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graphkit-learn: A Python Library for Graph Kernels Based on Linear Patterns

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ABSTRACT

This paper presents `graphkit-learn`, the first Python library for efficient computation of graph kernels based on linear patterns, able to address various types of graphs. Graph kernels based on linear patterns are thoroughly implemented, each with specific computing methods, as well as two well-known graph kernels based on non-linear patterns for comparative analysis. Since computational complexity is an Achilles' heel of graph kernels, we provide several strategies to address this critical issue, including parallelization, the trie data structure, and the FCSP method that we extend to other kernels and edge comparison. All proposed strategies save orders of magnitudes of computing time and memory usage. Moreover, all the graph kernels can be simply computed with a single Python statement, thus are appealing to researchers and practitioners. For the convenience of use, an advanced model selection procedure is provided for both regression and classification problems. Experiments on synthesized datasets and 11 real-world benchmark datasets show the relevance of the proposed library.

1. Introduction

Graph kernels have become a powerful tool in bridging the gap between machine learning and graph representations. Graph kernels can be constructed by explicit feature maps or implicit ones using the kernel trick (Kriege et al., 2019). Many graph kernels have been proposed by manipulating measurements of different sub-structures of graphs (Ghosh et al., 2018; Gaüzère et al., 2015a). Of particular interest are graph kernels based on linear patterns, since they have acceptable accuracy on many benchmark datasets with competitive computational complexity compared to kernels based on non-linear patterns. Moreover, they have been serving as a baseline for designing new kernels. These kernels have been constructed using either walk patterns (*i.e.*, based on alternating sequences of vertices and edges) or path patterns (*i.e.*, walks without repeated vertices), including the common walk kernel (Gärtner et al., 2003), the marginalized kernel (Kashima et al., 2003), the generalized random walk kernel (Vishwanathan et al., 2010), the shortest path kernel (Borgwardt and Kriegel, 2005), the structural shortest path kernel (Ralaivola et al., 2005) and the path kernel up to length h (Suard et al., 2007).

Although several open-source libraries for graph kernels have been published, only parts of the aforementioned kernels have been implemented so far and only limited types of graphs were tackled. In this paper, we present the new open-source Python library `graphkit-learn`, implementing all the kernels based on linear patterns and a wide selection of graph datasets. Table 1 compares our library with other libraries that implement graph kernels based on linear patterns, showing the completeness of our library. For comparison, two graph kernels based on non-linear patterns are also implemented, namely the Weisfeiler-Lehman (WL) subtree kernel (Shervashidze et al., 2011; Morris et al., 2017) and the treelet kernel (Gaüzère et al., 2015b; Bougleux et al., 2012; Gaüzère et al., 2012). Additionally, we propose several computing methods and tricks to improve specific kernels, as well as auxiliary functions to preprocess datasets and perform model selection. The library is publicly available to the community on GitHub: <https://github.com/jajupmochi/graphkit-learn>, and can be installed by `pip install graphkit-learn`.

The remainder of this paper is organized as follows: Section 2 introduces the `graphkit-learn` library in detail. Section 3 presents three strategies applied in the library to reduce the computational complexity of graph kernels. Experiments and analyses are shown in Section 4. Finally, Section 5 concludes the paper.

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Table 1. Libraries available online including graph kernels based on linear patterns.

Libraries	Kernels implemented									Languages
	Common walk	Marginalized	Random walk Sylvester eq.	Random walk conj. grad.	Random walk fixed-point iter.	Random walk spectral decomp.	Shortest path (SP)	Structural SP	Path up to length h	
GraKeL ^a	✓	✗	✗	✗	✗	✗	✓	✗	✗	Python
pykernels ^b	✗	✗	✗	✓	✗	✗	✓	✗	✗	Python
ChemoKernel ^c	✗	✓	✗	✗	✗	✗	✗	✗	✓	C++
graphkernels ^d	✓	✗	✗	✗	✗	✗	✓	✗	✗	Python (C++ core)
graph-kernels ^e	✓	✗	✗	✗	✗	✗	✗	✗	✗	C++, R (C++ core)
graphkit-learn ^f (this paper)	✓	✓	✓	✓	✓	✓	✓	✓	✓	Python

a: <https://github.com/ysig/GraKeL>

b: <https://github.com/gmun/pykernels>

c: <https://github.com/bgauzere/ChemoKernel>

d: <https://github.com/BorgwardtLab/GraphKernels>

e: <https://github.com/BorgwardtLab/graph-kernels>

f: <https://github.com/jajupmochi/graphkit-learn>

2. The graphkit-learn Library

The graphkit-learn library is written in Python. Fig. 1 shows the overall architecture of the library in 3 main parts:

- Methods to load graph datasets from various formats and to process them before computing graph kernels, which are implemented respectively by the function `loadDataset` in the module `utils.graphfiles` and the function `get_dataset_attributes` in the module `utils.graphdataset`.
- Implementations of 9 graph kernels based on linear patterns and 2 on non-linear patterns in the module `kernels`, which are the major contributions of the library.
- Methods to perform model selection with cross-validation (*i.e.*, hyper-parameter tuning), which are implemented in the module `model_selection_precomputed`.

The remainder of this section describes these contents in detail.

2.1. Graph Data Processing

In graphkit-learn, the NetworkX package is applied to handle graphs (Hagberg et al., 2008), which supports rather comprehensive graph attributes, including symbolic and non-symbolic labels on vertices and edges, edge weights, directness, etc. A dataset in graphkit-learn is represented as a list of graphs, where each graph is represented by a `networkx.Graph` class if undirected or a `networkx.DiGraph` class if directed. Located in the `gklearn.utils` module, `graphfiles.loadDataset` loads raw data from several widely-used graph dataset formats and transforms the data into NetworkX graphs. The `graphdataset.get_dataset_attributes` extracts the properties of a dataset, such as its size, the average vertex number and edge number, the average vertex degree, whether the graphs are directed, labeled symbolically and non-symbolically on their vertices and edges, etc. These attributes are useful to graph kernels, because the kernels may utilize different computing methods according to them.

2.2. Implementations of Graph Kernels

The main contribution of graphkit-learn is the implementations of graph kernels, within the module `gklearn.kernels`. Our implementations provide the ability to address various types of graphs, including unlabeled graphs, vertex-labeled graphs, edge-labeled and fully-labeled graphs, directed and

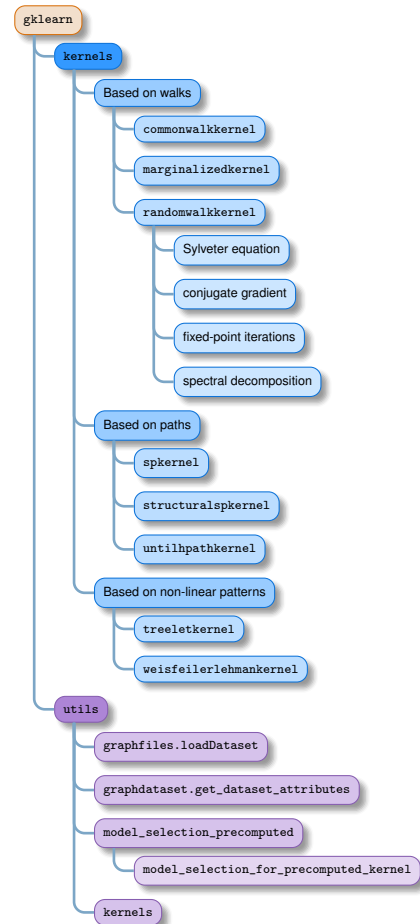


Fig. 1. The overall architecture of graphkit-learn library.

undirected graphs, and edge-weighted graphs. Only parts of these types have been tackled by other available libraries. Table 2 shows the types of graphs that each kernel can process.

Each kernel method takes a list of NetworkX graph objects as the input, and returns a Gram matrix whose entries are the evaluations of the kernel on pairs of graphs from the list. Other arguments can be chosen by the users to specify the computing methods and to serve as the tunable hyper-parameters of the kernel, according to the definition of the kernel. The computation is then carried out with a single Python statement. The specific implementation of each graph kernel is described next.

`commonwalkkernel` implements the common walk kernel. Two computing methods are provided based on exponential se-

Table 2. Comparison of graph kernels.

Kernels	Labeling				Directed	Edge weighted	Weighting	Implementations
	symbolic		non-symbolic					
	vertices	edges	vertices	edges				
Common walk	✓	✓	✗	✗	✓	✗	a priori	commonwalkkernel
Marginalized	✓	✓	✗	✗	✓	✗	✗	marginalizedkernel
Random walk: Sylvester equation	✗	✗	✗	✗	✓	✓	a priori	randomwalkkernel
Random walk: Conjugate gradient	✓	✓	✓	✓	✓	✓	a priori	randomwalkkernel
Random walk: Fixed-point iterations	✓	✓	✓	✓	✓	✓	a priori	randomwalkkernel
Random walk: Spectral decomposition	✗	✗	✗	✗	✓	✓	a priori	randomwalkkernel
Shortest path	✓	✗	✓	✗	✓	✓	✗	spkernel
Structural shortest path	✓	✓	✓	✓	✓	✗	✗	structuralspkernel
Path kernel up to length h	✓	✓	✗	✗	✓	✗	✓	untilhpathkernel
Treelet	✓	✓	✗	✗	✓	✗	✓	treeletkernel
Weisfeiler-Lehman (WL) subtree	✓	✗	✗	✗	✓	✗	✗	weisfeilerlehmankernel

“Weighting” indicates whether the substructures can be weighted in order to obtain a similarity measure adapted to a particular prediction task.

ries and geometric series as introduced by Gärtner et al. (2003). The direct product of labeled graphs is implemented for the convenience of computation.

`marginalizedkernel` computes the marginalized kernel with the recursion algorithm (Kashima et al., 2003). The users can set the argument `remove_totters=True` to remove tottering with the method introduced by Mahé et al. (2004).

The generalized random walk kernel is implemented by `randomwalkkernel`. Four possible computing methods are provided: Sylvester equation, conjugate gradient, fixed-point iterations, and spectral decomposition, as introduced by Vishwanathan et al. (2010). The argument `compute_method` allows to select one of the four methods. For conjugate gradient and fixed-point iterations, the labels of vertices at the two ends of an edge are added to both sides of the corresponding edge labels.

The shortest path kernel is computed by `spkernel`. The Floyd-Warshall’s algorithm (Floyd, 1962) is employed to transform the original graphs into shortest-paths graphs (Borgwardt and Kriegel, 2005). `structuralspkernel` computes the structural shortest path kernel introduced by Ralaivola et al. (2005). The Fast Computation of Shortest Path Kernel (FCSP) method is applied for both kernels. See Section 3.1 for details.

`untilhpathkernel` computes the path kernel up to length h . Two normalization kernels can be chosen, the Tanimoto kernel and the MinMax kernel, studied by Suard et al. (2007). It is recommended to choose the trie data structure to store paths according to h and structure properties of graphs (see Section 3.3).

Two graph kernels based on non-linear patterns are implemented: `treeletkernel` for the treelet kernel (Gaüzère et al., 2015b) and `weisfeilerlehmankernel` for the Weisfeiler-Lehman (WL) subtree kernel (Shervashidze et al., 2011).

Besides, user-defined vertex kernels and/or edge kernels of labeled graphs are supported in the shortest path kernels, the structural shortest path kernel, and the generalized random walk kernel computed by conjugate gradient and fixed-point iterations methods. These kernels allow using simultaneously symbolic and non-symbolic labels in graph kernels, which enables graph kernels to tackle more types of graph datasets. The module `utils.kernels` contains several pre-defined kernels between labels of vertices or edges, in which the function

`deltakernel` computes the Kronecker delta function between symbolic labels, the function `gaussiankernel` computes the Gaussian kernel between non-symbolic labels, the function `kernelsum` and `kernelproduct` are respectively the sum and product of kernels between symbolic and non-symbolic labels. Moreover, edge weights can be included in the shortest path kernel, the structural shortest path kernel, and the generalized random walk kernel computed by Sylvester equation and spectral decomposition methods.

2.3. Model Selection and Evaluation

For the convenience of use, a complete model selection and evaluation procedure is implemented in the module `gklearn.utils.model_selection_precomputed`, in which all work is carried out by `model_selection_for_precomputed_kernel`. This method first preprocesses the input dataset, then computes Gram matrices and performs the model evaluation with machine learning methods from the `scikit-learn` library (Pedregosa et al., 2011). Support Vector Machines (SVM) are applied for classification tasks and kernel ridge regression for regression (Schölkopf and Smola, 2002). A two-layer nested cross-validation (CV) is applied to select and evaluate models, where the outer CV randomly splits the dataset into 10 folds with 9 as validation set, and the inner CV then randomly splits the validation set to 10 folds with 9 as training set. The whole procedure is performed 30 times, and the average performance is computed over these trails. The kernel parameters are tuned within this procedure. This design allows the users to perform model selection in a single Python statement. Demos to use the library are provided in the `notebooks` folder.

3. Strategies to Reduce the Computation Complexity

The computational complexity limits the practicability and scalability of graph kernels. In this section, we consider 3 strategies to reduce the computing time and memory usage to compute graph kernels: the Fast Computation of Shortest Path Kernel method, parallelization, and the trie structure. Datasets and environment settings applied in this section are described in Section 4.2.

3.1. The Fast Computation of Shortest Path Kernel Method

To compute the shortest path kernel between 2 graphs G_1 and G_2 , shortest paths between all pairs of vertices in both graphs are compared. Each time we compare 2 shortest paths, both their corresponding pairs of vertices are compared once, causing significant redundancy during the vertex comparison procedure. If G_1 has n_1 vertices and G_2 has n_2 vertices, then there are at most n_1^2 shortest paths in G_1 and n_2^2 shortest paths in G_2 , thus $n_1^2 n_2^2$ comparisons between shortest paths and $2n_1^2 n_2^2$ comparisons between vertices are required to compute the kernel. Each pair of vertices is compared $2n_1 n_2$ times on average.

The Fast Computation of Shortest Path Kernel (FCSP) reduces this redundancy (Xu et al., 2014). Instead of comparing vertices during the procedure of comparing shortest paths, FCSP first compares all pairs of vertices between 2 graphs, and then stores the comparison results in an $n_1 \times n_2$ matrix named shortest path adjacency matrix; finally when comparing shortest paths, comparison results of corresponding vertices are retrieved from the matrix. This method reduces vertex comparisons to at most $n_1 n_2$ times, with an additional memory usage of size $O(n_1 n_2)$. In practice, FCSP can reduce the time complexity up to several orders of magnitudes.

In our implementation, we apply this vertex comparing method to the shortest path kernel, as recommended by Xu et al. (2014). Moreover, we also extend this strategy and apply it to the structural shortest path kernel, which allows reducing more redundancy since this kernel requires comparisons between all vertices on each pair of shortest paths. If the average length of the shortest paths in G_1 and G_2 is h , the new method is at most $n_1 n_2 h$ times faster than direct comparison.

We further extend this strategy to edge comparison when computing the structural shortest kernel. If G_1 has m_1 edges and G_2 has m_2 edges, then it requires $m_1 m_2$ times of edge label comparisons, compared to $n_1^2 n_2^2 h$ times by the original method.

3.2. Parallelization

Parallelization may significantly reduce the computational complexity. The basic concept of parallelization is to split a set of computation tasks into several pieces, and then carry them out separately on multiple computation units such as CPUs or GPUs. We implement parallelization with Python’s multiprocessing.Pool module in two aspects: In cross-validation, parallelization is carried out over the set of trials; parallelization is performed on pairs of graphs when computing Gram matrices of graph kernels (except for the WL subtree kernel due to the special structure of the kernel).

Many factors may influence the efficiency of parallelization, such as the number of computation cores, the transmission bandwidth between these cores, the method to split the data, the computational complexity to tackle one piece of data, etc. Fig. 2 reveals the influence of parallelization and CPU core numbers (7 versus 28), on runtime to compute Gram matrices and to perform model selections for the shortest path kernel on 8 datasets. Moreover, we present the ratio between runtimes to compute the Gram matrices on 28 and 7 cores. The values of this ratio for large-scale datasets are around 4, which turns out to be the inverse ratio of the number of CPU cores (28/7). It is

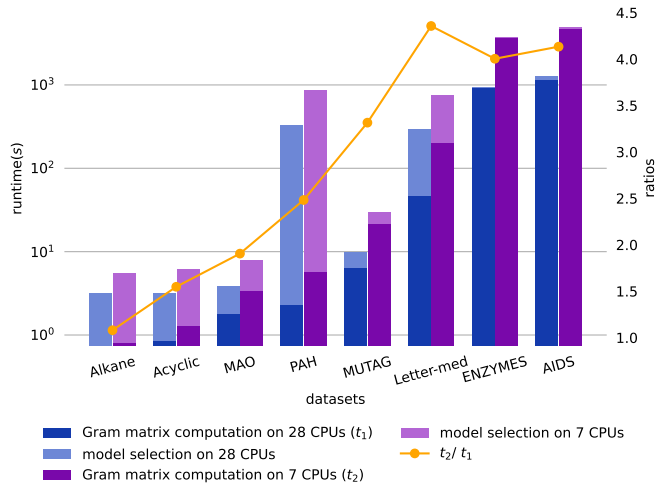


Fig. 2. Left y-axis: Runtimes (in seconds) to compute Gram matrices (bottom of each pillar) and perform model selections (top of each pillar) for the shortest path kernel on each dataset on 28 CPU cores (blue pillar) and 7 CPU cores (magenta pillar) with parallelization. Right y-axis: The orange dots are the ratios between the runtimes to compute Gram matrices of each dataset on 28 and 7 cores.

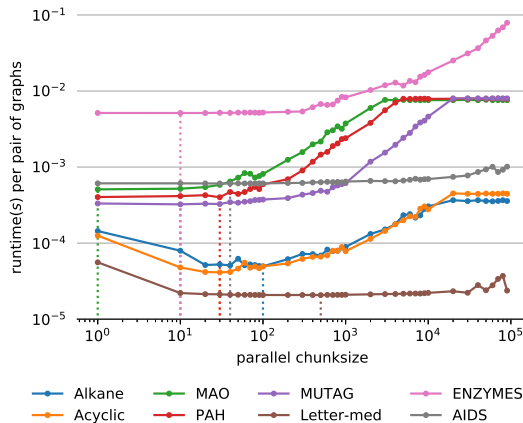


Fig. 3. Runtimes to compute the Gram matrices of the shortest path kernel on each dataset on 28 CPU cores with different chunksize values.

worth noting that the *Letter-med* dataset has the largest number of graphs (but with relatively “small” graphs), and *Enzymes* has the “average-largest” graphs (the second one being *PAH*).

Ideally, parallelization is more efficient when more computation cores are applied. However, this efficiency may be suppressed by the parallel procedure required to distribute data to computation cores and collect returned results. Parallelizing relatively small graphs to a large number of computation cores may be more time consuming than non-parallel computation. For instance, Fig. 2 shows that it takes almost the same time to compute the Gram matrix of the small dataset *Alkane* on 28 and 7 CPU cores, indicating that the time efficiency raised by applying more CPU cores is nearly neutralized by the cost to allocate these cores. To tackle this problem, it is essential to choose an appropriate chunksize, which describes how many data are grouped together as one piece to be distributed to a single computation core.

	common walk	marginalized	Sylvester equation	conjugate gradient	fixed-point iterations	spectral decomposition	shortest path	structural SP	path up to length h	treelet	Wt. subtree
Alkane	1.09	24.94	8.1	23.14	24.22	1.71	20.39	23.29	2.75	2.51	1.02
Acyclic	1.24	25.19	8.9	19.11	18.27	1.51	20.36	22.56	4.89	2.72	1.02
MAO	1.68	24.59	4.32	1.14	1.06	7.25	20.96	24.91	6.46	2.0	1.03
PAH	1.32	26.05	5.17	1.15	1.16	10.19	24.98	26.98	2.06	3.26	1.04
Mutag	1.16	27.23	12.09	1.39	1.57	5.69	25.43	27.47	13.5	6.17	1.01
Letter-med	1.43	1.54	14.83	1.46	1.65	1.61	2.63	2.37	31.54	30.35	1.01
Enzymes	1.43	14.66	1.85	2.03	1.73	inf	14.52	inf	16.23	17.22	1.01
AIDS	1.08	1.59	2.0	1.07	1.08	inf	1.8	2.15	1.8	21.04	1.01
NCI1	inf	1.17	1.94	inf	inf	inf	1.27	inf	4.14	23.94	1.07
NCI109	inf	1.27	1.93	inf	inf	inf	1.3	inf	6.04	32.0	1.07
D&D	inf	inf	inf	inf	inf	inf	inf	inf	inf	inf	1.01

Fig. 4. The ratio between runtimes of the worse and the best chunksize settings for each graph kernel on each dataset. Darker color indicates a better result. Gray cells with the “inf” marker indicate that the computation of the graph kernel on the dataset is omitted due to much higher consumption of computational resources than other kernels.

In Fig. 3, runtimes to compute the Gram matrices of the shortest path kernel with different chunksize values are compared on 28 CPU cores. When chunksizes are too small, the runtimes become slightly high, as the parallel procedure costs too much time; as chunksizes become bigger, the runtimes turn smaller, and then reach the minima; after that, the runtimes may become much bigger as chunksizes continue growing, due to the waste of computational resources. The minimum runtime of each dataset (shown with the vertical dot lines) varies due to the time and memory consumed to compute Gram matrices. Computations with wise chunksize choices could be more than 20 times faster than the worst choices. In our experiments, for convenience of implementations and comparisons, the chunksize to compute an $N \times N$ Gram matrix on n_\square CPU cores is set to 100 if $N^2 > 100n_\square$; and N^2/n_\square otherwise. The value 100 is chosen since the corresponding runtimes are close enough to their minima on all the datasets.

The ratio between runtimes of the worse and the best chunksize settings for each graph kernel on each dataset is shown in Fig. 4. On all available settings, the proper choices of the chunksizes speed up the computation. Some are more than 30 times faster than the worse chunksize settings (i.e., the path kernel up to length h and the treelet kernel on *Letter-med*).

3.3. The trie Structure

In some graph kernels that require comparison of paths (i.e., the path kernel up to h), the paths are pre-computed for the sake of time complexity. However, for large datasets, when the maximum limits of the lengths of paths are high, storing these paths becomes memory consuming. Ralaivola et al. (2005) proposed a suffix tree data structure for fast computation of path kernels. Inspired by that, we employ the trie data structure (Fredkin, 1960) to store paths in order to tackle the memory problem.

The trie combines the common prefixes of paths together to reduce space complexity. Take the path kernel up to h for example. Let n be the average vertex number of each graph, d be

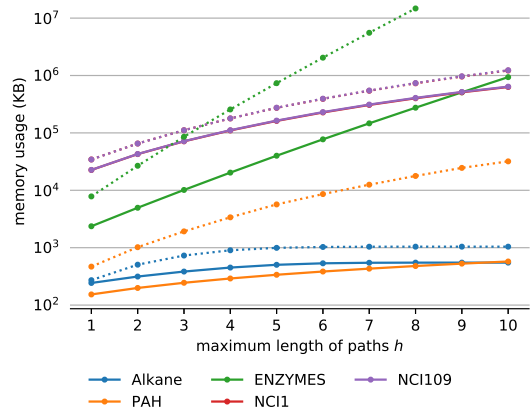


Fig. 5. Memory usages to store paths in all graphs in each dataset under different maximum length of paths h . Dot lines represent explicit storage of paths, and solid lines represent storage using the trie structure. Note that lines of datasets *NCI1* and *NCI109* overlap.

Table 3. Experimental settings.

Environments	Settings
CPU	Intel(R) Xeon(R) E5-2680 v4 @ 2.40GHz
# CPU cores	28
Memory (in total)	252 GB
Operating system	CentOS Linux release 7.3.1611, 64 bit
Python version	3.5.2

the average vertex degree, and l the different vertex labels in total (for conciseness, only symbolic vertex labels are considered here). When paths are stored explicitly in memory (i.e., using the Python list object), the space complexity to store paths in one graph is in $O(n(1 + d + \dots + d^h))$; The trie reduces it to $O(l(1 + l + \dots + l^h))$, making it very efficient for large datasets and graphs, and when h is high. See Fig. 5 for a comparison.

Although saving paths to the trie structure and retrieving paths from it require extra computing time, less memory usage may avoid possible swapping between memory and hard disk, which may save more time in practice. As a result, the users should use trie structure according to the limits of their computing resources. In *graphkit-learn*, the trie structure is implemented for the path kernel up to h .

4. Experiments

To show the effectiveness and the practicability of the *graphkit-learn* library, we tested the library on synthesized graphs and several real-world datasets. A two-layer nested CV is applied to select and evaluate models, which is described in detail in Section 2.3. Table 3 summarizes the settings used in the experiments.

4.1. Performance on Synthesized Graphs

In this section, the performance and properties of each graph kernel are studied using synthesized graphs, with runtimes estimated on the Gram matrix computations.

First, we study the scalability of the kernels by increasing the number of graphs in the dataset (from 100 to 1000), where the

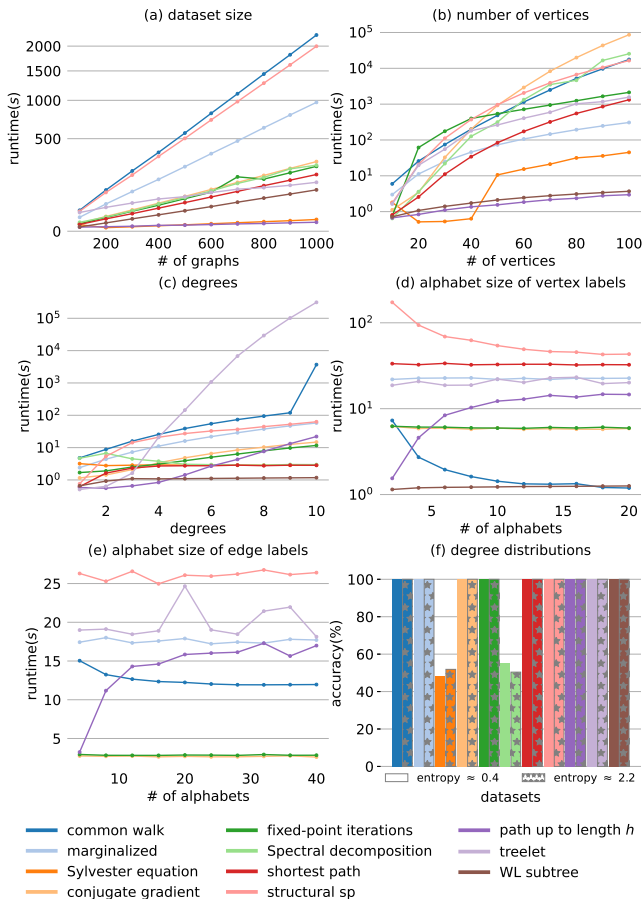


Fig. 6. Performance of all graph kernels on synthesized graphs.

generated unlabeled graphs consist of 20 vertices and 40 edges randomly assigned to pairs of vertices. Fig. 6(a) shows the runtimes for all kernels. Since all the lines are linear with the y-axis being in square root scale, this indicates that the runtimes are quadratic in the number of graphs.

The scalability is also analyzed by increasing the number of vertices (from 10 to 100), where 10 datasets of 100 unlabeled graphs each were generated. The average degree of all generated graphs is equal to 2 and the edges are randomly assigned to pairs of vertices. Fig. 6(b) shows the runtimes increasing in the numbers of vertices, for all kernel. The path kernel up to length h kernel and the WL subtree kernel have the best scalability.

To study the scalability of the kernels w.r.t. the average vertex degree, we generated unlabeled graphs consisting of 20 vertices with increasing degrees (from 1 to 10). The edges are randomly assigned to pairs of vertices. For each of the 10 degree values, we generated 100 graphs. Fig. 6(c) shows that most kernels have good scalability to the degrees, the worst being the treelet kernel, as the number of treelets in each graph increases rapidly with the degree.

To study the scalability of the kernels w.r.t. the alphabet sizes of symbolic vertex labels, we generated unlabeled graphs of 20 vertices and 40 edges randomly assigned to pairs of vertices. The vertices are symbolically labeled with increasing alphabet sizes, and the edges are unlabeled. For each alphabet size

(from 0 to 20), we generated 100 graphs. As Fig. 6(d) shows, the runtimes of the path kernel up to path h increases significantly with the alphabet size. This is because the trie structures to store paths become bigger, and it requires more time to construct and compare them. On the contrary, the runtimes of the common walk kernel and the structural shortest path kernel become smaller when the alphabet size becomes bigger. The former is related to smaller direct product graphs (see (Gärtner et al., 2003)), and the latter is caused by the reduced comparison between vertex labels through the shortest paths.

The scalability of the kernels w.r.t. the alphabet sizes of edge labels is studied in the same way, except that the edges are symbolically labeled with increasing alphabet sizes, and the vertices are unlabeled. For each alphabet size (0, 4, 8, ..., 40), we generated 100 graphs. According to Fig. 6(e), the runtimes of the path kernel up to path h increase with the alphabet sizes, caused by the aforementioned reason concerning the trie structures. In general, the influence of the alphabet size on the runtime is small for all kernels.

Finally, we studied the classification performances of the kernels on graphs with different amounts of entropy on degree distributions. For this reason, we generated two sets of 200 graphs with 40 vertices. Graphs of the first set have low entropy on degree distributions, while graphs of the second set have high entropy (0.4 versus 2.2 on average). Each set has two classes, one consisting of half of the graphs with one label on vertices and the other class another label. A classification task is performed on each set using the SVM classifier, and the accuracy is evaluated. Fig. 6(f) shows that all graph kernels achieve equivalent accuracy on the both degree distributions. Except for the generalized random walk kernels computed by either Sylvester equation or spectral decomposition that cannot deal with labels, all graph kernels achieve high accuracy. It indicates that these graph kernels are suitable for various degree distributions.

As a conclusion, the dataset size and the number of vertices have the most significant effect on the computation runtimes of the aforementioned graph kernels. For the treelet kernel, the vertex degree is also important. These effects should be examined carefully before using the kernels.

4.2. Real-world Datasets

In the following experiments, 11 well-known real-world datasets are considered for regression and classification tasks. These datasets come from different fields: *Alkane* (Cherqaoui and Villemin, 1994), *Acyclic* (Cherqaoui et al., 1994), *MAO* (Brun, 2018), *PAH* (Brun, 2018), *Mutag* (Debnath et al., 1991), *Enzymes* (Schomburg et al., 2004; Borgwardt et al., 2005), *AIDS* (Riesen and Bunke, 2008), *NCII* (Wale et al., 2008), *NCII09* (Wale et al., 2008) and *D&D* (Dobson and Doig, 2003) are chemical compounds and proteins from the bio/cheminformatics fields; *Letter-med* (Riesen and Bunke, 2008) involves graphs of distorted letter drawings, within the category of image recognition. *Alkane* and *Acyclic* are concerned with the determination of the boiling point using regression. The other datasets are related to classification tasks. These datasets have a wide range of graph properties, by including labeled and unlabeled graphs, symbolic and non-symbolic attributes, different average vertex numbers, linear and non-linear patterns, etc.

	common walk	marginalized	Sylvester equation	conjugate gradient	fixed-point iterations	spectral decomposition	shortest path	structural SP	path up to length h	treelet	WL subtree
Alkane	15.52	43.75	8.97	11.13	12.78	12.95	7.81	8.65	9.0	2.53	26.42
Acyclic	12.93	18.77	32.5	13.15	14.2	33.05	9.03	13.1	6.66	5.99	19.8
MAO	93.0	85.62	84.52	88.57	73.71	77.67	87.81	91.62	85.43	91.19	93.05
PAH	71.8	57.67	71.5	73.93	58.33	70.73	69.4	74.5	75.27	66.3	75.93
Mutag	85.96	76.11	82.77	86.18	86.58	84.05	81.84	86.26	88.47	90.79	87.18
Letter-med	36.16	5.2	37.27	93.12	91.3	36.38	93.72	94.88	43.83	inf	36.13
Enzymes	42.81	45.92	23.24	60.89	63.11	23.68	70.09	inf	57.49	52.23	50.76
AIDS	94.71	inf	92.42	98.93	98.57	87.21	99.26	98.84	99.65	99.54	98.63
NC11	inf	inf	59.76	71.34	inf	inf	inf	79.88	84.84	64.84	84.63
NC1109	inf	inf	60.62	67.6	67.25	inf	inf	79.04	83.94	63.46	85.47
D&D	inf	inf	inf	inf	inf	inf	inf	inf	81.4	inf	77.3

Fig. 7. Accuracy achieved by graph kernels, in terms of regression error (the upper table) and classification rate (the lower table). Red color indicates the worse results and dark green the best ones. Gray cells with the “inf” marker indicate that the computation of the graph kernel on the dataset is omitted due to much higher consumption of computational resources than other kernels.

The diversity of these particularities allows to explore the behavior of the graph kernels on different types of graphs and the coverage of graphs that `graphkit-learn` is able to manage. See (Kersting et al., 2016) for details on these datasets.

4.3. Performance on the Real-world Datasets

Fig. 7 shows the accuracy achieved by the aforementioned graph kernels. Each row corresponds to a dataset and each column to a graph kernel. All kernels achieve better results compared with random assignment, where kernels based on paths and non-linear patterns outperform those based on walks on most datasets. Kernels based on paths achieve equivalent or even better results than those on non-linear patterns, where the path kernel up to length h dominates on most datasets with symbolic labels; while when non-symbolic labeled graphs are given, kernels based on shortest paths achieve the best results (such as *Letter-med* and *Enzymes*).

These results confirm `graphkit-learn`’s ability to tackle various types of graphs, which are labeled or unlabeled, with symbolic and/or non-symbolic attributes, linear and/or non-linear patterns, and have a wide range of average vertex numbers from 4 (*Letter-med*) to 284 (*D&D*). Kernels based on linear patterns achieve competitive accuracies on graphs with non-linear patterns compared to kernels based on non-linear patterns. Along with the preceding analyses, these facts prove that these kernels can serve as reliable methods for classification and regression problems on graphs, as well as qualified benchmark kernels for future graph kernels design.

Besides accuracy, we furthermore examined the computational complexity of each kernel. Fig. 8 displays the time consumed to compute the Gram matrix of each kernel on each dataset. The results are consistent with the computational complexities of graph kernels. In most cases, the computation is

	common walk	marginalized	Sylvester equation	conjugate gradient	fixed-point iterations	spectral decomposition	shortest path	structural SP	path up to length h	treelet	WL subtree
Alkane	0.48	0.51	-0.42	-0.18	-0.22	-0.19	-0.12	0.02	-0.29	-0.3	0.16
Acyclic	0.36	0.62	-0.18	-0.04	-0.11	-0.1	-0.08	0.24	-0.3	-0.31	0.34
MAO	0.81	0.69	-0.47	-0.11	-0.03	0.14	0.25	0.88	-0.14	-0.28	-0.25
PAH	1.56	1.05	-0.42	0.14	0.25	0.37	0.36	1.32	-0.28	-0.24	-0.03
Mutag	1.28	1.36	-0.3	0.44	0.53	0.77	0.69	1.84	-0.07	-0.24	0.19
Letter-med	2.01	2.08	1.13	1.97	1.85	1.78	1.57	1.62	1.08	inf	2.02
Enzymes	3.9	3.18	0.72	2.62	2.79	3.4	2.85	inf	2.16	2.08	1.41
AIDS	2.83	inf	1.37	2.91	3.03	3.74	2.95	3.9	1.59	0.87	2.22
NC11	inf	inf	2.3	3.96	inf	inf	inf	5.12	2.04	1.48	3.02
NC1109	inf	inf	2.3	4.37	4.38	inf	inf	5.13	2.05	1.48	1.48
D&D	inf	inf	inf	inf	inf	inf	inf	inf	2.67	inf	2.95

Fig. 8. Computational time to compute Gram matrices of graph kernels (in \log_{10} of seconds). Same color legends as Fig. 7 are used.

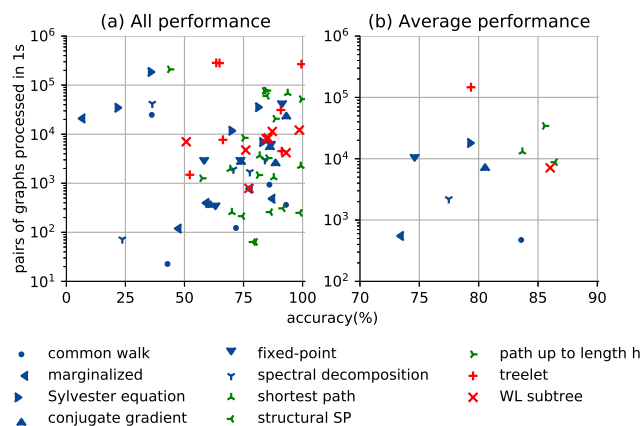


Fig. 9. Comparison of computational complexity versus accuracy of all graph kernels on all datasets (a), as well as the average performance of each kernel over all datasets (b). Markers correspond to different kernels; Colors blue, green and red depict graph kernels based on walks, paths and non-linear patterns, respectively.

efficient and it takes seconds or minutes to compute the whole Gram matrix. On the largest dataset (*i.e.*, *D&D*, which contains 1178 graphs with 284 vertices and 715 edges per graph average), two graph kernels can still be computed in tolerable time. For example, the path kernel up to length h can be computed within 8 minutes on *D&D*, which benefits from not only its relatively lower computational complexity, but also the trie structure applied to it (see Section 3.3). Notice that it takes too much time to compute some graph kernels on some large datasets. For instance, the computational complexity of the common walk kernel is in $O(n^6)$ per pair of graphs. To this end, it is irrational to apply this kernel on graphs with large amounts of vertices. In conclusion, these analyses illustrate the practicability of the `graphkit-learn` library.

The joint performance of the computational complexity and accuracy of each graph kernel on each dataset is shown in

Fig. 9. Performances that cannot be acquired in reasonable time are omitted. In Fig. 9(b), the performance of each kernel is averaged on at least 5 datasets. Fig. 9 provides a helpful guidance for the users to find the best trade-offs for each kernel. According to this, our implementations of graph kernels can tackle various types of graphs within reasonable time and memory usage. The users can freely make use of the kernels or combine them with self-developed methods.

5. Conclusion and Future Work

In this paper, we presented the Python library `graphkit-learn` for graph kernel computations. It is the first library that provides a thorough coverage of graph kernels based on linear patterns (9 kernels based on linear patterns and 2 on non-linear patterns for comparison). We provided 3 strategies to reduce the computational complexity, including the extension of the FCSP method for other kernels and edge comparison. Experiments showed that it is easy to take advantage of the proposed library to compute graph kernels, in conjunction with the well-known `scikit-learn` library for Machine Learning. Future work includes implementations of other non-linear kernels, a more thorough test of graph kernels on a wider range of benchmark datasets, a C++ implementation bound to Python interface for faster computation, and integrating more machine learning tools for graphs in the library, such as graph edit distance methods and tools to solve the graph pre-image problem. Meanwhile, we encourage interested users and authors of graph kernels to commit their implementations to the library.

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Appendix A. Examples to Use the Library

In this appendix we show usage examples of the library. The dataset *MUTAG* and the path kernel up to length h are used as the example.

First, a single Python statement allows to load a graph dataset:

```
1 from gklearn.utils.graphfiles import loadDataset
2
3 graphs, targets = loadDataset('DATA_FOLDER/MUTAG/
4 MUTAG_A.txt')
```

“DATA_FOLDER” is the user-defined folder to store the datasets.

With the loaded graphs, the Gram matrix can be computed as following:

```
1 from gklearn.kernels import untilhpathkernel
2
3 gram_matrix, run_time = untilhpathkernel(
4     graphs, # The list of input graphs.
5     depth=5, # The longest length of paths.
6     k_func='MinMax', # Or 'tanimoto'.
7     compute_method='trie', # Or 'naive'.
8     n_jobs=1, # The number of jobs to run in
9     parallel.
10    verbose=True)
```

The Gram matrix and the time spent to compute it are returned.

Besides kernel computation, a complete model selection and evaluation procedure using a 2-layer nested cross-validation can be performed by the following code:

```
1 from gklearn.utils import
2   model_selection_for_precomputed_kernel
3 from gklearn.kernels import untilhpathkernel
4 import numpy as np
5
6 # Set parameters.
7 datafile = 'DATA_FOLDER/MUTAG/MUTAG_A.txt'
8 param_grid_precomputed = {
9     'depth': np.linspace(1, 10, 10),
10    'k_func': ['MinMax', 'tanimoto'],
11    'compute_method': ['trie']}
12 param_grid = {'C': np.logspace(-10, 10, num=41,
13    base=10)}
14
15 # Perform model selection and classification.
16 model_selection_for_precomputed_kernel(
17     datafile, # The path of dataset file.
18     untilhpathkernel, # The graph kernel used for
19     estimation.
20     param_grid_precomputed, # The parameters used
21     to compute gram matrices.
22     param_grid, # The penelty Parameters used for
23     penelty items.
24     'classification', # Or 'regression'.
25     NUM_TRIALS=30, # The number of the random
26     trials of the outer CV loop.
27     ds_name='MUTAG', # The name of the dataset.
28     n_jobs=1,
29     verbose=True)
```

The “param_grid_precomputed” and the “param_grid” arguments specify grids of hyper-parameter values used for grid search in the cross-validation procedure. The results will be automatically saved.

More demos and examples can be found in the notebooks directory and the `gklearn.examples` module of the library.