Leveraging Soft Functional Dependencies for Indexing Multi-dimensional Data

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ABSTRACT
Recent work proposed learned index structures, which learn the distribution of the underlying dataset to improve their performance. The initial work on learned indexes has repeatedly shown that by learning the cumulative distribution function of the data, index structures such as the B-Tree can improve their performance by an order of magnitude while having a smaller memory footprint.

We propose a new learned index for multidimensional data that instead of learning the distribution of keys, learns from correlations between columns of the dataset. Our approach is driven by the observation that in many datasets, the values of two (or multiple) columns are correlated. Databases traditionally already exploit correlation between the columns and more specifically soft functional dependencies (FDs) in query optimisers to predict the selectivity of queries and thus to find better query plans. We want to take the learned functional dependencies a step further and use them to create more efficient indexes. In this paper, we consequently use learned functional dependencies to reduce the dimensionality of the datasets. With this attempt we work around the curse of dimensionality — which in the context of spatial data stipulates that with every additional dimension, the performance of an index deteriorates further — to accelerate query execution.

More precisely, we learn how to infer one (or multiple) attributes from the remaining attributes and hence no longer need to index it. This reduces the dimensionality and hence makes the index more efficient. We show experimentally that by predicting correlated attributes in the data, rather than indexing them, we can improve the query execution time and reduce the memory overhead of the index at the same time. In our experiments, we are able to reduce the execution time by 25% while shrinking the memory footprint of the index by four orders of magnitude.

PVldb Reference Format:
Behzad Ghaffari, Ali Hadian, Thomas Heinis. Leveraging Soft Functional Dependencies for Indexing Multi-dimensional Data. PVLDB, 09(xxx): xxxx-yyyy, 2020.

DOI: https://doi.org/10.14778/xxxxxxx.xxxxxxx

1. INTRODUCTION
Multidimensional data plays a crucial role in many different applications, be it in spatial data analytics or data analytics in general. Indexing multidimensional data, however, is challenging as the curse of dimensionality hits: with every additional dimension indexed, performance of the index degrades. Therefore, multidimensional data calls for novel approaches in modelling and indexing large spatial data. A promising approach to tackle the curse of dimensionality is using machine learning techniques and exploit patterns in data distribution for more efficient indexing.

For example, learned indexes automatically model and use the distribution of the underlying data to find locate the data records. Recent work proposed learned index structures, which learn from attributes of the full or a subset of the dataset to improve performance of the index structure. Our approach is motivated by the observation that in real datasets, correlation between two or more attributes of the data is a common occurrence. We argue that by taking learned indexes to the multidimensional case, in addition to learning from CDF of the data, we also have the opportunity to learn from relationships between attributes of the data such as correlation between id and timestamp, a common case in real-world datasets; or between flight distance and flight time in an airline dataset, which is derived from physical phenomenons.

The idea of learning from attributes, i.e., learning the relationships between columns of data, has already been used to improve estimate the selectivity of a given query and thus to improve query optimisers. We take this idea a step further to indexing multidimensional data.

More precisely, we develop models that explain correlations in the attributes of the data and we show that we consequently do not need to index every dimension, thereby effectively reducing the dimensionality of the dataset. We only need to store one dimension for each group of correlated attributes. In case a query with a "missing" dimension is executed, we use our model to check which range of values in the indexed dimensions correlate with the query and scan the indexed attribute instead. As we show experimentally, the suggested approach significantly shrinks the
memory footprint of the index, by 1.5 to 5 orders of magnitude depending on the number of the FDs and their degree of correlation, while improving the overall lookup time of the indexes at the same time.

The remainder of the paper is structured as follows. We first discuss related work in section 2 and then provide an overview of our approach in section 3. Further we discuss how to detect, model, and index the correlated attributes in section 4. In section 7 we discuss our experimental setup and, more importantly, the experimental results. We finally conclude the paper in 8 where we also discuss future work.

2. RELATED WORK

The ideas in this paper build upon various research directions including learned data structures, partial indexes, model estimation, interpolation search and grid-based data structures.

We refer to the paper by Kraska et al. 11 which first introduced and explored the idea of the learned index. In a learned index, the CDF of the key distribution is learned by fitting a model; then the learned model is used as a replacement to the conventional index structures (such as B+-tree) for finding the physical location of the query results. Index learning frameworks such as the RMI model 11 13 are capable of learning arbitrary models 13, though further research and a recent experimental benchmark 8 has shown that simple models such as linear splines are very effective for most real-world datasets 8 4 6 12. Our work is partially inspired by hybrid learned indexes that combine machine learning with traditional indexes structures 5 4 6 12. Hybrid learned indexes have recently been well explored in the one-dimensional case. For example, RadixSpline 8 uses radix-trees as the top-level model while FITing-tree 4 and IFB-tree 5 use B+-tree as the top-level index structure. Then they use a series of piecewise linear functions in the leaf level. Such a model- assisted index design limits the worst case inefficiencies of the model. Furthermore, adaptability and updatability of learned indexes have been explored in a similar area 3 5. Finally, in the multivariate area, learning from a sample workload has also shown interesting results 14.

Despite focusing on different problems, our work is particularly inspired by FITing-tree, which uses a fraction of keys rather than the full key set to build the index. It then makes up for the reduced accuracy of the index by predicting any key’s position that is not indexed. This prediction is achieved using piecewise linear functions that are responsible for interpolation for different sections of data. The FITing-Trees, maintains a minimum and maximum error term for its models that are updated on inserts.

3. APPROACH OVERVIEW

As outlined previously, we are interested in exploiting correlations in a multidimensional dataset to build a more efficient index. Therefore, the structure of the key steps of our approach, illustrated in Figure 1 are as follows:

- **Learning the correlations.** We first implement a method that automatically detects whether a functional dependency exists between two or more columns, and evaluates whether the dependency can be effectively modelled in the presence of noise.

- **Primary index.** We then apply a pre-processing step to our data. We use the learned correlations to separate data that agree with the learned dependency from the remaining points that are regarded as outliers. We will create a primary index on those data points that have up to a certain deviation from the learned correlation (i.e. those that are within a certain tolerance margin around the fitted line). The primary index only indexes one column per each set of correlated columns. For the rest of the correlated columns, a model is learned to represent the correlation between indexed attributes and learned attributes will be used to execute queries. If a query targets a dependent column $C_d$ that is not indexed but is correlated with another indexed column $C_i$, then the learned correlation model automatically converts the query constraints targeting $C_d$ to an equivalent constraint on $C_i$.

- **Secondary index.** Data points that do not fall within the tolerance margin of the soft FD model are excluded from the primary index and are indexed with all dimensions in a secondary index, which is a typical multidimensional index structure like R-tree or Grid index.

- **Query translation.** As the data in the primary index is now highly correlated, we define a model to predict any correlated dimensions in the data i.e. we predict learned attributes using the set of indexed attributes. By doing so, we show that an index on the key, informative dimensions along with a learned model that
predicts remaining indexed dimensions can achieve up to 25% better execution performance while reducing the index size by an order of 10,000X.

4. DEPENDENCY DETECTION

Learned index structures — and indexes in general — typically work by predicting where a queried record might be located in storage space and scan near the prediction to find any matching results. Because of this, models used by an index structure must be able to achieve sufficient accuracy in predicting every point that is indexed, otherwise a lookup might take an unexpected amount of time to execute. In the context of this paper, it means that when looking for correlations, our goal is not to find a model that minimises the distance to every point in the dataset. Rather, we are interested in a model that is sufficiently close to a sizeable portion of data points. Put differently, we must pick any sufficiently large subset of all points in our dataset and find a model that best explains these points while ignoring the remaining points, i.e., the outliers. We also aim to keep the process of learning models as efficient as possible to avoid significant retraining delays in the case that our model loses its accuracy after a high number of inserts.

Motivated by minimising the training time and error in our model, the main contribution in our method for detecting correlation is that we only consider centres of dense areas in a sample drawn from the dataset. More precisely, we overlay a multidimensional grid on the key space (spanning minimum and maximum points along each dimension) and measure the weight of each cell (bucket) by counting the number of points that intersect with the cell. We then filter out any cells that do not reach a threshold in their weights and consider our training data to be the weighted centres of the remaining cells. This approach is similar to observing a heat map and deciding where a correlation can be seen. Figure 2 shows the heatmap of a pair of correlated columns, together with the buckets’ centres that reach the minimum threshold.

After the training set (bucket centres) is found, in order to learn correlations between multiple attributes, we recursively consider unique pairs of columns and attempt to use a Monte Carlo sampler to check whether a linear model fits the training points (Algorithm 1). If two columns are found to be correlated, we save the resulting pair along with their model parameters. In the final step we merge all groups that have a dimension in common and pick one column in each group to be the predictor responsible for estimating the remaining columns in its group (or context in alternative terminology). Later in section 5 we show how the predictor columns can be used to reduce the dimensionality of an index while allowing queries on all columns.

Parameters. The suggested method leaves a few parameters that can be tuned to boost performance. For example, we can use larger samples in combination with smaller buckets and a lower bucket acceptance threshold to increase our models’ accuracy. We will leave tuning these parameters as future work.

5. PREDICTING DEPENDENT ATTRIBUTES

Let us consider the simple case where we want to answer queries on two columns C1 and C2. We define a query by a rectangle characterised by its lowermost left-point \((q_{1\text{low}}, q_{2\text{low}})\) and uppermost rightmost point \((q_{1\text{high}}, q_{2\text{high}})\). Note that with this setting, we can express the case where, for example, only the first dimension is queried by defining \(q_{2\text{high}} = \infty\) and \(q_{2\text{low}} = -\infty\). Similarly we can express point queries by defining the lower and upper points to be equal. With this we only need to implement a search strategy for the full query, i.e., where \((q_{1\text{low}}, q_{2\text{low}})\) and \((q_{1\text{high}}, q_{2\text{high}})\) are defined and unequal, to cover all cases.

Suppose that the columns to be indexed (C1 and C2) are correlated, i.e., a soft functional dependency between C1 and C2 can be learned. In this case, an index range can be built on only one of the attributes, and any query constraint that target a non-indexed attribute can be mapped to equivalent query constraints on the indexed column using

![Figure 2: An error margin can be defined by considering the the correlation model of the data (left) and the density of the data points around the model (right).](image)

![Heatmap](image)
the prediction model and its error bounds. To do this without loss in accuracy, we need to define an oracle function \( \psi : C_1 \to C_2 \) that calculates the exact value of \( C_2 \) based on a given \( C_1 \) for each row in the dataset. Because in practice finding such an oracle function may prove impossible for real-world datasets, we must relax this concept and allow our model to instead predict the approximate value for \( C_2 \).

As in the case with other approaches in learned index structures \([11, 3, 10]\), using an approximation without any bounds is impractical since we want to avoid scanning the entire dataset when only the learned dimension is queried. We must therefore define tight error bounds for the approximation. To do so, we argue that once a significant majority of the values of the learned attribute \( C_2 \) are learned, i.e., the corresponding data points are located along a line, we can define a margin (minimum and maximum error bounds) thus characterising a distribution close to a straight line. We then only keep the points that fall between these bounds and leave outliers aside to be inserted into a secondary partial index. Put differently, for any point \((p_1, p_2) \in (C_1, C_2)\) in our primary index we have:

\[
p_2 \in [\psi(p_1) - \epsilon_{\text{min}}, \psi(p_1) + \epsilon_{\text{max}}]
\]  

(1)

Where \( \epsilon_{\text{min}}, \epsilon_{\text{max}} \) are the error bounds, or as illustrated graphically, the distances at which the data separators have been drawn on both directions. Figure 4 shows the process of defining the two parallel lines characterising the minimum and maximum error bounds and the role of our primary and secondary index. Reiterating that these maximum error terms are small enough, when asked to create a multidimensional index on \( C_1 \) and \( C_2 \), we only need to sort our rows based on the \( C_2 \) column and argue that the other dimension was not informative enough. To answer a range query targeting both dimensions, we will need to (1) calculate which range of positions in the indexed dimension correspond to the queried range for the missing dimension and (2) scan the intersection of the the queried ranges projected on the indexed dimension.

Put differently, because the data in the primary index is now perfectly linear, we will be able to immediately tighten the minimum and maximum bounds of our query for each of correlated dimensions making the overall scanned range smaller. As illustrated in Figure 3 with a 2D example, we need to find the intersection points of the query rectangle with our minimum and maximum thresholds. We can then scan the points in the indexed attribute \((C_2)\) between the more selective bounds (drawn as solid vertical lines in Figure 3):

\[
[\max(\psi(q_{1,\text{low}}), q_{2,\text{low}} - \epsilon_{\text{min}}), \min(\psi(q_{1,\text{high}}), q_{2,\text{high}} + \epsilon_{\text{max}})]
\]  

(2)

### 6. INDEX LAYOUT

In order to evaluate differences in performance when predicting dimensions, we need to build an index on indexed dimensions. We implement our index on top of Grid Files \([15]\) with a few modifications. In particular we choose boundaries for each cell based on quantiles along each dimension and use the same number of grid lines for each attribute. Addresses for all cells are sorted using the original ordering of columns in the dataset. Furthermore, each cell stores points in a continuous block of virtual memory in a row store format. Finally, rows within each page are sorted based on a given function similar to the approach proposed in Flood \([14]\). Sorting the rows inside pages means that we can reduce the dimensionality of the grid by one. This is because instead of having grid lines for the particular sorted attribute we can use binary search to locate items (or a scan between two bounding binary searches in a range query).

Note that picking grid lines based on distribution of the dataset does not mean that we have regular cells. Although doing so does reduce the standard deviation in cell lengths for non uniform datasets, bucket lengths are still allowed to grow arbitrarily large. Figure 4 shows the variation in cell lengths in one of our experiments.

The combination of predicting attributes and having a sorted dimension means that for a dataset with \( n \) dimensions and \( m \) predicted attributes, we only need an index with \( n - m - 1 \) dimensions. Due to this reduced dimensionality we will show in section 7.2.3 that the resulting index makes much more efficient use of memory. Such an effect is also
illustrated in Figure 4.

7. EVALUATION

7.1 Experimental Setup

7.1.1 Implementation and Runtime Environment

We implement the online section of our index in C and compile it using Clang 10.0.0. All of the mentioned indexes in our experiments including the R-Tree and Grids run in a single thread and use single precision floating point values. For the offline data processing sections, we use Python and the pydec3 library [2] for model estimations. We run our measurements on a machine with Intel Core i5-8210Y CPU running at 3.6 GHz (L1: 128KB, L2: 512KB, L3: 4MB) and 8GB of RAM.

7.1.2 Datasets

We run our experiments on two real world datasets:

- **Open Street Map (OSM)**: we use 4 dimensions of the OSM data for the US Northeast region [1] which contains 105M records; The Id and Timestamp attributes in the OSM dataset are correlated and its Latitude and Longitude coordinates contain multiple dense areas. For this dataset we group (Id, Timestamp) for the case of learned index.

- **Airlines**: data from US Airlines flights from 2000 up to 2009, which has 8 attributes and 80M records. The airline dataset is more interesting for our experiments because it contains many correlated dimensions. Example grouping in this dataset in our experiments usually consists of (Distance, TimeElapsed, AirTime) and (ArrTime, DepTime, ScheduledArrTime). We can reduce the grid dimensionality to 2-4 in the case of the learned grid. Table 1 summarises the key aspects of the datasets.

We generate the queries by picking a random point from the data. Then, we look at knn nearby points and take the minimum and maximum values corresponding to each dimension. Our range queries are rectangles and target all columns in the index. Figure 5 shows the distribution of the result count in our query set.

7.1.3 Baselines

We refer to our implementation explained throughout this paper as the Learned grid. We compare our suggested method with R-Tree, arguably the most broadly used index for multidimensional data, and two grid structures as baselines: the uniform grid and column files.

**Uniform grid**: or equivalently the full grid, is a hash structure that breaks down each attribute into uniformly sized grid cells between their minimum and maximum values. The address for each cell is stored independently and no adjacent cells are "shared/merged" explicitly. In memory, addresses for all cells are sorted using the original ordering of columns in the dataset. Furthermore, each cell stores points in a continuous block of virtual memory in a row store format.

**Column files**: Essentially a non uniform grid, uses the CDF of the data to align/arrange its cell boundaries and sorts data within each cell based on one of the attributes in the data, thus reducing the dimensionality of the index by one. In a lookup on the sorted dimension, we use binary search in each cell to get the range that needs to be scanned. Column files is indeed similar to the approach [14] with the difference that it does not assume that the query workload is known and hence uses the data distribution to arrange and align the grid layout.

**Full scan**: Every item in the dataset is scanned and checked against each query.

7.2 Results

7.2.1 Tuning

In this experiment we measure and compare the execution time for all indexes. We use the configuration that performs best for each index. This configuration consists of chunk size for the full grid, chunk size and sort dimension for the column files and the learned grid, and the node capacity (non-leaf and leaf capacity) of the R-Tree. For example, we evaluated different node capacities between 2 to 32 for the for the R-Tree index and the best performance for each experiment (i.e. point queries and individually for each selectivity rate in range queries) was used. The best node size for R-Tree was between 8 and 12 for each test.

Note that because of memory constraints we limit any index from using unreasonable amount of memory overhead. More specifically, we limit any index that would require more memory overhead for its index directory than memory occupied by the underlying data itself. Memory usage of the indexes is shown later in Section 7.2.4.

We evaluate our results using range queries and point queries that are drawn randomly from each dataset. We define a point query as a range query where the lower bound and upper bound in the matching hyper rectangle are equal.

7.2.2 Point and range queries

As seen in Figure 6, the learned grid outperforms both the R-Tree and full grid. Note that the main drawback in the case of full grid is the higher index dimensionality and the

| Count       | Airline | OSM  |
|-------------|---------|------|
| Key Type    | float   | float|
| Dimensions  | 8       | 4    |
| Correlated Dimensions | (3, 3) | 2    |
| Indexed Dimensions (Learned) | 2-4 | 3    |
| Primary Index Ratio | 92% | 73%  |

Table 1: Dataset characteristics

Figure 5: Example distribution of query selectivity in Airline data

![Figure 5: Example distribution of query selectivity in Airline data](image-url)
This is because with a skewed dataset, most grid cells become empty or very small in size. In addition, in comparison to column files, the learned grid benefits from smaller number of memory lookups. The decreased total number of cells in a learned grid also translates to binary search on larger ranges in each cell, which makes the learned grid even more efficient.

7.2.3 Effect of selectivity in range queries

In addition to this, we run the same experiment with the range queries with selectivity sizes. In this experiment we use the airline data for the year 2008 only and plot the results in Figure 7 showing that the Learned Grid does not lose performance on larger/shorter queries. Note that, we can check whether the query intersects with the primary, the secondary, or both indexes; and run it against the appropriate indexes. For queries with larger selectivities, it is hence more likely for both indexes to be invoked which results in more invocation and larger overhead from the secondary index.

7.2.4 Memory Usage

Figure 8 plot the range query performance against memory overhead in the case of the learned grid, column files and the R-Tree. As seen, all grid indexes have a sweet spot. This is because as we increase the number of cells, although we are likely to scan fewer items, after a certain point the increased pointer lookups starts to hurt performance mainly because there is diminishing returns in reducing the actual items considered when increasing the grid size. In other words, it takes a lot of effort to improve the accuracy of an unlearned grid after a certain point for skewed datasets. This effect is illustrated in Figure 4.

8. CONCLUSIONS & FUTURE WORK

In this paper we address the degradation of performance/query execution time for every additionally indexed dimension (also referred to as the curse of dimensionality). Instead of indexing all dimensions, we learn soft functional dependencies, i.e., the correlation between different dimensions/attributes. By doing so, we no longer have to index the learned attributes and can thus reduce the number of dimensions indexed, thereby accelerating query execution and reducing memory overhead. In case the learned attribute is queried for, we use the model (as well as the secondary index) to find a starting point for scanning the data. As we show experimentally, our approach uses substantially less memory and also executes queries faster.

This work only studied the case where the correlation can essentially be learned using a line. Our idea could be extended to cases where data points are split between two separate parallel lines. In such a case, multiple models can be learned. Alternatively, we can learn a mixture of models such as where dense points and linear models lie and index them separately. We leave this as future work.
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