Institut für Informatik, Universität Zürich

MSc Project Report

Implementing Learned Indexes on 1 and 2 Dimensional Data

Neeraj Kumar, Nivedita Nivedita, Xiaozhe Yao

Matrikelnummer: 19-759-570

Email: xiaozhe.yao@uzh.ch

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supervised by
Prof. Dr. Michael H. Böhlen and
Mr. Qing Chen

University of Zurich[UZH]

Department of Informatics

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B-tree and KD-tree are the two of the indexes used in 1-dimensional and 2-dimensional data. In this master project we implement them from scratch and analyse their complexity. Afterwards we introduce the learned indexes that replace these tree structures with a machine learning approach.

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 hand-engineered data structures and algorithms, such as B-Tree, KD-Tree, Hash Table, etc. These indexes have played an important role in databases and have been widely used in modern data management systems (DBMS). Despite their success, they do not consider the distribution of the database entries, which might be helpful in designing faster indexes.

For example, if the dataset contains integers from 1 to 1 million, the key can be used directly as an offset. With the key used as an offset, the values with the key can be retrieved in $\mathcal{O}(1)$ time complexity. Compared with B-Tree, which always takes $\mathcal{O}(\log n)$ time complexity for the same query. At the same time, by using the key as an offset directly, we do not need any extra overhead regarding memory space, where the B-Tree needs extra $\mathcal{O}(n)$ space complexity to save the tree.

From the above example, we found there are two promising advantages of learned indexes over hand-engineered indexes:

1. Learned indexes may be faster when performing queries, especially when the number of entries in the database are extremely huge.

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

We will explore and analyse these two advantages qualitatively in the *chapter 5*.

Nowadays, to leverage these two advantages, 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. This approach has been shown to be powerful and competitive compared with hand-engineered indexes, such as B-Tree.

In this report, we explore the development of database indexes, from hand-engineered indexes to 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. **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	
X	
Hyper-Parameters	
V	something
Functions	
$\mathcal{LR}$	Linear Regression function

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.

1.3 Motivation

In traditional database indexes, the complexity for locating an item is usually bounded by some function related to the total number of elements. For example, with a B-Tree, an item can be found within $\mathcal{O}(\log n)$ time complexity. In the meantime, saving a B-Tree as index takes n space complexity. With the rapid growing of the volume of data, n becomes much larger than ever before. Hence, the big data era is calling for a database index that have constant complexity in both time and space.

To achieve such a goal, the distribution of the data is important. For example, assume that the data is fixed-length records over a set of continuous integers from 1 to 100 million, the conventional B-Tree index can be replaced by the keys themselves, making the query time complexity an $\mathcal{O}(1)$ rather than $\mathcal{O}(\log n)$. Similarly, the space complexity would be reduced

from $\mathcal{O}(n)$ to $\mathcal{O}(1)$. This example shows that with the knowledge of the distribution of the data, it is possible to locate the item in database in constant time.

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**.

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.

Even though there might be potential advantages, the learned index model has several assumptions, as listed below.

1. All data records are stored in memory.
2. All data records are sorted by X.
3. All data records are stored statically in database, hence we do not take insertion and deletion into consideration.

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. For example, the PostgreSQL uses B-Tree as its index. B-Trees can be considered as a natural generalisation of binary search tree. In binary search tree, there is only one key and two children possible in it's internal node. However, an internal node of B-Tree 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 an multi-way decision based on comparisons with the keys stored at the node x. The image below illustrates a simple B-Tree.

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

Motivation

In computers, the memories are organised in an hierarchical way. For example, a classical computer system consists three layers of memory: the CPU cache, main memory and the hard disk. In such a system, the CPU cache is the fastest but the most expensive while and hard disk is the cheapest but also the slowest. When querying for an item, the CPU will first try to fetch it from the CPU cache. If not there the CPU will then try to fetch it from the main memory, and then the hard disk.

At the same time, the traditional hard disk drive (HDD) is made by a moving mechanical parts.

In summary, there are two properties in classical computer systems that we need to take into account:

1. The memory is not flat, meaning that memory references are not equally expensive.
2.

Definition and Terms

Before we formally define B-Trees, we assume the following terms:

- **Keys**: The key in database is a special attribute that could identify a row in the database. In our work, each key corresponds to a **value** and forms a key-value pair.

- **Internal Node**: An internal node is any node of the tree that has child nodes.
- **Leaf Node**: A leaf node is any node that does not have child nodes.

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 nondecreasing 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.

Insertion of B-Tree

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

2.1.2 Baseline Learned Index

Motivation

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 n entries are allocated in the

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.

Definitions

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 1: Training of Recursive Model Index

```
input: num_of_stages; num_of_models; types_of_models; x; y
trainset=[[(x,y)]]
stage← 0
while stage <num_of_stages do
    while model <num_of_models[stage] do
        model.train(trainset[stage][model])
        models[stage].append(model)
    end
    if not last stage then
        for i ← 0 to len(x) do
            model=models[output from previous stage]
            output=model.predict(x[i])
            next=output * num_of_models[stage+1]/max_y
            trainset[stage+1][next].add((x[i],y[i]))
        end
end
```

Prediction

Algorithm 2: 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
```

2.2 Two Dimensional Data

2.2.1 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 use machine learning models through several steps and generate a learned index for spatial data to reduce the storage consumption and IO cost compared to existing indexes such as R-Tree.

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 cumulative distribution function (CDF) over the key search space. However, 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.

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 partially monotonic function according to the borders of cells to map the data from $\mathbb{R}^d$ into $\mathbb{R}$.

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 equal number of cells. If a point (x,y)'s mapped value is larger than those of the keys stored in the first i cells, i.e. $M(x, y) > \sup \bigcup_{j=0}^{i-1} M(C_j)$, we store (x,y) in cell i. Subsequently, for a query rectangle qr = $[l_0, u_0) \times [l_1, u_1)$, we only need to predict i_1 and i_2, the indices of (l_0, l_1) and (u_0, u_1), respectively, scan the keys in i_2 - i_1 + 1 cells, and those keys that fall in the query rectangle qr .

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 M is a partially monotonic 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 $x_1 \leq y_1$

Training

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

1. The training dataset, notated as (X, Y) with entries notated as (x, y). X represents the two dimensional key values, and Y represents the corresponding data item value.

2. This number represents the number of cells(pages) into which the key space mapped values will be divided. It is an integer variable. Pages or cells will be used interchangeably in the next section to represents the subset of keys in a particular cell.

During training, sort all keys according to their mapped values, divide the keys into equal sized cells(pages), and store the mapped values of first and last key for each page into an array. For prediction, find the page corresponding to mapped value of query point, and scan this page sequentially.

Algorithm 3: Training Algorithm for Lisa Baseline Method

```
input: num_of_cells;x;y
trainset=[(x,y); x ∈ R^2; y ∈ R]
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
```

Prediction

Algorithm 4: Prediction Algorithm for Lisa Baseline Model

```
input: x_test:  Key Value to be searched
x_test.mapped_value = x_test[0]+x_test[1]
for i ← 0 to len(denseArray) do
 | if ((x_test.mapped_value ≥ denseArray[i].lower)&(x_test.mapped_value ≤
 |   denseArray[i].upper)) then
 |  | Key is in Page i
 |  | break
end
Sequentially search for x_test in page j
```

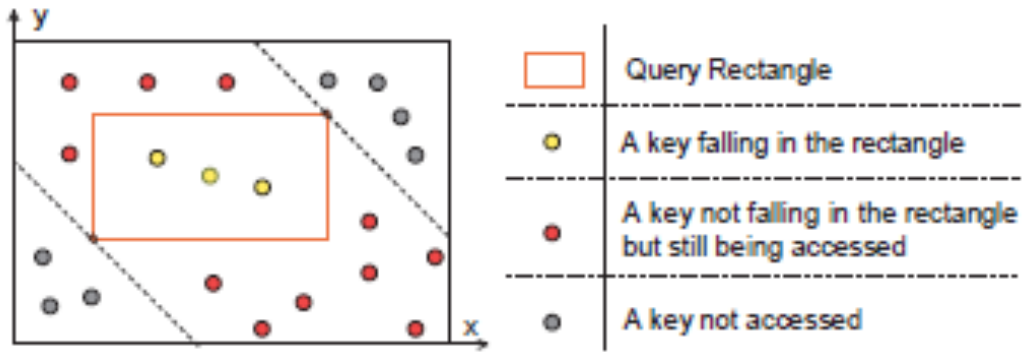

Figure 2.1: Baseline Method Limitation

Limitation

Prediction cost in baseline method consists of following two parts.

1. Search cost for the page which contains the key. If page size is small, this cost will be high as keys will be divided into larger number of pages
2. Scan cost of all the keys in a particular page to match the query point. If page size is large, number of pages will be smaller, number of keys per page will be higher, resulting in higher cost of sequential scan with in the page.

Consider the example in figure 2.1. 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 14 keys in the triangle.

Lisa Overview

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

This section presents the additional definition for Lisa model.

1. **Shard**.shard S is the preimage of an interval $[a, b) \subseteq [0, +1)$ under the mapping function M, i.e., $S = M^{-1}([a.b))$.
2. **Local Model**. local model L_i is a model that processes operations within a shard Si . It keeps dynamic structures such as the addresses of pages contained by S_i . Will add further details as we start working on corresponding modules.

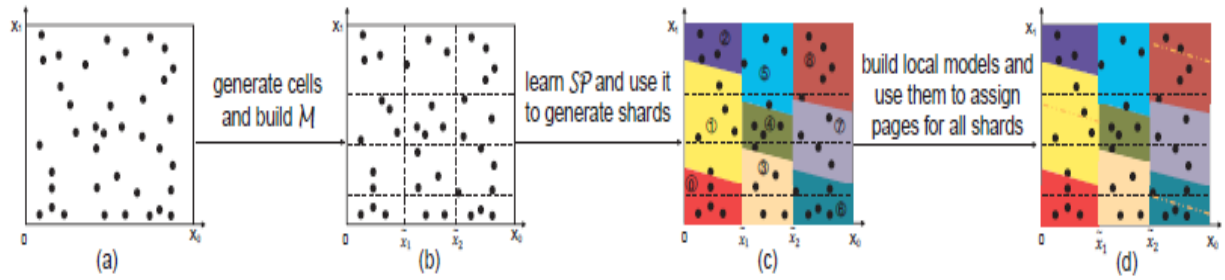

Figure 2.2: Lisa Framework

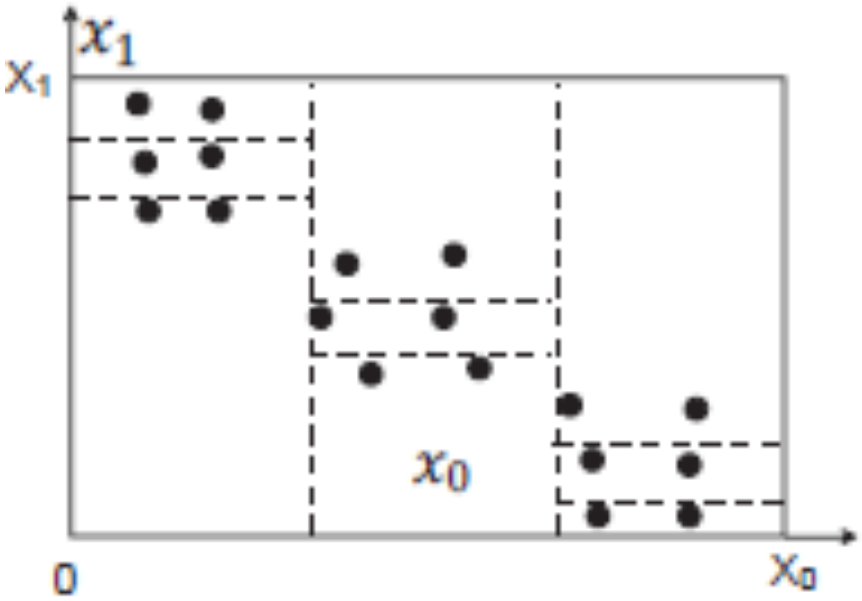

Figure 2.3: Cell Partition Strategy

Lisa Design

Grid Cells Generation 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 and numbering the cells also along these axes. 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, i.e. mapped value of all keys in cell i will be less than mapped values of keys in cell j, if i <j. Consider the example shown in the figure 2.3 total number of keys are 18, and we decided to partition the key space into 9 cells, resulting in 2 keys per cell. To partition the key space, we first sort the keys values according to 1^{st} dimension, divide the keys into 3 cells each containing 6 keys. Then for each cell, we sort the keys again according to 2^{nd} dimension, and divide the keys in each cell into 3 new cells.

Algorithm 5: 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**
        Store the 2nd dimensional coordinates of first and last key for each cell.
    end
end

3 Evaluation

4 Insights and Findings

5 Conclusion

Bibliography

[KBC+18] Tim Kraska, Alex Beutel, Ed H Chi, Jeffrey Dean, and Neoklis Polyzotis. The case for learned index structures. In *Proceedings of the 2018 International Conference on Management of Data*, pages 489–504, 2018.