
A Structural Smoothing Framework For Robust Graph-Comparison

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Abstract

In this paper, we propose a general smoothing framework for graph kernels by taking *structural similarity* into account, and apply it to derive smoothed variants of popular graph kernels. Our framework is inspired by state-of-the-art smoothing techniques used in natural language processing (NLP). However, unlike NLP applications which primarily deal with strings, we show how one can apply smoothing to a richer class of inter-dependent sub-structures that naturally arise in graphs. Moreover, we discuss extensions of the Pitman-Yor process that can be adapted to smooth structured objects thereby leading to novel graph kernels. Our kernels are able to tackle the diagonal dominance problem, while respecting the structural similarity between sub-structures, especially under the presence of edge or label noise. Experimental evaluation shows that not only our kernels outperform the unsmoothed variants, but also achieve statistically significant improvements in classification accuracy over several other graph kernels that have been recently proposed in literature. Our kernels are competitive in terms of runtime, and offer a viable option for practitioners.

1 Introduction

In many applications we are interested in computing similarities between structured objects such as graphs. For instance, one might aim to classify chemical compounds by predicting whether a compound is active in an anti-cancer screen or not. A kernel function which corresponds to a dot product in a reproducing kernel Hilbert space offers a flexible way to solve this problem [18]. R-convolution [10] is a framework for computing kernels between discrete objects where the key idea is to recursively decompose structured objects into sub-structures. Let $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ denote a dot product in a reproducing kernel Hilbert space, \mathcal{G} represent a graph and $\phi(\mathcal{G})$ denote a vector of sub-structure frequencies. The kernel between two graphs \mathcal{G} and \mathcal{G}' is computed by $k(\mathcal{G}, \mathcal{G}') = \langle \phi(\mathcal{G}), \phi(\mathcal{G}') \rangle_{\mathcal{H}}$. Many existing graph kernels can be viewed as instance of R-convolution. For instance, the graphlet kernel [21] decomposes a graph into graphlets, Weisfeiler-Lehman Subtree kernel (referred as Weisfeiler-Lehman for the rest of the paper) [22] decomposes a graph into subtrees, and the shortest-path kernel [1] decomposes a graph into shortest-paths. However, R-convolution based graph kernels suffer from a few drawbacks. First, the size of the feature space often grows exponentially. As size of the space grows, the probability that two graphs will contain similar sub-structures becomes very small. Therefore, a graph becomes similar to itself but not to any other graph in the training data. This is well known as the *diagonal dominance problem*, and the resulting kernel matrix is close to the identity matrix. In other words, the graphs are orthogonal to each other in the feature space. Second, lower order sub-structures tend to be more numerous while a vast majority of the sub-structures occur very rarely. In other words, a few sub-structures dominate the distribution which exhibits a strong power-law behavior and results in underestimation of the true distribution.

Third, the sub-structures used to define a graph kernel are often related to each other. However, an R-convolution kernel only respects exact matchings. This problem is particularly important when noise is present in the data since considering partial similarity between sub-structures might alleviate the noise problem.

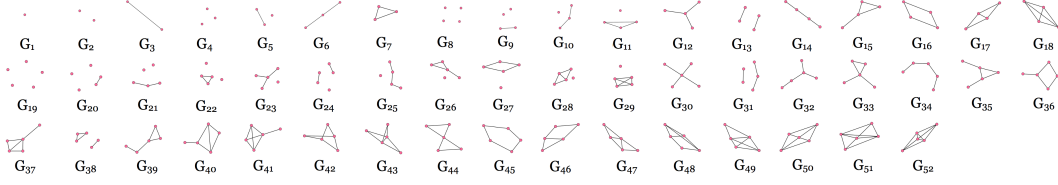


Figure 1: Graphlets of size $k \leq 5$.

Our solution: In this paper, we propose to tackle the above problems by using a general framework to *smooth* graph kernels that are defined using a frequency vector of decomposed structures. We use *structure* information by encoding relationships between lower order and higher order sub-structures in order to derive our method. Consequently, our smoothing algorithm not only respects the dependency between sub-structures but also tackles the diagonal dominance problem by distributing the probability mass across features. Moreover, we discuss extensions of the Pitman-Yor process that can be adapted to smooth subgraph distributions. In our experiments, the smoothed graph kernels outperform their base variants, especially in the presence of noise in edges or labels.

2 Graph kernels

Existing graphs kernels based on R-convolution can be categorized into three major families: graph kernels based on limited-sized subgraphs [e.g. 21], graph kernels based on subtree patterns [e.g. 17, 20], and graph kernels based on walks [e.g. 26] or paths [e.g. 1].

Graph kernels based on subgraphs: A *graphlet* G [16] is non-isomorphic sub-graph of size- k , (see Figure 1). Given two graphs \mathcal{G} and \mathcal{G}' , the kernel [21] is defined as $\mathcal{K}_{GK}(\mathcal{G}, \mathcal{G}') = \langle \mathbf{f}^{\mathcal{G}}, \mathbf{f}^{\mathcal{G}'} \rangle$ where $\mathbf{f}^{\mathcal{G}}$ and $\mathbf{f}^{\mathcal{G}'}$ are vectors of normalized counts of graphlets, that is, the i -th component of $\mathbf{f}^{\mathcal{G}}$ (resp. $\mathbf{f}^{\mathcal{G}'}$) denotes the frequency of graphlet G_i occurring as a sub-graph of \mathcal{G} (resp. \mathcal{G}').

Graph kernels based on subtree patterns: Weisfeiler-Lehman [20] is a popular instance of graph kernels that decompose a graph into its subtree patterns. This kernel simply iterates over each vertex in a graph, and compresses the label of the vertex and labels of its neighbors into a multiset label. The vertex is then relabeled with the compressed label to be used for the next iteration. Algorithm concludes after running for h iterations, and the compressed labels are used for constructing a frequency vector for each graph. Formally, given \mathcal{G} and \mathcal{G}' , this kernel is defined as $\mathcal{K}_{WL}(\mathcal{G}, \mathcal{G}') = \langle \mathbf{l}^{\mathcal{G}}, \mathbf{l}^{\mathcal{G}'} \rangle$ where $\mathbf{l}^{\mathcal{G}}$ contains the frequency of each compressed label occurring in h iterations.

Graph kernels based on walks or paths: Shortest-path graph kernel [1] is a popular instance of this family. This kernel simply compares the sorted endpoints and the length of shortest-paths that are common between two graphs. Formally, let $\mathbb{P}_{\mathcal{G}}$ represent the set of all shortest-paths in graph \mathcal{G} , and $p_i \in \mathbb{P}_{\mathcal{G}}$ denote a triplet (l_s, l_e, n_k) where n_k is the length of the path and l_s and l_e are the labels of the starting and ending vertices, respectively. The kernel between graphs \mathcal{G} and \mathcal{G}' is defined as $\mathcal{K}_{SP}(\mathcal{G}, \mathcal{G}') = \langle \mathbf{p}^{\mathcal{G}}, \mathbf{p}^{\mathcal{G}'} \rangle$ where i -th component of $\mathbf{p}^{\mathcal{G}}$ contains the frequency of i -th triplet occurring in graph \mathcal{G} (resp. $\mathbf{p}^{\mathcal{G}'}$).

3 Smoothing multinomial distributions

In this section, we briefly review smoothing techniques for multinomial distributions. Let e_1, e_2, \dots, e_m represent a sequence of n discrete events drawn from a ground set $\mathcal{A} = \{1, 2, \dots, V\}$.

4.2 Designing the DAG

In order to construct a DAG for smoothing structured objects, we first construct a vocabulary V that denotes the set of all unique sub-structures that are going to be *smoothed*. Each item in the vocabulary V represents a node in the DAG. V can be generated statically or dynamically based on the type of sub-structure the graph kernel exploits. For instance, it requires a one-time $O(2^k)$ effort to generate the vocabulary of size $\leq k$ graphlets for graphlet kernel. However, one needs to build the vocabulary dynamically in Weisfeiler-Lehman and Shortest-Path kernels since the sub-structures depend on the node labels obtained from the datasets. After constructing the vocabulary V , parent/child relationship between sub-structures needs to be obtained. Given a sub-structure s of size k , we apply a *transformation* to find all possible sub-structures of size $k - 1$ that s can be reduced into. Each sub-structure s' that is obtained by this transformation is assigned as a *parent* of s . After obtaining the parent/child relationship between sub-structures, the DAG is constructed by drawing a directed edge from each parent to its children nodes. Since all descendants of a given sub-structure at depth $k - 1$ are at depth k , this results in a topological ordering of the vertices, and hence the resulting graph is indeed a DAG. Next, we discuss specific details of constructing the DAG for different graph kernels.

Graphlet Kernel: We construct the vocabulary V for graphlet kernel by enumerating all canonical graphlets of size up to k^2 . Each canonically-labeled graphlet is a node in the DAG. We then apply a transformation to infer the parent/child relationship between graphlets as follows: we place a directed edge from graphlet G to G' if, and only if, G can be obtained from G' by deleting a node. In other words, all edges from a graphlet G of size $k - 1$ point to a graphlet G' of size k . In order to assign weights to the edges, given a graphlet pair G and G' , we count the number of times G can be obtained from G' by deleting a node (call this number $n_{GG'}$). Recall that G is of size $k - 1$ and G' is of size k , and therefore $n_{GG'}$ can at most be k . Let \mathcal{C}_G denote the set of children of node G in the DAG, and $n_G := \sum_{G' \in \mathcal{C}_G} n_{GG'}$. Then we define the weight $w_{GG'}$ of the edge connecting G and G' as $n_{GG'}/n_G$. The idea here is that the weight encodes the proportion of different ways of extending G which results in the graphlet G' . For instance, let us consider G_{15} and its parents G_5, G_6, G_7 (see Figure 2 for the DAG of graphlets with size $k \leq 5$). Even if graphlet G_{15} is not observed in the training data, it still gets a probability mass proportional to the edge weight from its parents in order to overcome the sparsity problem of unseen data.

Weisfeiler-Lehman Kernel: The Weisfeiler-Lehman kernel performs an *exact matching* between the compressed multiset labels. For instance, given two labels ABCDE and ABCDF, it simply assigns zero value for their similarity even though two labels have a partial similarity. In order to smooth Weisfeiler-Lehman kernel, we first run the original algorithm and obtain the multiset representation of each graph in the dataset. We then apply a transformation to infer the parent/child relationship between compressed labels as follows: in each iteration of Weisfeiler-Lehman algorithm, for each multiset label of size k in the vocabulary, we generate its *power set* by computing all subsets of size $k - 1$ while keeping the root node fixed. For instance, the parents of a multiset label ABCDE are {ABCD, ABCE, ABDE, ACDE}. Then, we simply construct the DAG by drawing a directed edge from parent labels to children. Notice that considering only the set of labels generated from the Weisfeiler-Lehman kernel is not sufficient enough for constructing a valid DAG. For instance, it might be the case that none of the possible parents of a given label exists in the vocabulary simply due to the sparsity problem (e.g. out of all possible parents of ABCDE, we might only observe ABCE in the training data). Thus, restricting ourselves to the original vocabulary leaves such labels orphaned in the DAG. Therefore, we consider so-called *pseudo parents* as a part of the vocabulary when constructing the DAG. Since the sub-structures in this kernel is data-dependent, we use a uniform weight between a parent and its children.

Shortest-Path Kernel: Similar to other graph kernels discussed above, shortest-path graph kernel does not take partial similarities into account. For instance, given two shortest-paths ABCDE and ABCDF (compressed as AE5 and AF5, respectively), it assigns zero for their similarity since their sink labels are different. However, one can notice that the sub-structures of shortest-path kernels exhibit a strong dependency relationship. For instance, given a shortest-path $p_{ij} = \{ABCDE\}$ of size k , one can derive the following shortest-paths: {ABCD, ABC, AB} of size $< k$ as a result

²We used Nauty [12] to obtain canonically-labeled isomorphic representations of graphlets.

of the *optimal sub-structure* property, that is, one can show that all sub-paths of a shortest-path are also shortest-paths with the same source node [6]. In order to smooth shortest-path kernel, we first build the vocabulary by computing all shortest-paths for each graph. Let p_{ij} be a shortest-path of size k and $p_{ij'}$ be a shortest-path of size $k - 1$ that is obtained by removing the sink node of p_{ij} . Let l_{ij} be the compressed form of p_{ij} that represents the sorted labels of its endpoints i and j concatenated to its length (resp. $l_{ij'}$). Then, in order to build the DAG, we draw a directed edge from $l_{ij'}$ of depth $k - 1$ to l_{ij} of depth k if and only if $p_{ij'}$ is a sub-path of p_{ij} . In other words, all ascendants of l_{ij} consist of the compressed labels obtained from sub-paths of p_{ij} of size $< k$. Similar to Weisfeiler-Lehman kernel, we assign a uniform weight between parents and children.

5 Pitman-Yor Smoothing

Pitman-Yor processes are known to produce power-law distributions [8]. [24] proposed a novel interpretation of interpolated Kneser-Ney as approximate inference in a hierarchical Bayesian model consisting of Pitman-Yor processes [15]. By following a similar spirit, we extend our model to adapt Pitman-Yor process as an alternate smoothing framework for those cases where the *feature space is finite*. We will only give a very high level overview of a Pitman-Yor process and refer the reader to the excellent papers by [24] and [8] for more details. A Pitman-Yor process P on a ground set \mathcal{G}_{k+1} of size- $(k+1)$ graphlets is defined via $P_{k+1} \sim PY(d_{k+1}, \theta_{k+1}, P_k)$ where d_{k+1} is a discount parameter, $0 \leq d_{k+1} < 1$, $\theta > -d_{k+1}$ is a strength parameter, and P_k is a base distribution. The most intuitive way to understand draws from the Pitman-Yor process is via the Chinese restaurant process (also see Figure 3).

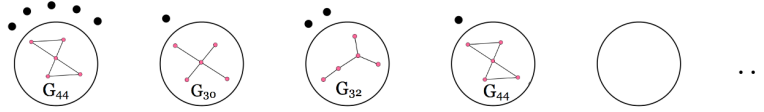


Figure 3: An illustration of table assignment, adapted from [9]. In this example, labels at the tables are given by $(l_1, \dots, l_4) = (G_{44}, G_{30}, G_{32}, G_{44})$. Black dots indicate the number of occurrences of each label in 10 draws from the Pitman-Yor process.

Algorithm 1 Insert a Customer

Input: $d_{k+1}, \theta_{k+1}, P_k$
 $t \leftarrow 0$ // Occupied tables
 $c \leftarrow ()$ // Counts of customers
 $l \leftarrow ()$ // Labels of tables
if $t = 0$ **then**
 $t \leftarrow 1$
 append 1 to c
 draw graphlet $g_i \sim P_k$ // Insert customer in parent
 draw $g_j \sim w_{ij}$
 append g_j to l
 return g_j
else
 with probability $\propto \max(0, c_j - d)$
 $c_j \leftarrow c_j + 1$
 return l_j
 with probability proportional to $\theta + dt$
 $t \leftarrow t + 1$
 append 1 to c
 draw graphlet $g_i \sim P_k$ // Insert customer in parent
 draw $g_j \sim w_{ij}$
 append g_j to l
 return g_j
end if

Algorithm 2 Delete a Customer

Input: d, θ, P_0, C, L, t
with probability $\propto c_l$
 $c_l \leftarrow c_l - 1$
 $g_j \leftarrow l_j$
if $c_l = 0$ **then**
 $P_k \propto 1/w_{ij}$
 delete c_l from c
 delete l_j from l
 $t \leftarrow t - 1$
end if
return g

Consider a restaurant with an infinite number of tables. Customers enter the restaurant one by one. The first customer sits at the first table, and is seated at the first table. Since this table is occupied for the first time, a graphlet is assigned to it by drawing a sample from the base distribution. The label of the first table is the first graphlet drawn from the Pitman-Yor process. Subsequent customers when they enter the restaurant decide to sit at an already occupied table with probability proportional to $c_i - d_{k+1}$, where c_i represents the number of customers already sitting at table i . If they sit at an already occupied table, then the label of that table denotes the next graphlet drawn from the Pitman-Yor process. On the other hand, with probability $\theta_{k+1} + d_{k+1}t$, where t is the current number of occupied tables, a new customer might decide to occupy a new table. In this case, the base distribution is invoked to label this table with a graphlet. Intuitively the reason this process generates power-law behavior is because popular graphlets which are served on tables with a large number of customers have a higher probability of attracting new customers and hence being generated again. In a hierarchical Pitman-Yor process (HYPY), the base distribution P_k is recursively defined via a Pitman-Yor process $P_k \sim PY(d_k, \theta_k, P_{k-1})$. In order to label a table, we need a draw from P_k , which is obtained by inserting a customer into the corresponding restaurant. However, adopting the traditional HYPY is not straightforward in our case since the *size* of the context differs between levels of hierarchy, that is, a *child* restaurant in the hierarchy can have more than one *parent* restaurant to request a label from. In other words, P_{k+1} is defined over \mathcal{G}_{k+1} of size n_{k+1} while P_k is defined over \mathcal{G}_k of size $n_k \leq n_{k+1}$. Therefore, one needs a *transformation function* to transform base distributions of different sizes. We incorporate edge weights between parent and child restaurants by using the same weighting scheme in Section 4.2. This changes the Chinese Restaurant process as follows: When we need to label a table, we will first draw a size- k graphlet $g_i \sim P_k$ by inserting a customer into the corresponding restaurant. Given g_i , we will draw a size- $(k+1)$ graphlet g_j proportional to w_{ij} , where w_{ij} is obtained from the DAG. Deletion of a customer is handled similarly.

6 Related work

A survey of most popular graph kernel methods is already given in previous sections. Several methods proposed in smoothing structured objects [4], [19]. Our framework is similar to dependency tree kernels [4] since both methods are using the notion of smoothing for structured objects. However, our method is interested in the problem of smoothing the count of structured objects while the smoothing itself is achieved by using a DAG where the DAG is discarded once the counts are smoothed. Another related work to ours is propagation kernels [13] that defines graph features as counts of similar node-label distributions on the respective graphs by using Locality Sensitive Hashing (LSH). Our framework not only considers node label distributions, but also explicitly incorporates structural similarity via the DAG. Another similar work to ours is recently proposed framework by [28] which learns the co-occurrence relationships between sub-structures by using neural language models. However, their framework do not respect the structural similarity between sub-structures, which is an important property to consider especially in the presence of noise in edges or labels.

Table 1: Comparison of classification accuracy (\pm standard deviation) of Shortest-path (SP), Weisfeiler-Lehman (WL), Graphlet (GK) kernels with their smoothed variants, SMTH SP, SMTH WL, SMTH GK, respectively, along with PYP Smoothed Graphlet (PYP GK) kernel. Ramon & Gärtner (RAM & GÄR), p -random walk (p -RANDWALK) and Random Walk (RANDWALK) kernels are included for comparison where $> 72\text{H}$ indicates the computation did not finish in 72 hours.

METHOD/DATASET	MUTAG	PTC	ENZYMES	PROTEINS	NCI1	NCI109
SP	85.22 \pm 2.43	58.24 \pm 2.44	40.10 \pm 1.50	75.07 \pm 0.54	73.00 \pm 0.24	73.00 \pm 0.21
SMTH SP	87.94 \pm 2.58	60.82 \pm 1.84	42.27 \pm 1.07	75.85 \pm 0.28	73.26 \pm 0.24	73.00 \pm 0.31
WL	82.22 \pm 1.87	60.41 \pm 1.93	53.88 \pm 0.95	74.49 \pm 0.49	84.13 \pm 0.22	83.83 \pm 0.31
SMTH WL	87.44 \pm 1.95	60.47 \pm 2.39	55.30 \pm 0.65	75.53 \pm 0.50	84.66 \pm 0.18	84.72 \pm 0.21
GK	81.33 \pm 1.02	55.56 \pm 1.46	27.32 \pm 0.96	69.69 \pm 0.46	62.46 \pm 0.19	62.33 \pm 0.14
SMTH GK	83.17 \pm 0.64	58.44 \pm 1.00	30.90 \pm 1.51	69.83 \pm 0.46	62.48 \pm 0.15	62.48 \pm 0.11
PYP GK	83.11 \pm 1.23	57.44 \pm 1.44	29.63 \pm 1.30	70.00 \pm 0.80	62.50 \pm 0.20	62.68 \pm 0.18
RAM & GÄR	84.88 \pm 1.86	58.47 \pm 0.90	16.96 \pm 1.46	70.73 \pm 0.35	56.61 \pm 0.53	54.62 \pm 0.23
P-RANDWALK	80.05 \pm 1.64	59.38 \pm 1.66	30.01 \pm 1.00	71.16 \pm 0.35	$> 72\text{H}$	$> 72\text{H}$
RANDWALK	83.72 \pm 1.50	57.85 \pm 1.30	24.16 \pm 1.64	74.22 \pm 0.42	$> 72\text{H}$	$> 72\text{H}$

7 Experiments

The aim of our experiments is threefold. First, we want to show that smoothing improves the classification accuracy of various graph kernels. Second, we want to show that the smoothed kernels are comparable to or outperform state-of-the-art graph kernels in terms of classification accuracy, while remaining competitive in terms of computational requirements. Third, we want to show that our methods significantly outperforms base kernels when edge or label noise is presence. In the main body of the paper we primarily focus on classification accuracy, and relegate runtime comparisons to Appendix ??.

Datasets We experimented with the following standard benchmark datasets used in graph kernels: MUTAG, PTC, ENZYMES, PROTEINS, NCI1 and NCI109. MUTAG is a dataset of 188 mutagenic aromatic and heteroaromatic nitro compounds [5] with 7 discrete labels. PTC [25] is a dataset of 344 chemical compounds has 19 discrete labels. NCI1 and NCI109 [27] are two balanced datasets of chemical compounds having size 4110 and 4127 with 37 and 38 labels, respectively. ENZYMES is a dataset of 600 protein tertiary structures obtained from [2], and has 3 discrete labels. PROTEINS is a dataset of 1113 graphs obtained from [2] where nodes are secondary structure elements (SSEs) and there is an edge between two nodes if they are neighbors in the amino acid sequence or in 3D space, having 3 discrete labels. See Appendix ?? for more information on the datasets.

Experimental setup We compare our framework against representative instances of major families of graph kernels in the literature. Other than base kernels of our framework; the Weisfeiler-Lehman kernel [21], the graphlet kernel [21], and the shortest-path kernel [1], we also compare our smoothed kernels with the random walk kernel [7], the subtree kernel [17], and p -step random walk kernel [23]. The Random Walk, p -step Random Walk and Ramon-Gärtner kernels are written in Matlab and were obtained from the authors of [21]. All other kernels were coded in Python³. We used a parallel implementation for smoothing the counts of Weisfeiler-Lehman kernel for efficiency purposes. In order to ensure a fair comparison, all experiments are performed on the same hardware. All kernels are normalized to have a unit length in the feature space. Moreover, we use 10-fold cross validation with a binary C -Support Vector Machine (SVM) to test classification performance. The C value for each fold is independently tuned using training data from that fold. In order to exclude random effects of the fold assignments, this experiment is repeated 10 times and average prediction accuracy of 10 experiments with their standard deviations are reported. See Appendix ?? for a detailed discussion of parameter selection procedure for each algorithm and the parameters used in our experiments.

³Implementations of original and smoothed versions of the kernels are publicly available at <http://web.ics.purdue.edu/~ypinar/nips>.

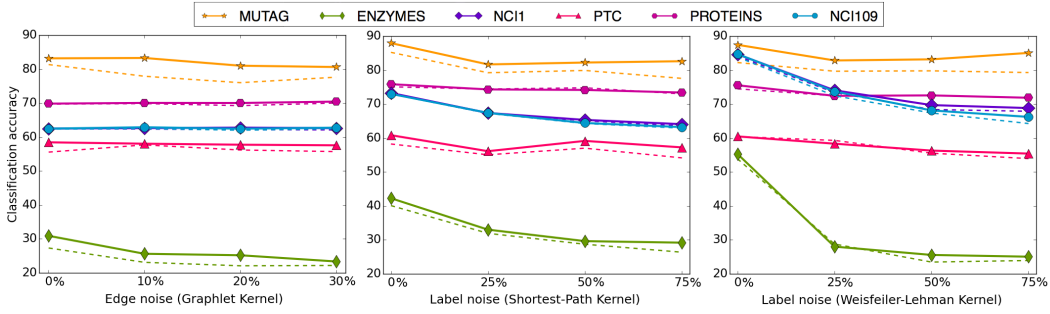


Figure 4: Classification accuracy vs. noise for base graph kernels (dashed lines) and their smoothed variants (non-dashed lines).

7.1 Results

In our first experiment, we compare the graphlet kernel, the Weisfeiler-Lehman kernel, and the shortest-path kernel with their smoothed variants. The results are in Table 1 where smoothed variants that are statistically significant over the base kernels are shown in bold as measured by a t -test with a p value of ≤ 0.05 . As can be seen on *every dataset*, smoothing improves the classification accuracy of *every base kernel*.

In our second experiment, we picked the best smoothed kernel, in terms of classification accuracy, for each of our datasets from Table 1, and compared their performance with the state-of-the-art graph kernels (see Table 1). As can be seen, the smoothed kernels outperform other methods on all datasets, and the results are statistically significant on every dataset except PTC.

In our third experiment, we compared Pitman-Yor smoothed graphlet kernels to base graphlet kernel. As can be seen from Table 1, Pitman-Yor smoothed graphlet kernels are able to improve the performance of all datasets while achieving statistically significant improvements over a majority of them. However, it can also be seen that Pitman-Yor smoothed graphlet kernels are outperformed by Smoothed graph kernels introduced in Section 3.

Finally, as our fourth experiment, we test the performance of graph kernels when *edge* and *label* noise is present where we randomly removed and added $\{10\%, 20\%, 30\%\}$ of the edges in each graph for edge-noise and randomly flipped $\{25\%, 50\%, 75\%\}$ of the node labels in each graph for label-noise by respecting the label-distribution. Figure 4 shows the performance of smoothed graph kernels under noise. As can be seen from the figure, smoothed graph kernels are able to significantly outperform their base variants.

8 Conclusion and Future Work

We presented a novel framework for smoothing graph kernels inspired by smoothing techniques from natural language processing and applied our method to state-of-the-art graph kernels. Our framework is rather general, and lends itself to many extensions. For instance, by defining domain-specific parent-child relationships, one can construct different DAGs with different weighting schemes for smoothing. Another interesting extension of our smoothing framework would be to apply it to graphs with continuous labels. While we restricted ourselves to graph kernels in this paper, our framework is applicable to any R-convolution kernel that uses a frequency-vector based representation.

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