to further study distributed representations of graphs. In summary, this paper makes the following contributions:

- Provide an overview of Geo2DR, a unified set of modules for constructing systems capable of learning distributed representations of graphs and its substructures. (Section 4.)
- A modular design of the individual modules of the library so that they may be used independently of the other stages of our design methodology. For example, one can seamlessly use the decomposition algorithms and the output substructure patterns with the GenSim library [24] for distributive modelling if a user does not want to use the implemented neural language models. Conversely, the implemented PyTorch models may be used on other discrete structure beyond graphs. In other words, whilst the main intention of our toolkit is for graph learning, they may be re-purposed for other projects. (Section 4 and 6.)
- We open a repository of reference implementations for published methods such as: Narayanan et al.’s Graph2Vec [2], DGK-WL, -SP, -GK by Yanardag and Vishwanathan [3], and Anonymous Walk Embeddings by Ivanov and Burnaev [13] to help new users create their own distributed vector space models of graphs. It also includes reference implementations for graph kernel methods that may be used with the kernel methods in Sci-kit Learn [25] and LibSVM [26] to construct variants of the DGK models. (Section 4.)
- A comprehensive comparative study of existing systems for graph classification under homogeneous experimentation scenarios. This allows a fairer constructive analysis of these systems and empirical evaluation on the correctness of re-implementation created via Geo2DR. Throughout we show a high ability to reproduce results produced in published systems. (Section 5.)

1 https://github.com/paulmorio/geo2dr
2 Preliminaries on graphs and graph kernels

We adopt the following definition and notation for describing graphs and graph kernels. A graph is an abstract structure which defines a set of entities which are related in some way. Graphs contain nodes representing said entities with related nodes being connected by an edge which records the relation. We define \( G = (V, E) \) as a graph where \( V \) is a set of nodes and \( E \subseteq (V \times V) \) is a 2-tuple set of edges in the graph. Hence if \( u \) and \( v \) are nodes in \( G \), their relation is recorded with an edge as \((u, v) \in E\). The neighbours of a node \( v \) in graph \( G = (V, E) \), is the set of nodes which share an edge with \( v \), denoted \( \mathcal{N}(v) = \{u|(u, v) \in E\} \).

Graphs can be categorised depending on the attributes of the nodes and edges. A labelled graph is a graph whose nodes or edges have labels, which may or may not be unique. Nodes and/or edges can be labelled, with the graphs then being called node- or edge-labelled graphs respectively. Otherwise the graph is simply known as an unlabelled graph. Edges can either be directed or undirected. Directed edges are uni-directional relations from starting node \( u \) to a target node \( v \) and recorded as \((u, v) \in E\) and \((u, v) \neq (v, u)\).

As mentioned previously, the ability to quantify the similarity of graph topologies is central to graph learning systems. As topological patterns are not intuitively well represented using classic feature vectors, considerable effort has focused on using kernel methods for machine learning tasks. Kernel methods are machine learning algorithms which rely on a kernel for the pattern recognition task. Kernels are functions which define a relation or more contextually, a similarity over pairs of observations using their raw representations. Consequently, using a kernel function over graphs generates a gram or kernel matrix which can be used with kernel methods such as SVMs to perform the intended machine learning task [4].

Ideally a kernel would be a similarity function \( \text{sim}(G, G') = d, d \in \mathbb{R}^+ \) where \( d \) or the "distance" between graphs \( G \) and \( G' \) is small if they have similar structural properties and larger otherwise. Due to the high computational complexity of directly assessing the comparability of graphs, as evidenced by the graph isomorphism test [27], numerous flexible kernels based on approximate and inexact matching of graphs have been proposed in literature. For a comprehensive review we refer the reader to Vishwanathan et al. [4].

3 Related work

Representation learning of graphs using neural networks has turned into a large and exciting hub of research driven by successive proposals of graph representation learning models and proliferation of datasets to apply them onto. A significant part of the activity has been focused on Graph Convolutional Neural Networks (GCNN). Such neural networks are characterised by graph convolutional operators [28] [6] [7] that serve as useful inductive biases for learning representations of nodes and other graph substructures. Gilmer et al. [29] generalised the convolution operator over irregular domains as a message passing scheme summarised in Equation [1]

\[
\mathbf{h}_i^{(k)} = \gamma^{(k)} \left( \mathbf{h}_i^{(k-1)}, \Lambda_{j \in \mathcal{N}(i)} \phi^{(k)} \left( \mathbf{h}_i^{(k-1)}, \mathbf{h}_j^{(k-1)}, \mathbf{e}_{i,j} \right) \right),
\]

where \( \mathbf{h}_i^{(k)} \in \mathbb{R}^f \) represents the \( f \)-dimensional feature vector of node \( i \) in the \( k \)-th layer of the GCNN, \( \mathbf{e}_{i,j} \in \mathbb{R}^D \) represents edge features from node \( i \) to \( j \), \( \Lambda \) represents some differentiable permutation invariant function such as a sum, mean or max. \( \gamma \) and \( \phi \) are differentiable functions including neural networks.

Representations of entire graphs are then created through the successive application of graph convolution operations followed by different pooling methods [6] [9] [11] which aggregate node representations towards a single vector representation for the entire graph.

The difficulty of reliably constructing GCNN models has driven the need for toolkits and libraries to facilitate their development for replication, extension and creation of new models. Several such libraries have been made such as: Graph Nets introduced by Battaglia et al. [16], DGL by Wang et al. [17], GEM by Goyal et al. [18], and most recently PyTorch Geometric by Fey and Lenssen [19]. These libraries have greatly contributed to lowering the barrier of entry into GCNN research, fueling the development of novel methods and libraries supporting them in a healthy feedback cycle.
Alongside ongoing research into GCNNs and their variants, another approach has focused on extending graph kernel methods [4] with neural language embedding methods [30, 21, 22] that exploit the distributive hypothesis to learn representations of graphs. However, as far as the authors are aware there is no library currently available designed to support the construction of such models. The approach towards distributive modelling of graphs was pioneered by Yanardag and Vishwanathan [3]. They observed that most graph kernel methods can be formulated as instances of the R-Convolutional framework. Here the similarity between different graphs is computed by decomposing graphs into discrete substructure patterns such as graphlets, shortest paths, and rooted subgraphs. This produces $|V|$-dimensional bag-of-words or pattern frequency vectors for each graph where $V$ is the set of the unique patterns induced over all the graphs in a dataset. The graphs and its induced substructure patterns, are input into a kernel function, such as counting the common substructures across pattern frequency vectors, that defines the relation or similarity measure between the graphs to construct the kernel matrix for use with SVMs.

Yanardag and Vishwanathan [3] further observed that as the specificity of substructure patterns to be induced from graphs increases (via lengthening walks/path, increasing the number of nodes in graphlet patterns) graphs are represented by extremely high dimensional occurrence frequency vectors. As a result, only few substructure patterns are common across any given set of graphs producing sparse solutions where each graph is more similar to itself, a phenomenon known as diagonal dominance. To tackle this issue the authors proposed using neural language models which exploit the distributive hypothesis [12] to learn dense low dimensional vector representations of the substructures and construct graph kernel matrices. This was quickly followed up by works such as the aptly named Graph2Vec [2] and Anonymous Walk Embeddings [13] (AWE) which proposed different substructure patterns graphs could be reduced to and the use of Doc2Vec variants [22] to build distributed representations of whole graphs directly.

Geo2DR provides various modules that can be used as "building blocks" to construct systems capable of learning such distributed representations of both substructure patterns and whole graphs of arbitrary size. This is inherently different to learning of representations centered around the message-passing and pooling approaches. Existing libraries [16, 17, 18, 19] supporting this approach would require substantial shift in their design methodologies and philosophies to accommodate intuitive distributive model construction. Hence Geo2DR is a complementary library alongside existing toolkits enabling researchers a broader range of representation learning opportunities.

4 Overview of the Geo2DR library

Building upon the theoretical framework in Yanardag and Vishwanathan [3], we can characterise the process through which representations are learned in Deep Graph Kernels [3], Graph2Vec [2] and Anonymous Walk Embeddings (specifically AWE-DD) as a two stage process.

The first stage consists of inducing discrete substructure patterns for each graph across a dataset of graph to create a corpus which associates each graph its substructures. This defines a vocabulary and a language which can be utilised by a neural language model such as Skipgram [21] to learn substructure pattern embeddings or its generalization PV-DBOW [22] to learn graph level embeddings. This characterises the second stage in which training of the neural language model creates distributed vector representations of the graphs that are contextualised by the substructure patterns within it, with respect to the other patterns found in the other graphs of the dataset. This notion is analogous to the distributive modelling of other discrete structures such as text.

Geo2DR is a library built to support this two stage pipeline for the construction of models and systems capable of learning distributed representations of graphs. Substructure decomposition algorithms and neural language models found in [3, 2, 13] are implemented as separate modules that can be seen as "building blocks" that may be combined in different ways. Furthermore useful tools are provided to preprocess datasets of popular public benchmark datasets [23] and a corpus object which handles the various definitions of context and data loading into our embedding methods implemented in PyTorch. This provides a unified design pipeline that can help users focus on improving individual parts, or quickly construct existing models instead of carefully analysing and repurposing the original reference implementations which used different language versions, datastructures, data pipelines, etc. Figure 1 is a diagrammatic sketch of the two stage process from raw data from the graph datasets to
the creation of the substructure or graph embeddings along with the various support modules also included to help facilitate the process.

Practically, the library is centered around three subpackages under Geo2DR. The first, data, contains modules for transforming the data formats used by popular dataset repositories such as Kersting et al. [23] into formats used by the decomposition algorithms implemented in Geo2DR. In Geo2DR, we chose to use the GEXF (Graph Exchange XML Format) as permanent storage format for individual instances of the graphs. This is because the format is compatible with network analysis software such as Gephi and NetworkX. The modules within the decomposition subpackage contain all the algorithms for inducing the substructure patterns in the graphs and forming vocabularies. The outputs of these algorithms are directly compatible with our PyTorch implementations of neural language models as well as those in Gensim [24]. This essentially describes the packages and modules necessary for stage 1 of the process. The final subpackage embedding_methods contains modules for constructing corpus datasets and neural language models to build the distributed representation learning system of stage 2. Several trainer classes are included which are battery-included corpus and neural net combinations that can be used to reconstruct common architecture setups.

As an example, we will describe the pipeline using specific modules of the subpackages above. This will go through the steps of downloading the MUTAG benchmark dataset from Kersting et al. [23] repository[2] to re-implementing the Graph2Vec [2] model and learning distributed representation of the graphs. To start, we need transform source data into a format usable with Geo2DR. The data.TU_Gexf_formatter module can be used to process the data format used by Kersting et al. and produce individual graph files in the GEXF format. The decomposition.weisfeiler_lehman_patterns module can be used to induce rooted subgraph patterns using Shervashidze et al.’s [31] multiset node relabelling algorithm across the GEXF files representing the dataset. This also constructs a vocabulary of the different patterns found across the dataset. This achieves step 1 of the two stage process. A useful side-effect is the construction of text documents for each graph in the dataset. These text documents record the patterns within each graph as string literals along with the context definition rules chosen by each substructure decomposition algorithm [3][13]. This permanence allows for subsequent study on the distribution of the substructure patterns or skipping expensive pattern decomposition stages within end-to-end systems as many decomposition algorithms such as the Weisfeiler-Lehman node relabelling algorithm are deterministic.

Subsequently we require the construction of corpus datasets and training distributive neural language models upon these to achieve stage 2 and obtain the desired vector representations of the graphs. Different constructions of corpus datasets set the desired definitions of target-context pairs for learning the distributed representations. For re-implementing Graph2Vec we use the embedding_methods.PVDBOW_corpus to create a dataset where each target observation consists of a graph \( G_i \in G \), where \( G \) is the set of all the graphs in the dataset, a context substructure pattern \( t_j \).
Table 1: List of substructure patterns that can be induced in the graphs, and the neural language models implemented within the first release of Geo2DR.

| Induced substructure patterns               | Neural language models |
|---------------------------------------------|------------------------|
| Graphlets (size 2-8 nodes)                  | Skipgram [21]          |
| Shortest paths                              | CBOW [21]              |
| Weisfeiler-Lehman (WL) rooted subgraphs     | PV-DM [22]             |
| Random walks                                | PV-DBOW [22]           |
| Anonymous walks                             |                        |

that is observed within the graph and \( t_j \in V \) where \( V \) is the vocabulary of substructure patterns, and a negative context sample \( n \in V \) forming \((G_i, t_j, n)\) and the corpus dataset of all such observations is designated \( D \). These observations can be used within the Skipgram model with negative sampling under embedding.methods.skipgram which optimises:

\[
\mathcal{L} = \sum_{G_i \in G} \sum_{t \in V} \left| \{(G_i, t) \in D\} \right| (\log \sigma(\Phi_i \cdot S_t) + k \cdot \mathbb{E}_{t_N \in P_D} \left[ \log \sigma(-\Phi_i \cdot t_N) \right])
\] (2)

Where \( \Phi \in \mathbb{R}^{|G| \times \delta} \) is the \( \delta \) dimensional matrix of graph embeddings we desire of the graph dataset \( G \), and \( \Phi_i \) is embedding for \( G_i \in G \). Similarly, \( S \in \mathbb{R}^{|V| \times \delta} \) are the \( \delta \) dimensional embeddings of the substructure patterns in the vocabulary \( V \) so \( S_t \) represents the vector embedding corresponding to substructure pattern \( t \). The embeddings of the substructure patterns are also tuned but ultimately not used, as we are interested in the graph embeddings in \( \Phi \). \( k \) is the number of negative samples with \( t_N \) being the sampled context pattern, drawn according to the empirical unigram distribution \( P_D(t) = \frac{|\{(G_i, G, t) \in D\}|}{|D|} \). This completes stage 2 of the pipeline using the corpus construction, neural language model and training modules. Downstream classification can be done with any algorithm operating on the graph embeddings.

In this first release we allow the induction of all 5 types of substructure patterns across graph datasets as used by Yanardag and Vishwanathan’s Deep Graph Kernels, Narayanan et al.’s Graph2Vec, and Ivanov and Burnaev’s Anonymous Deep Walk Embeddings. Geo2DR also contains PyTorch implementations of the neural language models used by each these systems, named after the original word2vec and doc2vec architectures upon which they are based. These are listed in Table 1. The DGK methods learn substructure embeddings which are later used to compute a kernel function for graphs based on the embeddings of the substructures. This kernel can then be used with a SVM to perform graph classification. Graph2Vec and AWE-DD use variants of the PV-DBOW and PV-DM respectively to learn graph embeddings directly. Table 2 is a succinct summary of the different combinations used in these systems which make up the most popular and powerful graph embedding methods.

A critical aspect of learning distributed representations is the definition of context for the substructure patterns. In particular, for embedding of substructure patterns and using the PV-DM model for graph embeddings, the definition of context is highly important as it dictates which target-context pairs form the corpus dataset. To this aspect we have adopted the cooccurrence rules of substructure patterns as described in Yanardag and Vishwanathan’s Deep Graph Kernels [3] which is also borrowed in the subsequent works Graph2Vec [2] and Anonymous Walk Embeddings [13].

5 Empirical evaluation

As a form of validation for the various implemented modules, we empirically evaluate re-implementations of existing models using our library. Table 2 describes the induced substructure pattern and neural language model driving each method. Here we perform a series of common benchmark graph classification tasks under homogeneous data and evaluation scenarios giving a fairer picture of how they compare. To validate the re-implementations, classification datasets were chosen by their use in the original publications as well as some that were not used for better comparability.

All datasets were downloaded from the benchmark dataset repository by Kersting et al. [23] and processed into the format used by Geo2DR with the included data formatter. In each of the datasets the
Table 2: Table characterising each of the existing published methods by the substructure patterns induced and associated embedding method to create the graph kernel matrix (for DGK models) or graph embeddings.

| Method     | Induced substructure pattern | Embedding method | Object embedded |
|------------|-----------------------------|------------------|-----------------|
| DGK-WL     | WL rooted subgraphs         | Skipgram or CBOW | Substructures   |
| DGK-SP     | Shortest paths              | Skipgram or CBOW | Substructures   |
| DGK-GK     | Graphlets                   | Skipgram or CBOW | Substructures   |
| Graph2Vec  | WL rooted subgraphs         | PV-DBOW          | Whole graphs    |
| AWE-DD     | Anonymous walks             | PV-DM            | Whole graphs    |

Table 3: Random-split 10 fold cross-validation performance of SVM using RBF kernel on bag-of-words vectors of normalised frequencies of induced substructure patterns. OOM is out-of-memory.

| Substructure pattern | MUTAG     | ENZYMES   | PROTEINS  | NCI1      | REDDIT-B   | IMDB-M    |
|---------------------|-----------|-----------|-----------|-----------|------------|-----------|
| WL Rooted Subgraphs | 88.95 ± 7.96  | 56.33 ± 6.18 | 74.29 ± 2.55 | 83.94 ± 1.99 | 77.35 ± 4.35 | 48.60 ± 4.33 |
| Shortest Paths      | 83.68 ± 7.24  | 41.67 ± 4.83 | 74.73 ± 2.04 | 70.95 ± 1.95 | 78.25 ± 2.71 | 44.40 ± 4.17 |
| Graphlets           | 83.16 ± 6.16  | 25.33 ± 3.48 | 70.36 ± 3.59 | 54.09 ± 7.61 | 78.25 ± 2.71 | OOM       |
| Anonymous Walks     | 80.53 ± 6.68  | 27.33 ± 6.23 | 71.87 ± 2.05 | 66.08 ± 2.21 | 81.30 ± 2.49 | 38.20 ± 3.91 |

Discrete node labels are exposed, but not the edge labels. For unlabelled datasets such as REDDIT-B, the node was labelled by their degree following practice of Shervashidze et al. [31] to enable methods such as the WL rooted subgraph decomposition to induce patterns in the graphs; this was also applied to methods which can directly handle unlabelled graphs for conformity.

For all experiments, attempts were made to follow the hyper-parameter setup of the original systems used to publish the results, and used small hyper-parameter search spaces where additional details were unknown. As we look at several kernels and embedding models we leave the specific hyperparameter ranges in Appendix A. In all cases, the same off-the-shelf C-Support Vector Machine implemented in SciKit-learn [25] was used with an RBF kernel trick for the supervised classification task on the graph embeddings learned. C values were estimated over the set (0.001, 0.01, 0.1, 1, 10, 100). We report the average score of 10 iterations of training and applying 10 fold cross validation using the SVM over random data splits with individual training restarts in all cases. The exact setups of the experiments here can be replicated using the code provided at the GitHub repository [4].

Graph kernels: We start with an experiment suite based on the substructure patterns alone, using the decomposition algorithms to construct normalised bag-of-words frequency vectors for each of the graphs. Table 3 records the mean and standard deviation of randomly split 10 fold cross validation using the SVM described above. The results closely match that of the published methods in [3][31][34][13]. Generally, we see that the WL rooted subgraphs perform well consistently across the classification task in comparison to the other substructures with the shortest paths following closely behind. However, the fact that different substructure patterns excel in classifying some datasets and do not perform as well in others suggests that topological characteristics which are useful for characterising graphs are not found in just one substructure pattern.

Deep graph kernels and graph embeddings: Most of our experiments in Table 4 show a high reproducibility of the results published by the original proposers. Small discrepancies are to be expected due to the homogenised set up, smaller hyper-parameter spaces, and initial random seeds, but they do not deviate significantly from published results. The increased performance of the DGK models over its kernel counterparts affirms the suggestion by Yanardag and Vishwanathan that using substructure pattern embeddings is a useful addition to the construction of the graph kernel. Nonetheless, the performances of Graph2Vec and AWE-DD also suggest that useful representations can also be found directly. They perform similarly and sometimes even better than the DGK models, whilst also providing the flexibility of using the graph embeddings for other downstream tasks. Generally, the ranking of the different methods here follow the behaviour of the substructure patterns they are based on in the graph kernel results. Graph2Vec and DGK-WL perform well across the board, compared to the methods using "linear" patterns such as walks and paths which have variable performance behaviour. The discrepancies between our results and the results published

[4]https://github.com/paulmorio/geo2dr/tree/master/replication
Table 4: Graph classification performance over random-split 10 fold cross validation in each of the re-implemented systems with standard deviation. OOM is out-of-memory.

| Method       | MUTAG     | ENZYMES   | PROTEINS  | NCI1      | REDDIT-B | IMDB-M |
|--------------|-----------|-----------|-----------|-----------|----------|--------|
| DGK-WL       | 88.42 ± 8.42 | 41.00 ± 1.83 | 72.08 ± 0.74 | 77.54 ± 3.91 | OOM      | 47.82 ± 0.79 |
| DGK-SP       | 84.03 ± 7.16  | 44.27 ± 2.26 | 76.93 ± 2.56 | 69.22 ± 5.29 | OOM      | 49.71 ± 1.18 |
| DGK-GK       | 84.21 ± 6.74  | 23.61 ± 3.14 | 69.77 ± 3.13 | 53.92 ± 4.81 | 78.32 ± 1.92 | 44.40 ± 4.18 |
| Graph2Vec    | 84.91 ± 2.79  | 51.77 ± 1.75 | 74.05 ± 2.28 | 71.34 ± 2.12 | 81.25 ± 2.64 | 45.71 ± 0.91 |
| AWE-DD       | 79.29 ± 2.92  | 23.76 ± 1.74 | 69.70 ± 1.29 | 63.54 ± 1.82 | 81.46 ± 1.75 | 40.53 ± 6.42 |

Table 5: Total training run time (seconds) over 100 epochs on MUTAG. Bold text refers to lowest time taken for training, bolded are also times which are within error of being the best.

| Method       | Original reference implementation | Only Geo2DR PyTorch modules | Geo2DR with compatible libraries Gensim/Tensorflow |
|--------------|-----------------------------------|-----------------------------|-----------------------------------------------|
| DGK-WL       | 3.06 ± 0.15                        | 3.33s ± 0.07s               | 3.19 ± 0.08                                  |
| DGK-SP       | 6.95 ± 0.23                        | 6.86 ± 0.27s               | 7.39 ± 0.08                                  |
| DGK-GK       | 9.46s ± 0.69s                      | 19.41s ± 0.49s             | 9.89 ± 0.74                                  |
| Graph2Vec    | 8.86s ± 0.05s                      | 10.64s ± 0.11s             | 8.88s ± 0.06s                                |
| AWE-DD       | 1231.75s ± 21.81s                  | 314.84s ± 8.91s            | —                                             |

in Anonymous Walk Embeddings are larger in both kernels and the distributed representations. We can attribute this discrepancy our selection of hyper-parameters which were not fully described in the original paper. Furthermore, in studying the AWE-DD implementation their evaluation script outputs the best result in a ten fold cross-validation which must have been averaged across their multiple runs, rather than the Monte-Carlo average of average scores in 10 fold cross validation, hence our scores will underestimate theirs. Direct comparison between the original implementation and the Geo2DR re-implementation on the same hyperparameters bears similar results.

**Runtime experiments and improvements in Geo2DR:** Table 5 contains the average total training times incurred over 100 epochs, performed ten times with one standard deviation on a single quad-core Intel 4690 CPU. Comparison is drawn between the original reference implementation made available by each of the original proposing papers and its re-implemented counter part in Geo2DR. All methods were trained over the MUTAG dataset as this is the only graph dataset included in the available reference implementations within the format that is directly usable with their implementations. Furthermore, none of the original reference implementations have scripts or tools to transform the publicly available datasets they used into the formats used by their own implementations, making reproduction difficult. This is why we have included data processing tools directly into the Geo2DR library to address this common limitation for the future. Furthermore, we also include a simple script which recreates the data format used by the DGK implementation based on its descriptions provided by its author. This script is also available in our repository. As each of original proposers approached their implementations in different ways, we use the discussion section to discuss comparisons of the implementations in more detail.

### 6 Discussion on implementations

The DGK models directly store their datasets in memory and expose it to the Gensim library to use the Skipgram/CBOW models. Gensim benefits from highly optimised data access and numerical computations that make it fast for training on multi-core CPUs compared to similar Python data + Tensorflow/PyTorch implementations on the same hardware. We can only expect significant speed up using our PyTorch models when considering the use of GPU on high dimensional, large batch-size training regimes. For this purpose each of the decomposition algorithms in Geo2DR can

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3[https://github.com/nd7141/AWE](https://github.com/nd7141/AWE)

4[https://github.com/nd7141/AWE, accessed February 2020](https://github.com/nd7141/AWE)

5[www.mit.edu/~pinary/kdd unfortunately no longer exists, but can be obtained from the authors directly.](www.mit.edu/~pinary/kdd)
also output the substructure pattern corpus in the format used by Gensim directly to benefit from these optimised routines as in the third column of Table 5 which brings similar run time performance to the original.

Graph2Vec’s original reference implementation\(^7\) loads its datasets directly into memory and uses a strict computational graph implemented in Tensorflow \(^37\) to achieve admirable speeds. The re-implementation follows suit with loading the dataset into memory within a custom PyTorch dataset object which interfaces with the dataloader to perform the batching and loading into our PV-DBOW model. The preset computational graph and efficient optimisers provided by Tensorflow results in a small but nonetheless significant speed up over the Geo2DR PyTorch implementation. As a result, the data_formatter in Geo2DR was designed to produce datasets that are fully compatible with Narayanan et al’s Tensorflow implementation. This allows us to obtain the same training times in the third column.

AWE-DD’s reference implementation\(^8\) relies on a dataloader which loads batches of target-context pairs of the dataset iva reading substructure pattern files on the harddrive into a Tensorflow computational graph. As such, the training speed of their implementation is bottlenecked through the dataloading and access routines. Similar times can be found in Geo2DR if we use the same approach with the disk loading corpus. However substantial speed up can be obtained by loading the dataset into memory first as shown in the second column. For the sake of this study, we have also forked all of the original reference implementations without modification, so that they may be compared with our work, at the time of development.

7 Conclusion

Through the characterisation of existing methods, and the reproduction of their results in Geo2DR, we have shown that Geo2DR is a successful amalgation of the various components that enable learning distributed representations. Using the simple design methodology, one can quickly re-implement existing models, which is becoming an increasingly important part of reproducible research and designing novel architectures. By exploiting the modular structure and compatibility with other software and libraries the set of tools for constructing learning systems is broadened without having to deal with different data structures, language paradigms and workflows used by individual implementations. Using a host of re-implemented methods allows for more homogenised experiment suites that can be used to more fairly compare existing and new methods in future research efforts. Geo2DR is now released publicly, but will continue to evolve to add new components, compatibility with other libraries, tutorials, and accommodate new developments in the field.

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A Hyper-parameter selections of re-implemented methods

For each of the methods described in Section 5 we prescribed a gridsearch over the following hyper-parameter settings inspired by the settings of the original papers:

A.1 Graph Kernels

- **WL Rooted Subgraphs**: Rooted subgraphs of up to depth 2 induced.
- **Shortest Paths**: Shortest paths of all pairs of nodes induced.
- **Graphlets**: Graphlets of size 7 induced, sampling 100 graphlets per graph.
- **Anonymous Walks**: Anonymous walks of length 10 induced exhaustively from each node in the graph.

A.2 Deep graph kernels and graph embeddings

- **DGK-WL**: Rooted subgraphs of up to depth 2 induced. Trained Skipgram model with negative sampling using 10 negative samples with an Adam optimiser for 5 and 100 epochs using batch sizes of 10000 and 1000 with an initial learning rate of 0.1 and 0.01 adjusted by a cosine annealing scheme. Substructure embedding sizes of 2, 5, 10, 25, 50 dimensions were generated. Graph kernels were constructed using the formulation described in Yanardag and Vishwanathan [3].
- **DGK-SP**: Shortest paths of all pairs of nodes induced. Trained Skipgram model with negative sampling using 10 negative samples with an Adam optimiser for 5 and 100 epochs using batch sizes of 10000 and 1000 with an initial learning rate of 0.1 and 0.01 adjusted by a cosine annealing scheme. Substructure embedding sizes of 2, 5, 10, 25, 50 dimensions were generated. Graph kernels were constructed using the formulation described in Yanardag and Vishwanathan [3].
- **DGK-GK**: Graphlets of size 7 induced, sampling 2, 5, 10, 25, and 50 graphlets for each graph. Trained Skipgram model with negative sampling using 10 negative samples with an Adam optimiser for 5 and 100 epochs using batch sizes of 10000 and 1000 with an initial learning rate of 0.1 and 0.01 adjusted by a cosine annealing scheme. Substructure embeddings of 2, 5, 10, 25, 50 dimensions were generated. Graph kernels were constructed using the formulation described in Yanardag and Vishwanathan [3].
- **Graph2Vec**: Rooted subgraphs of up to depth 2 induced. Trained over PV-DBOW (Skipgram) model with negative sampling using 10 negative samples with an Adam optimiser for 25, 50, 100 epochs and batch sizes of 512, 1024, 2048, 10000 with an initial learning rate of 0.1 adjusted by a cosine annealing scheme. Graph embeddings of 128 and 1024 dimensions were learned.
- **AWE-DD**: Anonymous walks of length 10 induced exhaustively. Trained over PV-DM architecture with negative sampling using 10 negative samples with an Adagrad optimiser (as in reference implementation) for 100 epochs with batch sizes 100, 500, 1000, 5000, 10000 with an initial learning rate of 0.1. Window-sizes of 4, 8, 16 were used to extract context anonymous walks around the target anonymous walk in the PV-DM architecture.