course:

Searching the Web (NDBI038)

Searching the Web and Multimedia Databases (BI-VWM)

lecture 10:

Approximate similarity search

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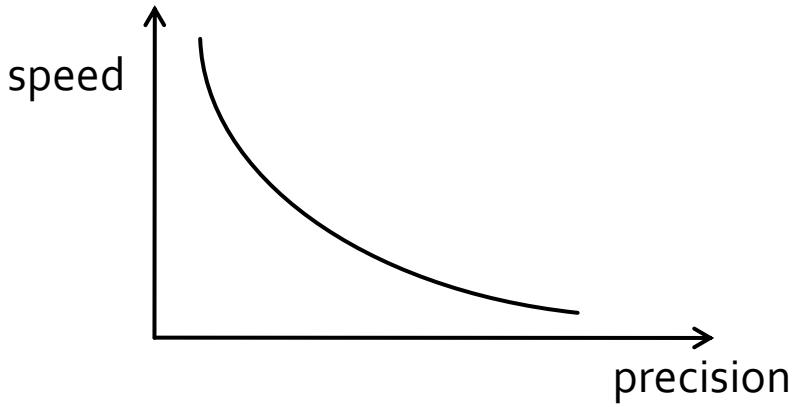
Today's lecture outline

- motivation
  - indexability
- mapping techniques
  - pivot space (simple usage of pivot tables)
  - FastMap
- approximate kNN search using M-tree
  - exact kNN algorithm
  - approximate kNN variants
- probabilistic queries using pivot tables
- permutation indexes

Motivation – exact search

- "exact" similarity search could be too slow
  - even when indexing technique is employed
- we might want to trade the retrieval precision for the speed
  - huge gain in speed usually expected (orders of magnitude) while only small loss in retrieval precision (several percent)

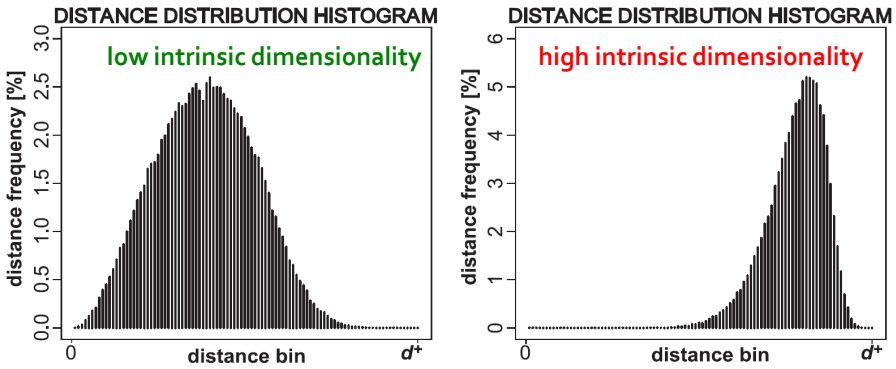


Motivation – exact search

- what is "too slow" exact search?
  - metric postulates alone do not ensure efficient indexing/search
  - also data distribution in space is very important
  - indexability = ability of structuring the database into distinct classes, such as clusters
    - **intrinsic dimensionality** – an indexability indicator

Motivation – exact search

- **intrinsic dimensionality** $\rho(S,d) = \mu^2 / 2\sigma^2$
  (μ is **mean** and σ^2 is **variance** of distance distribution in S)
- low ρ (e.g., below 10) means the dataset is **well-structured** – i.e. there exist tight clusters of objects
- high ρ means the dataset is **poorly** structured – i.e. objects are almost equally distant
  - intrinsically high-dimensional datasets are hard to organize
  - **exact search using any MAM becomes inefficient!** (the same as sequential scan)



Motivation – imperfect similarity

- moreover, similarity function often does not mimic perfectly the human perceived similarity (especially in multimedia databases)
  - even sequential search is thus subjectively approximate!
- hence, approximate search techniques only increase the subjective error of retrieval
  - i.e., just quantitative change, not a "change of category"

Motivation – approximate search

- what is "approximate"?
  - guarantee of a bound (strongest)
    - every object in query result is relevant to some extent
  - probabilistic estimates
    - every object in query result is relevant with some probability
    - i.e., on average, some percentage of objects is relevant, the rest could be completely wrong
  - no guarantee (weakest)
    - just experimental observation based on sampling, etc.

Motivation – approximate search

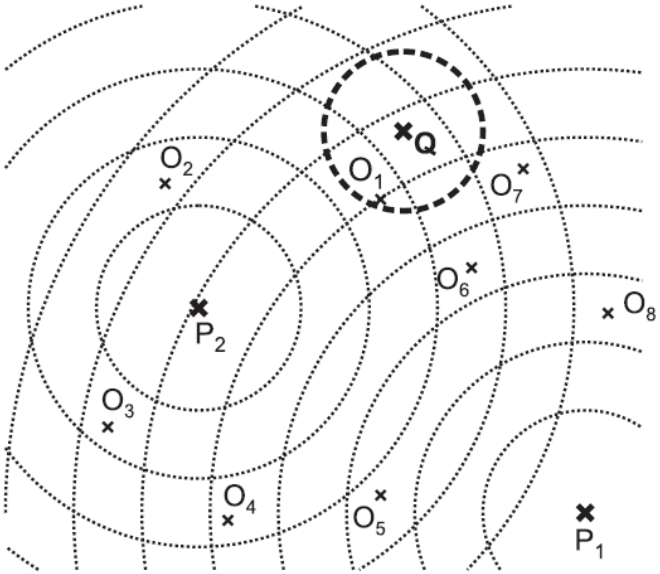
- how to speedup search?
  - realtime cost is crucial
    - indexing to reduce the distance computation (more aggressive than exact search)
    - transformation of the metric space into a simpler but only approximate target (vector) space
      - sequential search in the target space or a kind of indexing again

Mapping techniques

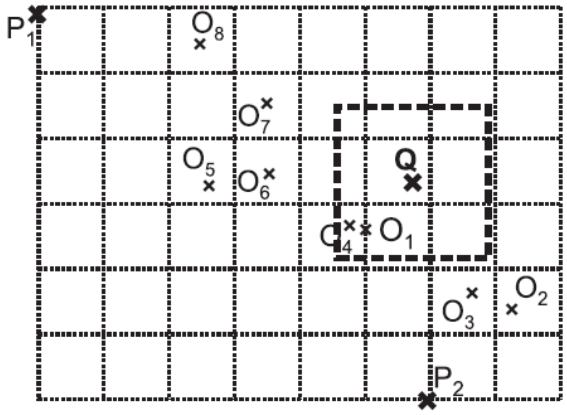
- expensive distance function δ in an arbitrary metric space could be replaced by cheap L_p distance
  - the metric space is embedded into a suitable vector space
- pre-processing of the database
  - mapping the database
    - mostly static (the embedding scheme is data-dependent)
    - some dynamic (the scheme is data-independent, e.g., simple **pivot tables**)
  - indexing the target space by metric access methods (or spatial access methods)
- many mapping techniques for metric spaces developed
  - mostly mapping to Euclidean vector space
  - metric multidimensional scaling (best but slow)
  - faster methods: **FastMap**, MetricMap, SparseMap

Mapping techniques – pivot tables

- the pivot tables (LAESA) could be used as a simple approximate method based on mapping (omitting the refinement step)
  - coordinate axis = distances to a pivot
  - using $L_\infty()$ as an approximation of $\delta()$



2NN query:
result = {O_1, O_4}



	P_1	P_2	$L_\infty(q,O_i)$
O_1	5	2.6	0.7
O_2	7.2	1.4	2.1
O_3	6.7	1.6	1.8
O_4	4.8	2.7	1
O_5	2.6	3.2	3.1
O_6	3.6	3.5	2.2
O_7	3.6	4.5	2.2
O_8	2.5	5.5	3.2

Mapping techniques – pivot tables

- will this work?
  - L_∞ in the pivot space lower-bounds δ in the metric space
  - the more (good) pivots, the tighter lower bound
    - and thus better approximation
  - limiting the need of distance $\delta(*,*)$ computations to
    - mapping the query object into the pivot space
    - optionally, re-ranking
      - e.g., 100NN query in the pivot space + re-ranking to 10NN result in the metric space
  - reasonable number of good pivots needed
  - no guarantee of retrieval precision (just empirical)

Mapping techniques – FastMap

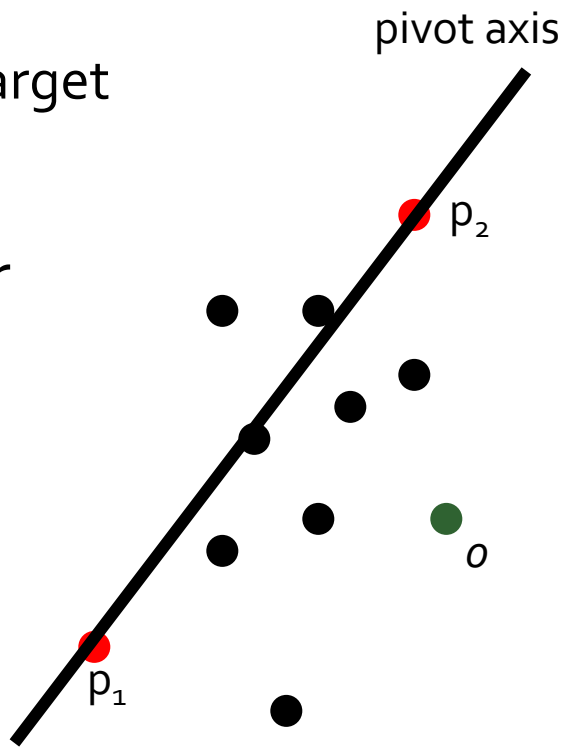
- considering an arbitrary metric space
  as an "unknown" Euclidean space
  (of user-defined dimensionality)

- the (assumed) coordinates are "recovered" by use of
  - establishing artificial coordinate system using pairs of pivots (each pair means one **pivot axis**)
  - **cosine law** and **Pythagorean theorem**,
    allowing to **project** the database objects onto the "pivot axis" (taking into account the orthogonal hyperplane formed by the already established pivot axes)

Mapping techniques – FastMap

the FastMap algorithm:

- step 0:
  - let *k* be the number of dimensions of the target Euclidean space we construct
- step 1: select first (next) best pivot pair
  - select object *o* at random
  - find p_1 being the furthest from *o*
  - find p_2 being the furthest from p_1
  - we have virtual "axis" (p_1, p_2), i.e., first (next) dimension was established



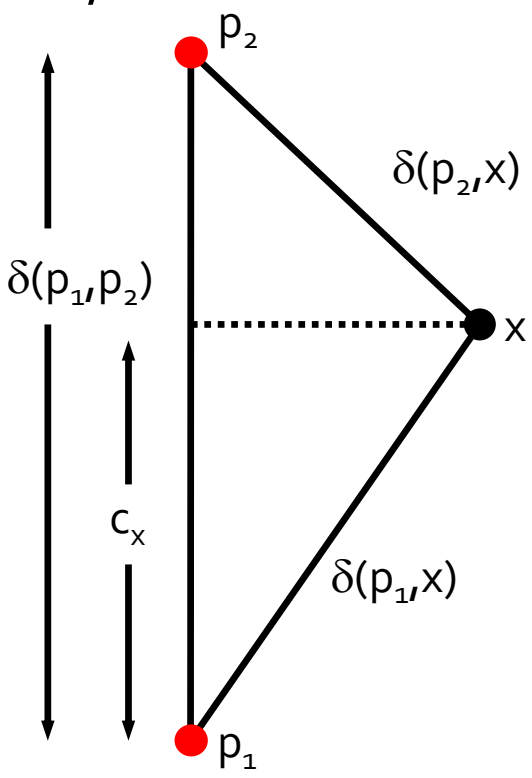
Mapping techniques – FastMap

- step 2:
  - given pivots (p_1, p_2), for any database point x, we use the **cosine law** to determine the relation of x along the axis p_1p_2

$$\delta(p_2, x)^2 = \delta(p_1, x)^2 + \delta(p_1, p_2) - 2c_x\delta(p_1, p_2)$$

$$c_x = \frac{\delta(p_1, x)^2 + \delta(p_1, p_2) - \delta(p_2, x)^2}{2\delta(p_1, p_2)}$$

c_x is the (next) coordinate of x in the target space, created by pseudo-projection

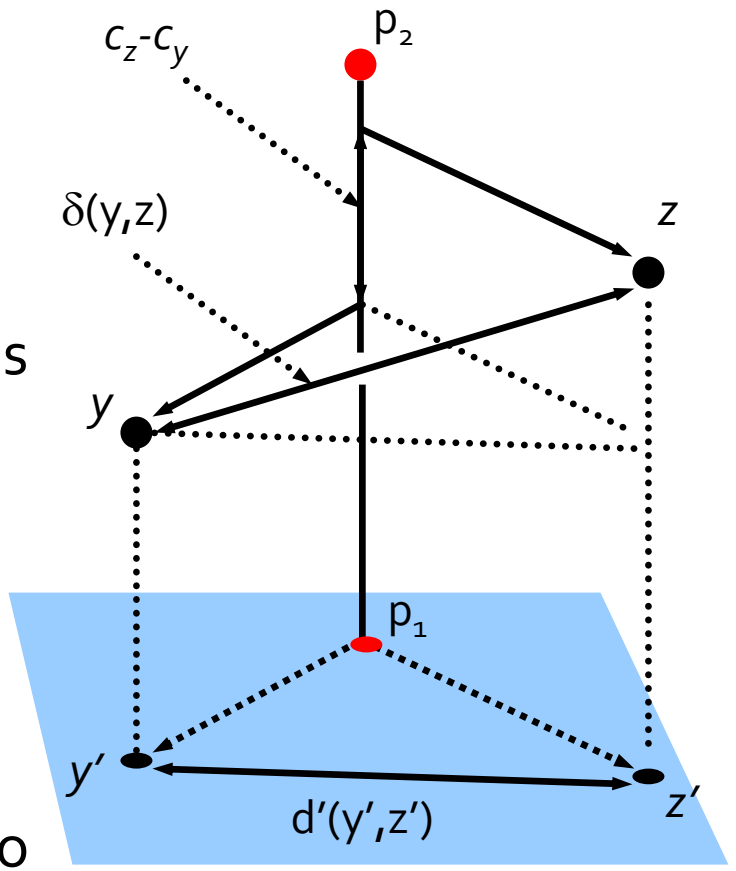


Mapping techniques – FastMap

- step 3:
  - we need to update the function $\delta(*,*)$ in order to include the already established coordinates of database objects
  - we can compute distances within the "orthogonal hyperplane" using the Pythagorean theorem

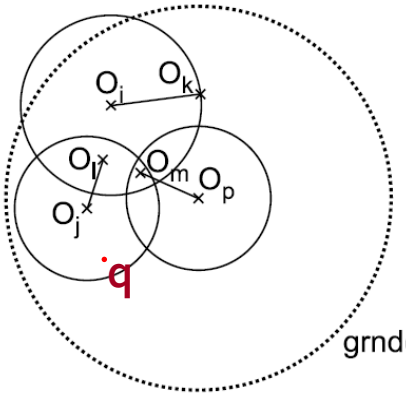
$$d'(y',z') = \sqrt{\delta(y,z)^2 - (c_z - c_y)^2}$$

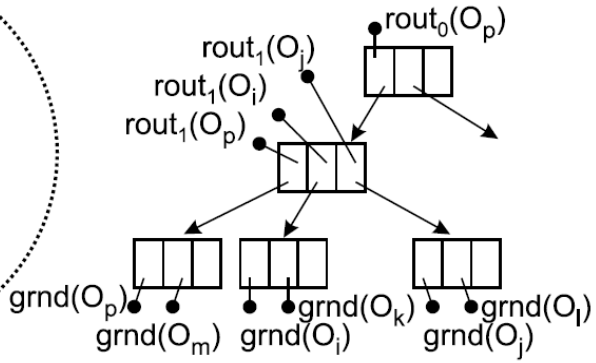
  - hence, let **$\delta(*,*)$:= d'(*,*)** and goto step 1 (or terminate if all k dimensions have been established)



M-tree

- M-tree is a metric index consisting of recursively nested ball regions (see previous lecture)
  - idea of R-tree generalized to metric spaces
- algorithm for exact kNN search developed (branch-and-bound)
  - based on a **priority queue PR** that maintains the nodes that cannot be excluded from the search
    - ordering of nodes by their (balls') lower-bound distances to q
  - kNN candidates + their distances to q are stored in a **NN array**
    - includes also candidate nodes (and upper-bound distances to q)
    - the k^{th} entry of NN means the dynamic query radius

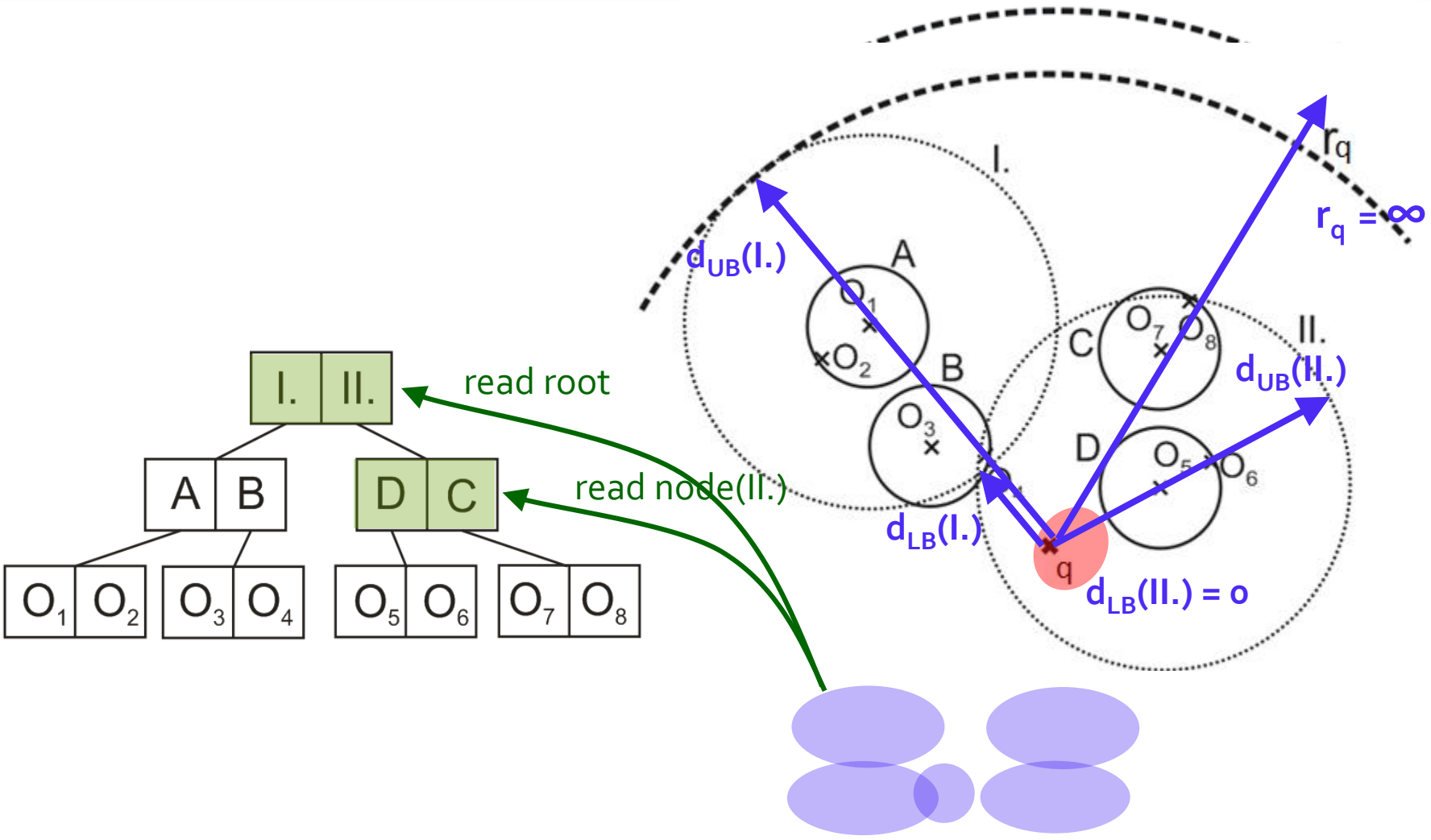




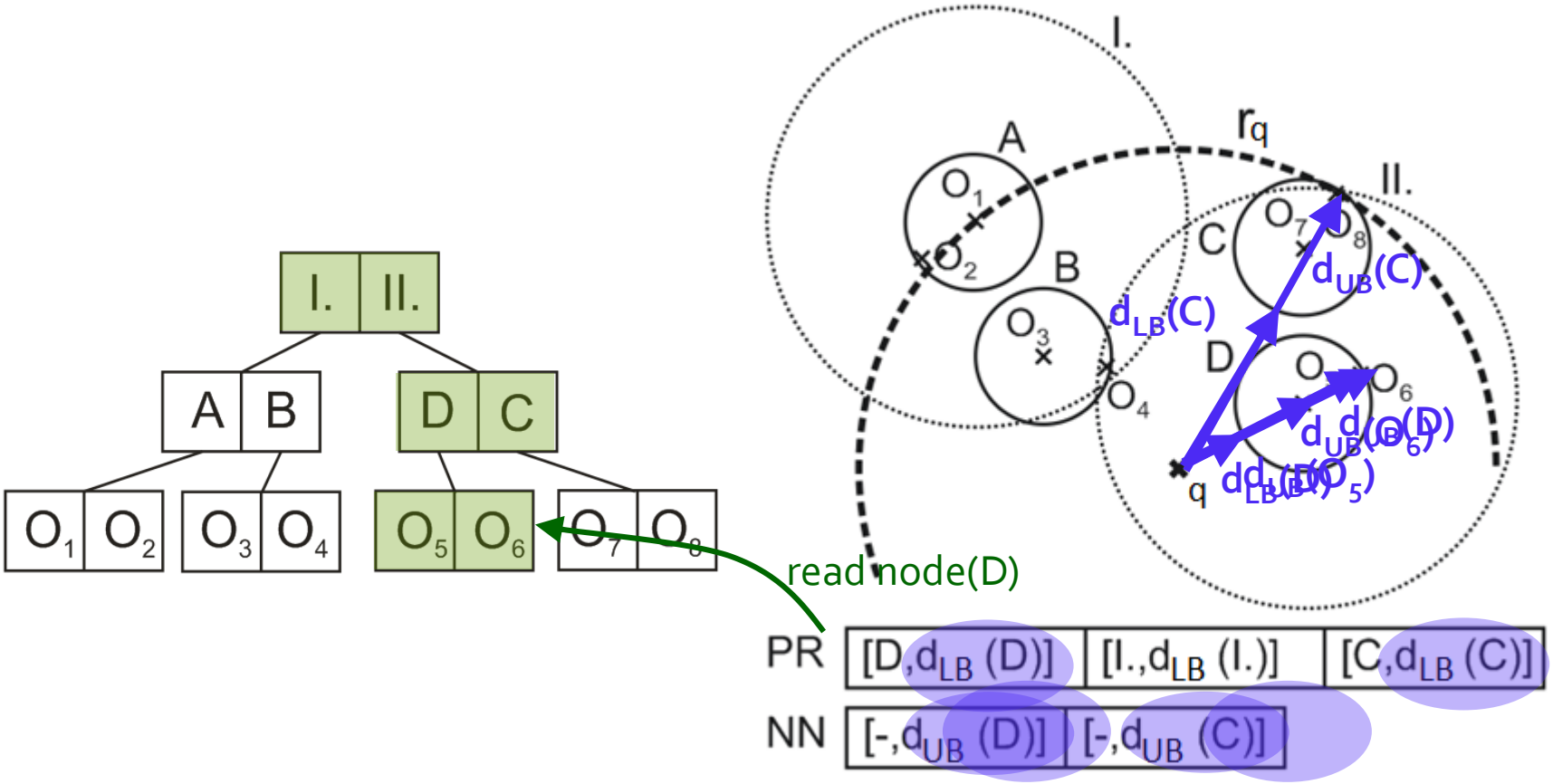
M-tree – exact kNN search

- the idea
  - consider a range query **(q, r_q)** processing,
    however the query radius **r_q** is dynamic
  - at the beginning the dynamic radius **r_q** is infinite,
    PR queue contains just the M-tree root, and **NN array** is empty
  - the M-tree is traversed, inserting into the priority queue PR nodes that have to be processed (i.e., the query ball overlaps the nodes' balls)
    - for each node in PR, its lower-bound distance (to the ball) is also stored
  - in the NN array, candidates to k nearest neighbors are stored
    - either directly objects (and distances to q)
      or candidate balls (and upper-bound distances to q)
    - NN[k] determines the dynamic query radius
  - during kNN processing, nodes are fetched from PR, updating PR and NN
    - note that NN[k] is decreasing, so that some nodes in PR are pruned prior to their fetch

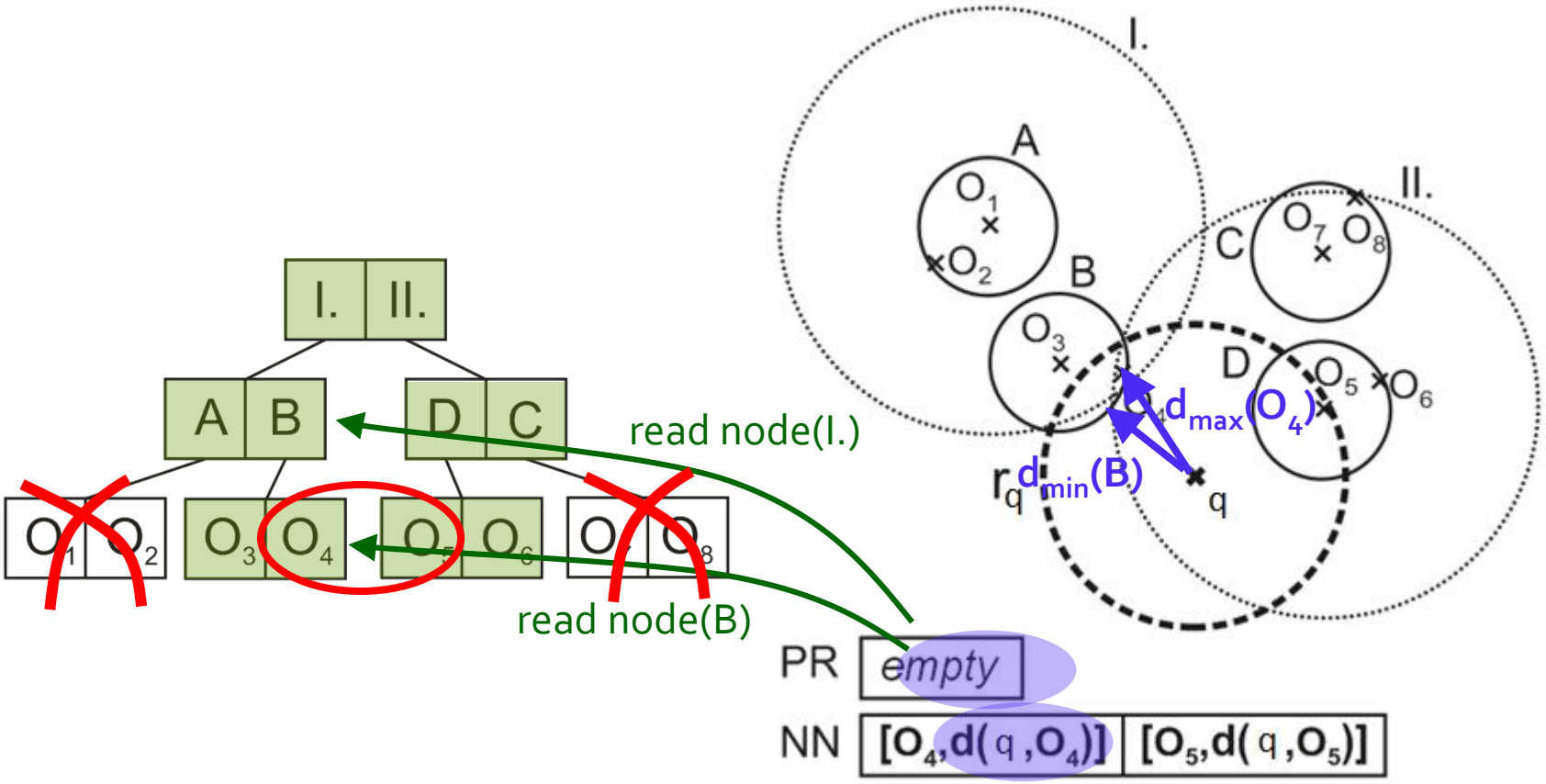
Example: exact 2NN search in M-tree



Example: exact 2NN search in M-tree



Example: exact 2NN search in M-tree

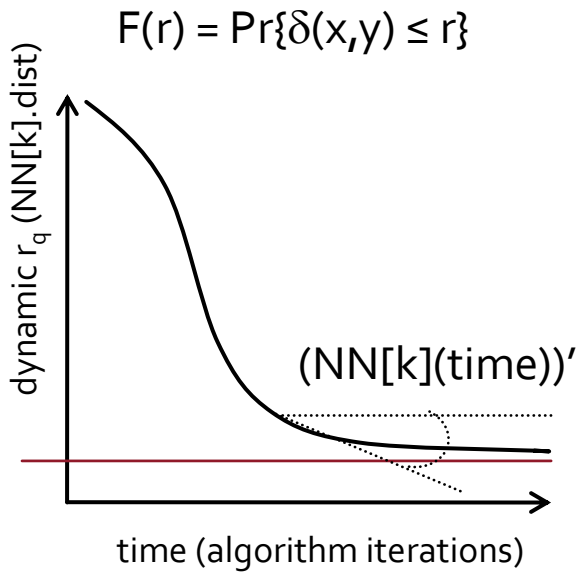


M-tree – approximate kNN search

- the exact kNN algorithm could be adjusted to provide faster approximate search
- we consider four heuristics
  - slowdown of improvements
    - if the NN array changes only slowly, let's terminate
  - approximately correct search
    - returned k nearest neighbors are guaranteed to be not much further than the true k nearest neighbors
  - good fraction approximation
    - if the distance to the candidate k^{th} neighbor is likely to represent small enough portion of the database, let's terminate
  - PAC queries (probably approximately correct queries)

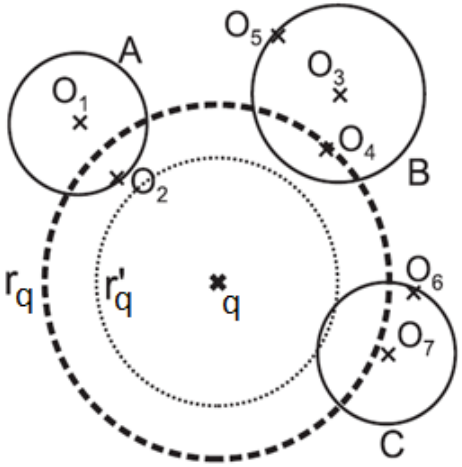
M-tree – approximate kNN search

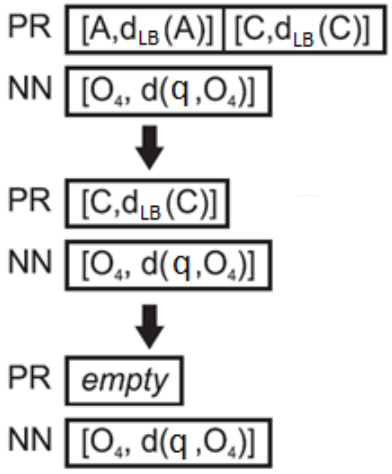
- slowdown of improvements
  - consider the function NN[k] in time, i.e., how the dynamic query radius improves during the kNN processing
  - given a user-defined parameter κ, let's terminate the kNN search as soon as the first derivative (absolute value) of NN[k](time) falls below κ
    - i.e., the small improvements of the result are not worth the effort



M-tree – approximate kNN search

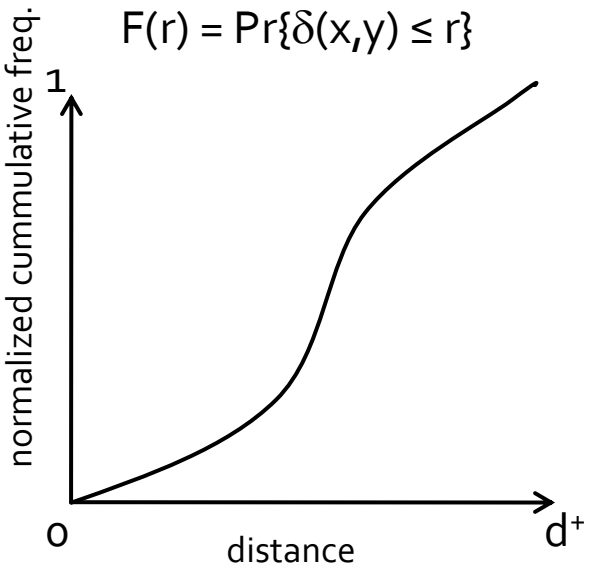
- approximately correct search
  - consider a user-defined error threshold ε, while relaxing the task of kNN search to $(1+\varepsilon)$kNN search
    - i.e., the neighbor returned is allowed to be up to $(1+\varepsilon)$ times further from **q** than the real one
  - algorithm adjustment
    - nodes from PR are filtered more aggressively using $r_q' = r_q/(1+\varepsilon)$ instead of r_q





M-tree – approximate kNN search

- good fraction approximation
  - given query object **q** and a user-defined fraction **κ** (of the database) that has to be inspected during a (kNN) search
  - for a range query **(q, r)**, let's estimate the fraction of database falling into **(q, r)**
  - then, in the kNN algorithm we test if the database fraction estimated for the actual **(q, NN[k])** is greater than **κ**
    – if so, terminate
    - the database fraction for (q, r) is computed as $F(r) = Pr\{\delta(x,y) \leq r\}$ using the cummulative distance distribution histogram

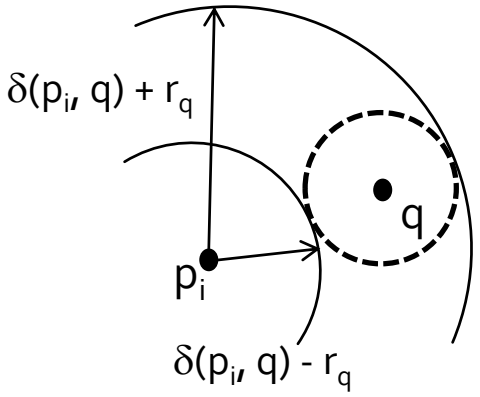


M-tree – approximate kNN search

- PAC queries
  - probably approximately correct queries
  - combination of the probabilistic and approximately correct methods
    - e.g., the two previous methods
  - in M-tree's kNN algorithm
    - nearest neighbors are searched, but guaranteeing only probability κ that the result objects will be at least $(1+\varepsilon)$ nearest neighbors
    - the terminating condition in the kNN algorithm
      - estimate the distance to k^{th} nearest neighbor (query radius $\mathbf{r_q}$)
        - by testing $F(r_q)$, until $F(r_q)$ * size of the database = k
      - nodes from PR are filtered using $r_q' = r_q/(1+\varepsilon)$

Approximate search in pivot tables

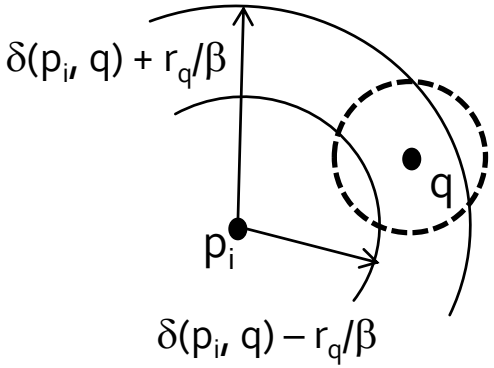
- consider pivot tables and a range query **(q, r_q)**
- using pivots, the exact search algorithm must check all objects that are within all the rings obtained by the pivots and the ranqe query (see on the right)



- in the approximate version, consider a user-defined threshold δ, that guarantees that the search is correct with the probability δ
  - the rings are "thinned" using β, computed as

$$\beta \leq \frac{r_Q \sqrt{1-(1-\delta)^{\frac{1}{p}}}}{\sqrt{2}\sigma}$$

where p is number of pivots, and σ is the variance over the distance distribution



Permutation indexes

- consider a set of *k* pivots p_i and a pivot table (distance matrix)
- instead of using the distance matrix, let's create for each database object u a permutation of pivots Π_u, represented as an ordered set of pivots' indices
- hence, no distances are stored in the index, just the ordering of pivots
- allows compact storage
  - $kn \log_2 k$ bits
    instead of $32kn$ bits used by pivot tables

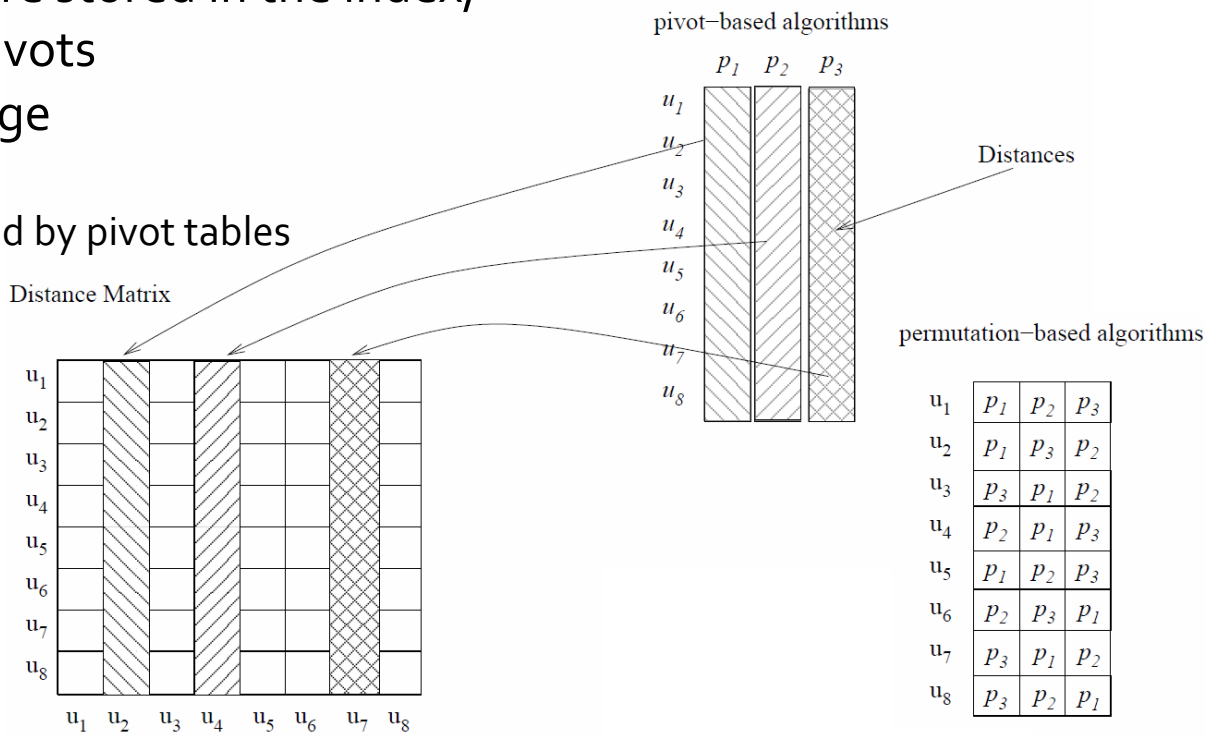


image from Chávez et al., Effective Proximity Retrieval by Ordering Permutations, IEEE Tran. on Patt. Anal. and Mach. Int., 30(9), 2008

Permutation indexes

- similarity for permutations
  - Spearman Rho

$$S_\rho(\Pi_u, \Pi_q) = \sum_{1 \le i \le k} \left(\Pi_u^{-1}(i) - \Pi_q^{-1}(i)\right)^2$$

  - Spearman Footrule

$$F(\Pi_u, \Pi_q) = \sum_{1 \le i \le k} |\Pi_u^{-1}(i) - \Pi_q^{-1}(i)|$$

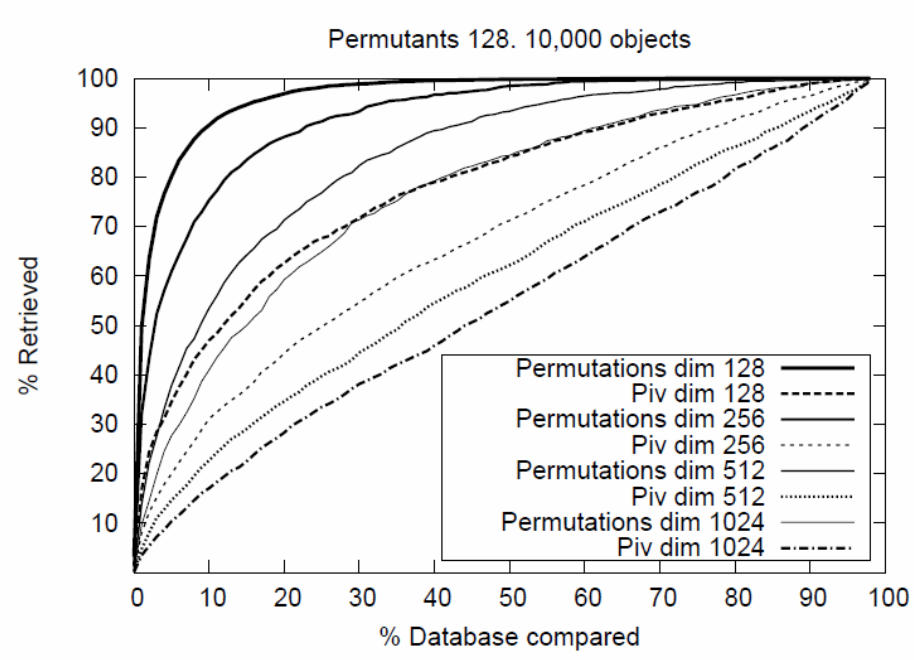
  where $\Pi^{-1}{}_u(i)$ is the position of pivot p_i in the permutation Π_u

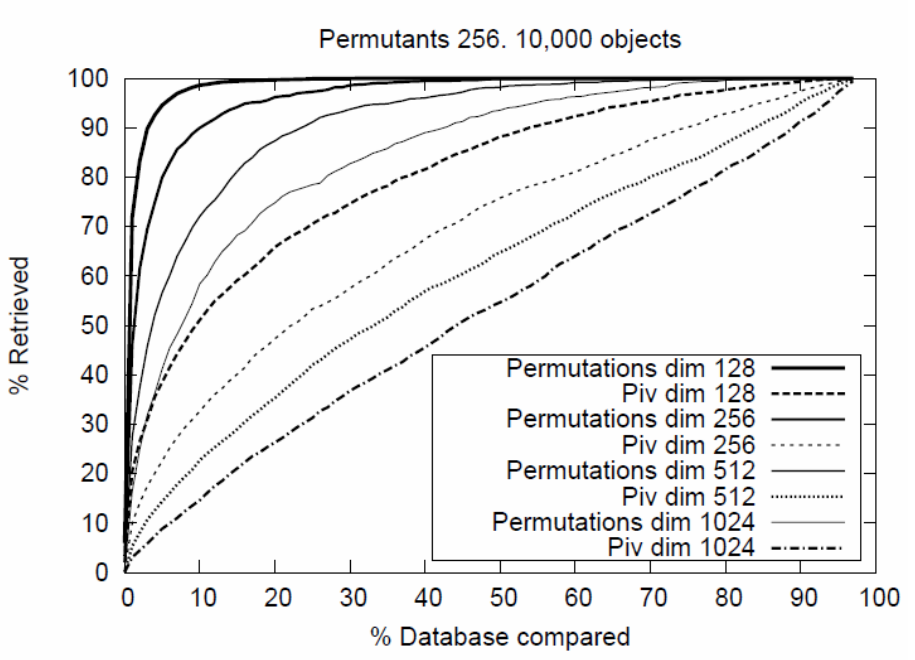
- thus, instead of the **geometric** framework the **combinatorial** framework is used

Permutation indexes

- the approximate queries using permutation indexes are, in fact, similar to the pivot-table ones
- instead of L_∞ on vectors in pivot space, the Spearman Rho/Footrule on pivot permutations is used for sorting the objects in the first step
- the second (refinement) step is the same, using some early termination condition

Permutation indexes





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