Motif-based Convolutional Neural Network on Graphs

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Abstract

This paper introduces a generalization of Convolutional Neural Networks (CNNs) to graphs with irregular linkage structures, especially heterogeneous graphs with typed nodes and schemas. We propose a novel spatial convolution operation to model the key properties of local connectivity and translation invariance, using high-order connection patterns or motifs. We develop a novel deep architecture Motif-CNN that employs an attention model to combine the features extracted from multiple patterns, thus effectively capturing high-order structural and feature information. Our experiments on semi-supervised node classification on real-world social networks and multiple representative heterogeneous graph datasets indicate significant gains of 6-21% over existing graph CNNs and other state-of-the-art techniques. An updated, published version of this paper can be found here [Sankar et al., 2019b].

1 Introduction

CNNs [LeCun et al., 1998] have achieved immense success in various machine learning tasks where the underlying data representation is grid-structured, such as image classification, object detection etc. [LeCun et al., 2015]. Their efficacy has inspired the study of CNN paradigm in non-euclidean domains such as Natural Language [Kim, 2014], Graphs [Bruna et al., 2014] and Manifolds [Masci et al., 2015].

Two fundamental properties utilized in the design of CNNs are local connectivity and translation invariance. The neurons in a CNN model spatial locality by extracting features from small localized regions called receptive fields and achieve weight-sharing across spatial locations thus capturing translation invariance. This enables them to significantly reduce the number of parameters without sacrificing the ability to extract informative patterns.

In many scenarios, we encounter data lying in irregular domains that are naturally represented as graphs encoding interactions between various real-world entities. For instance, an academic citation network (such as DBLP) is composed of multiple types of nodes, viz. authors, papers and venues inter-connected in different relationships.

Direct generalizations of CNNs to graphs is non-trivial since real-world graphs do not share the same locality patterns as in grid-structured data. For example, convolutional filter design in images directly follows from the structure of the data manifold where every pixel has eight neighbors with precise spatial locations. Graphs however possess irregular neighborhood structures with variable neighbors per node, rendering standard notions of connectivity and translation in-applicable. Besides, most modern graphs are heterogeneous, comprising nodes of several types with diverse feature sets, that entails fine-grained modeling of interactions between different types subject to the schema and domain semantics.

The two properties identified earlier for traditional CNNs are quite relevant and in fact necessary for graphs. The goal of graph convolution is to model a target node of interest by extracting features from semantically relevant context nodes, which is precisely captured by the property of local connectivity. Consider a heterogeneous graph where not every pair of node types can connect directly (e.g., in DBLP, an author does not link to another author; they connect through a paper). For an author node, her co-authors and published venues are examples of high-order context nodes that provide relevant features. In addition, the role of various context nodes must be appropriately differentiated to accurately capture different semantics. Thus, we seek to realize the two key properties via appropriate definitions of spatial locality and weight-sharing, which leads to two key requirements:

R1 Spatial locality to identify the receptive field around a node, subject to the diversity of node types, semantics and heterogeneous interactions.
R2 Weight-sharing scheme to assign nodes the same weight in different locations of the receptive field if and only if their semantic roles (position in the receptive field) are identical.

Though the requirements outlined above seem natural, existing graph CNNs fall short of addressing them satisfactorily. Recent work on graph CNNs fall into two categories: spectral and spatial. Spectral techniques focus on defining convolution using an element-wise product in the Fourier domain, while spatial techniques define convolution through weight-sharing among local neighborhoods of the graph.

Spectral CNNs employ the analogy between classic Fourier transforms and projection onto the eigenbasis of the graph Laplacian to define spectral filtering [Bruna et al., 2014; Defferrard et al., 2016]. However, the spectral filters are functions of the Laplacian eigenbasis and thus incapable of application on another graph with a different structure.
On the other hand, spatial CNNs define spatial locality (R1) based on adhoc definitions of neighborhood proximity that operate on the immediate neighbors of each node [Kipf and Welling, 2017, Atwood and Towsley, 2016, Such et al., 2017]. While immediate neighbors are adequate to model regular grid-structured data, the notion of closeness on graphs is application dependent. As illustrated earlier, we require a high-order notion of locality that is not limited to immediate neighbors to extract relevant features for an author in DBLP. Furthermore, existing spatial CNNs are type-agnostic, thus failing to capture semantic dependencies between nodes of different types. Thus, an appropriate definition of spatial locality, subject to graph heterogeneity and semantics is the 

**first key challenge** in designing an effective graph CNN.

Weight-sharing schemes (R2) proposed by previous spatial CNNs fail to distinguish semantic roles of nodes in the receptive field. Existing schemes work by: hop distance from a node [Atwood and Towsley, 2016], linearizing the neighborhood through a canonical ordering [Niepert et al., 2016], or aggregation of immediate neighborhood [Kipf and Welling, 2017, Such et al., 2017, Hamilton et al., 2017]. However, they operate under the assumption of a homogeneous neighborhood structure and fail to account for varying semantics of different context nodes, especially in expressive heterogeneous graphs. We identify the definition of a weight-sharing scheme that clearly delineates the semantic roles of nodes in the receptive field as our **second key challenge**.

To address the above challenges, we propose **motifs** to model the receptive field (the central notion of a CNN) around a target node of interest. Motifs, also known as high-order structures, are fundamental building blocks of complex networks. [Milo et al., 2002], that describe small subgraph patterns with specific connections among different node types. We identify two key insights captured by the use of motifs:

1. **High-order locality**: Unlike adhoc definitions of local neighborhood, motifs specify the context nodes relevant to a target node of interest linked via certain paths, thus providing a principled framework capturing high-order locality, such as an author (target) connecting to another author (context) through a paper they coauthored.

2. **Precise semantic role**: Motifs enable accurate discrimination of semantic roles of various nodes in the receptive field based on their types and structural linkage patterns, such as distinguishing the roles of a co-author (context) and publication venue (context) in characterizing a target author.

Conceptually, motifs are similar to metagraphs [Fang et al., 2016] that have been successfully used to model semantic proximity in heterogeneous graphs, and hence can be described through domain knowledge. We use this as our basis to develop a novel graph CNN architecture **Motif-CNN**. We summarize the main contributions of our paper below:

1. We use motifs to define the receptive field around a target node of interest modeling the key aspects of local connectivity and translation invariance, thus capturing high-order semantics in homogeneous and heterogeneous graphs alike.

2. We present a novel motif-based convolution operation that delineates the semantic roles of various nodes in the receptive field and extracts features across motif instances in the local neighborhood. To the best of our knowledge, we are

![Figure 1: (a) Sample Motifs in DBLP - Types: Author (A), Paper (P) and Venue (V) with target in red and context in blue (b) Example graph with instances of $M_1$ for target $a$.](image)

**2 Motif-based Convolutional Neural Network**

We first introduce notations used throughout the paper.

### 2.1 Preliminaries

A graph is defined as $G = (V, E)$ with node type mapping $l : V \mapsto \mathcal{L}$ where $V = \{v_1, \ldots, v_N\}$ is the set of $N$ nodes, $E$ is the set of edges and $\mathcal{L}$ is the node type set. We exclude link types for the sake of brevity. The nodes are collectively described by a feature matrix $X \in \mathbb{R}^{N \times D}$ where $D$ is the number of features. Since different node types in a heterogeneous graph may not share the same feature space, we concatenate the features of all types (with zero padding) to get a joint representation of $D$ features.

### 2.2 Properties of Convolution

In this section, we revisit the key properties of a CNN to motivate and establish the foundation of our model.

A conventional CNN models the locality of a pixel (receptive field) using a ‘square-grid’ of fixed size and extracts translationally invariant features by scanning a filter across the grid-structured input. In graphs, the goal is to characterize a specific node of interest, **target node**, through features of semantically relevant neighboring nodes, **context nodes**.

**Local Connectivity**: Let us revisit, e.g., DBLP, with the goal of predicting the research area of an author. Though an author is linked only to papers, the venues and citations of her published papers provide strong cues in identifying her research area. It is thus necessary to look beyond the immediate neighbors to model local connectivity through high-order structures or motifs that encode specific linkage patterns.

Conventionally, a motif (or metagraph) has been defined as a pattern of edges among different node types [Benson et al., 2016, Fang et al., 2016]. To model locality specific to a node type, we use a motif to characterize the interaction of a target node with a (possibly) different context type through semantically relevant patterns of connections. In Fig. 1(a) motif $M_1$ is a pattern that describes the interaction of a target node $A$ with context nodes $V_3$ through auxiliary paper nodes $P_1$ and $P_2$, i.e., high-order structure $M_1$ indicates that $P_1$, $P_2$ and $V_3$ provide relevant features to characterize $A$. We use
lower-case letters (e.g., $a$) to denote nodes in $G$ and upper-case letters (e.g., $A$) for node types. In Fig. 1(a), the subscript under a node gives the node index, e.g., $P_1$ and $P_2$ are two different nodes of type $P$. An author node $a$ is now characterized via different instances of motif $M_1$ in $G$ with $a$ as target (illustrated in Fig. 1(b)), i.e., $a$ is locally connected with the context nodes $v_1$ and $v_2$ in the two marked instances.

**Translation Invariance:** Consider Fig. 1(b) where $a_1$ and $a_2$ are linked to target node $a$ via motif $M_2$. They represent co-authors who are expected to share a similar relationship with $a$. Generalizing this idea, we posit that nodes linked via certain patterns of connections share the same semantic roles relative to the target node. Since a motif contains one context node and multiple auxiliary nodes, it is essential to delineate their semantic roles relative to the target node to accurately model weight-sharing. In motif $M_2$ (Fig. 1(a)), it is evident that the roles of $P_1$ and $P_2$ relative to target $A$ are different, while the roles of $P_1$ and $P_2$ are indistinguishable in $M_1$. Thus, two nodes in the receptive field share the same semantic roles in motif $M$ if and only if they are of the same type and are structurally symmetric relative to the target node.

We formalize this by using a motif to define a receptive field specific to a node type. A motif $M$ is defined as a subgraph composed of a designated target node $t_M$, context node $c_M$ and auxiliary nodes $B_M$, with $K_M$ unique semantic roles.

**Definition 1:** A motif $M$ with target node $t_M$, context node $c_M$ and auxiliary nodes $B_M$ is defined as $M = (V_M, E_M, B_M, t_M, c_M, \phi_M)$ with motif type mapping $\psi_M : V_M \mapsto \mathcal{L}$ where $V_M$ is the set of all nodes with $t_M, c_M \in V_M$ and $B_M \subseteq V_M - \{t_M, c_M\}$. $E_M$ is the set of edges, $\phi_M : V_M - \{t_M\} \mapsto \{1, \ldots, K_M\}$ is a role mapping function that returns the semantic role of a node and $\forall x \in V_M, l_M(x) \in \mathcal{L}$.

Since the semantic roles of various nodes w.r.t. target node $t_M$ in motif $M$ can be easily deduced from the structure and types of nodes in $M$, we include it in the definition of a motif. The number of unique roles $K_M$ is at most $1 + |B_M|$.

We define an instance $S_M$ of motif $M$ with target $u$ in $G$ as a subgraph induced by $M$ with $u$ as the target node.

**Definition 2:** An instance $S_M = (V_S, E_S)$ of motif $M$ with target node $u$ in $G$ is a subgraph of $G$ where $V_S \subseteq V$ and $E_S \subseteq E$, such that there exists a bijection $\psi_S : V_S \mapsto V_M$ satisfying (i) $u \in V_S$, $\psi_S(u) = t_M$ (ii) $\forall x \in V_S$, $l(x) = l_M(\psi_S(x))$ and (iii) $\forall x, y \in V_S$, $(x, y) \in E_S$ if $(\psi_S(x), \psi_S(y)) \in E_M$.

The receptive field around a target node $t_M$ is defined by the context node $c_M$ and auxiliary nodes $B_M$ in motif $M$. We define a tensor to model role-specific motif connectivity.

**Motif-adjacency Tensor:** We define $\mathcal{A}_M$, a tensor of $K_M$ matrices to encode the occurrences of nodes in each unique semantic role $k$ over all instances of $M$ in the graph $G$. $\mathcal{A}_{kij}$ is the number of times node $v_i$ appeared in an instance of $M$ in role $k$ with $v_j$ as target. Formally,

$$\mathcal{A}_{kij} = \sum_{S_M \in \mathcal{S}_M} I(\phi(V_S, E_S, v_i, v_j) = k)$$

where $I(\cdot)$ is the indicator function. We define a diagonal matrix $D_M \in \mathbb{R}^{N \times N}$ to store the number of motif instances at each node (as target), i.e., $D_{ii} = |I_M^{v_i}| = l_i \forall 1 \leq i \leq N$.

For any graph-based learning task, it is necessary to use a combination of multiple relevant motifs to achieve good performance. A single motif describes a specific semantic connection pattern among different node types that is permissible by the schema. Unlike conventional filters that extract features around each pixel in an image, a motif is useful only for certain nodes in the graph, e.g., a triangular motif can model the context around densely connected nodes but would fail for nodes with only one neighbor and not all node types can be covered by a single motif in heterogeneous graphs. Furthermore, the underlying task at hand may require multiple semantic patterns for optimal performance. Thus, we employ multiple domain-specific relevant motifs as input.

We consider a motif relevant if the context node can provide useful features to model the target node. Let us consider, e.g., the interaction between a pair of author nodes in DBLP. Since the schema does not permit a direct A-A link, $M_1$ is an example of a motif that describes a co-authorship relation. Since such relevance depends on the specific domains (e.g., authors and publications) and applications (e.g., classifying authors’ areas), our framework assumes a set of motifs as input, which are specified by domain experts to capture the relevance between different types of nodes. In our experiments, we explore all relevant motifs of up to 5 nodes.

**Problem Definition:** Given a set of $U$ motifs $U_M = \{M_1, \ldots, M_U\}$ as input along with their respective motif-adjacency tensors, our goal is to learn a prediction model on the nodes of $G$ given task-specific supervision. In this paper, we focus on the application of semi-supervised node classification, where we are given a set $Y_i$ of nodes with labels.

### 2.3 Motif-based Convolution

In this section, we propose a novel motif-based spatial convolution operation to extract local features for a specific node type, capturing the above described properties.

Specifically, we are given motif $M$ with target type $T = l(t_M)$ and a target node $v_i \in V$ with $l(v_i) = T$ as input. For ease of explanation, we restrict our initial definitions to a single feature ($D = 1$) and single filter per motif ($F = 1$).

**Motif Filter:** A motif filter (on $M$) is defined by a weight $w_0$ for target $t_M$ and a weight vector $w \in \mathbb{R}^{K_M}$ for the $K_M$ roles, i.e., each weight in $w$ differentiates the semantic roles of context and auxiliary nodes in the receptive field.

**Convolutional Unit:** To define convolution at node $v_i$, the features of all nodes locally connected through motif $M$ are weighted according to their semantic roles and normalized by the diagonal matrix that reduces the bias introduced by highly connected nodes, giving rise to:

$$h^M(v_i) = \sigma \left( w_0 + \frac{1}{D_{ii}} \sum_{j=1}^{N} \sum_{k=1}^{K_M} w_k \mathcal{A}_{kij}^M \right)$$

| Dimensions | Description |
|------------|-------------|
| $N$        | Scalar | Number of nodes |
| $D$        | Scalar | Number of input features |
| $K$        | Scalar | Number of unique semantic roles in motif $M$ |
| $U$        | Scalar | Number of motifs/Conv. units in one layer |
| $X$        | $N \times D$ | Input Feature Matrix |
| $K_M$      | $N \times F$ | Activations at Conv. unit $j$ (motif $M_j$) in layer $l$ |
| $\mathcal{A}$ | $K_M \times N \times N$ | Motif-adjacency tensor for motif $M$ |
| $W$        | $(K_M + 1) \times D \times F$ | Filter weight tensor for motif $M$ |
In each layer, the activations of all Conv. Units are combined where
\[ M \in \mathbb{R} \times K \]
and applies the softmax activation function to obtain a first-order feature map. Since different motifs are to use a set of \( K \) weight parameters for motif \( M \) and \( H^M \in \mathbb{R}^{X \times F} \) is the output of the Conv. Unit.

### 2.4 Combining Multiple Motifs

So far, we have described a Conv. Unit that uses a single motif as a sum over each node \( v \) in the context of target \( v_j \), thus reducing to Eqn. [1]. Thus, Eqn. [5] provides an interpretation of Eqn. [1] as a standard convolution over motif instances, followed by mean pooling. This provides a strong basis for our motif-based formulation, since it generalizes primitives of conventional convolution and pooling operations to graphs.

For multi-label classification, we use \( K \) sigmoid units in the output layer and apply the binary cross-entropy loss function.

### 2.5 Complexity analysis

We analyze the complexity of our model in two parts:

#### Pre-Computation of \( \mathcal{A}^M \):

The Motif-Adjacency Tensor, which is independent of the architecture is pre-computed for all motifs. In this paper, we focus on motifs of up to 3 nodes. The cost of computing \( \mathcal{A}^M \) for triangles is \( O(|E|^{1.5}) \) [Latapy, 2008]. For non-triangle 3-node motifs, each pair of neighbors can be examined for all nodes giving a complexity of \( \Theta(\sum_j d_j^2) \) (\( d_j \) is the degree of node \( v_j \)), with superior efficient algorithms in practice [Lai et al., 2015].

For larger motifs, subgraph matching can be used with approximate sampling strategies for practical efficiency.

#### Model Training:

The complexity of single layer is a function of the number of motifs \( U \) (typically < 5) and density of each \( \mathcal{A}^M \), given by \( O(\sum_{i<j} |\mathcal{A}^M| |DF|) \). In practice, the number of roles \( K_M \) is at most 3 and the role-specific matrices are sparser than the original adjacency matrix, giving an average-case complexity \( O(U|DF|) \). Thus, we observe linear scaling with \( U \) in comparison to GCN with \( O(|DF|) \).

An efficient implementation of Motif-CNN using sparse-dense matrix operations in Tensorflow [Abadi et al., 2016] is publicly available.

### 2.6 Discussion on Motif-based Convolution

In this section, we demonstrate that our motif-based convolution (described in Eqn. [1]) can be expressed as standard convolution over motif instances followed by mean pooling.

Recall that a conventional CNN scans a square filter to extract features through an inner product between the filter parameters and features. Similarly, we interpret the motif filter as scanning the local neighborhood of a target node to compute an inner product over each instance. The output of the standard convolution operation at node \( v_i \) and motif \( M \), \( h^M_{s,v_i} \), at each instance \( S_{v_i} = (V_S, E_S) \in F_{v_i}^M \) is given by:

\[
    h^M_{s,v_i} = w_0 v_i + \sum_{v_j \in V_S(v_i)} w_{\phi_M}(S_{v_j}) y_j \quad \forall S_{v_i} \in F_{v_i}^M
\]

Using a mean pooling operation to aggregate the outputs of convolution similar to traditional CNN architectures, we get:

\[
    h^M_{\text{new},v_i} = \sigma \left( \text{pool}\left\{ h^M_{s,v_i} : S_{v_i} \in F_{v_i}^M \right\} \right) = \sigma \left( \frac{1}{|F_{v_i}^M|} \sum_{s,v_i} h^M_{s,v_i} \right)
\]

where \( h^M_{\text{new},v_i} \) is the output at node \( v_i \) after pooling.

For careful inspection of Eqn. [6] we can express the second term as a sum over each node \( v_j \) in \( G \) weighted by the occurrence count of \( v_j \) in the context of target \( v_i \) in role \( k \), thus reducing to Eqn. [1]. Thus, Eqn. [5] provides an interpretation of Eqn. [1] as a standard convolution over motif instances, followed by mean pooling. This provides a strong basis for our motif-based formulation, since it generalizes primitives of conventional convolution and pooling operations to graphs.

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[1] https://github.com/aravindsankar28/Meta-GNN
that in the trivial case of using an “edge” as the only motif, our model (Eqn. 2) approximately reduces to GCN [Kipf and Welling, 2017]. Thus, Motif-CNN generalizes state-of-the-art graph CNNs through high-order structures or motifs.

3 Experiments

In this section, we present experiments on homogeneous and heterogeneous graph datasets. We compare against three graph CNN methods a) DCNN [Atwood and Towsley, 2016] b) GCN [Kipf and Welling, 2017] and c) Graph-CNN [Such et al., 2017]. We exclude spectral methods as they have been shown inferior to GCN. We also compare against a simpler model Motif-CNN-A that uses a weighted combination of motifs instead of attention in each layer. We additionally compare against multiple state-of-the-art node classification techniques to present a comprehensive evaluation.

3.1 Homogeneous Graphs

We conduct experiments on social network datasets with node attributes on semi-supervised node classification. We use two real-world social media datasets from Flickr [Tang and Liu, 2009] and LinkedIn [Sankar et al., 2019a] in our experiments. In Flickr, the graph is described by the friendship network among users, node attributes by user interest tags and classes by user interest groups. LinkedIn is a set of ego-networks with node attributes given by user profiles and classes by tags assigned by the ego-user to his friends into various categories, such as classmates, colleagues, etc. We only include ego-networks with at least 10% labels per class. Flickr corresponds to a multi-label scenario, while LinkedIn is multi-class. Table 2 illustrates the statistics of the two datasets.

**Experimental setup:** In each dataset, we randomly sample 20% of the labeled examples for training, 10% for validation and the rest for testing. We repeat this process 10 times, and report the average performance in terms of both Micro-F1 and Macro-F1. Unless otherwise stated, we train a 3-layer Motif-CNN with ReLU activations and tune hyper-parameters (learning rate, dropout rate and number of filters per motif) based on the validation set. We train all graph CNNs for a maximum of 200 epochs using Adam [Kingma and Ba, 2014] with windowed early stopping on the validation set. Since we expect motifs such as triangles (Δ) to be discriminative in social networks, we experiment with Δ and (Δ + edge). Additionally, we compare against two standard baselines for SSL: ICA [Sen et al., 2008] and Planetoid [Yang et al., 2016].

**Experimental results:** We summarize the classification results in Table 3. Motif-CNN (Δ + edge) outperforms other benchmark algorithms and achieves gains of 6% in Flickr and 11% in LinkedIn (Macro-F1) over the next-best method. Motif-CNN (Δ) suffers from sparsity for nodes of low degree, which is offset by Motif-CNN (Δ+edge) which uses both edge and triangle patterns. This highlights the ability of Motif-CNN in learning feature associations through triangle patterns that are important in social networks. Motif-CNN outperforms the basic model Motif-CNN-A, justifying the choice of dynamically weighting the features from multiple motifs.

### Table 2: Statistics of Flickr and LinkedIn social networks

| Dataset   | |V| | |E| | |D| | |Classes |
|-----------|-------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Flickr    | 13,696                        | 1,354,461       | 1000            | 10              |
| LinkedIn  | 7124                          | 39,649          | 2394            | 3               |

### Table 3: Classification results on Flickr and LinkedIn

| Method      | Flickr Micro-F1 | Flickr Macro-F1 | LinkedIn Micro-F1 | LinkedIn Macro-F1 |
|-------------|-----------------|-----------------|-------------------|-------------------|
| DCNN        | 46.39           | 46.96           | 70.27             | 54.81             |
| GCN         | 41.71           | 42.24           | 71.91             | 57.53             |
| Graph-CNN   | 40.61           | 41.86           | 70.02             | 53.57             |
| Planetoid   | 31.53           | 31.39           | 62.49             | 43.63             |
| ICA         | 28.53           | 22.45           | 63.39             | 47.55             |
| Motif-CNN (Δ) | 47.05         | 47.45           | 72.13             | 58.75             |
| Motif-CNN-A (Δ+ edge) | 46.29        | 46.94           | 74.42             | 63.51             |
| Motif-CNN (Δ+ edge) | 49.10         | 49.56           | 74.75             | 63.57             |

### Table 4: Statistics of heterogeneous graph datasets

| Dataset   | |V| | |E| | |L| | |Classes |
|-----------|-------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| DBLP-A     | 11,170                        | 24,846          | 3               | 4               |
| DBLP-P     | 35,770                        | 131,636         | 3               | 10              |
| Movie      | 10,441                        | 99,509          | 4               | 6               |

**3.2 Heterogeneous Graphs**

We conduct classification experiments on heterogeneous graphs using three real-world datasets (statistics in Table 4): DBLP-A: This is a bibliographic citation graph composed of 3 node types: author (A), paper (P) and venue (V), connected by three link types: P→P, A→P and P→V. We use a subset of DBLP [Sun et al., 2011] with text features of papers to classify authors based on their research areas.

**DBLP-P:** This dataset has the same schema as DBLP, but the task is to classify research papers. The categories of papers are extracted from Cora [McCallum et al., 2000].

**Movie:** We use MovieLens [Harper and Konstan, 2016] to create a graph with 4 node types: movie (M), user (U), actor (A) and tag (T) linked by 4 types: U-M, A-M, U-T and M-T, with features available for actors and movies, for movie genre prediction which is multi-label classification.

**Experimental setup:** We sample 10% of the labeled examples for training, 10% for validation and the rest for testing. For node types that do not have features, we assume 1-hot encoded inputs for the graph convolutional models. For Motif-CNN, we use all relevant 3-node motifs that indicate semantic closeness based on the graph schema. We provide the details of these motifs online. We also present comparisons against multiple heterogeneous SSL baselines given below:

**LP-Metapath:** SSL algorithm that utilizes metapath-specific Laplacians to jointly propagate labels and learn weights for different metapaths [Wan et al., 2015].

**LP-Metagraph:** SSL algorithm based on an ensemble of metagraph guided random walks [Jiang et al., 2017].

**Column Network (CLN):** Deep neural network for classification in multi-relational graphs [Jiang et al., 2017].

**metapath2vec:** Heterogeneous network embedding model that uses metapath-based random walks [Dong et al., 2017].

For metapath-based methods, we provide all relevant metapaths and for LP-Metagraph, we use all metagraphs with ≤ 4 nodes and report the best performance among their three ensemble methods. Note that LP-Metagraph and LP-Metagraph

3https://sites.google.com/site/motifcnn/
Experimental results: From Table 5, we observe that Motif-CNN achieves gains of 7% and 21% (Macro-F1) over other graph CNN models while gaining 4% and 4% overall in DBLP-A and DBLP-P respectively. Since the task of classifying research papers in DBLP-P is more fine-grained, the attention mechanism significantly improves performance by appropriately weighting the importance of different motifs. In DBLP-P, DCNN does not scale due to $O(N^2)$ space complexity with the authors’ implementation. In Movie, Motif-CNN performs the best with gain of 14% Macro-F1 and 12% Micro-F1 over graph CNN models. Thus, Motif-CNN convincingly outperforms all graph CNN models on heterogeneous datasets, while gaining over other state-of-the-art classification methods by a smaller margin. The relatively higher gains in heterogeneous datasets shows the power of capturing high-order features through relevant patterns.

3.3 Computational Efficiency

We report running times on an Intel(R) Xeon(R) CPU E5-2699 v4 2.20 GHz system with 8 cores and 64 GB memory.

Computation Time: We compare the model training time per epoch of Motif-CNN versus other graph CNNs on the heterogeneous graph datasets in Fig. 3. We find that Motif-CNN is quite efficient in practice and comes second only to GCN (which is expected - see Sec 2.6) while Graph-CNN is orders of magnitude slower since it entails dense matrix operations.

We evaluate the efficiency of different models by comparing the total running time till convergence. Although the pre-computation cost is a noticeable (but not substantial) portion of the total time, Motif-CNN is reasonably close to GCN as its rapid convergence trades off the cost of pre-computation.

Convergence: We compare the convergence rates of different graph CNNs by depicting the validation set loss in Fig. 4 on using the same model configuration and hyper-parameters. Overall, Motif-CNN achieves lower error and faster convergence in comparison to other graph CNNs since it leverages multiple relevant patterns simultaneously.

4 Related work

We organize related work in three sections: a) Graph CNNs b) Graph Motifs and c) Semi-supervised classification.

Graph CNNs can be categorized in two general directions:

Spectral: Convolution is defined via the Fourier Transform described by eigenvectors of the Graph Laplacian [Bruna et al., 2014, Defferrard et al., 2016]. As noted in Sec 1, spectral CNNs cannot be transferred across different graphs.

Spatial: These methods directly generalize convolution in the graph domain through immediate neighborhood proximity [Atwood and Towsley, 2016; Niepert et al., 2016; Such et al., 2017; Kipf and Welling, 2017]. As discussed in Sec 1, all these methods are limited to learning just a single type of filter through convolution, rendering them incapable of modeling semantic relevance in heterogeneous graphs.

Graph Motifs: Motifs are high-order structures that are crucial in many domains such as neuroscience [Sporns and Kötter, 2004], bioinformatics [Pržulj, 2007; Sankar et al., 2017] and social networks. Recent work has explored motifs in clustering [Benson et al., 2016], clique detection [Hu et al., 2019], strong tie detection [Rotabi et al., 2017], graph classification [Dutta, 2017] and ranking [Zhao et al., 2018]. In contrast, we employ motifs to define the receptive field around a target node of interest for graph convolution.

Semi-supervised node classification: In this paper, we focus on graph-based SSL which has been well-studied for homogeneous graphs and is often termed Collective Classification [Sen et al., 2008] with node features.

In heterogeneous graphs, metapaths [Wan et al., 2015] and metagraphs [Fang et al., 2016] have been leveraged to develop skip-gram [Dong et al., 2017] and deep learning models [Pham et al., 2017] for SSL [Jiang et al., 2017]. All these techniques use metapaths or metagraphs to model just the similarity between a pair of nodes of the same type but cannot utilize the features of all node types for classification. In contrast, we propose a unified framework to extract local features through more general high-order structural patterns.

5 Conclusion and Future Work

In this paper, we have introduced a novel convolution operation that uses motifs to capture the key aspects of local connectivity and translation invariance in graphs. We proposed Motif-CNN that effectively fuses information from multiple patterns to learn high-order features through deeper layers. Our experiments demonstrate significant gains over existing graph CNNs especially on heterogeneous graphs.

We identify multiple interesting directions for future work. To scale the model to large graphs, sampling methods [Hamil-
can be explored to approximate motif-based neighborhoods. Further avenues for future work include extensions of our framework to temporally evolving graphs [Sankar et al., 2018] and user behavior modeling for recommender systems [Krishnan et al., 2017].

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