STRUCTURAL LANDMARKING AND INTERACTION MODELLING: ON RESOLUTION DILEMMAS IN GRAPH CLASSIFICATION

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Paper under double-blind review

ABSTRACT

Graph neural networks are promising architecture for learning and inference with graph-structured data. However, generating informative graph level features has long been a challenge. Current practice of graph-pooling typically summarizes a graph by squeezing it into a single vector. This may lead to significant loss of predictive, iterpretable structural information, because properties of a complex system are believed to arise largely from the interaction among its components. In this paper, we analyze the intrinsic difficulty in graph classification under the unified concept of "resolution dilemmas" and propose "*SLIM*", an inductive neural network model for Structural Landmarking and Interaction Modelling, to remedy the information loss in graph pooling. We show that, by projecting graphs onto end-to-end optimizable, and well-aligned substructure landmarks (representatives), the resolution dilemmas can be resolved effectively, so that explicit interacting relation between component parts of a graph can be leveraged directly in explaining its complexity and predicting its property. Empirical evaluations, in comparison with state-of-the-art, demonstrate promising results of our approach on a number of benchmark datasets for graph classification.

1 INTRODUCTION

Complex systems are ubiquitous in natural and scientific disciplines, and how the relation between component parts gives rise to global behaviour of a system is a central research topic in many areas such as system biology (Camacho et al., 2018), neural science (Kriegeskorte, 2015), and drug and material discoveries (Stokes et al., 2020; Schmidt et al., 2019). Recently, graph neural networks provide a promising architecture for representation learning on graphs – the structural abstraction of a complex system. State-of-the-art performances are observed in various graph mining tasks (Bronstein et al., 2017; Defferrard et al., 2016; Hamilton et al., 2017; Xu et al., 2019; Velickovic et al., 2017; Morris et al., 2019; Wu et al., 2020; Zhou et al., 2018; Zhang et al., 2020). However, due to the non-Euclidean nature, important challenges still exist in graph classification. For example, in order to generate a fixed-dimensional representation for a graph of arbitrary size, *graph pooling* is typically adopted to summarize the information from each each node. In the pooled form, the whole graph is squeezed into a "super-node", in which the identities of the constituent sub-graphs and their inter-connections are mixed together. Is this the best way to generate graph-level features? From a complex system's view, mixing all parts together may hurt interpretability and model prediction, because properties of a complex system arise largely from the *interactions* among its components (Hartwell et al., 1999; Debarsy et al., 2017; Cilliers, 1998).

The choice of the "collapsing"-style graph pooling roots deeply in the lack of natural alignment among graphs that are not isomorphic. Therefore pooling sacrifices structural details for feature (dimension) compatibility. Recent years, substructure patterns[1] draw considerable attention in graph mining, such as motifs (Milo et al., 2002; Alon, 2007; Wernicke, 2006; Austin R. Benson, 2016) and graphlets (Shervashidze et al., 2009). It provides an intermediate scale for structure comparison or counting, and has been applied to node embedding (Lee et al., 2019; Ahmed et al., 2018), deep graph kernels (Yanardag & Vishwanathan, 2015) and graph convolution (Yang et al., 2018). However, due to

[1]Informally, substructure in this paper means a connected subgraph and will be used interchargeably with it.

combinatorial nature, only substructures of very small size (4 or 5 nodes) can be considered (Yanardag & Vishwanathan, 2015; Wernicke, 2006), greatly limiting the coverage of structural variations; also, handling substructures as discrete objects makes it difficult to compensate for their similarities, and so the risk of overfitting may rise in supervised learning scenarios (Yanardag & Vishwanathan, 2015).

We view these intrinsic difficulties as related to *resolution dilemmas* in graph-structured data processing. Resolution is the scale at which measurements can be made and/or information processing algorithms are conducted, and here we will discuss two types of resolution and related dilemma: spatial resolution and structural resolution. *Spatial resolution* relates to the geometrical scale of the "elementary component" of a graph on which an algorithm operates. In GNN, since graph pooling compresses the whole graph into a single vector, node/edge identities are mixed together and the spatial resolution drops to the lowest. We call this **vanishing spatial resolution**. On the other hand, *structural resolution* is the fineness level in differentiating between two substructures. Current practice of exact matching makes it computationally intractable to handle exponentially many subgraphs, and the risk of overfitting may also rise as observed in deep graph kernels (Yanardag & Vishwanathan, 2015) and dictionary learning (Marsousi et al., 2014). We call this over-delicate substructure profiling an **exploding structural resolution**. In fact, these two resolution dilemmas are not isolated, and both originated from the way we perform identification and alignment of substructures.

Our contribution. In this paper, we propose a simple neural architecture called "Structural Landmarking and Interaction Modelling" - or SLIM, for inductive graph classification. Our key contribution is to allow graphs to be projected onto a set of end-to-end optimizable, well-aligned structural landmarks, so that identities of graph substructures and their interactions can be modelled explicitly to explain the complexity and improve graph classification. This is in contrast to existing graph-pooling techniques, which typically collapse the whole graph into a single node and thus suffer from important information loss. We show that by resolving the resolution dilemmas and subsequently respecting the structural organization of complex systems, SLIM can be more interpretable, accurate, and provides new insights in graph representation learning.

In the rest of the paper, we will first define the resolution dilemmas of graph classification in Section 2, together with the discussion of related works. We then cover in Section 3, 4 and 5 the design, analysis, and performance of SLIM, respectively. Finally, the last section concludes the paper.

2 Resolution Dilemmas in Graph Classification

A complex system is often composed of many parts interacting with each other in a non-trivial way. Since graphs are structural abstraction of complex systems, accurate graph classification depends on how global properties of a system relate to its structure. It is believed that property of a complex system arises from interactions among its components (Debarsy et al., 2017; Cilliers, 1998). Consequently, accurate interaction modelling should benefit prediction. However, it is non-trivial due to resolution dilemmas, as described in the following subsections.

2.1 Spatial Resolution Diminishes in Graph Pooling

Graph neural networks (GNN) for graph classification typically involves two key blocks, graph convolution and graph pooling (Kipf & Welling, 2017; Hamilton et al., 2017; Xu et al., 2019), at significantly different spatial resolutions. The goal of convolution is to pass information among neighboring nodes in the general form of

$$h_v = \texttt{AGGREGATE}\left(\{h_u, u \in \mathcal{N}_v\}\right),$$

where $\mathcal{N}_v$ is the neighbors of v (Hamilton et al., 2017; Xu et al., 2019). Here, the spatial resolution is controlled by the number of convolution layers: more layers capture lager substructures/sub-trees and can lead to improved discriminative power (Xu et al., 2019). In other words, the spatial resolution in the convolution stage can be controlled easily, and multiple resolutions may be even combined together via `CONCATENATE` function (Hamilton et al., 2017; Xu et al., 2019) for improved modelling.

The goal of graph pooling is to generate compact, graph- or subgraph-level representations that are compatible across graphs. Due to the lack of natural alignment between non-isomorphic graphs, graph pooling typically "squeezes" a graph $\mathcal{G}$ into a single vector (or "super-node") in the form of

$$h_{\mathcal{G}} = \texttt{READOUT}\left(\{f(h_v), \forall v \in \mathcal{V}\}\right),$$

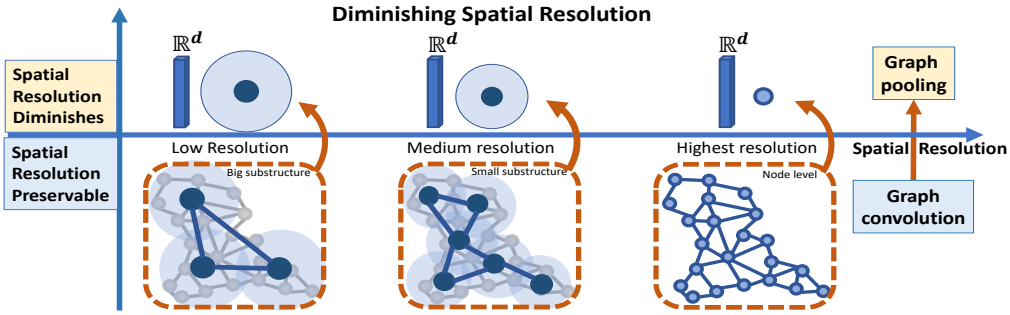

Figure 1: Spatial resolution vanishes after graph pooling.

where $\mathcal{V}$ is the vertex set of $\mathcal{G}$. The readout functions include: max-pooling (Cangea et al., 2018), sum-pooling (Xu et al., 2019), some other pooling functions (Hamilton et al., 2017), or deep sets (Zaheer et al., 2017); attention has been used to evaluate node importance in attention pooling (Lee et al., 2019) and gPool (Gao & Ji, 2019); hierarchical pooling has also been investigated (Ying et al., 2018).

A crucial resolution bottleneck occurs in graph pooling, as shown in Figure 1. Since all the nodes are mixed into one, subsequent classifier can no longer identify any individual substructure nor their interactions, regardless of the spatial resolution used in the convolution stage. We call this "diminishing spatial resolution", which can be undesirable. For example, in molecule classification problems, the label of the graph usually hinges heavily on the functional modules and how they are organized in a molecule (Stokes et al., 2020); a coarse spatial resolution will mix up functional modules and conceal their interaction, leading to important loss of structural information.

2.2 Structural Resolution Explodes in Substructure Identification

Substructures are the basic unit to accommodate interacting relations. A global criterion to identify and align substructures is the key to preserving substructure identities and comparing the inherent interactions across graphs. Again, the granularity in determining whether two substructures are "similar" or "different" is subject to a wide spectrum of choices, which we call "structural resolution".

We illustrate the concept in Figure 2. The right end denotes the finest resolution in differentiating substructures: exact matching, as we manipulate motif/graphlet (Milo et al., 2002; Alon, 2007; Wernicke, 2006; Yang et al., 2018; Shervashidze et al., 2009). The exponential configuration of subgraphs will finally lead to an "exploding" structural resolution, because maintaining a large number of unique substructures is computationally infeasible, and easily overfits (Yanardag & Vishwanathan, 2015). The left end of the spectrum treats all substructures the same and underfits the data. We are interested in a medium structural resolution, where similar substructures are mapped to the same identity, which we believe can benefit the generalization performance (empirical evidence in Fig. 4).

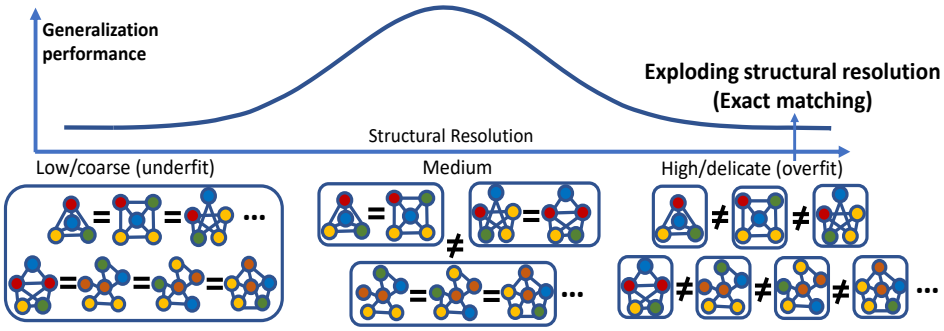

Figure 2: Over-delicate structural resolution may hamper the generalization performance.

Relation between Spatial and Structural Resolution Dilemmas. The two dilemmas are closely related. Due to difficulty of characterizing discrete subgraphs, exact matching is typically used and

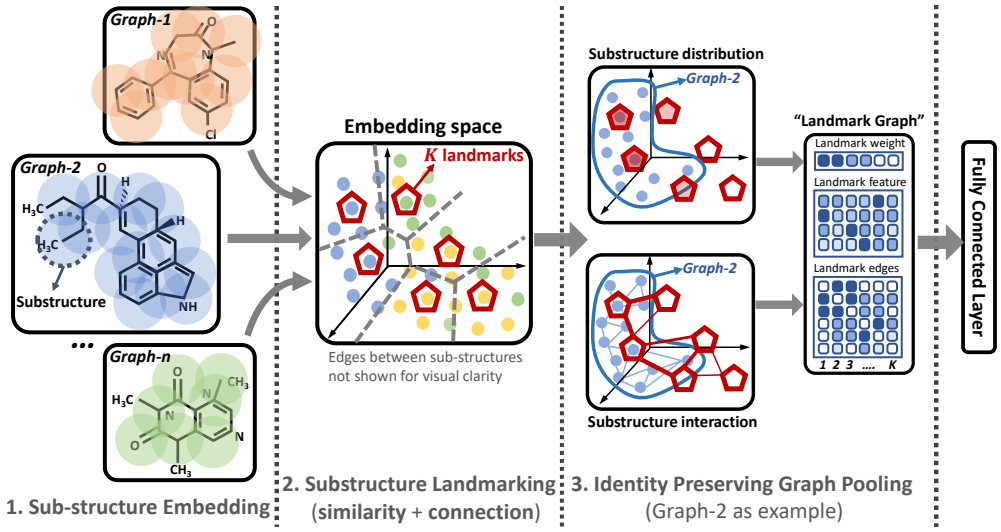

Figure 3: The three main steps of the SLIM network illustrated in molecule graph classification.

causes an **exploding structural resolution**. Such an over-delicate granularity makes it infeasible to align/categorize the exponential amount of substructures. As a result, graph pooling has to collapse each graph into a single node to generate compatible graph-level features, causing **vanishing spatial resolution**. Next, we show how to resolve the challenge chain by controlling structural resolution.

3 Structural Landmarking and Interaction Modelling (SLIM)

Considering the difficulty in manipulating substructures as discrete objects, we embed them in a continuous space, so that most of the structure-related operations can be transformed from discrete and off-the-shelf version to a continuous and optimizable counterpart. The key idea of SLIM is the learning of discriminative structural landmarks in this new space, via both unsupervised compression and supervised fine-tuning, and through the distribution of embedded substructures from across the training graphs. Structural landmarking resolves resolution dilemmas and allows explicit interaction modelling in graph classification.

Problem Setting. Give a set of labeled graphs $\{\mathcal{G}_i, y_i\}$'s for $i = 1, 2, ..., n$, with each graph defined on the node/edge set $\mathcal{G}_i = (\mathbf{V}_i, \mathbf{E}_i)$ with adjacency matrix $\mathbf{A}_i \in \mathbb{R}^{n_i \times n_i}$ where $n_i = |\mathbf{V}_i|$, and $y_i \in \{\pm 1\}$. Assume that nodes are drawn from c categories, and the node attribute matrix for $\mathcal{G}_i$ is $\mathbf{X}_i \in \mathbb{R}^{n_i \times c}$. Our goal is to train an inductive model to predict the labels of the testing graphs.

The SLIM network has three main steps: (1) substurcture embedding, (2) substructure landmarking, and (3) identity-preserving graph pooling, as shown in Figure 3. Detailed discussion follows.

3.1 Substructure Embedding

The goal of substructure embedding is to extract substructure instances and embed them in a metric space. One can employ multiple layers of graph convolution (Hamilton et al., 2017; Xu et al., 2019) to model substructures (in fact, rooted sub-trees growing from each node). In Figure 3, sub-graphs in each shaded circle represents a substructure instance associated with one atom.

More specifically, we extract one sub-graph instance from each node using an h-hop breadth-first search. Let $\mathbf{A}_i^{(k)}$ be the kth-order adjacency matrix, i.e., the pq^{th} entry equals 1 only if node p and q are within k-hops away. Since each sub-graph is associated with one node, the sub-graphs extracted from $\mathcal{G}_i$ can be represented as $\mathbf{Z}_i = \mathbf{A}_i^{(k)}\mathbf{X}_i$, whose j^{th} row is a c-dimensional vector summarizing counts of the c node-types in the sub-graph around the jth node. Again, different variations of graph convolution (Kipf & Welling, 2017; Hamilton et al., 2017) can be adopted (see Appendix A).

Next we consider embedding the substructure instances (i.e., rows of $\mathbf{Z}_i$'s) from each graph jointly into a latent space so that statistical manipulations become feasible. The embedding should preserve important proximity relations to facilitate subsequent landmarking: if two substructures are similar, or they frequently inter-connect with each other, their embeddings should be close. In other words, the embedding should be smooth with regard to both structural similarities and geometrical interactions.

A parametric transform on $\mathbf{Z}_i$'s with controlled complexity can guarantee the smoothness of embedding w.r.t. structural similarity, e.g., an autoencoder (with one hidden-layer)

$$f(\mathbf{Z}_i) = \sigma\left(\mathbf{Z}_i \cdot \mathbf{T} + \mathbf{b}\right). \tag{1}$$

Let $\mathbf{H}_i = f(\mathbf{Z}_i) \in \mathbb{R}^{n_i \times d}$ be the embedding of the n_i sub-graph instances extracted from $\mathcal{G}_i$. To maintain the smoothness of $\mathbf{H}_i$'s w.r.t. geometric interaction, we maximize the log-likelihood of the co-occurrence of substructure instances in each graph, similar to word2vec (Mikolov et al., 2013)

$$\max \sum_{i=1}^{n} \sum_{j=1}^{n_i} \sum_{l \in \mathcal{N}_j^i} \log \left(\frac{\exp\langle \mathbf{H}_i(j,:), \mathbf{H}_i(l,:) \rangle}{\sum_{l'} \exp\langle \mathbf{H}_i(j,:), \mathbf{H}_i(l',:) \rangle} \right) \tag{2}$$

Here $\mathbf{H}_i(j,:)$ is the jth row of $\mathbf{H}_i$, $\langle , \rangle$ is inner product, and $\mathcal{N}_j^i$ are the neighbors of node j in graph $\mathcal{G}_i$. This loss function tends to embed strongly inter-connecting substructures close to each other.

3.2 Substructure Landmarking

The goal of structural landmarking is to identify a set of informative structural landmarks in the continuous embedding space such that these landmarks have: (1) high statistical coverage, namely, they should faithfully recover distribution of the substructures from the input graphs, so that we can generalize them to new substructure examples from the distribution; and (2) high discriminative power, namely the landmarks should be able to reflect discriminative interaction patterns for classification.

Let $\mathbf{U} = \{\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, ..., \boldsymbol{\mu}_K\}$ be the set of structural landmarks. In order for them to be representative of the substructures from the input graphs, it is desirable that each sub-graph instance can be faithfully approximated by the closest landmark in $\mathbf{U}$. Thus, we minimize the following distortion loss

$$\sum_{i=1}^{n} \sum_{j=1}^{n_i} \min_{k=1,2,\ldots,K} \|\mathbf{H}_i(j,:) - \boldsymbol{\mu}_k\|^2. \tag{3}$$

Here $\mathbf{H}_i(j,:)$ denotes the jth row (substructure) from graph $\mathcal{G}_i$. In practice, we implement soft assignment by using a cluster indicator matrix $\mathbf{W}_i \in \mathbb{R}^{n_i \times k}$ for each graph $\mathcal{G}_i$, whose jk^{th} entry is the probability that the jth substructure of $\mathcal{G}_i$ belongs to the kth landmark $\boldsymbol{\mu}_k$. Inspired by deep embedding clustering (Xie et al., 2016), $\mathbf{W}_i$ is parameterized by a Student's t-distribution

$$\mathbf{W}_i(j,k) = \frac{(1 + \|\mathbf{H}_i(j,:) - \boldsymbol{\mu}_k\|^2/\alpha)^{-\frac{\alpha+1}{2}}}{\sum_{k'} (1 + \|\mathbf{H}_i(j,:) - \boldsymbol{\mu}'_k\|^2/\alpha)^{-\frac{\alpha+1}{2}}},$$

and the loss function can be greatly simplified by minimizing the KL-divergence

$$\min_{\mathbf{U}, \mathbf{H_i's}} \sum_i \mathrm{KL}\left(\mathbf{W}_i, \widetilde{\mathbf{W}}_i\right), \quad \text{s.t. } \widetilde{\mathbf{W}}_i(j,k) = \frac{\mathbf{W}_i^2(j,k)/\sum_l \mathbf{W}_i(l,k)}{\sum_{k'} [\mathbf{W}_i^2(j,k')/\sum_l \mathbf{W}_i(l,k')]}. \tag{4}$$

Here, $\widetilde{\mathbf{W}}_i$ is a self-sharpening version of $\mathbf{W}_i$, and minimizing the KL-distance forces each substructure instance to be assigned to only a small number of landmarks similar to sparse dictionary learning. Besides the unsupervised regularization in (3) or (4), learning of the structural landmarks is also affected by the classification loss, guaranteeing the discriminative power of the landmarks.

3.3 Identity-and-Interaction-Preserving Graph Pooling

The goal of identity-and-interaction-preserving graph pooling is to project structural details of each graph onto the common space of landmarks, so that a compatible, graph-level feature can be obtained that simultaneously preserves the identity of the parts (substructures) and models their interactions.

The structural landmarking mechanism allows computing rich graph-level features. First, we can model substructure distributions. The density of the K substructure landmarks in graph $\mathcal{G}_i$ can be

computed as $\mathbf{p}_i = \mathbf{W}_i' \cdot \mathbf{1}_{n_i \times 1}$. Furthermore, the first-order moment of substructures belonging to each of the K landmarks in $\mathcal{G}_i$ is $\mathbf{M}_i = \mathbf{X}_i' \cdot \mathbf{W}_i \cdot \mathbf{P}_i^{-1}$ where $\mathbf{P}_i = \text{diag}(\mathbf{p}_i)$, and the kth column of $\mathbf{M}_i$ is the mean of $\mathcal{G}_i$'s substructure instances belonging to the kth landmark. Second, we can model how the K landmarks interact with each other in graph $\mathcal{G}_i$. To do this, we can project the adjacency matrices $\mathbf{A}_i$'s onto the landmark sets and obtain an $\mathbb{R}^{K \times K}$ interaction matrix $\mathbf{C}_i = \mathbf{W}_i \cdot \mathbf{A}_i \cdot \mathbf{W}_i'$, which encodes the interacting relations (geometric connections) among the K structural landmarks.

These features can be used together for final classification. For example, they can be concatenated to feed into fully-connected layer. One can also combine them together and transform each graph $\mathcal{G}_i$ into a constant-sized "landmark" graph with node feature $\mathbf{M}_i$, node weight $\mathbf{p}_i$, and edge weights $\mathbf{C}_i$. Then the standard graph convolution can be applied to the landmark graphs to generate graph-level features (without pains of graph alignment anymore). In experiments, for simplicity, we will compute the normalized interaction matrix $\tilde{\mathbf{C}}_i = \mathbf{P}_i^{-1}\mathbf{C}_i\mathbf{P}_i^{-1}$ and use it as features, which works pretty well on all the benchmark datasets. More details can be found in Appendix H.

4 Discussions

4.1 Structural Resolution from Coding Perspective

The structural resolution is controlled by the landmark size K, which can be deemed as the number of basis in dictionary learning. Note that graphs can be considered as constructed from (inter-connected) substructure instances, each instance $\mathbf{z}$ represented by the landmarks as $\mathbf{z} = \sum_k \alpha_k \boldsymbol{\mu}_k$. In other words, the structural landmarks can be deemed as code vectors (or basis) in a dictionary.

In dictionary learning, it is known that in general neither too small nor too large dictionary is desirable. A too small number of code-vectors fail to recover basic data structures, whereas too many basis may result in overfitting (Marsousi et al., 2014). In particular, when the redundancy of the basis vectors, as measured by the "mutual coherence", exceeds a certain range, the probability of a faithful signal recovery diminishes due to instability of sparse coding (Donoho & Huo., 2001; Mehta & Gray, 2013).

We have very similar observations on the choice of structural resolution K. Note that in case of exact sub-structure matching, which corresponds to a maximal K due to the combinitorial nature of substructures, the redundancy in structural landmarks increases significantly, which violates the recovery condition and leads to inferior performance. This is why we prefer a reasonable control on the structural resolution, in contrast to exact sub-structure matching as in graphlets or motif discovery. In the Appendix B (Theorem 1), we provide a more detailed theoretic analysis on how the mutual coherence of the structural landmarks depends on the choice of structural resolution K.

4.2 Comparison with Related Methods

Here we briefly discuss how our approach differs from existing ones, and leave more comprehensive discussion to the Appendix (which also includes more topics in the choice of resolution, interpretability, hierarchical and semi-supervised version, etc.).

Graph Isomorphism. GNNs have great potential in graph isomorphism test by generating injective node embedding, thanks to the theoretic foundation in (Xu et al., 2019; Morris et al., 2019). SLIM provides new insight here: (1) it finds a tradeoff in handling similarity and distinctness; while graph isomorphism network (Xu et al., 2019) tries to discern even the slightest difference of sub-structures, SLIM network groups similar sub-structures (using tunable granularity), so that graphs can be projected onto structural landmarks; (2) it explores new ways of generating graph-level features: instead of aggregating all parts together, it taps into the vision of complex systems so that interaction relation is leveraged to explain the complexity and improve the learning (more in Appendix I).

Graphlets, Graph Kernels, and Embedding Methods. Graphlets and Graph kernels both exploit substructures to characterize graphs and their similarity. The SLIM network has some key differences. First, we consider sub-structure landmarks that are **end-to-end optimizable** for generating discriminative, graph-level interacting patterns, while graph kernels or graphlets typically enumerate sub-structures offline. Second, SLIM models interaction between sub-structures, which is very different from graph kernels. Third, interpretation is challenging due to nonlinearity of kernel methods and exponential number of sub-graphs/graphlets; while SLIM computes a small number of discriminative

substructure landmarks that are easier to interpret. Finally, embedding-type methods mostly focus on node- or edge-level representations (Mikolov et al., 2013; Ahmed et al., 2018), so our key innovation of landmark learning and interaction modelling is an orthogonal direction (more in Appendix J).

Other Aggregation or Pooling Methods. Hierarchical pooling (Ying et al., 2018; Gao & Ji, 2019; Lee et al., 2019; Khasahmadi et al., 2020) can fully exploit non-flat graph organization, but the final output is still in the form of a single, aggregated node vector for feature compatibility. Other aggregation strategies: Sortpooling re-arranges graph nodes in a linear chain and perform 1d-convolution (Zhang et al., 2018); SEED uses distribution of multiple random walks to capture graph structures (Wang et al., 2019); Deep graph kernel evaluates graph similarity by subgraph counts (Yanardag & Vishwanathan, 2015). Explicit modelling of the interaction between constituent parts of the graph, however, is still not considered in these approaches.

5 EXPERIMENTS

Benchmark data. We have used a number of popular benchmark data sets for graph classification. (1) MUTAG: chemical compound data set with 188 instances and two classes; there are 7 node/atom types, and 3 edge/bound types (bond types are ignored). (2) PROTEINS: protein molecule data set with 1,113 instances and three classes; there are 3 node types (secondary structure elements). (3) NCI1: chemical compounds data set for cancer cell lines with 4,110 instances and two classes. (4) PTC: chemical compound data set for toxicology prediction with 417 instances and 8 classes. (5) D&D: enzyme classification with 1,178 instances and two classes. (6) IMDB-B: movie collaboration date set with 1,000 instances and two classes. (7) IMDB-M: movie collaboration date set with 1,500 instances and three classes derived from actor/actress and genre information of movies on IMDB; and (8) COLLAB: scientific collaboration network of researchers from 3 physics fields (classes).

Competing methods. We have incorporated a number of competitive methods in recent years for comparison: (1) Graph neural tangent kernel (GNTK) (Du et al., 2019); (2) Graph Isomorphism Network (GIN) (Xu et al., 2019); (3) End-to-end graph classification (DCGNN) (Zhang et al., 2018); (4) Hierarchical and differential pooling (DiffPool) (Ying et al., 2018); (5) Self-attention Pooling (SAG) (Lee et al., 2019); (6) Convolutional network for graphs (PATCHY-SAN) (Niepert et al., 2016); (7) Graphlet kernel (GK) (Shervashidze et al., 2009); (8) Weisfeiler-Lehman Graph Kernels (WLGK) (Shervashidze et al., 2011); and (9) Propagation kernel (PK) (Neumann et al., 2016). For method (4),(6),(7),(8),(9) we directly cited their reported results (averaged 10-fold corss-validated error) due to unavailability of their codes; for other competing methods we run their codes and report the results.

Experimental setting. Following the experimental setting in (Xu et al., 2019) and (Niepert et al., 2016), we evenly split the data into 10 folds and report the average and standard deviation of the accuracies from each of the 10 rounds (9-fold training vs 1-fold testing). In the SLIM network, the spatial resolution is controlled by a BFS with 3-hop neighbors; the structural resolution is set to $K = 100$; the FC-layer has one hidden layer with dimension 64; cross-entropy is used for classification; and weights for the loss term (2) and (4) are set to 0.01. No drop-out or batch-normalization is used considering the size of the benchmark data. The hyper-parameters for the SLIM network are selected using a small portion of the training splits as validation set, including: (1) the number of hidden units in the autoencoder Eq.(1) is chosen from $\{d, d/2, 2d, 8, 16\}$ where d is the input dimension of the encoder; (2) the optimizer is chosen from SGD and Adagrad, with learning rate $\{1e-2, 5e-2, 1e-3, 5e-3, 1e-4\}$; (3) local graph representation, including node distribution, layer-wise distribution, and weighted layer-wise summation (see Appendix A for details).

Structural Resolution. In Figure 4, we examine the performance of SLIM against different choices of structural resolution (landmark set size K). As can be seen, the accuracy-vs-K curve is bell-shaped. When K is either too small (underfitting) or too large (coherent landmarks that overfit), the accuracy is inferior, and the best performance is typically obtained around a median K value. This justifies our conjecture, as well as the usefulness of structural landmarking in improving graph classification.

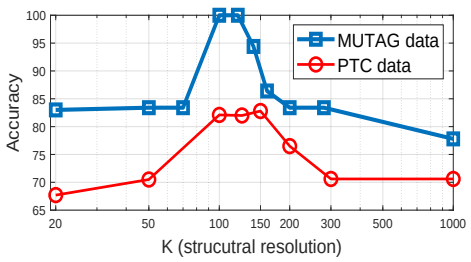

Figure 4: Accuracy vs structural resolution K.

Table 1: Averaged algorithm performance on 8 benchmark data-sets (bioinformatics & social-net).

ALG.	MUTAG	PTC	NCI1	Protein	D&D	IMDB-B	IMDB-M	COLLAB
GK	81.38±1.74	55.65±0.46	62.49±0.27	71.39±0.31	74.38±0.69	65.87±0.98	43.89±0.38	72.84±0.28
PK	76.00±2.69	59.50±2.44	82.54±0.47	73.68±0.68	78.25±0.51	—	—	—
WLGK	84.11±1.91	57.97±2.49	**84.46±0.45**	74.68±0.49	78.34±0.62	73.40±4.63	49.33±4.75	79.02±1.77
PC-SAN	92.63±4.21	60.00±4.82	78.59±1.89	75.89±2.76	77.12±2.41	71.00±2.29	45.23±2.84	72.60±2.15
DGCNN	85.83±1.66	58.59±2.47	74.46±0.47	75.54±0.94	79.37±1.03	70.03±0.86	47.83±0.85	73.76±0.49
DiffPool	90.52±3.98	—	76.53±2.23	75.82±3.56	78.95±2.40	78.08±4.24	53.13±4.70	79.70±1.84
GNTK	90.12±8.58	67.92±6.98	75.20±1.53	75.61±4.24	**79.42±2.18**	76.90±3.60	52.80±4.60	**83.60±1.22**
SAG	73.53±9.68	69.67±3.12	74.18±1.29	71.86±0.97	76.91±2.12	78.10±4.20	53.80±4.08	79.88±1.02
GIN	90.03±8.82	64.60±7.00	79.84±4.57	71.28±2.65	77.58±2.94	75.10±5.10	52.30±2.80	80.21±1.92
SLIM	**93.28±3.36**	**74.41±6.92**	80.53±2.01	**77.47±4.34**	**79.61±2.66**	**80.20±2.10**	**54.00±4.02**	78.22±2.02

Table 2: Averaged ranking of different algorithms on the 8 benchmark data-sets.

ALG.	GK	PK	WLGK	PC-SAN	DGCNN	DiffPool	GNTK	SAG	GIN	SLIM
Rank	8.7	6.4	5.6	5.8	5.8	4.1	3.7	4.7	4.6	**1.9**

Classification Performance. We compare the performance of different methods in Table 1. We use eight well-known data sets consisting of three social network data sets (IMDB-B, IMDB-M, COLLAB) and five bioinformatics data sets (MUTAG, PTC, NCI1 PROTEINS, DD). As can be seen, in Table 1, overall, neural network-based approaches are more competitive than graph kernels, except that graph kernels have lower fluctuations, and the WL-graph kernel perform the best on the NCI1 dataset. For social network data, the SLIM network gains a competitive score on IMDB-B and IMDB-M. From Table 2, SLIM yields the highest average ranking in terms of accuracy among all the 8 benchmark datasets.

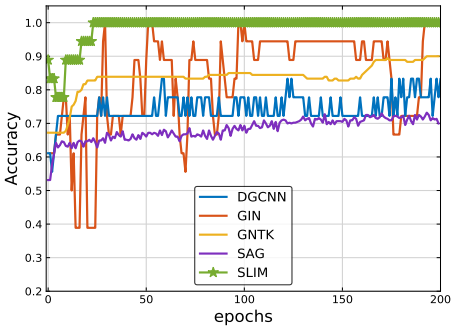

Figure 5: Algorithm stability on the `Mutag` dataset. **More examples in Appendix G**.

Algorithm Stability (Evolution of Accuracy). In Figure 5 (more results in Appendix G, Figure 7), we have plotted the evolution of the testing accuracy versus the number of epochs on the benchmark datasets, so as to have a more comprehensive evaluation on algorithm stability. As can be seen, our approach not only generates accurate classification, but also the accuracy converges relatively faster and remains more stable with respect to the epochs. This signifies a small variance during the training process and makes it practically easy to determine when to stop training. Other GNN algorithms can also attain a high accuracy on some of the benchmark datasets, but the prediction performance fluctuates significantly across the training epochs (even by using very large mini-batch sizes). In such cases, determining when to stop can be challenging.We speculate that stability of the SLIM network arises from explicit modelling of the sub-structure distributions. In Figure 5, it is also worthwhile to note that on the MUTAG data the proposed method produces a classification with 100% accuracy on more than half of the runs across different folds, and converges to the perfect classification steadily. It demonstrates the power of the SLIM network in capturing important graph-level features.

Visualization Example. Finally, we visualize embedding of the learned substructure landmarks and the interacting patterns on top of them, using MUTAG as an example (Appendix F, Figure 6).

6 Conclusion

Graph neural networks provide a popular state-of-the-art computational architecture for graph mining. In this paper, we designed the SLIM network that employs structural landmarking to resolve resolution dilemmas in graph classification and capture inherent interactions in graph-structured systems. Encouraged by the promising experimental results, we expect this attempt to open up possibilities in designing GNNs with informative structural priors.

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A Representation of Substructures

Here we list a few simple variations used for representing the sub-graph that is grown from each node, including (1) emphasize the center node, $\mathbf{Z}_i = [\mathbf{X}_i;\ \mathbf{A}_i\mathbf{X}_i]$ as inspired by (Xu et al., 2019); (2) layer-wise node type distribution $\mathbf{Z}_i = [\tilde{\mathbf{A}}_i^{(1)}\mathbf{X}_i;\ \tilde{\mathbf{A}}_i^{(2)}\mathbf{X}_i;\ \ldots\ \tilde{\mathbf{A}}_i^{(k)}\mathbf{X}_i]$, where $\tilde{\mathbf{A}}_i^{(k)}$ specifies whether two nodes in $\mathcal{G}_i$ are *exactly* k-hops away; or (3) weighted Layer-wise summation $\mathbf{Z}_i = \alpha_k \sum_k \tilde{\mathbf{A}}_i^{(k)}\mathbf{X}_i$, where α_k's are non-negative weighting that decays with k, which is a more delicate summary of node-type distributions on each layer of BFS.

B Mutual Coherence of Structural Landmarks

In the following, we quantify a lower-bound of the coherence as a factor of the landmark size K in clustering-based basis selection, since the sparse coding and k-means algorithm generate very similar code vectors (Coates & Ng, 1993).

Theorem 1. *The lower bound of the squared mutual coherence of the landmark vectors increases monotonically with K, the number of landmarks in clustering-based sparse dictionary learning.*

$$\mu^2(\mathbf{U}) \quad \geq \quad 1 - \frac{4C_dC_p}{u_{max}^2 K^{\frac{1}{d}}} \left(\left\lfloor \left(\frac{K}{2} \right)^{\frac{1}{d}} \right\rfloor^{-1} + 1 \right)$$

Here, d is the dimension, $C_d = \frac{3}{2}\left(1 + \log(d)/d\right)\gamma_d V_d$, where $\gamma_d = 1 + d\log(d\log(d))$ and $V_d = 2\Gamma(\frac{1}{2})^d / d\Gamma(\frac{d}{2})$ is the volume of the d-dimensional unit ball; u_{max} is the maximum ℓ_2-norm of (a subset) of the landmark vectors $\boldsymbol{\mu}_k$'s, and C_p is a factor depending on data distribution $p(\cdot)$.

Proof. Suppose we have n spatial instances embedded in the d-dimensional latent space as $\{\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_n\}$, and the landmarks (or codevectors) are defined as $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, ..., \boldsymbol{\mu}_K$. Let $p(\mathbf{z})$ be the density function of the instances. Define the averaged distance between the instance and the closest landmark point as

$$s = \frac{1}{n} \sum_{i=1}^{n} \|\mathbf{z}_i - \boldsymbol{\mu}_{c(i)}\|_2, \tag{5}$$

where $c(i)$ is the index of the closest landmark to instance i. As expected, s will decay with the number of landmarks with the following rate (Ron Meir, 1999)

$$s \leq C_d C_p \left(\left\lfloor \left(\frac{K}{2} \right)^{\frac{1}{d}} \right\rfloor^{-1} + 1 \right) K^{-\frac{1}{d}} \tag{6}$$

where C_d is a dimension-dependent factor $C_d = \frac{3}{2}\left(1 + \frac{\log(d)}{d}\right)\gamma_d$, with $V_d = 2\Gamma(\frac{1}{2})^d / d\Gamma(\frac{d}{2})$ the volume of the unit ball in k-dimensional Euclidean space and $\gamma_d = 1 + d\log(d\log(d))$; $C_p = \left(\int p(\mathbf{z})^{\frac{d}{d+1}} d\mathbf{z}\right)^{\frac{d+1}{d}}$ is a factor depending on the distribution p.

Since s is the average distortion error, we can make sure that there exists a non-empty subset of instances Ω_z such that $\|\mathbf{z}_i - \boldsymbol{\mu}_{c(i)}\| \leq s$ for $i \in \Omega_z$. Next we will only consider this subset of instances and the relevant set of landmarks will be denoted by Ω_u. For the landmarks $\boldsymbol{\mu}_p \in \Omega_u$, we make a realistic assumption that there are enough instances so that we can always find one instance $\mathbf{z}$ falling in the middle of $\boldsymbol{\mu}_p$ and its closest landmark neighbor $\boldsymbol{\mu}_p$. In this case, we have then bound the distance between the closest landmark pairs as

$$\|\boldsymbol{\mu}_p - \boldsymbol{\mu}_q\| \leq \|\boldsymbol{\mu}_p - \mathbf{z}\|_2 + \|\boldsymbol{\mu}_q - \mathbf{z}\|_2 \leq 2s.$$

For any such pair, assume that the angle spanned by them is θ_{pq}. we can bound the angle between the two landmark vectors by

$$\sin(\theta_{pq}) \leq \frac{2s}{\|\boldsymbol{\mu}_p\|}. \tag{7}$$

Let $u_{max} = \max_{\boldsymbol{\mu}_p \in \Omega_u} \|\boldsymbol{\mu}_p\|_2$, we can finally low-bound the normalized correlation between close landmark pairs, and henceforth the coherence of the landmarks, as

$$\begin{aligned}
\mu^2(\mathbf{U}) \quad &\geq \quad \max_{p,q \in \Omega_u} \cos^2(\theta_{pq}) \\
&= \quad \max_{p,q \in \Omega_u} 1 - \sin^2(\theta_{pq})^2 \\
&\geq \quad 1 - \frac{4s^2}{u_{max}^2} \\
&\geq \quad 1 - \frac{4C_d K^{-\frac{1}{d}}}{u_{max}^2} \left(\left\lfloor \left(\frac{K}{2} \right)^{\frac{1}{d}} \right\rfloor^{-1} + 1 \right)
\end{aligned}$$

This indicates that the squared mutual coherence of the landmarks has a lower bound that consistently increases when the number of the landmark vectors, K, increases in a dictionary learning process. □

This theorem provides important guidance on the choice of structural resolution. It shows that when a clustering-based dictionary learning scheme is used to determine the structural landmarks, the size of the dictionary K can not be chosen too large; or else the risk of overfitting can be huge. Note that exact sub-structure matching as is often practiced in current graph mining tasks corresponds to an extreme case where the number of landmarks, K, equals the number of unique sub-structures; therefore it should be avoided in practice. The structural landmarking scheme is a flexible framework to tune the number of landmarks, and to avoid overfitting.

C CHOICE OF SPATIAL AND STRUCTURAL RESOLUTIONS

The spatial resolution determines the "size" of the local sub-structure (or sub-graph), such as functional modules in a molecule. Small sub-structures can be very limited in terms of their representation power, while too large sub-structures can mask the right scale of the local components crucial to the learning task. An optimal spatial resolution can be data-dependent. In practice, we will restrict the size of the local sub-graphs to 3-hop BFS neighbors, considering that the "radius" of the graphs in the benchmark data-sets are usually around 5-8. We then further fine-tune the spatial resolution by assigning a non-negative weighting on the nodes residing on different layers from the central code in the local subgraph. Such weighting is shared across all the sub-graphs and can be used to adjust the importance of each layer of the BFS-based sub-graph. The weighting can be chosen as a monotonously decaying function, or optimized through learning.

The choice of structural resolution has a similar flavor in that too small or too large resolutions are neither desirable. On the other hand, it can be adjusted conveniently by tuning the landmark set size K based on the validation data. In our experiments, K can be chosen by cross validation; for simplicity, we fix $K = 100$.

Finally, note that geometrically larger substructures (or sub-graphs) are characterized by higher variations among instances due to the exponential amount of configuration. Therefore, the structural resolution should also commensurate with spatial resolutions. For example, substructures constructed by 1-hop-BFS may use a smaller landmark size K than those with 3-hop-BFS. In our experiments we do not consider such dependencies yet, but will study it in our future research.

D HIERARCHICAL VERSION

D.1 SUBTLETY IN SPATIAL RESOLUTION DEFINITION

First we would like to clarify a subtlety in the definition of spatial resolutions. In physics, resolution is defined as the smallest distance (or interval) between two objects that can be separated; therefore it must involve two scales: the scale of the object, and the scale of the interval. Usually these two scales are proportional. In other words, you cannot have a large intervals and small objects, or the opposite (a small interval and large object). For example, in the context of imaging, each object is a pixel and the size of the pixel is the same as the interval between two adjacent pixels.

In the context of graphs, each object is a sub-graph centered around one node, whose scale is manually determined by the order of the BFS-search centered around that node. Therefore, the interval between two sub-graphs may be smaller than the size of the sub-graph. For example, two nodes i and j are direct neighbors, and each of them haa a 3-hop sub-graph. Then, the interval between these two subgraphs, if defined by the distance between i and j, will be 1-hop; this is smaller than the size of the two sub-graphs, which is 3-hop. In other words, the two objects/subgraphs indeed overlap with each other, and the scale of the object and the scale of the interval between objects is no longer commensurate (large objects and small interval in this scenario).

This scenario makes it less complete to define spatial resolutions just based on the size of the sub-graphs (as in the main text), since there are actually two scales to define. To avoid unnecessary confusions, we skip these details. In practice, one has two choices dealing with the discrepancy: (1) requiring that the sub-graphs are not overlapping, i.e., we do not have to grow one k-hop subgraph around each node; instead, we just explore a subset of the sub-graphs. This can be implemented in a hierarchical version which we discuss in the next subsection; (2) we still allow each node to have a local sub-graph and study them together, which helps cover the diversity of subgraphs since

theoretically, an ideal choice of the subgraph is highly domain specific and having more sub-graph examples gives a better chance to include those sub-graphs that are beneficial to the prediction task.

D.2 HIERARCHICAL SLIM

We can implement a hierarchical version of SLIM so that sub-graphs of different scales, together with the interacting relation between sub-graphs under each scale, can be captured for final prediction. Note that in (Ying et al., 2018) a hierarchical clustering scheme is used to partition one graph, in a bottom up manner, to less and less clusters. We can implement the same idea and construct a hierarchy of scales each of which will host a number of sub-structures. The structural landmarking scheme will be implemented in each layer of the hierarchy to generate graph-level features specific to that scale. Finally these features can be combined together for graph classification.

E SEMI-SUPERVISED SLIM NETWORK

The SLIM network is flexible and can be trained in both fully supervised setting and semi-supervised setting. This is because the SLIM model takes a parametric form and so it is inductive and can generalize to any new samples; on the other hands, the clustering-based loss term in (4) can be evaluated on both labeled samples and unlabeled samples, rendering the extra flexibility to look into the distribution of the testing sample in the training phase, if they are available. This is in flavor very similar to the smoothness constraint widely used in semi-supervised learning, such as the graph-regularized manifold learning (Belkin et al., 2006). Therefore, the SLIM network can be implemented in the following modes

- Supervised version. Only training graphs and their labels are available during the training phase, and the loss function (4) is only computed on the training samples.
- Semi-supervised version. Both labeled training graphs and unlabeled testing graphs are available. The loss function (4) will be computed on both the training and testing graphs, wile the classification loss function will only be evaluated on the training graph labels.

F INTERPRETABILITY

The SLIM network not only generates accurate prediction in graph classification problems, but can also provide important clues on interpreting the prediction results, because the graph-level features in SLIM bear clear physical meaning. For example, assume that we use the interaction matrix $\mathbf{C}_i$ for the ith graph $\mathcal{G}_i$ as its feature representation; and the pq^{th} entry then quantifies the connectivity strength between the pth sub-structure landmark and the qth structure landmark. Then, by checking the K^2-dimensional model coefficients from the fully-connected layer, one can then tell which subset of substructure-connectivity (i.e., two substructures are directly connected in a graph) is important in making the prediction. To improve the interpretability one can further imposes a sparsity constraint on the model coefficient.

In traditional graph neural networks such as GraphSAGE of GIN, node features are transformed through many layers and finally mingled altogether through graph pooling. The resultant graph-level representation, whose dimension is manually determined and each entry pools the values across all the nodes in the graph, can be difficult to interpret.

In Figure 6, we illustrate the sub-structure embedding and the learned landmarks of SLIM network on the MUTAG dataset. Here, molecules belonging to different classes are marked with red and blue edges. As can be observed, the sub-structures landmarks can generate highly discriminative features for graph classification; furthermore, by examining the substructure instances associated with each landmark, domain experts can acquire valuable clues for interpretating the underlying mechanism of classification. In fact, discriminative roles of the landmarks are two-fold. First, landmark themselves can be discriminative by being associated with one class more often than the other. Second, even in scenarios where both classes may share some common sub-structure landmarks (which is possible in molecules due to some common functional modules), the interacting pattern defined among the landmarks can still serve as an effective discriminator. We believe the dual discriminating mechanism

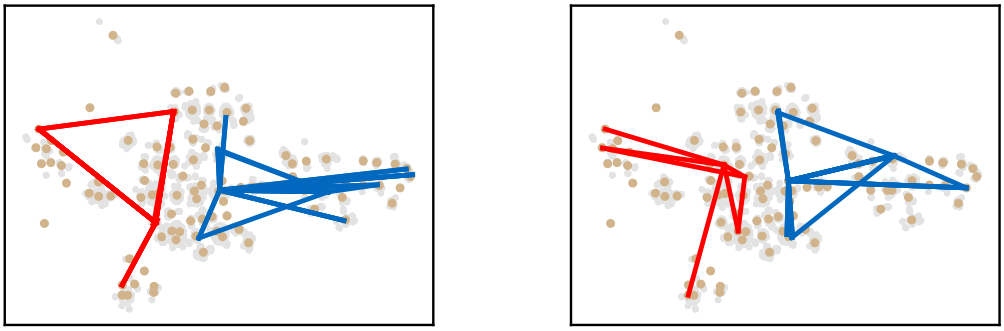
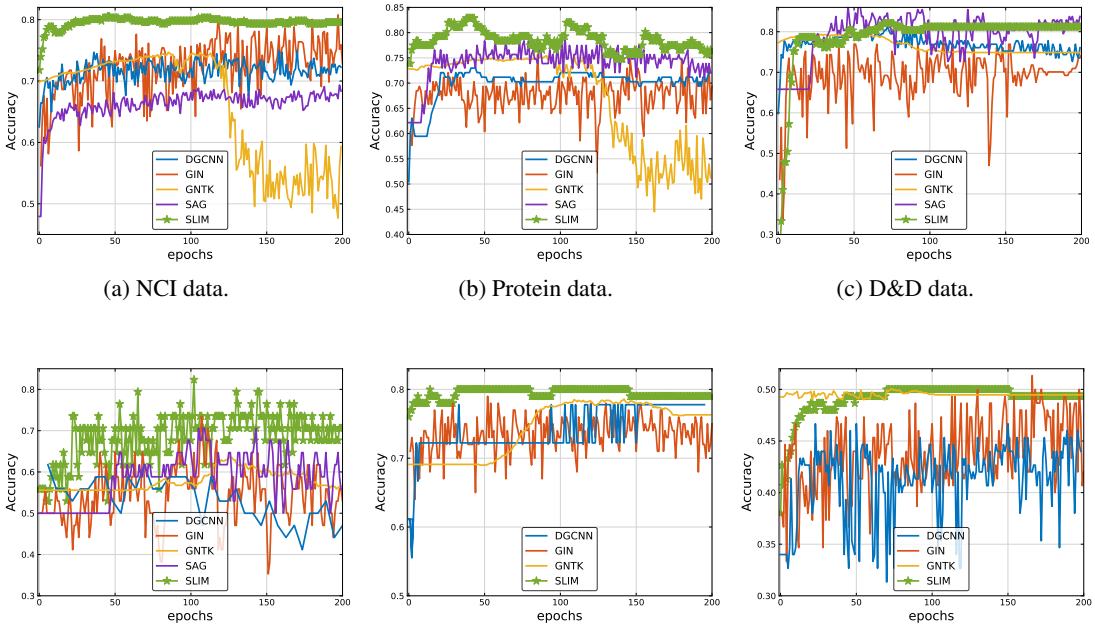


Figure 6: Two pairs of molecules from different classes of MUTAG data, with their respective substructure-interaction-patterns marked on top of the learned structural landmarks. Red and blue colors signify the class labels.



(a) NCI data. (b) Protein data. (c) D&D data.

(d) PTC data. (e) IMDB-B data. (f) IMDB-M data.

Figure 7: Testing accuracy of different algorithms over the training epochs.

using structural landmarks can be quite desirable in solving difficult graph classification problem, which we will investigate in more detail in our future studies.

G Algorithm Stability (Test Accuracy Evolution)

Here we have reported the evolution of the testing accuracies for a number of competing algorithms on more all the benchmark training data, as in Figure 7.

H THE PREDICTION LAYER

The SLIM network renders various possibilities to generate the prediction layer.

- Fully connected layer. The interaction matrix can be re-shaped into a vector, or transformed to a smaller matrix via bilateral dimension reduction before reshaped into a vector. Then a fully connected layer follows for the final prediction.
- Landmark Graph. Each graph $\mathcal{G}_i$ can be transformed into a landmark-graph a with fixed number of K (landmark) nodes, with $\mathbf{p}_i$ and $\mathbf{C}_i$ quantifying the weight of each node and the edge between every pair of nodes, and $\mathbf{M}_i$ the feature of each node (see definition in Section3.3). Then, this graph can be subject to a graph convolution such as $\mathbf{D}_i^{-1}\mathbf{C}_i\mathbf{M}_i$ generate a fixed-dimensional graph-level feature without having to take care of the varying graph size. We will study this in our future experiments.
- Riemannian manifold. When using the interaction matrix $\mathbf{C}_i$ or the normalized version as graph level features, we can treat each graph as a point in the Riemannian manifold due to the symmetry and positive semi-definiteness of the representation. Then the distance between two interaction matrices can be computed as the Wasserstein distance between two Gaussian distributions with the interaction matrix as covariances, which has a closed-form. We will study this in our future experiments.

I INTERACTION VERSUS INTEGRATION

The SLIM network and existing GNNs represent two different flavors of learning, namely, interaction modelling versus integration approach. Interaction modelling is based on mature understanding of complex systems and can provide physically meaningful interpretations or support for graph classification; integration based approaches bypass the difficulty of preserving the identity of sub-structures and instead focus on whether the integrated representation is an injective mapping, as typically studied in graph isomorphism testing.

Note that an ideal classification is different from isomorphism testing and is not injective. In a good classifier, the goal of deciding which samples are similar and which are not are equally important. Here comes the tradeoff between handling similarity and distinctness. The Isomorphism-flavor GNN's are aimed at preserving the differences between local sub-structures (even just a very minute difference), and then map the resultant embedding to the class labels. Our approach, on the other hand, tries to absorb patterns that are sufficiently close to the same landmark, and then map the landmark-based features to class labels. In the latter case, the structural resolution can be tuned in a flexible way to explore different fineness levels, thus tuning the balance between "similarity" and "distinctness"; in the meantime, the structural landmarks allow preserving sub-structure identities and exploiting their interactions.

J COMPARISON WITH RELATED METHODS

Graph kernels are powerful methods to measure the similarity between graphs. The key idea is to compare the sub-structure pairs from the two graphs and compute the accumulated similarity, where examples of substructures include random walks, paths, sub-graphs, or sub-trees. Among them, paths/sub-graphs/sub-trees are deterministic sub-structures in a graph, while random walks are stochastic sequences (of nodes) in a graph.

Although the SLIM network considers sub-structures as basic processing unit, it has a number of important differences. First, we consider sub-structure landmarks that are **end-to-end optimizable**, aimed at both reconstructing substructure distribution and generating discriminative interacting pattern for graph classification; while sub-structures in graph kernels or graphlets are typically identified offline. Second, graph kernels measure similarity between all possible pairs of sub-structures across two graphs; while SLIM network models interaction between sub-structures, i.e., the functional organization of a graph, which is very different from graph kernels. Third, interpretation is challenging due to nonlinearity of kernel methods and exponential number of candidates in graphlets; while SLIM maintains a reasonable amount of discriminative "landmark" sub-structures easier to interpret.

In recent years, embedding algorithms have drawn considerable attention that transform nodes (or sub-graphs) into a low-dimensional Euclidian space, as pioneered by the word-to-vector work (Mikolov et al., 2013). It is worthwhile to note that these algorithms focus on node- or edge-level embedding, while our target is graph-level classification. As a result, our approach emphasizes more on the innovation in modelling the interacting relation between component parts of a graph, as inspired by the views from complex systems. In fact, our most important contribution lies exactly in learning substructure landmarks jointly across graphs to enable identity-preserving graph pooling. This is rarely a consideration in algorithms whose main focus is just to embed the nodes or sub-graphs.

Here we use Role2Vec (Ahmed et al., 2018) as an example to illustrate the similarity and difference between our approach and embedding-type methods. Similarity: both methods embed nodes or subgraphs, and consider high-order subgraph features. Differences: (1) Tasks are different; Role2Vec is node-level embedding, while ours is graph-level classification; (2) Data are different; Role2Vec focuses on single graph, we simultaneously handle many graphs, i.e., align sub-structures from different graphs and project each graph onto shared structural landmarks - a new framework for graph pooling; (3) Methods are different; Role2Vec designs attributed random walk, we use KL to fit substructure distribution; R2V finds subgraph motifs offline like in graphlets, we optimize discriminative substructure landmarks in an end-to-end fashion.

Recent years, various hierarchical pooling strategies (Ying et al., 2018; Lee et al., 2019; Khasahmadi et al., 2020) have been proposed to fully exploit non-flat graph organization and show promising results in graph classification. However, despite the hierarchical process that reduces the number of nodes layer by layer, the final representation is still in the form of a single, aggregated node vector for feature compatibility, leading to potential loss of informative graph structural details. Note that hierarchical methods usually perform grouping inside each graph, while in our approach the substructure landmarks are identified by jointly clustering the substructure instances across all the graphs. Therefore our landmark set size is typically larger than the number of clusters in hierarchical methods, in order to accommodate the diversity in sub-structure distribution. Note that some of the hierarchical methods need to sort the nodes of the graph as a pre-processing procedure (Ying et al., 2018; Khasahmadi et al., 2020).

We are also aware some other types of aggregation strategies: Sortpooling re-arranges graph nodes in a linear chain and perform 1d-convolution (Zhang et al., 2018); SEED uses distribution of multiple random walks to capture graph structures (Wang et al., 2019); Deep graph kernel evaluates graph similarity by subgraph counts (Yanardag & Vishwanathan, 2015). Again, explicit modelling of the interaction between constituent parts of the graph is not considered in these approaches.