TOWARDS SUBGRAPH ISOMORPHISM COUNTING WITH GRAPH KERNELS

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ABSTRACT

Subgraph isomorphism counting is known as #P-complete and requires exponential time to find the accurate solution. Utilizing representation learning has been shown as a promising direction to represent substructures and approximate the solution. Graph kernels that implicitly capture the correlations among substructures in diverse graphs have exhibited great discriminative power in graph classification, so we pioneeringly investigate their potential in counting subgraph isomorphisms and further explore the augmentation of kernel capability through various variants, including polynomial and Gaussian kernels. Through comprehensive analysis, we enhance the graph kernels by incorporating neighborhood information. Finally, we present the results of extensive experiments to demonstrate the effectiveness of the enhanced graph kernels and discuss promising directions for future research.

1 INTRODUCTION

The objective of subgraph isomorphism counting is to determine the number of subgraphs in a given graph that match a specific *pattern* graph, i.e., that are isomorphic to it. This technique is highly valuable in knowledge discovery and data mining applications, such as identifying protein interactions in bioinformatics (Milo et al., 2002; Alon et al., 2008). Moreover, it is beneficial for analyzing heterogeneous information networks (HINs), including knowledge graphs (Shen et al., 2019), online social networks (Kuramochi & Karypis, 2004), and recommendation systems (Huang et al., 2016; Zhao et al., 2017). The diverse range of types within the HIN schema offers meaningful semantics, making subgraph counting a valuable component in various types of queries.

Numerous backtracking algorithms and indexing-based approaches have been proposed to tackle the challenges of subgraph isomorphisms (Ullmann, 1976; Cordella et al., 2004b; He & Singh, 2008; Han et al., 2013; Carletti et al., 2018; Klein et al., 2011). However, previous research on similar tasks often focuses on specific constraints, with limited discussions on general patterns in heterogeneous graphs. Due to the NP-hard nature of subgraph isomorphisms, researchers have also explored efficient approximations of the number of subgraph isomorphisms instead of exact counts, using techniques such as sampling (Jha et al., 2015) and color coding (Zhao et al., 2012). While these approximate solutions are relatively efficient, generalizing them to heterogeneous settings is challenging, especially considering the high memory consumption and dynamic programming complexity in heuristic rules.

Graph-based learning has recently gained significant interest, and graph kernel methods have been extensively applied in machine learning for graph classification (Kashima & Inokuchi, 2002; Glavaš & Šnajder, 2013; Zhang et al., 2013; Jie et al., 2014) and clustering (Clarisó & Cabot, 2018; Tepeli et al., 2020). These applications involve more *local* decisions, where learning algorithms typically make inferences by examining the local structures of a graph. Certain kernels are designed to capture the structural information of graphs, such as the Weisfeiler-Leman subtree kernel (WL kernel) (Shervashidze et al., 2011), which naturally lends itself to isomorphism testing (Weisfeiler & Leman, 1968). However, there exists a gap between isomorphism testing and subgraph isomorphism counting: the former is a binary problem, while the latter is a #P problem. Furthermore, isomorphism testing only considers the global structure histograms, whereas subgraph isomorphism counting requires analyzing the local structure combinations. Nonetheless, we can still utilize graph kernels to approximate the number of isomorphic subgraphs using kernel values among thousands of graphs to represent substructures implicitly. This solution could be feasible because kernel functions and Gram matrix construction are cost-effective. With neighborhood-aware techniques and kernel tricks, we

can further elevate the performance of graph kernels, making them comparable to neural networks. Code and data will be released upon publication.

2 Related Work

Subgraph isomorphism search, which involves finding all identical bijections, poses a more challenging problem and has been proven to be NP-complete. Numerous subgraph isomorphism algorithms have been developed, including backtracking-based algorithms and indexing-based algorithms. Ullmann's algorithm (Ullmann, 1976) is the first and the most straightforward, which enumerates all possible mappings and prunes non-matching mappings as early as possible. Several heuristic strategies have been proposed to reduce the search space and improve efficiency, such as VF2 (Cordella et al., 2004b), VF3 (Carletti et al., 2018), TurboIso (Han et al., 2013), and BoostIso (Ren & Wang, 2015). Some algorithms are specifically designed and optimized for particular applications and database engines Graph query languages, such as GraphGrep (Giugno & Shasha, 2002) and GraphQL (He & Singh, 2008), represent patterns as hash-based fingerprints and use overlapping label-paths in the depth-first-search tree to represent branches. Various composition and selection operators can be designed based on graph structures and graph algebras. Indexing techniques play a crucial role in this area, like gIndex (Yan et al., 2004), FG-Index (Cheng et al., 2007), and CT-Index (Klein et al., 2011). Another significant direction is approximating the number of subgraph isomorphisms, striking a balance between accuracy and efficiency. Sampling techniques (Wernicke, 2005; Ribeiro & Silva, 2010; Jha et al., 2015) and color coding (Alon et al., 1995; Bressan et al., 2019) are commonly employed. However, most methods focus on homogeneous graphs and induced subgraphs, which limits their applications in real scenarios.

Graph neural networks (GNNs) can capture rich structural information of graphs, and researchers have explored their potential in subgraph matching. The message passing framework is one such technique that leverages the representation of a neighborhood as a multiset of features and aggregates neighbor messages to find functional groups in chemical molecules (Gilmer et al., 2017). Additionally, certain substructures in social networks enhance the effectiveness of recommender systems (Ying et al., 2018). Subsequently, researchers have employed graph neural networks for subgraph counting and matching purposes. Liu et al. (2020) developed a comprehensive and unified end-to-end framework that combines sequence and graph models to count subgraph isomorphisms. Ying et al. (2020) utilized graph neural networks to embed vertices and employed a voting algorithm to match subgraphs using the acquired representations. Chen et al. (2020) conducted a theoretical analysis of the upper limit of k-WL and similar message passing variants.

Given that the message-passing framework simulates the process of the Weisfeiler-Leman algorithm, it is still under research whether general graph kernels can be used to predict the numbers of subgraph isomorphism. One of the mainstream paradigms in the design of graph kernels is to present and compare local structures. The principal idea is to encode graphs into sparse vectors, and similar topologies should have similar representations. For example, the represented objects can be bags of components, e.g., triangles (Shervashidze et al., 2009), paths (Borgwardt & Kriegel, 2005), or neighborhood (Shervashidze et al., 2011). However, simple structures have limited the discriminative power of classifiers because two different structures may result in the same representations. Therefore, people explore higher-order structures (Shervashidze et al., 2011; Morris et al., 2020). Higher-order structures usually come with exponential costs, so many other graph kernels turn to generalization (Schulz et al., 2022) and efficiency (Bause & Kriege, 2022) with the loose of guidance.

3 Background and Motivations

3.1 Problem Definition

Let $\mathcal{G} = (\mathcal{V}_\mathcal{G}, \mathcal{E}_\mathcal{G}, \mathcal{X}_\mathcal{G}, \mathcal{Y}_\mathcal{G})$ be a *graph* with a vertex set $\mathcal{V}_\mathcal{G}$ and each vertex with a different *vertex id*, an edge set $\mathcal{E}_\mathcal{G} \subseteq \mathcal{V}_\mathcal{G} \times \mathcal{V}_\mathcal{G}$, a label function $\mathcal{X}_\mathcal{G}$ that maps a vertex to a set of *vertex labels*, and a label function $\mathcal{Y}_\mathcal{G}$ that maps an edge to a set of *edge labels*. To simplify the statement, we let $\mathcal{Y}_\mathcal{G}((u,v)) = \emptyset$ (where $\emptyset$ corresponds an empty set) if $(u,v) \notin \mathcal{E}_\mathcal{G}$. A *subgraph* of $\mathcal{G}$, denoted as $\mathcal{G}_S$, is any graph with $\mathcal{V}_{\mathcal{G}_S} \subseteq \mathcal{V}_\mathcal{G}$, $\mathcal{E}_{\mathcal{G}_S} \subseteq \mathcal{E}_\mathcal{G} \cap (\mathcal{V}_{\mathcal{G}_S} \times \mathcal{V}_{\mathcal{G}_S})$ satisfying $\forall v \in \mathcal{V}_{\mathcal{G}_S}, \mathcal{X}_{\mathcal{G}_S}(v) = \mathcal{X}_\mathcal{G}(v)$ and $\forall e \in \mathcal{E}_{\mathcal{G}_S}, \mathcal{Y}_{\mathcal{G}_S}(e) = \mathcal{Y}_\mathcal{G}(e)$. One of the important properties in graphs is the *isomorphism*.

Definition 3.1 (Isomorphism) *A graph $\mathcal{G}_1$ is isomorphic to a graph $\mathcal{G}_2$ if there is a bijection $f : \mathcal{V}_{\mathcal{G}_1} \to \mathcal{V}_{\mathcal{G}_2}$ such that:*

- $\forall v \in \mathcal{V}_{\mathcal{G}_1}, \mathcal{X}_{\mathcal{G}_1}(v) = \mathcal{X}_{\mathcal{G}_2}(f(v))$,
- $\forall v' \in \mathcal{V}_{\mathcal{G}_2}, \mathcal{X}_{\mathcal{G}_2}(v') = \mathcal{X}_{\mathcal{G}_1}(f^{-1}(v'))$,
- $\forall (u, v) \in \mathcal{E}_{\mathcal{G}_1}, \mathcal{Y}_{\mathcal{G}_1}((u, v)) = \mathcal{Y}_{\mathcal{G}_2}((f(u), f(v)))$,
- $\forall (u', v') \in \mathcal{E}_{\mathcal{G}_2}, \mathcal{Y}_{\mathcal{G}_2}((u', v')) = \mathcal{Y}_{\mathcal{G}_1}((f^{-1}(u'), f^{-1}(v')))$.

When $\mathcal{G}_1$ and $\mathcal{G}_2$ are isomorphic, we use the notation $\mathcal{G}_1 \simeq \mathcal{G}_2$ to present this and name the function f as an *isomorphism*. A specific isomorphism f is $\{\} \to \{\}$ when considering two empty graphs with no vertices. In addition, the *subgraph isomorphism* is more general.

Definition 3.2 (Subgraph isomorphism) *If a subgraph $\mathcal{G}_{1_S}$ of $\mathcal{G}_1$ is isomorphic to a graph $\mathcal{G}_2$ with a bijection f, we say $\mathcal{G}_1$ contains a subgraph isomorphic to $\mathcal{G}_2$ and name f as a subgraph isomorphism.*

The problem of subgraph isomorphisms involves two types of subgraphs: node-induced subgraphs and edge-induced subgraphs. The former one corresponds to induced subgraph definition that requires $\mathcal{E}_{\mathcal{G}_S} = \mathcal{E}_{\mathcal{G}} \cap (\mathcal{V}_{\mathcal{G}_S} \times \mathcal{V}_{\mathcal{G}_S})$, while the latter one corresponds to the general definition of subgraphs. To make it easier to generalize, we assume that all subgraphs mentioned here are edge-induced.

3.2 Graph Isomorphism Test and Representation Power

Graph isomorphism tests are used to determine whether two graphs are isomorphic, which are useful in various fields such as computer science, chemistry, and mathematics.

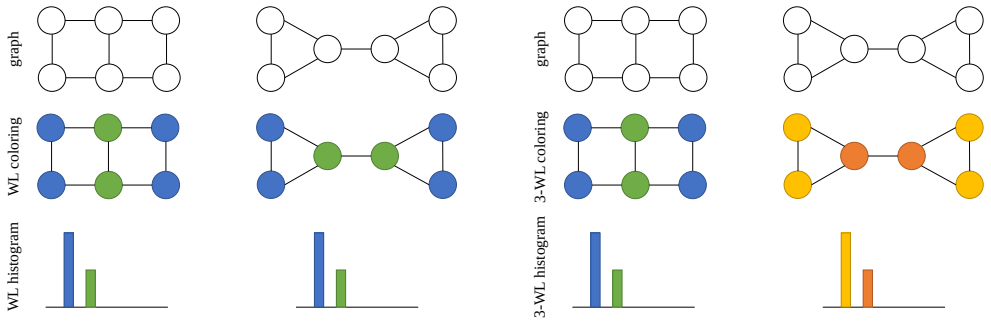
Definition 3.3 (Graph Isomorphism Test) *A graph isomorphism test is a function $\chi : \Sigma \times \Sigma \to \{0, 1\}$ that determines whether two graphs are isomorphic, where Σ is the graph set.*

Ideally, a perfect graph isomorphism test should be able to distinguish **all** graph pairs, i.e., $\forall \mathcal{G}_i, \mathcal{G}_j \in \Sigma : \chi(\mathcal{G}_i, \mathcal{G}_j) = 1 \Leftrightarrow \mathcal{G}_i \simeq \mathcal{G}_j$. The graph isomorphism problem is a well-known computational problem that belongs to the class of NP problems. Nonetheless, there are heuristic techniques that can solve the graph isomorphism tests for most practical cases. For example, the *Weisfeiler-Leman algorithm* (WL algorithm) (Weisfeiler & Leman, 1968) is a heuristic test for graph isomorphism that assigns colors to vertices of graphs iteratively:

$$
\begin{aligned}
c_v^{(t+1)} &= \texttt{Color}(c_v^{(t)}, \boldsymbol{N}_v^{(t)}), \\
\boldsymbol{N}_v^{(t)} &= \{\texttt{Color}(c_u^{(t)}, \{c_{(u,v)}^{(t)}\}) | u \in \mathcal{N}_v\}, \\
c_v^{(0)} &= \mathcal{X}_{\mathcal{G}}(v), \\
c_{(u,v)}^{(t)} &= \mathcal{Y}_{\mathcal{G}}((u, v)),
\end{aligned}
$$

where $c_v^{(t)}$ is the color of vertex v at the t-th iteration, $\mathcal{N}_v$ is v's neighbor collection, $\mathcal{X}_{\mathcal{G}}(v)$ is the vertex label of v in graph $\mathcal{G}$, $\mathcal{Y}_{\mathcal{G}}((u, v))$ is the edge label of (u, v) in graph $\mathcal{G}$, and $\texttt{Color}$ is a function to assign colors to vertices. The time complexity of color assignment is $\mathcal{O}(|\mathcal{E}_{\mathcal{G}}|)$ for each iteration. Given two graphs $\mathcal{G}_i$ and $\mathcal{G}_j$, the WL algorithm refines colors to vertices of $\mathcal{G}_i$ and $\mathcal{G}_j$ in parallel and then compares the resulting colors of vertices in the two graphs.

The WL algorithm is guaranteed to terminate after a finite number of iterations. It determines that two graphs are isomorphic only if the colors of vertices in both graphs are the same when the algorithm finishes, here "same" refers to having identical color histograms. However, the WL algorithm is unable to distinguish all non-isomorphic graphs, as demonstrated in Figure 1a. Therefore, it is crucial to comprehend the **representation power** of this algorithm. What makes the algorithm potent for isomorphism testing is its injective color refinement, which takes into account the neighborhood of each vertex. The neighbor collection $\mathcal{N}_v$ is defined based on the 1-hop neighborhood, meaning that color refinement relies solely on the local information of each vertex. Hence, an extension of the WL algorithm that considers higher-order interactions between vertices is expected to possess greater power for isomorphism testing, which are called *k-dimensional Weisfeiler-Leman algorithm* (Cai et al., 1992). It iteratively assigns colors to the k-tuples ($k \geq 2$) of $\mathcal{V}_{\mathcal{G}}^k$ as follows:



(a) Example of the non-isomorphic graphs with the same WL color histogram.

(b) Example of the non-isomorphic graphs with different 3-WL color histograms.

Figure 1: Example of the non-isomorphic graphs with the same WL color histogram but different 3-WL color histograms.

$$
\begin{aligned}
c_{\boldsymbol{v}}^{(t+1)} &= \texttt{Color}(c_{\boldsymbol{v}}^{(t)}, \boldsymbol{N}_{\boldsymbol{v}}^{(t)}), \\
\boldsymbol{N}_{\boldsymbol{v}}^{(t)} &= \bigcup_{j=1}^{k} \{\texttt{Color}(c_{\boldsymbol{u}}^{(t)}, \{c_{(\boldsymbol{u},\boldsymbol{v})}^{(t)}\}) | \boldsymbol{u} \in \mathcal{N}_{\boldsymbol{v}}^{j}\}, \\
c_{\boldsymbol{v}}^{(0)} &= \texttt{Color}(\mathcal{X}_{\mathcal{G}}(\boldsymbol{v}[k]), \{\mathcal{X}_{\mathcal{G}}(\boldsymbol{v}) | w \in \boldsymbol{v} - \{\boldsymbol{v}[k]\}\}), \\
c_{(\boldsymbol{u},\boldsymbol{v})}^{(t)} &= \begin{cases} \mathcal{Y}_{\mathcal{G}}((u,v)) & \text{if } u = \boldsymbol{v} - \boldsymbol{u} \text{ and } v = \boldsymbol{u} - \boldsymbol{v}, \\ \emptyset & \text{otherwise.} \end{cases},
\end{aligned}
$$

where $\boldsymbol{v}$ refers to a tuple of k vertices in $\mathcal{V}_{\mathcal{G}}$, $\boldsymbol{v}[j]$ denotes the j-th element of the tuple $\boldsymbol{v}$, $\mathcal{N}_{\boldsymbol{v}}^{j}$ $(1 \leq j \leq k)$ is the neighbor collection of $\boldsymbol{v}$ in which only the j-th elements are different (i.e., $\mathcal{N}_{\boldsymbol{v}}^{j} = \{\boldsymbol{u} | (\forall i \neq j \ \boldsymbol{u}[i] = \boldsymbol{v}[i]) \wedge (\boldsymbol{u}[j] = \boldsymbol{v}[j])\}$), $\mathcal{X}_{\mathcal{G}}(\boldsymbol{v}[k])$ is the vertex label of $\boldsymbol{v}[k]$ in graph $\mathcal{G}$, $\mathcal{X}_{\mathcal{G}}(\boldsymbol{v})$ is the vertex label of $\boldsymbol{v}$ in graph $\mathcal{G}$, $\mathcal{Y}_{\mathcal{G}}((u,v))$ is the edge label of (u,v) in graph $\mathcal{G}$, $\boldsymbol{v} - \boldsymbol{u}$ indicates the difference of two tuples, and $\texttt{Color}$ is a function to assign colors to tuples. The k-WL algorithm is also guaranteed to terminate after a finite number of iterations. Figure 1b demonstrates the same example in Figure 1a with different 3-WL color histograms, despite having the same WL color histogram. This suggests that the 3-WL algorithm can distinguish more non-isomorphic graphs than the WL algorithm, which is expected to obtain strictly stronger representation power. It is worth noting that the complexity of the k-WL algorithm increases exponentially because it constructs $|\mathcal{V}_{\mathcal{G}}|^{k}$ tuples and at most $|\mathcal{V}_{\mathcal{G}}|^{2k}$ connections, which are regarded as "vertices" and "edges" in the k-tuple graph. Thus, the complexity of color assignment becomes $\mathcal{O}(|\mathcal{V}_{\mathcal{G}}|^{2k})$.

3.3 Graph Kernels

However, there is a gap between the power of representation and subgraph isomorphisms. While the power aims to distinguish non-isomorphic graph pairs, counting subgraph isomorphisms presents a greater challenge, which is a combinatorial problem depending on substructures. Therefore, our objective is to approximate subgraph isomorphism counting through representation learning and optimization as regression. The isomorphism test can be seen as a hard indicator function that determines whether an isomorphism exists, which can be extended as a kernel function for subgraph isomprhism counting. A *kernel function* is designed to measure the similarity between two objects.

Definition 3.4 (Kernel) *A function $k : \Sigma \times \Sigma \to \mathbb{R}$ is called a kernel over an non-empty set Σ.*

An even more crucial concept is the selection of a kernel function k in a manner that allows for the existence of a *feature map* h from the set Σ to a Hilbert space $\mathbb{H}$ equipped with an inner product. This feature map should satisfy $\forall \mathcal{G}_i, \mathcal{G}_j \in \Sigma : k(\mathcal{G}_i, \mathcal{G}_j) = \langle h(\mathcal{G}_i), h(\mathcal{G}_j) \rangle$. This space $\mathbb{H}$ is referred to as the *feature space*. A group of kernel functions known as *graph kernels* (GKs) are employed to compute the similarity between two graphs by taking them as input.

Neural networks have been regarded as effective feature extractors and predictors, and sequence and graph neural networks can be aligned with the kernel functions (Lei et al., 2017; Xu et al., 2019). Liu et al. (2020) proposed a unified end-to-end framework for sequence models and graph models to

directly predict the number of subgraph isomorphisms rather than the similarities, further illustrating the practical success.

4 BEYOND THE REPRESENTATION POWER LIMITATION VIA IMPLICIT CORRELATIONS

Constructing neural networks to directly predict the number of subgraph isomorphisms has been shown effective and efficient (Liu et al., 2020; Yu et al., 2023). But transforming Σ to a limited-dimensional space $\mathbb{H}$ remains challenging in optimization, and it has been shown bounded in theory and practice (Chen et al., 2020; Liu & Song, 2022). Therefore, we turn to other directions to leverage implicit structure correlations to make predictions.

4.1 GRAM MATRIX CONSTRUCTION

Given a set of graphs $\mathcal{G}_1, \mathcal{G}_2, \cdots, \mathcal{G}_D \in \Sigma$, the *kernel matrix* $\boldsymbol{K}$ is defined as:

$$\boldsymbol{K} = \begin{bmatrix} k(\mathcal{G}_1, \mathcal{G}_1) & k(\mathcal{G}_1, \mathcal{G}_2) & \cdots & k(\mathcal{G}_1, \mathcal{G}_D) \\ k(\mathcal{G}_2, \mathcal{G}_1) & k(\mathcal{G}_2, \mathcal{G}_2) & \cdots & k(\mathcal{G}_2, \mathcal{G}_D) \\ \vdots & \vdots & \ddots & \vdots \\ k(\mathcal{G}_D, \mathcal{G}_1) & k(\mathcal{G}_D, \mathcal{G}_2) & \cdots & k(\mathcal{G}_D, \mathcal{G}_D) \end{bmatrix}, \tag{1}$$

$$s.t. \boldsymbol{K}_{ij} = k(\mathcal{G}_i, \mathcal{G}_j) = \langle h(\mathcal{G}_i), h(\mathcal{G}_j) \rangle. \tag{2}$$

The kernel matrix $\boldsymbol{K} \in \mathbb{R}^{D \times D}$ is also called the *Gram matrix*. Different kernel functions emphasize specific structural properties of graphs. For instance, *Shortest-path Kernel* (SP) (Borgwardt & Kriegel, 2005) decomposes graphs into shortest paths and compares graphs according to their shortest paths, such as path lengths and endpoint labels. Instead, Graphlet Kernels (Shervashidze et al., 2009) compute the distribution of small subgraphs (i.e., wedges and triangles) under the assumption that graphs with similar graphlet distributions are highly likely to be similar. The *Weisfeiler-Leman subtree kernel* (WL kernel) belongs to a family of graph kernels denoted as (k-WL) (Shervashidze et al., 2011), where k indicates the element size during the color assignment.

Let's take the WL kernel as an example. It is a popular graph kernel based on the WL algorithm mentioned in § 3.2 upon 1-hop neighborhood aggregation to assign finite integer labels $\mathbb{S}$, i.e., h_{KL}: $\mathcal{G} \rightarrow \Big\|_{s \in \mathbb{S}} \#\{v \in \mathcal{V}_{\mathcal{G}} | \boldsymbol{c}_v = s\}$ such that Color: $v \in \mathcal{V}_{\mathcal{G}} \rightarrow c_v \in \mathbb{S}$. Usually, the convergence of the colors for different graphs occurs in different iterations, so it is hard to determine a specific "finite" number of iterations. Thus, the WL kernel is often manually set to a particular number T:

$$k_{\text{WL}}(\mathcal{G}_i, \mathcal{G}_j) = \langle h_{\text{WL}}(\mathcal{G}_i), h_{\text{WL}}(\mathcal{G}_j) \rangle = \Big\langle \Big\|_{t=0}^{T} \boldsymbol{C}^{(t)}_{\mathcal{V}_{\mathcal{G}_i}}, \Big\|_{t=0}^{T} \boldsymbol{C}^{(t)}_{\mathcal{V}_{\mathcal{G}_j}} \Big\rangle, \tag{3}$$

where $\boldsymbol{C}^{(t)}_{\mathcal{V}_{\mathcal{G}_i}}$ is the color histogram (a color vector that counts the number of occurrences of vertex colors) of $\mathcal{G}_i$ at iteration t, i.e., $\boldsymbol{C}^{(t)}_{\mathcal{V}_{\mathcal{G}_i}} = \Big\|_{s \in \mathbb{S}} \#\{v \in \mathcal{V}_{\mathcal{G}_i} | \boldsymbol{c}^{(t)}_v = s\}$. Note that there is no overlap between the colors at different iterations such that color vectors $\{\boldsymbol{C}^{(t)}_{\mathcal{V}_{\mathcal{G}_i}} | 0 \leq t \leq T\}$ are orthogonal to each other. Hence, the kernel is efficient in computing by reducing a sum of inner products:

$$k_{\text{WL}}(\mathcal{G}_i, \mathcal{G}_j) = \sum_{t=0}^{T} \boldsymbol{C}^{(t)\top}_{\mathcal{V}_{\mathcal{G}_i}} \boldsymbol{C}^{(t)}_{\mathcal{V}_{\mathcal{G}_j}}. \tag{4}$$

It is worth noting that the Gram matrix does not explicitly maintain the graph structure and substructure information. But this information can be implicitly captured within the matrix.

The running time for a single color vector is $\mathcal{O}(T \cdot |\mathcal{E}_{\mathcal{G}_i}|)$, and the running time for the dot product is $\mathcal{O}(T \cdot (|\mathcal{V}_{\mathcal{G}_i}| + |\mathcal{V}_{\mathcal{G}_j}|))$. Therefore, the running time for the WL kernel and the Gram matrix is $\mathcal{O}(T \cdot M \cdot D + T \cdot N \cdot D^2)$, where N and M represent the maximum number of vertices and edges among the D graphs, respectively. For a k-WL kernel, the time complexity is $\mathcal{O}(T \cdot N^{2k} \cdot D + T \cdot N \cdot D^2)$.

Algorithm 1 Neighborhood-aware color assignment algorithm.

input a directed graph $\mathcal{G} = (\mathcal{V}_\mathcal{G}, \mathcal{E}_\mathcal{G}, \mathcal{X}_\mathcal{G}, \mathcal{Y}_\mathcal{G})$, a fixed integer T

initialize the color of each node v in $\mathcal{V}_\mathcal{G}$ as $c_v^{(0)} = \mathcal{X}_\mathcal{G}(v)$ and color of each edge e in $\mathcal{E}_\mathcal{G}$ as $c_e = \mathcal{Y}_\mathcal{G}(e)$
for iter t from 1 to T **do**
  create a new color counter $\mathcal{C}^{(t)}$ and initialize $\mathcal{C}^{(t)} = \emptyset$
  for each v in $\mathcal{V}_\mathcal{G}$ **do**
    create a color multi-set $\boldsymbol{N}_v^{(t)}$ and initialize $\boldsymbol{N}_v^{(t)} = \emptyset$
    for each neighbor u in v's neighbor set $\mathcal{N}_v$ **do**
      add the neighbor color $\texttt{Color}(c_u^{(t)}, \{c_{u,v}\})$ to $\boldsymbol{N}_v^{(t)}$
      calculate the pair-wise color $\texttt{Color}(c_v^{(t)}, \{\texttt{Color}(c_u^{(t)}, \{c_{u,v}\})\})$ and record it in the color counter $\mathcal{C}^{(t)}$
      //{neighborhood information recording}
    end for
    calculate the set-wise color $\texttt{Color}(c_v^{(t)}, \boldsymbol{N}_v^{(t)})$, record it in the color counter $\mathcal{C}^{(t)}$, and update $c_v^{(t+1)}$
    //{original color assignment}
  end for
end for
output the graph color histogram $\bigcup_{t=0}^{T}\{\mathcal{C}^{(t)}\}$

4.2 Neighborhood Information in the Hilbert Space

Since the graph kernel is a function of the graph representation, the graph structure is expected to be preserved in the Hilbert space. However, the hash function in the WL kernel family does not capture the neighbors of a node. For example, $c_u^{(t)}$ and $c_v^{(t)}$ would be different if $u \in \mathcal{V}_{\mathcal{G}i}$ and $v \in \mathcal{V}_{\mathcal{G}_j}$ have different neighbors (more precisely, at least one neighbor is different). Nevertheless, the subset of neighbors is essential for examining isomorphisms, as the inclusion relation is a necessary condition for subgraph isomorphisms. We modify the color assignment algorithm in the WL kernel family to incorporate neighborhood information in the Hilbert space or record it in the graph histogram. The modified WL kernel is called *neighborhood-information-extraction WL kernel* (NIE-WL kernel). The neighborhood-aware color assignment algorithm is described in Algorithm 1. The only change is the addition of pairwise colors to the color histogram. This pairwise color depends on the edges and the latest node colors, without affecting the original color assignment. As a result, the color histogram becomes more expressive, as it can record neighborhood information.

It is clear that the NIE-WL kernel should have the same expressive power as the WL kernel, but the histogram of the NIE-WL kernel records $|\mathcal{V}_\mathcal{G}| + |\mathcal{E}_\mathcal{G}|$ colors instead of $|\mathcal{V}_\mathcal{G}|$ colors. The additional $|\mathcal{E}_\mathcal{G}|$ colors (denoted as $\boldsymbol{C}_{\mathcal{E}_{\mathcal{G}_i}}^{(t)}$ for the t-th iteration) can be used in constructing the Gram matrix, where neighborhood information is preserved. If we decompose the NIE-WL kernel into the WL kernel and the neighborhood-information-extraction kernel (denoted as NIE), we can get:

$$
\begin{aligned}
k_{\text{NIE-WL}}(\mathcal{G}_i, \mathcal{G}_j) &= \left\langle \left\| \sum_{t=0}^{T} \boldsymbol{C}_{\mathcal{V}_{\mathcal{G}_i}}^{(t)} || \boldsymbol{C}_{\mathcal{E}_{\mathcal{G}_i}}^{(t)}, \left\| \sum_{t=0}^{T} \boldsymbol{C}_{\mathcal{V}_{\mathcal{G}_j}}^{(t)} || \boldsymbol{C}_{\mathcal{E}_{\mathcal{G}_j}}^{(t)} \right\rangle = \sum_{t=0}^{T} (\boldsymbol{C}_{\mathcal{V}_{\mathcal{G}_i}}^{(t)} || \boldsymbol{C}_{\mathcal{E}_{\mathcal{G}_i}}^{(t)})^\top (\boldsymbol{C}_{\mathcal{V}_{\mathcal{G}_j}}^{(t)} || \boldsymbol{C}_{\mathcal{E}_{\mathcal{G}_j}}^{(t)}) \right. \right. \\
&= \sum_{t=0}^{T} \boldsymbol{C}_{\mathcal{V}_{\mathcal{G}_i}}^{(t)\top} \boldsymbol{C}_{\mathcal{V}_{\mathcal{G}_j}}^{(t)} + \sum_{t=0}^{T} \boldsymbol{C}_{\mathcal{E}_{\mathcal{G}_i}}^{(t)\top} \boldsymbol{C}_{\mathcal{E}_{\mathcal{G}_j}}^{(t)} = k_{\text{WL}}(\mathcal{G}_i, \mathcal{G}_j) + k_{\text{NIE}}(\mathcal{G}_i, \mathcal{G}_j). \qquad (5)
\end{aligned}
$$

In other words, the NIE-WL kernel is the linear combination of the WL kernel and the neighborhood-information-extraction kernel. This also implies that the NIE-WL kernel is a hybrid kernel function, incorporating information beyond feature transformations.

4.3 Kernel Tricks

Graph kernels are typically characterized as *positive semi-definite kernels*. Consequently, these kernels $\boldsymbol{K}$ possess the *reproducing property*:

$$
\theta(\mathcal{G}_i) = \sum_{j=1}^{D} \boldsymbol{K}_{ij} \theta(\mathcal{G}_j) = \langle \boldsymbol{K}_i, \boldsymbol{\theta} \rangle, \qquad (6)
$$

where θ is a function belonging to a new feature space $\mathbb{H}'$, and $\boldsymbol{\theta} = [\theta(\mathcal{G}_1), \theta(\mathcal{G}_2), \cdots, \theta(\mathcal{G}_D)]$ is the vectorized representation of θ. The space $\mathbb{H}'$ is known as the *reproducing kernel Hilbert space* (RKHS) and does not require explicit construction.

Based on the definition of kernels and the reproducing property, a graph $\mathcal{G}_i$ can be represented as $\boldsymbol{g}_i$ in the Hilbert space (more precisely, RKHS) according to Eq. (6). We then embed the resulting graph representation into another Hilbert space, $\mathbb{H}'$, using another kernel function k'. We consider the following two popular kernel functions.

Polynomial Kernel The *polynomial kernel* is defined as $k_{\text{Poly}}(\mathcal{G}_i, \mathcal{G}_j) = (\boldsymbol{g}_i^\top \boldsymbol{g}_j + 1)^p$, where $p \in \mathbb{N}$ is a positive integer. In practice, explicitly computing the polynomial kernel matrix such that $\boldsymbol{K}_{i,j} = k_{\text{Poly}}(\boldsymbol{g}_i, \boldsymbol{g}_j)$ is infeasible due to the high dimensionality of the Hilbert space. Instead, we employ the kernel trick to compute the polynomial kernel matrix implicitly:

$$k_{\text{Poly}}(\mathcal{G}_i, \mathcal{G}_j) = (\boldsymbol{g}_i^\top \boldsymbol{g}_j + 1)^p = \sum_{k=0}^{p} \frac{p!}{k!(p-k)!} (\boldsymbol{g}_i^\top \boldsymbol{g}_j)^{p-k} 1^k = (\boldsymbol{K}_{i,j} + 1)^p. \tag{7}$$

Gaussian Kernel A polynomial kernel transforms the graph representation into a higher dimensional space $\binom{|\Sigma|+p}{p}$. However, the polynomial kernel is sensitive to the parameter p, which may result in an overflow issue when p is too large. A popular kernel function that maps the graph representation into an infinite-dimensional space is named *Gaussian kernel* or *radial basis function kernel*, i.e., $k_{\text{RBF}}(\mathcal{G}_i, \mathcal{G}_j) = \exp(-\frac{\|\boldsymbol{g}_i - \boldsymbol{g}_j\|^2}{2\sigma^2})$, where σ is a positive real number. We also have a trick to compute the Gaussian kernel matrix implicitly:

$$k_{\text{RBF}}(\mathcal{G}_i, \mathcal{G}_j) = \exp(-\frac{\|\boldsymbol{g}_i - \boldsymbol{g}_j\|^2}{2\sigma^2}) = \exp(-\frac{\boldsymbol{g}_i^\top \boldsymbol{g}_i - 2\boldsymbol{g}_i^\top \boldsymbol{g}_j + \boldsymbol{g}_j^\top \boldsymbol{g}_j}{2\sigma^2}) = \exp(-\frac{\boldsymbol{K}_{i,i} - 2\boldsymbol{K}_{i,j} + \boldsymbol{K}_{j,j}}{2\sigma^2}). \tag{8}$$

By employing the aforementioned implicit computation tricks, the kernel transformations become efficient and scalable through matrix operations. Hybrid kernel functions can be obtained by combining different graph kernels. For instance, a hybrid kernel function with the WL kernel and RBF kernel is Eq. (9), where $\boldsymbol{K}_{\text{WL}}$ is the Gram matrix with respect to the WL kernel.

$$k_{\text{WL,RBF}}(\mathcal{G}_i, \mathcal{G}_j) = \exp(-\frac{\boldsymbol{K}_{\text{WL}i,i} - 2\boldsymbol{K}_{\text{WL}i,j} + \boldsymbol{K}_{\text{WL}j,j}}{2\sigma^2}). \tag{9}$$

5 Experiment

5.1 Experimental Setup

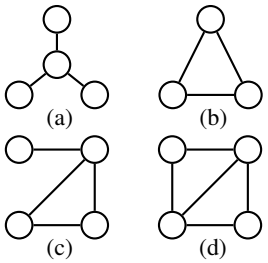


Figure 2: Patterns considered in experiments: (a) 3-star, (b) triangle, (c) tailed triangle, and (d) chordal cycle.

Evaluation We regard subgraph isomorphism counting with graph kernels as a machine learning problem. Since we model subgraph isomorphism counting as a regression problem with Gram matrices, we use the SVM (Chang & Lin, 2011) and Ridge (Hoerl & Kennard, 1970) implemented in the scikit-learn package. We assess models based on the root mean squared error (RMSE) and the mean absolute error (MAE). We collect the most popular datasets for graph classification, as graph properties are often determined by substructures within the graph. In order to obtain meaningful and challenging predictions, we enumerate all vertex label permutations and edge permutations from the 3-stars, triangles, tailed triangles, and chordal cycles. Furthermore, to enhance the quality of the data, we filter out patterns with an average frequency of less than 1.0 across the entire dataset. Detailed settings can be found in Appendix A. Our approach to graph kernels involves substructures from different levels:

- **Paths**: Shortest-path Kernel (Borgwardt & Kriegel, 2005) decomposes graphs into shortest paths and compares these paths.
- **Wedges and triangles**: Graphlet Kernels (Shervashidze et al., 2009) compute the distribution of graphlets of size 3, which consist of wedges and triangles.
- **Whole graphs**: Weisfeiler-Leman Optimal Assignment Kernel (WLOA) (Kriege et al., 2016) improves the WL kernel by capitalizing on the theory of valid assignment kernels.

- **High-order neighborhood**: k-WL Kernels (Shervashidze et al., 2011) measure the histogram of k-combinations by assigning colors to k-tuples, while δ-k WL kernels record the number of k-tuples with the same color. δ-k-LWL and δ-k-LWL$^+$ focus on local structures of the graph instead of the whole graph (Morris et al., 2020).

We also apply polynomial and Gaussian kernel transformations to the kernels mentioned above. Besides, we incorporate the neighborhood-aware color assignment to k-WL Kernels and their variants. We provide two trivial baselines and neural baselines as references (please refer to Appendix B.1).

Efficient Implementation Graph kernels are implemented in C++ with C++11 features and the -O2 flag. In addition to the technical aspects, we also focus on training efficiency. The simplest input for regressors is the original graph kernel matrix of size $D \times D$. However, this kernel matrix only contains graphs in the entire dataset, without any information about patterns. It is necessary to incorporate pattern structure information during training. Assuming we have Q patterns, we need to repeatedly construct Q kernel matrices of size $(1 + D) \times (1 + D)$. In fact, the $D \times D$ submatrix is the same for all Q kernel matrices because it is irrelevant to the patterns. Therefore, it is recommended that we construct a matrix of size $(Q + D) \times (Q + D)$ only once and then repeatedly slice the submatrix to obtain information about the D graphs and the specific pattern for prediction.

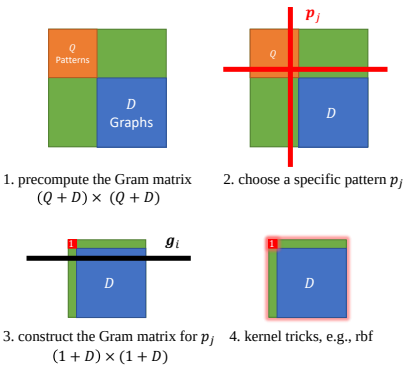


Figure 3: Efficient implementation.

5.2 Empirical Results

5.2.1 SVM vs. Ridge

We begin by comparing the performance of SVM and Ridge (precisely, Kernel Ridge) regression without kernel tricks on subgraph isomorphism counting. This is a common practice to evaluate the performance of these two regressors. As shown in Figure 4 and Appendix B.2, the performance of the two regressors is comparable, with Ridge performing slightly better. There are two main reasons. First, Ridge is solved by Cholesky factorization in the closed form, which typically achieves better convergence than the iterative optimization of SVM. Second, the objective of Ridge is to minimize the sum of squared errors, which is more straightforward and suitable for the regression task than the ϵ-insensitive loss function of SVM. Therefore, we mainly report the results of Ridge.

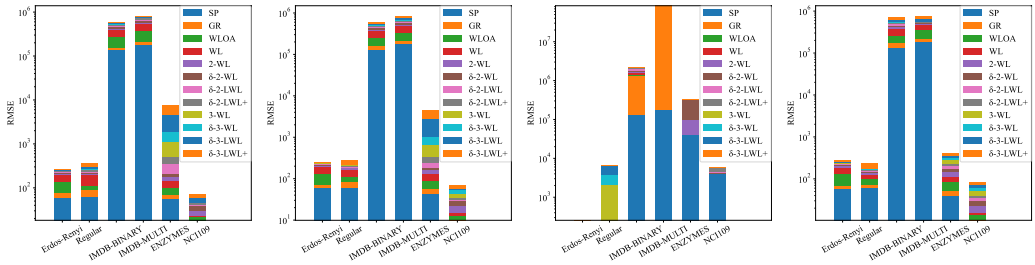
5.2.2 Kernel Tricks for Implicit Transform

In addition, we also observe an increase in errors with the polynomial kernel trick from Figure 4. The number of matched subgraphs is typically small but can be very large for specific structures, such as complete graphs or cliques. The polynomial kernel trick can easily lead to fluctuations due to extreme values, resulting in performance fluctuations and even overflow.

5.2.3 Effectiveness of Neighborhood Information Extraction

Explicit neighborhood information extraction (NIE) is a crucial component for handling homogeneous data by providing edge colors. However, this method is not as beneficial when applied to synthetic *Erdős-Renyi* and *Regular* datasets because the uniform distribution of neighborhoods results in uniform distributions of edge colors. As demonstrated in Table 1, incorporating NIE consistently enhances the performance of both linear and RBF kernels.

Overall, the RBF kernel combined with NIE proves to be more effective for homogeneous data, while the linear kernel is substantially improved when applied to heterogeneous data. The most significant enhancements are observed on the highly challenging *IMDB-BINARY* and *IMDB-MULTI* datasets, where the RMSE is dramatically reduced from 30,527.764 to 757.736 and from 21,910.109 to 833.037, respectively. When compared to naive baselines that predict either zeros or the training sets' expectations, the RMSE is diminished to a mere 0.5%. In addition, some kernel methods, such as GR and the 2-WL family, can provide the same or even more reliable predictions as neural methods.



(a) SVM, Linear. (b) Ridge, Linear. (c) Ridge, Poly. (d) Ridge, RBF.

Figure 4: Illustration on approximation errors, where the out-of-memory (OOM) is omitted in plots.

Table 1: Performance on subgraph isomorphism counting, where k-WL‡ represents the best model in the kernel family, and the best and second best are marked in red and blue, respectively.

Models	Homogeneous								Heterogeneous			
	Erdős-Renyi		*Regular*		IMDB-BINARY		IMDB-MULTI		*ENZYMES*		*NCI109*	
	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE	RMSE	MAE
Zero	92.532	51.655	198.218	121.647	138262.003	37041.171	185665.874	33063.770	64.658	25.110	16.882	7.703
Avg	121.388	131.007	156.515	127.211	133228.554	54178.671	182717.385	53398.301	59.589	31.577	14.997	8.622
TXL	10.861	7.105	15.263	10.721	15369.186	3170.290	19706.248	3737.862	25.912	11.284	5.482	2.823
RGCN	9.386	5.829	14.789	9.772	46074.355	13498.414	69485.242	12137.598	23.715	11.407	**1.217**	0.622
RGIN	6.063	3.712	13.554	8.580	31058.764	6445.103	26546.882	4508.339	**8.119**	**3.783**	**0.511**	**0.292**
CompGCN	6.706	4.274	14.174	9.685	32145.713	8576.071	26523.880	7745.702	14.985	6.438	1.271	0.587
Ridge, Linear												
SP	58.721	34.606	60.375	41.110	131672.705	56058.593	181794.702	54604.564	43.007	14.422	4.824	2.268
GR	14.067	7.220	23.775	12.172	30527.764	7894.568	30980.135	6054.027	14.557	5.595	5.066	2.066
WLOA	58.719	34.635	25.905	17.003	96887.226	28849.659	117828.698	25808.362	28.911	11.807	3.142	1.142
WL	58.719	34.635	56.045	33.891	107500.276	41523.359	147822.358	49244.753	46.466	14.920	1.896	0.746
2-WL‡	9.921	4.164	8.751	5.663	33336.019	9161.265	47075.541	13751.520	26.903	10.079	2.584	1.068
3-WL‡	**4.096**	**1.833**	**3.975**	**2.277**	39237.071	7240.730	76218.966	9022.754	335.940	13.790	3.872	1.375
Ridge, Linear, NIE												
WLOA	58.719	34.635	25.905	17.003	33625.086	6009.372	20858.288	2822.391	23.478	10.037	3.203	1.133
WL	58.719	34.635	56.045	33.891	66414.032	17502.328	70013.402	13266.318	20.971	8.672	1.772	0.704
2-WL‡	9.921	4.164	8.751	5.663	14914.025	3671.681	37676.903	9930.398	97.024	7.191	1.259	**0.539**
3-WL‡	**4.096**	**1.833**	**3.975**	**2.277**	**1808.841**	**264.480**	**1346.608**	**123.394**	380.480	19.073	OOM	OOM
Ridge, RBF												
SP	58.721	34.606	60.375	41.110	131672.705	56058.593	181794.702	54604.564	38.945	14.712	5.474	2.224
GR	11.670	5.663	12.488	5.012	42387.021	5110.985	41171.761	4831.495	**12.883**	**5.073**	4.804	1.944
WLOA	58.719	34.635	25.906	17.002	92733.105	28242.033	137300.092	34067.513	32.827	12.230	3.215	1.261
WL	58.719	34.635	25.905	17.003	109418.159	32350.523	112515.690	25035.268	26.313	10.933	2.227	0.837
2-WL‡	10.500	4.630	8.495	5.634	40412.745	5351.789	21910.109	2982.532	29.560	11.878	5.001	1.799
3-WL‡	**4.896**	**2.536**	**4.567**	**2.745**	89532.736	21918.757	91445.323	17703.656	43.908	18.509	10.925	5.320
Ridge, RBF, NIE												
WLOA	58.719	34.635	25.906	17.002	31409.659	6644.798	19456.664	3892.678	24.429	10.354	3.163	1.189
WL	58.719	34.635	25.905	17.003	48568.177	17533.158	71434.770	20472.124	23.155	9.302	2.026	0.805
2-WL‡	10.500	4.630	8.495	5.634	15241.302	3289.949	30093.401	6593.717	33.838	13.947	6.619	2.807
3-WL‡	**4.896**	**2.536**	**4.567**	**2.745**	**757.736**	**148.417**	**833.037**	**75.286**	43.918	18.491	OOM	OOM

Moreover, NIE attains state-of-the-art performance on homogeneous data, with a relative gain of 72.1% compared with the best neural networks. As for the remaining two heterogeneous datasets, neighborhood information is still not comparable to the GR kernel in *ENZYMES*. This observation is aligned with the performance of CompGCN (Vashishth et al., 2020), where such the node-edge composition may hurt the structure presentation. RGIN (Liu et al., 2020) significantly outperforms graph kernels, indicating the future direction of advanced subset representations. These significant findings serve as a foundation for further research and advancements in the field of graph kernels, as well as other representation learning methods like graph neural networks.

6 Conclusion

We are the first to concentrate on the representation of patterns and subgraphs by utilizing a variety of graph kernels to tackle the challenge of subgraph isomorphism counting. While most graph kernels are designed for substructures, their application in approximating subgraph isomorphism counting is not straightforward. Instead, we propose constructing the Gram matrix to leverage implicit correlations. Experimental results demonstrate the effectiveness of graph kernels and kernel tricks. Additionally, neighborhood information extraction (NIE) could relieve overfitting by additional pair-wise histograms and obtain significant improvement in challenging datasets.

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