

Manifold Learning and Graph Kernels

Third Assignment of the course in Artficial Intelligence held by Prof. Torsello

Bernardi Riccardo - 864018

Index:

Manifold Learning and Graph Kernels

Index:

- 1. Problem Statement
- 2. Introduction
- 3. The Graph Kernel
 - 3.1 What is a kernel
 - 3.2 What is a Graph kernel
 - 3.3 The available kernels

Random Walk

Graphlet Kernel, Petri et al.

Weisfeiler-Lehman Kernel

DSGK - Dominant Set Graph Kernel

4. The Manifold Technique

- 4.1 What is a Manifold Technique
- 4.2 The available Manifold Techniques

PCA

Isomap

Locally-linear embedding

5. Comparison

- 4.1 Training without Manifold
- 4.2 Training with Manifold
- 4.2 Results

6. Conclusions

Bibliography

Appendix

Appendix 1

1. Problem Statement

Read this article presenting a way to improve the disciminative power of graph kernels.

Choose one graph kernel among

- Shortest-path Kernel
- Graphlet Kernel
- Random Walk Kernel
- Weisfeiler-Lehman Kernel

Choose one manifold learning technique among

- Isomap
- Diffusion Maps
- Laplacian Eigenmaps
- Local Linear Embedding

Compare the performance of an SVM trained on the given kernel, with or without the manifold learning step, on the following datasets:

- PPI
- Shock

Note: the datasets are contained in Matlab files. The variable G contains a vector of cells, one per graph. The entry am of each cell is the adjacency matrix of the graph. The variable labels, contains the class-labels of each graph.

NEW I have added zip files with csv versions of the adjacecy matrices of the graphs and of the lavels. the files graphxxx.csv contain the adjacency matrices, one per file, while the file labels.csv contais all the labels

- PPI
- Shock

2. Introduction

We are going to explain in this paper the experiments we run over the two datasets provided, they are called PPI and SHOCK. The PPI dataset deals with the Protein Protein Interaction, It consists of 86 graphs that repesent proteins and between them we would like to discover interesting similarities. The second dataset contains 150 graphs and we would like as before to find a way to efficiently compute similarities between them. In the chapter 3 we are going to introduce the kernels and the graph kernels, also we are going to propose a library that provides them. In the chapter 4 we are going to look inside the possible manifold learning techniques to reduce the visited space of our algorithm and also to visualize our result in 2Dimensions. The 5th chapter talks about the Comparisons that we made and we will discuss about possible

improvements. In the last chapter that is the 6th we will draw the conclusions. The other chapters at the very end of this paper are the bibliography and the appendix.

Disclaimer:

This assignment was done only by Riccardo Bernardi(864018@stud.unive.it), both the code, the report and the experiments.

During this assignment was also created the Dominant Set Graph Kernel, this was both invented and implemented by Riccardo Bernardi(864018@stud.unive.it).

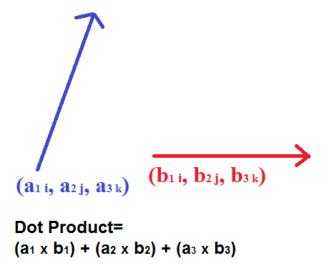
3. The Graph Kernel

We are going here to answer these questions:

- what is a kernel and how to create one?
- what is a graph kernel?
- which kernels are available and where?

3.1 What is a kernel

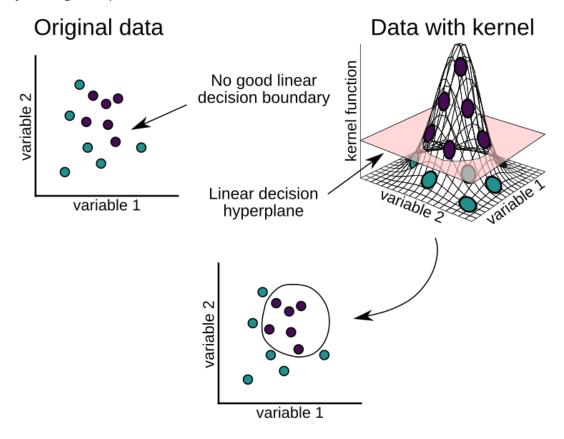
Kernel is a way of computing the dot product of two vectors \mathbf{x} and \mathbf{y} in some (possibly very high dimensional) feature space, which is why kernel functions are sometimes called "generalized dot product". Suppose we have a mapping $\varphi:\mathbb{R}n\to\mathbb{R}m$ that brings our vectors in \mathbb{R}^n to some feature space \mathbb{R}^m . Then the dot product of \mathbf{x} and \mathbf{y} in this space is $\varphi(x)^T\varphi(y)$. A kernel is a function k that corresponds to this dot product, i.e. $k(x,y)=\varphi(x)^T\varphi(y)$. So Kernels give a way to compute dot products in some feature space without even knowing what this space is and what is φ .



For example, consider a simple polynomial kernel $k(x,y)=(1+x^Ty)^2$ with $x,y\in R^2$. This doesn't seem to correspond to any mapping function φ , it's just a function that returns a real number. Assuming that x=(x1,x2) and y=(y1,y2), let's expand this expression:

$$k(x,y) = (1+x^Ty)^2 = (1+x_1y_1+x_2y_2)^2 = = 1+x_1^2y_1^2+x_2^2y_2^2+2x_1y_1+2x_2y_2+2x_1x_2y_1y_2$$

Note that this is nothing else but a dot product between two vectors $(1,x_1^2,x_2^2,\sqrt{2}x_1,\sqrt{2}x_2,\sqrt{2}x_1x_2)$ and $(1,y_1^2,y_2^2,\sqrt{2}y_1,\sqrt{2}y_2,\sqrt{2}y_1y_2)$. So the kernel $k(x,y)=(1+x^Ty)^2=\varphi(x)^T\varphi(y)$ computes a dot product in 6-dimensional space without explicitly visiting this space.



Another example is Gaussian kernel $k(x,y) = exp(-\gamma ||x-y||^2)$. If we Taylor-expand this function, we'll see that it corresponds to an infinite-dimensional codomain of ϕ .

This operation is often computationally cheaper than the explicit computation of the coordinates. This approach is called the "kernel trick". Kernel functions have been introduced for sequence data, graphs, text, images, as well as vectors.

The kernel trick avoids the explicit mapping that is needed to get linear learning algorithms to learn a nonlinear function or decision boundary.

The key restriction is that the dot product must be a proper inner product. On the other hand, an explicit representation for ϕ is not necessary, as long as V is an inner product space. The alternative follows from Mercer's theorem: an implicitly defined function ϕ exists whenever the space X can be equipped with a suitable measure ensuring the function k satisfies Mercer's condition.

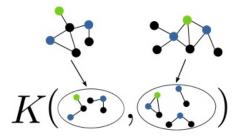
K is said to be non-negative definite (or positive semidefinite) if and only if:

$$\sum_{i=1}^n \sum_{j=1}^n K(x_i,x_j) c_i c_j \geq 0$$

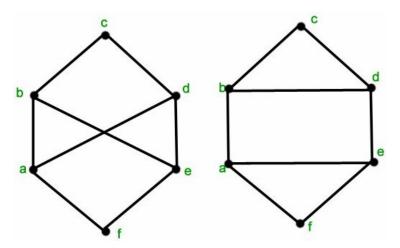
Theoretically, a Gram matrix K∈Rn×n with respect to {x1,...,xn} (sometimes also called a "kernel matrix"[3]), where Kij=k(xi,xj), must be positive semi-definite (PSD).[4] Empirically, for machine learning heuristics, choices of a function k that do not satisfy Mercer's condition may still perform reasonably if k at least approximates the intuitive idea of similarity.[5] Regardless of whether k is a Mercer kernel, k may still be referred to as a "kernel".

3.2 What is a Graph kernel

A graph kernel is a kernel function that computes an inner product on graphs. Graph kernels can be intuitively understood as functions measuring the similarity of pairs of graphs. They allow kernelized learning algorithms such as support vector machines to work directly on graphs, without having to do feature extraction to transform them to fixed-length, real-valued feature vectors.



All starts with Graph isomorphism: Find a mapping f of the vertices of G1 to the vertices of G2 such that G1 and G2 are identical;



i.e. (x,y) is an edge of G1 iff (f(x),f(y)) is an edge of G2. Then f is an isomorphism, and G1 and G2 are called isomorphic. No polynomial-time algorithm is known for graph isomorphism. Neither is it known to be NP-complete.

We can move to Subgraph isomorphism. Subgraph isomorphism asks if there is a subset of edges and vertices of G1 that is isomorphic to a smaller graph G2. Subgraph isomorphism is NP-complete.

Drawbacks:

- Excessive runtime in worst case
- Runtime may grow exponentially with the number of nodes
- For larger graphs with many nodes and for large datasets of graphs, this is an enormous

problem

The more common way to proceed though is to create a kernel function that should perform a reasonable approximation of the graph isomorphism problem and can tell at the end of the process how much two graphs are similar to each other. The way it works is extracting some patterns that we believe are really important and can characterize well the graph such that they can be something like a fingerprint and such that it can be compared. This approach is called graph kernel through bag of patterns. The Pros are that we can control the precision and the computational cost moving from easier of more complex extractions of patterns. The Contras is that the right algorithm can be different based on the domain of the problem(i.e.: chemistry may prefer a more local approach for feature extraction instead physics a more general one)

Graph kernels based on bags of patterns

- (1) Extraction of a set of patterns from graphs,
- (2) Comparison between patterns,
- (3) Comparison between bags of patterns.

3.3 The available kernels

The kernels we used come from GraKel [125]. It is a library that provides implementations of several well-established graph kernels. The library unifies these kernels into a common framework. Furthermore, it provides implementations of some frameworks that work on top of graph kernels. Specifically, GraKeL contains 15 kernels and 2 frameworks.

Also we introduced a brand new kernel called Dominant-Set Graph Kernel. This kernel is crafted, implemented and invented by the author of this report.

Random Walk

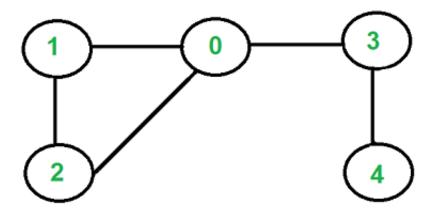
The principle is to count common walks in two input graphs G and G', walks are sequences of nodes that allow repetitions of nodes. The Pros are that walks of length k can be computed by looking at the k-th power of the adjacency matrix, easy. Some Disadvantages are Runtime, Tottering and Halting. Some potential solutions are presented in [68][79][81]. So the direct computation takes $O(n^6)$. The solution is to cast computation of random walk kernel as Sylvester Equation, these can be solved in $O(n^3)$. The equation:

$$AX + XB = C$$
.

The Vec-Operator flattens an n x n matrix A into an n^2 x1 vector vec(A). It stacks the columns of the matrix on top of each other, from left to right. The Kronecker Product is the product of two matrices A and B in which each element of A is multiplied with the full matrix B. An example here:

$$\begin{bmatrix} 1 & 2 \\ 3 & 1 \end{bmatrix} \otimes \begin{bmatrix} 0 & 3 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 1 \cdot 0 & 1 \cdot 3 & 2 \cdot 0 & 2 \cdot 3 \\ 1 \cdot 2 & 1 \cdot 1 & 2 \cdot 2 & 2 \cdot 1 \\ 3 \cdot 0 & 3 \cdot 3 & 1 \cdot 0 & 1 \cdot 3 \\ 3 \cdot 2 & 3 \cdot 1 & 1 \cdot 2 & 1 \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 & 3 & 0 & 6 \\ 2 & 1 & 4 & 2 \\ 0 & 9 & 0 & 3 \\ 6 & 3 & 2 & 1 \end{bmatrix}$$

The phenomenon of tottering occurs when walk allow for repetitions of nodes. A heavy problem can consist in a walk that can visit the same cycle of nodes all over again. Here in the image it can be that the partition visited remains only the one comprised in the cycle.



Another problem lies on the fact that a kernel measures similarity in terms of common walks. Hence a small structural similarity can cause a huge kernel value.

Random walk graph kernel has been used as an important tool for various data mining tasks including classification and similarity computation. Despite its usefulness, however, it suffers from the expensive computational cost which is at least $O(n^3)$ or $O(m^2)$ for graphs with n nodes and m edges. A more efficient way to compute it is its variant called Ark that exploits the low rank structure to quickly compute random walk graph kernels in $O(n^2)$ or O(m) time.

Computing Random Walk Graph Kernel can be done with these methods:

- Naive Method. The naive algorithm is to com- pute the Equation (2.1) by inverting the n2 × n2 matrix W. Since inverting a matrix takes time proportional to the cube of the number of rows/columns, the running time is $O(n^6)$.
- Sylvester Method. If the weight matrix can be decomposed into one or two sums of Kronecker products, Sylvester method solves the Equation in $O(n^3)$ time. However, there are two drawbacks in Sylvester method. First, the method requires the two graphs to have the same number of nodes, which is often not true. Second, the theoretical running time of Sylvester method on the weight matrix composed of more than two Kronecker products is unknown.
- ullet Spectral Decomposition Method. For unlabeled and unnormalized matrices, spectral decomposition method runs in $O(n^3)$ time. The problem of spectral decomposition method is that it can't run on the labeled graph or normalized matrix.
- Conjugate Gradient Method. Conjugate gradient (CG) method is used to solve linear systems efficiently. To use CG for computing random walk graph kernel,we first solve (I–cW)x=p for x using CG, and compute qT x. Each iteration of CG takes $O(m^2)$ since the most expensive operation is the matrix-vector multiplication. Thus CG takes $O(m^{2iF})$ time where iF denote

- the number of iterations. A problem of the CG method is its high memory requirement: it requires $O(m^2)$ memory.
- Iteration method first solves (I cW)x = p for x by iterative matrix-vector multiplications, and then computes qT x to compute the kernel. Note that the fixed point iteration method converges only when the decay factor c is smaller than $|\xi 1|-1$ where $\xi 1$ is the largest magnitude eigenvalue of W . Similar to CG, the fixed point iteration method takes $O(m^{2iF})$ time for iF iterations, and has the same problems of requiring $O(m^2)$ memory.

Graphlet Kernel, Petri et al.

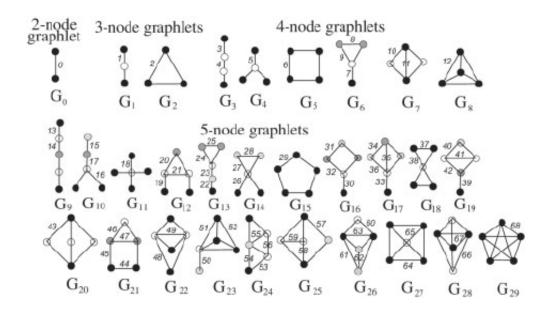
Graphlets are small connected non-isomorphic induced subgraphs of a large network. An induced subgraph must contain all edges between its nodes that are present in the large network, while a partial subgraph may contain only some of these edges.

The principle is to count subgraphs of limited size k in G and G', these subgraphs are referred to as graphlets and then define a graph kernel that counts isomorphic graphlets in two graphs. More formally we let be $G = \{graphlet(1), \ldots, graphlet(Nk)\}$ be the set of size-k graphlets and G be a graph of size n. Define a vector fG of length Nk whose i-th component corresponds to the frequency of occurrence of graphlet(i) in G, $\#(graphlet(i) \subseteq G)$. We will call fG the k- spectrum of G. This statistic is the foundation of our novel graph kernel. Given two graphs G and G' of size $n \ge k$, the graphlet kernel kg is defined as $kg(G,G') := fG \cdot fG'$.

As our goal is to develop scalable graph kernels, we study graphlet kernels based on the 3-, 4- and 5- spectra of graphs here. In order to account for differences in the sizes of the graphs, which can greatly skew the frequency counts fG, we normalize the counts to probability vectors:

Clearly, if G = G', then fG = fG'. But is the reverse true? It has been shown that when n = k+1 and $n \le 11$, equality of k-spectra implies isomorphism. For n > 11, it is still a conjecture whether a graph of size n = 1.

The runtime problems are that the pairwise test of isomorphism is expensive and another one is that the number of graphlets scales as O(nk). Two solutions on unlabeled graphs are to precompute isomorphisms and to extract sample graphlets. One disadvantage is that the same solutions not feasible on labeled graphs.



Weisfeiler-Lehman Kernel

the kernel comes directly from the Weisfeiler-Lehman Isomorphism test that is explained here below.

Here is the algorithm for the Weisfeiler-Lehman Isomorphism Test. It produces for each graph a canonical form. If the canonical forms of two graphs are not equivalent, then the graphs are definitively not isomorphic. However, it is possible for two non-isomorphic graphs to share a canonical form, so this test alone cannot provide conclusive evidence that two graphs are isomorphic.

Algorithm 1 One iteration of the 1-dim. Weisfeiler-Lehman test of graph isomorphism

- 1: Multiset-label determination
 - For i = 0, set $M_i(v) := l_0(v) = \ell(v)$.
 - For i > 0, assign a multiset-label $M_i(v)$ to each node v in G and G' which consists of the multiset $\{l_{i-1}(u)|u \in \mathcal{N}(v)\}$.
- 2: Sorting each multiset
 - Sort elements in $M_i(v)$ in ascending order and concatenate them into a string $s_i(v)$.
 - Add $l_{i-1}(v)$ as a prefix to $s_i(v)$ and call the resulting string $s_i(v)$.
- 3: Label compression
 - Sort all of the strings $s_i(v)$ for all v from G and G' in ascending order.
 - Map each string $s_i(v)$ to a new compressed label, using a function $f: \Sigma^* \to \Sigma$ such that $f(s_i(v)) = f(s_i(w))$ if and only if $s_i(v) = s_i(w)$.
- 4: Relabeling
 - Set $l_i(v) := f(s_i(v))$ for all nodes in G and G'.

When using this method to determine graph isomorphism, it may be applied in parallel to the two graphs. The algorithm may be terminated early after iteration i if the sizes of partitions of nodes partitioned by compressed labels diverges between the two graphs; if this is the case, the graphs are not isomorphic.

Example of the Weisfeiler-Lehman Isomorphism Test:

We demonstrate here the Weisfeiler-Lehman isomorphism test using the example graphs from above. The graphs are shown again here for completeness.

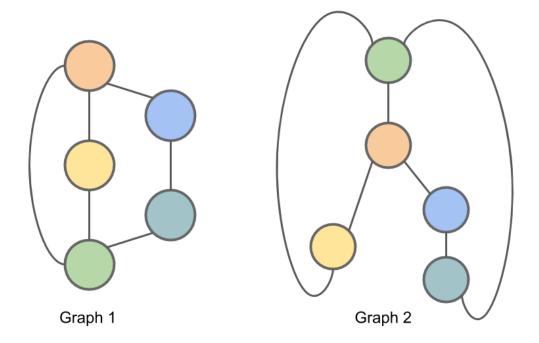
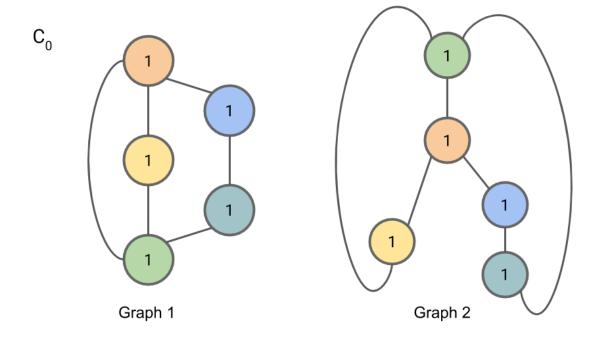
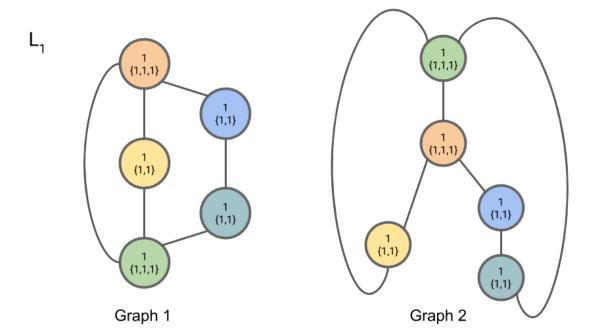


Figure: Graph 1 and Graph 2 are isomorphic. We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.

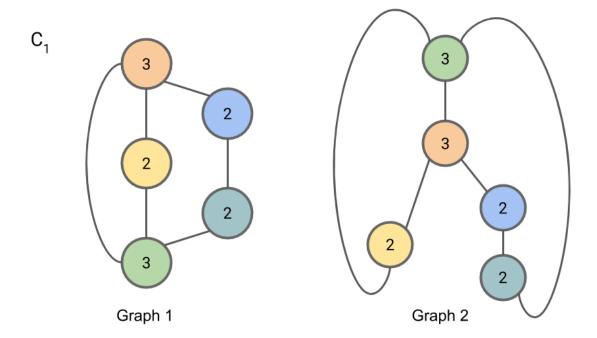
To initialize the algorithm (Step 1), we set C0,n=1 for all nodes n.



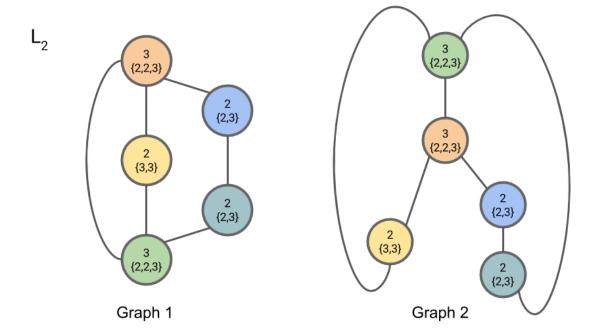
For iteration 1, Step 2, we compute L1. The first part of a node's L is the node's old compressed label; the second part of a node's L is the multiset of the neighboring nodes' compressed labels.



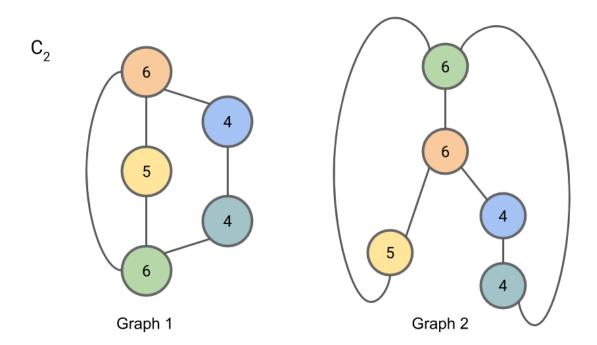
For iteration 1, Step 3, we introduce "compressed" labels C1 for the nodes:



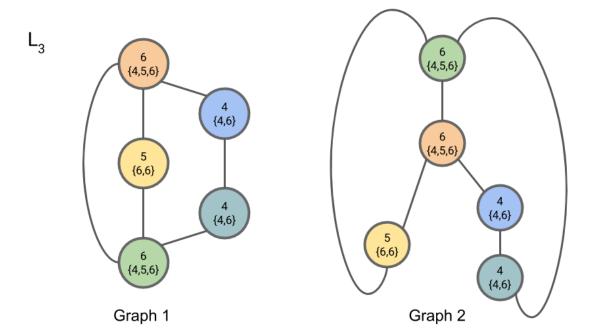
We now begin iteration 2. In iteration 2, Step 2, we compute L2:



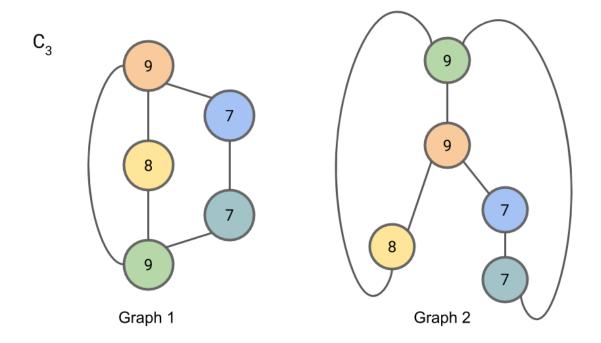
In iteration 2, Step 3, we compute C2:



In iteration 3, Step 2, we compute L3:



In iteration 3, Step 3, we compute C3:



Since the partition of nodes by compressed label has not changed from C2 to C3, we may terminate the algorithm here.

Concretely, the partition of nodes by compressed label may be represented as the number of nodes with each compressed label. That is: **"2 7s, 1 8, and 2 9s"**. This is the canonical form of our graph. Since both Graph 1 and Graph 2 have this same canonical form, we cannot rule out the possibility that they are isomorphic (they *are* in fact isomorphic, but the algorithm doesn't allow us to conclude this definitively.)

DSGK - Dominant Set Graph Kernel

The Dominant set graph kernel came out spontaneously while trying to improve the performances of the graph kernels, in particular it seemed in some cases that the weisfeiler-lehman kernel could have been the best kernel with respect to the others in the classification. The successive hypothesis was that an improvement could have been done if the algorithm could have worked on the **dominant** graphs discarding the ones that were only noise. Stating this hypothesis we used an algorithm to compute the dominant sets on an adjacency matrix through the replicator dynamic technique and after that we computed the weisfeiler-lehman kernel on the dominant set. Intuitively this improves the generality of the prediction because you are going to compute the kernel not on all the points that can be also noisy but on a set that you are guaranteed to be a robust cluster. The experiments are below and show that this algorithms works well in practice being the best one over all the other algorithms.

The algorithm computes only the triangular superior matrix of similarity, in this way it is faster. There are some auxiliary functions such as the "from_set_to_adj" and the "from_adj_to_set". These are auxiliary functions needed to be compliant with the SVM and the GraKel libraries. For sure these operations can be improved in a future version of the kernel.

```
class DomSetGraKer():
    def __init__(self):
        self.train_graphs = None

def similarity(self,gladj,g2adj):
    # launch similarity measure Weisfeiler-lehman kernel
    # the inputs are 2 adj matrices of the 2 graphs to be compared
    # the output is the value of similarity

def fit_transform(self, graphs):
    # return the kernel matrix given the adj matrix of the given set

def transform(self, graphs):
    # return the kernel matrix given the training set and the test set
```

4. The Manifold Technique

We are going here to answer these questions:

- what is a manifold technique and how to use one?
- which manifold techniques are available and where?

4.1 What is a Manifold Technique

It is also called Nonlinear dimensionality reduction. High-dimensional data, meaning data that requires more than two or three dimensions to represent, can be difficult to interpret. One approach to simplification is to assume that the data of interest lie on an embedded non-linear manifold within the higher-dimensional space. If the manifold is of low enough dimension, the data can be visualised in the low-dimensional space.

Consider a dataset represented as a matrix (or a database table), such that each row represents a set of attributes (or features or dimensions) that describe a particular instance of something. If the number of attributes is large, then the space of unique possible rows is exponentially large. Thus, the larger the dimensionality, the more difficult it becomes to sample the space. This causes many problems. Algorithms that operate on high-dimensional data tend to have a very high time complexity. Many machine learning algorithms, for example, struggle with high-dimensional data. This has become known as the curse of dimensionality. Reducing data into fewer dimensions often makes analysis algorithms more efficient, and can help machine learning algorithms make more accurate predictions. Humans often have difficulty comprehending data in many dimensions. Thus, reducing data to a small number of dimensions is useful for visualization purposes.

The reduced-dimensional representations of data are often referred to as "intrinsic variables". This description implies that these are the values from which the data was produced. For example, consider a dataset that contains images of a letter 'A', which has been scaled and rotated by varying amounts. Each image has 32x32 pixels. Each image can be represented as a vector of 1024 pixel values. Each row is a sample on a two-dimensional manifold in 1024-dimensional space (a Hamming space). The intrinsic dimensionality is two, because two variables (rotation and scale) were varied in order to produce the data. Information about the shape or look of a letter 'A' is not part of the intrinsic variables because it is the same in every instance. Nonlinear dimensionality reduction will discard the correlated information (the letter 'A') and recover only the varying information (rotation and scale).

PCA (a linear dimensionality reduction algorithm) is used to reduce this same dataset into two dimensions, the resulting values are not so well organized.

By comparison, if Principal component analysis, which is a linear dimensionality reduction algorithm, is used to reduce this same dataset into two dimensions, the resulting values are not so well organized. This demonstrates that the high-dimensional vectors (each representing a letter 'A') that sample this manifold vary in a non-linear manner.

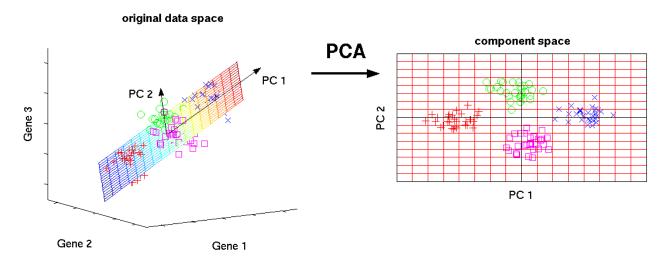
4.2 The available Manifold Techniques

PCA

Principal component analysis (PCA) is a technique that is useful for the compression and classification of data. The purpose is to reduce the dimensionality of a data set (sample) by finding a new set of variables, smaller than the original set of variables, that nonetheless retains most of the sample's information.

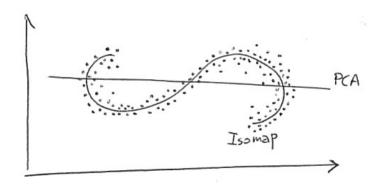
By information we mean the variation present in the sample, given by the correlations between the original variables. The new variables, called principal components (PCs), are uncorrelated, and are ordered by the fraction of the total information each retains.

More formally: given a sample of n observations on a vector of p variables. Define the first principal component of the sample by the linear transformation $z_1=a_1^Tx$ where the vector $a_1=(a_{11},\ldots,ap1)$ is chosen such that is maximum the $Var[z_1]$. You continue adding other dimensions but constraining the successive dimension being orthogonal to the previous one so having zero correlation. Another constraint is the fact that $a_k^Ta_k=1$.



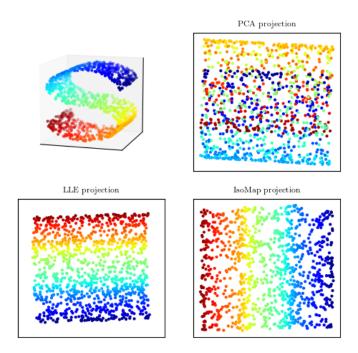
Isomap

Isomap is a combination of the Floyd–Warshall algorithm with classic Multidimensional Scaling. Classic Multidimensional Scaling (MDS) takes a matrix of pair-wise distances between all points and computes a position for each point. Isomap assumes that the pair-wise distances are only known between neighboring points, and uses the Floyd–Warshall algorithm to compute the pair-wise distances between all other points. This effectively estimates the full matrix of pair-wise geodesic distances between all of the points. Isomap then uses classic MDS to compute the reduced-dimensional positions of all the points.



Locally-linear embedding

Locally-Linear Embedding (LLE) has several advantages over Isomap, including faster optimization when implemented to take advantage of sparse matrix algorithms, and better results with many problems. LLE also begins by finding a set of the nearest neighbors of each point. It then computes a set of weights for each point that best describes the point as a linear combination of its neighbors. Finally, it uses an eigenvector-based optimization technique to find the low-dimensional embedding of points, such that each point is still described with the same linear combination of its neighbors. LLE tends to handle non-uniform sample densities poorly because there is no fixed unit to prevent the weights from drifting as various regions differ in sample densities.



5. Comparison

Train an SVM with the kernel chosen applying the manifold technique or not and show the difference

4.1 Training without Manifold

Training without Manifold

4.2 Training with Manifold

Training with Manifold

4.2 Results

Results of Manifold Techniques

	method	PPI_score	SHOCK_score
0	SPK-precomputed-no-RED	Acc: 49.17%	Acc: 0.0%
1	SPK-linear-no-RED	Acc: 75.14%	Acc: 43.0%
2	SPK-rbf-no-RED	Acc: 62.22%	Acc: 31.5%
3	WLK-precomputed-no-RED	Acc: 42.64%	Acc: 3.0%
4	WLK-linear-no-RED	Acc: 75.56%	Acc: 38.5%
5	WLK-rbf-no-RED	Acc: 47.78%	Acc: 26.0%
6	STK-precomputed-no-RED	Acc: 41.94%	Acc: 1.5%
7	STK-linear-no-RED	Acc: 73.47%	Acc: 42.5%
8	STK-rbf-no-RED	Acc: 67.36%	Acc: 39.5%
9	DSGK-precomputed-no-RED	Acc: 36.25%	Acc: 3.5%
10	DSGK-linear-no-RED	Acc: 79.17%	Acc: 42.0%
11	DSGK-rbf-no-RED	Acc: 67.5%	Acc: 30.0%
12	SPK-linear-ISO	Acc: 62.92%	Acc: 32.0%
13	SPK-rbf-ISO	Acc: 75.83%	Acc: 34.5%
14	WLK-linear-ISO	Acc: 53.47%	Acc: 22.5%
15	WLK-rbf-ISO	Acc: 64.03%	Acc: 33.0%
16	STK-linear-ISO	Acc: 56.81%	Acc: 17.0%
17	STK-rbf-ISO	Acc: 57.22%	Acc: 29.5%
18	DSGK-linear-ISO	Acc: 66.25%	Acc: 23.0%
19	DSGK-rbf-ISO	Acc: 73.19%	Acc: 33.0%
20	SPK-linear-LLE	Acc: 53.33%	Acc: 18.0%
21	SPK-rbf-LLE	Acc: 53.33%	Acc: 18.0%
22	WLK-linear-LLE	Acc: 53.33%	Acc: 19.5%
23	WLK-rbf-LLE	Acc: 53.33%	Acc: 19.5%
24	STK-linear-LLE	Acc: 53.33%	Acc: 11.0%
25	STK-rbf-LLE	Acc: 53.33%	Acc: 12.5%
26	DSGK-linear-LLE	Acc: 53.33%	Acc: 22.0%
27	DSGK-rbf-LLE	Acc: 53.33%	Acc: 22.0%

28	SPK-linear-TSNE	Acc: 56.67%	Acc: 39.5%
29	SPK-rbf-TSNE	Acc: 57.08%	Acc: 41.5%
30	WLK-linear-TSNE	Acc: 70.83%	Acc: 27.5%
31	WLK-rbf-TSNE	Acc: 70.83%	Acc: 41.5%
32	STK-linear-TSNE	Acc: 48.75%	Acc: 15.0%
33	STK-rbf-TSNE	Acc: 53.33%	Acc: 36.5%
34	DSGK-linear-TSNE	Acc: 61.67%	Acc: 25.5%
35	DSGK-rbf-TSNE	Acc: 74.31%	Acc: 33.5%

6. Conclusions

Explain here...

Bibliography

- 1. Manifold Learning and Dimensionality Reduction for Data Visualization... Stefan Kühn https://www.youtube.com/watch?v=j8080l9Pvic
- 2. Unsupervised Learning Explained (+ Clustering, Manifold Learning, ...) https://www.youtube.com/watch?v=-OEgiMH5aok
- 3. Unfolding Kernel Embeddings of Graphs https://www.dsi.unive.it/~atorsell/Al/graph/Unfolding.pdf
- 4. Graph Kernels https://www.dsi.unive.it/~atorsell/Al/graph/kernels.pdf
- 5. Manifold Learning https://scikit-learn.org/stable/modules/manifold.html
- 6. In-Depth: Manifold Learning https://jakevdp.github.io/PythonDataScienceHandbook/05.10-manifold-learning.html
- 7. What Is Manifold Learning? https://prateekvjoshi.com/2014/06/21/what-is-manifold-learning/
- 8. Manifold Learning: The Theory Behind It https://towardsdatascience.com/manifold-learning-the-theory-behind-it-c34299748fec
- 9. Introduction to manifold learning https://onlinelibrary.wiley.com/doi/pdf/10.1002/wics.122
 2
- 10. Is Manifold Learning for Toy Data only? https://www.stat.washington.edu/mmp/Talks/mani-mmp516.pdf
- 11. Proximity graphs for clustering and manifold learning https://papers.nips.cc/paper/2681-pr oximity-graphs-for-clustering-and-manifold-learning.pdf

- 12. Manifold Learning https://indico.in2p3.fr/event/6040/attachments/29587/36427/Manifold_learning.pdf
- 13. GRAPH CONSTRUCTION FOR MANIFOLD DISCOVERY https://people.cs.umass.edu/~ccarey/pubs/thesis.pdf
- 14. Machine Learning on Graphs: A Model and Comprehensive Taxonomy https://arxiv.org/pdf /2005.03675.pdf
- 15. Manifold Learning and Spectral Methods http://mlss2018.net.ar/slides/Pfau-1.pdf
- 16. Manifold Learning in the Age of Big Data https://www.stat.washington.edu/mmp/Talks/mani-sppexa19.pdf
- 17. manifold learning with applications to object recognition https://people.eecs.berkeley.edu/ ~efros/courses/AP06/presentations/ThompsonDimensionalityReduction.pdf
- 18. Representation Learning on Graphs: Methods and Applications https://www-cs.stanford.ed u/people/jure/pubs/graphrepresentation-ieee17.pdf
- 19. Data Analysis and Manifold Learning (DAML) http://perception.inrialpes.fr/people/Horaud/Courses/DAML_2011.html
- 20. Spectral Methods for Dimensionality Reduction http://cseweb.ucsd.edu/~saul/papers/smdr
 _ssl05.pdf
- 21. Robust Principal Component Analysis for Computer Vision http://files.is.tue.mpg.de/black/p apers/rpca.pdf
- 22. K-means Clustering via Principal Component Analysis http://ranger.uta.edu/~chqding/papers/KmeansPCA1.pdf
- 23. K-means Clustering & PCA https://www.inf.ed.ac.uk/teaching/courses/inf2b/labs/learn-lab3.
 pdf
- 24. Charting a Manifold https://papers.nips.cc/paper/2165-charting-a-manifold.pdf
- 25. Learning High Dimensional Correspondences from Low Dimensional Manifolds https://repository.upenn.edu/cgi/viewcontent.cgi?article=1131&context=ese_papers
- 26. Is manifold learning for toy data only?, Marina Meila https://www.youtube.com/watch?v=dd hbjCLljho
- 27. Locally Linear Embedding https://www.youtube.com/watch?v=scMntW3s-Wk&list=PL_AYx6i
 B_DjTXmIN126hH2wZc1aGWb0u9
- 28. A Global Geometric Framework for Nonlinear Dimensionality Reduction http://www.robots.cox.ac.uk/~az/lectures/ml/tenenbaum-isomap-Science2000.pdf
- 29. Laplacian Eigenmaps for dimensionality reduction and data representation http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.9.5888&rep=rep1&type=pdf
- 30. Non-linear dimension reduction http://statweb.stanford.edu/~tibs/sta306bfiles/isomap.pdf
- 31. Isomap Isometric feature mapping https://www.cise.ufl.edu/class/cap6617fa17/ISOMAP.p
 ptx.pdf
- 32. Pattern Search Multidimensional Scaling https://arxiv.org/pdf/1806.00416.pdf
- 33. An Introduction to Locally Linear Embedding https://cs.nyu.edu/~roweis/lle/papers/lleintro.
 pdf
- 34. Nonlinear Dimensionality Reduction by Locally Linear Embedding http://www.robots.ox.ac.uk/~az/lectures/ml/lle.pdf
- 35. Manifold Learning: The Price of Normalization http://www.jmlr.org/papers/volume9/goldberg08a.pdf
- 36. Dimensionality Estimation, Manifold Learning and Function Approximation using Tensor Voting http://www.jmlr.org/papers/volume11/mordohai10a/mordohai10a.pdf
- 37. Riemannian Manifolds An Introduction to Curvature https://www.maths.ed.ac.uk/~v1ranic

- k/papers/leeriemm.pdf
- 38. Adaptive Neighboring Selection Algorithm Based on Curvature Prediction in Manifold Learning https://arxiv.org/pdf/1704.04050.pdf
- 39. Nonlinear Manifold Learning Part One: Background, LLE, IsoMap http://web.mit.edu/6.454/www/www_fall_2003/ihler/slides.pdf
- 40. Sparse Manifold Clustering and Embedding http://cis.jhu.edu/~ehsan/Downloads/SMCE-NI
 PS11-Ehsan.pdf
- 41. Sampling Methods for the Nystrom Method http://www.jmlr.org/papers/volume13/kumar1 2a/kumar12a.pdf
- 42. On the Nystro'm Method for Approximating a Gram Matrix for Improved Kernel-Based Learning http://www.jmlr.org/papers/volume6/drineas05a/drineas05a.pdf
- 43. Ensemble Nystro"m Method https://papers.nips.cc/paper/3850-ensemble-nystrom-method.
 pdf
- 44. Revisiting the Nystr"om method for improved large-scale machine learning http://proceedings.mlr.press/v28/gittens13.pdf
- 45. Spectral Grouping Using the Nystro"m Method https://people.eecs.berkeley.edu/~malik/papers/FBCM-nystrom.pdf
- 46. LAURENS VAN DER MAATEN
- 47. http://lvdmaaten.github.io/drtoolbox/
- 48. Dimensionality Reduction: A Comparative Review. http://lvdmaaten.github.io/publications/papers/TR_Dimensionality_Reduction_Review_2009.pdf
- 49. Visualizing Data using t-SNE http://lvdmaaten.github.io/publications/papers/JMLR_2008.pdf
- 50. Laplacian Eigenmaps for Dimensionality Reduction and Data Representation https://www2.imm.dtu.dk/projects/manifold/Papers/Laplacian.pdf
- 51. Laplacian eigenmaps and spectral techniquesfor embedding and clustering http://web.cse. ohio-state.edu/~belkin.8/papers/LEM_NIPS_01.pdf
- 52. Diffusion Maps: Analysis and Applications https://core.ac.uk/download/pdf/1568327.pdf
- 53. Computing and Processing Correspondences with Functional Maps http://www.lix.polytech.nique.fr/~maks/fmaps_SIG17_course/notes/siggraph17_course_notes.pdf
- 54. Vector Diffusion Maps and the Connection Laplacian http://citeseerx.ist.psu.edu/viewdoc/doinent-10.1.1.435.8939&rep=rep1&type=pdf
- 55. Nonlinear Dimensionality Reduction II: Diffusion Maps https://www.stat.cmu.edu/~cshalizi/350/lectures/15/lecture-15.pdf
- 56. Understanding the geometry of transport: diffusion maps for Lagrangian trajectory data unravel coherent sets https://arxiv.org/pdf/1603.04709.pdf
- 57. Diffusion Maps, Spectral Clustering and Eigenfunctions of Fokker-Planck Operators https://papers.nips.cc/paper/2942-diffusion-maps-spectral-clustering-and-eigenfunctions-of-fokker-planck-operators.pdf
- 58. Diffusion Maps for Signal Processing http://www.eng.biu.ac.il/~gannot/articles/Diffusion%2
 0Magazine.pdf
- 59. Applications of Diffusion Wavelets https://core.ac.uk/reader/1145976
- 60. Diffusion Wavelets and Applications http://helper.ipam.ucla.edu/publications/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5/mgaws5-5164.pdf
- 61. Value Function Approximation with Diffusion Wavelets and Laplacian Eigenfunctions https://people.cs.umass.edu/~mahadeva/papers/nips-paper1-v5.pdf
- 62. Wavelet methods in statistics: Some recent developments and their applications https://arxiv.org/pdf/0712.0283.pdf

- 63. StatQuest: t-SNE, Clearly Explained https://www.youtube.com/watch?v=NEaUSP4YerM
- 64. Shortest-path kernels on graphs https://www.dbs.ifi.lmu.de/~borgward/papers/BorKri05.p df
- 65. Generalized Shortest Path Kernel on Graphs https://arxiv.org/pdf/1510.06492.pdf
- 66. Shortest-Path Graph Kernels for Document Similarity https://www.aclweb.org/anthology/D
 17-1202.pdf
- 67. An Introduction to Graph Kernels https://ethz.ch/content/dam/ethz/special-interest/bsse/b orgwardt-lab/documents/slides/CA10_GraphKernels_intro.pdf
- 68. Fast shortest-path kernel computations using approximate methods http://publications.lib. chalmers.se/records/fulltext/215958/215958.pdf
- 69. Shortest-path kernels on graphs https://www.dbs.ifi.lmu.de/Publikationen/Papers/borgwar dt.pdf
- 70. Graphlet Kernels https://ethz.ch/content/dam/ethz/special-interest/bsse/borgwardt-lab/documents/slides/BNA09_3_4.pdf
- 71. Efficient graphlet kernels for large graph comparison http://proceedings.mlr.press/v5/sherv ashidze09a/shervashidze09a.pdf
- 72. The Graphlet Spectrum http://members.cbio.mines-paristech.fr/~nshervashidze/publicatio ns/KonSheBor09.pdf
- 73. Efficient graphlet kernels for large graph comparison https://people.mpi-inf.mpg.de/~mehlhorn/ftp/AISTATS09.pdf
- 74. Generalized graphlet kernels for probabilistic inference in sparse graphs http://citeseerx.ist
 .psu.edu/viewdoc/download?doi=10.1.1.720.557&rep=rep1&type=pdf
- 75. Graphlet Decomposition: Framework, Algorithms, and Applications https://nickduffield.net/download/papers/KAIS-D-15-00611R2.pdf
- 76. Efficient Graphlet Counting for Large Networks https://www.cs.purdue.edu/homes/neville/papers/ahmed-et-al-icdm2015.pdf
- 77. Halting in Random Walk Kernels https://papers.nips.cc/paper/5688-halting-in-random-walk-kernels.pdf
- 78. Graph Kernels http://www.jmlr.org/papers/volume11/vishwanathan10a/vishwanathan10a.
- 79. Fast Random Walk Graph Kernel http://www.cs.cmu.edu/~ukang/papers/fast_rwgk.pdf
- 80. GRAPH KERNELS https://sites.cs.ucsb.edu/~xyan/tutorial/GraphKernels.pdf
- 81. Fast Computation of Graph Kernels https://pdfs.semanticscholar.org/4459/336b270333c36 66310a332acfb2641b27c0d.pdf
- 82. Weisfeiler-Lehman Graph Kernels http://www.jmlr.org/papers/volume12/shervashidze11a/shervashidze11a/shervashidze11a.pdf
- 83. The Weisfeiler-Lehman Kernel https://ethz.ch/content/dam/ethz/special-interest/bsse/borg wardt-lab/documents/slides/CA10 WeisfeilerLehman.pdf
- 84. Wasserstein Weisfeiler-Lehman Graph Kernels https://papers.nips.cc/paper/8872-wasserst ein-weisfeiler-lehman-graph-kernels.pdf
- 85. Global Weisfeiler-Lehman Kernels https://arxiv.org/pdf/1703.02379.pdf
- 86. A Persistent Weisfeiler–Lehman Procedure for Graph Classification http://proceedings.mlr.
 press/v97/rieck19a/rieck19a.pdf
- 87. A Fast Approximation of the Weisfeiler-Lehman Graph Kernel for RDF Data https://work.del aat.net/awards/2013-09-23-paper.pdf
- 88. RDRToolbox A package for nonlinear dimension reduction with Isomap and LLE. https://www.bioconductor.org/packages/release/bioc/vignettes/RDRToolbox/inst/doc/vignette.pdf

- 89. An Introduction to Diffusion Maps https://inside.mines.edu/~whereman/talks/delaPorte-He rbst-Hereman-vanderWalt-DiffusionMaps-PRASA2008.pdf
- 90. Convergence of Laplacian Eigenmaps http://papers.neurips.cc/paper/2989-convergence-of-laplacian-eigenmaps.pdf
- 91. Laplacian Eigenmap for Image Retrieval http://people.cs.uchicago.edu/~niyogi/papersps/papersps/paper.pdf
- 92. Quantum Laplacian Eigenmap https://arxiv.org/pdf/1611.00760.pdf
- 93. Laplacian Eigenmaps from Sparse, Noisy Similarity Measurements https://arxiv.org/pdf/160 3.03972.pdf
- 94. Laplacian eigenmaps for multimodal groupwise image registration <a href="https://www.google.com/url?sa=t&rct=j&q=&esrc=s&source=web&cd=&ved=2ahUKEwjlwqKVvqvqAhVU6qYKHeM7AA4QFjAKegQlChAB&url=https%3A%2F%2Frepub.eur.nl%2Fpub%2F100364%2FRepub_100364_O-A.pdf&usg=AOvVaw2xVygozmBAE735xOQ8m_rQ
- 95. Nonlinear Dimensionality Reduction I: Local Linear Embedding https://www.stat.cmu.edu/~cshalizi/350/lectures/14/lecture-14.pdf
- 96. A NOTE ON THE LOCALLY LINEAR EMBEDDING ALGORITHM https://core.ac.uk/reader/2174
 7186
- 97. LOCALL Y LINEAR EMBEDDING ALGORI THM http://jultika.oulu.fi/files/isbn9514280415.pdf
- 98. Truly Incremental Locally Linear Embedding http://ai.stanford.edu/~schuon/learning/inclle.pdf
- 99. Supervised locally linear embedding http://rduin.nl/papers/icann_03_lle.pdf
- 100. Me gusta en YouTube: On Graph Kernels https://www.youtube.com/watch?v=xwVOarJGD7
 Q
- 101. Embedding & Manifold Learning https://moodle.unive.it/mod/resource/view.php?id=17667
 3
- 102. Wednesday 29/4/2020 https://drive.google.com/file/d/1jQfGEqw9CYOHYAiIIdxmG7zc-7GKh_5sy/view
- 103. Monday 27/4/2020 https://drive.google.com/file/d/1IM9csbR7s-ec2_1_ck1GzOoZeaRAaFGx/v iew
- 104. Wednesday 22/4/2020 https://drive.google.com/file/d/1wzkmQJ344orELbQKoVL1P-yrAMofi3v8/view
- 105. On Graph Kernels https://www.youtube.com/watch?v=xwVOarJGD7Q
- 106. Weisfeiler-Lehman Neural Machine for Link Prediction <a href="https://www.youtube.com/watch?v="https://www.youtube.com/watch?
- 107. Deep Graph Kernels https://www.youtube.com/watch?v=hqbMbTlTpXU
- 108. Graph Theory FAQs: 03. Isomorphism Using Adjacency Matrix https://www.youtube.com/w atch?v=UCle3Smvh1s
- 109. Deep Graph Kernels https://dl.acm.org/doi/pdf/10.1145/2783258.2783417
- 110. GRAPHLET COUNTING http://evlm.stuba.sk/APLIMAT2018/proceedings/Papers/0442_Hocevar.pdf
- 111. Graphlet based network analysis https://docs.lib.purdue.edu/cgi/viewcontent.cgi?article=22
 07&context=open_access_dissertations
- 112. Graphlet Counting for Topological Data Analysis https://webthesis.biblio.polito.it/7641/1/tesi.pdf
- 113. Estimating Graphlet Statistics via Lifting https://arxiv.org/pdf/1802.08736.pdf
- 114. GEM https://github.com/palash1992/GEM
- 115. awesome-graph-classification https://github.com/benedekrozemberczki/aweso/me-graph-c

- <u>lassification</u>
- 116. node2vec: Embeddings for Graph Data https://towardsdatascience.com/node2vec-embedd ings-for-graph-data-32a866340fef
- 117. Graph Embedding Graph Analysis and Graph Learning https://maelfabien.github.io/machi nelearning/graph_5/#
- 118. DeepWalk: Implementing Graph Embeddings in Neo4j https://neo4j.com/blog/deepwalk-im-plementing-graph-embeddings-in-neo4j/
- 119. Inference on Graphs with Support Vector Machines http://members.cbio.mines-paristech.fr /~jvert/talks/040206insead/insead.pdf
- 120. sklearn.manifold.SpectralEmbedding https://scikit-learn.org/stable/modules/classes.html# module-sklearn.manifold)
- 121. sklearn.manifold.LocallyLinearEmbedding https://scikit-learn.org/stable/modules/generate d/sklearn.manifold.LocallyLinearEmbedding.html#sklearn-manifold-locallylinearembedding
- 122. Graph Classification https://www.csc2.ncsu.edu/faculty/nfsamato/practical-graph-mining-with-R/slides/pdf/Classification.pdf
- 123. SVMS and kernel methods for graphs https://courses.cs.ut.ee/2011/graphmining/Main/KernelMethodsForGraphs
- 124. Graph Representation Learning and Graph Classification https://www.cs.uoregon.edu/Reports/AREA-201706-Riazi.pdf
- 125. GraKeL: A Graph Kernel Library in Python https://github.com/ysig/GraKeL
- 126. Fast Subtree kernels on graphs https://papers.nips.cc/paper/3813-fast-subtree-kernels-on-graphs.pdf
- 127. weisfeiler lehman isomorphism test https://davidbieber.com/post/2019-05-10-weisfeiler-lehman-isomorphism-test/
- 128. A tutorial on Principal Components Analysis http://www.cs.otago.ac.nz/cosc453/student_tutorials/principal_components.pdf

Appendix

Appendix 1

NP-completeness

A decision problem C is NP-complete iff

- C is in NP
- C is NP-hard, i.e. every other problem in NP is reducible to it.