course:

Searching the Web (NDBI038)

Searching the Web and Multimedia Databases (BI-VWM)

lecture 9:

Indexing metric similarity for efficient multimedia retrieval

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Today's lecture outline

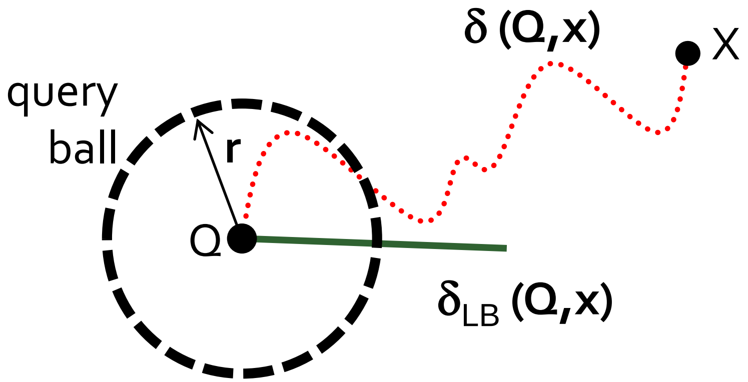
- metric access methods
  - motivation
  - pivot tables
    - AESA, LAESA
  - hierarchical structures
    - GNAT, M-tree
  - hashed indexes
    - D-index
  - hybrid structures
    - PM-tree, M-index
- performance measures
  - distance computations, I/O cost, internal cost, realtime cost

Motivation

- similarity search
  - effective (quality of similarity measure)
  - **efficient = fast**
- lower-bounding
  - general mechanism for efficient similarity search
  - using cheap lower bound instead of expensive distance
- metric space model
  - lower-bounding based on pivots and metric postulates
  - allows partitioning of the space
  - database indexing based on metric space model
    - metric access methods

General lower-bounding

- a cheap determination of **lower-bound distance** $\delta_{LB}(*,*) \leq \delta(*,*)$
- provides a mechanism how to quickly filter irrelevant objects from search
  - consider query ball **(Q, r)** and data object **x**
  - if $\delta_{LB}(Q,x) > r$, **x** is irrelevent
- **tight** lower bound needed
  - increasing probability that $\delta_{LB}(*,*) > r$
  - e.g., near-zero LB is useless



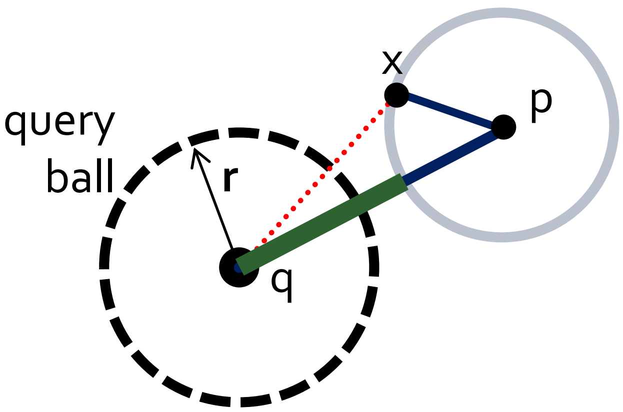
Metric postulates

- metric postulates support common assumptions on similarity
  - reflexivity – object is maximally similar to itself
  - non-negativity – two distinct objects are somehow dissimilar
  - symmetry – the direction of similarity judgement is not important
  - triangle inequality – similarity is transitive

$$
\begin{array}{rcllc}
\delta(x,y) & = & 0 & \Leftrightarrow x = y & \text{reflexivity} \\
\delta(x,y) & > & 0 & \Leftrightarrow x \neq y & \text{non-negativity} \\
\delta(x,y) & = & \delta(y,x) & & \text{symmetry} \\
\delta(x,y) + \delta(y,z) & \geq & \delta(x,z) & & \text{triangle inequality}
\end{array}
$$

Metric lower-bounding

- metric space model provides a specific means of lower-bounding
  - **pivot objects** – static objects (selected from the database)
  - triangle inequality for lower bound construction (using a pivot)
  - precomputed distances from objects to pivots
    - stored in a metric index



<u>The task:</u> check if **x** is inside query ball

•we know **δ(q,p)**

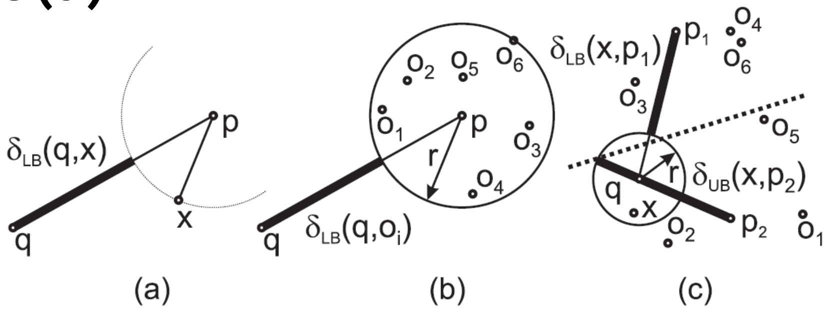
•we know **δ(x,p)**

•we do not know **δ(q,x)**

•we do not have to compute **δ(q,x)**, because its lower bound |δ(q,p)-δ (p,x)| is larger than **r**, so **x** surely cannot be in the query ball, so **x** is ignored

Metric lower-bounding

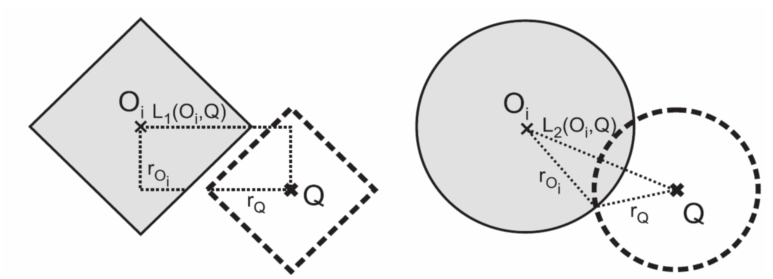
- lower bound to a database object **(a)**
  - basic concept
- lower bound to a region **(b)**
  - ball-shaped regions
  - logical combinations of predicates
- combination of lower and upper bounds **(c)**
  - hyper-plane partitioning



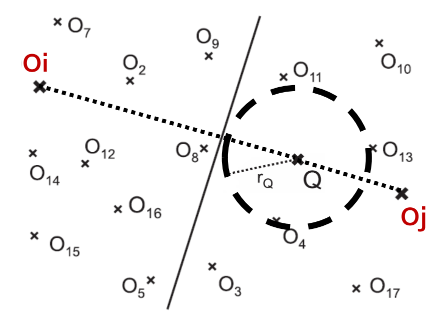
- usage: filtering whole regions (or directly the objects)
  - the search is then performed just in several partitions (subset of objects), while computing as few distance computations of **δ(q,x)** as possible → **efficient search**

Filtering metric regions

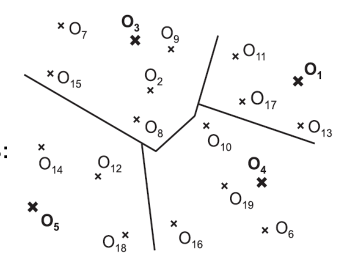
- ball-shaped regions
  - for two balls (O_i, r_{Oi}) and (q, r_q) it holds:
    if $\delta(O_i, q) > r_{Oi} + r_q$, then
    the balls do not overlap (and vice versa)



- hyperplane-separated regions
  - for two regions determined by a hyperplane between O_i ,O_j, it holds:
    if $\delta(O_i, q) - r_q > \delta(O_j, q) + r_q$, then
    first (Oi) region does not overlap query
    if $\delta(O_j, q) - r_q > \delta(O_i, q) + r_q$, then
    second (Oj) region does not overlap query
    - simply: if lower-bound distance to query from one pivot is greater than upper-bound distance to query from the second pivot, the first region does not overlap

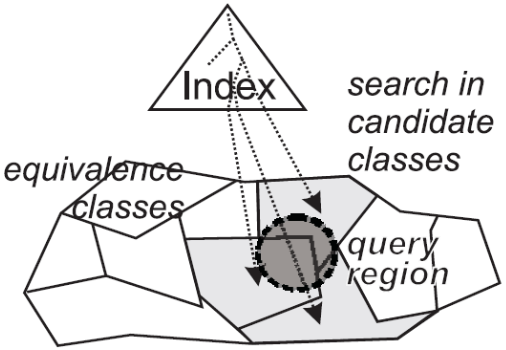


generalization
to multiple pivots:



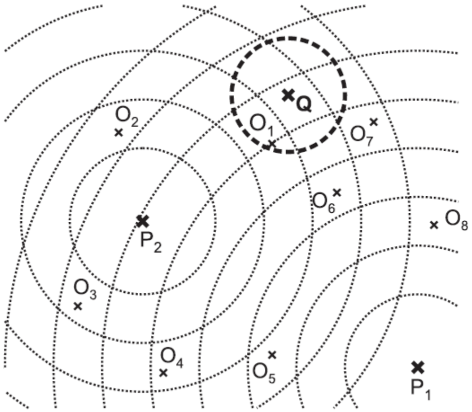
Metric access methods – motivation

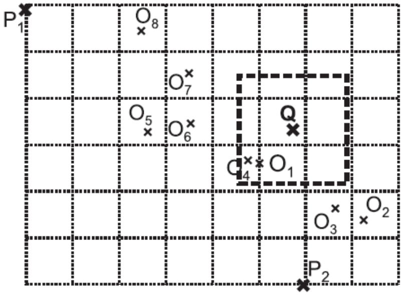
- metric access methods (MAM), or metric indexes
  - database methods for **fast similarity search in database S**
  - various types of cost measuring the "fast"
    (realtime, number of distance comp., I/O, internal, etc.)
- the means: **metric indexing**
  - based on lower-bounding using pivots
  - general metric space assummed
    (i.e., only distances could be used for indexing, not the actual object content)
  - metric postulates needed (the similarity function must be metric distance)
- various structural MAM designs
  - flat indexes (pivot tables)
  - hierarchical indexes (trees)
  - hashed indexes
  - hybrid indexes
  - index-free methods



Pivot tables

- class of indexes using mapping of data to the pivot space
  - each data object **x** maps to a vector **v**
  - i.e., we get distance matrix
- originally AESA/LAESA
  (Linear) Approximating and Eliminating Search Algorithm
- AESA
  - every data object is regarded as a pivot, i.e., we have square matrix of size **O(|S|²)**
  - empirical average **O(1)** time for nearest neighbor search, expensive construction
- LAESA
  - only some **k** data objects selected as pivots, i.e., matrix size **O(|S|)**
- contractive mapping
  - L_∞ distance in pivot space is lower bound to the original distance δ

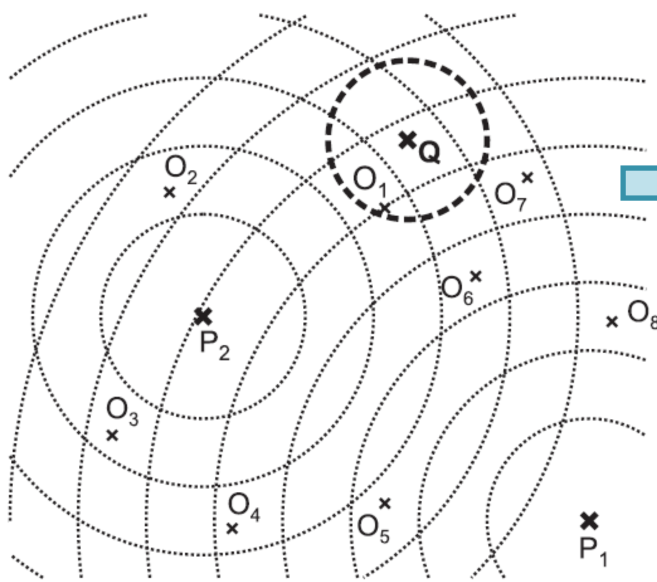


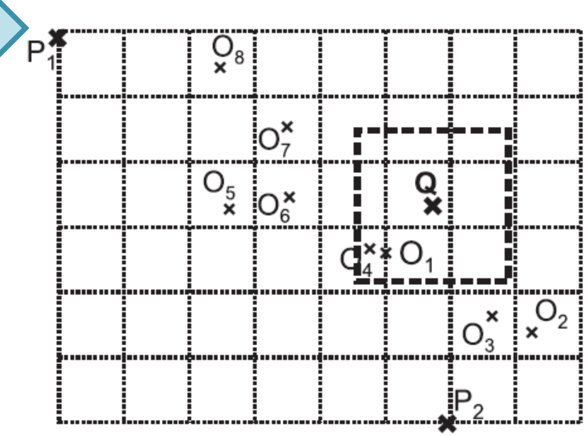


LAESA range query

	P_1	P_2
O_1	5	2.6
O_2	7.2	1.4
O_3	6.7	1.6
O_4	4.8	2.7
O_5	2.6	3.2
O_6	3.6	3.5
O_7	3.6	4.5
O_8	2.5	5.5

- simple 2 phases
  - sequential processing of the distance matrix, filtering
  - the non-filtered candidates must be refined in the original space





LAESA nearest neighbor query

- one-phase (as in AESA, see next slide)
  - suitable for large number of pivots
- two-phase
  1. the entire query vector $\mathbf{v}_q$ is determined from the query object
  2. the database objects $\mathbf{o}_i \in \mathbf{S}$ are sorted asc. w.r.t $\mathbf{L}_\infty(\mathbf{v}_q, \mathbf{v}_{oi})$
  3. in this order the $\delta(\mathbf{q}, \mathbf{o}_i)$ is being computed, updating the NN candidate $\mathbf{o}_{nn}$
     - if $\delta(\mathbf{q}, \mathbf{o}_{nn}) < \mathbf{L}_\infty(\mathbf{v}_q, \mathbf{v}_{oi})$, the filtering terminates (there is no better candidate than $\mathbf{o}_{nn}$)

AESA nearest neighbor query

- **problem:**
  cannot compute the entire query vector because all database objects are pivots (i.e., would result in naive sequential search)

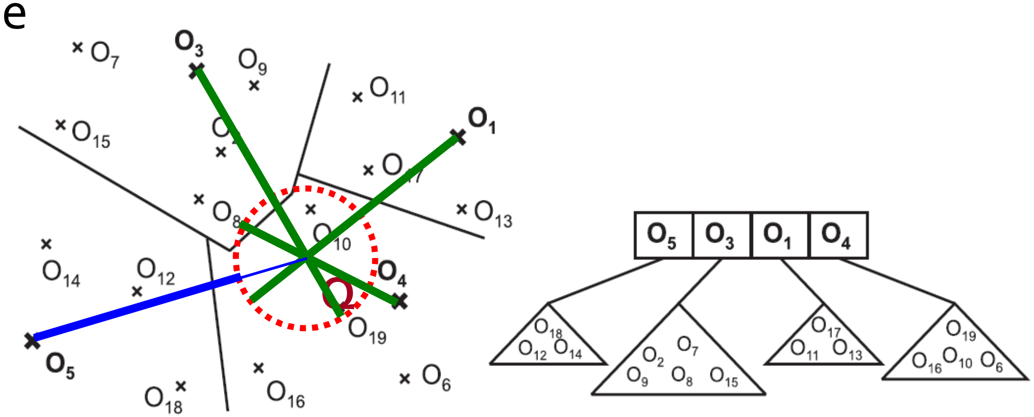
- **the idea:**
  - multiple passes of the matrix, each considering one more column (pivot), starting with one column (random)
  - after each pass
    - the lower bounds are increasing, because we get more pivots
    - because of that also more objects is filtered from search

Hierarchical metric access methods

- partitioning on the metric space, creating a hierarchy of metric regions
  - direct partitioning – close objects are in the same partition
    - either balls (e.g., **M-tree**) or hyperplane-separated subspaces (e.g., **GNAT**)
  - recursive – partitions are decomposed the same way as the whole database
  - using **local** pivots, instead of **global** pivots
    - local pivot is context-dependent, e.g., selected from objects in a subtree
    - local pivots are not fixed for the index lifetime,
they could be replaced as the database is being updated
- natural approach (inspired by R-tree, kd-tree, etc.), but
  - problem of huge volume of regions
  - problem of overlaps between sibling regions
  - problem of the shape of regions

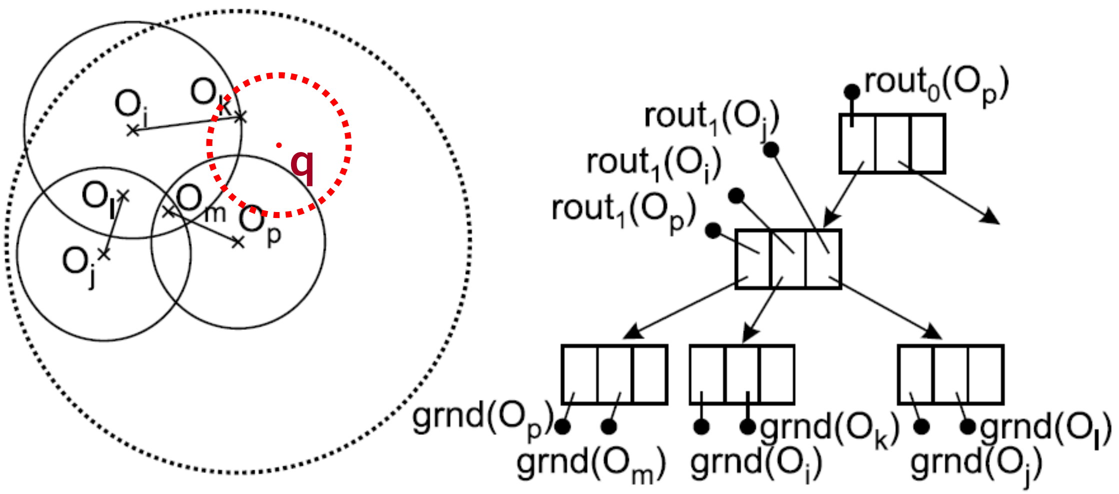
GNAT

- base on hyperplane partitioning of the space
- generalization of gh-tree into n-ary tree
  - multiple pivots in each node
  - some other extensions
    - distance ranges
- range query processing
  - test overlap of all partitions
  - recursively proceed down the hierarchy in the overlapping partitions
  - filtering of partition/subtree belonging to $\mathbf{O_5}$ (in the example):
    - if the **closest possible object** inside the query (w.r.t $\mathbf{O_5}$) is more distant than the **furthest possible object** inside the query (w.r.t. any of $\mathbf{O_1}$, $\mathbf{O_3}$, $\mathbf{O_4}$), then the subtree can be filtered out



M-tree

- inspired by R-tree – modification into metric spaces
  - hierarchy of nested balls; balanced, paged, dynamic index
  - suitable for secondary storage
  - compact hierarchy is necessary, ball overlaps lead to inefficient query processing
  - many descendants – e.g., M*-tree, PM-tree, Slim-tree, etc.
- query processing
  - traversing the hierarchy, accessing just the overlapping nodes/subtrees



Metric access methods based on hashing

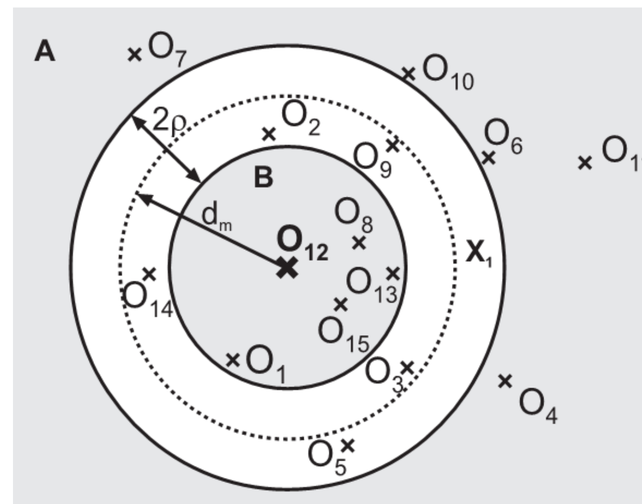
- similarity hashing function is crucial
  - each object is hashed into a bucket
  - locality-sensitive hashing function – close object should be hashed to the same bucket
  - could be only achieved based on distance to a (set of) pivot(s)
    - remember, the content of the object is not accessible to MAMs
- having the hashing function, the index design can use different structures
  - plain hash tables
  - hierarchical hash tables (e.g., **D-index**)
  - etc.

D-index

- D-index = hash-based index

- based on hashing functions $bps^{1,\rho,j}$ (ball-partitioning split functions), where $\mathbf{p_j}$ is pivot, $\mathbf{d_m}$ is median distance from $\mathbf{p_j}$ to the objects $\mathbf{o_i}$, and $\boldsymbol{\rho}$ is a splitting parameter

- the function assigns to an object o_i:
  - 2 , if it is inside the ring (p_j, d_m-ρ, d_m+ρ)
  - 1, if it is outside the greater ball (p_j, d_m+ρ)
  - 0, if it is inside the smaller ball (p_j, d_m-ρ)

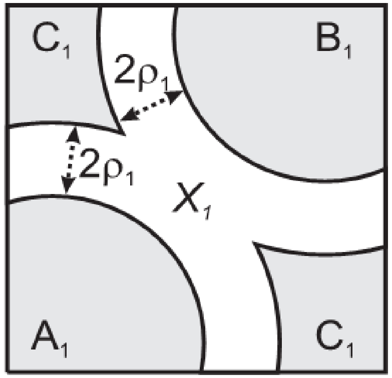


$$bps^{1,\rho,j}(O_i) = \begin{cases} 0 & \text{if } d(O_i, P_j) \le d_m - \rho \\ 1 & \text{if } d(O_i, P_j) > d_m + \rho \\ 2 & \text{otherwise} \end{cases}$$

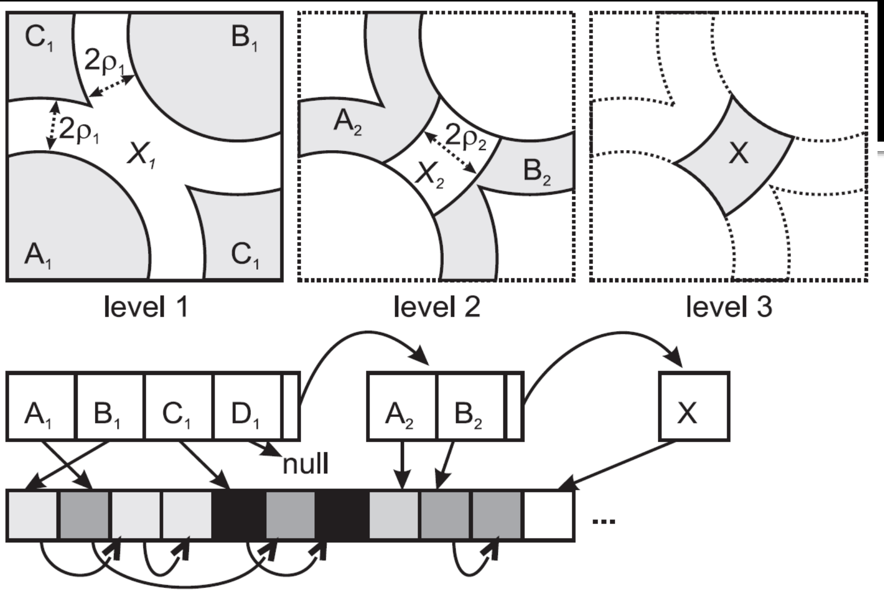
D-index

- the $bps^{1,\rho,j}$ functions can be combined
- if there **is no** 2 in the hash of the combined function, the string 0, 1 is a binary code of a partition (up to 2^n)
- if there **is a 2** in the hash code, the hashed object belongs to so-called exclusion set

- the motivation is to keep the partitions separated by the region of exclusion set
- the exclusion set is hashed again (based on different $bps^{1,\rho,j}$ functions), recursively, until it gets sufficiently small



D-index



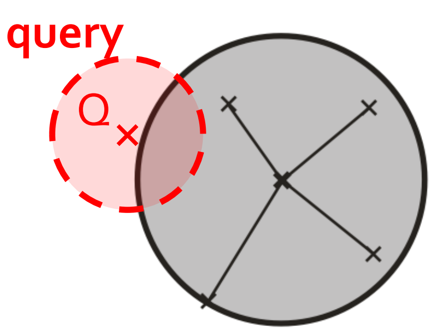
- D-index structure
  - hashed regions are organized in buckets on the disk
  - the rehashing of exclusion set defines another level of D-index
- advantages
  - for small query radius (**r < ρ**), at most one bucket is accessed at each level
  - if the whole query lies inside a region, only that bucket is accessed
  - if the whole query lies inside the exclusion set, no bucket at that level is accessed and the query processing proceeds at the next level
- disadvantages
  - selection of the parameters ρ, d_m is difficult and/or D-index is not balanced
  - the ρ parameter should be very small, in order to not become everything into the exclusion set (i.e., suitable only for small and point queries)

Hybrid metric access methods

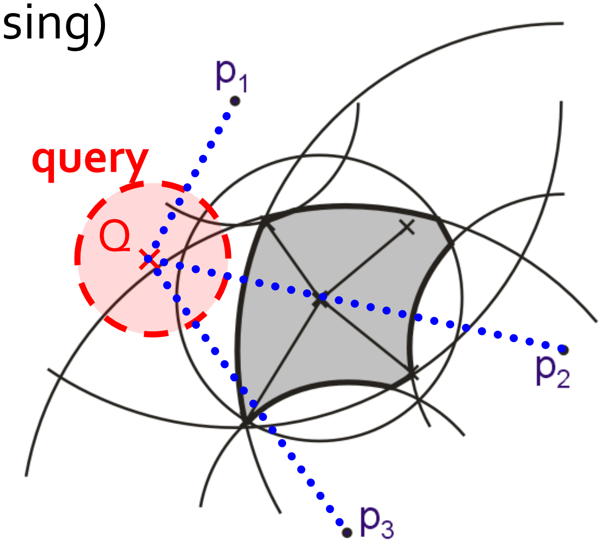
- combinations of different principles
  - pivot tables with hierarchical indexes
    - e.g., PM-tree
  - even more complex, combining pivot tables,
    hierarchical ball-shaped + hyperplane-based indexes, and hashing
    - e.g., M-index
- synergistic effect
  - different principles are most efficient under different conditions,
    so let's employ them all

PM-tree

- PM-tree = M-tree additionally using a set of ***p*** global pivots
- each ball region is further reduced by ***p*** rings, centered in the pivots
- smaller volume of regions
  - better filtering (faster query processing)

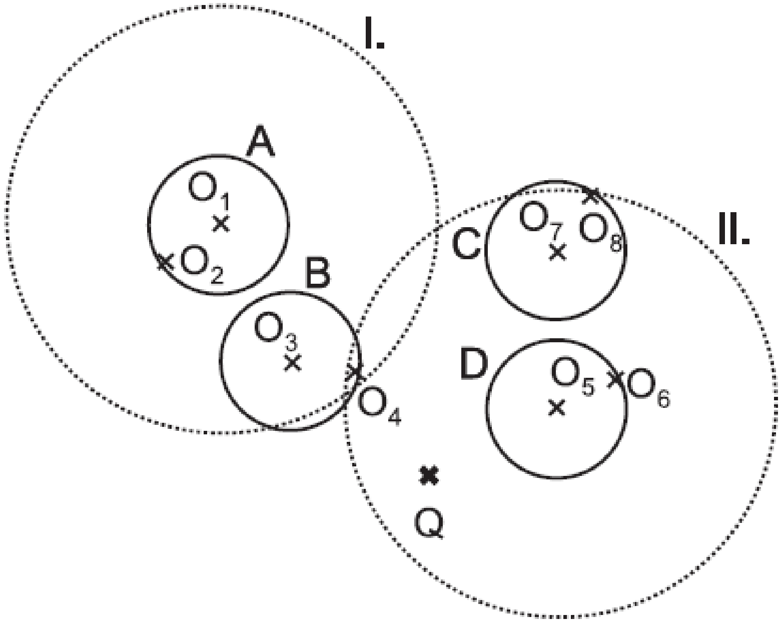


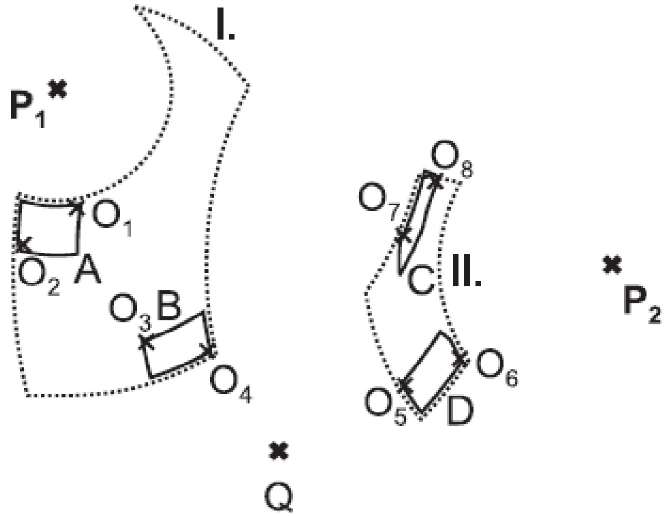
M-tree region



PM-tree region

M-tree vs. PM-tree hierarchy



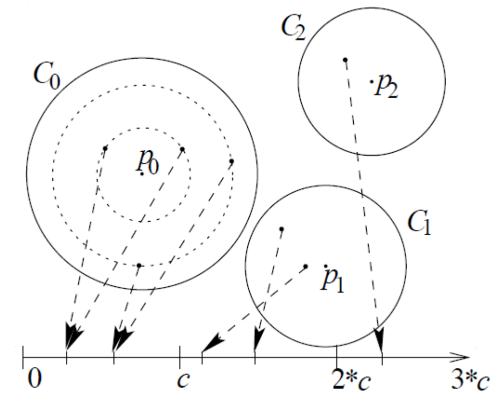


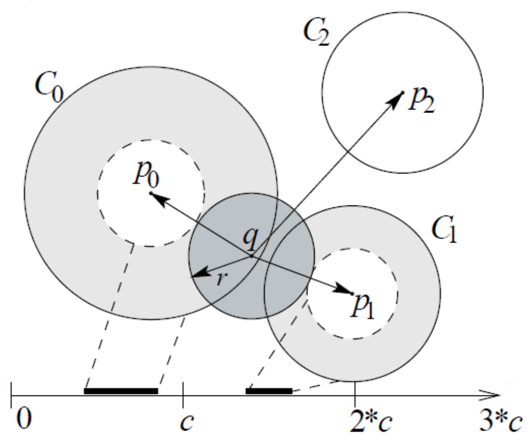
M-index

- combines all of the principles used in MAMs so far
  - pivot tables (for each object the distances to global pivots are stored)
  - hyperplane partitioning
  - ball partitioning
  - hashing (even preserving order)
- the index itself could be any database structure maintaining linear ordering of keys
  - e.g., B+-tree

M-index

- inspired by iDistance (mapping scheme into 1D)
  - select **n** pivots $\mathbf{p_i}$ as centers of clusters $\mathbf{C_i}$
  - let's divide the real axis among **n** intervals <i*c, (i+1)*c>, where **i** is the Id of cluster $\mathbf{C_i}$
  - each object **o** is mapped (hashed) to the Id **i** of the nearest pivot
  - the distance is added to the integer key as the fractional part $iDist(o) = d(p_i, o) + i \cdot c$
    - suppose c=1 and distances normalized to 0..1
  - a range query is then transformed into a set of intervals that have to be searched





(images from Novak and Batko, Metric Index: An Efficient and Scalable Solution for, Similarity Search, SISAP 2009)

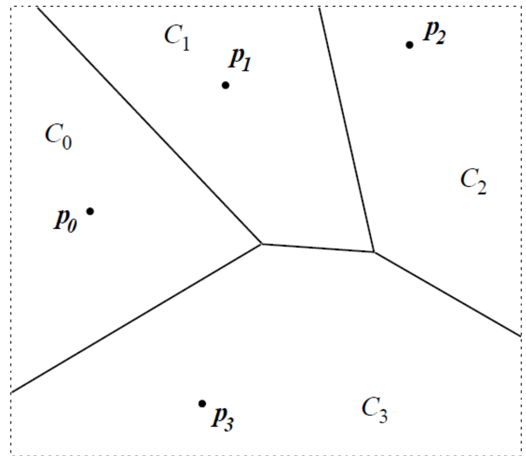
M-index

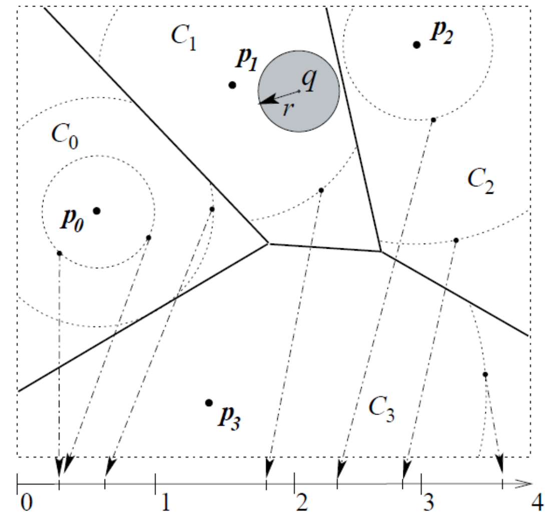
(images from Novak and Batko, Metric Index: An Efficient and Scalable Solution for, Similarity Search, SISAP 2009)

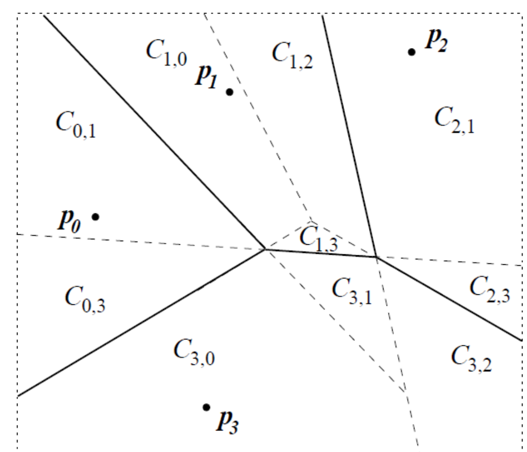
- because the data objects are partitioned among the nearest pivots, the clusters can be filtered as in GNAT

- as in GNAT, recursive partitioning is considered in M-index (so-called **multi-level M-index**), leading to recursive splitting of the intervals on the real axis. The final key of an object **o** is then:

$$key_l(o) = d(p_{(0)_o}, o) + \sum_{i=0}^{l-1} (i)_o \cdot n^{(l-1-i)}$$

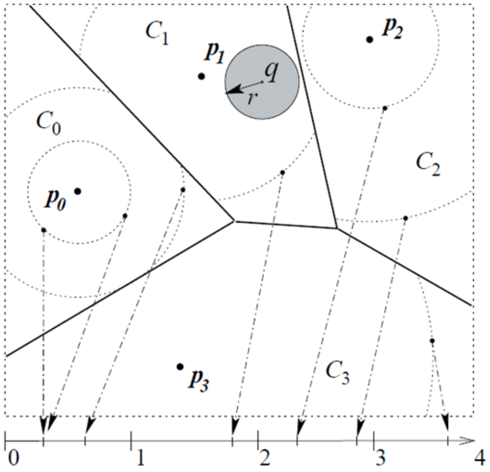






M-index

- in addition to the mapping to real axis, the M-index stores information for additional filtering
  - for each object a vector of distances to the pivots is stored, allowing to consider the non-filtered candidates as a pivot table
  - for each cluster the minimal and maximal radius is stored, to allow ball filtering (as used in M-tree)



Performance measures

- performance of MAM in terms of
  - indexing
  - querying
- cost measures
  - logic cost
    - number of distance computations
    - I/O cost (disk access)
    - internal cost (task-specific algorithms, internal data structures)
    - other (networking, synchronization of parallel processes, etc.)
  - physical overall cost
    - realtime (wall clock time, the response time)

Performance measures

- optimization of the total (index+query) cost
  - sequential scan as reference method
    - no indexing and linear cost queries
  - in database scenario =
    index cost is amortized by reduced query cost
    - frequent queries and not frequent updates
    - outperforms sequential scan in long term
- cost measure selection
  - logic cost measures used in specific evaluation should be dominant components in the realtime
    - other logic cost measures ignored
    - wall clock realtime ignored (affected by external factors)

Distance computations (DC)

- DC = number of distance **δ(*,*)** computations
- DC dominating component in the realtime when
  - expensive distance function is used
    - ≥ $O(n^2)$ and/or large object size (n)
  - rather small database is used
    - fits in main memory

I/O cost (disk accesses)

- classic database-oriented cost (also transactions/per second)
- example comparison HDD vs. SSD for 100 MB index, 4kB disk page, i.e., 25,600 pages
  - HDD (magnetic drive technology)
    - 1990
      - seek time + latency = **65ms**, transfer **600 kB/s** (Seagate ST 225 20MB)
      - sequential scan, **100% pages**, contiguous access = **167 sec**
      - a hierarchical MAM, **1% pages**, random access = **16.6 sec seek + 1.6 sec read = 18.2 sec** (**~9.2x speedup**)
    - 2020
      - seek time + latency = **6ms**, transfer **100 MB/s**
      - sequential scan, **100% pages**, contiguous access = **1 sec**
      - a hierarchical MAM, **1% pages**, random access = **1.5 sec seek + 0.01 sec read = 1.51 sec** (**~0.66x slowdown**)
  - SSD (solid-state drive)
    - sequential read **2150 MB/s**, random read **300k IO/s** (4kB IO, M.2 NAND NVMe), 2020
    - sequential scan, **100% pages**, contiguous access = **45 ms**
    - a hierarchical MAM, **1% pages**, random access = **0.85 ms** (**~52x speedup** vs. 100x theoretical best)

  - hierarchical indexing (random access) makes sense again in SSD (or RAM)!
    - optimized sequential scan could be a surprise in HDD

Internal cost

- more sophisticated MAM $\rightarrow$ more internal overhead
  - various auxiliary main-memory structures + processing
  - overhead data in the index + processing
- examples
  - incremental kNN processing (Hjaltason and Samet)
    - optimal in DC (w.r.t. equivalent range query), **but**
    - huge time/space overhead when managing the heap of requests
  - pivot tables (basic LAESA)
    - scanning the distance matrix
    - consider, e.g., 128 dimensional vector dataset + any L_p distance, 128 pivots $\rightarrow$ distance matrix processing means the **same or worse than simple sequential query (!)**

Realtime cost

- realtime cost (wall-clock time)
  - **cons:**
    - **optimization- and platform-dependent**
    - **harder to set up fair comparison**
  - **pros:**
    - **the only objective measure when it comes to real-world application!**
- real-world example
  - database of up to 5.6 million peptide spectra (pieces of proteins), dim ≈ 32 (intrinsic dim. ≈ 3)
  - **O(n)** variant of Hausdorff distance