國立臺灣大學電機資訊學院資訊工程研究所
碩士論文
Department of Computer Science and Information Engineering
College of Electrical Engineering and Computer Science
National Taiwan University
Master Thesis

利用正交轉換在分散式環境中尋找 K 個最近鄰居
kNN-Search with Orthogonal Transformation in the Distributed
Environment

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國立臺灣大學
資訊工程研究所

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王瑞斌 撰

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  —台灣大學論文 LATEX 樣版原創者黃子桓的教學網頁
- LaTeX 常用語法及論文範本
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- 使用 LaTeX 做出精美的論文
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- 李果正-大家來學 LATEX—建議先看完前四章
- WIKIBOOKS-LATEX—好用的線上工具書
- Working with a .bib file using JabRef
- Using BibDesk - A short tutorial
- LaTeX for Physicists

III. 下載 LaTeX 整合發行套件，可參考 TeX Collection：
1. MacTeX: For **MacOSX**，下載 MacTeX.pkg
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4. CTAN: The Comprehensive TeX Archive Network.

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       可參考 Working with a .bib file using JabRef 或是 Google 及 YouTube
    2. BibDesk (For Mac)
       可參考 Using BibDesk - A short tutorial 或是 Google 及 YouTube
- 方程式編輯器：Daum Equation Editor (Chrome App，必須使用 Google 瀏覽器)

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1. `xelatex thesis`
   對 thesis.tex 進行第一次 XeLaTeX 編譯，產生 thesis.pdf 以其他檔案
2. `bibtex thesis`
   對 thesis.tex 進行 BibTeX 編譯，產生 bbl 檔以及 blg 檔
3. `xelatex thesis`
   對 thesis.tex 進行第二次 XeLaTeX 編譯，產生目錄、圖表連結及參考文獻
4. `xelatex thesis`
   對 thesis.tex 進行第三次 XeLaTeX 編譯，產生參考文獻連結，完成編譯

注意！此範本使用 cite 套件，可依據你利用文獻管理系統所整理好的 thesisbib.bib 檔在論文最後產生參考文獻頁面，若你的系所規定要在每個章節的後面產生參考文獻，則可以用 chapterbib 套件，來對每個有附參考文獻的章節 tex 檔進行一次 BibTeX 編譯產生 bbl 檔，如範例的 introduction.tex、THM.tex 和 EXP.tex，如果有這需要請把 thesis.tex 檔裡使用 cite 套件的指令利用註解符號 % 來取消使用 cite 套件，並刪去出現在使用 chapterbib 套件指令前面的註解符號 % 來啟動使用 chapterbib 套件

```
\usepackage{cite}
%\usepackage{chapterbib}
```
改成

```
%\usepackage{cite}
\usepackage{chapterbib}
```

再來利用註解符號%取消會把參考文獻放在論文最後的指令

```
\bibliographystyle{unsrt}
\addcontentsline{toc}{chapter}{\bibname}
\bibliography{thesisbib}
```
改成
```
%\bibliographystyle{unsrt}
%\addcontentsline{toc}{chapter}{\bibname}
%\bibliography{thesisbib}
```

再把用來輸入章節檔案的 \input 指令改成 \include 指令

```
\input{introduction}  =>  \include{introduction}
\input{THM}           =>  \include{THM}
\input{EXP}           =>  \include{EXP}
```

最後記得在每個有附參考文獻的章節加上產生參考文獻的指令，即在introduction.tex、THM.tex和EXP.tex三個檔案裡最後啟動下面兩行指令

```
%\bibliographystyle{unsrt} => \bibliographystyle{unsrt}
%\bibliography{thesisbib}  =>  \bibliography{thesisbib}
```

而編譯時則需要對有附參考文獻的introduction.tex、THM.tex和EXP.tex各做一次 BibTeX 編譯，編譯流程如下

1. `xelatex thesis`
   對 thesis.tex 進行第一次 XeLaTeX 編譯，產生 thesis.pdf 及其他檔案
2. `bibtex introduction`
   對 introduction.tex 進行 BibTeX 編譯，產生 bbl 檔以及 blg 檔
3. `bibtex THM`
   對 THM.tex 進行 BibTeX 編譯，產生 bbl 檔以及 blg 檔
4. `bibtex EXP`
   對 EXP.tex 進行 BibTeX 編譯，產生 bbl 檔以及 blg 檔
5. `xelatex thesis`
   對 thesis.tex 進行第二次 XeLaTeX 編譯，產生目錄、圖表連結及參考文獻

6. `xelatex thesis`
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  `%\makecertification`

  編譯完後就可以產生審定書格式。口試通過後，請把已經簽名的審定書掃描成 pdf 檔，再取代原本的cert.pdf，即可放上已簽名的審定書。處理審定書出現的指令在 thesis.tex 裡

  ```
  %----------- generate the certification ...
  %\makecertification
  %----------- includepdf by using package ...
  \addcontentsline{toc}{chapter}{口試委員會審定書}
  \includepdf[pages={1}]{cert.pdf}
  ```

- 浮水印：
  資料夾已經附上浮水印檔案了，若學校有更改，到請到台大圖書館網頁的電子論文服務下載pdf 格式的浮水印到此範本所在資料夾。若要開啟關閉浮水印功能，即自行刪去或加上下面位於thesis.tex指令的註解符號%

  ```
  %\CenterWallPaper{0.174}{watermark.pdf}
  %\setlength{\wpXoffset}{6.1725cm}
  %\setlength{\wpYoffset}{10.5225cm}
  ```

- 單面印刷與雙面印刷：
  此範本為單面印刷，若論文頁數超過 80 頁，依規定需要用雙面印刷，此時只需把 thesis.tex 裡的

  ```
  \documentclass[a4paper, 12pt, oneside]{book}
  ```
  改成
  ```
  \documentclass[a4paper, 12pt, twoside]{book}
  ```

- 如何加入附錄?

在 thesis.tex 裡，依需求選擇 input 或 include，刪去 % 符號來輸入附錄章節

```
%----------- Input your appendix here  -----------
%\input{AppendixA}
%or %chapter cite  == \include
%\include{AppendixA}
```

在章節檔 AppendixA.tex 裡，開頭打

```
\chapter{First appendix title}
```

即可，以此類推。

- 系上規定論文圖表須全部放到最後獨立出來的章節，且章節不出現在目錄中：

在 thesis.tex 裡，依需求選擇 input 或 include，刪去 % 符號來輸入圖表章節

```
%----------- Input your Figure chapter here  -----------
%\input{EndFigTab}
%chapter cite  == \include
%\include{EndFigTab}
```

在章節檔 EndFigTab.tex 裡有範例和說明可供參考，要注意正文的圖表和附錄的圖表要分清楚，即在 EndFigTab.tex 內

```
\renewcommand{\thefigure}{\arabic{chapter}.
\arabic{figure}}
\renewcommand{\thetable}{\arabic{chapter}.
\arabic{table}}
%--- Input your main figures and tables here  ---
```

這幾行之後章節計數器格式已切換為 1…9，放正文的圖表，

```
\renewcommand{\thefigure}{\Alph{chapter}.
\arabic{figure}}
\renewcommand{\thetable}{\Alph{chapter}.
\arabic{table}}
%--- Input your appendix figures and tables here  ---
```

這幾行之後章節計數器格式已切換為 A…Z，放附錄的圖表。另外要取消圖表的浮動功能，才能讓圖表按照指令出現順序排好，即把平常使用的圖表指令

```
\begin{figure}[htb]
...
\begin{table}[htb]
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\begin{figure}[!]
...
\begin{table}[!]
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剩下的只要注意章節圖表的計數器設定即可。\ref 和 \label
指令可以在此圖表章節與正文章節使用。

- 如果我想要修改 margin(文字邊界) 的話，可以從哪裡下手呢?
  請打開ntu.sty修改下面這行的上下左右參數即可：

  ```
  \RequirePackage[top=3cm,left=3cm,bottom=2cm,right=3cm]
  {geometry}
  ```

- 我想引用 Twomey (1974): Pollution and planetary albedo 這篇論文，
  如何用 \cite 引用它的時候在內文顯示 Twomey (1974) [編號]？
  建議使用 natbib 套件，參考資料如下：
  LaTeX/Bibliography Management
  Overview of Bibtex-Styles
  Reference sheet for natbib usage

- X\=E\=TEX：
  此範本中文字體使用X\=E\=TEX 轉換，細節請參考Hitripod寫的XeTeX：
  解決 LaTeX 惱人的中文字型問題。

- 如何輸入英文 ‘單引號’ 和 “雙引號” 以及不同長度的破折號？
  可以參考李果正 -大家來學 LATEX第 17 頁針對標點符號的遊戲規
  則，範例如下，輸入以下指令：

  ```
  ‘單引號’\\
  ‘‘雙引號’’\\
  -hyphen\\
  --en-dash\\
  ---em-dash\\
  ```

  則顯示：
  ‘單引號’
  “雙引號”

-hyphen
–en-dash
—em-dash

中文摘要

請打開並編輯abstractCH.tex

關鍵字：壹、貳、參、肆、伍、陸、柒

Abstract

Open and edit abstractEN.tex

Key words:A, B, C, D, E, F, G

Contents

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Chapter 1

Introduction

Due to the advance of technology, query by similarity for various kinds of datasets among distributed machines like mobile devices becomes an increasingly common and important task. In this distributed environment where a large amount of local machines are involved in computation and storage, our goal in most case is to minimize the amount of transmission cost during finding the answer from these machines. Therefore, this paper aims to generalize the current state-of-the-art on distributed pattern matching from only workable for "time series" datasets to more types of dataset such as "images" and "music" while significantly reducing the communication cost.

Consider the first scenario in which, through a program installed on mobile devices, a company about data mining could obtain some unusual and potentially profitable images and want to know quickly whether a similar image exsists in someone's cell phone or tabelet. To do so, it is required to find the similar images among a large amount of distributed devices for the final answer. Moreover, this company could construct a platform which allows users to search among the images of other cell phones as long as they also provide their images. With this platform, each user could use their images to find the similar images from other cell phones. On the other hand, beside of the images, this platform could also deal with other type of data like music.

Since this paper is generalized from the work [1] called LeeWave and our work [2] called MsWave, our model could also apply to those scenarios such as the abnormal detection and work on the time series datasets. Although our discussions in the following

chapters would focus on the problem of handling a single query and finding the k nearest neighbors among these distribued devices, we could deal with multiple queries and the k farthest neighbors like MsWave only with a little modifications.

However, to design a framework which could handle these scenarios would requires addressing some challanges. First, our goal is to find the *exact k* nearest neighbors instead of approximate k nearest neighbors. So, we find the answer according to their exact similarity. Second, the number of distributed devices could be very large. It would cause huge communication cost to get our answers from them. Third, since there could be a large amount of users on that platform, we also have to handle a extremely long sequence of queries. Forth, to achieve the cost saving in communication, we have to extract valuable information from queries to send to machines instead of the whole query. It is a important question to define the valuable information and then discard impossible candidates only with the help of these information. Finally, since in many situations there are bandwidth limitations and concerns of energy consumption as well as communication cost, it is crucial to design an framework that needs as little communication cost among distributed machines as possible. This paper would overcome these problems on the basis of the ideas proposed by LeeWave.

Although the state-of-the-art method, LeeWave in [1] could solve some of the challenges above, there are still some problems for it to deal with. The most important problem is that the way LeeWave to prune the candidates is not effective when the datasets are not time series. Since the bounds of LeeWave comes from the Haar wavelet transformation, which is a kind of transformation usually applied on time series, these bounds would be no longer tight when the data we deal with is not time series. Another problem is that the cost of the pruning procedure in LeeWave grows linearly with the number of total instances in these distrubited devices. When the number of instances is large, its communication cost would be too expensive.

We summarize our main contributions as follows:

1. We propose a general communication-efficient framework which could find kNN and kFN instances given multiple queries for various types of datasets which are

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distributed in a large amount of devices.

2. In the part of methodology, based on the ideas of upper bounds and lower bounds of similarity in [1], we derive new bounds with the help of the orthogonal transformation. And these new bounds enhance the power of pruning is the main source to achieve the goal of cost saving in communication.

3. Since it would be expensive to find the threshold used in the pruning procedure if the number of total instances in these machines is large, we give a method that could make this cost be indenpendent of this number.

4. We propose a method to estimate the communication cost which allows us to dynamically adjust how much information we need to send for the current query according to the history of the past queries.

5. We conduct extensive experiments for various types of datasets to demonstrate that our model could achieve the goal of saving communication cost.

1.1 Thesis Overview

We organize this paper as follows: In the chapter 2, we discuss about the related papers and their limitations. Then, in the chapter 3, we propose the details of our framework. In the chapter 4, we provide the results of the experiments for the datasets of images, music, and time series. Finally, in the chapter 5, we discuss the results and our future work.

Chapter 2

Related Works

In this chapter, we talk about the works which are related to these scenarios.

2.1 Concurrent Processing

Concurrent Processing (CP) [3] is the baseline of this problem. First, the server would send the whole query to every local machine. Each machine calculates the distance between this query and every instance on it. Then, every machine return the top k instances with the lowest distance back to the server. By these $m \times k$ instances, the server could know which k instances are the k nearest neighbors of the query. We could easily notice that much communication cost is waste in this framework.

2.2 Probabilistic Processing

There is another method named Probabilistic Processing (PRP) in [3] that we could take it as an improvement of CP. The most important characteristic of PRP is that it guarantee to find the answers in two rounds with less communication cost than CP. In the first round, the server also sends the whole query to every local machines. But, instead of return the top k instances like CP does, each machine only return the top $\left\lfloor \frac{k}{m} \right\rfloor + 1$ instances back to the server where m is the number of total local machines. With these

$m \times (\lfloor \frac{k}{m} \rfloor + 1) = k + m$ instances, the server could prune some machines which are impossible to obtain the final k answers and then ask the other machines for the final answers in the second rounds. Although PRP might able to prune some machines in the first round, it still spends too much cost in the second round.

2.3 LeeWave

Now let's talk about the state-of-the-art method, LeeWave [1], which is the starting point of our framework. The spirit of LeeWave is to iteratively pruning impossible candidaites until only k instances left by transforming a raw feature vector into an error tree like TODO with the help of the Haar wavelet transformation. Although the total number of coefficients in an error tree would be equal to length of the raw feature vector, the coefficients at the upper levels would be more important than those in the lower levels. The importance defined here is the chance to contibute more to the final Euclidean distance, And it could also be observed from the way to calculate the Euclidean distance from the error trees, the higher level the coefficient is, the heavier weight it has to multiply.

Once we have the importance of the coefficients, LeeWave sends coefficents according to their levels in the error tree transformed from the query q, from upside to down. In each round, LeeWave would send those coefficients in one level of the tree to each candidate machines. Then, these machines would return some information that allows the server to compute the bounds between q and the instances in these machines. With the help of these bounds, the server could prune some instances that they are impossible to be the final answers. If there are exactly k instances left after pruning, then we just achive our goal to find the kNN/kFN. Otherwise, the server would send the next level and repeat the pruning process until finding the answers or sending every level of this tree.

2.4 MsWave

MsWave [2] is our previous work which is also extended from LeeWave but toward a different direction. While the main contibution of this paper is to generalize the ideas

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of LeeWave to various types of datasets, the contribution of MsWave focus on how to modify the bounds in LeeWave for multiple queries and finding k farthest neighbors. We could say that LeeWave is a special case of MsWave for a single query only with some slightly difference. Since the foundation of MsWave and this paper is the same, we could easily apply our all improvements in this paper to the scenarios in MsWave. That is, we could also solve the cases of multiple queries and find k farthest neighbors with our new bounds. Because there are detailed discussions about the situation of multiple queries and differences between finding kNN and kFN, we only conduct the experiments for the case of a single query and finding kNN.

2.5 Others

Due to the population of the P2P paradigm [4, 5], there are some methods which use the distributed computing to do similarity search over a set of machines. For example, [6–8] are P2P approaches proposed for similarity search, but they are designed for one dimensional data, not high dimensional data. SWAM [9] is a family of *Small World Access Methods*, whose goal is to build a network topology which could collect peers with similar content. However, in this framework, each peer could only obtain a single data, which is not suitable with our problem for a large amount of data. VBI-tree and SkipIndex both rely on tree-based approaches that could not scale when the dimensions of data are high. [10] leverage on LSH-based approaches for similarity search over structured P2P network for high dimensional data. Nevertheless, it only provides the approximate results, not exactly solution. But the biggest difference between these papers and our framework is the setting of the network. While their framework apply on a more general P2P system, our setting is that every local machine is only able to communicate with a single server.

Chapter 3

Methodology

HiHi Iam r44 . The organization of this thesis is as follows. In chapte **??**, the theoretical background and definition of surface plasmon will be included [1]. Chapte 4 contains description of experiment methods such as atomic force microscopy and scanning electron microscopy.

3.1   Problem Setup

There are a query set $Q = \{q_1, q_2, ..., q_T\} \subset \mathbb{R}^D$ at the server P and a dataset $X_i \subset \mathbb{R}^D$ on each local machine M_i. For each coming query q_t, we want to find its k_{th} nearest neighborhood among these distributed datasets while reducing the transmission cost between P and each M_i.

3.2   Overview of Our Framework

In this section, we describe the overall framework of our work. Then, we will give the details about the framework in the following sections.

Figure 3.3 is the overall flow on our framework. There are two main phases in our framework. For each X_i, the first phase only needs to be done for once. On the other hand, we need to run the second phase for each new query q_t.

The first phase is an preprocessing procedure for the second phase. Its goal is to im-
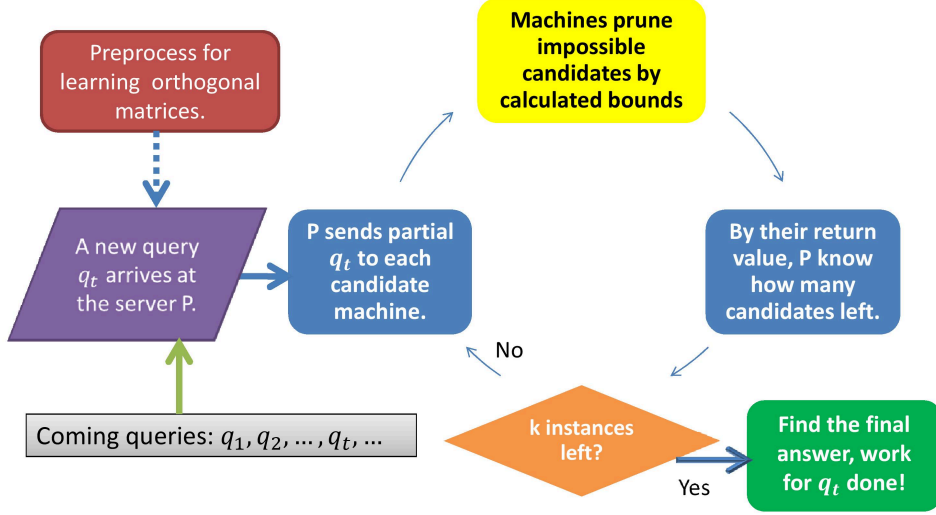
Figure 3.1: The overall flow of our framework.

prove the performance of pruning in the second phase. We will prove in the section 3.5.2 that this pruning power is highly correlated to the distribution of the norm of the feature vectors. As a result, each M_i would learn an othorogal matrix W_i for its X_i to fit our desired distribution and then send each W_i back to P. We can notice that this phase is only dependent on X_i and independent of q_t. Therefore, we only need to do the first phase for once. we give the details about how to learn W_i, how to send it back to P in the section 3.3.

The second phase is the main procedure of our framework. Note that P have already got W_i for each X_i in the beginning of the second phase. For each coming query q_t, we iteratively prune some candidates which are impossible to be the kNN of q_t to reduce the search space until there are only k candidates left.

To prune candidates iteratively, we divide the second phase into several rounds. For each round j, we use a $Select$ function $S_i(q_t, j; \theta_t)$ to generate the values for trasmitting from P to M_i, where S_i is the importance-selecting function of M_i and θ_t is its parameters for q_t. (We put the details of S_i at the section **??**.) By these values, each M_i could calculate

8

the bounds between each candidate x_l and q_t. With these bounds, P would be able to determine which candidates are definitely not our answer and then disregards them in the following rounds. By these pruning, we could achieve the goal of saving transmission cost from avoiding to consider the unnecessary candidates.

Note that we could use the square of the Euclidean distance instead of the origin Euclidean distance to find kNN as it is non-negative. So we will use the former one in our framework.

3.3   Orthogonal Transformation

Since the In this section, we describe the overview of this thesis.

3.3.1   Definition of Ortohogonal Transformation

Definition 1. *A matrix $W \in \mathbb{R}^{D \times D}$ is orthogonal if whose columns and rows are orthogonal vectors, i.e.*

$$W^T W = W W^T = I$$

where I is the identity matrix.

3.3.2   Property of Orthogonal Transformation

Property 1. *Let $x, y \in \mathbb{R}^{D \times 1}$, and $W \in \mathbb{R}^{D \times D}$ be an orthogonal matrix. Then,*

$$Dist(x, y) = \sum_{d=1}^{D} (x[d] - y[d])^2 = \sum_{d=1}^{D} (W[d, :]x - W[d, :]y)^2 = Dist(Wx, Wy)$$

where $W[d, :]$ is the d_{th} row of W.

We will use this important property in the section **??**.

3.4 Enhance the Bounds by the Orthogonal Transformation

In the section 3.2, we mentioned that the first phase is an auxiliary step for the second phase. After the introduction of the orthogonal transformation, we introduce this powerful tool into the first phase in our framework.

3.4.1 The Goal of the First Phase

Our goal in the first phase is to reduce the ranges of the bounds used in the second phase. Since we will use a threshold to prune the impossible candidates according to their bounds in the pruning procedure, the ranges of the bounds would be one of the most influential factor of the pruning power. It is easy to understand that when the ranges of their bounds is short, more candidates would be pruned than those with long ranges of the bounds. In other words, the shorter the range of the bound, the higher chance this candidate would be pruned if it is not our final answer of kNN.

Moreover, we would prove in the section 3.4.5 that to reduce the range of the bounds, the final goal of the first phase would become to learn an orthogonal transformation W which could make each raw feature vector $x \in \mathbb{R}^D$ (the orange vector in the figure below) transformed to be Wx (the red vector in the figure below) which would make the absolute values of elements in the forward part of the vector larger and those in the later part smaller.
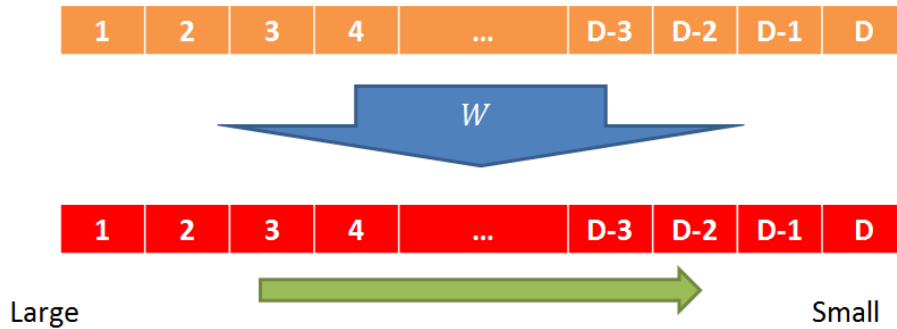

Figure 3.2: The goal of the first phase.

3.4.2 Definition of the Bounds

First, we need to define the bounds for the pruning. Recall that given a query q_t, our goal is to find its kNN in these distributed datasets X_i. Intuitively, we need to calculate the square of the Euclidean distance $Dist(q_t, x), \forall x \in \cup_i X_i$. However, to cacluate $Dist(q_t, x)$, we need to send the whole q_t to the local machines or send the whole x to P, which causes a huge transmission cost. Therefore, instead of the exact value of Euclidean distances, our propsed framework uses bounds to find the kNN.

Definition 1. $\forall x, y \in \mathbb{R}^D$, *a lower bound $LB(x, y)$ and a upper bound $UB(x, y)$ must satisfy the following inequation:*

$$LB(x, y) \le Dist(x, y) \le UB(x, y)$$

3.4.3 Relation Between the Norms and the Bounds

To acheive the goal of reducing the length of the ranges of the bounds, we could look into the derivation of the bounds. Suppose there are two vectors $x, y \in \mathbb{R}^D$, but we could only observe the first s dimensions of x and $\sum_{d=s+1}^{D} x[d]^2$, which is the square of two norm of the unobserved part $x[s + 1 : D]$. In the section 3.5.2, we give the bounds as

$$LB(x, y) = \sum_{d=1}^{s} (x[d] - y[d])^2.$$

$$\begin{aligned}
UB(x, y) = & \sum_{d=1}^{s} (x[d] - y[d])^2 \\
+ & \sum_{d=s+1}^{D} x[d]^2 + \sum_{d=s+1}^{D} y[d]^2 \\
+ & 2 \times \sqrt{\sum_{d=s+1}^{D} x[d]^2 \times \sum_{d=s+1}^{D} y[d]^2}.
\end{aligned}$$

Therefore, we could get the length of the range by the substraction.

$$Len = UB(x,y) - LB(x,y)$$

$$= \sum_{d=s+1}^{D} x[d]^2 + \sum_{d=s+1}^{D} y[d]^2$$

$$+2 \times \sqrt{\sum_{d=s+1}^{D} x[d]^2 \times \sum_{d=s+1}^{D} y[d]^2}.$$

Since the term $\sum_{d=s+1}^{D} x[d]^2$ is given, all we could do is to reduce the length with the help of the $\sum_{d=s+1}^{D} y[d]^2$ term. If we could reduce $\sum_{d=s+1}^{D} y[d]^2$, the term $\sum_{d=s+1}^{D} x[d]^2 \times \sum_{d=s+1}^{D} y[d]^2$ would also decrease and then make Len smaller. Therefore, our goal now becomes to make the term $\sum_{d=s+1}^{D} y[d]^2$ as small as possible, which is the square norm of the vector $y[s+1:D]$.

Note that the lower (upper) bounds is non-decreasing (non-increasing) as s becomes larger and $LB(x,y) = UB(x,y)$ when $s = D$. This means that LB and UB would be exactly equal to $\sum_{d=1}^{D} (x[d] - y[d])^2$ eventually.

To reduce the length of the ranges Len for each s, we hope to make $\sum_{d=s+1}^{D} y[d]^2$ as small as possible. However, since the feature vector y is given from datasets, the value of $\sum_{d=s+1}^{D} y[d]^2$ is already determined when s is given. As a result, we introduce the orthogonal transformation to achieve this goal.

3.4.4 Equivalent Bounds After Transformation

From the section 3.3.2, we know the distance of two vectors won't be changed after an orthogonal transformation. Now we use this property to achieve our goal to reduce the length of the ranges Len given s.

Given an orthogonal transformation $W \in \mathbb{R}^{D \times D}$, we have $Dist(x,y) = Dist(Wx, Wy)$. This means that the bounds we derivated before could also be the bounds for $Dist(Wx, Wy)$. That is,

$$LB(x,y) \leq Dist(x,y) = Dist(\hat{x}, \hat{y}) \leq UB(x,y)$$

where $\hat{x} = Wx$.

This also means that we could use the same way to derivate the lower bounds and

upper bounds for $Dist(Wx, Wy)$ and these bounds are also the bounds for $Dist(x, y)$. That is,

$$LB(\hat{x}, \hat{y}) \le Dist(x, y) = Dist(\hat{x}, \hat{y}) \le UB(\hat{x}, \hat{y})$$

So, we could use the bounds $LB(\hat{x}, \hat{y}), UB(\hat{x}, \hat{y})$ for $Dist(x, y)$ and the length of range we want to reduce becomes

$$
\begin{aligned}
\hat{Len}(W) &= UB(\hat{x}, \hat{y}) - LB(\hat{x}, \hat{y}) \\
&= \sum_{d=s+1}^{D} \hat{x}[d]^2 + \sum_{d=s+1}^{D} \hat{y}[d]^2 \\
&\quad + 2 \times \sqrt{\sum_{d=s+1}^{D} \hat{x}[d]^2 \times \sum_{d=s+1}^{D} \hat{y}[d]^2}.
\end{aligned}
$$

which becomes a function of W.

As a result, instead of trying to reduce $\sum_{d=s+1}^{D} y[d]^2$ which is impossible as we mentioned in the section 3.4.3, our goal becomes to reduce $\sum_{d=s+1}^{D} \hat{y}[d]^2$ with the help of W.

3.4.5 Reduce the Norm with Orthogonal Transformation

For $y \in \mathbb{R}^{D \times 1}$ and $W \in \mathbb{R}^{D \times D}$, given s, we want to reduce $\sum_{d=s+1}^{D} \hat{y}[d]^2$ as much as possible. However, since s is unknown while deciding W in the first phase of our framework, we have to handle all possible values which s could be. Moreover, since $\sum_{d=1}^{D} \hat{y}[d]^2$ is equal to $\sum_{d=1}^{D} y[d]^2$, which is independent with W, if the $\sum_{d=s+1}^{D} \hat{y}[d]^2$ decreases with some W, the term $\sum_{d=1}^{s} \hat{y}[d]^2$ must increase. Here, we use a more general strategy to deal with these problems.

We could look the term $\sum_{d=s+1}^{D} \hat{y}[d]^2$ from a different angle. Actually, this term is the square norm of the latter part of the vector $\hat{y}$. Therefore, although $\sum_{d=1}^{D} \hat{y}[d]^2$ is a constant for W, we could reduce the square norm of the latter part by increasing the forward part of it. In other words, we move the norm of the latter part of y to its forward part. To accomplish it, we design an objective function and then optimize this function to find our

ideal W.

$$f(W;y) = \sum_{d=1}^{D} w_d \times \hat{y}[d]^2 = \sum_{d=1}^{D} w_d \times (W[d,:]y[d])^2 \tag{3.1}$$

where $w_d = d, \forall d = 1 : D$.

Because w_d would give the larger penalty as d increases, the elements in the latter part of $\hat{y}$ would be forced to become small while minimizing this objective function. This is exactly our goal to reduce $\sum_{d=s+1}^{D} \hat{y}[d]^2$. Therefore, our question becomes how to optimize this objective function with the constraints that W must be an orthogonal matrix.

3.4.6 Optimize with Orthogonal Constraints

Finally, we could introduce this concept of reducing the norms into our framework. In the first phase, we solve the following optimization problem to learn an orthogonal matrix W_i for each machine Mi.

$$\begin{aligned} \underset{W}{\text{minimize}} \quad & F_i(W) \\ \text{subject to} \quad & W^T W = W W^T = I \end{aligned} \tag{3.2}$$

where

$$F_i(W) = \sum_{x \in X_i} f(W;x) = \sum_{x \in X_i} \sum_{d=1}^{D} d \times (W[d,:]x[d])^2 \tag{3.3}$$

.

This is an optimization problem with constraints that its solution must be an orthogonal matrix. We could solve it efficiently with the help of the package from [11] as long as we have its gradient.

After we get the optimal W_i^* for each M_i, we send these matrices back to the server P. Since the learning of W_i^* is independent with the queries in the future, we only have to go through the procedure of learning W_i^* for once if X_i doesn't change too much.

3.4.7 Reduce the Cost of Sending Matrices

However, the cost to sending an orthogonal matrix $W \in \mathbb{R}^{D \times D}$ is $D \times D$, which is too expensive. Therefore, in this section, we prove that we could reduce this cost to $\frac{D \times (D-1)}{2}$.

First, we introduce a lemma which would be used in our proof.

Lemma. For all vector $\mathbf{x} = (x_1, x_2, \ldots, x_D) \in \mathbb{R}^D$, we could use a spherical coordinate system with a radial coordinate r and $D-1$ angular coordinates $\phi_1, \phi_2, \ldots, \phi_{D-1}$ to represent it as

- $x_1 = r \cos(\phi_1)$

- $x_2 = r \sin(\phi_1) \cos(\phi_2)$

- $x_3 = r \sin(\phi_1) \sin(\phi_2) \cos(\phi_3)$

- $\vdots$

- $x_{D-1} = r \sin(\phi_1) \ldots \sin(\phi_{D-2}) \cos(\phi_{D-1})$

- $x_D = r \sin(\phi_1) \ldots \sin(\phi_{D-2}) \sin(\phi_{D-1})$

where $\phi_i \in [0, \pi]$, $\forall i = 1, 2, \ldots, D-2$ and $\phi_{D-1} \in [0, 2\pi)$. ∎

Since these row vectors $w_1, w_2, w_3, \ldots, w_D$ in W are orthonomal vectors, their r in this lemma is 1, which allows us to represent an orthonomal vector in $\mathbb{R}^D$ with $D-1$ parameters ($\phi_1, \phi_2, \ldots, \phi_{D-1}$ in the lemma). Moreover, since they are orthogonal to each other ($w_i w_j^T = 0$, $\forall i \neq j$), our goal becomes how to represent D vectors in $\mathbb{R}^D$ which are orthogonal to each other.

Now we are ready to give the proof by mathematical induction.

Theorem. Given D orthonomal vectors $w_1, w_2, w_3, \ldots, w_D \in \mathbb{R}^D$, we could use $\frac{D \times (D-1)}{2}$ parameters to represent them.

Proof. *Base case*: If $d = 2$, we could use a single parameter θ for w_1, w_2 as

$$
\begin{aligned}
w_1 &= (\cos(\theta), \sin(\theta)) \\
w_2 &= (\cos(\theta + \frac{\pi}{2}), \sin(\theta + \frac{\pi}{2}))
\end{aligned}
$$

(3.4)

Therefore, the total number of parameters here is 1 and equal to $\frac{2 \times (2-1)}{2}$.

To be clear, we give one more base case here.

Base case-2:

When $d = 3$, we need to represent three vectors $w_1, w_2, w_3 \in \mathbb{R}^3$.

In the beginning, by the lemma above, we could use $3 - 1 = 2$ parameters to represent w_3.

Then, since w_1 and w_2 are orthogonal to w_3, they must lie in the plane whose normal vector is w_3. Since we already have w_3 (with two parameters), this plance is fixed. All we need to do is to decide w_1 and w_2 on this $\mathbb{R}^2$ plane. By projecting the x axis in the $\mathbb{R}^3$ to this plane, we could build a Cartesian coordinate system in two dimensions on this plane. And we know that we could use one parameter to decide w_1 and w_2 in an $\mathbb{R}^2$ plane from the base case above.

So, the total number of parameters for $\mathbb{R}^3$ case is $2 + 1 = 3$ and equal to $\frac{3 \times (3-1)}{2}$

Inductive hypothesis:

Suppose the theorem holds for all values d up to some k, $k > 3$

Inductive step:

Let $d = k + 1$, we need to represent $k + 1$ vectors $w_1, w_2, w_3, \ldots, w_{k+1} \in \mathbb{R}^{k+1}$. We could use similar way like $d = 3$ to do it.

First, by the lemma above, we could use $(k+1) - 1 = k$ parameters to represent w_{k+1}. Then, our problem becomes to decide $w_1, w_2, \ldots, w_k$ on this hyperplane. From the inductive hypothesis, we know it needs $\frac{k \times (k-1)}{2}$ parameters.

So, the total number of parameters for $\mathbb{R}^{k+1}$ case is

$$k + \frac{k \times (k-1)}{2} = \frac{k \times (k+1)}{2} \ldots \blacksquare$$

3.5 Pruning by the Bounds

Now we start to discuss the second phase of our framework. In this section, we talk about how to prune the candidates if we already have bounds. Note that this mechanism is the most crucial part to achieve our goal to save the transmission cost.

3.5.1 Pruning the Candidates with the Bounds

For the query q_t, if we already know $LB(q_t, x)$ and $UB(q_t, x)$ $\forall x \in \cup_i X_i$, we could use the k_{th} smallest upper bounds and directly prune those x whose lower bounds are higher than this value thr. I.e., we want to prune

$$\{x | LB(q_t, x) > thr, \forall x \in \cup_i X_i\}$$

where thr is the k_{th} largest $UB(q_t, x)$ $\forall x \in \cup_i X_i$. The following figure is an example of how we prune instances.
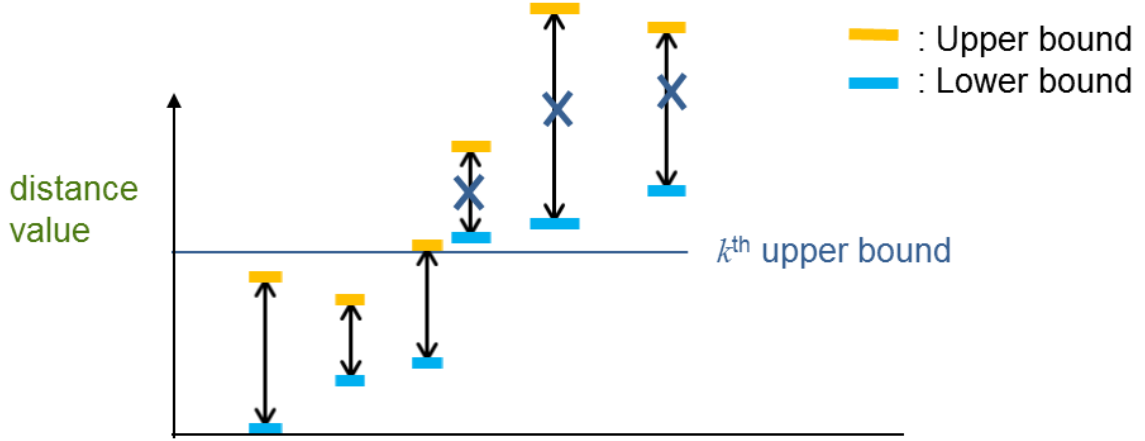

Figure 3.3: The procedure of pruning impossible candidates.

We will talk about the details to generate these bounds and find the threshold in the section 3.5.4.

3.5.2 Derivation of our Bounds

Suppose there are two vectors $x, y \in \mathbb{R}^D$, we know the square of their Euclidean distance is

$$Dist(x, y) = \sum_{d=1}^{D} (x[d] - y[d])^2 \tag{3.5}$$

However, if we could only observe the first s dimensions of x, we could decompose their distance as

$$Dist(x, y) = \sum_{d=1}^{D} (x[d] - y[d])^2$$
$$= \sum_{d=1}^{s} (x[d] - y[d])^2 + \sum_{d=s+1}^{D} (x[d] - y[d])^2.$$

Since the first component of (**??**) is already known, all we need to do is to deal with the second term. Therefore, we further expand the second term as below:

$$\sum_{d=s+1}^{D} (x[d] - y[d])^2 = \sum_{d=s+1}^{D} x[d]^2 + \sum_{d=s+1}^{D} y[d]^2 - \sum_{d=s+1}^{D} 2 \times x[d] \times y[d].$$

By this analysis, we find the final term is the inner product between two partial vector $x[s+1 : D]$ and $y[s+1 : D]$, which could be approximated by Cauchy–Schwarz inequality

$$\sum_{d=s+1}^{D} x[d] \times y[d] \leq \sqrt{\sum_{d=s+1}^{D} x[d]^2 \times \sum_{d=s+1}^{D} y[d]^2}. \tag{3.6}$$

After combing with (**??**) and (3.6), we derive the bounds as

$$LB(x, y) = \sum_{d=1}^{s} (x[d] - y[d])^2. \tag{3.7}$$

$$UB(x, y) = \sum_{d=1}^{s} (x[d] - y[d])^2$$
$$+ \sum_{d=s+1}^{D} x[d]^2 + \sum_{d=s+1}^{D} y[d]^2$$
$$+ 2 \times \sqrt{\sum_{d=s+1}^{D} x[d]^2 \times \sum_{d=s+1}^{D} y[d]^2}. \tag{3.8}$$

We could notice that the calculation of the bounds only needs the first s dimensions of

x and $\sum_{d=s+1}^{D} x[d]^2$. Therefore, we only need one more number to get the bounds for the unobserved part $x[s+1:D]$.

3.5.3 Calculation of our Bounds

After the derivation of the bounds, we describe the procedure of caculating them in our framework.

For the query q_t, at the first round (i.e. $j = 1$), P sends the first s_1 dimensions of q_t and $\sum_{d=s_1+1}^{D} q_t[d]^2$ to each M_i . With these values, each M_i would able to calculate the lower bounds $LB(q_t, x)$ and upper bounds $UB(q_t, x)$ for each $x \in X_i$. Then, after P getting the k_{th} smallest upper bounds as thr, we could run the pruning procedure.

In each following round (i.e. $j > 1$), P sends the next s_j dimensions of q_t to each M_i whose instances were not pruned completely. These M_i will update their bounds as follows:

$$LB_j(x, y) = LB_{j-1}(x, y) + \sum_{d=p_{j-1}+1}^{p_j} (x[d] - y[d])^2. \qquad (3.9)$$

$$\begin{aligned} UB_j(x, y) = &\ LB_j(x, y) \\ &+ \sum_{d=p_j+1}^{D} x[d]^2 + \sum_{d=p_j+1}^{D} y[d]^2 \\ &+ 2 \times \sqrt{\sum_{d=s+1}^{D} x[d]^2 \times \sum_{d=s+1}^{D} y[d]^2}. \qquad (3.10) \end{aligned}$$

where $p_j = \sum_{i=1}^{j} s_i$, LB_j and UB_j indicate the lower bounds and upper bounds at the round j repectively.

We call those p_j as pivots, which mean that each machine would observe the first p_i elements of q_t at the round j.

3.5.4 Finding the Threshold in Distributed Machines

The question now is to find the threshold thr for pruning. In [2], we directly send these bounds computed in each M_i back to the server P. However, it would make the transmission cost grow linearly with the number of total instances in these distributed

machines and lead to expensive cost when our dataset is extremely huge. As a result, we propose a method that could make the growth of the cost independent with the number of total instances.

To be simplified, we could think this problem as follows: given many distributed numbers N_i, we want to find the k_{th} largest number among these N_i. The N_i here actually means the upper bounds at the machine M_i in our framework. Once we model this problem as this, we could solve it through modifying the work of [3].

In [3], there are also many phases to find the kNN. In the first phase, the server P would send the whole query to every machine. Then, in the following phases, it just focuses on finding the instances with the k_{th} largest distance with the query. To make it fit our problem, we can only use the phases of PRP except the first phase to find the k_{th} largest upper bound as our threshold thr. Its cost is linear to

$$ m \times (\left\lfloor \frac{k}{|M|} \right\rfloor + 1) = m + k, $$

which is much lower than [2] when the number of total instances is very large.

3.6 Decision of the Pivots

The remaining problem is to decide how many dimensions (i.e. s_j) of q_t we have to send from the server P in each round j. If we send too few dimensions, the bounds would be too loose to prune any candidates and we will spend much unnecessary cost in finding the thresholds. On the other hand, if we send too many dimensions, although it could allow us to prune many candidates at once, it would send too many dimensions to some candidates which could be pruned by much fewer dimensions. That would also lead to the waste the transmission cost. Therefore, in this section, we propose a simple but effective method to decide how many dimensions of q_t we should send from P in each round.

3.6.1   Estimation of the Number of Residual Machines

From the discussion above, we could notice that the decision of pivots is highly dependent on the transmission cost. Therefore, if we could estimate the cost as a cost function of the pivots p_j, we could decide these pivots by optimizing this function.

However, to estimate the cost, we need to know the number of residual candidates sites before sending those dimensions of q_t in each round. But it is almost impossible to know how many sites would be left after we send part of q_t before we actually send the part of q_t. Therefore, we estimate a vector called $EstResMach \in \mathbb{R}^D$ where $EstResMach[j]$ indicates our estimate of the number of residual machines *after* we send $q_t[1:j]$ to each local machine.

To allow P to estimate this vector $EstResMach$ without causing any more transmission cost, we use the history information from $q_1, ..., q_t$. Suppose that we just finish finding the answer for q_t, during the procedure, we would collect some such pairs of information $(index_j, ResMach_j)$ for some j where $index_j$ means each candidate machine would observe the first $index_j$ dimensions of q_t at the round j and $ResMach_j$ indicates the number of residual machines after pruning by $q_t[1:index_j]$. For those dimensions which are not in these pairs, we use linear interpolation to estimate their $ResMach$.

Here(fig?) is an example for the above procedure.

We use the following procedure to maintain this vector $EstResMach$:

3.6.2   Estimation of the Transmission Cost

Once we have the vector $EstResMach$, we are ready to estimate the transmission cost *before* sending the query. For a query q, we could estimate its transmission cost in the first round

$$Cost_1 = TotalNumOfMach \times s_1 + Cost_{PRP}(TotalNumOfMach)$$

And for those round $j > 1$ as follows,

$$Cost_j = EstResMach[p_{j-1}] \times s_j + Cost_{PRP}(EstResMach[p_{j-1}])$$

where $p_j = \sum_{i=1}^{j} s_i$.

Give some explanation.

Therefore, we could solve this optimization problem to get the optimal pivots that could get the minimal total cost.

However, there are too many variables to decide in this problem. According to our experiments, the most crucial variable is the number of dimensions which will be sent in the first round, which is s_1 in this optimization problem. The other s_j don't have such huge influence like s_1. Therefore, we make all s_j be equal and then simplifiy this optimization problem as follows,

$$Cost_1 = TotalNumOfMach \times StartD + Cost_{PRP}(TotalNumOfMach)$$

And for those round $j > 1$,

$$Cost_j = EstResMach[p_{j-1}] \times EachLenD + Cost_{PRP}(EstResMach[p_{j-1}])$$

where $p_j = StartD + (j - 1) \times EachLenD$.

Thus, the final optimization becomes as below,

$$\begin{aligned}
\underset{StartD, EachLenD}{\text{minimize}} \quad & \sum_j Cost_j(StartD, EachLenD) \\
\text{subject to} \quad & StartD, EachLenD \in \mathbb{N}
\end{aligned} \tag{3.11}$$

where $p_j = StartD + (j - 1) \times EachLenD$.

3.6.3   Coordinate Descent to Decide the Pivots

Now we have reduced the number of variables to only two variables: $StartD$ and $EachLenD$. To solve this optimization problem efficiently, we apply the Coordinate Descent method as follows for each query.

algorthm?

After solving the optimal $StartD$ and $EachLenD$ for this query, we are able to decide its pivots as below:

$$p_j = StartD + (j-1) \times EachLenD \tag{3.12}$$

Since the vector $EstResMach$ would be updated for every new query, we will use Coordinate Descent to solve these pivots also for every new query.

3.7   Importance-Selecting Function and Overall Framework

At each round j for q_t, we need to decide what to send from P to each M_i and then calculate the bounds at M_i.

Note that we will find the kNN after all dimensions of q_t are sent.....

$$S_i(q_t, \; j, \; \theta_t; \; W_i) = \; \hat{q}_t[p_{j-1}^t + 1 : p_j^t] \cup Meta$$

where

$$\hat{q}_t = W_i q_t, \theta_t = (StartD_t, LenD_t)$$
$$p_j^t = min\{D, StartD_t + LenD_t \times (j-1)\}, \; \forall j \geq 1, \; \forall t \tag{3.13}$$
$$p_0^t = 0, \; \forall t$$
$$Meta = \sum_{d=StartD_t+1}^{D} \hat{q}[d]^2 \; \; if \; j = 1$$
$$else = 0$$

In this section, we describe the overview of our framework.

Input: $X_1, X_2, X_3, \ldots, X_m$
Output: $W_1, W_2, W_3, \ldots, W_m$

1 **for** $i = 1; i \leq m; i = i + 1$ **do**
2 $\quad$ M_i: Compute W_i with X_i by solving...;
3 $\quad$ M_i: Send W_i back to P;
4 **end**

Algorithm 1: First Phase

Input: q_t, k
Output: kNN of q_t

1 $P.CandidateMach(m) = True$;
2 $P.Counter = N$;
3 P: Solve θ_t;
4 **for** $j = 1; P.Counter > k; j = j + 1$ **do**
5 $\quad$ **for** $i = 1; i \leq m; i = i + 1$ **do**
6 $\quad\quad$ **if** $(CandidateMach(i) == True)$ **then**
7 $\quad\quad\quad$ P: Send the values of $S_i(q_t, \ j, \ \theta_t; \ W_i)$ to M_i.;
8 $\quad\quad\quad$ M_i: $\forall x \in X_i$, compute bounds by solving...;
9 $\quad\quad$ **end**
10 $\quad$ **end**
11 $\quad$ P: Use PRP to find the threshold thr and send it to every candidate machine.;
12 $\quad$ $P.Counter = 0$.;
13 $\quad$ **for** $i = 1; i \leq m; i = i + 1$ **do**
14 $\quad\quad$ **if** $(CandidateMach(i) == True)$ **then**
15 $\quad\quad\quad$ M_i: Prune instances by thr, return number of residual instances n_i back to P.;
16 $\quad\quad\quad$ **if** $(n_i == 0)$ **then**
17 $\quad\quad\quad\quad$ $P.CandidateMach(i) = False$;
18 $\quad\quad\quad$ **end**
19 $\quad\quad\quad$ $P.Counter+ = n_i$;
20 $\quad\quad$ **end**
21 $\quad$ **end**
22 **end**
23 return $con(r_i)$;

Algorithm 2: Second Phase

Chapter 4

Experiment

4.1 Experiment Setup

In this section, we discuss the resluts of our experiments. There are four parts in our experiments. First, we compare our framework with other frameworks in the communication cost. Second, since there are several stages of improvement in our framework, we discuss each of their influence to our final model. Third, we consider the amortization of transmitting the orthogonal matrices. Finally, we compare the power of pruning among different bounds. For every experiment, we average the results of 100 experiments by randomly picking our 100 instances as the queries.

4.2 Data Description

The table 4.1 is the description of those datasets we used in our experiments. Note that the $n \times m$ in the final column means that there are n instances placed in each machine and m machines used in this experiments. For instance, for the image dataset ANN with SIFT feature, there are totally 5000 machines and each has 200 instances in our experiments.

4.2.1 Time Series Data

The time series datasets we used is a synthetic dataset. We use the random walk data model in [12]. Each time series is generated by a random walk whose every step size is

Table 4.1: Summary for each dataset

Type	Dataset	Feature	Num of Dimensions	Num of Instances
Time Series	Random Walk	$N(0,1)$	128	200×5000
Image	ANN	SIFT	128	200×5000
	Flickr	CSD	256	500×2000
		SCD	256	500×2000
Audio	Million Songs	MVD	480	500×1900
		TRH	480	500×1900

a normal distributed random number with mean 0 and standard deviation 1. We also use this model to generate the synthetic dataset in the experiments of MsWave [2].

4.2.2 Image Data

We use two datasets in our experiments for images. First is the data provied in [13], which is a widely used dataset for evaluate the performance of approximate nearest neighbors search algorithms. The another one is the Flickr datasets with two kind of features used in [14]. The dataset is also a widely used dataset in the task of image retrieval. The CSD indicates *Color Structure Descriptor* while the SCD means *Scalable Color Descriptor*.

4.2.3 Audio Data

Here we use the audio data named Million Song Dataset from [15] which is a free-available collection of audio features for a million contemporary popular music tracks. For the features, MVD means *Modulation Frequency Variance Descriptor* and TRH is *Temporal Rhythm Histograms*. Please refer to [16–18] to see the details about how these features were extracted.

4.3 Comparison Among all Frameworks

$k = 10$, $|Q| = 500$, $M = 500, 1000, 1500, ...$ compare all diff frameworks for all data here. remember to add Mat cost.

4.3.1 Frameworks for Comparison

We compare our framework with LeeWave, *LeeWave*, *Naive*,

CP, *PRP*, CP

Note that the cost of our framework here does not include the cost of sending the orthogonal matrices. We will prove in the section ref that the total cost including the matrices could be amortized by enough queries and thus to achieve the cost here. That is, we could see the cost of our framework here as the cost after amortized by enough queries. Due to the time limitations, we didn't conduct enough number of queries to achieve the amortized results.

4.3.2 Results of Different Frameworks

4.4 Comparison Among our Framework with Different Configurations

There are many stages of algorithms which lead to the final version of our framework. Therefore, in this section, we would like to discuss the performance of our framwork with or without.

From **??** to our framework, we have enhanced it

4.4.1 Different Configurations for Comparison

4.4.2 Results of Different Configurations

4.4.3 Influence of the Orthogonal Transformation

NoW

4.4.4 Influence of the Threshold-Finding Procedure

NoPRP

4.4.5   Influence of the Coordinate Descent for Deciding Pivots

NoCD

4.5   Power of the Pruning Procedure

Comp among LeeWave, NoW, Main for ResSite.

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