Institut für Informatik, Universität Zürich

MSc Project Report

Implementing Learned Indexes on 1 and 2 Dimensional Data

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Databases use indexes to find records efficiently. Among these indexes, B-tree and KD-tree are the two indexes used for 1-dimensional and 2-dimensional data. In this project, we first implement these two indexes from scratch and then we implemented the learned indexes, including a fully connected neural network and a recursive model for 1-dimensional data [KBC+18] and the LISA model for 2-dimensional data [LLZ+20]. Afterwards, we conduct several experiments to evaluate the performance of learned indexes. In addition to the implementation and evaluation, we then theoretically analyse some properties that the learned indexes hold. Beyond that, we also explore and discuss the properties that the learned indexes should hold.

As an extension to the existing learned indexes, we explore the possibilities of using convolution operation and convolutional neural network as learned indexes.

Contents

1. Introduction

Over the years, indexes have been widely used in databases to improve the speed of data retrieval. In the past decades, the database indexes generally fall into the hand-engineered data structures, such as B-Tree, KD-Tree, etc. These indexes have played a crucial role in databases and have been used widely in modern data management systems (DBMS) such as PostgreSQL. Despite their huge success, a shortcoming of these data structures is the lack of consideration of how the database records distributed. We use an example to demonstrate how distributions can affect the efficiency of database indexes.

Example 1.1 For example, if the dataset contains integers from 1 to 1 million, then the keys can be used directly as offsets. With the keys used as offsets, the value with a given key can be retrieved in $\mathcal{O}(1)$ time complexity while B-Tree requires $\mathcal{O}(\log n)$ time complexity for the same query. From the perspective of space complexity, we do not need any extra overhead by using the key as an offset directly, while the B-Tree needs extra $\mathcal{O}(n)$ space complexity to save the tree. ♣

From the above example, we found that there are two promising advantages of leveraging the distribution of the data:

1. It may be faster when performing queries, especially when the number of entries in the database are rather huge.

2. It may take less memory space, as we only need to save the model with constant size.

Nowadays, to learn the distribution and apply it to database indexes, researchers proposed learned indexes [KBC+18], where machine learning techniques are applied to automatically learn the distribution of the database entries and build the data-driven indexes. In this project, we implemented hand-engineered indexes and the learned index. After that, we explore the possibilities of using complex convolutional neural networks as database indexes. This report is organised into the following chapters:

1. **Introduction**. In this chapter, we illustrate the organisation of this report. Besides, we go through the modern computer systems and introduce the general information about database indexes.

2. **Implementation**. In this chapter, we thoroughly describe the implementation of one and two dimensional indexes, including B-Tree, baseline learned index, recursive model, KD-Tree and LISA.

3. **Evaluation**. In this chapter, we perform evaluation among the indexes we implemented with different evaluation dataset.

4. **Insights and Findings**. We demonstrate our findings during the implementation in this chapter. Besides, we also discuss the advantages and disadvantages of different indexes.

5. **Convolution and CNN for Learned Indexes**. In this chapter we explore the possibilities of using convolution operation and convolutional neural network to build learned indexes.

6. **Conclusions**.

1.1. Notations

In this report, we will use the following notations:

Sets and Spaces	
$\mathbb{R}$	The set of real numbers
$\mathbb{R}^d$	The set of d dimensional real space
Random Variables	
$\boldsymbol{X}$	A vector or matrix
x	A single value in $\mathbf{X}$
(x, y)	A tuple contains two values
Hyper-Parameters	
N	A pre-set hyper parameter
Functions	
$\mathcal{LR}$	Linear Regression Function
$\mathcal{P}$	Polynomial Function
$\mathcal{M}$	Mapping Function
$\mathcal{O}$	Big-O notation for complexity
$\mathcal{SP}$	Shard Prediction Function
$\mathcal{Q}$	Range Query
$\mathcal{K}$	KNN Query
Others	
♣	End of Example
■	End of Proof

1.2. Terminologies

In the following chapters, we will use the following terminologies

Index model is a function that maps the index of a row of data into the location (e.g. page index) of the data. For example, in one-dimensional case, the index models include B-Tree, Linear Regression models, etc.

Key is a special attribute in the database that could identify a record. In our work, the key could be a scalar in one-dimensional case, or a (x, y) pair in two-dimensional case.

Order of a tree is the maximum number of children that a node can have.

Internal node is any node of a tree that has child nodes and is not a root node.

Leaf node is any node that does not have child nodes.

Level of a node is defined as the number of edges between this node and the root node.

1.3. Assumptions

Formally, we define the index of each record as x and the corresponding location as y and we represent the whole data as (X, Y) pairs with the total number of pairs defined as N. We could then normalise the Y into $\tilde{Y} \in [0, 1]$ so that the $\tilde{y}$ represents the portion of the y among the whole Y. With these definitions, we can then define a function $F : X \to \tilde{Y}$ that maps the index into the portion of the y. We have $y = F(x) * N$. As the output of this function can be considered as the probability of $X \leq x$, we can regard this function $F(x)$ as the cumulative distribution function (CDF) of X, i.e. $F(x) = \mathbb{P}(X \leq x)$. Now that N is determined by the length of data records, we only need to learn such CDF and we called the learned CDF function as **learned index model**.

Example 1.2 From the perspective of the distribution of data records, our previous example can be rephrased as following. Our data records are (X, Y) pairs with a linear relation, i.e. $y = x, \forall y \in Y$. We are looking for a function F such that $y = x = F(x) * N$, and hence we end up with $F(x) = \frac{1}{N} * x$. If we use this linear function $F(x)$ as the index model, then we could locate the data within $\mathcal{O}(1)$ time complexity and we only need to store the total number of records as the only parameter. Compared with B-Tree and other indexes, the advantages are enormous. ♣

In order to ensure the learned index model to be the desired CDF, we need to make the following assumptions:

1. All data records are stored statically in database, hence we do not take insertion and deletion into consideration. If there is some insertion or deletion, then the total size of the data records, N, will be different. Therefore, if insertion or deletion are involved, we cannot calculate the position as we show above.

2. All data records are sorted according to theirs keys $\boldsymbol{X}$. Only when the data records are sorted according to the keys, we can regard the index model as CDF, i.e. $F(x) = \mathbb{P}(X \leq x)$.

3. For simplicity, we assume that our data records are stored in a continuous memory space. In other words, the indices of pages in this project is continuous integers and all the data records are loaded into memory.

2. Implementation

2.1. One Dimensional Data

2.1.1. B-Tree

B-Tree and its variants have been widely used as indexes in databases. B-Trees can be considered as a generalisation of binary search tree: In binary search tree, there is only one key and two children at most in the internal node. B-Tree extends the nodes such that each node can contain several keys and children. The keys in a node serve as dividing points and separate the range of keys. With this structure, we make a multi-way decision based on comparisons with the keys stored at the node x.

In this section, we introduce the construction and search processes of B-Trees and then analyse their properties.

Attributes

Each node in a B-Tree has the following attributes:

- $x.n$ is the number of keys currently stored in the node x.
- Inside each node, the keys are sorted in non decreasing order, so that we have $x.keys_1 \leq x.keys_2 \leq \cdots \leq x.keys_{x.n}$.
- $x.leaf$, a Boolean value determines if current node is a leaf node.

With these properties, A B-Tree T whose root is $T.root$ have the following properties:

- Each internal node x contains $x.n+1$ children. We assume the children are $x.c_1, \cdots, x.c_{x.n+1}$.
- The nodes in the tree have lower and upper bounds on the number of keys that can contain. These bounds can be expressed in terms of a fixed integer t.

When inserting keys into a binary search tree, we search for the leaf position at which to insert the new key. However, with B-Tree, we cannot simply find the position, create a new node and insert the value because the tree will be imbalanced again. Hence, in this section, we illustrate an operation that splits a full node around its median key

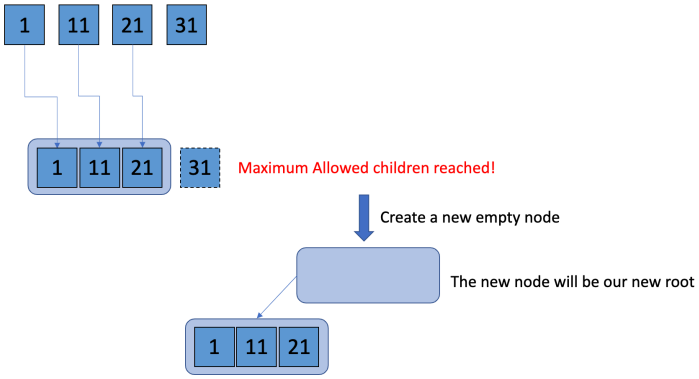


Figure 2.1.: B-Tree key insertion

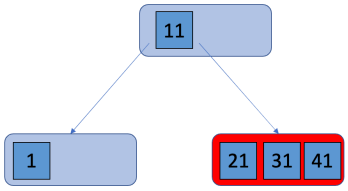


Figure 2.2.: B-Tree key insertion

Insertion in a B-Tree

Algorithm 1: Algorithm for B-Tree insertion

Input: m:`order_of_tree` ,(k, v):`(key, value)`, N:`Node;`
Output: `B-Tree`

if *N is a leaf and not yet full* **then**
  `insert` (k, v) `into` N
else
  `create new Node N'`
  `Find the median of the node`
  `Add the value at the median location to the new node N'`
end
if *N is root with no children and not full* **then**
  `insert` (k, v) `into` N
end

There are two conditions in insertion:

- **When the node is empty or not created at all**: In the algorithm, initially when the first key is inserted and there is no root to the tree it will check the condition if there are any nodes and if not create a new one. It will insert the new key in the node and keeps inserting the new keys until it is one less than the order of the B-Tree being created.
- **When the node is full**: As soon as the maximum number of allowed children has reached for the root node a new empty node is created. Suppose we have inserted

[1,11,21] to a node of a B-Tree with degree 4. Now if we want to insert a new value 31 into the tree, since it has reached the maximum number of children it will find the median of the existing node [1,11,21] which is 11 and increase the level of the B-tree to 2 and make [1] and [21] child nodes of [11]. So now if a new value is to be inserted it can be inserted. Splitting of the node happens each time it reaches it's maximum allowed keys. Now 31 will be compared with 11 and since 31 > 11 it will be inserted in the right child and it will have an updated value of [21,31]. More keys can then be inserted until it reaches it's maximum and splits again. Once the node is split it's parent is also updated to the median value i.e., [11] in this case for nodes [1] and [21,31,41] as can be seen in 2.2.

2.1.2. Baseline Learned Index

Overview

The B-Tree can be regarded as a function $\mathcal{F}$ that maps the key x into its corresponding page index y. It is known to us that the pages are allocated in a way that the every S entries are allocated in a page where S is a pre-defined parameter. For example, if we set S to be 10 items per page, then the first page will contain the first 10 keys and their corresponding values. Similarly, the second 10 keys and their corresponding values will be allocated to the second page.

If we know the CDF of X as $F(X \leq x)$ and the total number of entries N, then the position of x can be estimated as $p = F(x) * N$ and the page index where it should be allocated to is given by

$$y = \lfloor \frac{p}{S} \rfloor = \lfloor \frac{F(x) * N}{S} \rfloor$$

Example 2.1 For example, if the keys are uniformly distributed from 0 to 1000, i.e. the CDF of X is defined as $F(X \leq x) = \frac{x}{1000}$ and we set $S = 10, N = 1001$. Then for any key x, we immediately know it will be allocated into $y = \lfloor \frac{1000}{10} * \frac{x}{1000} \rfloor = \lfloor \frac{x}{10} \rfloor$. Assume that we have a key 698, then we can calculate $y = \lfloor \frac{698}{10} \rfloor = 69$. By doing so, the page index is calculated in constant time and space.

In this example, we see that the distribution of X is essential and our goal of learned index in one-dimensional data is to learn such distribution. To do so, we apply two different techniques as the baseline, the polynomial regression and fully connected neural network. ♣

To train such a learned index, we first manually generate the X with respect to a certain distribution. We then save the generated X into a dense array with the length N. Then we use the proportional index, i.e. the index of each x divided by N as the expected output y.

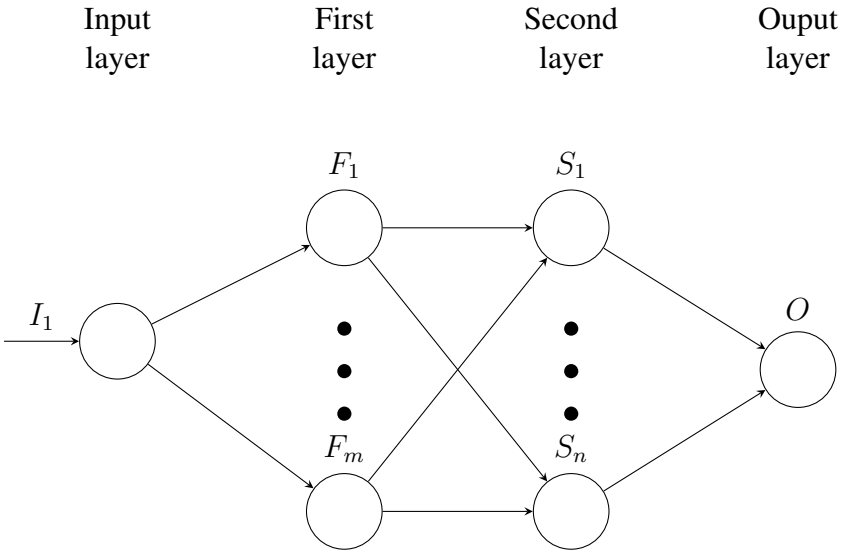


Figure 2.3.: The architecture of the fully connected neural network used as baseline learned index. In this neural network, we use only 2 fully connected layers. The input of this neural network is only one neuron such that it represents the given query key. The output of this neural network is limited to 1 neuron such that it represents the predicted proportional position of the key-value pair.

Fully Connected Neural Network

After generating the training dataset X and its corresponding Y, we build a fully connected neural network as the baseline learned index. The architecture of the fully connected neural network is illustrated in Figure 2.3.

We apply the Rectified Linear Unit (ReLU) activation function at the end of F_i and S_i. Formally, assume the output of F_i is $\boldsymbol{a}$, then we define the output of $\textit{ReLU}(F_i)$ as $y = \max(\boldsymbol{a}, 0)$ where max returns the larger value between each entry of $\boldsymbol{a}$ and 0. Then we train this fully connected neural network with standard stochastic gradient descent (SGD), and we set the learning rate to be $\alpha = 0.001$. We use the mean square error (MSE) $\ell = \frac{1}{n}\sum(y - \hat{y})^2$ as the loss function.

Formally, we can induce the output of this fully connected neural network as following:

1. In the input layer, we have the input as a scalar value x.
2. The first fully connected layer has m nodes, and the output is defined as $\boldsymbol{y_1} = \boldsymbol{w_1}x + \boldsymbol{b_1}$ where $\boldsymbol{w_1}$ and $\boldsymbol{b_1}$ is a $m \times 1$ matrix. Hence, the output of the first fully connected layer is a $m \times 1$ matrix. Then we apply the ReLU activation function to $\boldsymbol{y_1}$ and we get $\boldsymbol{z_1} = \max(\boldsymbol{y_1}, 0)$.
3. The second fully connected layer has n nodes, and the output is defined as $\boldsymbol{y_2} = \boldsymbol{w_2}\boldsymbol{z_1} + \boldsymbol{b_2}$. Similarly, after the ReLU operation, we get $\boldsymbol{z_2} = \max(\boldsymbol{y_2}, 0)$.
4. For the output layer, in order to get a scalar as output, we apply a n node fully connected layer here. The final output is defined as $\hat{y} = \boldsymbol{w_3}\boldsymbol{z_2} + \boldsymbol{b_3}$ where $\boldsymbol{w_3}$ is a $1 \times n$ matrix.

In summary, the output of the fully connected neural network can be calculated as

$$\hat{y} = \boldsymbol{w_3}\text{max}(\boldsymbol{w_2}\text{max}(\boldsymbol{w_1}x + \boldsymbol{b_1}, 0) + \boldsymbol{b_2}, 0) + \boldsymbol{b_3} \tag{2.1}$$

In the above fully connected neural network, there are 6 parameters to optimise: $\boldsymbol{w_1}, \boldsymbol{w_2}, \boldsymbol{w_3}$ and $\boldsymbol{b_1}, \boldsymbol{b_2}, \boldsymbol{b_3}$ and we apply the gradient descent and back propagation to optimise them. Formally, the steps are illustrated below:

1. **Initialisation**. For $\boldsymbol{w_i}$ and $\boldsymbol{b_i}$ of the shape $m \times n$, we randomly initialise the values of each entry using a uniform distribution $U(-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}})$.

2. **Forward Pass**. With the initialised $\boldsymbol{w_i}$ and $\boldsymbol{b_i}$, we calculate the output as formulated be the equation 2.1. We then calculate the error as $\ell = \frac{1}{n}\sum(y - \hat{y})^2$.

3. **Backward Pass**. After getting the error, we start from the last layer to perform the backward propagation operation. Formally, we do the following operations:
   a) We first calculate the partial derivatives: $\frac{\partial \ell}{\partial \boldsymbol{w_3}} = \boldsymbol{z_2}^T$, $\frac{\partial \ell}{\partial \boldsymbol{b_3}} = 1$ and $\nabla_3 = \frac{\partial \ell}{\partial \boldsymbol{z_2}} = \boldsymbol{w_3}^T$. Then we can update $\boldsymbol{w_3}$ and $\boldsymbol{b_3}$ as $\boldsymbol{w_3}^{\text{new}} = \boldsymbol{w_3} - \alpha * \frac{\partial \ell}{\partial \boldsymbol{w_3}}$ and $\boldsymbol{b_3}^{\text{new}} = \boldsymbol{b_3} - \alpha * \frac{\partial \ell}{\partial \boldsymbol{b_3}}$.
   b) Then we pass the ∇_3 to previous layer, and calculate the partial derivatives as $\frac{\partial \ell}{\partial \boldsymbol{w_2}} = \boldsymbol{z_2}^T\nabla_3$, $\frac{\partial \ell}{\partial \boldsymbol{b_2}} = \nabla_3$ and $\nabla_2 = \frac{\partial \ell}{\partial \boldsymbol{z_1}} = \nabla_3\boldsymbol{w_2}^T$. Then we update $\boldsymbol{w_2}$ and $\boldsymbol{b_2}$.
   c) After that, we pass the ∇_2 to the first layer, and calculate the partial derivatives as $\frac{\partial \ell}{\partial \boldsymbol{w_1}} = x^T\nabla_2$, $\frac{\partial \ell}{\partial \boldsymbol{b_1}} = \nabla_2$. Then we update $\boldsymbol{w_1}$ and $\boldsymbol{b_1}$.

4. **Loop between 2 and 3**. We perform the forward pass and the backward several times until the loss is acceptable or a maximum number of loops reached.

We will discuss more findings and insights about the baseline model in the *Chapter 4*.

2.1.3. Recursive Model Index

In our baseline models, it is not very difficult to reduce the mean square error from millions to thousands. However, it is much harder to reduce it from thousands to tens. This is the so called last-mile problem.

In order to solve this problem, recursive model index was proposed [KBC+18]. The idea is to split the whole set of data into smaller pieces and assign each piece an index model. By doing so, each model is only responsible for a small range of keys. Ideally, in each smaller range, the keys are distributed in a way that is easier to be learned by our index models, such as polynomial model, fully connected model or even traditional B-Tree model.

As shown in Fig. 2.4. A recursive model can be regarded as a tree structure, which contains a root model that receives the full dataset for training. Then the root model will split the dataset into several parts. Each sub-model will then receive one part of the full dataset. Then we train the sub-models one by one with the partial training dataset.

Example 2.2 For example, in the Fig. 2.4, the full dataset will be split into three parts and each sub-model receives one part. To train this recursive model, we first train the root model with the whole dataset. Then the root model will split the dataset into 3 parts according to the predicted value of each data point in the dataset. Then each sub-model will receive one part and we train the sub-model accordingly. ♣

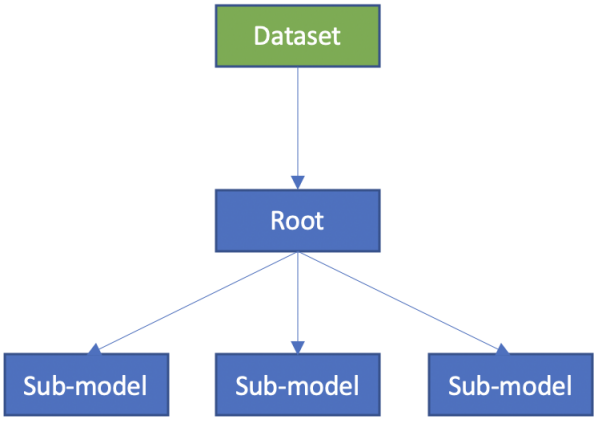


Figure 2.4.: An example recursive model index with one root model and three leaf model.

Properties

Similar to a tree, we define the following terms in a recursive model:

1. **Node Model**. Every node is responsible for making decisions with given input data. In one dimensional case, it can be regarded as a function $f : \mathbb{R} \to \mathbb{R}, x \to y$ where x is the input index and y is the corresponding page block. In principle, each node can be implemented as any machine learning model, from linear regression to neural network, or a traditional tree-based model, such as B-Tree.

2. **Internal Node Model**. Internal nodes are all nodes except for leaf nodes and the root node. Every internal node receives a certain part of training data from the full dataset, and train a model on it.

In the following sections, we will use the notations defined below:

1. $N_M^{(i)}$ is the number of models in the ith stage.

Training

In order to construct a recursive model, we need to have several parameters listed below:

1. The training dataset, notated as (X, Y) with entries notated as (x, y).

2. The number of stages, notated as N_S. It is an integer variable.

3. The number of models at each stage, notated as N_M. It is a list of integer variable. $N_M^{(i+1)}$ represents the number of models in the ith stage.

The training process of recursive model is an up-bottom process. There will be only one root model that receives the whole training data. After the root model is trained, we iterate over all the training data and predict the page by the root model. After the iteration, we get a new set of pairs (X, Y_0). Then we map $\forall y_0 \in Y_0$ into the selected model id in next stage by $\texttt{next} = y_0 * N_M^{(i+1)} / \texttt{max(Y)}$.

Algorithm 2: Training of Recursive Model Index

```
  input: num_of_stages; num_of_models; types_of_models; x; y
1 trainset=[[(x,y)]]
2 stage← 0
3 while stage <num_of_stages do
4 |   while model <num_of_models[stage] do
5 |   |   model.train(trainset[stage][model])
6 |   |   models[stage].append(model)
7 |   end
8 |   if not last stage then
9 |   |   for i ← 0 to len(x) do
10|   |   |   model=models[output from previous stage]
11|   |   |   output=model.predict(x[i])
12|   |   |   next=output * num_of_models[stage+1]/max_y
13|   |   |   trainset[stage+1][next].add((x[i],y[i]))
14|   |   end
15 end
```

Polynomial Internal Models

In the recursive model index, we use internal models to learn the CDF of a part of the full training data. In order to learn the CDF, we need to know or assume the distribution of a specific part of the data. In this report, we support the following distributions.

Linear Regression	$wx + b$
Quadratic Regression	$ax^2 + bx + c$
B-Tree	N/A
Fully Connected Neural Network	N/A

Here we describe how we fit a polynomial model.

The polynomial regression model with degree m can be formalised as

$$\hat{y}_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_m x_i^m$$

and it can be expressed in a matrix form as below

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^m \\ 1 & x_2 & x_2^2 & \cdots & x_2^m \\ \vdots & & & & \\ 1 & x_n & x_n^2 & \cdots & x_n^m \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_m \end{bmatrix}$$

which can be written as $Y = \boldsymbol{X}\boldsymbol{\beta}$.

Proof 2.1 Our goal is to find β such that the sum of squared error, i.e.

$$\mathrm{S}(\boldsymbol{\beta}) = \sum_{i=1}^{n} (\hat{y} - y)^2$$

is minimal. This optimisation problem can be resolved by ordinary least square estimation as shown below.

First we have the error as

$$\begin{aligned} \mathrm{S}(\boldsymbol{\beta}) = ||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}|| &= (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^T (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) \\ &= \boldsymbol{y}^T\boldsymbol{y} - \boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{y} - \boldsymbol{y}^T\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} \end{aligned} \tag{2.2}$$

Here we know that $(\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{y})^T = \boldsymbol{y}^T\boldsymbol{X}\boldsymbol{\beta}$ is a 1×1 matrix, i.e. a scalar. Hence it is equal to its own transpose. As a result we could simplify the error as

$$\mathrm{S}(\boldsymbol{\beta}) = \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{y} + \boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} \tag{2.3}$$

In order to find the minimum of $S(\boldsymbol{\beta})$, we differentiate it with respect to $\boldsymbol{\beta}$ as

$$\nabla_{\boldsymbol{\beta}} S = -2\boldsymbol{X}^T\boldsymbol{y} + 2(\boldsymbol{X}^T\boldsymbol{X})\boldsymbol{\beta} \tag{2.4}$$

By let it to be zero, we end up with

$$\begin{aligned} &-\boldsymbol{X}^T\boldsymbol{y} + (\boldsymbol{X}^T\boldsymbol{X})\boldsymbol{\beta} = 0 \\ \implies\ &\boldsymbol{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \end{aligned} \tag{2.5}$$

■

2.2. Two Dimensional Data

2.2.1. KD-Tree

KD-Tree is a space partitioning structure that can be used to organise data points in k dimensional space. We have fixed our dimensions of data points to 2-dimensions and their values are stored as a scalar. In our implementation, KD-Tree is a binary tree with every node having data points partitioned in 2-dimensional space. A KD-Tree is a binary tree since each node has two children and when the keys are multidimensional each node is partitioned at split axis based on the depth of the tree and the dimension of the key which in turn determines the number of split axis the tree will have. For example for a 3-dimensional space the first split axis is x-coordinate and then at the next level it will be y-coordinate and lastly z-coordinate.

Properties

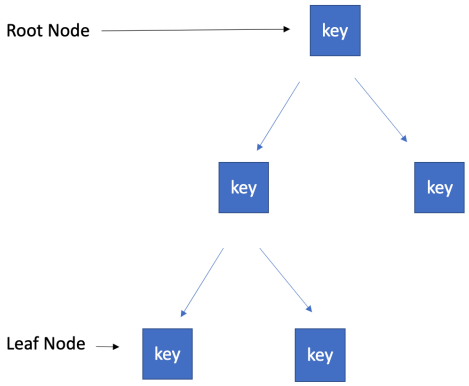


Figure 2.5.: KD-Tree

1. **Node**: Node of a KD-Tree is essentially a 2-dimensional data point. It can be k-dimensional for KD-Tree. Node is called a Root Node when it is at the top level as can be seen in Fig. 2.5 and does not have a parent. A node is called a Leaf Node when it has no children and is at the bottom level.

2. **Levels**: Nodes are at the same level when they have the same distance from root. Hence, a level increases as the distance of the nodes increase from root. In the 2.5 we can see the key at root is at level 1 and then we have level 2 and level 3.

3. **Dimensions**: Every KD-Tree can be structured in such a way that the data points are divided into k-dimensions. Each node is recursively cut into as many dimensions as is mentioned in the dimensions. In our case the data points are 2-dimensional and hence the space is divided into 2-dimensions alternatively until a leaf is reached.

Algorithm 3: Construction Algorithm for KD-Tree

Input : pointList; Keys=[$(x, y); x \in \mathbb{R}; y \in \mathbb{R}$], dimension = 2, split_axis; 0 or 1
Output: KD-Tree

```
for i ← 0 to len(pointList) do
    int split_axis := split_axis mod dimension // Select the split_axis
     based on depth
    Sort point list and choose median
    Create node at median
    node.leftChild := kdtree(points in pointList before
     median, split_axis+1); //SubTree Creation
    node.rightChild := kdtree(points in pointList after
     median, split_axis+1);
    return node
end
```

For constructing the KD-Tree we have the following constraints:

1. As one moves down the tree, one cycles through the axes used to select the splitting planes. For example, in a 2-dimensional plane we split the data on x-axis at the root and then split it on y-axis for it's children. We then split the grandchildren on x-axis again and so on.

2. Points are inserted by selecting the median of the points being put into the subtree, with respect to their coordinates in the axis being used to create the splitting plane. This ensures that the tree is balanced. A balanced tree is the one in which leaf node is approximately the same distance from the root.

In the algorithm above, we first sort all the values obtained in the Point list. We initialise the first split axis to 0 and then toggle between 0 and 1 as we increase the depth. Once the data points are sorted, their median is chosen.

Example 2.3 For example if we have points sorted as
$((1, 2), (3, 4), (5, 6), (7, 8), (9, 10)$
we will take the median as $(5, 6)$ and assign $(3, 4)$ to the left and $(7, 8)$ to the right. The reason node.leftChild = $(3, 4)$ is because $3 < 5$ and node.rightChild = $(7, 8)$ is because $7 > 5$ i.e., we compare the x-axis of the points to the root when we create the subsequent nodes. Now if we want to add point $[1, 2]$ to the above tree it will check the x-coordinate at the root and since $1 < 5$ it will go the left. In the left since we already have a node $(3, 4)$ it will check the y-coordinate of the points i.e., $4 > 2$ and so it will go and check in the left of the node if this point can be added there and since it's empty it is added in the left. Further points are added in the same way by checking the x-coordinate and y-coordinate alternatively. This process is then carried out recursively and subtrees are created on the left and right until all the points are added to the tree. Similarly point $(9, 10)$ is added in the right subtree as the rightChild of node $(7, 8)$. $(None)$ is added when the rightChild or

leftChild of the node is empty. The tree will now look like

$$(((1,2),(None),(3,4)),((None),(9,10),(7,8)),(5,6))$$

Points are added to left and right subtree as follows:
left subtree points: $((1,2)(3,4))$,
right subtree points: $(7,8),(9,10)$
centre being the root: $(5,6)$.
([Left Subtree, Right subtree, Root Point]) ♣

Construction time and space complexity of 2-dimensional KD-Tree:

The most expensive part of the construction of KD-Tree is sorting the points on both the axis. Instead of working with more complex algorithm to find the median we first presorted the values on x-axis and then on y-axis.
$T(n) = O(n)$, if $n = 1$
$O(n) + 2T(n/2)$, if $n > 1$
The above equations then solve to $O(nlogn)$.

Since KD-Tree is A binary tree, and every leaf and internal node uses $O(1)$ storage, hence the total storage is $O(n)$.

2.2.2. LISA: Learned Index for Spatial Data

Spatial data and query processing have become ubiquitous due to proliferation of location-based services such as digital mapping, location-based social networking, and geo-targeted advertising. Motivated by the performance benefits of learned indices for one-dimensional data, this section explores the application of learned index for spatial data. The main motivation is to map spatial data into one-dimensional data through several steps and apply machine learning techniques to generate a learned index for the one-dimensional data.

Motivation

In the last section, we described a recursive model index (RMI) that consists of a number of machine learning models staged into a hierarchy to enable synthesis of specialised index structures, termed learned indexes. Provided with a search key x, RMI predicts the position of x's data with some error bound, by learning the CDF over the key search space. However, as shown in Fig. 2.6, the idea of RMI is not applicable in the context of spatial data as spatial data invalidates the assumption required by RMI that the data is sorted by key and that any imprecision can be easily corrected by a localised search. Although it is possible to learn multi-dimensional CDFs, such CDFs will result in searching local regions qualified on one dimension but not all dimensions.

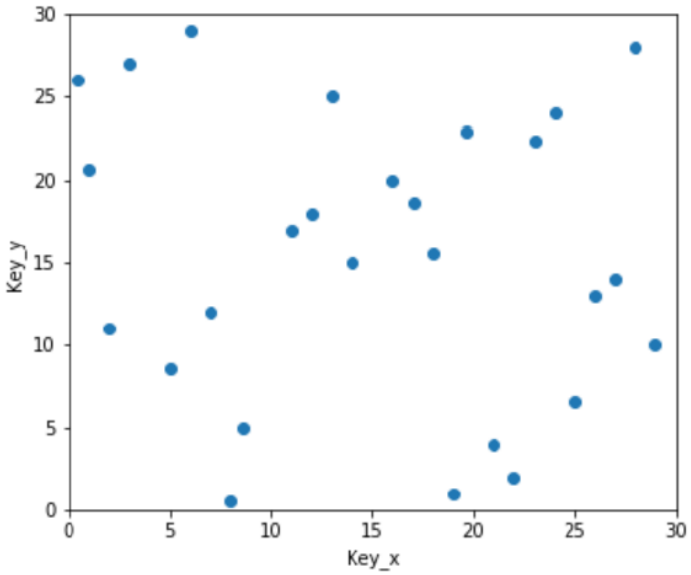


Figure 2.6.: Key Distribution in 2 dimensional case:Idea of learned indexes is not applicable in the context of spatial data as data is not sorted by key. Learning multidimensional CDFs will result in searching local regions qualified on one dimension but not all dimensions.

Example 2.4 For example, consider the joint cumulative function of two random variables X and Y defined as $F_{XY}(x, y) = P(X \leq x, Y \leq y)$. The joint CDF satisfies the following properties:

- $F_X(x) = F_{XY}(x, \infty)$, for any x (marginal CDF of X)
- $F_Y(y) = F_{XY}(\infty, y)$, for any y (marginal CDF of Y)
- if X and Y are independent, then $F_{XY}(x, y) = F_X(x)F_Y(y)$

♣

Need to find a solid argument to explain why learning multi dimensional CDFs will result in searching local regions qualified on one dimension.

LISA solves this problem by partitioning search space into a series of grid cells based on the data distribution and building a function map the data from $\mathbb{R}^d$ into $\mathbb{R}$, in our case, we have $d = 2$. We call this function as *Mapping Function*.

Definitions

This section presents the definition

1. **Key**. A key k is a unique identifier for a data record with $k = (x_0, x_1) \in \mathbb{R}^2$.
2. **Cell**. A grid cell is a rectangle whose lower and upper corners are points $(l_0, l_1) and (u_0, u_1)$, i.e., cell = $(l_0, u_0) \times [l_1, u_1)$

3. **Mapping Function**. A mapping function $\mathcal{M}$ is a function on the domain $\mathbb{R}^2$ to the non-negative range, i.e $M : [0, X_0] \times [0, X_1] \rightarrow [0, +\infty)$ such that $M(x_0, x_1) \leq M(y_0, y_1)$ when $x_0 \leq y_0$ and $x_1 \leq y_1$.

2.2.3. Baseline Method

We can extend the learned index method for range queries on spatial data by using a mapping function. This baseline method works as follows. We first sort all keys according to their mapped values and divide the mapped values into some cells such that each cell contains the same number of keys (except the last one). If a point (x, y)'s mapped value is larger than those of the keys stored in the first i cells, i.e. $\mathcal{M}(x, y) > \sup \bigcup_{j=0}^{i-1} M(C_j)$, we store (x, y) in the $(i + 1)$th cell.

For a range query, we have a query rectangle $qr = [l_0, u_0) \times [l_1, u_1)$, we only need to predict the indices of (l_0, l_1) and (u_0, u_1) namely i_1 and i_2 respectively. Then we scan the keys in $i_2 - i_1 + 1$ cells, and find those keys that fall in the query rectangle qr.

Example 2.5 As shown in Fig. 4.1, the key space is divided into 3 cells using the mapping function $\mathcal{M}((x, y)) = x + y$. The query rectangle consisting of only 1 key, falls inside the second part. During prediction, we need to find out the cells to which our query rectangle belongs (the 2^{nd} cell in our example). Once the cell is found, we need to compare the key of the query point, against all the possible keys in that cell until a match is found. This results in 8 irrelevant points accessed for the range query that only contains one relevant key. ♣

Training

The training dataset for the baseline model can be notated as $(\boldsymbol{X}, Y)$ with entries notated as $(\boldsymbol{x}, y)$. $\boldsymbol{X}$ represents the two dimensional key coordinates, and Y represents the corresponding data item.

In order to construct the baseline model, we need to have several parameters listed below:

1. N, which represents the number of cells into which the key's mapped value space will be divided.

As described in Algorithm 6, during training, we perform the following operations:

1. Sort all keys according to their mapped values.
2. Divide the keys into equal sized cells
3. Store the mapped values of first and last key for each cell into an array

Algorithm 4: Training Algorithm for Lisa Baseline Method

input : num_of_cells; trainset=[$(x, y); x \in \mathbb{R}^2; y \in \mathbb{R}$]
Output: M:Mapped Function

```
for i ← 0 to len(x) do
    x[i].mapped_value = x[i][0]+x[i][1]
end
Sort x based on x.mapped_value
Divide x into equal size pages according to num_of_cells
Store mapped value of first and last key for each page
for i ← 0 to num_of_cells do
    denseArray[i].lower = first key in page i
    denseArray[i].upper = last key in page i
end
```

For prediction, we find the cell corresponding to mapped value of the query point using binary search, scan this cell sequentially and compare the values of keys in the cell against the query point, until a match is found.

Prediction

Algorithm 5: Prediction Algorithm for Lisa Baseline Model

input: `x_test`: Key; `d`: the denseArray

```
x_test.mapped_value = x_test[0]+x_test[1]
for i ← 0 to len(denseArray) do
    if M(x_test) ∈ [d[i].lower, d[i].upper] then
        Key is in Page i
        break
    end
end
Sequentially search for x_test in page j
```

2.2.4. Lisa Overview

Given a spatial dataset, we generate the mapping function $\mathcal{M}$, the shard prediction function $\mathcal{SP}$. Based on them, we build our index structure, LISA, to process range query and KNN query. LISA consists of four parts: the representation of grid cells, the mapping function $\mathcal{M}$, the shard prediction function $\mathcal{SP}$, and the local models for all shards. As illustrated in the Fig 2.7. the procedure of building LISA is composed of four parts.

1. Grid cell partition.
2. Mapping spatial coordinates into scalars, i.e. $\mathbb{R}^d \to \mathbb{R}$.
3. Build shard prediction function $\mathcal{SP}$.
4. Build local models.

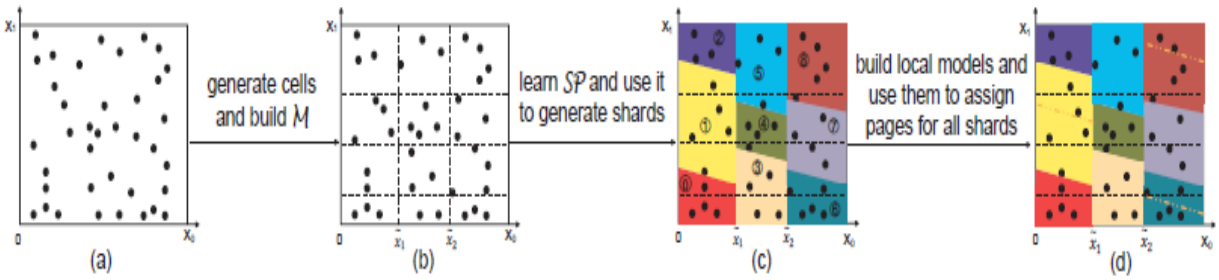


Figure 2.7.: Lisa Framework

Definitions

This section presents the additional definition specific to Lisa implementation.

4. **Shard**. The shard S is the pre-image of an interval $[a, b) \subseteq [0, +1)$ under the mapping function $\mathcal{M}$, i.e., $S = M^{-1}([a.b))$.
   Given an initial data set, we divide the key space into cell grids based on the data distribution, map keys values to an one dimensional space using mapping function, followed by learning several monotonic shard prediction functions. After sorted, the one dimensional mapped value space is then divided into equal-length intervals, and one shard prediction function is learned for each interval, to partition the keys belonging to a particular interval, into different shards. As keys are sorted by mapped values before partitioning them into equal sized intervals, and all shards exhibit a total order with respect to their corresponding intervals in the mapped range(Shard Prediction function for each interval is monotonically increasing), following relationship holds
   $inf(M(S_i)) > sup(M(S_j))$ when $i > j$.

5. **Local Model**. Local model L_i is a model that processes operations within a shard S_i . It keeps dynamic structures such as the addresses of pages contained by S_i .

2.2.5. Design and Implementation Details

Grid Cells Generation

The first task in Lisa implementation is to partition the 2 dimensional key space into a series of grid cells based on the data distribution along a sequence of axes. Then we number the cells along these axes as well. The principal idea behind this partition strategy is to divide the key space into cell boundaries and apply a mapping function to create monotonically increasing mapping values at the cell boundaries.

$M(x_i \in V) < M(x_j \in V)$ when $i < j$, where $x_i \in C_i$ and $x_j \in C_j$

i.e. mapped value of a key in cell i will always be less than mapped values of a key in cell j, if $i < j$.

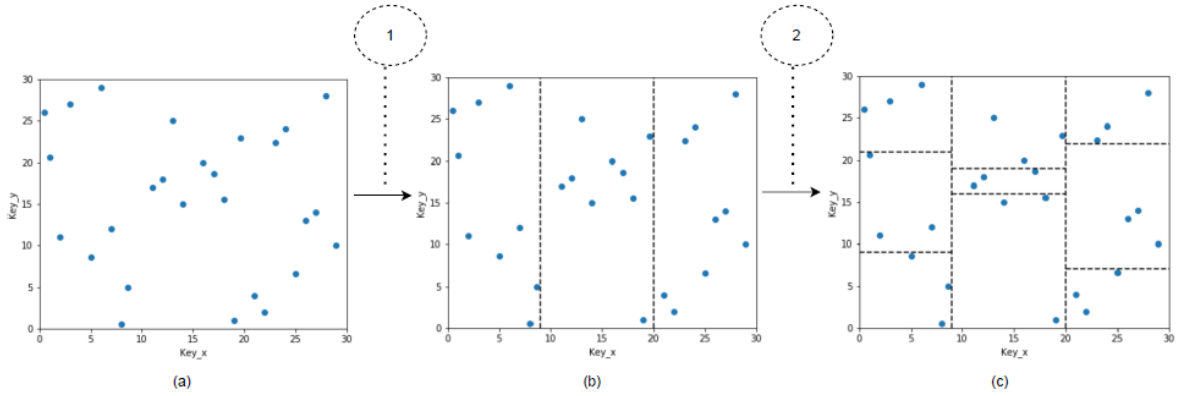


Figure 2.8.: Cell Partition Strategy:
1) : Sort Keys on x dimension and divide into 3 vertical columns each containing 9 keys
2) : Sort each vertical column keys on y dimension and divide into 3 horizontal columns each containing 3 keys

Example 2.6 Consider the example shown in the figure 2.8: 27 keys are partitioned into 9 cell, resulting in 3 keys per cell. To partition the key space, we first sort the keys values according to 1^{st} dimension and divide the keys into 3 vertical columns each containing 9 keys. Then for each vertical column of 9 keys, we sort the keys again according to 2^{nd} dimension, and divide the keys in each column into 3 new cells. The number of cells N into which the keys space is divided, is a hyper-parameter and found empirically using grid search.

♣

We need to sort the key space along the sequence of axis before we partition the keys value along that axis to make sure that cells don't contain overlapping keys.

Algorithm 6: Grid Cell Generation Algorithm for Lisa Method

input: num_of_cells; x; y

trainset=[$(x, y); x \in \mathbb{R}^2; y \in \mathbb{R}$]

$keysPerPage = len(x)/num\_of\_cells$

Sort x based on first dimension x[:][0]]

In first for loop, divide the keys into equal size subsets based on first dimension

for $i \leftarrow 0$ **to** $\sqrt{(num\_of\_cells)}$ **do**

  Store the 1st dimensional coordinates of first and last key for each cell. Each such cell will contain $keysPerPage * sqrt(num\_of\_cells)$ keys

end

Sort keys in each cell based on 2nd dimension,x[:][1]

for $i \leftarrow 0$ **to** $\sqrt{num\_of\_cells}$ **do**

  for $j \leftarrow 0$ **to** $\sqrt{(num\_of\_cells)}$ **do**

  end

  Store the 2nd dimensional coordinates of first and last key for each cell.

end

Mapping Function

A mapping function $\mathcal{M}$ is a function on the domain $\mathbb{R}^2$ to the non-negative range, i.e $M : [0, X_0] \times [0, X_1] \rightarrow [0, +\infty)$ such that $M(x_i \in V) < M(x_j \in V)$ if $i < j$, where $x_i \in C_i$ and $x_j \in C_j$. That means the mapped value of a key in cell i will always be less than mapped values of a key in cell j, if $i < j$.

Suppose $x = (x_0, x_1)$ and $x \in C_i = [\theta_{i_0}^{(0)}, \theta_{i_0+1}^{(0)}) \times [\theta_{i_1}^{(1)}, \theta_{i_1+1}^{(1)})$ then we define

$$M(x) = i + \frac{\mu(H_i)}{\mu(C_i)}$$

where $H_i = [\theta_{i_0}^{(0)}, x_0) \times [\theta_{i_1}^{(1)}, x_1)$ and μ is the Lebesgue measure on $\mathbb{R}^2$.

As shown in figure 2.9, in 2-dimensional case, $\frac{\mu(H_i)}{\mu(C_i)}$ represents the fraction of the area covered by the key(x_0, x_1) to the total area of the cell. Since we are adding i, the index of the cell, to this fraction, the mapped value of a key in cell i will always be less than mapped values of a key in cell j, if $i < j$. After calculating the mapped values of the data set, we sort the keys in each cell according to the mapped value. This results in the whole key space to be sorted according to the mapped value. Figure 2.10 shows the mapping of 2 dimensional key space to one dimensional CDF.

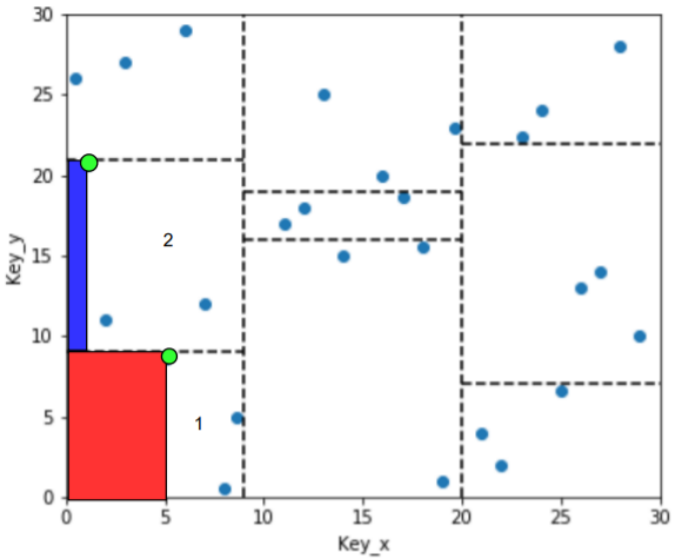


Figure 2.9.: Lebesgue Measure Representation for 2 dimensional data
1) Lebesgue Measure for the green point in first cell will be ratio of area of red rectangle divided by the total area of 1^{st} cell
1) Lebesgue Measure for the green point in second cell will be ratio of area of blue rectangle divided by the total area of 2^{nd} cell

Shard Prediction Function

After the mapping function, we get a dense array of mapped values. Then we partition them evenly into U parts and let $\boldsymbol{M}_p = [m_1, \cdots, m_U]$. We train linear regression functions $\mathcal{F}_i$ on each interval and suppose $V+1$ is the number of mapped values that each $\mathcal{F}_i$ needs to process and Ψ is the average number of keys falling in a shard. With these definitions, we know that each $\mathcal{F}_i$ generates $D = \lceil \frac{V+1}{\Psi} \rceil$ shards.

Example 2.7 For example, assume we have a dense array of mapped values as

$$[1, 1.2, 2.2, 3, 3.4, 4]$$

We want to partition it into 2 parts, so we have $\boldsymbol{M}_p = [3]$ and $V + 1 = 3$. In this case we will train 2 linear regression functions. Suppose that the average number of keys in a shard is $\Psi = 2$, then each $\mathcal{F}_i$ generates $D = \lceil \frac{V+1}{\Psi} \rceil = \lceil \frac{3}{2} \rceil = 2$ shards. ♣

Then with a given x, the predicted shard is given by $\mathcal{SP}(x) = \mathcal{F}_i(x) + i \times D$, where $i = \text{binary-search}(\boldsymbol{M}_p, x)$. More specifically, we first determine i by using binary search. The result tells which interval this x should belong to. Then we find the corresponding linear regression function $\mathcal{F}_i$ and calculate $\mathcal{F}_i(x)$, which is the predicted shard.

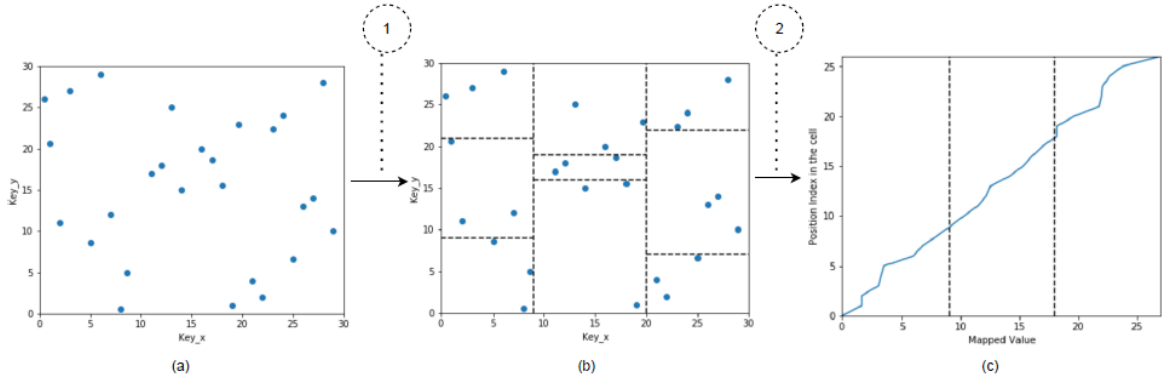


Figure 2.10.: Mapping 2 dimensional key Values to one dimensional cdf
1) Generate grid cells, and apply Lebesgue Measure to each cell.
2) Sort key in each cell according to mapped value. Mapped values in consecutive cells are already sorted by mapping function definition. Plot the cdf of mapped values.

Example 2.8 In the above example, given a key $x = 2.2$, we first perform binary search in $\boldsymbol{M}_p$ and we found $i = 1$. Then we find the first linear regression function $\mathcal{F}_1$ and calculate $\mathcal{F}_1(x)$. Since each linear regression function will yield $D = \lceil \frac{V+1}{\Psi} \rceil = 2$ shards, the shards that the first linear regression function generates will be from 0 to 1 and the shards that the second linear regression function generates will be from 2 to 3. Hence, the predicted shard id is given by

$$\mathcal{SP}(x) = \mathcal{F}_i(x) + i \times D$$

♣

Then the problem left is to train the linear regression functions $\mathcal{F}_i$. Let $\boldsymbol{x} = (x_0, \cdots, x_v)$ be the keys' mapped value that fall in $[m_{i-1}, m_i)$. Suppose that $\boldsymbol{x}$ is sorted, i.e. $x_i \leq x_j, \forall 0 \leq i < j \leq v$. Let $\boldsymbol{y} = (0, \cdots, V)$. Then we build a piecewise linear regression function f_i with inputs $\boldsymbol{x}$ and ground truth $\boldsymbol{y}$. For a given point with mapped value $m \in [m_{i-1}, m_i)$, its shard id is given by $\lceil \frac{f_i(m)}{\Psi} \rceil + i \times D$, i.e. $\mathcal{F}_i(x) = \frac{f_i(m)}{\Psi}$.

Example 2.9 In our previous example, in the interval $[0, 3)$, we have $\boldsymbol{x} = (1, 1.2, 2.2)$ and $\boldsymbol{y} = (0, 1, 2)$. Then for a point with the mapped value $m = 1.2$, the expected output will be $f_i(m) = 1$ and the shard id is given by $\lceil \frac{1}{2} \rceil + 0 \times 2 = 1$. Hence, the point with mapped value $m = 1.2$ will be allocated to the first shard. Then the problem is to train a continuous piecewise linear regression function in each interval. We constrain the piecewise linear regression function to be continuous so that it is guaranteed be monotonic. ♣

Formally, a piecewise linear function can be described as

$$f(x) = \begin{cases} b_0 + \alpha_0(x - \beta_0) & \beta_0 \leq x < \beta_1 \\ b_1 + \alpha_1(x - \beta_1) & \beta_1 \leq x < \beta_2 \\ \vdots & \\ b_\sigma + \alpha_\sigma(x - \beta_\sigma) & \beta_\sigma \leq x \end{cases} \tag{2.6}$$

In order to make this piecewise linear function continuous, the slopes and intercepts of each linear region depend on previous values. Formally, let $\bar{a} = b_0$, then Eq. (2.6) reduces to

$$f(x) = \begin{cases} \bar{\alpha} + \alpha_0(x - \beta_0) & \beta_0 \leq x < \beta_1 \\ \bar{\alpha} + \alpha_0(x - \beta_0) + \alpha_1(x - \beta_1) & \beta_1 \leq x < \beta_2 \\ \cdots & \\ \bar{\alpha} + \alpha_0(x - \beta_0) + \alpha_1(x - \beta_1) + \cdots + \alpha_\sigma(x - \beta_\sigma) & \beta_\sigma \leq x \end{cases} \tag{2.7}$$

Then to make Eq. (2.7) monotonically increasing, we only need to ensure that

$$\sum_{i=0}^{\eta} \alpha_i \geq 0, \forall 0 \leq \eta \leq \sigma$$

Let $\boldsymbol{\alpha} = (\bar{\alpha}, \alpha_0, \cdots, \alpha_\sigma)$, the square loss function $L(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_{i=1}^{V}(f(x_i) - y_i)^2$. We then optimise $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ iteratively.

Assume that $\boldsymbol{\beta} = \hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \hat{\beta}_1, \cdots, \hat{\beta}_\sigma)$ is fixed, then $\boldsymbol{\alpha}$ can be regarded as the least square solution of the linear equation $\boldsymbol{A\alpha} = \boldsymbol{y}$, where

$$\boldsymbol{A} = \begin{bmatrix} 1 & x_0 - \hat{\beta}_0 & \left(x_0 - \hat{\beta}_1\right) 1_{x_0 \geq \hat{\beta}_1} & \cdots & \left(x_0 - \hat{\beta}_\sigma\right) 1_{x_0 \geq \hat{\beta}_\sigma} \\ 1 & x_1 - \hat{\beta}_0 & \left(x_1 - \hat{\beta}_1\right) 1_{x_1 \geq \hat{\beta}_1} & \cdots & \left(x_1 - \hat{\beta}_\sigma\right) 1_{x_1} \geq \hat{\beta}_\sigma \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N - \hat{\beta}_0 & \left(x_V - \hat{\beta}_1\right) 1_{x_V \geq \hat{\beta}_2} & \cdots & \left(x_V - \hat{\beta}_\sigma\right) 1_{x_V \geq \hat{\beta}_\sigma} \end{bmatrix}$$

where $1_{x_0 \geq \hat{\beta}_1}$ equals to 1 if $x_0 \geq \hat{\beta}_1$, otherwise it equals to 0.
We have

$$\begin{aligned} L(\boldsymbol{\alpha}, \boldsymbol{\beta}) = (\boldsymbol{y} - \boldsymbol{A\alpha})^T(\boldsymbol{y} - \boldsymbol{A\alpha}) &= \boldsymbol{y}^T\boldsymbol{y} - \boldsymbol{\alpha}^T\boldsymbol{A}^T\boldsymbol{y} - \boldsymbol{y}^T\boldsymbol{A\alpha} + \boldsymbol{\alpha}^T\boldsymbol{A}^T\boldsymbol{A\alpha} \\ &= \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{\alpha}^T\boldsymbol{A}^T\boldsymbol{y} + \boldsymbol{\alpha}^T\boldsymbol{A}^T\boldsymbol{A\alpha} \end{aligned} \tag{2.8}$$

and if we let

$$\begin{aligned} \frac{\partial L(\boldsymbol{\alpha}, \boldsymbol{\beta})}{\boldsymbol{\alpha}} &= 2\boldsymbol{A}^T\boldsymbol{A\alpha} - 2\boldsymbol{A^T y} = 0 \\ &\implies \boldsymbol{\alpha} = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{Ay} \end{aligned} \tag{2.9}$$

we get the $\boldsymbol{\alpha}$ with the given fixed $\boldsymbol{\beta}$. Clearly, different $\boldsymbol{\beta}$ give rise to different optimal parameters. Let $\boldsymbol{\alpha}^\star(\boldsymbol{\beta})$ be the optimal $\boldsymbol{\alpha}$ for a particular $\boldsymbol{\beta}$, then we want to find $\boldsymbol{\beta}$ such that

$$L(\boldsymbol{\alpha}^\star(\boldsymbol{\beta}^\star), \boldsymbol{\beta}^\star) = \min\{L(\boldsymbol{\alpha}^\star(\boldsymbol{\beta}), \boldsymbol{\beta}) | \boldsymbol{\beta} \in \mathbb{R}^{\sigma+1}\} \tag{2.10}$$

For $\boldsymbol{\beta}$, we define $\boldsymbol{r} = \boldsymbol{A\alpha} - \boldsymbol{y}$ and

$$\boldsymbol{K} = \text{diag}(\bar{\alpha}, \alpha_0, \cdots, \alpha_\sigma), \boldsymbol{G} = \begin{bmatrix} -1 & -1 & \cdots & -1 \\ p_0^{(0)} & p_0^{(1)} & \cdots & p_0^{(V)} \\ p_1^{(0)} & p_1^{(1)} & \cdots & p_1^{(V)} \\ \vdots & \vdots & \ddots & \vdots \\ p_\sigma^{(0)} & p_\sigma^{(1)} & \cdots & p_\sigma^{(V)} \end{bmatrix}$$

where $p_i^{(l)} = -1_{x_l \geq \beta_i}$. Then

$$\boldsymbol{KG} = \begin{bmatrix} -\bar{\alpha} & -\bar{\alpha} & \cdots & -\bar{\alpha} \\ 0 & \alpha_0 p_0^{(1)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \alpha_\sigma p_\sigma^{(V)} \end{bmatrix}$$

then we have

$$g = \frac{\partial L(\boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = 2\boldsymbol{KGr}, Y = \frac{\partial g}{\partial \boldsymbol{\beta}} = 2\boldsymbol{KGG}^T\boldsymbol{K}^T \tag{2.11}$$

Show how these are calculated

As $g = \nabla_{\boldsymbol{\beta}} L$, $-g$ specifies the steepest descent direction of $\boldsymbol{\beta}$ for L. However, the convergence rate of $-g$ is low as it does not consider the second order derivative of L. Hence, we use Newton's method to perform the update along the direction of second derivative, $s = -\boldsymbol{Y}^{-1}g$. Newton's method assumes that the loss L is twice differentiable and uses the approximation with Hessian The geometric interpretation of Newton's method is that at each iteration, it amounts to the fitting of a paraboloid to the surface of $L(\boldsymbol{\alpha}, \boldsymbol{\beta})$ at the trial value β_k, having the same slopes and curvature as the surface at that point, and then proceeding to the maximum or minimum of that paraboloid. Hessian matrix, Y in our case is positive semidefinite and hence can be inverted.

$$Y = \frac{\partial g}{\partial \boldsymbol{\beta}} = 2\boldsymbol{KGG}^T\boldsymbol{K}^T = 2(\boldsymbol{KG})(\boldsymbol{G}^T\boldsymbol{K}^T) = 2(\boldsymbol{G}^T\boldsymbol{K}^T)^T(\boldsymbol{G}^T\boldsymbol{K}^T) = 2(\boldsymbol{M}^T\boldsymbol{M}) \tag{2.12}$$

Show how these are calculated Y is a full rank matrix as columns of Y are linearly independent (all keys are independent of each other). To prove that Y is positive definite, we need to show that $x^TYx > 0, \forall x \neq 0$.
$x^TYx = x^TM^TMx = (Mx)^T(Mx) = \|Mx\|_2^2 \geq 0, \forall x \neq 0$

In the beginning, we set $\beta^{(0)} = x_0$ and $\beta_i^{(0)} = x_{\lfloor i \times \frac{V}{\Psi} \rfloor}, \forall i \in [1, \sigma]$. Then we can obtain $\boldsymbol{\alpha}$ by solving Eq. (2.9). Then at each step, we perform a grid search to find the step $lr^{(k)}$ such that the loss L is minimal. Then at the next iteration, we increase k by one and set

$$\boldsymbol{\beta}^{(k+1)} = \boldsymbol{\beta}^{(k)} + lr^{(k)} s^{(k)}$$

As described in Algorithm 7, we perform following operations during shard training, :

1. Divide the sorted mapped values into equal sized U intervals.
2. Suppose V +1 is the number of mapped values in each interval and ψ is the estimated average number of keys falling in a shard.
3. For each interval, we want to build a monotonic regression model $\mathcal{F}_i$ whose domain is $[m_{i-1}, m_i]$
4. Each $\mathcal{F}_i$ generates D = $\lceil \frac{V+1}{\Psi} \rceil$ number of shards
5. $x = [x_0, \cdots, x_V]$ specifies the keys' mapped values in interval i, $[m_{i-1}, m_i]$
6. Given V +1 sorted mapped values $x = [x_0, \cdots, x_V]$ and their indices $y = [0, \cdots, V]$, each $\mathcal{F}_i$ is built and trained with the procedure mentioned in the algorithm 7.

Algorithm 7: Shard Training Algorithm

input: M_p, Ψ, U

Partition M_p into equal length U intervals $\boldsymbol{M}_p = [m_1, \cdots, m_U]$

for $i \leftarrow 0$ **to** U **do**

  $x = [x_0, \cdots, x_V]$ be the keys' mapped values in interval i

  $y = [0, \cdots, V]$

  Initialize $\beta^{(0)}$ as $\beta^{(0)} = x_0$ and $\beta_i^{(0)} = x_{\lfloor i \times \frac{V}{\Psi} \rfloor}, \forall i \in [1, \sigma]$

  while $k <$ *1000* **do**

    Initialize $A^{(k)}$ according to (2.7)

    $\alpha^{(k)} = ((A^{(k)})^T A^{(k)})^{-1} (A^{(k)})^T y$

    Calculate $g^{(k)}, Y^{(k)}$

    $s^k = -(Y^{(k)})^{-1} g^{(k)}$,

    Find update step $lr^{(k)}$ such that

    $\mathrm{L}(\alpha^\star(\beta^k + lr^{(k)} s^k), \beta^k + lr^{(k)} s^k) = \min\{L(\alpha^\star(\beta^k + lr^{(k)} s^k), \beta^k + lr^{(k)} s^k)\}$

    $\beta^{k+1} = \beta^k + lr^{(k)} s^k$

  end

end

Local Models for Shards

Local models are not relevant to our implementation as all the data is contained in the memory.

2.3. Queries

2.3.1. Point Query

A point query is a database operation that finds the records that exactly match our query conditions. In this project, we perform point query on 1-dimensional data. In addition, we assign the database records into pages, predict the page index with the index models and then perform sequential search on the predicted page. In order to evaluate the errors that different index models are making, we focus on predicting the page indices and ignore the sequential search operation on a specific page.

Example 2.10 For example, assume we have an 1-dimensional array $[1, 2, 3, 4]$ and two pages such that $[1, 2] \in P_0$ and $[3, 4] \in P_1$. A point query for $x = 2$ is expected to return 0 as the page index. ♣

Point Query with B-Tree

Point query in a B-Tree is basically the comparison of the value of the key that needs to be searched with the keys in the node. It first linearly checks the value in the root key and looks for a key value which is greater than the searched key. As soon as it finds a key greater than the searched key it will search in the child of the key before it. For example if we were to search of key [41] in the example of the B-Tree used above, we would first check the value [11] and since it smaller than [31] and there are no keys greater than this in the root node it will search in the right child of the root node. It will then linearly search the node and locate it's associated value and return it.

Algorithm 8: Algorithm for B-Tree Search

```
Input: k ; key, root ; Root of the B-Tree
Output: Value associated with key
for i ← 0 to len(RootNode) do
    if keys in root greater than k then
        SEARCH_CHILD(key) //Search linearly the child associated with the key
         location one before
        if Child is a leaf then
            Linearly search until the key is reached
        else
            SEARCH_CHILD(key)
        end
    end
end
```

Point Query with Baseline Index Model

Point Query with Recursive Model Index

Algorithm 9: Training of Recursive Model Index

```
input: x; models; num_of_stages; max_y
stage← 0
next_model← 0
while stage <num_of_stages do
    output = model.predict(x)
    next_model=output*len(models[stage+1])/max_y
    if last stage then
        y = next
end
```

2.3.2. Range Query

A range query is a database operation that retrieves all the records that lies in a range. In this project, we perform range query on 2-dimensional data only. In addition, we only consider a range query where the range is defined as a rectangle. Under these assumptions, a range query can be formalised as a query $\mathcal{Q}(\boldsymbol{l}, \boldsymbol{u})$ where $l, u \in \mathbb{R}^2$.

Example 2.11 For example, assume we have the points

$$[(1,2),(3,4),(3.5,4),(5,6)]$$

and the range query $\mathcal{Q}((2,3),(5,5))$, as shown below:

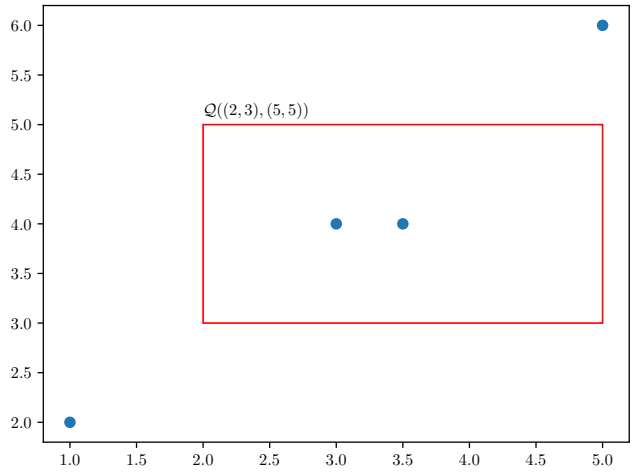


Figure 2.11.: A Range Query Example where $\mathcal{Q}(\boldsymbol{l}, \boldsymbol{u}) = \mathcal{Q}((2,3),(5,5))$

In this example, the range query should return the points that lies inside the red rectangle, i.e. $[(3, 4), (3.5, 4)]$.

Range Query with KD-Tree

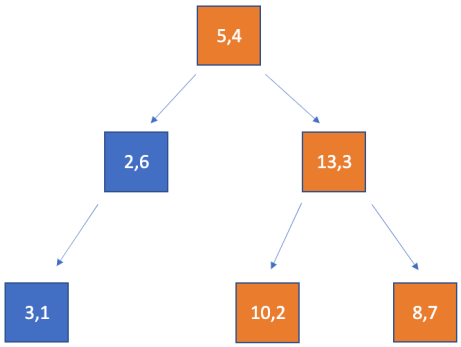


Figure 2.12.: KD-Tree for Range Query

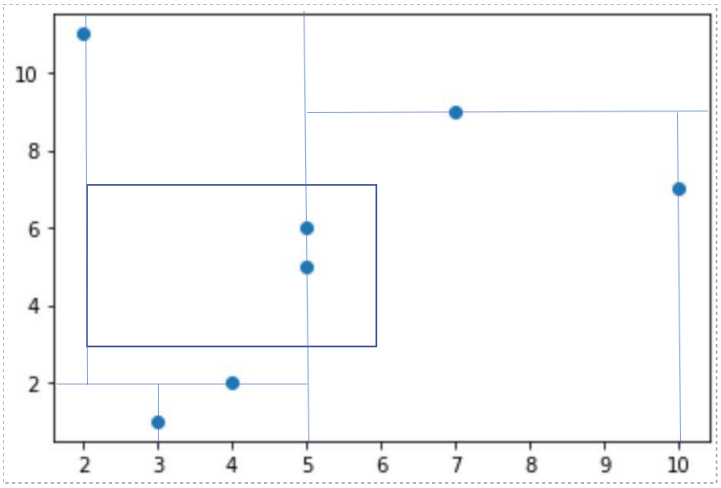


Figure 2.13.: KD-Tree Range Query Plot on 2-dimentional plane

We then check if the root of the tree lies within the range of the bounds and only then start traversing the tree.

Example 2.12 For example we have a tree with Point list as

$$((5, 6), (4, 2), (7, 9), (3, 1), (5, 5), (10, 7), (2, 11))$$

and with lower bound = $(2, 3)$ and upper bound = $(6, 7)$, we will get a tree as is shown in 2.12. We can see the points along with the rectangle range plotted in 2.13. Points $(5, 5)$ and $(5, 6)$ are returned in the query since they lie within the rectangle as seen in the plot.

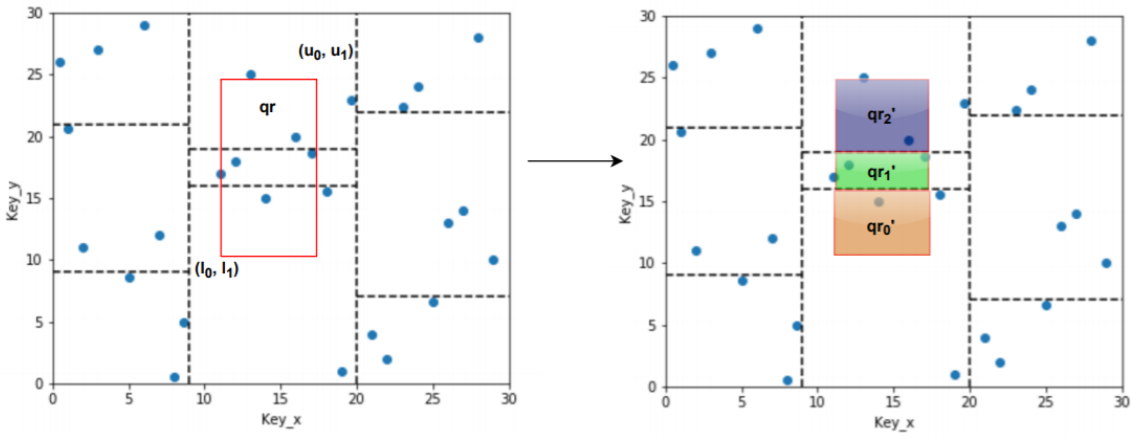


Figure 2.14.: Range Query Search in Lisa. 1) Find the cells that overlap with query rectangle qr.
2) Decompose qr into the unions of smaller query rectangles, each of which intersect one only one cell.
3) Find shards corresponding to lower and upper coordinates for each query rectangle, and perform a sequential search.

First the root point is checked and since the x-coordinate and y-coordinate both lie within the rectangle bounds i.e., $2 > 5 > 6$ and $3 > 6 > 7$. It then checks if the x-coordinate is lower than or greater than the lower bound x-coordinate. Since the value is larger than lower bound x-coordinate that is 2 it will then traverse to the left. In the left it has child node as $(4, 2)$ however, since the y-coordinate doesn't lie in the range of the upper bound this point is not selected. Therefore, it recursively traverses the tree and checks if the point lies within the bound until it reaches a leaf. ♣

Range Query with LISA

For a range query $\mathcal{Q}(\boldsymbol{l}, \boldsymbol{u})$, we first find the cells that overlap with $\mathcal{Q}$. Then we decompose $\mathcal{Q}$ into the union of smaller query rectangles $\bigcup \mathcal{Q}_i$ such that each smaller query rectangles intersects only one cell, as shown in the Fig. 2.14.

Suppose that $\mathcal{Q} = \bigcup \mathcal{Q}_i$ where $\mathcal{Q}_i = [l_{i_0}, u_{i_o}) \times [l_{i_1}, u_{i_1})$, i.e. we have $\mathcal{Q}_i$ representing the ith smaller query rectangles of one cell C_j.

Then we can calculate the mapped values of $\mathcal{Q}_i$, i.e. $\mathcal{M}(l_{i_0}, l_{i_1})$ and $\mathcal{M}(u_{i_0}, u_{i_1})$. For simplicity, we use $m_l^{(i)}$ and $m_u^{(i)}$ to denote $\mathcal{M}(l_{i_0}, l_{i_1})$ and $\mathcal{M}(u_{i_0}, u_{i_1})$ respectively.

After creating corresponding mapped values, we then apply the shard prediction function $\mathcal{SP}(m_l^i)$ and $\mathcal{SP}(m_u^i)$ to predict the shard that could possibly contain keys that lie in the query rectangle $\mathcal{Q}_i$. Then in each shard, we perform a sequential search to find the desired keys.

2.3.3. KNN Query

K-Nearest Neighbours (KNN), as the name suggests, is the process of finding K nearest neighbours to a given query point. In this project, the KNN query is only performed on 2-dimensional data. In addition, we only use ℓ_2 norm as the distance metric. A KNN query will be formalised as $\mathcal{K}(\boldsymbol{X})$ where $\boldsymbol{X} \in \mathbb{R}^2$.

KNN query with KD-Tree

As a baseline, we first perform KNN query with KD-tree.

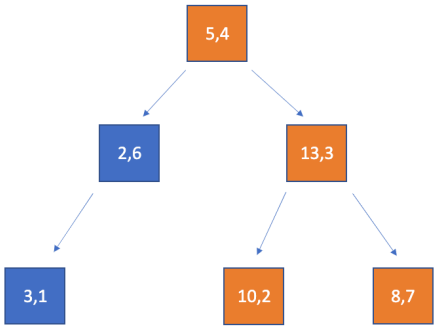


Figure 2.15.: KD-Tree for KNN Query

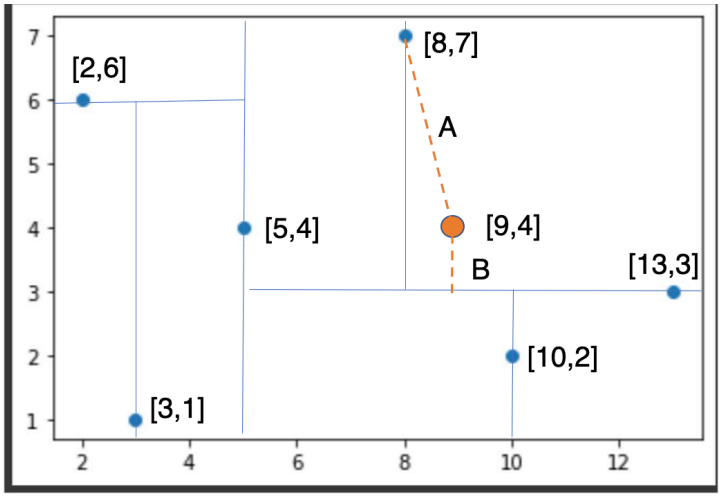


Figure 2.16.: KD-Tree KNN Plot on 2-dimentional plane

Example 2.13 For example, we have Point list as $((5,4),(2,6),(13,3),(8,7),(3,1),(10,2))$ then we will have a tree structure as shown in 2.15 and it's plot on 2-dimensional plane is shown in 2.16. As we can see in 2.16 that even though point $(8,7)$ is the leaf we will reach when we traverse the tree to search for point nearest to test point $(9,4)$ it is not infact the nearest point to the test data. In this case if we want to look for 4 nearest neighbour, we

first check the square of euclidean distance of $(9, 4)$ with the root of the tree i.e., $(5, 4)$ which is 16. It then calculates the distance with $(2, 6)$ and $(13, 3)$ which calculates to 53 and 17 respectively. It then keeps traversing to the right node while calculating distance until it reaches a leaf. After reaching the leaf it then checks the distance with $(8, 7)$ with a distance of 10 which is infact smaller than the previous shortest distance of 16 with the root. It adds these points to the list. It then makes a decision weather to go left from $(13, 3)$ based on the distance of the test point with leaf $(8, 7)$ i.e., A and the perpendicular distance with point $(13, 3)$ which is B. Since distance A > B as can be seen in the figure 2.16 there is a chance that there could a point in the subtree with a distance smaller than the previous points. In this case it will then check the distance with point $(10, 2)$ and the distance is the shortest(best distance) so far of 5. ♣

KNN Query with LISA

We do not know the analytical representation of shards, as we use machine learning model $\mathcal{SP}$ to generate shards. Thus,it is difficult to apply traditional KNN query pruning strategies applicable for KD-Trees, to LISA model.

Consider a query point $q_{knn} = x = (x_0, x_1)$, let $x^{'} \in V$ be the Kth nearest key to x in database at a distance value $\delta = \|x^{'} - x\|_2$. Lets define $\mathcal{Q}(x, \delta) \triangleq [x_0 - \delta, x_0 + \delta) \times [x_1 - \delta, x_1 + \delta)$ and $\mathcal{B}(x, \delta) \triangleq \{p \in V \mid \|x - p\|_2 \leq \delta\}$.We can create a query rectangle $qr = \mathcal{Q}(x, \delta + \epsilon)$ where $\epsilon \to 0$. As shown in Fig. 2.17, K nearest keys to x are all in $\mathcal{B}(x, \delta)$ and thus in qr. KNN query can be solved using the range query if we can estimate an appropriate distance bound δ for every query point.

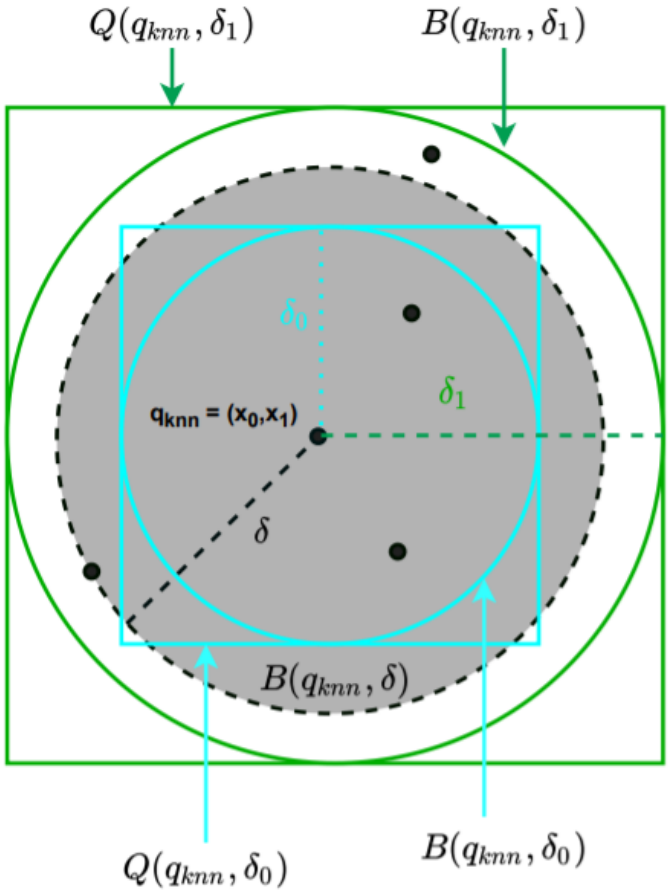


Figure 2.17.: KNN Query Implementation in Lisa(K=3)
1)q_{knn} represents the query point, $\mathcal{Q}(x, \delta) \triangleq [x_0 - \delta, x_0 + \delta) \times [x_1 - \delta, x_1 + \delta)$, represents query rectangle and $\mathcal{B}(x, \delta)$ represents the key space at distance δ containing K nearest keys.
2)KNN query can be solved by range query if we can estimate an appropriate distance bound δ for every query point

3. Evaluation

In order to evaluate the performance, we perform the evaluation on manually synthesised dataset.

3.1. One Dimensional Data and Indexes

For one dimensional data, the evaluation covers the following tasks:

- Find a structure for recursive model index empirically.
- Compares the performance between baseline model, recursive model and traditional B-Tree.

3.1.1. Dataset

For one dimensional case, we manually generate two columns of the data:

- The first column contains the keys X, which is randomly sampled from a given distribution.
- Then we assign the keys into different pages according to a preset parameter N_{page} for page size. Specifically, the first N_{page} keys will be assigned into the first page, the second N_{page} keys will be assigned into the second page and so on so forth. After the assignments, we set the second column Y to be the page index of the corresponding x.

Small Lognormal Distributed Data We first generate $10,000$ data points where X is from a lognormal distribution Lognormal$(0, 4)$. In the Fig 3.1, we illustrate the $x - y$ relations where X is randomly sampled from a lognormal distribution.

We use three groups to find the best recursive model for lognormal data.

- All models are fully connected neural networks. The number of second-level models are $200, 400$, and 600 respectively. The number of third-level models are $2000, 4000$ and 6000 for each number of second-level models.
- All models are linear regression models. The number of second-level models are $200, 400$, and 600 respectively. The number of third-level models are $2000, 4000$ and 6000 for each number of second-level models.

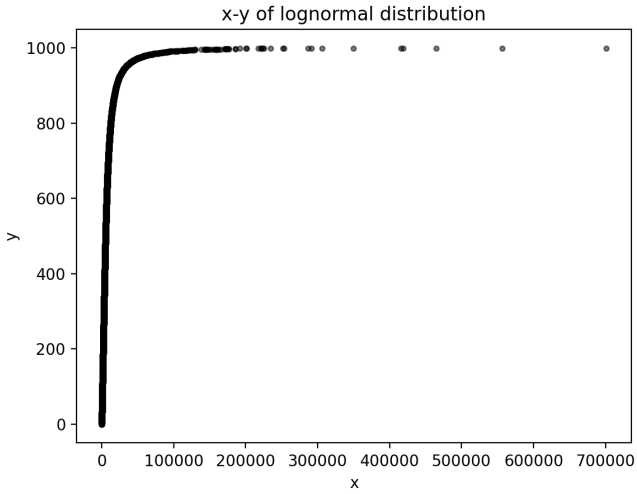
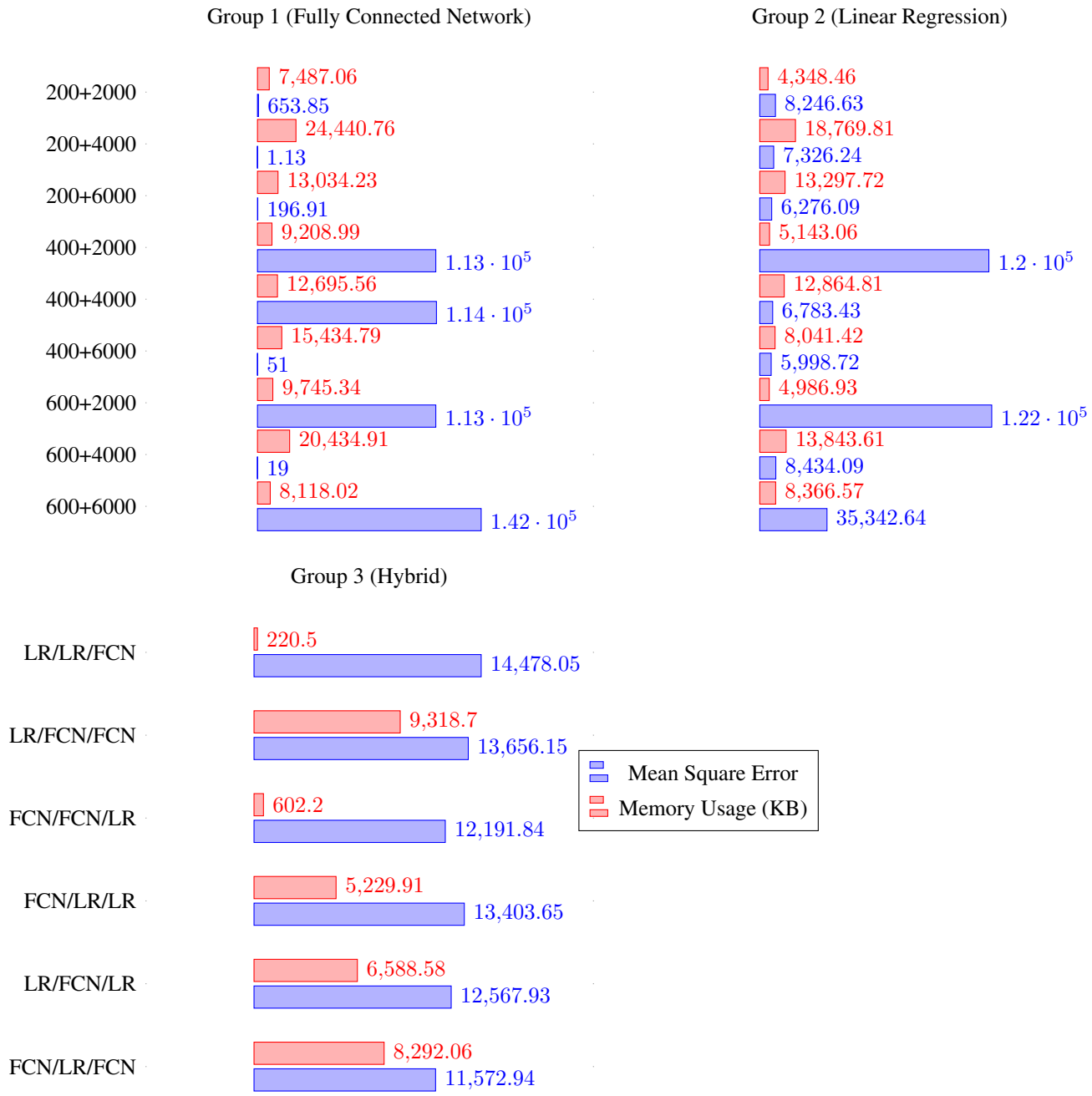


Figure 3.1.: The x-y graph where x is randomly sampled from a lognormal distribution

- Models are combinations of fully connected neural networks and linear regression models. The numbers of second-level and third-level models are determined by the best settings in previous two group.



From the experiment results, we found that the second setting in group 1 (1 FCN model as root, 200 FCN models as second level models and 4000 FCN models as third level models) is the best regarding the mean square error. We also have the following findings in this searching process.

- Generally, the average error in group 1, where all models are fully connected neural networks is less than the error in group 2. Fully connected neural networks have a potential to be more accurate, i.e. it could achieve a small error if we tuned the models parameters properly.

- Tuning a model is tedious and can be costly. There are lots of hyper-parameters to choose from, such as the number of models in each level, types of models in each level, number of levels, and the internal hyper-parameters in each model. Using grid search, as we did in this experiment can be costly and time-consuming.

Various Distributions and Sizes After the search process for a recursive model, we then conduct experiments on several different distributions and sizes datasets. During this process, we use the following settings:

Large Lognormal Distributed Data The last dataset that we used is a large dataset that contains 190 million key value pairs that are distributed under lognormal distribution.

3.2. Two Dimensional Data and Indexes

For two dimensional data, the evaluation covers the following tasks:

- Point Query for KD-Tree.
- Range Query for KD-Tree
- KNN Query for KD-Tree
- Find hyper-parameters for the Lisa model empirically.
- Compares the performance between kd-tree, baseline model and Lisa implementation.
- Find the hyper-parameters for the LISA model empirically.
- Compare the performance between KD-tree, baseline model and LISA implementation.

3.2.1. Dataset

For two dimensional case, we manually generate three columns of the data:

- The first two columns contain the 2 dimensional keys $\boldsymbol{X} \in \mathbb{R}^2$, which are independently sampled from a given distribution.
- Then we assign the keys into different pages according to a preset parameter N_{page} for page size. Specifically, the first N_{page} keys will be assigned into the first page, the second N_{page} keys will be assigned into the second page and so on so forth. After the assignments, we set the second column Y to be the page index of the corresponding x.

Training/Test Data Size	Query Size	Build Time(s)	Avg Query Time(s)	Memory Size(KB)	Evaluation Error(MSE)
10,000	1000	0.0653	1.88E-05	2459.02	0.0
10,000	2000	0.0653	1.87E-05	2459.02	0.0
10,000	2000	0.0653	1.87E-05	2459.02	0.0
10,000	2000	0.0653	1.87E-05	2459.02	0.0
100,000	1000	0.0739	1.82E-05	2459.02	0.0
100,000	2000	0.0739	1.80E-05	2459.02	0.0
100,000	2000	0.0739	1.80E-05	2459.02	0.0
100,000	2000	0.0739	1.80E-05	2459.02	0.0
10,00,000	1000	0.0654	1.82E-05	2630.2	0.0
10,00,000	1000	0.0654	1.82E-05	2630.2	0.0
10,00,000	1000	0.0654	1.82E-05	2630.2	0.0
10,00,000	2000	0.0654	1.80E-05	2630.2	0.0
10,000,000	1000	0.0677	1.91E-05	2631.6	0.0
10,000,000	1000	0.0677	1.91E-05	2631.6	0.0
10,000,000	1000	0.0677	1.91E-05	2631.6	0.0
10,000,000	2000	0.0677	1.88E-05	2631.6	0.0
19,000,000	1000	0.06968	1.87E-05	2631.6	0.0
19,000,000	1000	0.06968	1.87E-05	2631.6	0.0
19,000,000	1000	0.06968	1.87E-05	2631.6	0.0
19,000,000	2000	0.06968	1.86E-05	2631.6	0.0

Table 3.1.: Experimental results for KD Tree model(Range Query) for lognormal data

Training/Test Data Size	K Size	Build Time(s)	Avg Query Time(s)	Memory Size(KB)	Evaluation Error(MSE)
10,000	5	0.0653	0.000388	2459.02	0.0
10,000	10	0.0653	0.000173	2459.02	0.0
100,000	5	0.0737	0.00049	2621.76	0.0
100,000	10	0.0737	0.00017	2621.76	0.0
10,00,000	5	0.075	0.00043	2631.91	0.0
10,00,000	10	0.0759	0.000183	2631.91	0.0
10,000,000	5	0.0662	0.000417	2632.04	0.0
10,000,000	10	0.0662	0.00018	2632.04	0.0
19,000,000	5	0.0695	0.00039	2632.04	0.0
19,000,000	10	0.0695	0.000248	2632.04	0.0

Table 3.2.: Experimental results for KD Tree model(KNN Query) for lognormal data

3.2.2. Point Query KD-Tree

3.2.3. Range Query KD- Tree

3.2.4. KNN Query KD- Tree

3.2.5. Task 1 : Hyper-parameters Search

After generating dataset as mentioned in previous section, we sample a smaller subset from it. We repeat our experiments for 3 different sample sizes of 10000, 100000 and 1000000 points. Test and training data is same for all our experiments. For Baseline and Lisa models, final prediction is given by linear search through a range of values(identified as a Cell for Baseline and Shard for LISA model) and mean square error(MSE) is zero as test points are already learned during training. This is where Learned Index models differ from traditional machine learning models where model performance is evaluated on unseen data.

Hyper-parameter search for the baseline implementation

Baseline model has one hyper parameter: No_of_Cells specifying the number of equal length intervals into which mapped values are divided. As discussed in section, the query search consists of two parts, first is binary search to locate the cell into which the query key is located, followed by sequentially comparison of the query key value with keys in the found cell until a match is found. The time complexity of first search is $log_2 N_1$, where N_1 is the number of cells. The time complexity of second search is $\lceil N_2/2 \rceil$, where N_2 is the number of keys per cell. As shown in table, build time increases and query time decreases with increase in value of this hyper-parameter for all training data sizes.

Training/Test Data Size	Model	No. of cells	Build Time(ms)	Avg Query Time(ms)	Memory Size(KB)
10,000	Lisa Baseline	10	11.171	4.34261	313.77
10,000	Lisa Baseline	100	11.252	0.71891	315.85
10,000	Lisa Baseline	1000	13.542	0.32806	336.97

Table 3.3.: Experimental results for lisa baseline model: Training Data Size : 10,000 Points

Training/Test Data Size	Model	No. of cells	Build Time(ms)	Avg Query Time(ms)	Memory Size(KB)
100,000	Lisa Baseline	10	109.287	46.7233	3126.2
100,000	Lisa Baseline	100	111.596	4.8086	3128.3
100,000	Lisa Baseline	1000	111.978	0.7271	3149.4
100,000	Lisa Baseline	10000	128.496	0.3301	3168.7

Table 3.4.: Experimental results for lisa baseline model: Training Data Size : 100,000 Points

Training/Test Data Size	Model	No. of cells	Build Time(ms)	Avg Query Time(ms)	Memory Size(KB)
1,000,000	Lisa Baseline	10	1094.99	347.561	31251.3
1,000,000	Lisa Baseline	100	1099.68	40.145	31253.4
1,000,000	Lisa Baseline	1000	1104.65	4.473	31274.5
1,000,000	Lisa Baseline	10000	1143.73	0.669	31485.4
1,000,000	Lisa Baseline	100000	1273.56	0.294	31638.5

Table 3.5.: Experimental results for lisa baseline model: Training Data Size : 1,000,000 Points

Hyper-parameter search for the Lisa implementation

For Lisa model, we have 2 hyper parameters:

1. GridCellSize : Number of grid cells into which the key space is divided. In our implementation, we use a square grid cell, and total number of cells is given by $GridCellSize \times GridCellSize$.

2. NumberOfShardsPerInterval : Number of shards to learn per mapped interval.

Experiments results are consistent across all 3 training sizes and have following interpretation.

1. In general, average query time decreases and memory size increases with increasing values of GridCellSize and NumberOfShardsPerInterval.

2. For a particular value of GridCellSize, average query time decreases and memory size increases with increase in value of parameter NumberOfShardsPerInterval.

3. After shard prediction, we sequentially compare the query point key values with keys in the Shard. For query points at the Shard boundaries, if the query point is not found in the predicted shard, we continue our search in adjacent left and right shards. During test experiments we found that if Shard size is less than 30 keys then Shard prediction error can be more than 1. To avoid Shard Prediction error of more than 1 Shard, we limit minimum number of keys per Shard to be 30 keys. This is the reason that in table, we restrict the value of parameter NumberOfShardsPerInterval to 25 for GridCellSize of 25 and 30.

Range Query Experiments

Table shows evaluation results for LISA and KDTree models for range sizes of 10, 100, 1000, and 10000 for different training sizes. For a given range query size, we perform 20 trials and take the average. For each trial, we sample a random point from the test set and find the range from sampled point to the range query size.

Training/Test Data Size	Model	GridCellSize	No of Shards Per Interval	Build Time(s)	Avg Query Time(ms)	Memory Size(KB)
10,000	Lisa	4*4=16	5	4.335	1.13135	324.72
10,000	Lisa	4*4=16	10	3.370	0.96036	329.07
10,000	Lisa	4*4=16	20	1.127	0.86184	323.47

Table 3.6.: Point Query experimental results for LISA model, Training Data Size : 10,000 points

Training/Test Data Size	Model	GridCellSize	No of Shards Per Interval	Build Time(s)	Avg Query Time(ms)	Memory Size(KB)
100,000	Lisa	4*4=16	5	45.846	5.93345	3137.2
100,000	Lisa	4*4=16	10	42.398	3.29308	3141.6
100,000	Lisa	4*4=16	20	59.036	1.52851	3150.3
100,000	Lisa	4*4=16	50	122.64	1.51173	3176.6
100,000	Lisa	4*4=16	100	30.211	1.44518	3220.3
100,000	Lisa	6*6=36	5	24.428	3.19491	3149.4
100,000	Lisa	6*6=36	20	33.637	1.59742	3178.9
100,000	Lisa	6*6=36	50	66.375	1.55903	3238.1
100,000	Lisa	8*8=64	5	22.645	2.53317	3166.2
100,000	Lisa	8*8=64	20	35.638	1.52851	3218.7
100,000	Lisa	8*8=64	50	45.014	1.43397	3323.6

Table 3.7.: Point Query experimental results for LISA model, Training Data Size : 100,000 points

Training/Test Data Size	Model	GridCellSize	No of Shards Per Interval	Build Time(s)	Avg Query Time(ms)	Memory Size(KB)
1,000,000	Lisa	10*10=100	5	122.64	1.51173	3176.6
1,000,000	Lisa	10*10=100	10	30.211	1.44518	3220.3
1,000,000	Lisa	10*10=100	20	24.428	3.19491	3149.4
1,000,000	Lisa	10*10=100	50	33.637	1.52851	3178.9
1,000,000	Lisa	10*10=100	100	66.375	1.43397	3238.1
1,000,000	Lisa	20*20=400	25	22.645	2.53317	3166.2
1,000,000	Lisa	20*20=400	50	35.638	1.59742	3218.7
1,000,000	Lisa	25*25=625	25	45.014	1.55903	3323.6
1,000,000	Lisa	30*30=900	25	45.014	1.55903	3323.6

Table 3.8.: Point Query experimental results for LISA model, Training Data Size : 1,000,000 points

KNN Query Experiments

Table shows evaluation results for LISA and KDTree models for KNN Queries for various value of K and training sizes. For a given K value, we perform 20 trials and take the average of query time. For each trial, we sample a random point from the test set and find K neighbours around that point

4. Insights and Findings

4.1. General Discussions

Limitations

Though the learned index model, especially the recursive model has a potential to greatly reduce the memory usage and cost less time in making the query. It is still limited in several perspective.

- **Read-only database**. Current recursive model index assumes that the data is a static, read-only array. Only when this assumption is hold, we can regard the database index as the CDF. However, in reality, we usually need to insert and delete the data in the array and violates this assumption.

Requirements

For a learned index.

4.2. One Dimensional Learned Index

4.2.1. Baseline Learned Index

Activation Functions

- If we use identity activation function, i.e.$z^{(i)}(x) = x$, then no matter how many layers are there, the fully connected neural network falls back to a linear regression.

  Proof: The output of the first layer, with identity activation function, will be $z^{(1)}(w^{(1)}x + b^{(1)}) = w^{(1)}x + b^{(1)}$. Then the output will be the input of the next layer, and hence the output of the second layer will be $z^{(2)}(w^{(2)}(w^{(1)}x + b^{(1)}) + b^{(2)}) = w^{(2)}w^{(1)}x + w^{(2)}b^{(1)} + b^{(2)}$. Similar induction can be obtained for multiple layers. Hence if we use identity activation, the trained neural network will fall back to a linear regression. The visualization below shows our lemma is correct.

- With ReLU (Rectified Linear Unit) as activation function i.e. $z^{(i)}(x) = \max(0, x)$, then the fully connected neural network falls back to a piecewise linear function.

  Proof: The output with ReLU activation function, will be $z^{(1)}(w^{(1)}x+b^{(1)}) = \max(w^{(1)}x + b^{(1)}, 0)$. Then the output will be the input of the next layer, and hence the output of the second layer will be $z^{(2)}(w^{(2)}(w^{(1)}x+b^{(1)})+b^{(2)}) = \max(w^{(2)}w^{(1)}x+w^{(2)}b^{(1)}+b^{(2)}, 0)$.

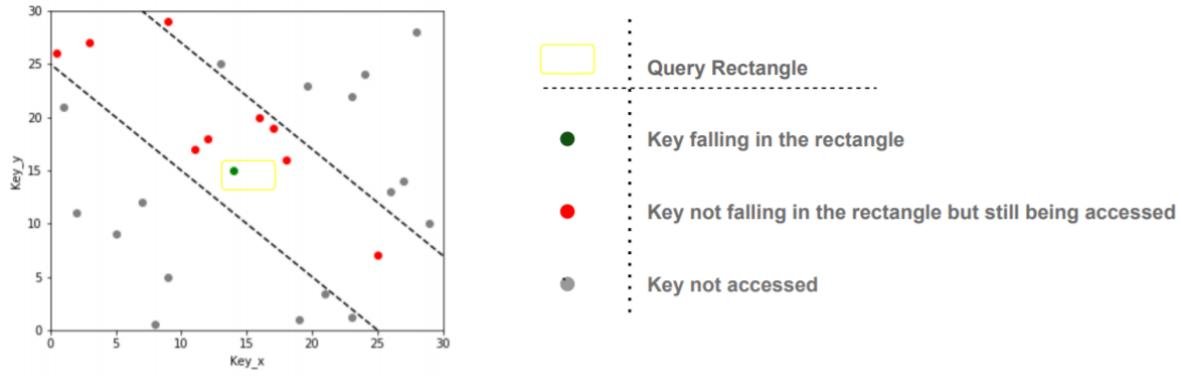


Figure 4.1.: Baseline Method Limitation

Similar induction can be obtained for multiple layers. Hence if we use identity activation, the trained neural network will fall back to a piecewise linear function. The visualization below shows our lemma is correct.

4.3. Two Dimensional Learned Index

Limitation

Prediction cost in baseline method consists of following two parts.

1. Search cost for the cell which contains the key. This cost will be equal to $log_2 N_1$, where N_1 is the number of cells into which mapped values are divided.

2. Cost associated with sequentially comparing the query point key value against keys inside the cell found in previous search. On average this cost will be equal to $N_2 \div 2$, where N_2 is the number of keys in a cell.

   If cell size is large, number of cells will be smaller, number of keys per cell will be higher, resulting in higher cost of sequential scan with in the cell.

Consider the example in figure 4.1. Dataset is divided into 3 sections based on the mapped values. Any point or range query in the second triangle(page) will result into a sequential scan through all 9 keys in the cells.

Lisa Baseline model search optimization

In case of high dimensional key values, key with in a page can not be searched with mapped value, as a large number of keys can have the same mapped value. However for the 2 dimensional scenario, we can get considerable savings in search cost by replacing sequential scan based on keys values to binary search based on mapped value. Once mapped value is found using binary search, we do a look up in its neighbourhood based on 2 dimensional key value. As shown in table **??**, we get significant savings in the query time with this approach.

Training/Test Data Size	Model	No. of cells	Build Time(ms)	Avg Query Time(ms)	Memory Size(KB)
10,000	Lisa Baseline	10	11.1208	0.284191	313.77
10,000	Lisa Baseline	100	12.0108	0.277918	315.85
10,000	Lisa Baseline	1000	12.7589	0.276572	336.97

Table 4.1.: Experimental results for baseline model with search optimization, Training Data Size : 10,000 points

Training/Test Data Size	Model	No. of cells	Build Time(ms)	Avg Query Time(ms)	Memory Size(KB)
100,000	Lisa Baseline	10	112.973	0.285525	313.77
100,000	Lisa Baseline	100	114.318	0.282053	315.85
100,000	Lisa Baseline	1000	116.699	0.280637	336.97

Table 4.2.: Experimental results for baseline model with search optimization, Training Data Size : 100,000 points

Training/Test Data Size	Model	No. of cells	Build Time(ms)	Avg Query Time(ms)	Memory Size(KB)
1,000,000	Lisa Baseline	10	1116.51	0.240508	313.77
1,000,000	Lisa Baseline	100	1118.85	0.235858	315.85
1,000,000	Lisa Baseline	1000	1134.88	0.234435	336.97

Table 4.3.: Experimental results for baseline model with search optimization, Training Data Size : 1,000,000 points

5. Convolution and CNN for Learned Indexes

6. Conclusion

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Appendices

A. Appendix

# id	Distributions	root model	second model	third models	Build Time (s)	Query Time (ms)	Evaluation Error (MSE)	Memory Size (KB)
1	log_normal	fcn	200 fcn	2000 fcn	418.9493798	0.970932583	653.8536667	7487.059896
2		fcn	200 fcn	4000 fcn	1141.521194	0.9675528	**1.134166667**	24440.75523
3		fcn	200 fcn	6000 fcn	688.8004486	1.07512705	196.9116667	13034.22656
4		fcn	400 fcn	2000 fcn	483.1734781	1.158343717	113246.196	9208.992183
5		fcn	400 fcn	4000 fcn	636.8463397	1.339095933	113652.3212	12695.55731
6		fcn	400 fcn	6000 fcn	742.0712694	1.243333667	51.00183333	15434.78905
7		fcn	600 fcn	2000 fcn	504.959355	1.06512235	113246.2647	9745.335942
8		fcn	600 fcn	4000 fcn	879.6010201	0.973031833	18.99766667	20434.90626
9		fcn	600 fcn	6000 fcn	373.6126809	1.11725315	142041.6877	8118.023442
10		lr	200 lr	2000 lr	262.5089284	1.280502367	8246.633985	4348.463542
11		lr	200 lr	4000 lr	869.7494701	1.304096217	7326.238372	18769.81252
12		lr	200 lr	6000 lr	655.0431077	1.318176683	6276.09111	13297.72135
13		lr	400 lr	2000 lr	275.3925674	1.31789575	120427.9247	5143.059892
14		lr	400 lr	4000 lr	601.7362665	1.453903583	6783.428749	12864.80731
15		lr	400 lr	6000 lr	388.5866734	1.623972083	5998.720313	8041.416654
16		lr	600 lr	2000 lr	267.8966881	1.861582733	121932.5051	4986.927088
17		lr	600 lr	4000 lr	558.531068	1.52717965	8434.091306	13843.60678
18		lr	600 lr	6000 lr	337.0881814	1.28034995	35342.6365	8366.570317
19		lr	200 lr	4000 fcn	34.86059083	1.63086885	14478.05283	**220.4973958**
20		lr	200 fcn	4000 fcn	410.2378013	1.653916983	13656.1507	9318.697933
21		fcn	200 fcn	4000 lr	38.131223	1.667702583	12191.8397	602.2005208
22		fcn	200 lr	4000 lr	238.9569197	1.663567483	13403.64758	5229.914058
23		lr	200 fcn	4000 lr	290.6430138	1.657428583	12567.93278	6588.58335
24		fcn	200 lr	4000 fcn	352.6849412	1.909310833	11572.93555	8292.059883

Table 6.1.

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