KDD 2021 Tutorial

High-Dimensional Similarity Query Processing for Data Science

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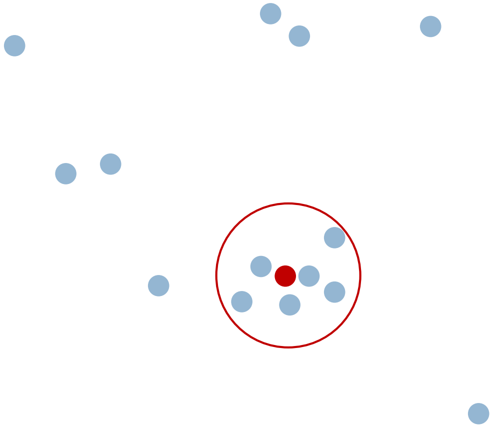
Outline

- Introduction
- Exact Query Processing
- Approximate Query Processing
- Selectivity Estimation
- Open Problems

Exact Query Processing

- Problem definition
  - Range-similarity query
    - Given:
      - a database *X* of high-dimensional vectors,
      - a query vector **q**,
      - a distance function *dist*(., .),
      - a threshold *t*.
    - <u>Return **ALL** the objects</u> **x** in *X* such that *dist*(**q**, **x**) ≤ *t*.
    - a.k.a. range-similarity query or t-selection problem
  - Given:
      - …
      - a number ***k***.
    - Return **ALL** the **k** objects R in X such that no other objects is closer to q than objects in R.
    - A.k.a. k nearest neighbor query



Motivation

- EXACT does not pose any uncertainty to the pipelines that apply similarity query processing as a component.
- It also simplifies empirical comparison as only speed and space consumptions are key evaluation criteria.
- Where is boundary of the exact and approximate query processing lies.

Challenge

- The curse of dimensionality
  - The computation of **exact NN** solution is very expensive.
  - Research effort has been attracted to **approximate NNS**.
    - Locality sensitive hashing (LSH)-based methods.
      - C2LSH, LSH-tree, SRS.
    - Product quantization (PQ)-based methods.
      - PQ, OPQ, LOPQ.
    - Neighborhood graph-based approaches.
      - KGraph, Small world Graph.

Opportunity

- Opportunity: the intrinsic dimensionality of real-life high dimensional data is usually much lower.
  - It is still feasible to develop efficient and practical exact NNS method.
  - Tree index-based method.
    - KD-tree, iDistance, Cover Tree.
  - Following the “filter and verify” paradigm.
    - PartEnum, HmSerach, MiH, GPH, Pigeonring.

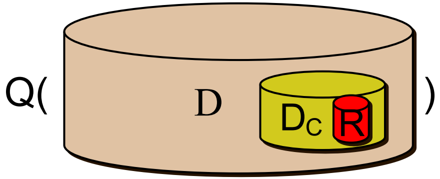
Outline

- Partitioning Methods. (Divide and conquer)
  - These methods partition the original space and bound the overall distance using the distance in each subspace.
- Dimensionality Reduction Methods
  - These methods project objects to another space to reduce dimensionality.
- Tree based methods (next part)
  - These methods partition the database in a hierarchical manner.

Partition based – Solve τ-selection Problem (Range Similarity Query)

Challenges:

- When D is large, straightforward searching is costly.
- D and f may be complex, and hard to be indexed directly.



General Solution: Divide and conquer

$$tS(D,Q,\tau) = Verify\left(tS\left(D_{(1)},Q_{(1)},\tau_1\right), tS\left(D_{(2)},Q_{(2)},\tau_2\right), \ldots\right)$$

Step 1: Decompose f into several parts, such that $f_1(x_1, q_1) + f_2(x_2, q_2) + \ldots + f_m(x_m, q_m) \le \tau$

Step 2: Perform candidate generation, such that CAND = $Q_1(D_1, q_1, f_1, \tau_1) \cup Q_2(D_2, q_2, f_2, \tau_2) \cup \ldots \cup Q_m(D_m, q_m, f_m, \tau_m)$.

Step 3: Verify x in CAND, such that $f(x, q) \le \tau$

Multi-Index Search (PartEnum VLDB2004, HmSearch SSDBM2012, MIH CVPR2012….)

- **Reduction** via pigeonhole principle

Number of partitions:

$m = 3$

$$HS(D,Q,\tau) = Verify(HS(\mathrm{D}_{(1)}, Q_{(1)}, \tau_1), HS(\mathrm{D}_{(2)}, Q_{(2)}, \tau_2), \ldots)$$

$$\tau_1 = \tau_2 = \tau_3 = \lfloor \frac{\tau}{m} \rfloor$$

$DB_{(1)}$ $\tau_1 = 1$

1	1	0
1	1	1
1	1	1
1	1	1
1	1	1
1	1	1

$Q_{(1)}$

$DB_{(2)}$ $\tau_2 = 1$

0	1	0
0	1	1
1	1	0
1	0	0
1	1	0
0	1	0

$Q_{(2)}$

$DB_{(3)}$ $\tau_3 = 1$

0	0	0	1
0	0	0	0
0	1	1	0
1	1	1	0
1	1	1	0
0	0	0	1

$Q_{(3)}$

Naïve Pigeonhole Principle (ICDE12, SSDBM13, CVPR 2012)

- **Tightness of divided-thresholds**

$$\tau_1 = \tau_2 = \tau_3 = \lfloor \frac{\tau}{m} \rfloor$$

	τ_1	τ_2	τ_3
$\tau = 5$	1	1	1
$\tau = 4$	1	1	1
$\tau = 3$	1	1	1

Same set of candidates

Naïve Pigeonhole Principle (CVPR 2012)

- **Vulnerable to *data skewness***
  - Data skewness is quite common
- Most solutions to data skewness
  - Do nothing, or
  - Shuffle the columns, and then sequential partitioning. Hopefully each partition is less likely to be extremely skewed [SSDBM13, CVPR12]

DB:	1	1	0	0	1	0	0	0	0	1
	1	1	1	0	1	1	0	0	0	0
	1	1	1	1	1	0	0	1	1	0
	1	1	1	1	0	0	1	1	1	0
	1	1	1	1	1	0	1	1	1	0
Q:	1	1	1	0	1	0	0	0	0	1

$\tau_1 = 1$ $\tau_2 = 1$ $\tau_3 = 1$

- All records in 1st partition are candidates ➔
- Verification for the entire DB, *irrespective of* other partitions

Achieve **Tight** Threshold Allocations General Pigeonhole Principle (GPH ICDE 2018)

- General Pigeonhole Principle
  - Allocate **different** thresholds to partitions
  - As long as the thresholds sum up to $\tau - m + 1$
  - Can be shown to be the tight
- $\tau_i \in \{-1, 0, 1, \ldots, \tau\}$
  - "-1" to allow discarding the partition
  - Correct and is the key to handle extreme skewness

$$\tau = 3$$

MIH thresholds:

$$\tau_1 = \left\lfloor \frac{\tau}{m} \right\rfloor = 1 \quad \tau_2 = \left\lfloor \frac{\tau}{m} \right\rfloor = 1 \quad \tau_3 = \left\lfloor \frac{\tau}{m} \right\rfloor = 1$$

GPH thresholds:

$\tau_1 = 0$ $\quad \tau_2 = 0$ $\quad \tau_3 = 1$

$\tau_1 = -1$ $\quad \tau_2 = 0$ $\quad \tau_3 = 2$

$\tau_1 = -1$ $\quad \tau_2 = 1$ $\quad \tau_3 = 1$

Adaptive Threshold Allocation (ICDE 2018)

- **Which threshold allocation is the best?**
  - Cost function:
    - Total number of candidates from the partitions
    - It upper bounds the query cost (up to some constant)
- Assumption:

  $CN(Q_i, u) \triangleq |HS(DB_{(i)}, Q_{(i)}, u)|$

  can be estimated $\forall i, u$

  - Use histogram, or
  - Use Machine Learning models

DB:

1	1	0	0	1	0	0	0	0	1
1	1	1	0	1	1	0	0	0	0
1	1	1	1	1	0	0	1	1	0
1	1	1	1	0	0	1	1	1	0
1	1	1	1	1	0	1	1	1	0

$<q_1, \tau_1>$ $<q_2, \tau_2>$ $<q_3, \tau_3>$

Q:

1	1	1	0	1	0	0	0	0	1

$\tau = 3$ $d = 10$

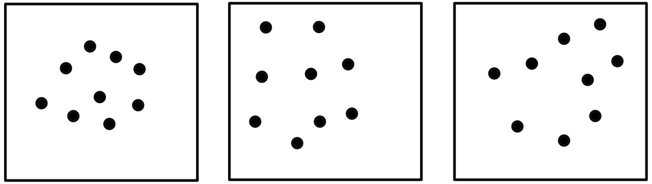
Minimize $CN(Q_{(1)}, u_1) + CN(Q_2, u_2) + CN(Q_{(3)}, u_3)$

Encourage Skewness (GPH ICDE 2018)

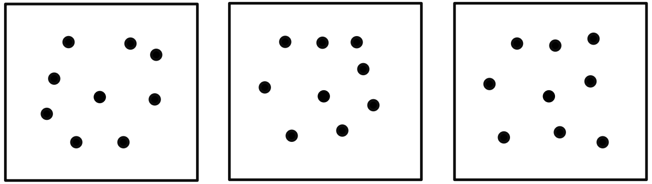
- **Let's make partitions more skewed !!**
  - Initial dimension partitioning
    - Greedy algorithm to minimize the total entropy of partitions
  - Refinement by local rearrangement
    - Move one dimension to another partition if it reduces the query cost

Dynamic Dimension Reduction

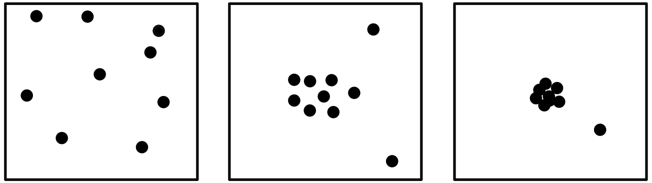
Origianl Data Partition



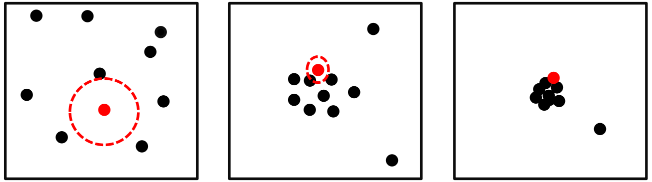
Random Shuffle Dimentions



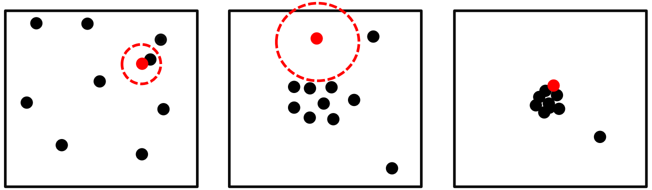
Skewnized Data Partition



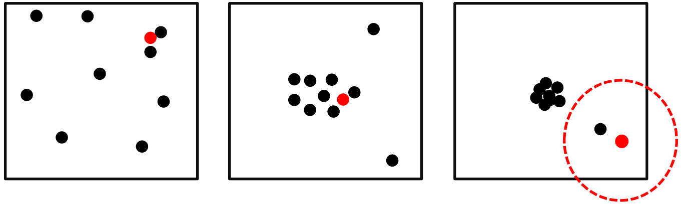
Query Q1, Allocate 1, 0 -1



Query Q2, Allocate 0, 1, -1

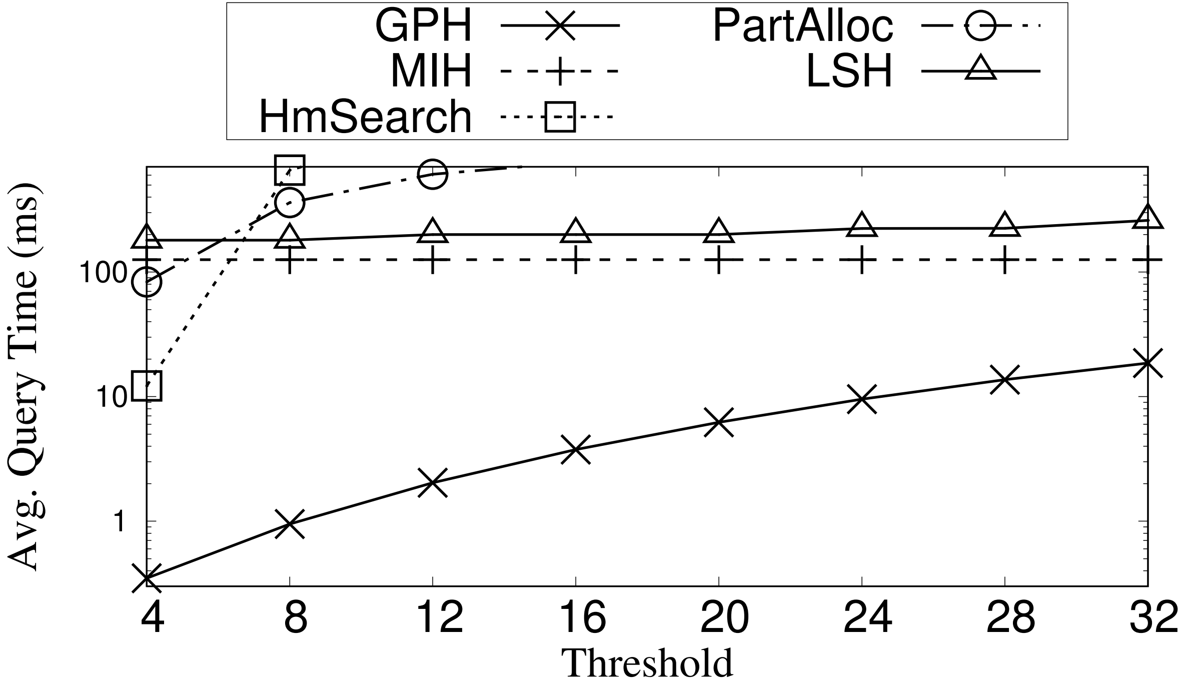


Query Q3, Allocate -1, -1, 2



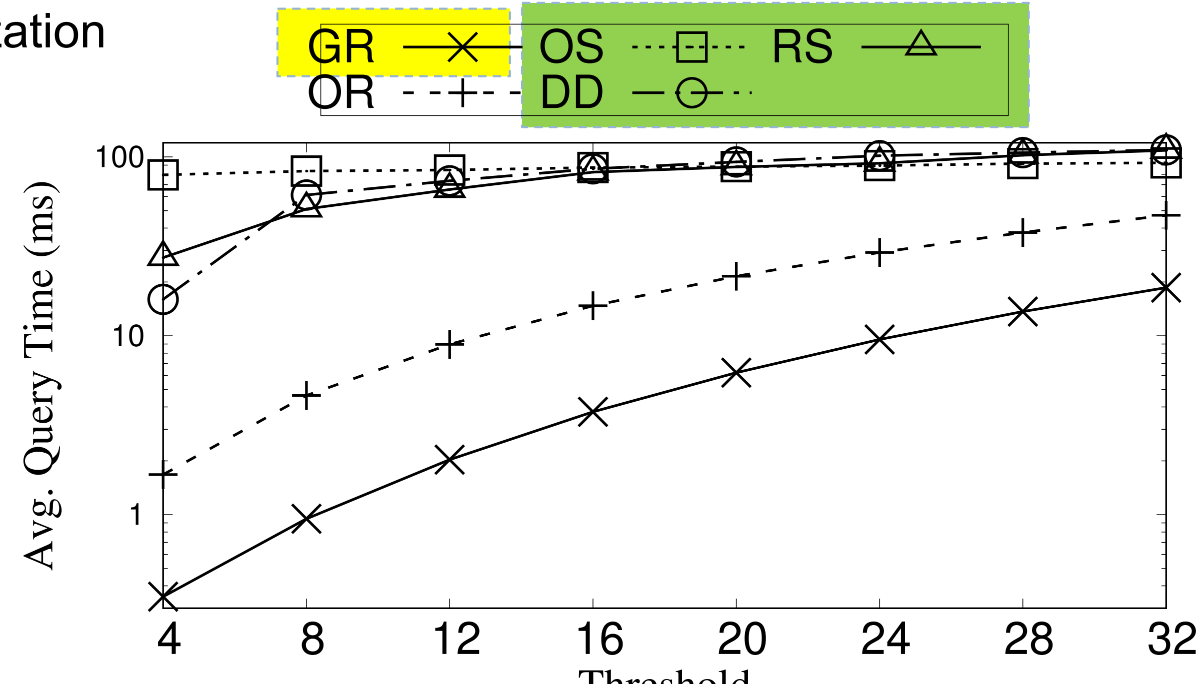
GPH Experiments - Running Time /2

- **PubChem dataset**
  - highly skewness ➔ existing methods lose their pruning power quickly

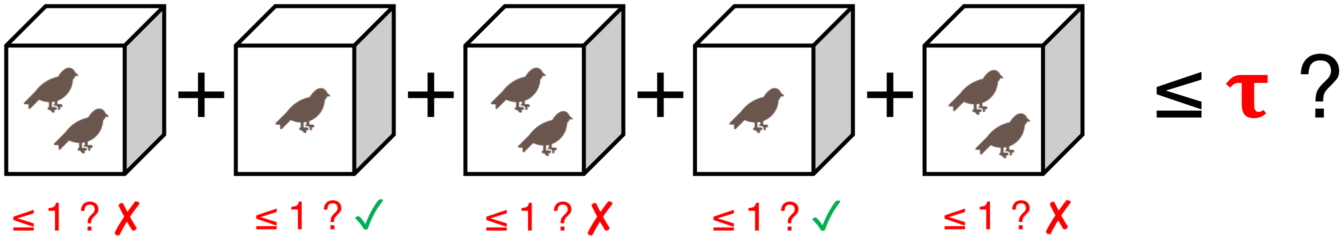


GPH Experiments - Dimension Partitioning (PubChem)

- OR: original dataset
- DD, OS, RS: existing methods that avoid skewness
- GR: Skewnization



Pigeonhole Principle (Multiple Boxes)



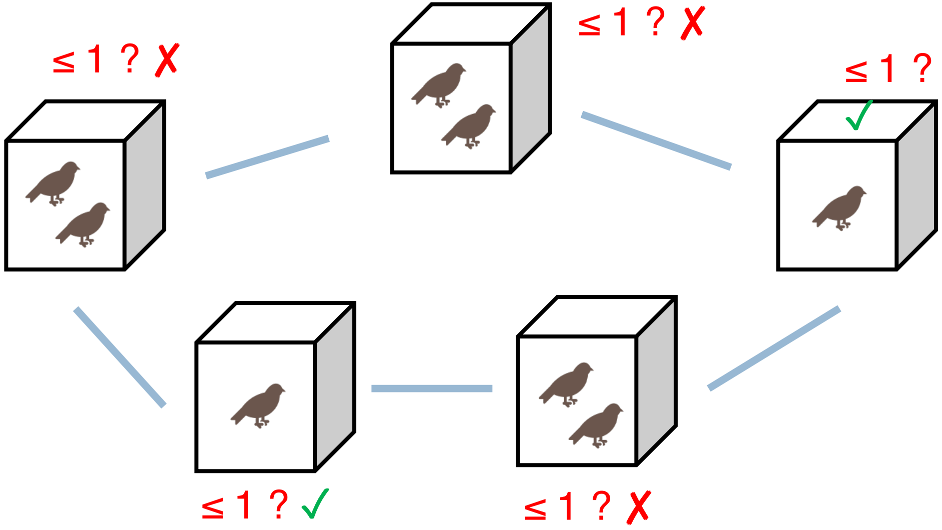
Basic Idea: Bound Multiple Boxes?

Problems: Exponential number of pigeonhole combinations.

- 20 combined 2 pigeonholes.
- 60 combined 3 pigeonholes.
- …

Pigeonring Principle: Basic form (VLDB19)

Dose m pigeonholes contain no more than τ pigeons?



l =1

≤ 5 ?

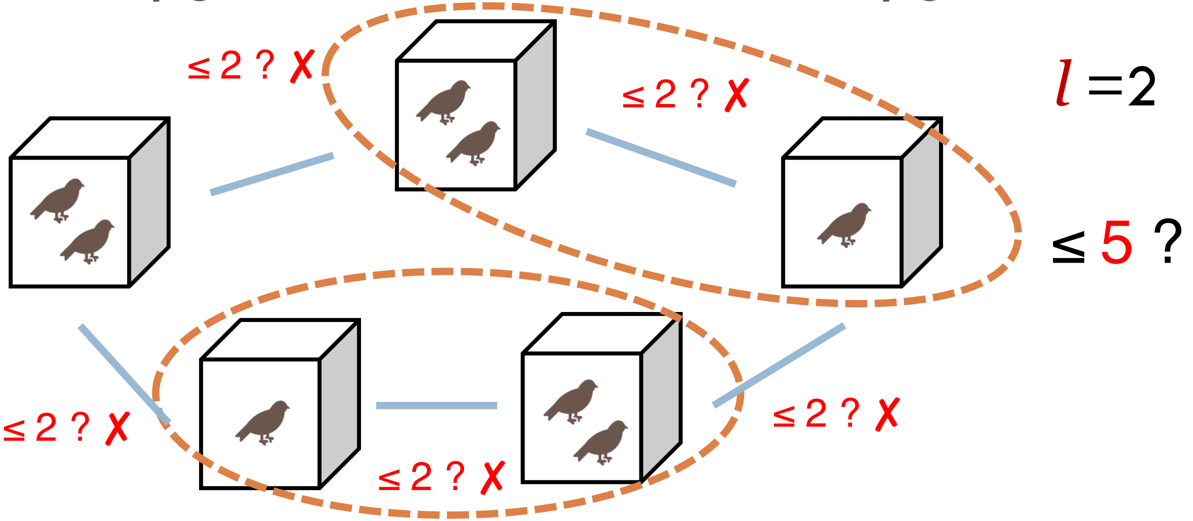
- Consider the adjacent partitions
- When l = 1, it is the same as General Pigeonhole Principle.

Define an order: Boxes are placed in a ring.

For every l in [1 .. m], there exist l consecutive boxes which contain a total of **no more than $l \cdot \tau / m$** pigeons.

Pigeonring Principle: Basic form. (VLDB19)

Dose m pigeonholes contain no more than τ pigeons?



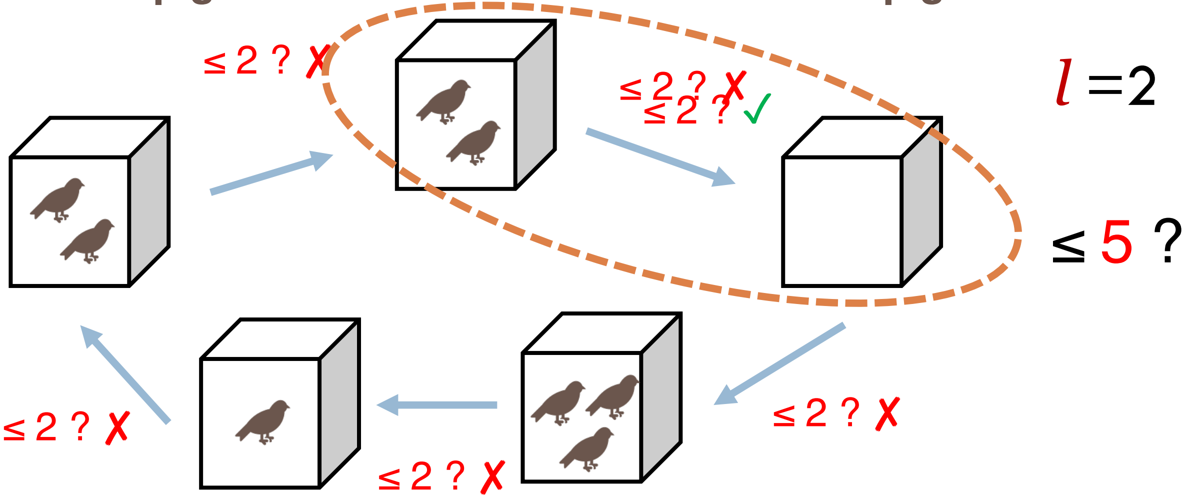
- Consider the adjacent partitions
- When l = 2, it is tighter than General Pigeonhole Principle.
- The record can be filtered!

Define an order: Boxes are placed in a ring.

For every l in [1 .. m], there exist l consecutive boxes which contain a total of **no more than $l \cdot \tau / m$** pigeons.

Pigeonring Principle: Strong form (VLDB19)

Dose m pigeonholes contain no more than τ pigeons?



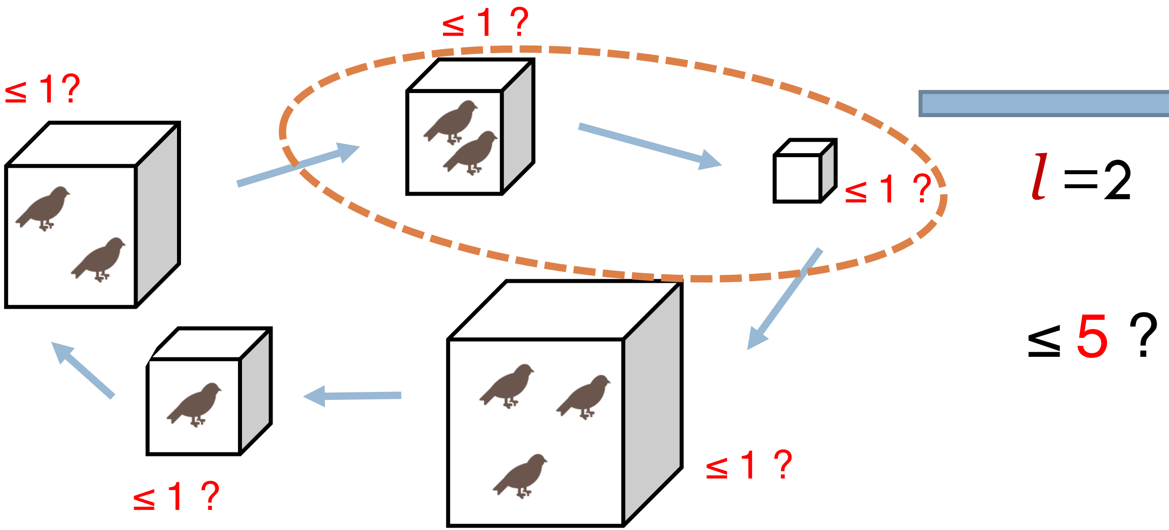
Add a direction, i.e., going clockwise.

- Consider the adjacent partitions
- When l = 2, it is tighter than General Pigeonhole Principle.
- The record can be filtered!

There exists a pigeonhole such that for **every** l in [1 .. m], starting from this pigeonhole and going clockwise, the l consecutive pigeonholes contain a total of no more than $l \cdot t/m$ pigeons.

Combine with GPH Threshold Allocation (VLDB19)

Dose m pigeonholes contain no more than τ pigeons?



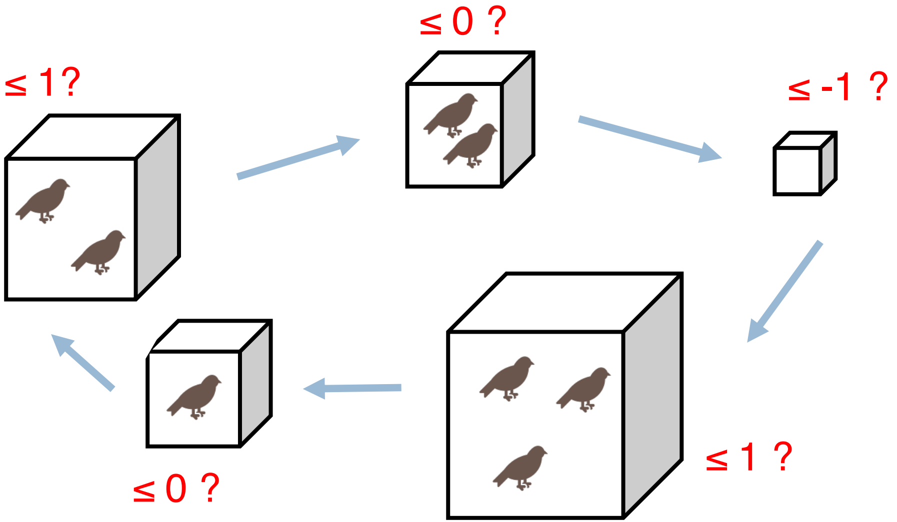
- Allocate 2 pigeons for the two holes
- Due to the non-uniform distribution of pigeons, even allocation is not good.

Not every pigeonhole is equal. **Non-uniform distribution.** i.e. Prefix Filtering

- Weak threshold allocation: every pigeonhole has equal τ/m partial threshold.
- GPH threshold allocation: We use an allocation vector $T = [\tau_0, \tau_1, \ldots, \tau_{m-1}]$.
  - Requires: $||T||_1 \geq \tau - m + 1$

Combine with GPH Threshold Allocation

Dose m pigeonholes contain no more than τ pigeons?



$l = 2$

≤ 5 ?

Pigeonring Principle +
GPH threshold allocation

Minimize

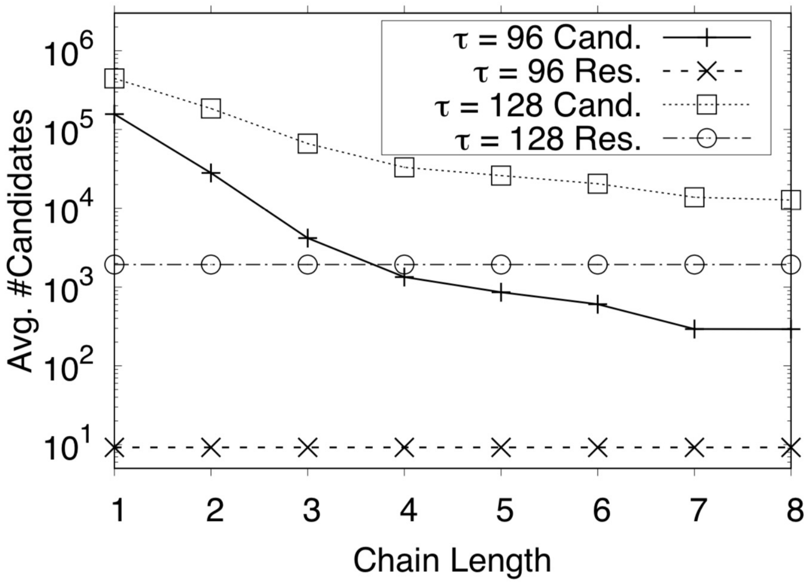
$$CN(q_1, \tau_1) + CN(q_2, \tau_2) + CN(q_3, \tau_3)$$

$$OPT[i,t] = \begin{cases} \min_{e=-1}^{t+i-1} OPT[i-1, t-e] + CN(q_i, e) & \text{if } i > 1 \\ CN(q_i, t) & \text{if } i = 1 \end{cases}$$

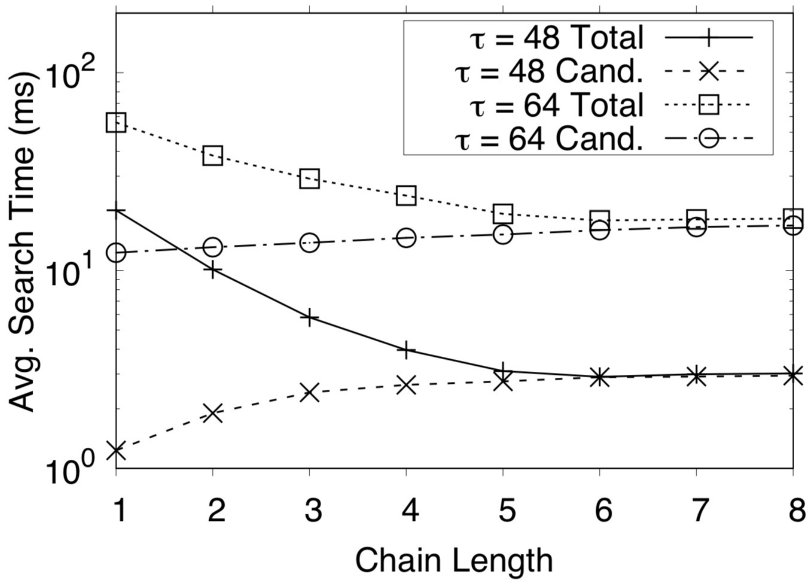
Not every pigeonhole is equal. **Non-uniform distribution.** i.e. Prefix Filtering

- Weak threshold allocation: every pigeonhole has equal τ/m partial threshold.
- GPH threshold allocation: We use an allocation vector $T = [\tau_0, \tau_1, \ldots, \tau_{m-1}]$.
  - Requires: $\|T\|_1 \geq \tau - m + 1$

Pigeonring – Experiment Study



(a) GIST, Candidate

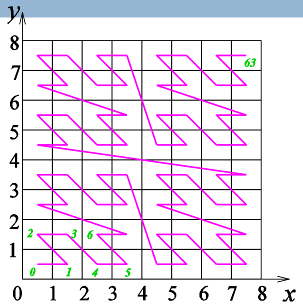


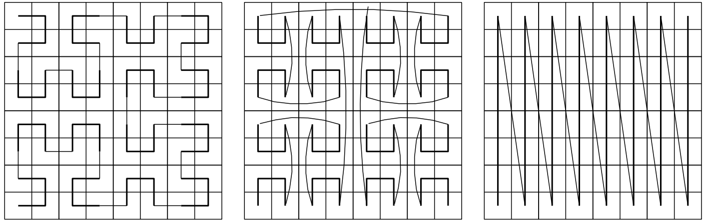
(b) GIST, Time

Effect of Chain Length on Hamming Distance Search

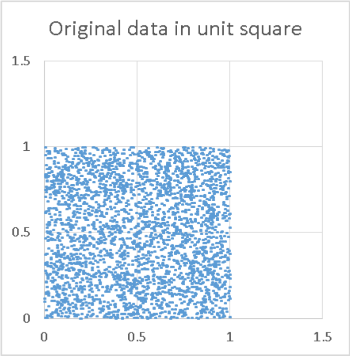
Other Dimension Reduction Based methods

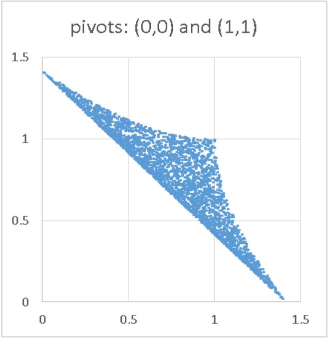
- Space Filling Curve
  - Not work for high

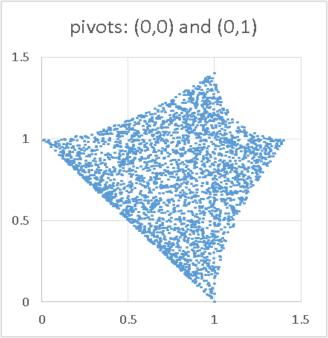




- Metric Space index (Pivot selection)







Neighboring corners are better than opposite corners!

Embedding Method with Guarantee (DASFAA 2018)

- An efficient distance lower bound
  - use the combination of linear and non-linear embedding.
- Dimensionality reduction
  - each point in a high dimensional space is embedded into a low dimensional space .
- Following "*filter-and-verify*" paradigm
  - develop an efficient exact NNS algorithm by pruning candidates using the new lower bounding,
  - hence reducing the cost of expensive distance computation in original space.

Summary of the Exact Techniques

Index	Disk-based / In-memory	Efficient query type	Dimensionality	Comments
R-tree	Disk-based	Point, window, kNN	Low	Disadvantage is overlap
K-d-tree	In-memory	Point, window, kNN(?)	Low	Inefficient for skewed data
Quad-tree	In-memory	Point, window, kNN(?)	Low	Inefficient for skewed data
Z-curve + B^+-tree	Disk-based	Point, window	Low	Order of the Z-curve affects performance
iDistance	Disk-based	Point, kNN	High	Not good for uniform data in very high-D
VA-File	Disk-based	Point, window, kNN	High	Not good for skewed data
GPH	Memory-based	Range, KNN	High	Good for Skewed data
Pigeonring	Memory-based	Range	High	Good for Skewed data
LNL	Disk-based	KNN	High	Good for Skewed data

Thank You!

Q & A