FAST GRAPH KERNEL WITH OPTICAL RANDOM FEATURES

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ABSTRACT

The graphlet kernel is a classical method in graph classification. It however suffers from a high computation cost due to the isomorphism test it includes. As a generic proxy, and in general at the cost of losing some information, this test can be efficiently replaced by a user-defined mapping that computes various graph characteristics. In this paper, we propose to leverage *kernel random features* within the graphlet framework, and establish a theoretical link with a mean kernel metric. If, at first glance, this method does not necessarily allow to reduce the computational complexity of the graphlet kernel *why do you say that? Isomorphism test is in exponential time; even without the OPU, the proposition of this paper is polynomial, so infinitely faster, no?*, we then incorporate *optical* random features that can compute such random features in *constant time*. Experiments show that the resulting algorithm is orders of magnitude faster that the graphlet kernel for the same, or better, accuracy.

Index Terms— Optical random features, Graph kernels

1. INTRODUCTION

In mathematics and data science, graphs are used to model a set of objects (the *nodes*) and their interactions (the *edges*). Given a set of pre-labeled graphs $(\mathcal{X} = \{\mathcal{G}_1, \ldots, \mathcal{G}_n\}, \mathcal{Y} = \{y_1, \ldots, y_n\})$, where each graph $\mathcal{G}_i$ belongs to the class with label y_i, graph classification consists in designing an algorithm that outputs the class label of a new graph. For instance, proteins can be modeled as graphs: amino acids are nodes and the chemical links between them are edges. They can be classified to enzymes and non-enzymes [1]. In social networks analysis, post threads can be modeled with graphs whose nodes are users and edges are replies to others' comment [2]. One task is then to discriminate between discussion-based and question/answer-based threads [3]. In addition to the graph structure, nodes and edges may have extra features. While it has been shown that node features are important to obtain high classification performance [4], here we focus on the case where one has only access to the graph structure.

Structure-based graph classification has been tackled with many algorithms. Frequent subgraphs based algorithms [5] analyze the graph dataset $\mathcal{X}$ to catch the frequent and discriminative subgraphs and use them as features. Kernel-based algorithms [6] can be used by defining similarity functions (kernels) between graphs. An early and popular example is the *graphlet kernel*, which computes frequencies of subgraphs. It is however known to be quite costly to compute [7], in particular due to the presence of graph isomorphism tests. While possible in particular cases [**?**], accelerating the graphlet kernel for arbitrary datasets remains open. Finally, Graph neural networks (GNNs) [**?**, **?**] have recently become very popular in graph machine learning. They are however known to exhibit limited performance when node features are unavailable [**?**].

In kernel methods, random features are an efficient method to approximate certain kernel functions [**?**, 8]. Recently, it has been shown*ref?* that *optical computing* can be leveraged to compute such random features in *constant time* in *any dimension* – within the limitations of the current hardware, here referred to as Optical Processing Units (OPUs). The main goal of this paper is to provide a proof-of-concept answer to the following question: can OPU computations be used to reduce the computational complexity of a combinatorial problem like the graphlet kernel? Drawing on a connection with mean kernels and Maximum Mean Discrepancy (MMD) [**?**], we show, empirically and theoretically, that a fast and efficient graph classifier can indeed be obtained with OPU computations.

* the biblio file is not up to date apparently *

* + good job with the intro! *

2. BACKGROUND

First, we present the concepts necessary to define the graphlet kernel. We represent a graph of size v by the adjacency matrix $\mathbf{A} \in \{0,1\}^{v \times v}$, such that $a_{i,j} = 1$ if there is an edge between nodes $\{i, j\}$ and 0 otherwise. Two graphs are said to be isomorphic ($\mathcal{G} \cong \mathcal{G}'$) if we can permute the nodes' labels of one such that their adjacency matrices are equal [9].

2.1. Isomorphic graphlets

In this paper, we will, depending on the context, manipulate two different notions of k-graphlets (that is, small graphs of size k), with or without discriminating isomorphic graphlets. We denote by $\bar{\mathfrak{H}} = \{\bar{\mathcal{H}}_1, ..., \bar{\mathcal{H}}_{\bar{N}_k}\}$ with $\bar{N}_k = 2^{\frac{k(k-1)}{2}}$ the set of all size-k graphs, where isomorphic graphs are counted multiple times, and $\mathfrak{H} = \{\mathcal{H}_1, ..., \mathcal{H}_{N_k}\} \subset \bar{\mathfrak{H}}$ the set of all

non-isomorphic graphs of size k. Its size N_k has a (quite verbose) closed-from expression [**?**], but is still exponential in k. In the course of this paper, we shall manipulate mappings $\varphi(\mathcal{H})$ and probability distributions (histograms) over graphlets. When the mapping φ is *permutation-invariant*, then the underlying space is $\mathfrak{H}$, otherwise it is $\bar{\mathfrak{H}}$. Using one or the other obeys a tradeoff: $\bar{\mathfrak{H}}$ is larger, while $\mathfrak{H}$ may necessitate costly isomorphism tests. In any case, assuming each isomorphic copies has equal probability, a probability distribution over $\bar{\mathfrak{H}}$ can easily be transformed into one over $\mathfrak{H}$, and both versions contains the same amount of information.

2.2. The graphlet kernel

The traditional graphlet kernel is defined as follows. We define the matching function $\varphi_k^{match}(\mathcal{F}) = \left[1_{(\mathcal{F}\cong\mathcal{H}_i)}\right]_{i=1}^{N_k} \in \{0,1\}^{N_k}$, where 1_Ω is the indicator function and $\mathcal{F}$ is a graph of size k. In words, $\varphi_k^{match}(\mathcal{F})$ is a one-hot vector of dimension N_k identifying $\mathcal{F}$ up to isomorphism. Note that the cost of evaluating φ_k^{match} once is $O\left(N_k C_k^{\cong}\right)$, where $C_k^{\cong}$ is the cost of the isomorphism test between two graphs of size k, for which no polynomial algorithm is known [10].

Given a graph $\mathcal{G}$, let $\mathfrak{F}_\mathcal{G} = \{\mathcal{F}_1, \mathcal{F}_2, \dots, \}$ be the set of subgraphs induced by all size-k subsets of nodes[1]. The following representation vector is called the k-spectrum of $\mathcal{G}$:

$$\mathbf{f}_\mathcal{G} = \frac{1}{|\mathfrak{F}_\mathcal{G}|} \sum_{\mathcal{F}\in\mathfrak{F}_\mathcal{G}} \varphi_k^{match}(\mathcal{F}) \in \mathbb{R}^{N_k} \tag{1}$$

For two graphs $\mathcal{G}, \mathcal{G}'$, the graphlet kernel is defined as $\mathbf{f}_\mathcal{G}^T \mathbf{f}_{\mathcal{G}'}$. For a graph of size v, the computation cost of $\mathbf{f}_\mathcal{G}$ is $C_{gk} = \mathcal{O}\left(\binom{v}{k} N_k C_k^{\cong}\right)$. This cost is usually prohibitively expensive, since each three terms are exponential in k.

Subgraph sampling is generally used as a first step to accelerate (and sometimes modify) the graphlet kernel [7]. Given a graph $\mathcal{G}$, we denote by $S_k(\mathcal{G})$ a sampling process that yields a random subgraph of $\mathcal{G}$, of which there exists many variants [**?**]. Then, sampling s iid subgraphs $\{F_1, ..., F_s\}$ of size k from $S_k(\mathcal{G})$, we define the estimator:

$$\hat{\mathbf{f}}_{\mathcal{G},S_k} = \frac{1}{s} \sum_{F\in\hat{\mathfrak{F}}_\mathcal{G}} \varphi_k^{match}(F). \tag{2}$$

you sum over $\hat{\mathfrak{F}}_\mathcal{G}$ that you have not defined. Do we really need the notation $\hat{\mathfrak{F}}_\mathcal{G}$? Perhaps we can say we sum over $\{F_1, ..., F_s\}$ and its expectation $\mathbf{f}_{\mathcal{G},S} = \mathbb{E}_{F\sim S_k(\mathcal{G})}\, \varphi_k^{match}(F)$, which is a probability distribution over the set of graphlets $\mathfrak{H}$. We refer to these expectations as graphlet kernels. In fact, in all generality, any choice of sampling procedure S_k yields a different definition of graphlet kernel. For instance, if one considers uniform sampling (S^{unif}: independently samples k nodes of $\mathcal{G}$ without replacement), then one obtains the original graphlet kernel of Eq. (1): $\mathbf{f}_{\mathcal{G},S^{\text{unif}}} = \mathbf{f}_\mathcal{G}$. Other choices of sampling procedures are possible [11]. In this paper, we will also use the random walk (RW) sampler, which, unlike uniform sampling, tends to sample connected subgraphs, which may be more informative about the graph structure.

The computation cost per graph of the approximate graphlet kernel with graph sampling of Eq. (2) is $C_{gk+gs} = \mathcal{O}\left(sC_S N_k C_k^{\cong}\right)$, where C_S is the cost of sampling one subgraph. For a fixed error in estimating $\mathbf{f}_{\mathcal{G},S}$, the required number of samples s is generally proportional to N_k *rather needs to be prop to N_k, no?* [7], which unfortunately still yields an unaffordable algorithm.

[1] $|\mathfrak{F}_\mathcal{G}|$ depends on $\mathcal{G}$ and is usually much smaller than N_k. Extreme examples are the complete and the empty graphs, where $|\mathfrak{F}_\mathcal{G}| = 1$.

3. GRAPHLET KERNEL WITH OPTICAL MAPS

3.1. Proposed algorithm

Algorithm 1: GSA-φ generic algorithm

Input: labeled graph dataset $\mathcal{X} = (\mathcal{G}_i, y_i)_{i=1,\dots,n}$
Tools *Graphlet sampler S_k, a function φ, linear classifier (ex. SVM)*
Hyperparameters *k: graphlet size, s: number of graphlet samples per graph, m: number of random features*
Output: Trained model to classify graphs
Algorithm
Random initialization of the SVM weights
for $\mathcal{G}_i$ *in* $\mathcal{X}$ **do**
  $\mathbf{z}_i = \mathbf{0}$ (null vector of size m)
  for $j = 1 : s$ **do**
    $F_{i,j} \leftarrow S_k(\mathcal{G}_i)$
    $\mathbf{z}_i \leftarrow \mathbf{z}_i + \frac{1}{s}\varphi(F_{i,j})$
$\mathcal{D}_\varphi \leftarrow (\mathbf{z}_i, y_i)_{i=1,\dots,n}$
Train the linear classifier on the new vector-valued dataset $\mathcal{D}_\varphi$

In this paper, we propose to deal with the main remaining bottleneck of the graphlet kernel, that is, the function φ_k^{match}. We therefore define a framework where it is replaced with a user-defined map $\varphi : \bar{\mathfrak{H}} \to \mathbb{R}^m$. The resulting algorithm (Alg. 1) is referred to as *graphlet sampling and Averaging $GSA - \varphi$*, and its cost per graph for a specific φ is $C_{GSA-\varphi} = \mathcal{O}\left(sC_S C_\varphi\right)$, where C_φ is the cost of applying φ on one graphlet.

Note that choosing $\varphi = \varphi_k^{match}$ and S_k as the uniform sampler, GSA-φ_k^{match} turns out to be the graphlet kernel with graphlet sampling. We see next that choosing φ as *kernel random maps* is both fast and efficient.

3.2. Efficiency of kernel random features with $GSA - \varphi$

A kernel κ associated to a random features (RF) decomposition is a positive definite function of two inputs that can be decomposed as follows [12]:

$$\kappa(\mathbf{x}, \mathbf{x}') = \mathbb{E}_{\mathbf{w}\sim p}[\xi_{\mathbf{w}}(\mathbf{x})\xi_{\mathbf{w}}(\mathbf{x}')^*] \quad (3)$$

where p is a probability distribution, and ξ is a real (or complex) function parameterized by $\mathbf{w}$. To approximate such kernels, we can emperically average m realizations of $\xi_{\mathbf{w}}(\mathbf{x})\xi_{\mathbf{w}}(\mathbf{x}')$. To do that, we define RF maps:

$$\varphi(\mathbf{x}) = \frac{1}{\sqrt{m}}(\xi_{\mathbf{w}_j}(\mathbf{x}))_{j=1}^m \in \mathbb{C}^m \quad (4)$$

where m is called here the number of features and the frequencies $\mathbf{w}_j$ are drawn identically and independently (iid) from p. Then, $\kappa(\mathbf{x}, \mathbf{x}') \approx \varphi(\mathbf{x})^T\varphi(\mathbf{x}')$.

For each kernel as in (3) , and for any two graphs $\mathcal{G}, \mathcal{G}'$, we define the MMD (Maximum Mean Discrepancy) metric between the two corresponding distrubutions $\mathbf{f}_{\mathcal{G},S_k}, \mathbf{f}_{\mathcal{G}',S_k}$ by:

$$MMD^2(\mathbf{f}_{\mathcal{G},S_k}, \mathbf{f}_{\mathcal{G}',S_k}) = \mathbb{E}_{\mathbf{w}}\Big(\big|\mathbb{E}_{S_k(\mathcal{G})}\xi_{\mathbf{w}}(F) - \mathbb{E}_{S_k(\mathcal{G}')}\xi_{\mathbf{w}}(F')\big|^2\Big)$$

The main property of the MMD is that, for so-called *characteristic kernels*, it is a true metric on distributions, *i.e.* $MMD(\mathcal{P}, \mathcal{Q}) = 0 \Leftrightarrow \mathcal{P} = \mathcal{Q}$. In addition, most usual kernels, like the Gaussian kernel, are characteristic [13].

The next theorem shows the efficiency of using RF maps as in (4) with our algorithm. It states that the Euclidean distance between the representation vectors $\mathbf{z}_{\mathcal{G}}, \mathbf{z}_{\mathcal{G}'}$ converges to the MMD metric between their distributions $\mathbf{f}_{\mathcal{G},S_k}, \mathbf{f}_{\mathcal{G}',S_k}$.

Theorem 1. *Let $\mathcal{G}$ and $\mathcal{G}'$ be two graphs, $\mathfrak{F}_{\mathcal{G}} = \{F_i\}_{i=1}^s$ (resp. $\mathfrak{F}_{\mathcal{G}'} = \{F_i'\}_{i=1}^s$) be iid size-k graphlet samples drawn from $S_k(\mathcal{G})$ (resp. $S_k(\mathcal{G}')$). Assume a random feature map as in* (4)*. Assume that $|\xi_{\mathbf{w}}(F)| \leq 1$ for any $\mathbf{w}, F$. We have for all $\delta > 0$ and with probability at least $1 - \delta$:*

$$\Big| \|\varphi(\mathfrak{F}_{\mathcal{G}}) - \varphi(\mathfrak{F}_{\mathcal{G}'})\|^2 - MMD(\mathbf{f}_{\mathcal{G},S_k}, \mathbf{f}_{\mathcal{G}',S_k})^2 \Big| \leq \frac{4\sqrt{\log(6/\delta)}}{\sqrt{m}} + \frac{8\left(1 + \sqrt{2\log(3/\delta)}\right)}{\sqrt{s}}$$

Proof. see Appendix. □

3.3. Considered choices of φ_{RF}

Gaussian maps φ_{Gs} applied on the adjacency matrix: φ_{Gs} is the RF map of the Gaussian kernel [12]. We for each subgraph $\mathcal{F}$ take its vectorized adjacency matrix $\mathbf{a}_{\mathcal{F}} = flatten(\mathbf{A}_{\mathcal{F}})$ as input. Then:

$$\varphi_{Gs}(\mathcal{F}) = \frac{1}{\sqrt{m}}\left(\sqrt{2}\cos(\mathbf{w}_j^T\mathbf{a}_{\mathcal{F}} + b_j)\right)_{j=1}^m \in \mathbb{R}^m \quad (5)$$

Graphlet kernel		$O(\binom{v}{k}N_kC_k^{\cong})$
GSA-φ with:	φ_k^{match}	$O(C_s s N_k C_k^{\cong})$
	φ_{Gs}	$O(C_s s m k^2)$
	$\varphi_{Gs+Eigen}$	$O(C_s s(mk + k^3))$
	φ_{OPU}	$O(C_s s)$

Table 1. Per-graph complexities of GSA-φ.

where the frequencies $\mathbf{w}_j \in \mathbb{R}^{k^2}$ are drawn from a Gaussian distribution with the inverse variance of the original kernel.

Gaussian maps φ_{Gs+Eig} applied on the sorted eigenvalues of the adjacency matrix: instead of passing the vectorized adjacency matrix as input, we pass the vector of its sorted eigenvalues $\boldsymbol{\lambda} \in \mathbb{R}^k$. The motive proposing φ_{Gs+Eig} is that it respects the isomorphism test since: i/ $\lambda(\mathbf{A}) = \lambda(\mathbf{PAP^T})$ for any permutation matrix $\mathbf{P}$, ii/ $F \cong F' \Rightarrow \exists \mathbf{P}, \mathbf{A}_F = P\mathbf{A}_{F'}P^T$. Thus, $F \cong F' \Rightarrow \varphi_{Gs+Eig}(F) = \varphi_{Gs+Eig}(F')$. φ_{Gs+Eig} maps isomorphic subgraphs to the same point in $\mathbb{R}^m$.

Optical random feature maps φ_{OPU}: This corresponds to the fastest version of our algorithm. OPUs (Optical Processing Units) technology was developed to compute a specific random features mapping in *constant time* $\mathcal{O}(1)$ in both m and k using light scattering [14]. Having the random matrix $\mathbf{W}$, traditional random maps (ex. φ_{Gs}) need $\mathcal{O}(mk^2)$ cost to compute $\mathbf{Wx}$ as in (5). An OPU computes its associated map at the speed of light, this map is modeled as follows [14]:

$$\varphi_{OPU}(\mathbf{x}) = |\mathbf{Wx} + \mathbf{b}|^2;\ \mathbf{W} \in \mathbb{R}^{m\times d}, \mathbf{b} \in \mathbb{R}^m, \mathbf{x} \in \mathbb{R}^d$$

Where $\mathbf{b}$ is a random bias vector, d is the input space dimension, the amplitude function $|\cdot|$ is taken element wise, and $\mathbf{W}$ is a random *iid* complex matrix with Gaussian real and imaginary parts. The complexities of the different mappings φ examined in this work are summarized in Table 1.

4. EXPERIMENTS

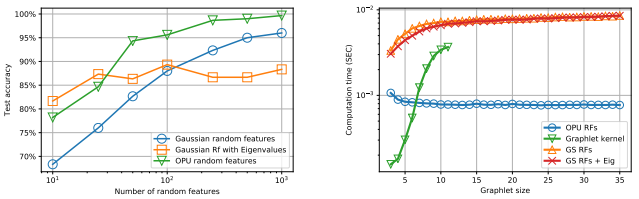
4.1. Setup

With respect to the performance and the computation cost, we compare different choices of map φ in $GSA - \varphi$. We benchmark the performance of $GSA - \varphi_{OPU}$ against GIN based graph convolutional network.

In all experiments except the last one, we use a synthetic dataset generated by a *Stochastic Block Model (SBM)* [15]. We generate 300 graphs, 240 for training and 60 for testing. Each graph has $v = 60$ nodes divided equally between six communities. Moreover, graphs are divided into two classes $\{0, 1\}$ based on the edges distribution considered. For each class we fix two values (p_{in}, p_{out}) which are the probabilities of generating an edge between any two nodes when they are in the same community and when they are in different ones, respectively. Besides, to prevent the classes

from being easily discriminated by the average degree, the pairs $(p_{in,i}, p_{out,i})_{i=0,1}$ are chosen such that all nodes have a fixed expected average degree equal to 10. Having one degree of freedom left, we fix $p_{in,1} = 0.3$, and we vary $r = (p_{in,1}/p_{in,0})$ the inter-class similarity parameter: the closer r is to 1, the more similar both classes are, and thus the harder it is to discriminate them.

On the other hand, D&D is a labeled dataset of size $n = 1178$ protein graphs [16]. Also, nodes have 7 features each, which are not used by our algorithms, *i.e.* we will try to classify the graphs just based on their structure. In what follows, unless otherwise indicated, we use uniform sampling and the adjacency matrix of subgraphs as input.



(a) RF maps (b) Computation cost

Fig. 1. Comparing different φ maps in $GSA - \varphi$. (a) test accuracy when using RF maps with $k = 6$ while varying m. (b) test accuracy of $GSA - \varphi_{OPU}$ and $GSA - \varphi_k^{match}$ fixing $k = 5$ while varying r. (c) Computation time as a function of k. If not specified: $r = 1.1$, $s = 2000$, $m = 5000$ and the Gaussian map variance $\sigma^2 = 0.01$.

4.2. Choice of feature map φ

Comparison of random features: Fig 1(a) shows that $GSA - \varphi_{OPU}$ applied on adjacency matrices gives better test accuracy with sufficiently large m than both $GSA - \varphi_{Gs}$ applied on adjacency matrices or $GSA - \varphi_{Gs+Eig}$ applied on its sorted eigenvalues. On the contrary, $GSA - \varphi_{Gs+Eig}$ performs best with a low number of random features, but increasing this number does not really improve the result and it is over-matched at high m. A possible justification is that the eigenvalues of the adjacency matrix lose information about the subgraphs, even though respecting the isomorphism means that we are working with a smaller histogram and less random features are required.

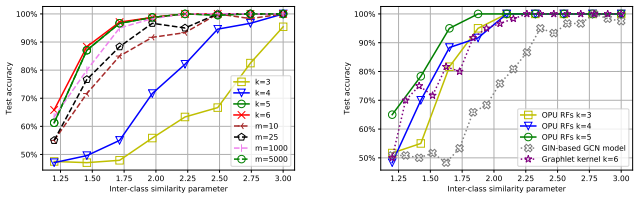
Comparing $GSA - \varphi_{OPU}$ to $GSA - \varphi_k^{match}$: from Fig 1(b) we observe that with the same limited number of samples s, $GSA - \varphi_{OPU}$ clearly outperforms the approximated graphlet kernel $GSA - \varphi_k^{match}$, so we conclude that $GSA - \varphi_{OPU}$ is more adapted in this case than the traditional graphlet kernel.

Computational time: Fig 1(c) shows the computation time of each of the previous methods with respect to the subgraphs size k. Other parameters are identically fixed for all methods. As expected, the execution time of the approximated graphlet kernel grows exponentially with k, and is polynomial for $GSA - \varphi_{Gs}$ and $GSA - \varphi_{Gs+Eig}$. On the contrary, it is almost constant for $GSA - \varphi_{OPU}$. We point out here that, with the current settings, there is a significant overhead between the point in time where we run our optimizer code on the OPUs server and the point when the OPU launches the computation. To be fair, this overhead time should be measured and subtracted from $GSA - \varphi_{OPU}$ computation time. As the technology comes into maturity, we can expect this additional time to be significantly reduced.

To summarize, $GSA - \varphi_{OPU}$ outperforms the traditional methods both in accuracy and computational cost.

4.3. Comparing $GSA - \varphi_{OPU}$ against GIN model

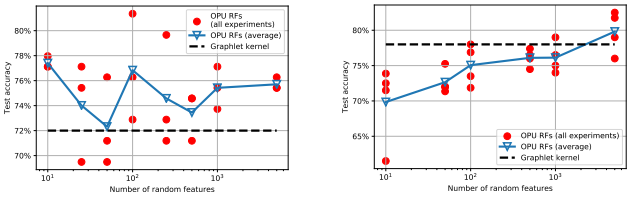
In Fig 2, we observe that for subgraphs sizes > 5, both RW and uniform sampling perform similarly well in $GSA - \varphi_{OPU}$, but RW sampling, as expected, provide more consistent results when the graphlet size k varies. Thus RW sampling is considered in this comparison. We see that $GSA - \varphi_{OPU}$ with RW performs better than the GIN model when the graphlet size is greater than 4. We note that we do not report the computational time for GIN, since it is highly dependent on high-speed graphical processing units (GPUs) to do the training process.



(a) φ_{OPU}& uniform sampling (b) φ_{OPU}& RW sampling

Fig. 2. Comparing test accuracies of $GSA - \varphi_{OPU}$ and GIN-based GCN network when varying the problem difficulty r. We used $GSA - \varphi_{OPU}$ with uniform sampling in (a) and with random walk sampling in (b). In both cases: $s = 2000$ and $m = 5000$. (c) The model consists of 5 GIN layers then 2 fully connected layers, the dimensions of hidden layers: 4.

In Fig 3, we have the test accuracy with varying value of m and fixed $s = 4000$, $k = 7$. For each value of m we conduct the experiment 5 times and take the average accuracy. Although we do not observe a clear, steady average improvement in accuracy when m grows, the results of the 5 corresponding experiments get more concentrated around the average value, giving a desirable reduced variance between experiments. On the other hand, accuracy results at low m show high variance between experiments, which might be accentuated by the fact that nodes features are ignored. However, using node features is without doubt necessary to reach state-of-the-art results, and it is an open question how to in-



(a) D&D (b) Reddit-Binary

Fig. 3. Bench-marking $GSA - \varphi$ against the graphlet kernel as a performance reference on real datasets with: s=4000,k=.

corporate that in our algorithm, but our goal here is mainly to test our algorithm on real data as a proof of concept.

5. CONCLUSION

We proposed a family of algorithms that combines graphlet sampling with efficient mappings. Then, we proposed to choose this mapping as kernel random maps, and showed a concentration of the random embedding around the MMD metric. Finally, while classical random features still require expensive matrix-vector multiplication, we used optical random features projections, which can be computed in $\mathcal{O}(1)$ to get the algorithm's fastest version. Our Experiments showed that it is significantly faster than traditional graphlet kernel and generally performs better while concentrating around the MMD metric. In our settings, it even outperformed a particular graph convolutional network on graph classification.

A major point left open to be analyzed is how to use our algorithm to classify graphs with node features. One promising possibility is to use our algorithm to generate features embeddings on the graph level, and then feed these embeddings with the nodes' features to a deep neural network. Doing this, we take advantage of the speed of both our algorithm and GPUs. On the theoretical side, the properties of the MMD metric could be further analyzed on particular models of graphs to get a concentration with higher certainty.

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Appendices

A. PROOF OF THEOREM 1

Proof. We decompose the proof in two steps.

Step 1: infinite s, finite m. First we define the random variables $x_j = |\mathbb{E}_{F\sim S_k(\mathcal{G})}\xi_{\mathbf{w}_j}(F) - \mathbb{E}_{F'\sim S_k(\mathcal{G}')}\xi_{\mathbf{w}_j}(F')|^2$, which are: i/independent, ii/have expectation $MMD(\mathcal{G},\mathcal{G}')^2$, /iii are bounded by the interval $[0,4]$ based on our assumption $|\xi_w| \leq 1$. Thus, as a straight result of applying Hoeffding's inequality with easy manipulation: with probability $1-\delta$

$$\left|\frac{1}{m}\sum_{j=1}^{m} x_j - MMD(\mathcal{G},\mathcal{G}')^2\right| \leq \frac{4\sqrt{\log(2/\delta)}}{\sqrt{m}} \tag{6}$$

Step 2: finite s and m. For any *fixed* set of random features $\{w_j\}_{1,\ldots,m}$ and based on our previous assumptions we have: i/ φ_{RF} is in a ball of radius $M = \frac{\sqrt{m}}{\sqrt{m}} = 1$, ii/ $\mathbb{E}_{F\sim S_k(\mathcal{G})}\,\varphi(F) = \mathbb{E}\left(\,\frac{1}{s}\sum_i \varphi(F_i)\,\right)$. Therefore, we can directly apply the vector version of Hoeffding's inequality on the vectors $\frac{1}{s}\sum_i \varphi(F_i)$ to get that with probability $1-\delta$:

$$\left\|\mathbb{E}_{F\sim S_k(\mathcal{G})}\varphi(F) - \frac{1}{s}\sum_i \varphi(F_i)\right\| \leq \frac{1+\sqrt{2\log\frac{1}{\delta}}}{\sqrt{s}} \tag{7}$$

Defining $J_{exp}(\mathcal{G},\mathcal{G}') = \|\mathbb{E}_{F\sim S_k(\mathcal{G})}\varphi(F) - \mathbb{E}_{F'\sim S_k(\mathcal{G}')}\varphi(F')\|$ and $J_{avg}(\mathcal{G},\mathcal{G}') = \|\frac{1}{s}\sum_i \varphi(F_i) - \frac{1}{s}\sum_i \varphi(F_i')\|$, then using triangular inequality followed by a union bound based on (7), we have the following with probability $1-2\delta$,

$$\left|J_{exp}(\mathcal{G},\mathcal{G}') - J_{avg}(\mathcal{G},\mathcal{G}')\right| \leq \frac{2}{\sqrt{s}}\left(1+\sqrt{2\log\frac{1}{\delta}}\right)$$

On the other hand, $J_{exp}(\mathcal{G},\mathcal{G}') + J_{avg}(\mathcal{G},\mathcal{G}') \leq 4$, so with same probability:

$$\left|J_{exp}(\mathcal{G},\mathcal{G}')^2 - J_{avg}(\mathcal{G},\mathcal{G}')^2\right| \leq \frac{8}{\sqrt{s}}\left(1+\sqrt{2\log\frac{1}{\delta}}\right) \tag{8}$$

Since it is valid for any fixed set of random features, it is also valid with *joint* probability on random features and samples, by the law of total probability.

Finally, combining (6), (8) with a union bound and a triangular inequality, we have with probability $1-3\delta$,

$$\left|\|\varphi(\mathfrak{F}_{\mathcal{G}}) - \varphi(\mathfrak{F}_{\mathcal{G}'})\|^2 - MMD(\mathcal{G},\mathcal{G}')^2\right| \leq \frac{4\sqrt{\log(2/\delta)}}{\sqrt{m}} + \frac{8}{\sqrt{s}}\left(1+\sqrt{2\log\frac{1}{\delta}}\right)$$

which concludes the proof by taking δ as $\delta/3$.

□