



Manifold Learning and Graph Kernels

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

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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

Isomap

Locally-linear embedding

Laplacian eigenmaps

Diffusion maps

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 discriminative 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 adjacency matrices of the graphs and of the labels. the files `graphxxx.csv` contain the adjacency matrices, one per file, while the file `labels.csv` contains 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 represent 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).

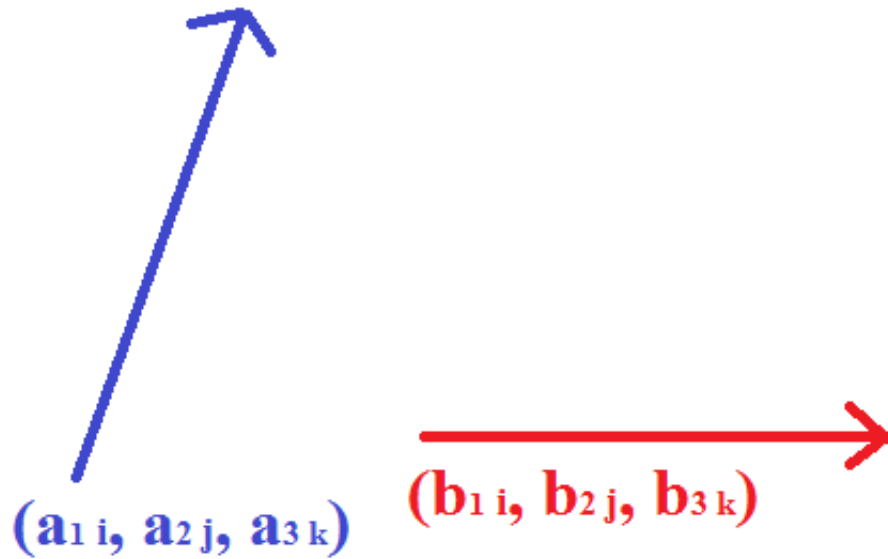
3. The Graph Kernel

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 $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^m$ 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 $\varphi(\mathbf{x})^T \varphi(\mathbf{y})$. A kernel is a function k that corresponds to this dot product, i.e. $k(\mathbf{x}, \mathbf{y}) = \varphi(\mathbf{x})^T \varphi(\mathbf{y})$. So Kernels give a way to compute dot products in some feature space without even knowing what this space is and what is φ .



Dot Product=

$$(a_1 \times b_1) + (a_2 \times b_2) + (a_3 \times b_3)$$

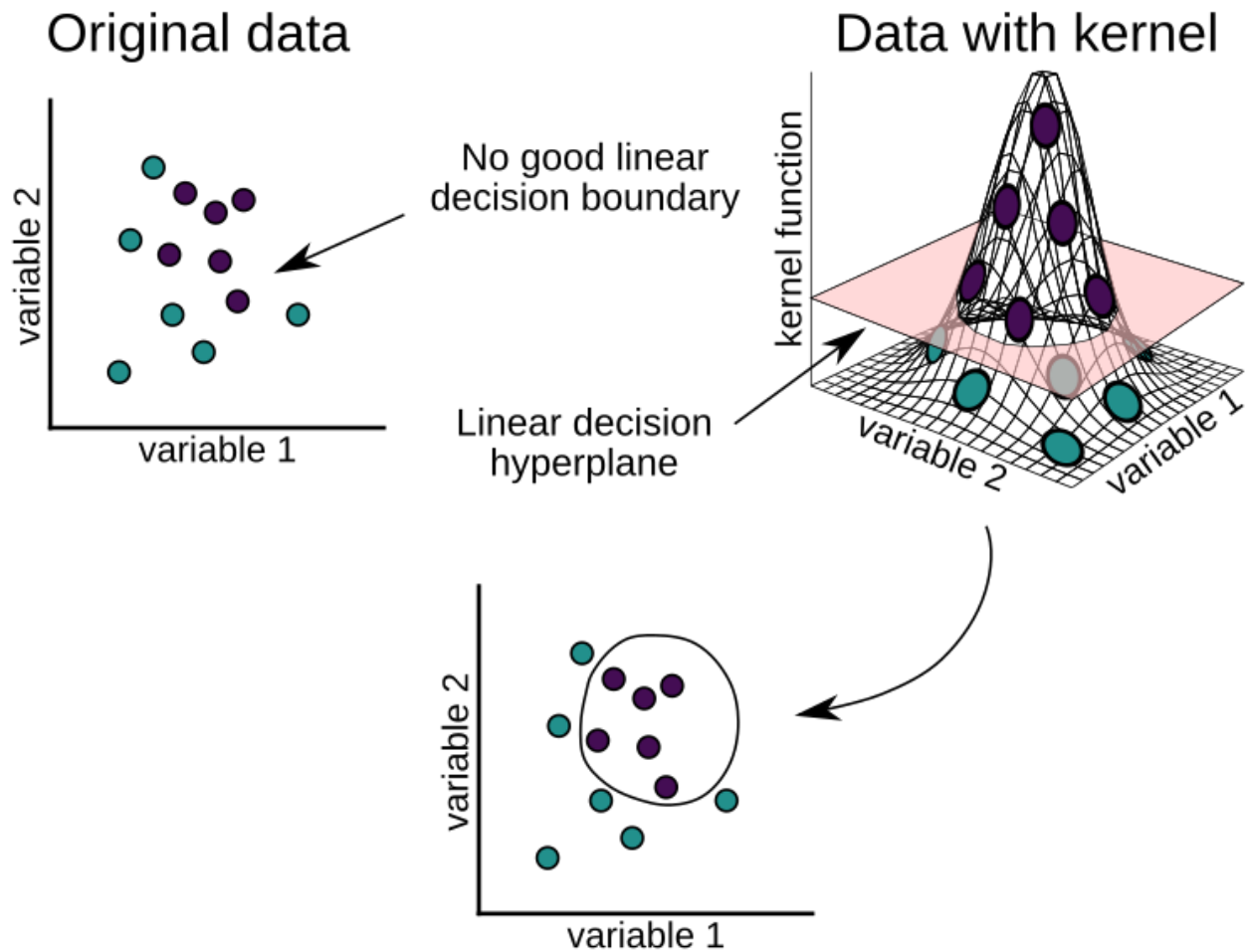
For example, consider a simple polynomial kernel $k(x, y) = (1 + x^T y)^2$ with $x, y \in R^2$. This doesn't seem to correspond to any mapping function φ , it's just a function that returns a real number. Assuming that $x=(x_1, x_2)$ and $y=(y_1, y_2)$, let's expand this expression:

$$k(x, y) = (1 + x^T y)^2 = (1 + x_1 y_1 + x_2 y_2)^2 = 1 + x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 y_1 + 2x_2 y_2 + 2x_1 x_2 y_1 y_2$$

Note that this is nothing else but a dot product between two vectors

$(1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2)$ and $(1, y_1^2, y_2^2, \sqrt{2}y_1, \sqrt{2}y_2, \sqrt{2}y_1 y_2)$. So the kernel

$k(x, y) = (1 + x^T y)^2 = \varphi(x)^T \varphi(y)$ 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:

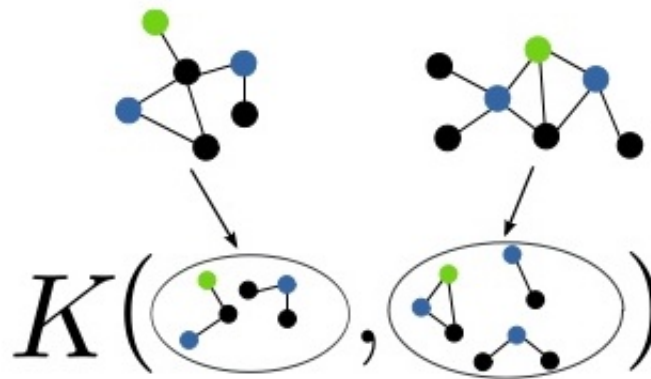
$$\sum_{i=1}^n \sum_{j=1}^n K(x_i, x_j) c_i c_j \geq 0$$

Theoretically, a Gram matrix $K \in \mathbb{R}^{n \times n}$ with respect to $\{x_1, \dots, x_n\}$ (sometimes also called a "kernel matrix"[3]), where $K_{ij} = k(x_i, x_j)$, 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

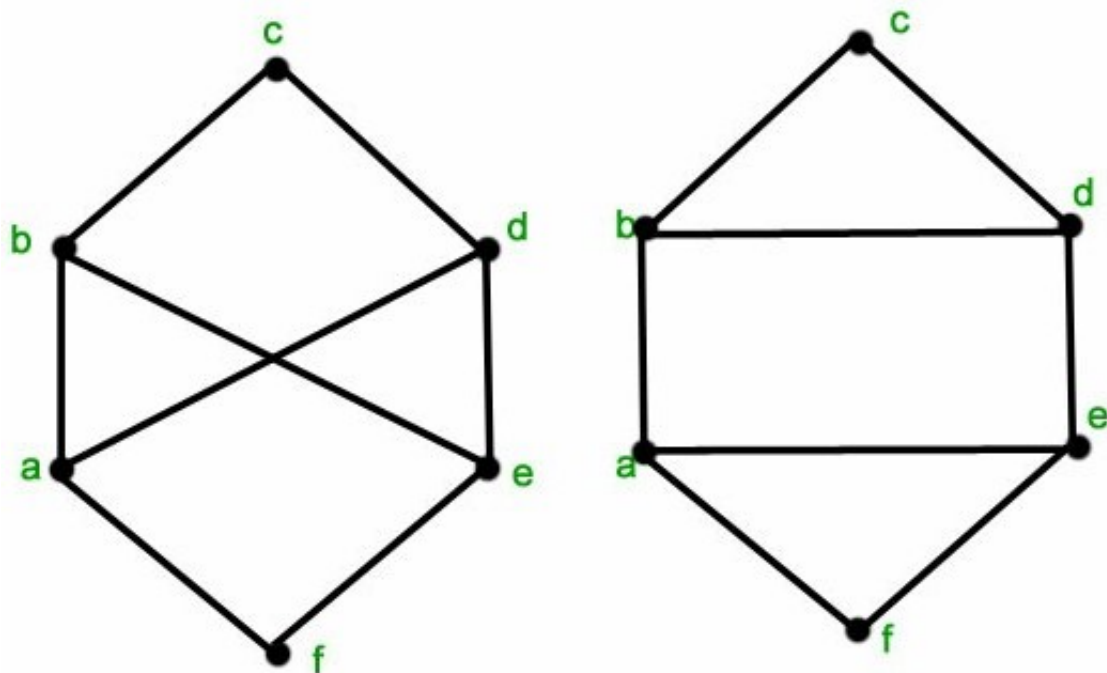
a Mercer kernel, k may still be referred to as a "kernel".

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 G_1 to the vertices of G_2 such that G_1 and G_2 are identical;



i.e. (x,y) is an edge of G_1 iff $(f(x),f(y))$ is an edge of G_2 . Then f is an isomorphism, and G_1 and G_2 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 G_1 that is isomorphic to a smaller graph G_2 . 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 Contrasts 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

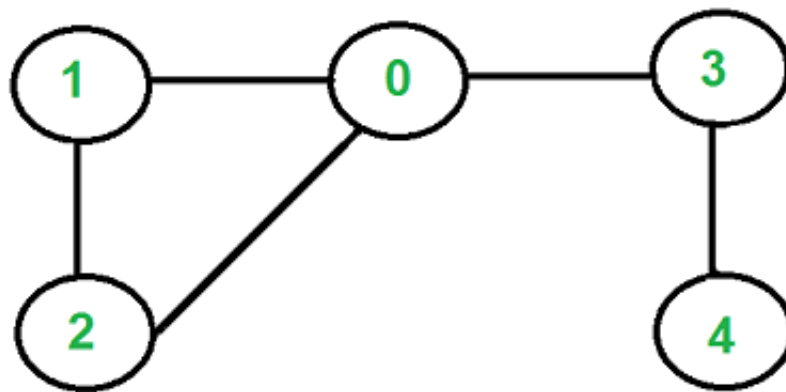
The principle is to count common walks in two input graphs G and G' , walks are sequences of nodes that allow repetitions of nodes. The Pros are that walks of length k can be computed by looking at the k -th power of the adjacency matrix, easy. Some Disadvantages are Runtime, Tottering and Halting. Some 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 $n \times n$ matrix A into an $n^2 \times 1$ vector $\text{vec}(A)$. 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 compute the Equation (2.1) by inverting the $n^2 \times n^2$ 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.
- 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 $q^T x$. Each iteration of CG takes $O(m^2)$ since the most expensive operation is the matrix-vector multiplication. Thus CG takes $O(m^{2i_F})$ time where i_F 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 $q^T x$ 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 ξ_1 is the largest magnitude eigenvalue of W . Similar to CG, the fixed point iteration method takes $O(m^{2i_F})$ time for i_F iterations, and has the same problems of requiring $O(m^2)$ memory.

Graphlet Kernel, Petri et al.

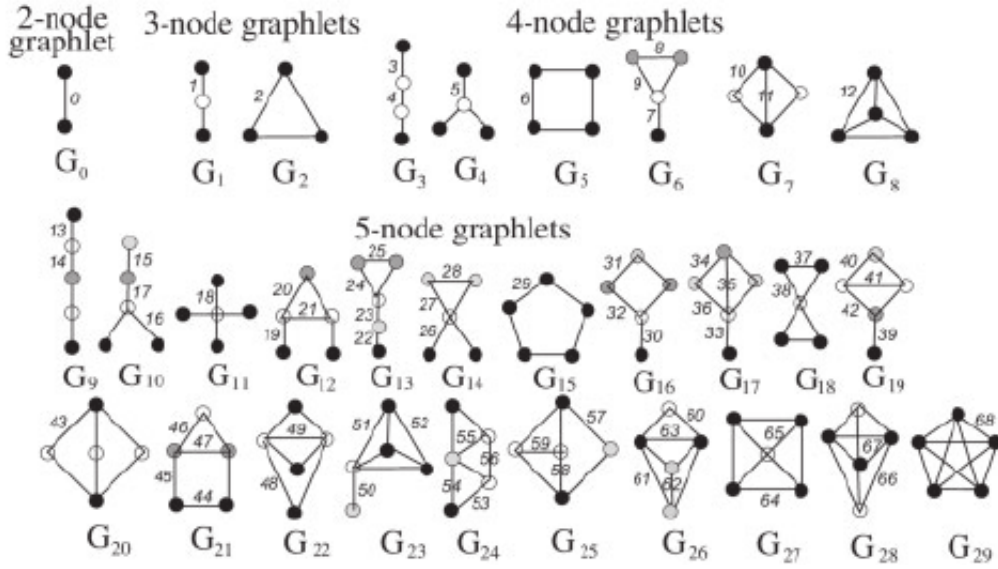
Graphlets are small connected non-isomorphic induced subgraphs of a large network. An induced subgraph must contain all edges between its nodes that are present in the large network, while a partial subgraph may contain only some of these edges.

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 $\mathcal{G} = \{\text{graphlet}(1), \dots, \text{graphlet}(N_k)\}$ be the set of size- k graphlets and G be a graph of size n . Define a vector f_G of length N_k whose i -th component corresponds to the frequency of occurrence of $\text{graphlet}(i)$ in G , $\#(\text{graphlet}(i) \subseteq G)$. We will call f_G the k -spectrum of G . This statistic is the foundation of our novel graph kernel. Given two graphs G and G' of size $n \geq k$, the graphlet kernel kg is defined as $kg(G, G') := f_G \cdot f_{G'}$.

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 f_G , we normalize the counts to probability vectors:

Clearly, if $G \cong G'$, then $f_G = f_{G'}$. But is the reverse true? It has been shown that when $n = k+1$ and $n \leq 11$, equality of k -spectra implies isomorphism. For $n > 11$, it is still a conjecture whether a graph of size n can be reconstructed from its subgraphs 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 $M_i(v) := l_0(v) = \ell(v)$.²
- 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 $f : \Sigma^* \rightarrow \Sigma$ such that $f(s_i(v)) = f(s_i(w))$ if and only if $s_i(v) = s_i(w)$.

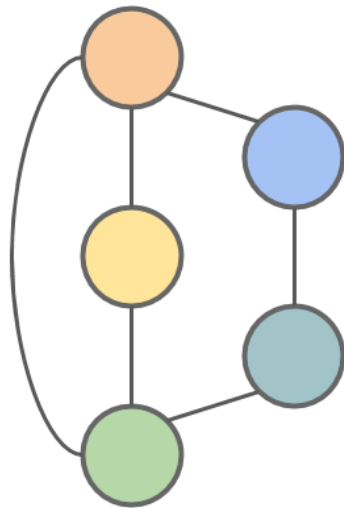
4: Relabeling

- Set $l_i(v) := f(s_i(v))$ for all nodes in G and G' .
-

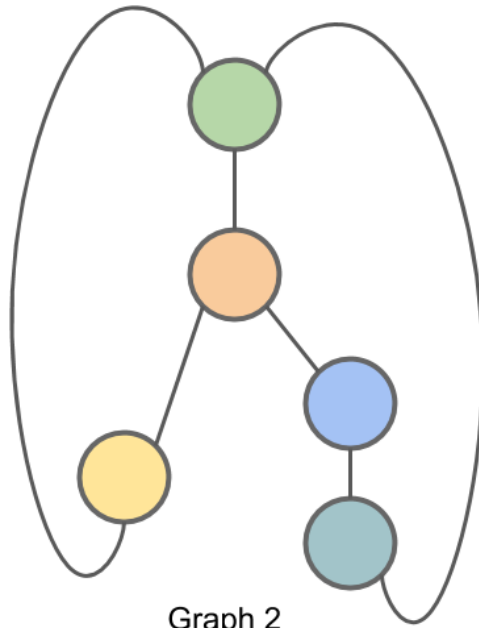
When using this method to determine graph isomorphism, it may be applied in parallel to the two graphs. The algorithm may be terminated early after iteration i if the sizes of partitions of nodes partitioned by compressed labels diverges between the two graphs; if this is the case, the graphs are not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



Graph 1

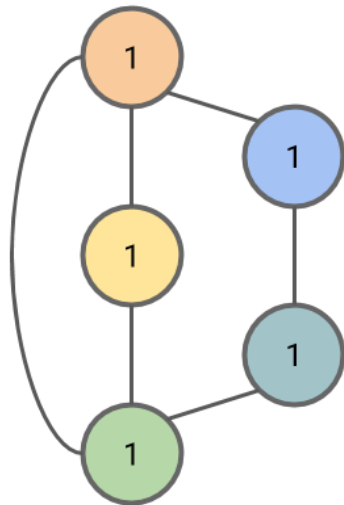


Graph 2

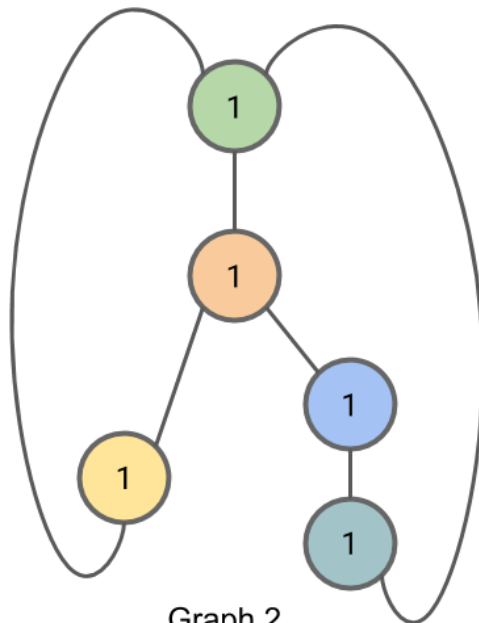
Figure: Graph 1 and Graph 2 are isomorphic. We will apply the Weisfeiler-Lehman isomorphism test to these graphs as a means of illustrating the test.

To initialize the algorithm (Step 1), we set $C_{0,n}=1$ for all nodes n .

C_0



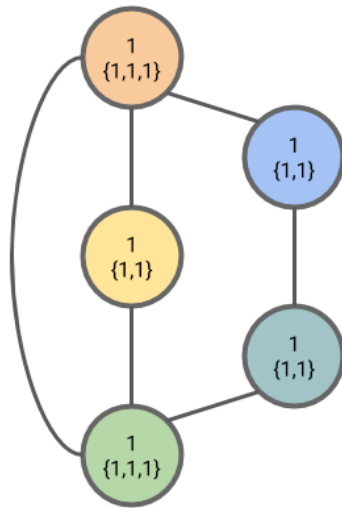
Graph 1



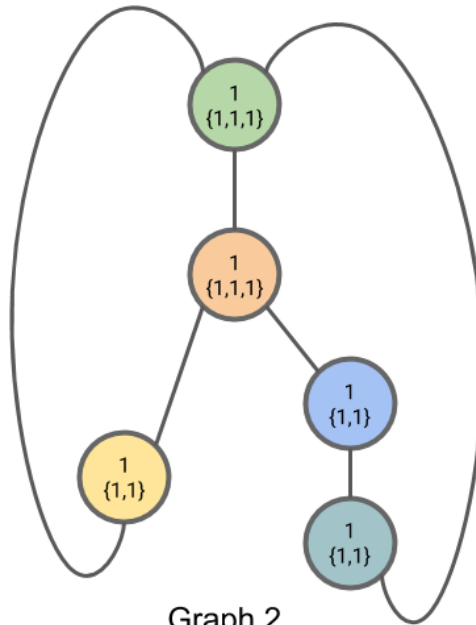
Graph 2

For iteration 1, Step 2, we compute L_1 . 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.

L_1



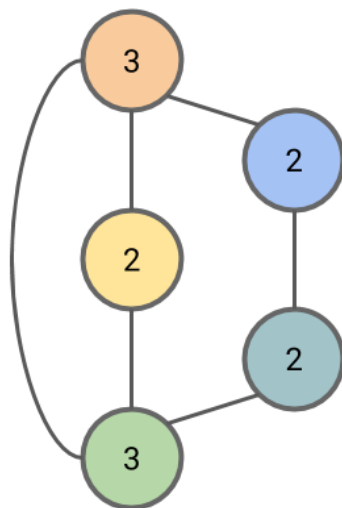
Graph 1



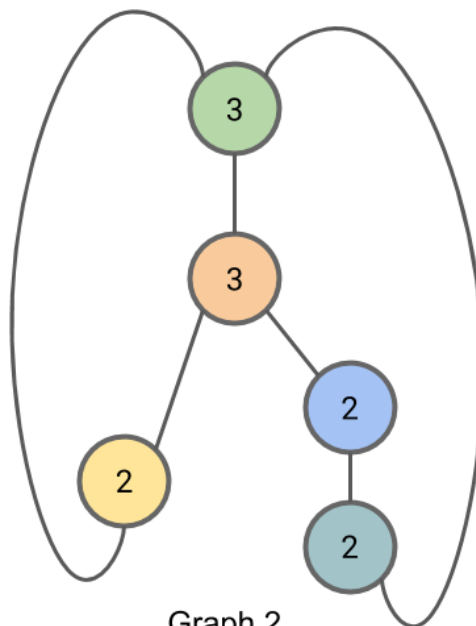
Graph 2

For iteration 1, Step 3, we introduce "compressed" labels C_1 for the nodes:

C_1



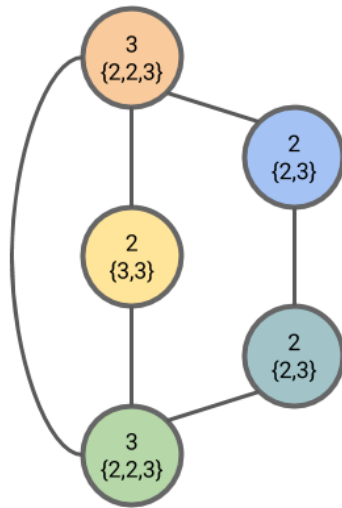
Graph 1



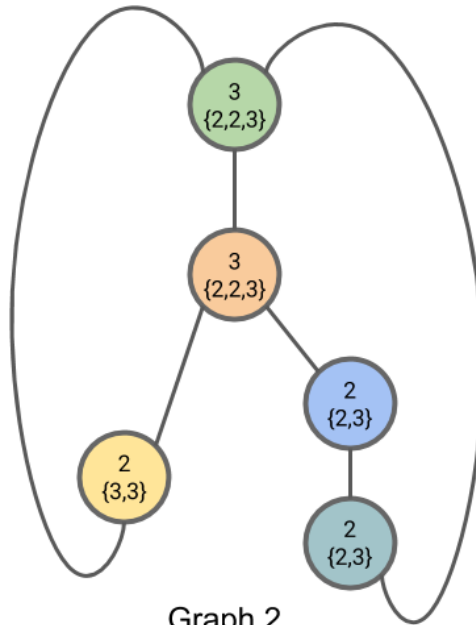
Graph 2

We now begin iteration 2. In iteration 2, Step 2, we compute L_2 :

L_2



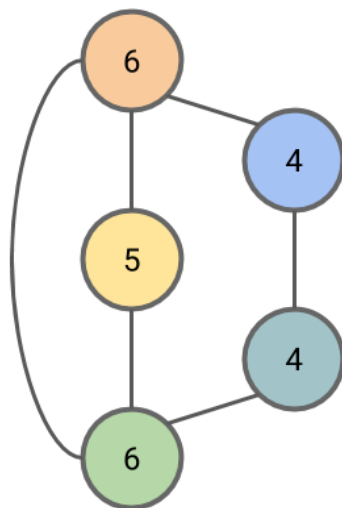
Graph 1



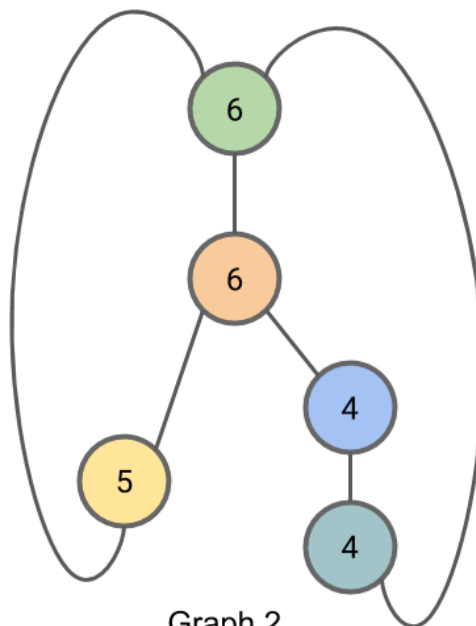
Graph 2

In iteration 2, Step 3, we compute C_2 :

C_2

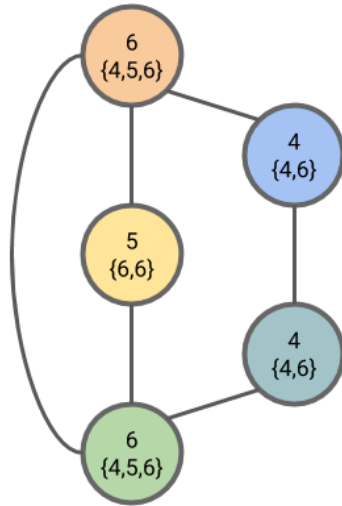


Graph 1

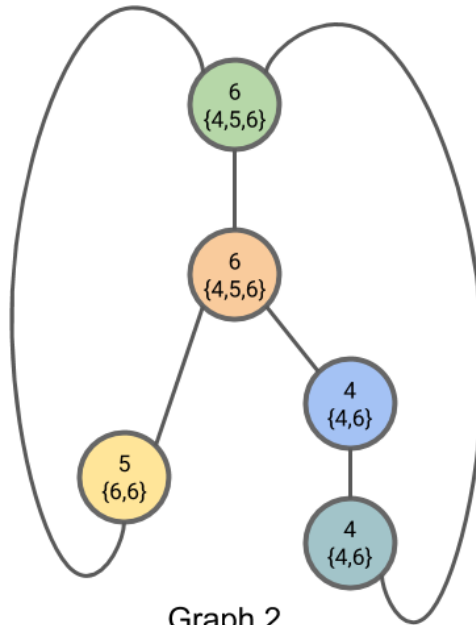


Graph 2

In iteration 3, Step 2, we compute L_3 :

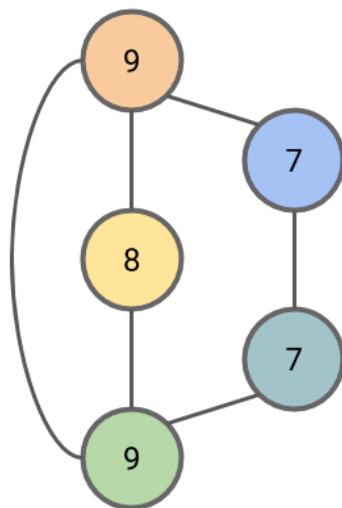
L_3 

Graph 1

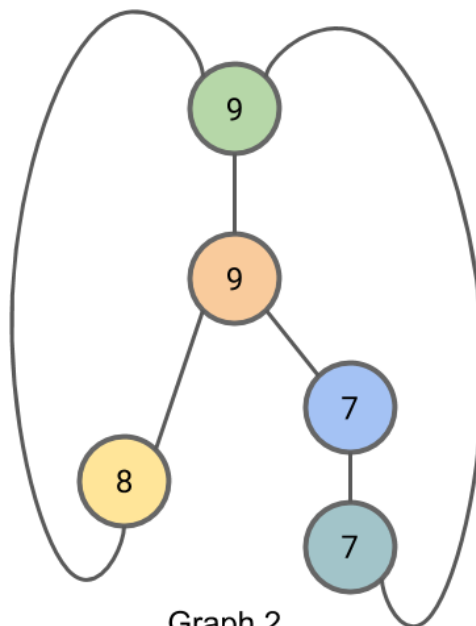


Graph 2

In iteration 3, Step 3, we compute C_3 :

 C_3 

Graph 1



Graph 2

Since the partition of nodes by compressed label has not changed from C_2 to C_3 , 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, g1adj, g2adj):
        # launch similarity measure Weisfeiler-lehman kernel

    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 ?

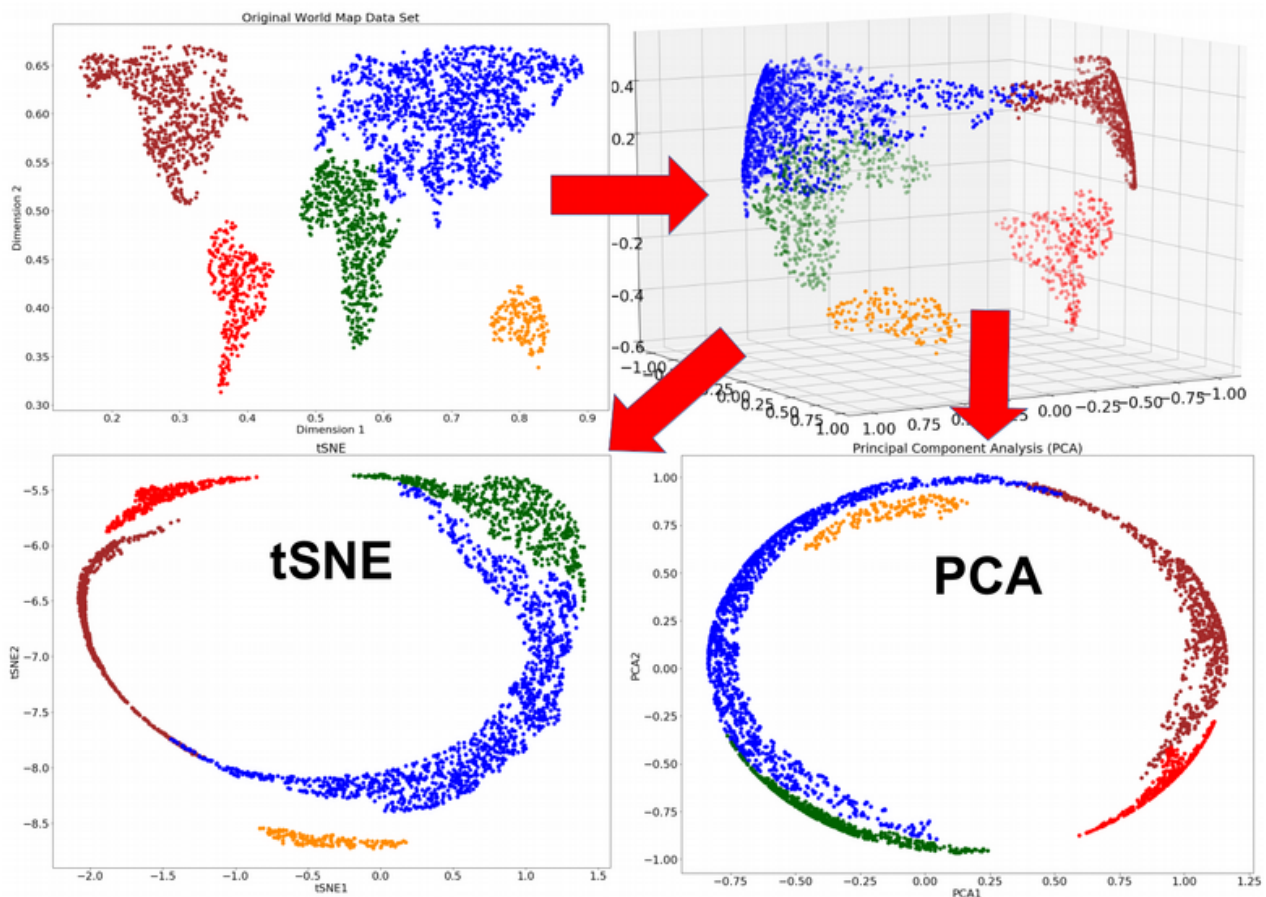
4.1 What is a Manifold Technique

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.

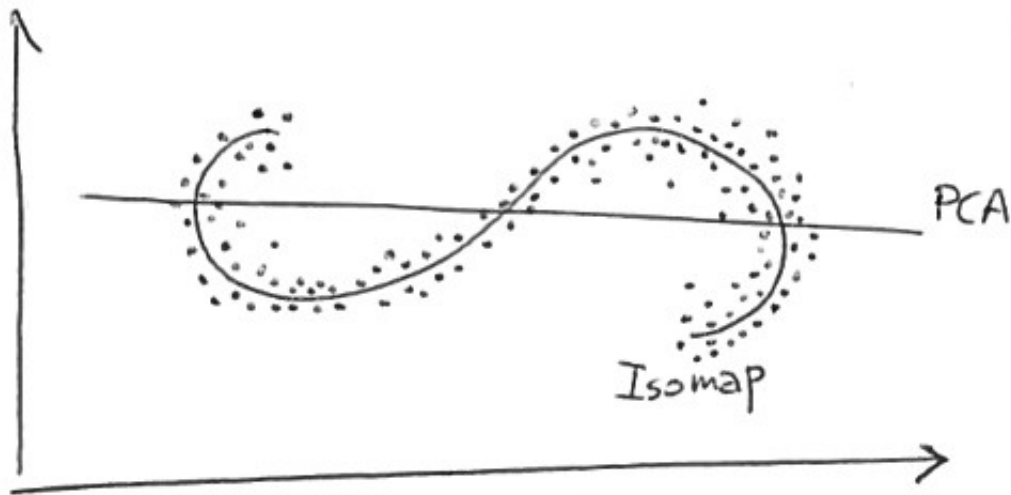


By comparison, if Principal component analysis, which is a linear dimensionality reduction algorithm, is used to reduce this same dataset into two dimensions, the resulting values are not so well organized. This demonstrates that the high-dimensional vectors (each representing a letter 'A') that sample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

4.2 The available Manifold Techniques

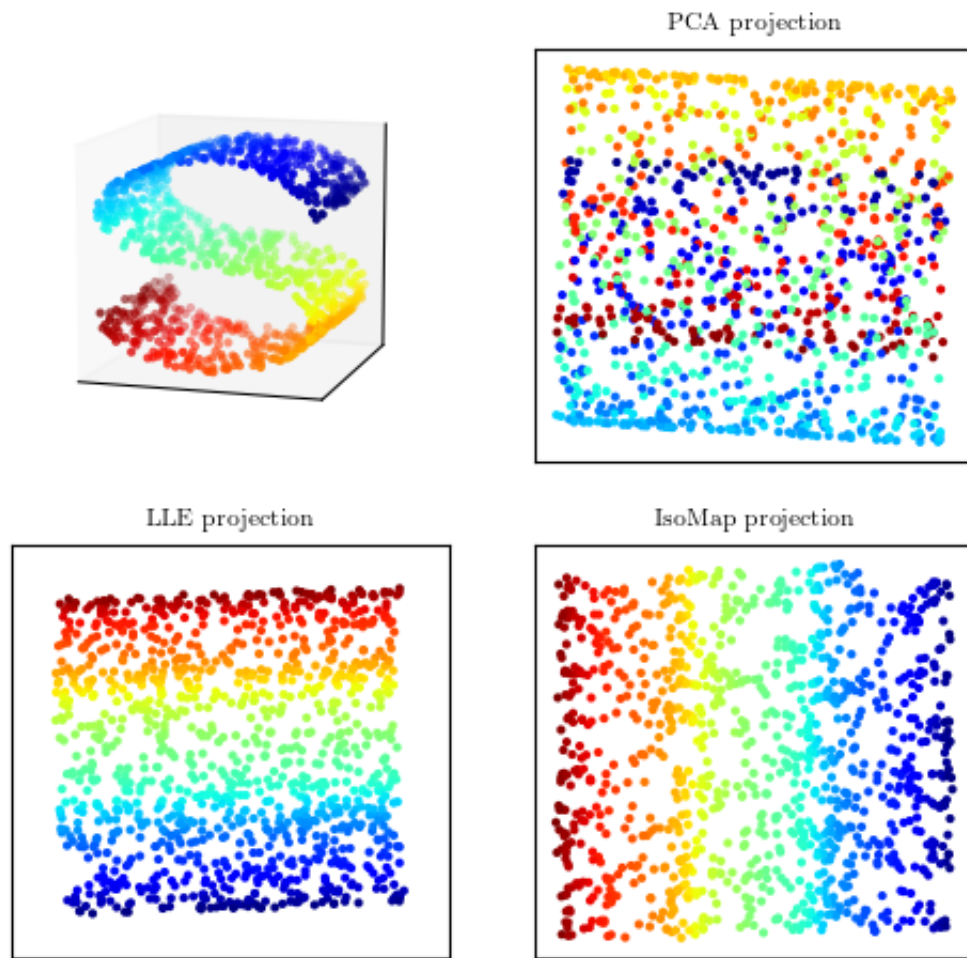
Isomap

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.



Laplacian eigenmaps

Laplacian Eigenmaps uses spectral techniques to perform dimensionality reduction. This technique relies on the basic assumption that the data lies in a low-dimensional manifold in a high-dimensional space. This algorithm cannot embed out-of-sample points, but techniques based on Reproducing kernel Hilbert space regularization exist for adding this capability.[9] Such techniques can be applied to other nonlinear dimensionality reduction algorithms as well.

Traditional techniques like principal component analysis do not consider the intrinsic geometry of the data. Laplacian eigenmaps builds a graph from neighborhood information of the data set. Each data point serves as a node on the graph and connectivity between nodes is governed by the proximity of neighboring points (using e.g. the k-nearest neighbor algorithm). The graph thus generated can be considered as a discrete approximation of the low-dimensional manifold in the high-dimensional space. Minimization of a cost function based on the graph ensures that points close to each other on the manifold are mapped close to each other in the low-dimensional space, preserving local distances. The eigenfunctions of the Laplace–Beltrami operator on the manifold serve as the embedding dimensions, since under mild conditions this operator has a countable spectrum that is a basis for square integrable functions on the manifold (compare to Fourier series on the unit circle manifold). Attempts to place Laplacian eigenmaps on solid theoretical ground have met with some success, as under certain nonrestrictive assumptions, the

graph Laplacian matrix has been shown to converge to the Laplace–Beltrami operator as the number of points goes to infinity.[10] Matlab code for Laplacian Eigenmaps can be found in algorithms[11] and the PhD thesis of Belkin can be found at the Ohio State University.[12]

In classification applications, low dimension manifolds can be used to model data classes which can be defined from sets of observed instances. Each observed instance can be described by two independent factors termed 'content' and 'style', where 'content' is the invariant factor related to the essence of the class and 'style' expresses variations in that class between instances.

[13]Unfortunately, Laplacian Eigenmaps may fail to produce a coherent representation of a class of interest when training data consist of instances varying significantly in terms of style.[14] In the case of classes which are represented by multivariate sequences, Structural Laplacian Eigenmaps has been proposed to overcome this issue by adding additional constraints within the Laplacian Eigenmaps neighborhood information graph to better reflect the intrinsic structure of the class.[15] More specifically, the graph is used to encode both the sequential structure of the multivariate sequences and, to minimise stylistic variations, proximity between data points of different sequences or even within a sequence, if it contains repetitions. Using dynamic time warping, proximity is detected by finding correspondences between and within sections of the multivariate sequences that exhibit high similarity. Experiments conducted on vision-based activity recognition, object orientation classification and human 3D pose recovery applications have demonstrate the added value of Structural Laplacian Eigenmaps when dealing with multivariate sequence data.[15] An extension of Structural Laplacian Eigenmaps, Generalized Laplacian Eigenmaps led to the generation of manifolds where one of the dimensions specifically represents variations in style. This has proved particularly valuable in applications such as tracking of the human articulated body and silhouette extraction.[16]

Diffusion maps

Diffusion maps leverages the relationship between heat diffusion and a random walk (Markov Chain); an analogy is drawn between the diffusion operator on a manifold and a Markov transition matrix operating on functions defined on the graph whose nodes were sampled from the manifold.[34](https://en.wikipedia.org/wiki/Nonlinear_dimensionality_reduction#cite_note-34) In particular, let a data set be represented by $X = [x_1, x_2, \dots, x_n] \in \Omega \subset \mathbb{R}^D$! $\{\mathbf{x}\} = [x_1, x_2, \dots, x_n] \in \Omega \subset \mathbb{R}^D$. The underlying assumption of diffusion map is that the high-dimensional data lies on a low-dimensional manifold of dimension d . Let X represent the data set and μ represent the distribution of the data points on X . Further, define a kernel which represents some notion of affinity of the points in X . The kernel k has the following properties[35]

k is symmetric

k is positivity preserving

Thus one can think of the individual data points as the nodes of a graph and the kernel k as defining some sort of affinity on that graph. The graph is symmetric by construction since the kernel is symmetric. It is easy to see here that from the tuple (X, k) one can construct a reversible Markov Chain. This technique is common to a variety of fields and is known as the graph Laplacian.

For example, the graph $K = (X, E)$ can be constructed using a Gaussian kernel.

In the above equation, $x_i \sim x_j$ denotes that x_i is a nearest neighbor of x_j . Properly, Geodesic distance should be used to actually measure distances on the manifold. Since the exact structure of the manifold is not available, for the nearest neighbors the geodesic distance is approximated by euclidean distance. The choice σ modulates our notion of proximity in the sense that if $\|x_i - x_j\|_2 \gg \sigma$ then $K_{ij} = 0$ and if $\|x_i - x_j\|_2 \ll \sigma$ then $K_{ij} = 1$. The former means that very little diffusion has taken place while the latter implies that the diffusion process is nearly complete. Different strategies to choose σ can be found in.[36]

In order to faithfully represent a Markov matrix, K must be normalized by the corresponding degree matrix D :

P now represents a Markov chain. $P(x_i, x_j)$ is the probability of transitioning from x_i to x_j in one time step. Similarly the probability of transitioning from x_i to x_j in t time steps is given by $P_t(x_i, x_j)$. Here P_t is the matrix P multiplied by itself t times.

The Markov matrix P constitutes some notion of local geometry of the data set X . The major difference between diffusion maps and principal component analysis is that only local features of the data are considered in diffusion maps as opposed to taking correlations of the entire data set.

K defines a random walk on the data set which means that the kernel captures some local geometry of data set. The Markov chain defines fast and slow directions of propagation through the kernel values. As the walk propagates forward in time, the local geometry information aggregates in the same way as local transitions (defined by differential equations) of the dynamical system.[35] The metaphor of diffusion arises from the definition of a family diffusion distance $\{D_t\}_{t \in \mathbb{N}}$

For fixed t , D_t defines a distance between any two points of the data set based on path connectivity: the value of $D_t(x, y)$ will be smaller the more paths that connect x to y and vice versa. Because the quantity $D_t(x, y)$ involves a sum over of all paths of length t , D_t is much more robust to noise in the data than geodesic distance. D_t takes into account all the relation between points x and y while calculating the distance and serves as a better notion of proximity than just Euclidean distance or even geodesic distance.

5. Comparison

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

	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%

4.1 Training without Manifold

Training without Manifold

4.2 Training with Manifold

Training with Manifold

4.2 Results

Results of Manifold Techniques

6. Conclusions

Explain here...

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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.