LARGE SCALE SEMI-SUPERVISED LEARNING

by

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(Under the Direction of Shannon Quinn)

ABSTRACT

Dealing with real world datasets can be difficult given the huge amounts in which they are available. Making predictions on such data can be challenging because the available ground truth is scarce. Given such a dataset, where available labeled data is far less than unlabeled data, we decide to adapt a large-scale semi-supervised learning eigenfunction approach to deal with such data. To serve the purpose of scalability, we simulate this approach in a distributed environment such as Apache Spark and provide a transductive as well as inductive approach to it. We also present a potential real world use case for this implementation. This use case deals with odor percept identification for millions of chemical substances composed of variant physicochemical properties that exist in nature. The end goal is to achieve a mapping of the chemical odors to their physicochemical properties.

INDEX WORDS: Eigenfunction, Semi-supervised Learning

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DEDICATION

To my parents, family, friends, colleagues and my advisor for their support, guidance and encouragement.

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I would like to thank Dr. Shannon Quinn for his immense guidance throughout this project and also during my academic career here at UGA. I thank him for introducing me to this ocean of Data Science and Machine Learning. I would also like to thank my colleagues and friends for their support and guidance during my graduate academic career.

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CHAPTER 1

INTRODUCTION

This chapter gives an introduction to the significance of semi-supervised learning and its potential applications. It discusses some of the different methods of semi-supervised learning.

1.1 Introduction

It is difficult to make predictions from real world datasets because of their large size and unstructured formats. A good example can be images from surveillance cameras. If predictions are to be made to detect objects in images, we need some ground truth to base our predictions on. But if these images are available in huge numbers, it is practically impossible to prepare ground truth by manually labeling more than a small fraction of the images. To make this problem somewhat more feasible, we can attempt to combine the small fraction of labeled data simultaneously with the unlabeled data in our model. In such a situation, where labeled data is orders of magnitude smaller than unlabeled data, a semi-supervised solution would work well.

Semi-supervised learning has two approaches, transductive and inductive learning.
In transductive learning, the whole dataset is used to build and train the model and predictions are made on all of the training data.

Inductive learning does not require the unseen data to be passed through the training phase again. Using the already trained model, predictions are made on unobserved data.

Our work is inspired by “Semi-supervised Learning in Gigantic Image Collections”, a 2009 paper by Fergus *et al*. The paper introduces an approach that is memory efficient for large scale processing. The approach is dominated by approximations to efficiently build a model for predictions. It uses semi-supervised learning approach by estimating a graph Laplacian matrix for the given dataset, numerically approximates the eigenfunctions, build interpolators and eventually derives the smoothness functions for the graph Laplacian. These smoothness functions are responsible for classifying unlabeled data into their corresponding classes depending on how smooth the function is with respect to the data points if they were depicted on a manifold.

The above description was the transductive learning approach offered by Semi-supervised learning. However, we anticipate the situation where we may wish to make predictions on future unobserved data without recomputing the entire semi-supervised model. Therefore, we have also implemented the inductive learning aspect of this approach. For a new unseen data point we interpolate this point using the interpolators we built during transductive learning and predict label for the interpolated values which are nothing but the smoothness functions.

This generic large scale semi-supervised learning algorithm could be used for other problems as well where known aspect of the data is very less as compared to the unknown aspect of the data. We also discuss the potential application of this approach on chemical olfactory data where we discuss the mapping of chemical substances to the odor perceptual space.

1.2 Major Contribution

We have implemented a large scale implementation of semi-supervised learning algorithm using the Eigenfunction approach as described in Fergus *et al* 2009. This algorithm is made to work in a distributed environment like Apache Spark which is capable of processing billions of data points using its parallel computing paradigm. The algorithm is a two stage algorithm where the first is the transductive learning part and second is the inductive learning part. The transductive learning part is in the form of a function called "fit ()". This function takes into consideration the labeled as well as unlabeled data available, builds a model and trains it on this data. Once trained, it first predicts the labels for the data used for training, using the labeled data to inform decisions on the unlabeled data. We make use of Expectation Maximization algorithm to predict labels for this data by clustering its resulting smoothness function values.

The next part of the algorithm is the inductive step. We have implemented a function "predict()" that works with new unobserved data points. It interpolates these points and predicts their labels. This part of the algorithm does not require the data points to go through the entire training process as explained in fit function. It just makes use of a few

parameters that were learned from the fit function and derives smoothness functions for the new data. Once we get those smoothness functions, we predict labels for them by clustering it using the previously trained expectation maximization model.
We also discuss the potential application of this algorithm on chemical olfactory data and present the computational olfaction as a case study.

The remainder of this document is structured as follows: CHAPTER 2 discusses the concept of semi-supervised learning using label propagation. CHAPTER 3 talks about available implementations of semi- supervised learning approaches and some background on semi-supervised learning with graph based methods. CHAPTER 4 discusses the algorithm in detail with the flowchart. CHAPTER 5 walks through the algorithm discussing its nuances with relevant results.
CHAPTER 6 sums up our approach with a conclusion. CHAPTER 7 discusses the potential use of this algorithm implementation in computational olfaction.

CHAPTER 2

SEMI-SUPERVISED LEARNING AND RELATED WORK

In this chapter, we discuss about Semi-supervised learning in general, work done on it and then discuss our approach in depth.

2.1 Motivation behind using the semi-supervised learning (SSL) approach

With less ground truth, it is infeasible to train a purely supervised classifier to accurately recognize the majority of possible data. Moreover, if we try to use unsupervised approach then we lose out on the information that the labeled data provides. Thus, we can say that semi-supervised learning works well on problems where there is a very small amount of labeled data relative to the amount of unlabeled data. Such algorithms are scalable and thus suitable for large datasets.

2.2 What is Semi-Supervised Learning?

Semi-supervised learning makes use of labeled as well as unlabeled data, and incorporating both into the initial training step of the model. Imagine n data points with d dimensions *(n <<< d)* which are independently and identically distributed. These n data points can be divided into 2 parts such that

$Xl := (x1, x2, \dots., xl);\ Yl := (y1, y2, \dots., yl) \dots..Xl, Yl\ are\ labeled\ points$

$Xu := x(l+1), \dots\dots, x(l+u) \dots\dots \mathit{are\ unlabeled\ points}$

The basic idea is, given a mapping of data points X to labels Y (f: X $\rightarrow$ Y), task is to learn a better predictor f by implicitly ordering these predictor functions f $\in$ F which is induced by the unlabeled data.

Ordinarily this ordering is interpreted as a prior over F or as a regularizer. But if after ordering, the target predictor function is found near the top of the ordering then you need less labeled data to learn this predictor function [2].

Semi-supervised learning can be interpreted in two forms, transductive learning and inductive learning. Given a set of labeled training set and an unlabeled test set, the idea of transduction is to perform predictions only for the test points. Whereas, in case of inductive learning the goal is to output a prediction function which is defined on the entire space X [4], therefore capable of predicting novel, unobserved data without rebuilding the entire model.

Semi-supervised learning was originally derived during estimation of the Fisher linear discriminant rule using unlabeled data was considered (Hosmer, 1973; McLachlan, 1977; O'Neill, 1978; McLachlan and Ganesalingam, 1982). Semi-supervised learning is suitable where each class-conditional density is Gaussian with equal covariance matrix. The likelihood of the model is then maximized using the labeled and unlabeled data with the help of clustering algorithms like expectation-maximization (EM) algorithm [18]. One essential prerequisite for semi-supervised learning is that the distribution of examples should be relevant to the classification problem especially with respect to the unlabeled data. Mathematically speaking, the information given by distribution $p(x)$ should prove to be useful in the inference of $p(y|x)$. Otherwise, the semi-supervised version would not prove to be more efficient over supervised version[4].

For semi-supervised learning to work efficiently, one of the following assumptions should hold.

1. Smoothness Assumption: Points that are close to each other are more likely to share the same label. "If two points $x1, x2$ in a high-density region are close, then so should be the corresponding outputs $y1, y2$." Thus the goal is to find smoothness function that fits the labeled data well. [4]
2. Cluster Assumption: If data clustering is known beforehand, then the points in the same cluster are more likely to share a label. Simply put, "if points are in the same cluster, they are likely to be of the same class". Cluster assumption can be thought of as a special case of smoothness assumption[4].
3. Manifold Assumption: "The high dimensional data lie roughly on a low dimensional manifold". This essentially means dimensionality reduction. The curse of dimensionality has been a bottleneck for most learning methods. In generative methods where data densities are used for estimation, data can grow exponentially with a higher number of dimensions. Also, there are discriminative methods which make use of pairwise distances. With high number of dimensions, these pairwise distances become less expressive and more correlated. "If the data happen to lie on a low-dimensional manifold, however, then the learning algorithm can essentially

operate in a space of corresponding dimension, thus avoiding the curse of dimensionality." [4].

Our approach is closely based on the Manifold Assumption since we will be dealing with data densities and a lot of numerical approximations at lower dimensions.

2.3 Methods in Semi-Supervised Learning

There are two main things to be addressed by a semi-supervised learning method: what implicit ordering of the functions is induced by the unlabeled data and how to find a predictor function at the top of this ordering that fits the labeled data well [2]. In simple words, we need to make a predictor that correctly identifies the data which we already know and makes well defined predictions on data that is not known. We take a look at different variations of semi-supervised learning in this section.

1. Generative Models: This method works on the assumption of joint probability distribution given by Bayes' rule, $p\langle x|y,\theta\rangle = p\langle y|\theta\rangle * p\langle x|y,\theta\rangle$, where $p\langle y|\theta\rangle$ is the class prior distribution and $p(x|y,\theta)$ is class conditional distribution. θ denotes the parameters of joint probability. Each θ is associated with a predictor function $f_\theta$such $f_\theta(x) = \underset{y}{\operatorname{argmax}}\, p\langle y|x,\theta\rangle$ and the chosen f_θ is the one that fits the labeled as well as unlabeled data well [2].
2. Low density Separation: Low density area is defined where there are fewer data points. A classic example of this would be transductive SVM. TSVM labels the unlabeled data that has maximal margin over all the data. TSVM then selects function $f^*(x) = h^*(x) + b$ by minimizing the following:

$$\underset{f}{\operatorname{argmin}} \frac{1}{l} \sum_{i=1}^{l} \max(1 - y_i f(x_i), 0) \; + \lambda_1 ||f||^2 + \lambda_2 \frac{1}{u} \sum_{i=l+1}^{l+u} \max\,(1 - |f(x)|, 0)$$

3. Graph-based methods: Graph based methods work on data in the form of a graph where every data point is a node in the graph. This graph can be constructed using either similarities between data points or connecting each point with its k nearest neighbors. The graph energy (Unnormalized Graph Laplacian) depicts how close or far two points are in the manifold space. This graph energy induces an implicit ordering of f ∈ F in ascending order [2]. The task comes down to finding functions that fit the labeled data well plus is ranked high in the order. These functions can be found by minimizing the following object function:

$$\underset{f}{\operatorname{argmin}} \frac{1}{l} \sum_{i=1}^{l} \mathrm{c}(f(x_i), y_i) \; + \lambda_1 ||f||^2 + \lambda_2 \sum_{i,j=1}^{l+u} w_{ij} \left(f(x_i) - f(x_j)\right)^2$$

It is essentially a convex optimization problem as the first term in the above equation is convex loss over labeled data, second is the regularizer term and third is the smoothness regularizer [2].

2.4 Semi-Supervised Learning Using Label Propagation

Label Propagation identifies community structures in the network. Because of this nature, it is best suited for a graph setting [17]. All densely connected components in the network carry same label. Every labeled node is initialized with a unique label which then propagates through the network. The Label Propagation algorithm is similar to labeling through k nearest neighbors. The graph based semi-supervised learning approach labels the unlabeled points using label propagation; the smoothness regularizer term observed in the previous section simulates the principle working of label propagation algorithm. Label Propagation is a memory efficient algorithm hence it works well with semi-supervised learning.

2.5 Existing work done on Large Scale Semi-supervised learning

This section talks about the existing work done on large scale semi-supervised learning that find workaround for direct construction of the graph Laplacian.

1. Prototype Vector Machine for large Scale Semi-Supervised Learning [14]: This method introduces a novel concept of prototypes vectors for better approximation on graph-based regularizer and model representation. These vectors essentially perform low rank approximation of the kernel matrix as well as help construct a model that can allow minimum information loss compared with the complete model. This low rank approximation prototypes help avoid the construction of complete *n x n* kernel matrix. And the label reconstruction prototypes work only on labels of k prototypes.

2. Large Graph Construction for Scalable Semi-Supervised Learning [15]: This paper introduces a workaround for the construction of the graph Laplacian but using anchor points that will cover the cloud of all points sufficiently. This paper tries to construct the Laplacian using the anchor points and adjacency matrix in combination. This approach constructs large sparse graphs over all the data.

CHAPTER 3

SEMI-SUPERVISED LEARNING - EIGENFUNCTION APPROACH (FERGUS, 2009)

This approach attempts labeling ~80 million images having 4 keywords and 3 labeled pairs for each keyword. The main assumption that the paper holds is that the original dimensions of the data are as independent as possible. They try to fulfil this assumption by rotating the data points using PCA.

They begin by building an unnormalized graph Laplacian $\mathrm{L} = \mathrm{D} - \mathrm{W}$ of the labeled dataset $(X_l, Y_l) = \{(x_1 y_1), \ldots., (x_l y_l)\}$ and an unlabeled dataset $X_u = \{x_{l+1}, x_n\}$. Where W defines the affinities between the nodes and D is a diagonal matrix formed by these affinities. Since this is a graph based SSL method, the minimizing equation is given by:

$$J(f) = f^T L f + \sum_{i=1}^{l} \lambda (f(i) - y_i)^2 = f^T L f + (f - y)^T \Lambda (f - y)$$

Where the smoothness regularizer is given by: $f^T L f = \frac{1}{2} \sum_{i,j} w_{ij} \left(f(i) - f(j)\right)^2$

And Λ is a diagonal matrix whose diagonal elements are $\Lambda_{ii} = \lambda$ if i is a labeled point and $\Lambda_{ii} = 0$ for unlabeled points [1]. The paper suggests that using the density distribution of the data, they can approximate the graph Laplacian without doing the $n \times n$ Laplacian computation. They propose that instead of diagonalizing the graph matrix to get the eigenvectors, they can calculate approximate eigenvectors by deriving k eigenfunctions for k smallest eigenvalues where $k << d$; d being total dimensions. The smoothness of an eigenvector is defined by its eigenvalue, so eigenvectors with small eigenvalues are smooth. Any vector can be written in the form $\sum_i \alpha_i^2 \sigma_i$. Thus the smoothness of the vector will be $f = \sum_i \alpha_i^2 \Phi_i$, so smooth vectors are a linear combination of eigenvectors with small values [1]. Here $\Phi_i \sigma_i$ are generalized eigenvectors and eigenvalues of the graph Laplacian L [1]. The following minimizing solution is proposed: $(\Sigma + U^T \Lambda U)\alpha = U^T \Lambda y$ which is a solution to a $k\ x\ k$ system of equations. Here, Σ is a covariance matrix, U is a k dimensional approximate eigenvector array, y is the label array, Λ are the coefficients for regularization and α is the minimizing factor that will eventually contain the meaningful coefficients that will give smooth functions which will turn out to be good predictors for the data. Using the linear equation, $f = U\alpha$, if we substitute the numerical solutions for U and α, we can find the smooth functions. Since U is n x k dimensional, α is vector with k coefficients, we will eventually get n 1-dimensional smooth functions which will help predict the labels for all n data points. Thus this algorithm helps reduce the complexity from $O(n^2)$ to $O(nk)$.

This paper introduces the novel concept of Eigenfunctions, or numerical approximations of analytical eigenvectors. To approximate the eigenvectors, the authors work on density distribution of the data points. They use smoothness operators derived from these densities which gives eigenfunctions of increasing smoothness. This smoothness operator is defined by:

$$L_p(F) = \frac{1}{2} \int \left(F(x_1) - \ (x_2)\right)^2 W(x_1 x_2) p(x_1) p(x_2)\, dx_1 x_2$$

where W defines the affinities and $p(x)$ defines the probability densities of data points. The product form of these densities depends on the assumption that the features are independent; hence, a rotation of the data is required to maximize pairwise independence of dimensions. We can obtain the eigenfunctions by minimizing the loss over this smoothness operator.

The paper defines a clear mapping between these approximated eigenfunctions and the generalized eigenvectors that we would get by building the actual graph Laplacian. As the number of data points *n* tends to infinity, the smoothness operator for the true graph Laplacian will approach the approximated smoothness operator $L_p(F)$ defined by the data densities. The minimization problems for eigenvector approach will also approach towards the minimization problem for eigenfunction approach. Hence as number of samples goes to infinity, eigenfunctions converge in the limit to the true eigenvectors [1].

The paper defines an approximate eigensolver that derives eigenfunctions from a *k x k* covariance matrix, thereby eliminating the costly diagonalization of the *n x n* Laplacian matrix. For practical purposes, these eigenfunctions can be estimated numerically by discretizing the densities in low dimensions using the following solver:

$$(\widetilde{D} - P\widetilde{W}P)g = \sigma P\widehat{D}g$$

where $\widetilde{W}$ is the affinity between the discrete points, P is a diagonal matrix whose diagonal elements give the density at the discrete points, and $\widetilde{D}$ is a diagonal matrix whose diagonal elements are the sum of the columns of $P\widetilde{W}P$, and $\widehat{D}$ is a diagonal matrix whose diagonal elements are the sum of the columns of P [1].

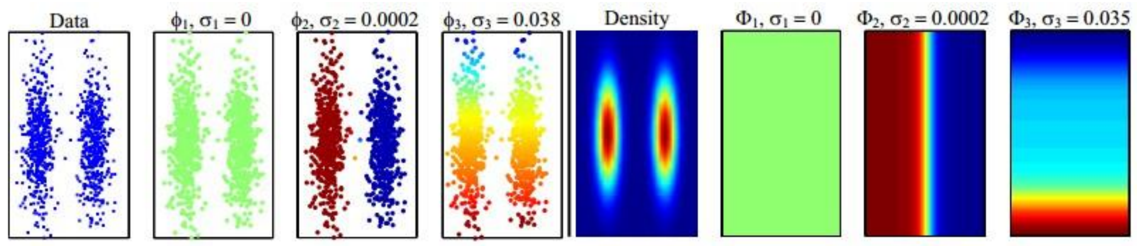


Figure 1: Far left: Original 2D toy data. Next three (left to right) are the first 3 eigenvectors, their values overlaid on the data. Next is the corresponding density plots of the data. Finally, the three rightmost panels are the numerical eigenfunctions of the data, which approximate the original eigenvectors [1].

Given the assumption that the components of the data are independent, the probability densities of the data can be expressed in a product form. Due to this, we need only *k* densities to get the approximate eigenfunctions. Below mentioned is the algorithm, reproduced from Fergus *et al* 2009:

a. Rotate data points to make them as independent as possible.
b. For each component, discretize data by building 1D histograms and add a smoothing constant to it.
c. Given these densities, solve numerically to get approximate eigenfunctions and solve generalized eigenvalue problem to get coefficients.
d. Order these eigenfunctions and select first *k*.

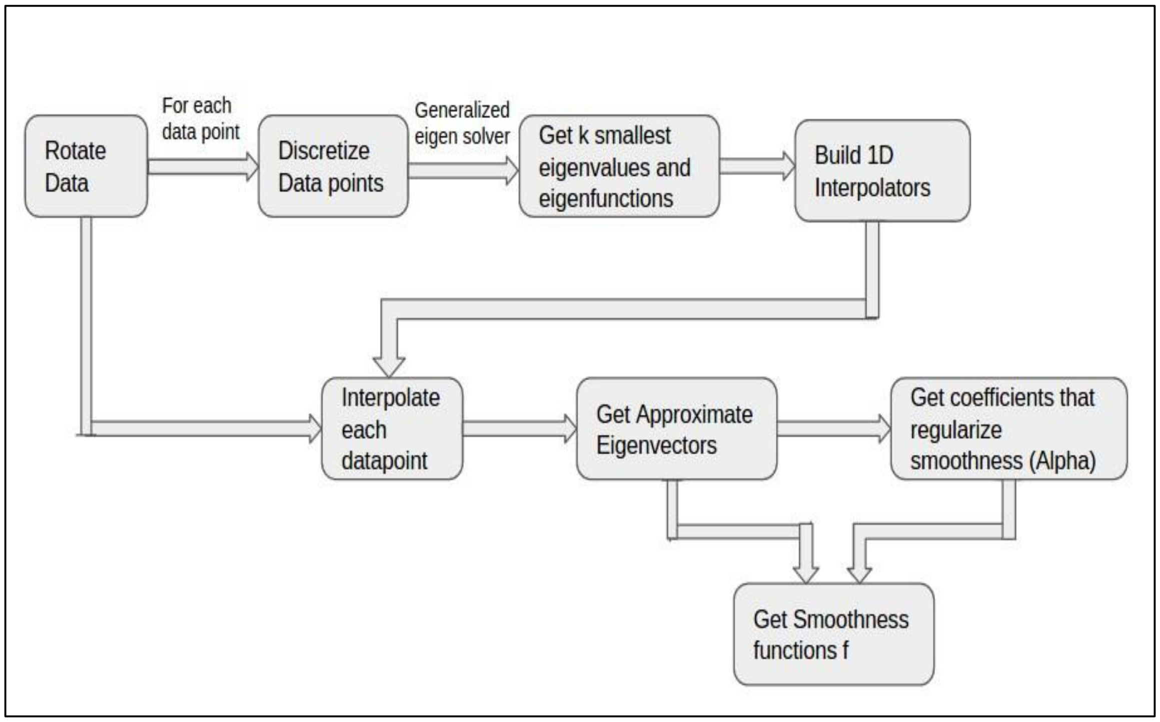

Rotate Data
For each data point
Discretize Data points
Generalized eigen solver
Get k smallest eigenvalues and eigenfunctions
Build 1D Interpolators
Interpolate each datapoint
Get Approximate Eigenvectors
Get coefficients that regularize smoothness (Alpha)
Get Smoothness functions f

Figure 2: Eigenfunction algorithm flow at a high level

Using linear interpolation in 1D, we interpolate each eigenfunction at labeled points. For data rotation, PCA is permitted because the change in the distance between the data points is not desired. Only the rotation is desired and this can be achieved with something like PCA.

So even if there are n data points, we just have to solve a *k x k* linear system of equations to get the eigenfunctions which will help get the approximate eigenvectors eventually.

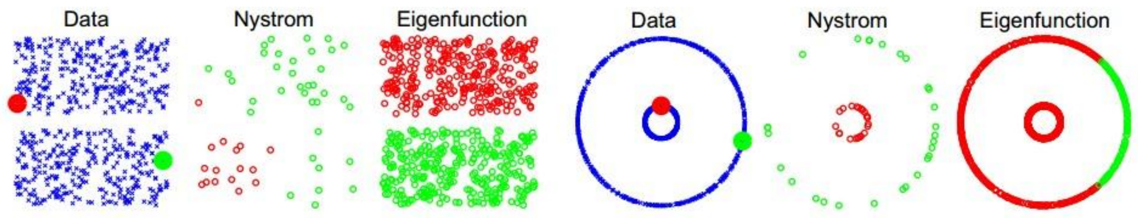


Figure 3: Comparison of Eigenfunction approach and Nystrom Method. Nystrom fails at low density areas. Eigenfunction approach fails when density is far from product form (Fergus, 2009, hence the need for an initial rotation step to make the dimensions independent).

For data above, the eigenfunction approach assumes the input data is linearly separable over the dimensions. Cases where this assumption fails, the eigenfunction approach does not work efficiently as shown in the above Fig. 5.

They tested their approach on CIFAR tiny image dataset of 79,302,017 images. They precomputed *k*=64 eigenfunctions on the whole dataset and then reduced data dimensions to 32D. Overall they had 4 classes with 3 pairs of labeled data for each class. In all 12 labeled data.

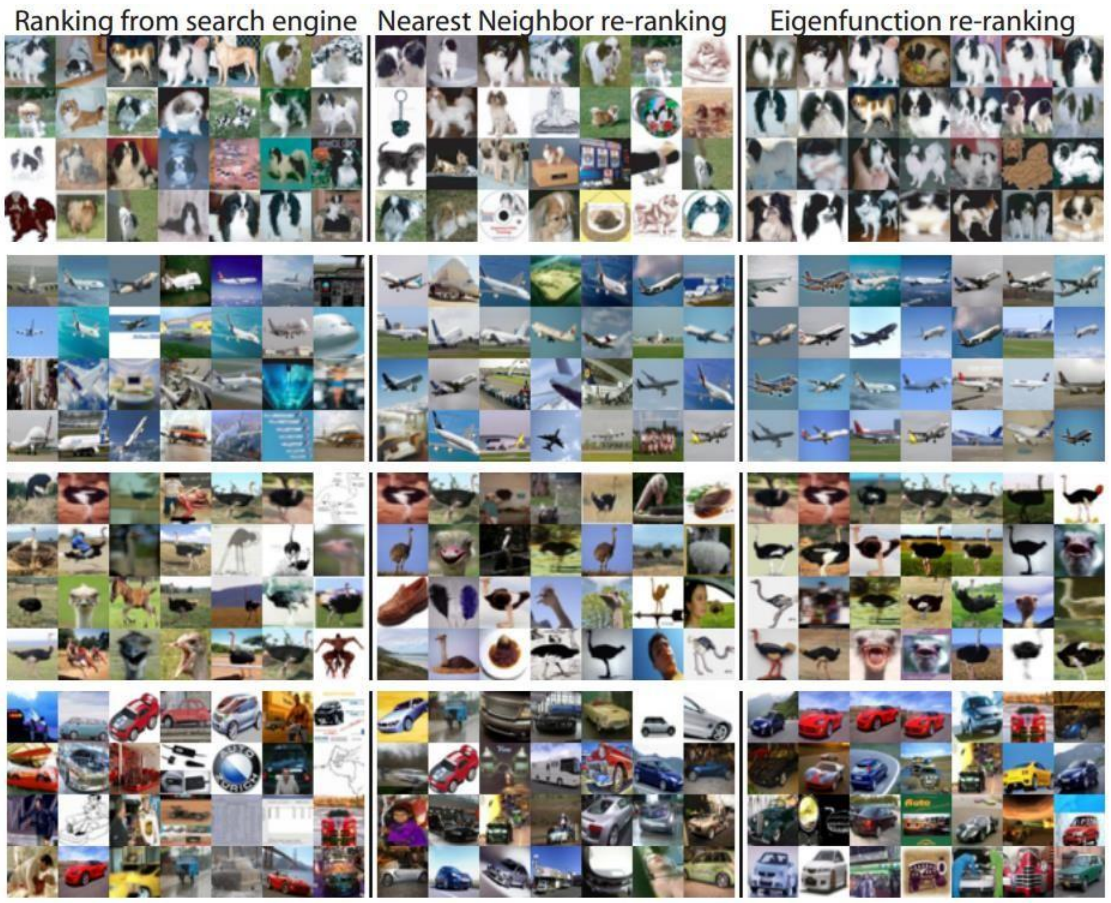


Figure 4: Comparison of Eigenfunction approach on the tiny images dataset [1].

CHAPTER 4

SYSTEM ARCHITECTURE AND OVERVIEW

This chapter discusses the architecture for the implemented fit and predict functions. It is a common practice to implement data science pipelines in this format where model is trained with a fit function and labels for unseen samples are predicted using a predict function. The predict function used the trained model parameters from the fit function to perform prediction. Our implemented pipeline is compatible with the distributed computing environment Apache Spark. Apache Spark provides a fault-tolerant, distributed computing environment which can handle huge amount of data because of its parallelism. It follows a master slave architecture where the execution begins from the driver machine (Master) and parallel jobs are distributed to worker machines (slaves).

The fit function implements the transductive learning aspect of semi-supervised learning while the predict function simulates the inductive learning aspect of it. Later we also discuss the challenges faced during the implementation of the architecture.

4.1 Fit Function

The implementation of this approach is programmed with respect to a distributed paradigm like Apache Spark. The fit function works as per the concept of transductive learning. It reads in the dataset with labeled as well as unlabeled data points and the corresponding labels. For unlabeled data points there has to be some dummy label which will not be counted as a relevant label. The function takes k and number of bins for discretization as input arguments, where parameter k is the number of dimensions to work on and number of bins is used to discretize the dimensions of the data points into histograms.

The function also takes data points and any known labels as input. As per the method, the data points are rotated doing a full Principal Component Analysis. After performing the PCA step, we retain all the dimensions, there by fulfilling the assumption that the data dimensions are independent and orthogonal with respect to each other. At a later point in the process, we will be required to work on one dimension of the data at a time. Hence the data which was in the form of a Resilient Distributed Dataset was converted to a more structured format such as a DataFrame, providing additional tools for inspecting and analyzing each dimension of the data in parallel. The number of dimensions, d, will always be far less than the total number of samples. Keeping this assumption in mind, it is feasible to make use of a structured format like a DataFrame.

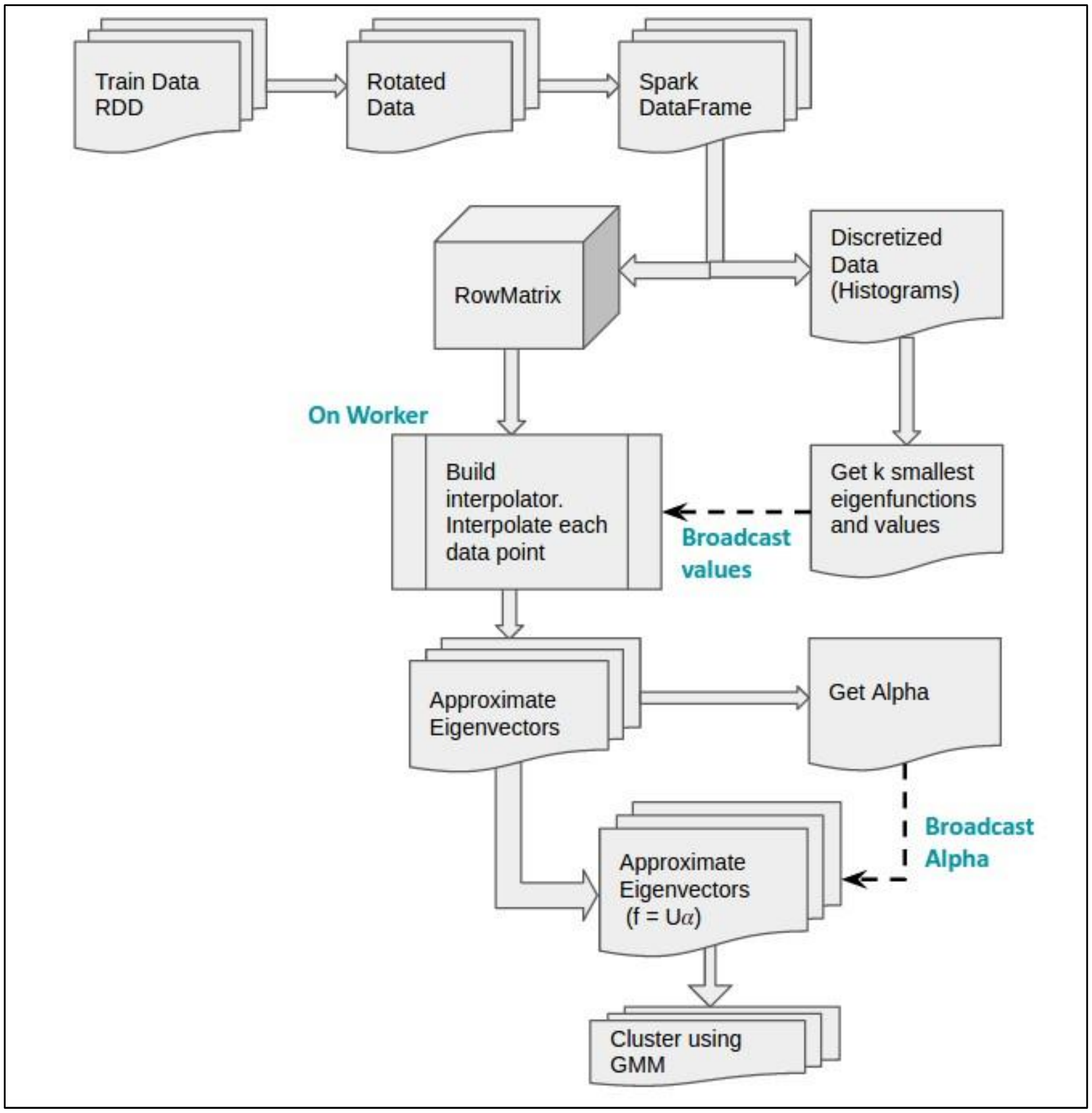
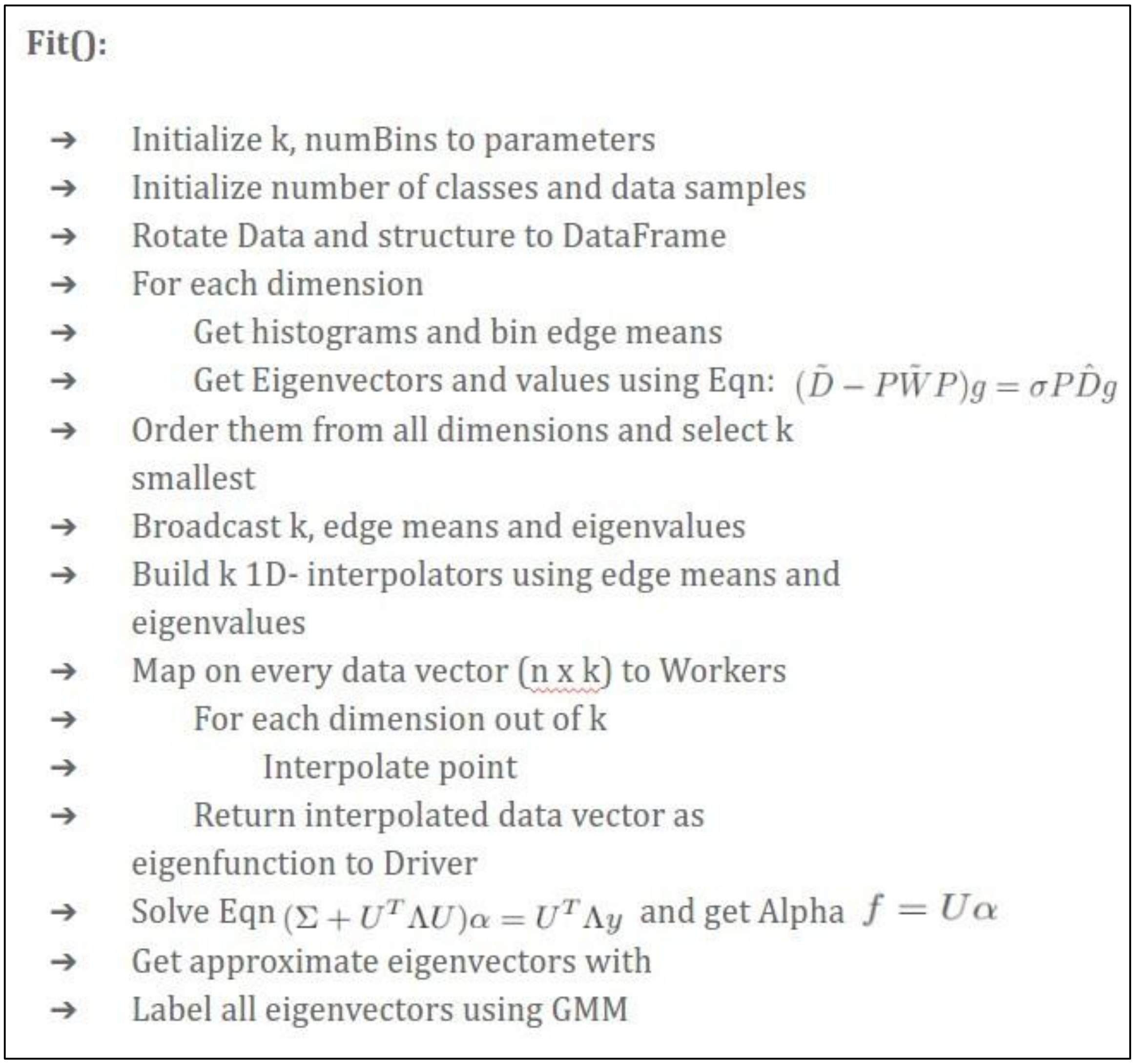

Train Data RDD
Rotated Data
Spark DataFrame
RowMatrix
Discretized Data (Histograms)
On Worker
Build interpolator. Interpolate each data point
Get k smallest eigenfunctions and values
Broadcast values
Approximate Eigenvectors
Get Alpha
Broadcast Alpha
Approximate Eigenvectors (f = Uα)
Cluster using GMM

Figure 5: Flow Process of the fit function

Below is the pseudo code:



```
Fit():

➔ Initialize k, numBins to parameters
➔ Initialize number of classes and data samples
➔ Rotate Data and structure to DataFrame
➔ For each dimension
➔     Get histograms and bin edge means
➔     Get Eigenvectors and values using Eqn: $(\tilde{D} - P\tilde{W}P)g = \sigma P\hat{D}g$
➔ Order them from all dimensions and select k
  smallest
➔ Broadcast k, edge means and eigenvalues
➔ Build k 1D- interpolators using edge means and
  eigenvalues
➔ Map on every data vector (n x k) to Workers
➔     For each dimension out of k
➔         Interpolate point
➔     Return interpolated data vector as
  eigenfunction to Driver
➔ Solve Eqn $(\Sigma + U^T \Lambda U)\alpha = U^T \Lambda y$ and get Alpha $f = U\alpha$
➔ Get approximate eigenvectors with
➔ Label all eigenvectors using GMM
```

Figure 6: Pseudo code for the fit function

This structured DataFrame will be primarily used to get the k smallest eigenfunctions and eigenvalues using the generalized eigensolver. Also, this DataFrame will be later required to interpolate each data point using the 1D interpolators.

For each dimension of data, we take all data points for that dimension, discretize them by binning them into a histogram. Here we make use of the number of bins parameter that was given as input to the function. Using the generalized eigensolver equation in Eigenfunction Approach [1], we obtain the eigenvectors and eigenvalues for that particular dimension using $\left(\widetilde{D} - P\widetilde{W}P\right)g = \sigma P\widehat{D}g$). For each dimension, there will be a corresponding, most significant, eigenvector and eigenvalue. So for d dimensions, there will be a (d x bins) vector of eigenvectors and corresponding vector of eigenvalues. After sorting the d eigenvalues in an ascending order, we select the top k eigenvalues and their corresponding eigenfunctions.

The next task is to obtain approximate eigenvectors from these k eigenfunctions. Since we do not build an actual n x n graph Laplacian, we are required to get approximate eigenvectors. For this purpose, we build 1D straightforward interpolators, one for each dimension of the data. These interpolators define a density area bounded by the k eigenfunctions. So once we get these k interpolators, we pass every data point through these interpolators, interpolate them and get values which are the numerically approximated eigenvectors. These approximated eigenvectors can be compared to the actual eigenvectors that we would get using the graph Laplacian. So we are getting the eigenvectors without having to do a complete n x n computation.

Next in the process we need coefficients that will help regularize the smoothness of the function such that the data points will fill well into the functions on the manifold. These coefficients can be obtained by solving the linear equation $(\Sigma + U^T \Lambda U)\alpha = U^T \Lambda y$ given in the Fergus *et al* paper that makes use of these approximated eigenvectors. We denote these coefficients with α (Alpha).

Eventually this alpha is going to be a 1D vector (*k x 1*). Using a linear combination of alpha and the approximate eigenvectors, we can get *n* 1D smoothness functions f which are the predictor functions. If we try to visualize these predictor functions, we can see a clustering pattern in the data.

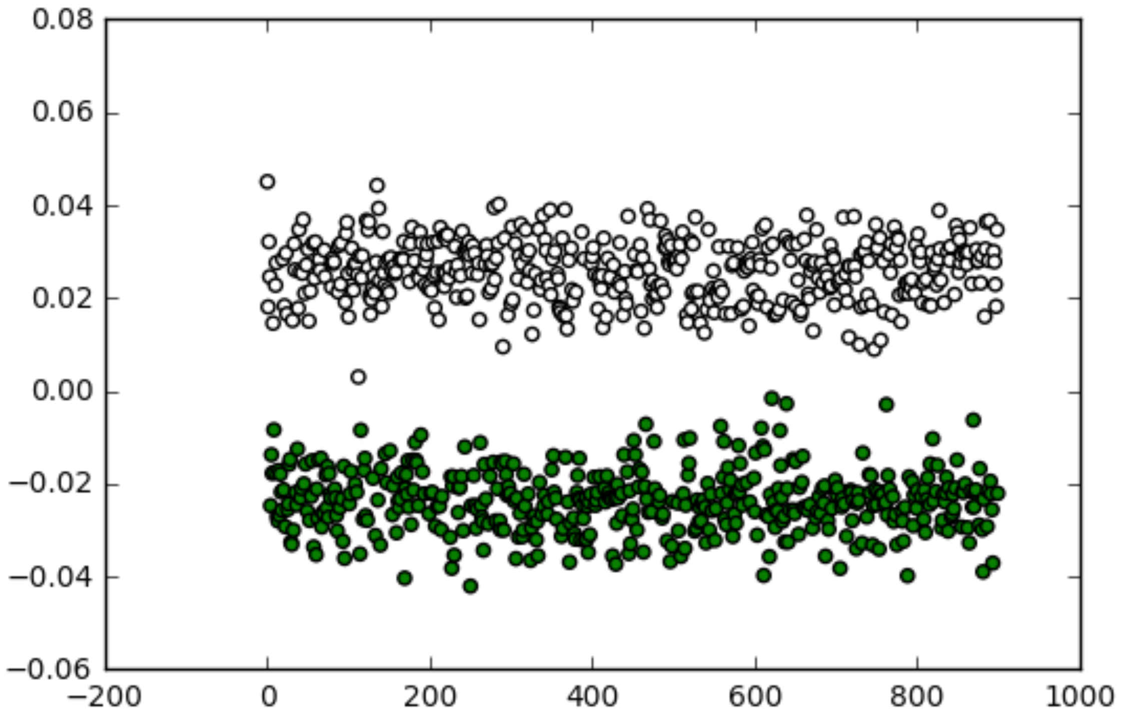


Figure 7: Clustering suggested by smoothness functions for 1000 data points with binomial clustering.

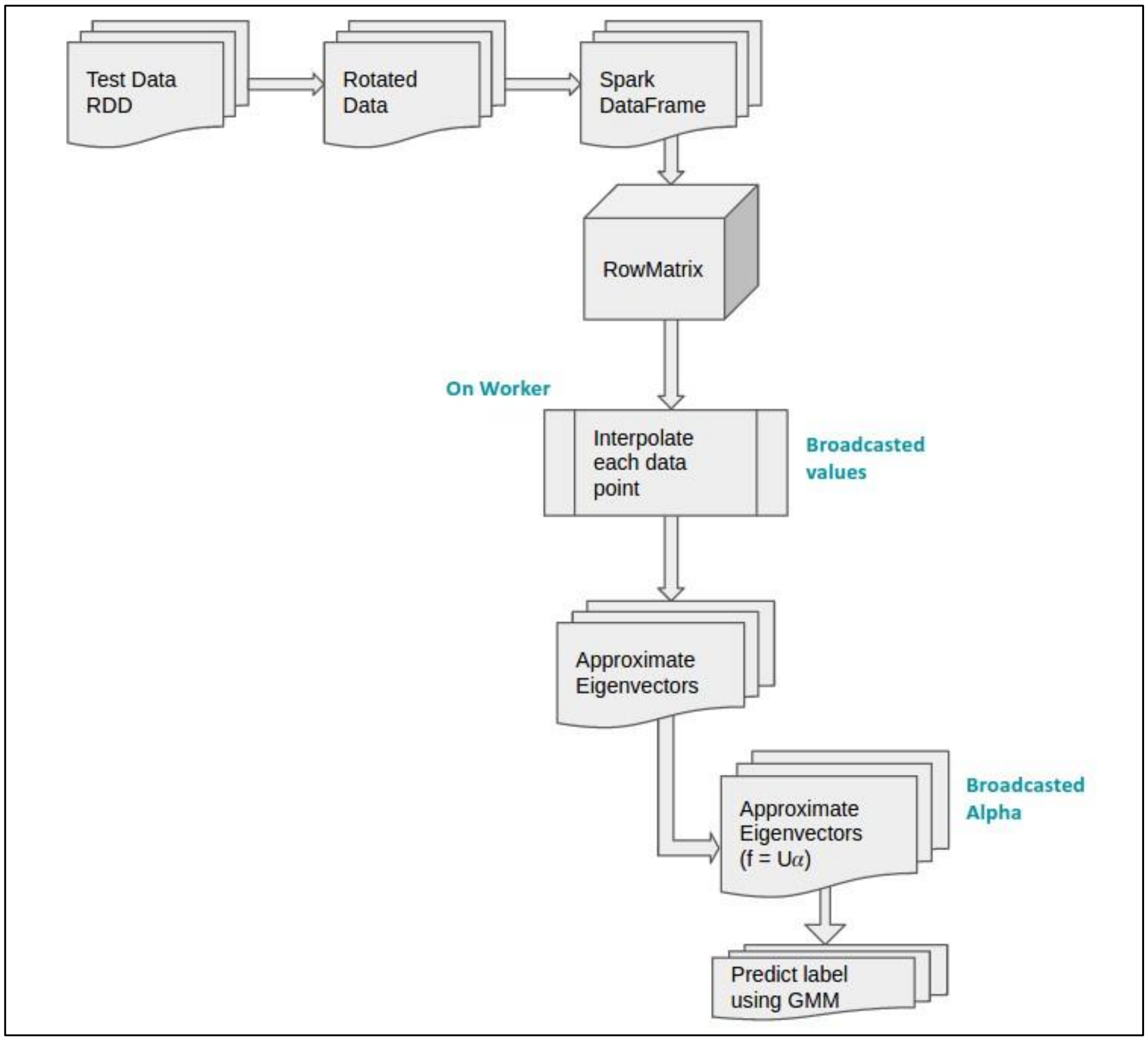
We then apply Gaussian Mixture Model (GMM) clustering that simulates expectation Maximization and clusters these predictor functions assigning hard label to them. Thus we present a transductive implementation where we end up labeling the same data that we used for training purpose.

For the purpose of reuse of parameters and a few variables, Apache Spark provides a broadcasting facility which enables sharing of variables among the workers. Parameters like alpha, k, bin edges which could be required on multiple workers are broadcasted for sharing purpose.

4.2 Predict Function

Predict function implements the inductive learning approach of this algorithm. It takes new, unobserved data samples as input, uses the trained model parameters, and outputs labels predicted for the new data. This prediction is performed without using the original training data, and without rebuilding the model. Data given as input is in the form of Resilient Distributed Dataset.

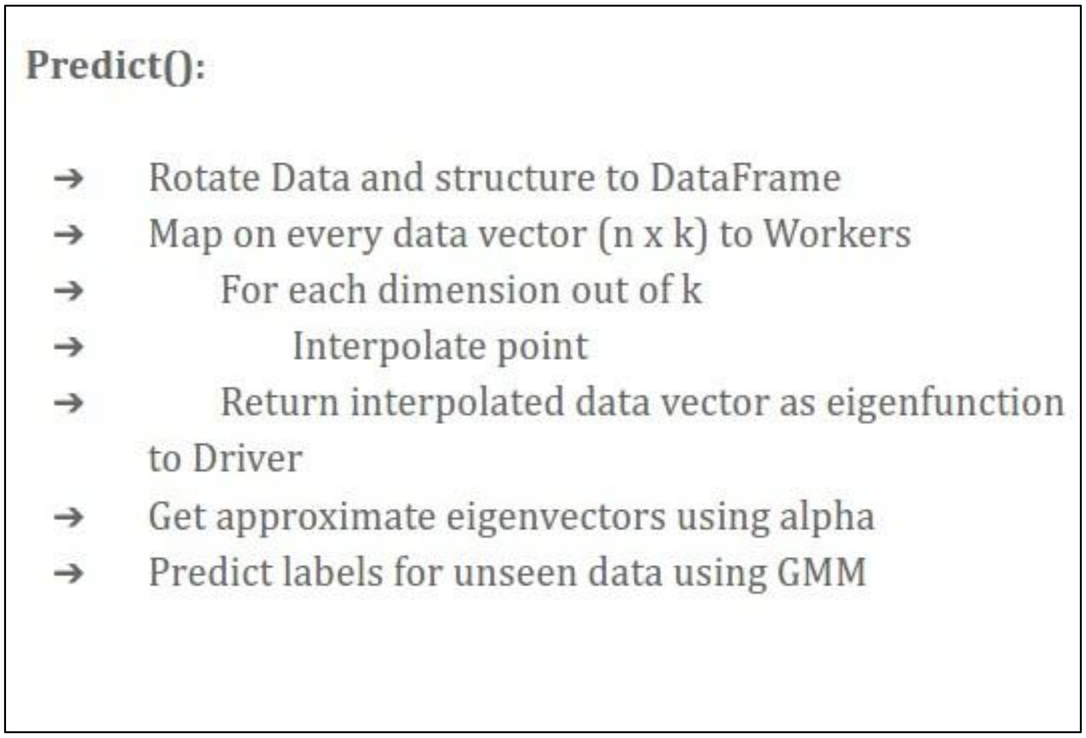
This data is first rotated using a full PCA (Principal Component Analysis). The rotated Data is transformed into a structured DataFrame. Then using the interpolators built during training phase, we interpolate each data point and get the approximate eigenvectors. It is to be noted here that we eliminate the phase of building interpolators and getting k



eigenfunctions. Since we reuse these interpolators and k eigenfunctions in the predict function to predict labels, we call these the learned parameters of the model.

Figure 8: Flow process for predict function

Below is the pseudo code:



```
Predict():

➔   Rotate Data and structure to DataFrame
➔   Map on every data vector (n x k) to Workers
➔       For each dimension out of k
➔           Interpolate point
➔       Return interpolated data vector as eigenfunction
    to Driver
➔   Get approximate eigenvectors using alpha
➔   Predict labels for unseen data using GMM
```

Figure 9: Pseudocode for Predict function

Again, using the alpha calculated in fit function, we take a linear combination of alpha and these approximate eigenvectors to calculate the smooth predictor functions. Here, alpha too can be named as a learned model parameter. We cluster these predictor functions to predict labels for all these unseen samples. This justifies the inductive learning approach as we predict label using the learned parameters of the model.

Again, we emphasize the inductive nature of the predict function: we make use of already trained models for PCA and GMM. Using these learned models from the fit function, we just transform test data in the predict function and predict labels for unseen data using GMM model. This is a typical data-science pipeline for using Machine-Learning

Algorithms. Using Python, these functions are made available as a module by the name "LabelPropagationDistributed".

4.3 Challenges

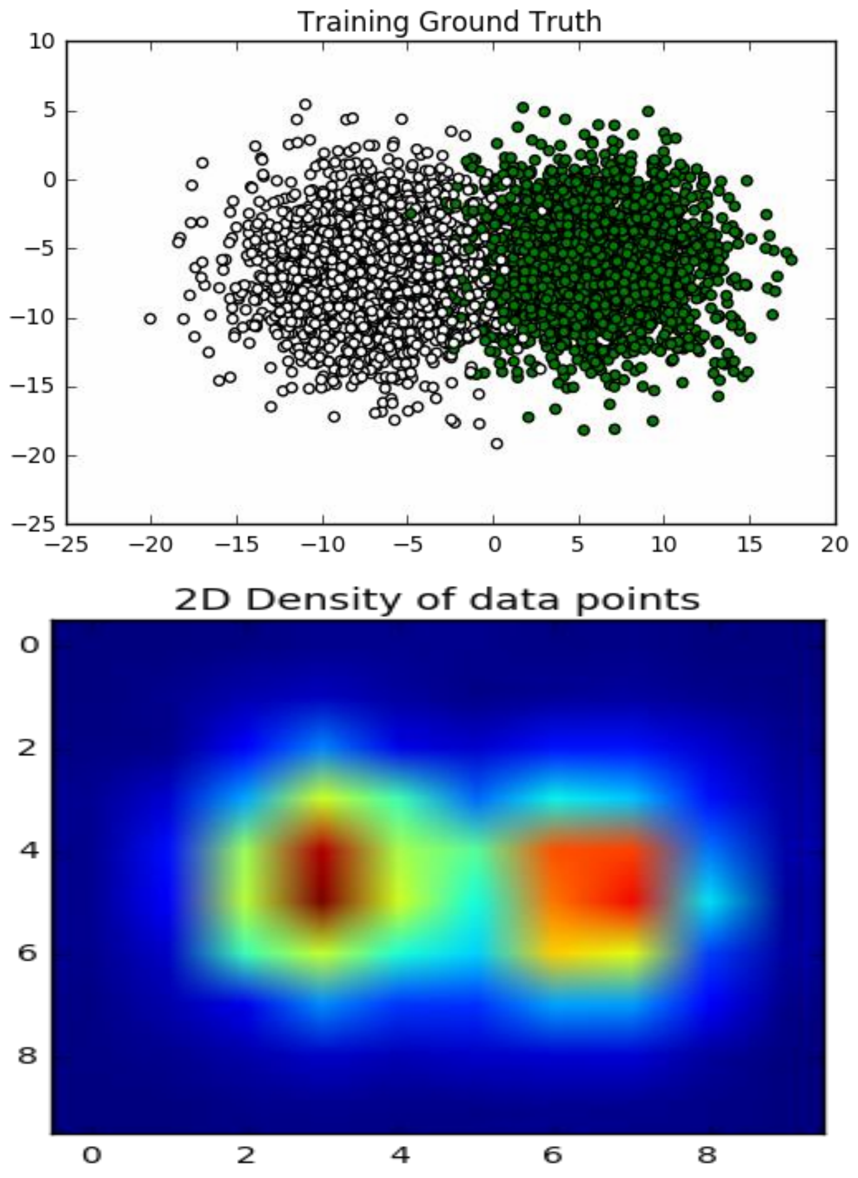
This algorithm has been implemented as a combination of functional as well as object oriented programming paradigms. Apache Spark uses functional programming to minimize network overhead, whereas well-known machine learning packages such as Scikit-learn use object-oriented programming to store learned model parameters. But to provide an implementation in the form of a package, the implementation had to be modularized. It was challenging to merge both programmatic into a single, standalone module.

Another challenge was related to the Eigenfunction approach as it was proposed by Fergus *et al* 2009. This approach does not discuss the inductive learning aspect of the algorithm. We were required to interpret and implement the inductive approach. There were issues for using class functions on the workers. If a function is specific to a class, sending it to worker sends the class object as well. This is not allowed as Spark cannot serialize - deserialize it. Solution was to declare them global.
This algorithm requires tweaking of three important parameters namely, k; the dimensions to work on, bins; the number of bins to build histograms and g; gamma to calculate affinities using the RBF kernel. We had to experiment to get the right combination of all three that gave us good results.

CHAPTER 5

EIGENFUNCTION APPROACH ANALYSIS

5.1 Data Densities

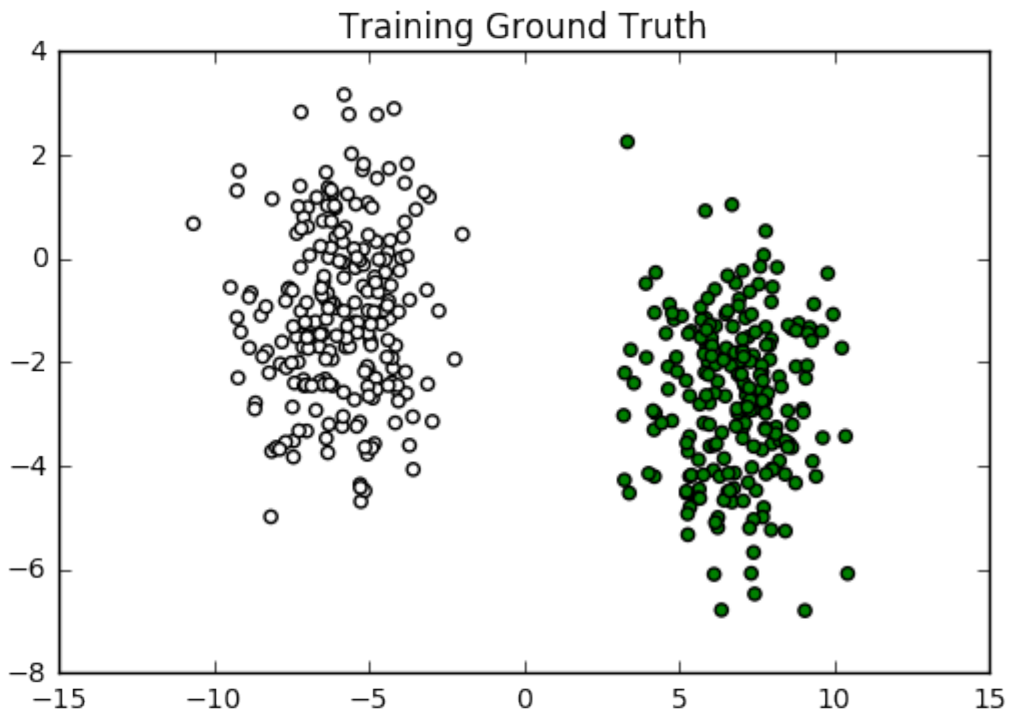


6 *Figure 10: Toy data blobs and the plot of their 2D densities using 2D histograms.*

Above is the plot of the first two dimensions of a toy dataset and its corresponding data densities. The dataset consisted of 10000 data points with a suggested 2 class clustering and 100 dimensions. These densities are the 2D histograms of the data points. This plot is just to give an idea as to how the interpolators would look like. The interpolators would be in 1D but this plot is in 2D for visualization purpose. The colors in the density plot change according to the density of points in that region.

5.2 Data points against Approximate Eigenvectors

Below is the plot of original data points against their approximate eigenvector values. This eigenvector is the second eigenvector and not the first. Because of minimal smoothness, the first eigenvector will always be flat.



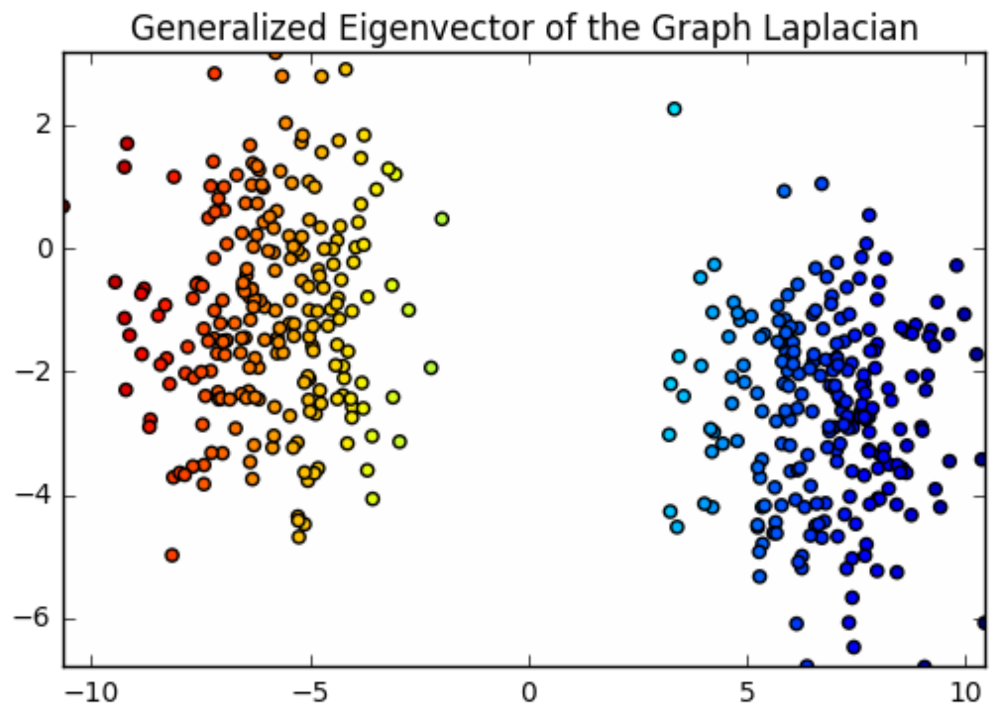


Figure 11: Toy dataset (above) and below is its plot against first Eigenvector for the data. Zeroth eigenvector will always be flat

5.3 Data points against smoothness functions

Below it is the plot of 2D densities of data against the final smoothness operator functions f. This plot depicts the interpolated area. Any new point can be interpolated into this density space and its corresponding label can be predicted depending on which labeled density it is nearer to.

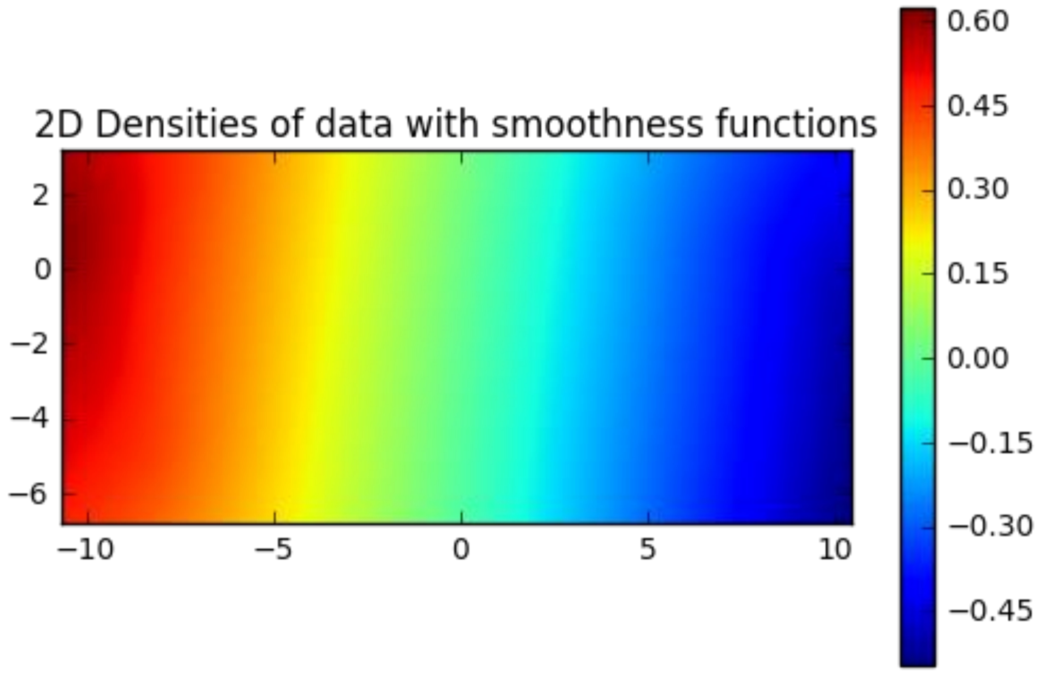


Figure 12: 2D densities of the corresponding toy dataset in the figure above versus its corresponding smoothness function values

CHAPTER 6

RESULTS

6.1 Results on Small dataset

Below are the results of the algorithm on a toy dataset. The dataset was in all of 100 points with 70 for training and 30 for testing. The dataset of 70 was used to train using the Fit function whereas the dataset with 30 points was used to test the predict function. This was a 2 dimensional data with number of bins as 50, k as 2 and gamma as 0.2. The classes were 2 as we can see below. The points marked in red are the labeled data points, that is, the ground truth which we already had.

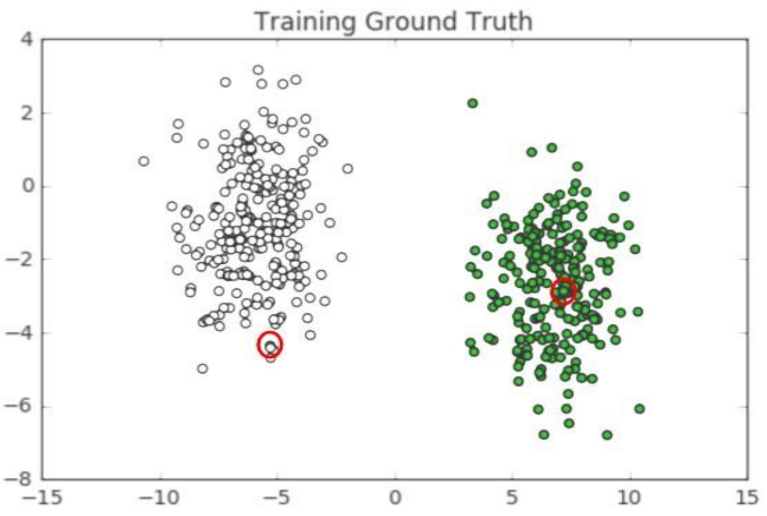


Figure 13: Transductive Learning. Train data ground truth

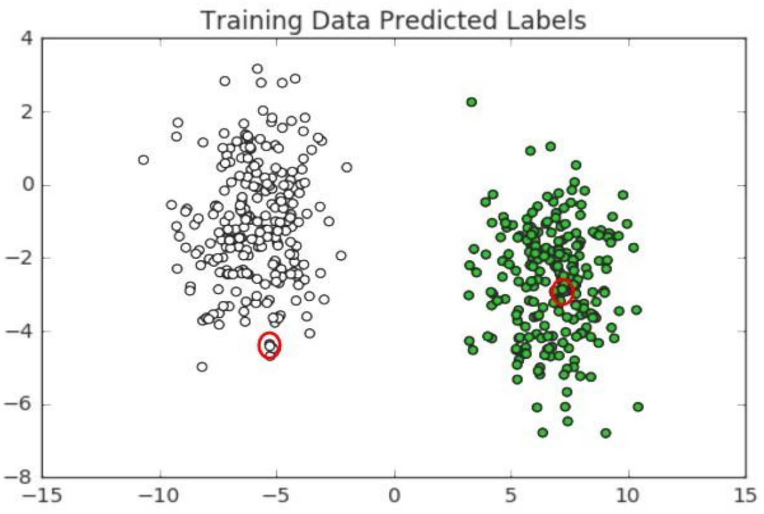


Figure 14: Inductive learning. Test data ground truth

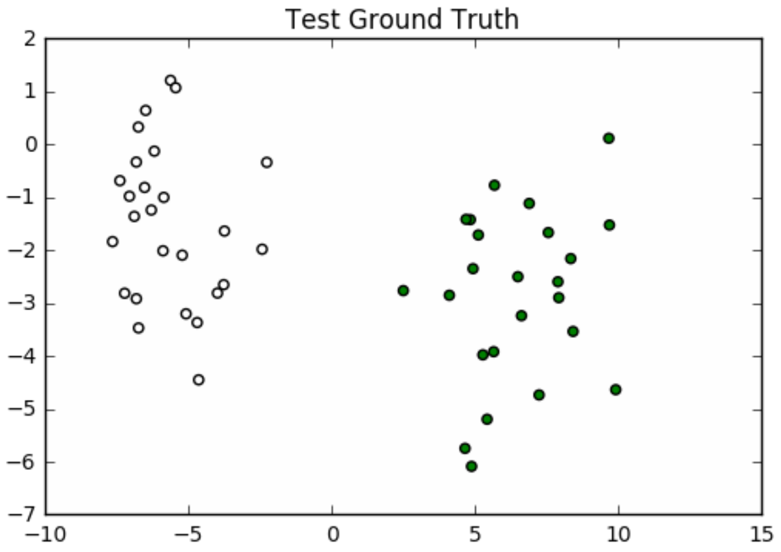


Figure 15: Transductive learning. Train data predicted labels

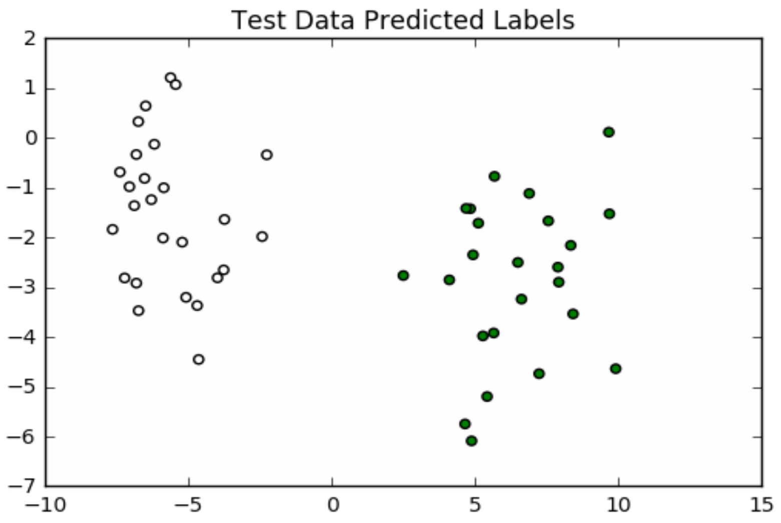


Figure 16: Inductive learning. Test data predicted labels.

Given the 2 labeled data points out of 70, it can be seen that the algorithm could label all 70 points correctly and the predict function could also label all the unseen 30 points with the same accuracy.

6.2 Results on Bigger Dataset

We then tried to use a dataset closer to a real-world scenario. The dataset size was 60000 with 10 classes and 100 dimensions. This dataset was a potential simulation to the olfactory dataset with 10 classes and 100 dimensions. (Though we will be dealing with 146 dimensions). Looking at the data distribution we decided to use a k of 20, number of bins as 2000 and a gamma for RBF kernel as 0.01. This algorithm is very sensitive to gamma, then bins and then k. Gamma decides the extent to which the label should be propagated. Out of the 60000 data, 54000 was training data and 6000 was for testing.

Below are the results for the same. The fit function resulted with an accuracy of 58.75% where 58.75% of the data points were correctly labeled when compared with the ground truth labels.

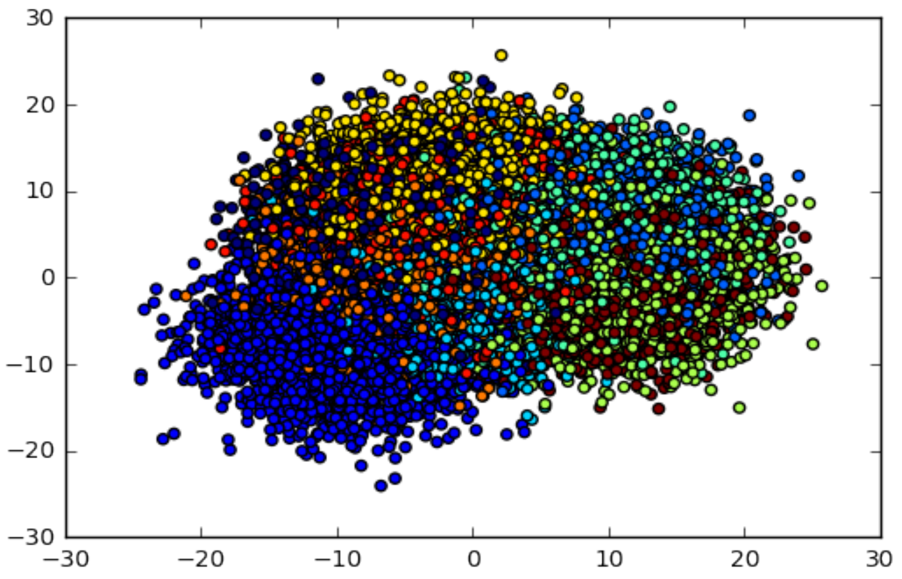


Figure 17: Training dataset with original clustering for first two dimensions.

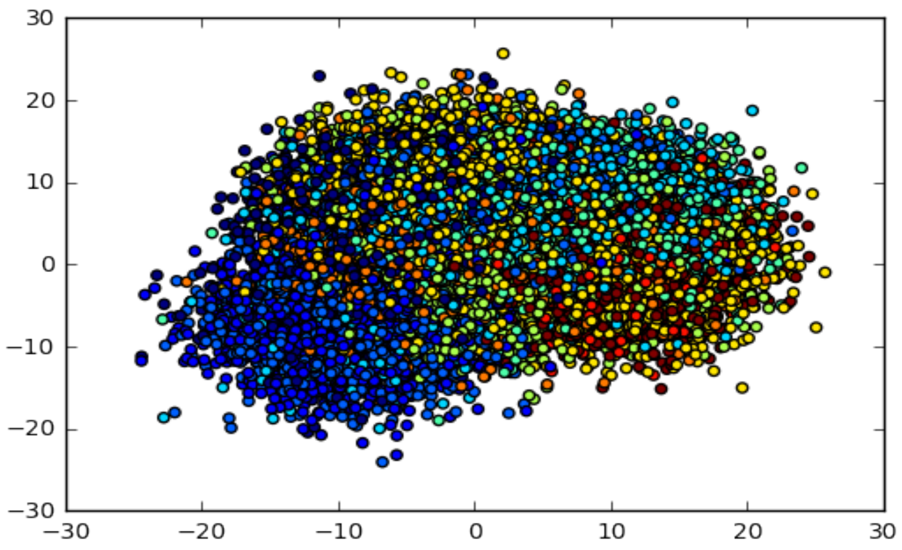


Figure 18: Labels propagated across the entire dataset with just 10 originally labeled points available. One label available for each class.

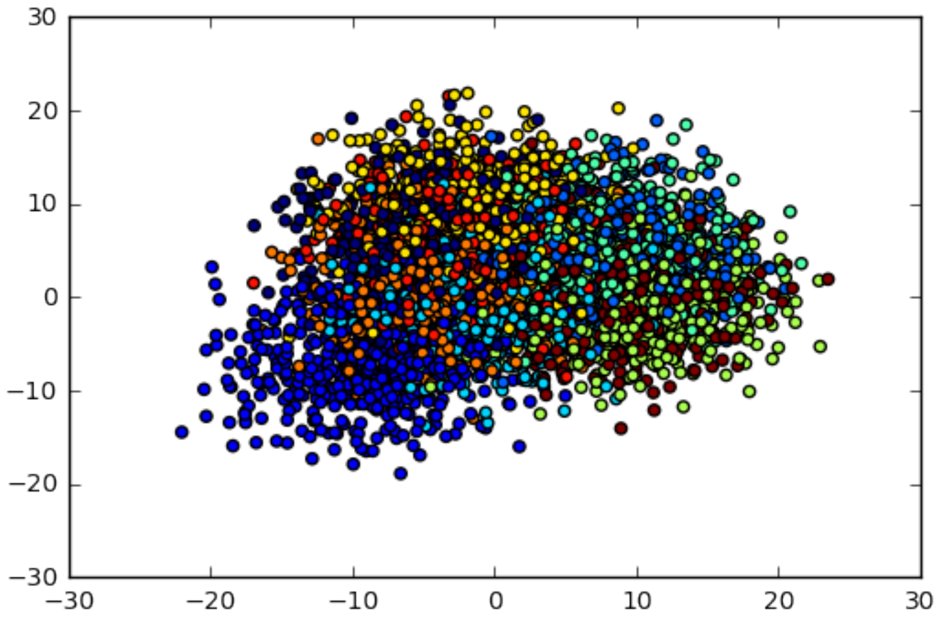


Figure 19: Test data set original clustering for first two dimensions.

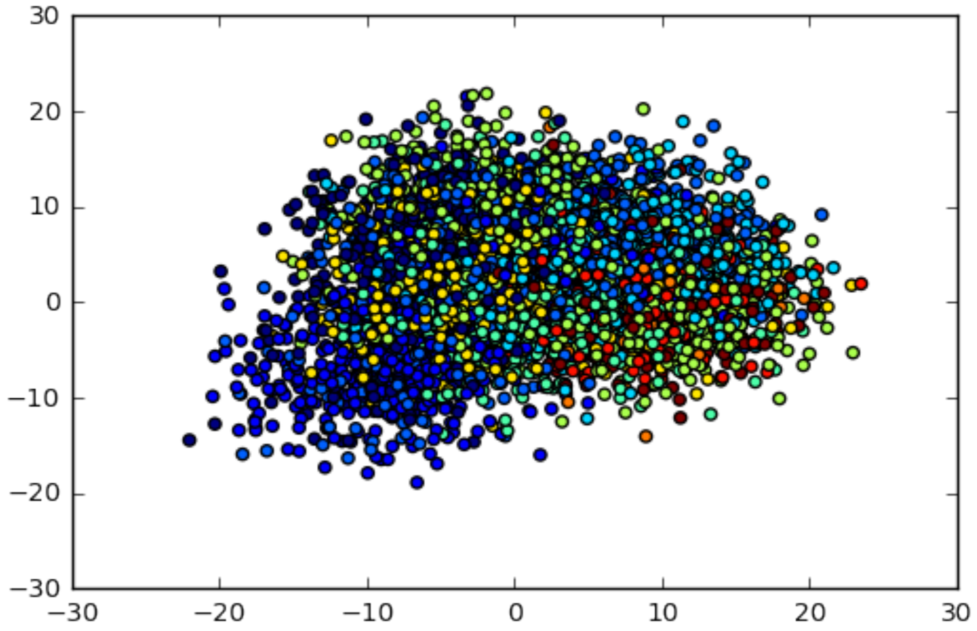


Figure 20: Label propagation after 1D interpolation of data using the learned model parameters during the training phase. This depicts the Inductive Learning.

6.3 Standalone Performance Vs Large-Scale Performance

PRECISION

We compared the accuracy of the algorithm implementation for the same size of dataset on the standalone implementation versus the large-scale implementation. We tried to test the algorithm on increasing datasets against their accuracy. Accuracy is measured in the form of F1-Measure, precision and recall. F1-Measure is the harmonic mean of precision and recall. We have presented the results in all three forms. It can be seen that the accuracies are almost the same for any given dataset when executed using both the algorithm implementations.

Table 1: Standalone Performance Vs Large-Scale Performance for Precision

Size	Standalone	Large-Scale
1000	1	1
2000	0.9641025641	0.9685863874
10000	0.983014862	0.9809926082
15000	0.9993284083	0.9993284083
20000	1	1
25000	1	1

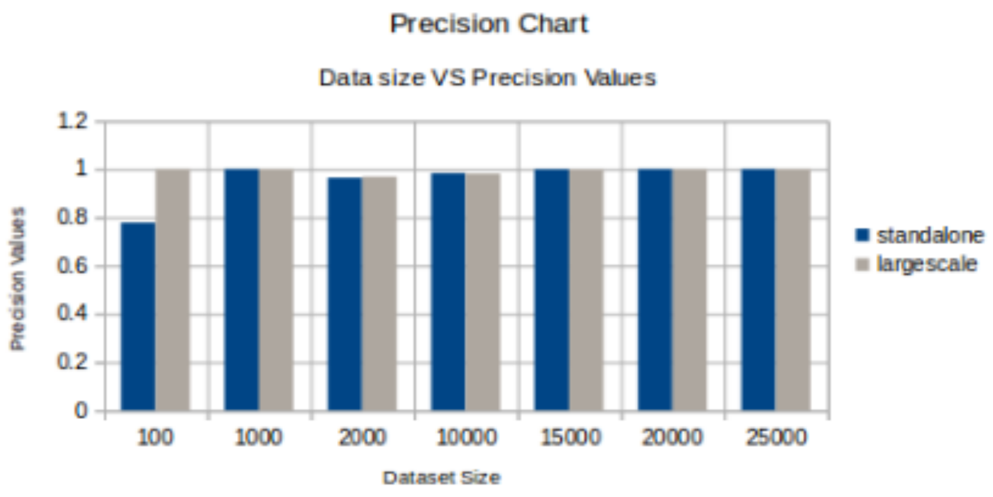


Figure 21: Precision comparison for standalone and largescale

RECALL

Table 2: Standalone Performance Vs Large-Scale Performance for recall

Size	Standalone	Large-Scale
1000	1	1
2000	0.9261083744	0.9113300493
10000	0.9159248269	0.918892186
15000	1	1
20000	1	1
25000	1	1

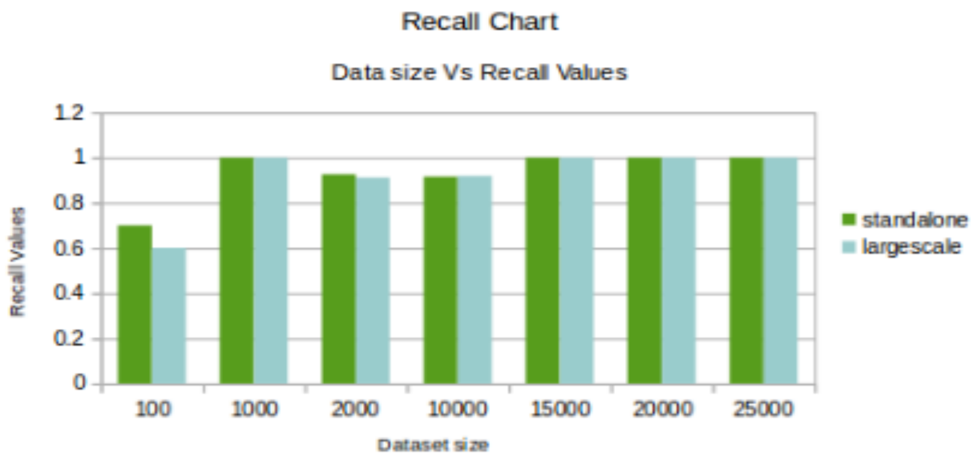


Figure 22: Recall comparison for standalone and largescale

F1-MEASURE

Table 3: Standalone Performance Vs Large-Scale Performance for F1-Measure

Size	Standalone	Large-Scale
1000	1	1
2000	0.9447236181	0.9390862944
10000	0.9482846902	0.948927477
15000	0.9996640914	0.9996640914
20000	1	1
25000	1	1

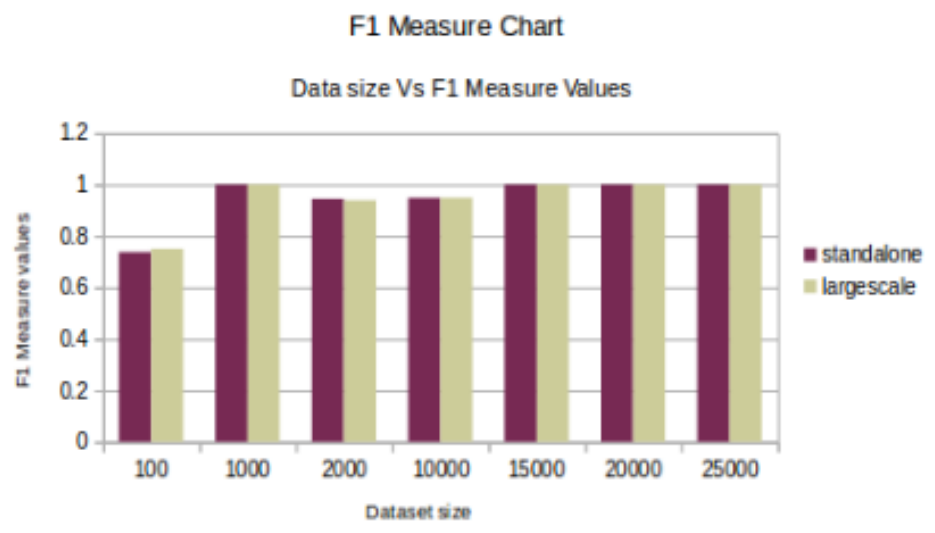
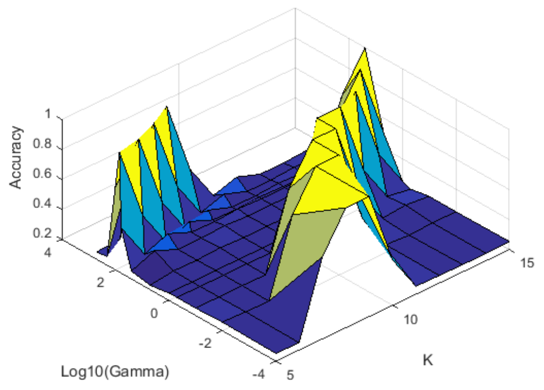


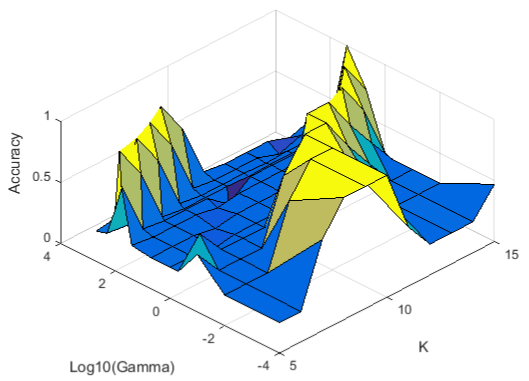
Figure 23: F1-Measure comparison for standalone and largescale

6.4 Parameters vs. Accuracy

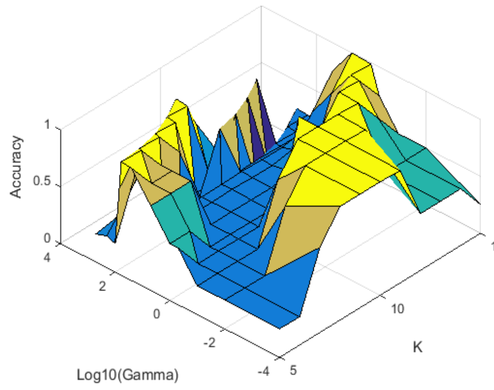
Here we try to tweak parameters like gamma, k and number of bins and compare the results with the accuracy. These parameters are very sensitive to the accuracy that we get. Starting with gamma, gamma is the RBF kernel affinity coefficient. The gamma decides the extent of label propagation towards its neighbors. The more scattered the intra-cluster points, the smaller gamma should be. Gamma corresponds to negative inverse of sigma in the RBF kernel. Parameter k decides how many dimensions to actually work on. The k dimensions are selected looking at the ordered eigenvalues. If the selected k is very large then a lot of noise gets introduced. If the k is very small the meaningful dimensions are not selected giving a bad clustering. Number of Bins depends on the data size to be dealt with. For each dimension we build histograms. So depending on the total data points, we can select number of bins for discretization. Few bins may not give a detailing of the densities. A larger number for bins may cause some bins to be empty thus again, not having a fair distribution. This algorithm needs a lot of tweaking of these 3 parameters to get the right combination which will give good accuracy in propagation. Below are some graphs depicting drop and rise in accuracy based on these 3 parameters.



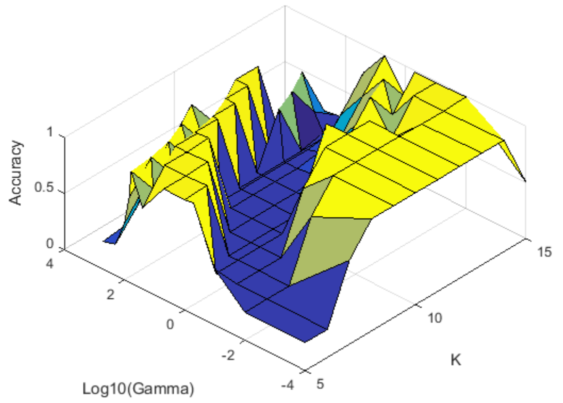
Bins = 100



Bins = 200



Bins = 400



Bins = 600

Figure 24: Effect of k and gamma values on Accuracy for different values of number of histogram bins. Accuracy is measured with F1-Measure. As number of bins increase, accuracy improves. The yellow region depicts the parameter combinations (k, bins, and gamma) where the accuracy is high.

It can be observed that as the number of bins increases, there seems to be more surface area (combination of gamma and k) that gives perfect accuracy. There is likely some threshold to this. But if the number of bins is increased beyond the threshold, the performance degrades.

6.5 Nodes Vs Time

Being a large-scale algorithm, we tested it on a cluster setup. In a distributed environment, the parallelism occurs depending on how my resources are allocated for the parallel execution. Keeping the dataset consistent, we tested the algorithm on variant nodes. As we increase the number of slave resources, the execution time reduces linearly. We tested with 1, 2 and 3 workers. Below are the statistics and graphs for these. All the times are Wall-times in seconds.

Table 4: Avg. performance gain for variant number of executors for fit function. (Time in seconds)

size	1 worker	2 workers	3 workers
1000	57.13766427	42.47342901	29.39921117
10000	80.71090465	56.49859133	38.41511018
50000	248.343311	170.8283744	119.0265084
100000	441.5165808	297.620228	196.867217
500000	2025.041952	1242.804394	822.3148522

Table 5: Avg. performance gain for variant number of executors for predict function. (Time in seconds)

size	1 worker	2 worker	3 worker
1000	82.64575286	60.66605968	40.80560379
10000	84.99851303	61.17617471	42.10171177
50000	93.39005802	61.2380533	45.61087728
100000	112.725675	72.51812732	54.20031161
500000	263.9568171	173.30298	123.6939093

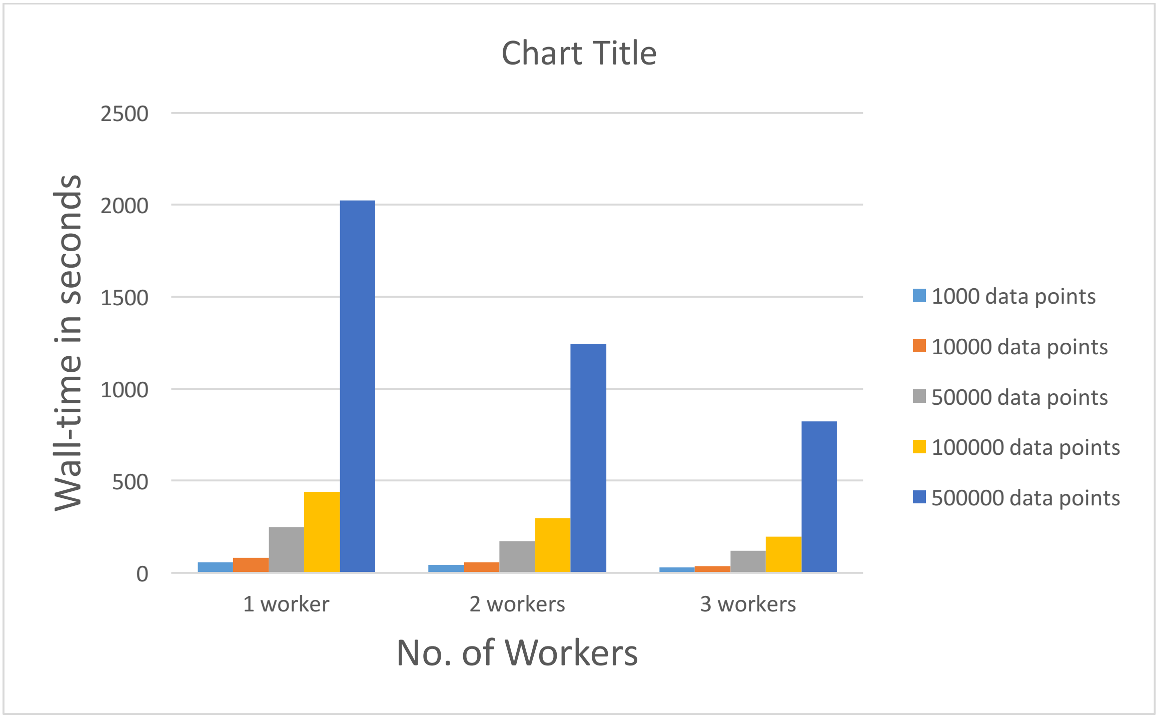


Figure 25: Scalability in seconds for variant data sizes against variant executors

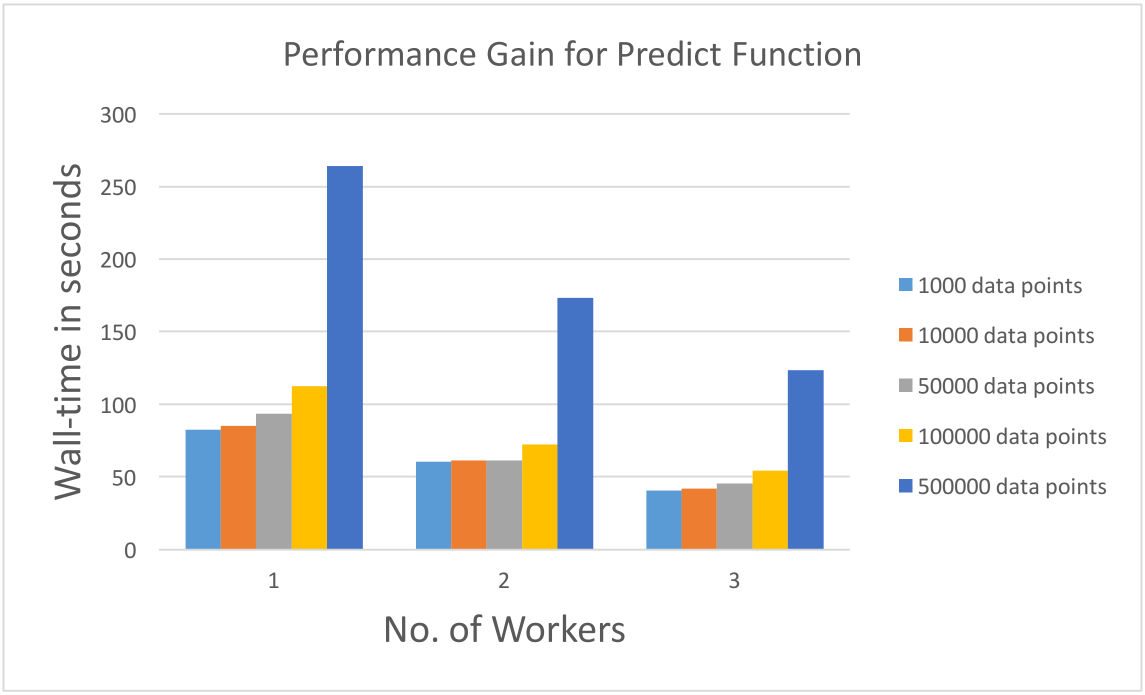


Figure 26: Scalability in seconds for variant data sizes against variant executors

CHAPTER 7

POTENTIAL USE CASE: COMPUTATIONAL OLFACTION

This chapter talks about the work done in olfaction so far. It talks about 3 different research work that will establish a ground truth for our work.

7.1 Introduction

The common dictionary definition of Olfaction is “sense of smell”. There can be disagreements in the descriptions of smells given by people. The perception of an odor for every person could be different as odors highly rely on hundreds of receptors in the brain. This concept is defined by the term Structure-Odor Relationship. It is difficult to map the physicochemical properties of Odors to perceptual representations[16]. The physicochemical properties are quantifiable, objective chemical properties of the molecule in question; e.g., color, texture, odor, number of atoms, melting point, boiling point and so on. Deriving a quantifiable mapping between these physicochemical properties and their resulting odor percepts is the driving question behind computational olfaction, and an ideal candidate for machine learning.

To achieve this, we choose the approach of applying Machine Learning techniques to map the physicochemical properties of chemical substances to the odor perceptual space. Machine Learning provides a statistically sound predictive analysis for the data which can be fairly trusted. Machine Learning has even proved its significance in numerous Healthcare prediction problems.

Our approach follows the semi-supervised learning pattern to do the desired mapping: it is expensive to acquire ground-truth perceptual odor descriptors for molecules, and impossible to do on a large scale. On the other hand, it is comparatively easy to derive physicochemical properties of small molecules. Thus, we are left in a situation with a large amount of unlabeled data and a small amount of labeled data, and need to learn a model: an ideal situation for semi-supervised learning.

There are data patterns that indicate the type of machine learning approach that can be undertaken to solve the issue at hand. In regards to that, looking at the data pattern that we are dealing with, semi-supervised learning approach may seem to work a lot better than either supervised or unsupervised learning approach alone. Another good reason to use ML approach is the availability of data characteristics. Data characteristics can be named as “features” in terms of Machine Learning language. The physicochemical properties are the features for our olfaction data.

The focus of this topic is on scaling the approach for huge amount of data. Given a set of Billions of chemical substances each with hundreds of physicochemical properties our large scale semi supervised approach can handle such huge amount of dataset. Being a generic algorithm, it is compatible with any real time dataset.

7.2 Computational Olfaction – Background

7.2.1 "Odor quality: semantically generated multidimensional profiles are stable" [5]

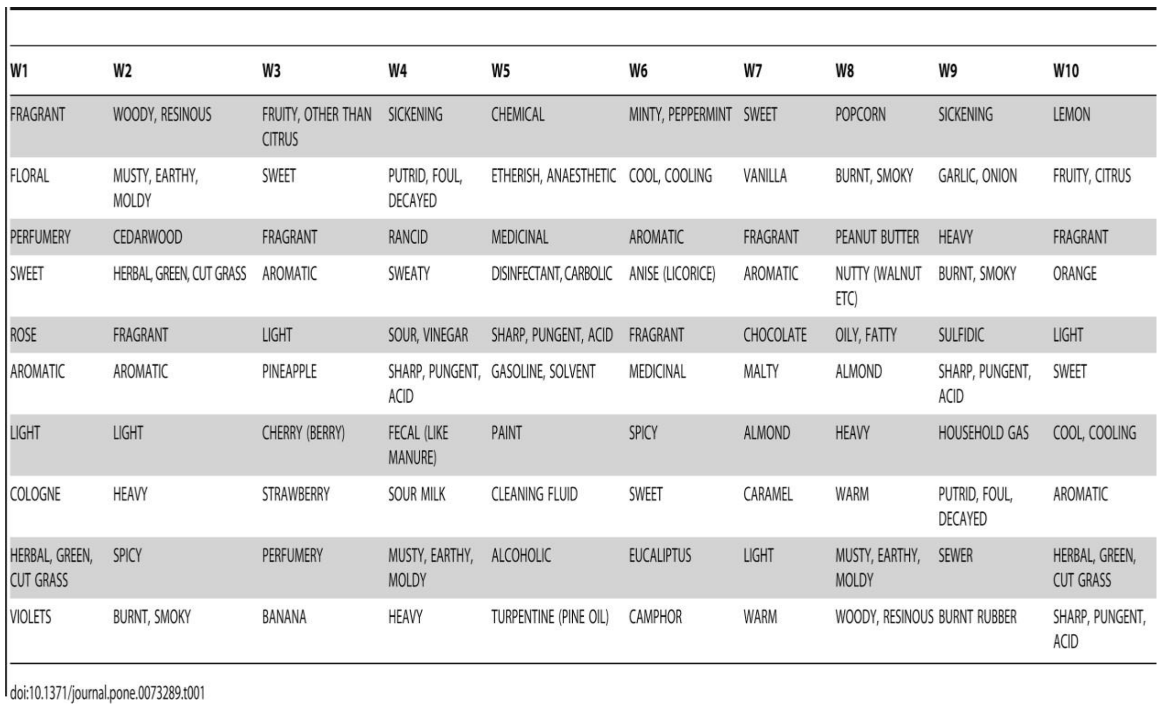
This paper talks about characterization of odors of 10 known compounds by 150 subjects using a list of 146 descriptors. There are two methods for identification of odor, reference odorant method and semantic method. As the name suggests, reference odorant method finds a reference to a similar odor whereas semantic method is to define or describe odor in terms of words. Around 150 subjects were asked to provide with a combination of descriptors for the 10 odorants. This combination was chosen out of the 146 descriptors given to them. A few of these 146 descriptors are Fruity, citrus, Lemon, Grapefruit, Orange, Fruity, non-citrus, Pineapple, Grape juice. The subjects were asked to provide scores for descriptors which they felt would be an appropriate combination for each of the 10 odorants. The score of every descriptor and the frequency of every descriptor were the deciding factors for the characterization of the odorants. The list of the 10 odorants is as follows: Acetophenone, Anethole, I-Butanol, I-Carvone, p-Cresylmethylether, Cyclohexanol, I-Heptanol, I-Hexanol, Phenylethanol, Pyridine.

7.2.2 "In search of the structure of human olfactory space" [6]

This paper investigates the structure of olfactory space defined by the responses of 150 human observers. They make use of responses for 144 odorants and represent it in a set of 146D vectors. These 146 dimensions are the descriptors that were established in the paper by Dravnieks(AOCP, 1985). Here they apply a PCA (Principal Component Analysis) on these odorants thereby reducing the dimensionality to a 2D curved surface which accommodates the 144 odorants. For 2D approximation, they relate the 2 parameters to the physicochemical parameters of odorant molecules. They also show that one of these parameters is related to the eigenvalues of molecules connectivity matrix, while the other is correlated with measures of molecules polarity[6]. The paper also established a mapping for the odour perceptual space and the physicochemical properties. They compared the resulting two co-ordinates to various physicochemical properties of odorants. They eventually worked with 126 physicochemical properties and established the correlation of these properties with the 2 perceptual dimensions.

7.2.3 "Categorical Dimensions of Human Odor Descriptor Space Revealed by Non- Negative Matrix Factorization" [7]

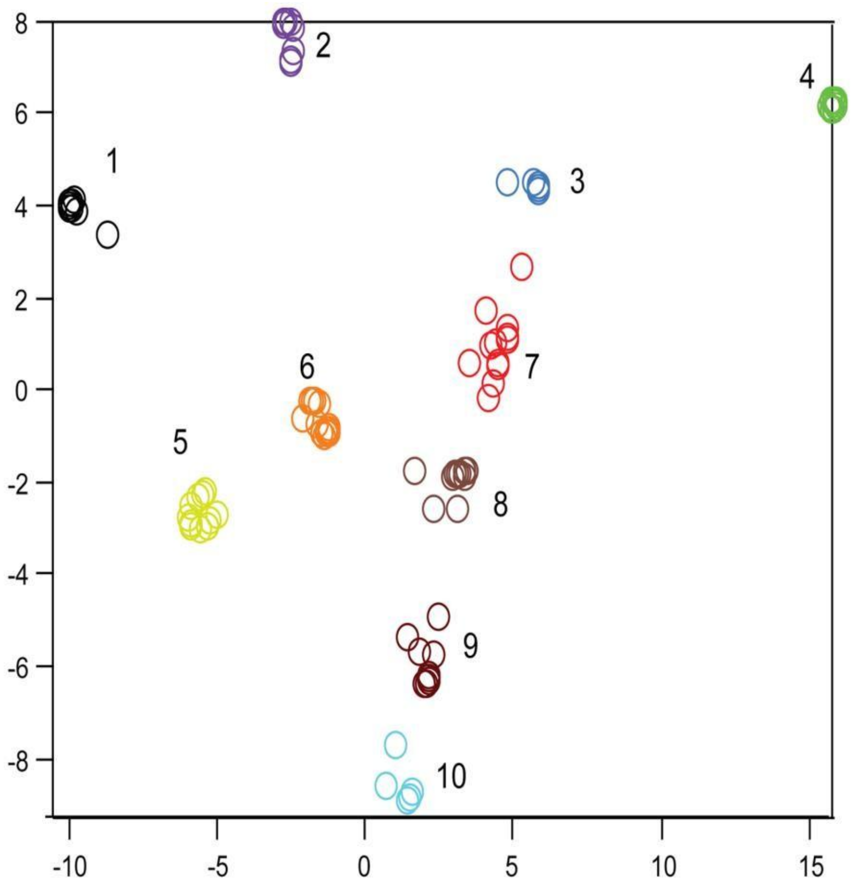
This paper talks about reducing the dimensions of odorants using a Non-Negative Matrix factorization to uncover the structure in a panel of odor profiles. Each odor is defined as a combination of these 146 descriptors. The paper also corroborates the theory that odor dimensions apply categorically; that the odor space is defined in a discrete and intrinsically clustered manner. They choose the NMF approach for dimensionality reduction based on the observation that all the descriptor values are non-negative. They reduce the 146 dimensional space to a 10 dimensional perceptual space. They worked on 144 monomolecular odors each represented as a 146 dimensional (descriptor) vector.



W1	W2	W3	W4	W5	W6	W7	W8	W9	W10
FRAGRANT	WOODY, RESINOUS	FRUITY, OTHER THAN CITRUS	SICKENING	CHEMICAL	MINTY, PEPPERMINT	SWEET	POPCORN	SICKENING	LEMON
FLORAL	MUSTY, EARTHY, MOLDY	SWEET	PUTRID, FOUL, DECAYED	ETHERISH, ANAESTHETIC	COOL, COOLING	VANILLA	BURNT, SMOKY	GARLIC, ONION	FRUITY, CITRUS
PERFUMERY	CEDARWOOD	FRAGRANT	RANCID	MEDICINAL	AROMATIC	FRAGRANT	PEANUT BUTTER	HEAVY	FRAGRANT
SWEET	HERBAL, GREEN, CUT GRASS	AROMATIC	SWEATY	DISINFECTANT, CARBOLIC	ANISE (LICORICE)	AROMATIC	NUTTY (WALNUT ETC)	BURNT, SMOKY	ORANGE
ROSE	FRAGRANT	LIGHT	SOUR, VINEGAR	SHARP, PUNGENT, ACID	FRAGRANT	CHOCOLATE	OILY, FATTY	SULFIDIC	LIGHT
AROMATIC	AROMATIC	PINEAPPLE	SHARP, PUNGENT, ACID	GASOLINE, SOLVENT	MEDICINAL	MALTY	ALMOND	SHARP, PUNGENT, ACID	SWEET
LIGHT	LIGHT	CHERRY (BERRY)	FECAL (LIKE MANURE)	PAINT	SPICY	ALMOND	HEAVY	HOUSEHOLD GAS	COOL, COOLING
COLOGNE	HEAVY	STRAWBERRY	SOUR MILK	CLEANING FLUID	SWEET	CARAMEL	WARM	PUTRID, FOUL, DECAYED	AROMATIC
HERBAL, GREEN, CUT GRASS	SPICY	PERFUMERY	MUSTY, EARTHY, MOLDY	ALCOHOLIC	EUCALIPTUS	LIGHT	MUSTY, EARTHY, MOLDY	SEWER	HERBAL, GREEN, CUT GRASS
VIOLETS	BURNT, SMOKY	BANANA	HEAVY	TURPENTINE (PINE OIL)	CAMPHOR	WARM	WOODY, RESINOUS	BURNT RUBBER	SHARP, PUNGENT, ACID

doi:10.1371/journal.pone.0073289.t001

Figure 27: 10 largest-valued descriptors for each of the 10 basis vectors obtained from non-negative matrix factorization [7]



Cluster 1

Aldehyde C-16, Allyl Caproate, iso-Amyl Acetate, Amyl Butyrate, Dimethyl Benzyl Carbinyl Butyrate , Ethyl Butyrate, Ethyl Propionate, Fructone, Methyl Anthranilate , Undecylenic Acid, gamma-Valerolactone

Cluster 2

Amyl Phenyl Acetate, Auralva, iso-Bornyl Acetate, Cashmeran, Dimethyl Phenyl Ethyl Carbinol, Hydroxy Citronellal, Indolene, beta-Ionone, alpha-Irone, Lyral, Methoxy-Naphthalene: 2-Methoxy, Naphthalene , Methyl Acetaldehyde Dimethyl Acetal, Musk Galaxolide, Musk T onalid, Phenyl Ethanol, Sandiff, Santalol

Cluster 3

dl-Camphor, l-Carvone, p-Cresyl Acetate, Eucalyptol, l-Menthol, Methyl Salicylate, Safrole

Cluster 4

Amyl Cinnamic Aldehyde Diethyl, Acetal, Citral, Citralva, Floralozone, Hexyl Cinnamic Aldehyde, Linalool, d-Limonene , Melonal, Myracaldehyde

Cluster 5

Anisole, 1-Butanol, m-Cresol, p-Cresol, p-Cresyl-iso-Butyrate, p-Cresyl Methyl Ether , Cyclohexanol , 2,5-Dimethyl, Pyrazine , Diola, Diphenyl Oxide, 1-Heptanol, 1-Hexanol, 3-Hexanol, Iodoform, Methyl Furoate, para-Methyl Quinoline , Nonyl Acetate, 1-Octanol, Phenyl Acetylene, Terpineol, Tetraquinone, Thymol, Toluene

Cluster 6

Adoxal, Andrane, iso-Butyl Quinoline Chlorothymol, Iso-Cyclocitral, Cyclotropal, Decahydro Naphthalene, Dibutyl Amine, Grisalva, Hexanal, Hydratropic Aldehyde Dimethyl Acetal, 2-Methyl-iso Borneol, Methyl iso-Nicotinate , Nootkatone, 1-Octen-3-OL, iso-Phorone, alpha-Pinene, iso-Propyl Quinoline, Propyl Sulfide, gamma-Undecalactone

Cluster 7

Abhexone, Acetophenone, Aldehyde C-18, Anethole, Benzalde-hyde, Dihydro Pyrone, Caryophyllene (beta and gamma Isomers) , Celeriax, Cinnamic Aldehyde, Coumarin, Cuminic Aldehyde , Eugenol, Furfural, trans-1-Hexenal, ortho-Tolualdehyde, Vanillin

Cluster 8

ortho-Acetyl Pyridine, Cyclotene, 2,4-trans-trans-Decadienal , 2,3-Dimethyl Pyrazine , 2,5-Dimethyl Pyrrole , 2-Ethyl Pyrazine, Furfuryl Mercaptan, Guaiacol, Heptanal, Thienopyrimidine, Zingerone

Cluster 9

Butyl Sulfide, Cyclodithalfarol, 2-Cyclohexanedione , Diethyl Sulfide, Dimethyl Trisulfide, Hexyl Amine , Pyridine, Tetrahydro Thiophene, Thioglycolic Acid, Thiophene

Cluster 10

Amyl Valerate, Butanoic Acid, Hexanoic acid, Hexyl Amine, Indole, Maritima, Methyl Thiobutyrate, Pentanoic Acid, 4-Pentenoic Acid, Phenyl Acetic Acid , Propyl Butyrate, Skatole, Trimethyl Amine, iso-Valeraldehyde, iso-Valeric Acid

Figure 28: 2D embedding of the odor perceptual space [7]

7.3 Challenges

1. Due to difficulty in interpretation of odors for chemical components, the known mappings for physicochemical features to components are very few. There is not enough established data available.
2. Moreover, it is impractical to manually identify odors of compounds for several reasons one of which being that it may be hazardous to do so. This strongly explains need for computational olfaction identification.
3. The semi-supervised approach given by Fergus et al makes a strong assumption that the data dimensions are as independent as possible. This won't be the case when dealing with olfaction dataset. The olfaction data is supposed to be a very high dimensional data. It is unlikely that the dimensions will be independent.

If we are able to find a numerical workaround to achieve independent dimensionality, we can apply eigenfunction approach to olfaction data.

CHAPTER 8

CONCLUSION

We have provided a large scale implementation of the eigenfunction approach using semi-supervised learning on a distributed framework like Apache Spark. We have discussed the transductive and inductive learning approaches provided by this approach. The approach implementation that we provide simulates the transductive as well as inductive parts of it. We have analyzed the eigenfunction approach and presented this analysis with the help of density plots. We have also discussed the background of computational olfaction and how this approach would be compatible with the olfaction data. We have presented this algorithm results on toy datasets and also analyzed the process. The main idea is to be able to apply this algorithm on large datasets. The motivation for this work was computational olfaction. The next step would be applying this algorithm on the olfaction data. The olfaction data is a data with 10 odor classes and is high-dimensional. If the dataset is dimensionally independent and proportionally labeled, an algorithm like eigenfunction can be aptly applied to such high dimensional data. Moreover, since this algorithm is linear with respect to the number of data points, the time required will be definitely lesser than that required by methods that construct a full n x n graph Laplacian. Given any such high-dimensional, dimensionally independent dataset with an appropriate proportion of labeled and unlabeled data, this algorithm can be used to predict labels for the unlabeled points by its transductive method and can also label any new unseen point by its inductive method.

The Eigenfunction approach is efficient in terms of computation time required but it lacks robustness since it is very sensitive to the three parameters k, bins, and gamma. A lot of tweaking is required if the data distribution and data pattern is unknown. But if we can study the data distribution, the clustering depicted by the ground truth, then it will be easier tweaking the parameters.

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