Indici per Query di Similarità

Sistemi informativi per le Decisioni

Slide a cura di Prof. Paolo Ciaccia

Plan of activities

- In the following we will go through 2 distinct topics, all of them being related by the common objective to provide efficient support to the execution of similarity queries

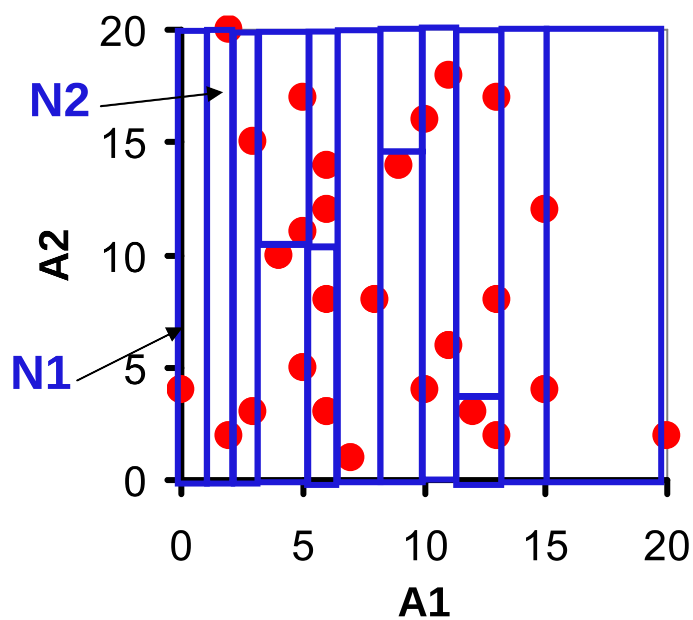
1. We will describe the *R-tree*, by detailing how to search within a vector space
2. Then, we will consider *metric trees*, which allow us to deal even with non-vector features and with distance functions other than (weighted) Lp-norms

Can we exploit indices to solve multi-dimensional queries?

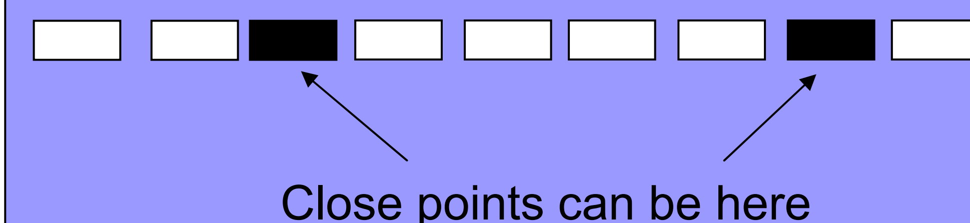
- As a first step we consider B+-trees, assuming that we have one multi-attribute index that organizes (sorts) the tuples according to the order A1,A2,…,AD
- Again, we must understand what this organization implies from a geometrical point of view…

The geometry of B+-trees

- Consider the list of leaf nodes of the B+-tree: N1→N2→N3 →…
- The 1st leaf, N1, contains the smallest value(s) of A1, the number of which depends on the maximum leaf capacity C (=2*B+-tree order) and on data distribution
- The 2nd leaf starts with subsequent values, and so on
- The "big picture" is that the attribute space **A** is partitioned as in the figure

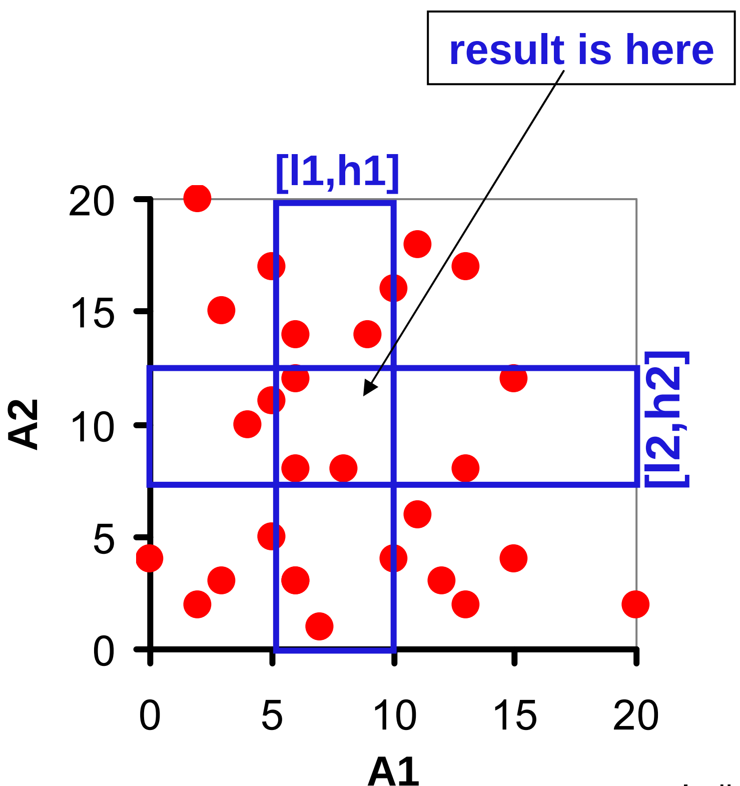


- No matter how we sort the attributes, searching for the k-NN of a point q will need to access too many nodes
- The basic reason is that "close" points of **A** are quite far apart in the list of leaves, thus moving along a coordinate (e.g., A1) will "cross" too many nodes



Another approach based on B+-trees

- Assume that we somehow know, e.g., using DB statistics (see [CG99]), that the k-NN of q are in the (hyper-)rectangle with sides [l1,h1]x [l2,h2]x…
- Then we can issue D independent range queries `Ai BETWEEN li AND hi` on the D indexes on A1,A2,…,AD, and then intersect the results



- Besides the need to know the ranges, with this strategy we waste a lot of work
- This is roughly proportional to the union of the results minus their intersection

Multi-dimensional (spatial) indices

- The multi-attribute B+-tree maps points of **A** $\subseteq \Re^D$ into points of $\Re$
- This "linearization" necessarily favors, depending on how attributes are ordered in the B+-tree, one attribute with respect to others
  - A B+-tree on (X,Y) favors queries on X, it cannot be used for queries that do not specify a restriction on X
- Therefore, what we need is a way to organize points so as to preserve, as much as possible, their "spatial proximity"

- The issue of "spatial indexing" has been under investigation since the 70's, because of the requirements of applications dealing with "spatial data" (e.g., cartography, geographic information systems, VLSI, CAD)
- More recently (starting from the 90's), there has been a resurrection of interest in the problem due to the new challenges posed by several other application scenarios, such as multimedia
- We will now just consider one (indeed very relevant!) spatial index…

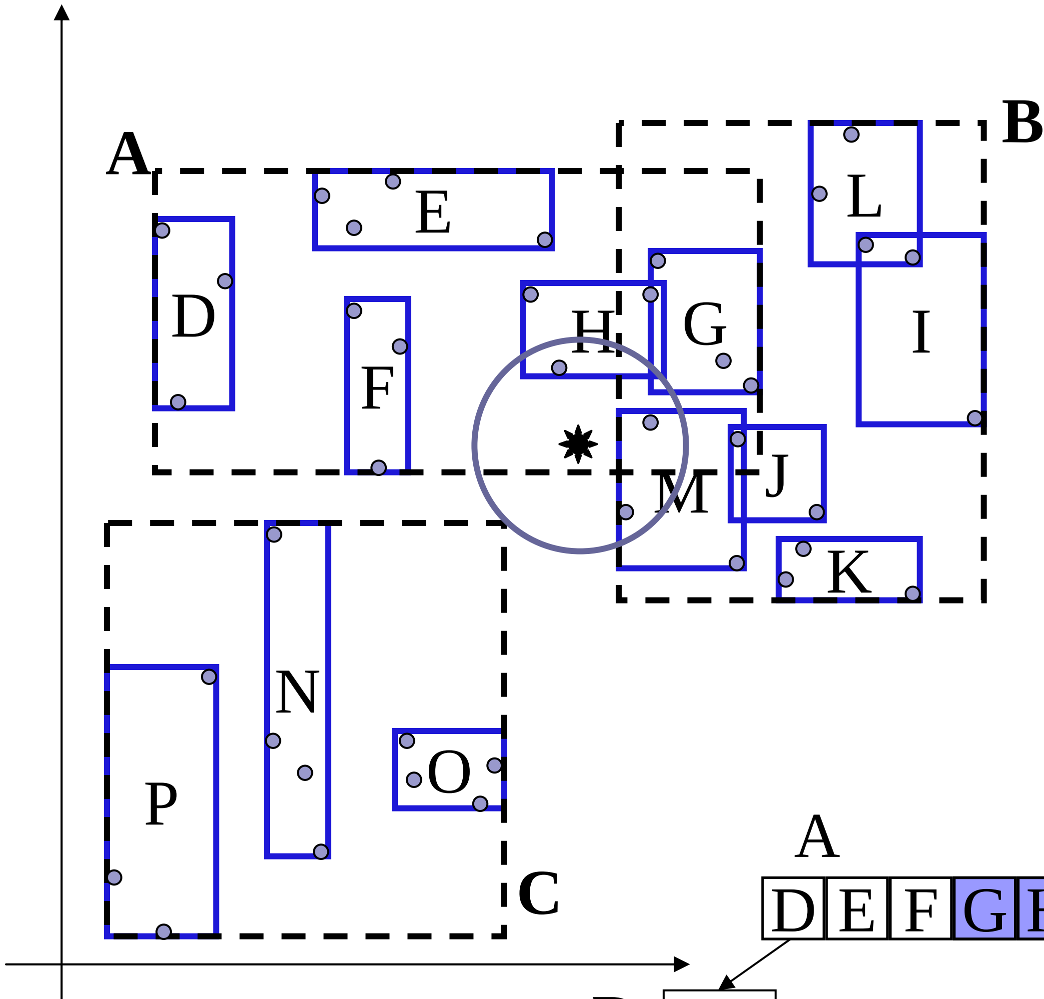
The R-tree (Guttman, 1984)

- The R-tree [Gut84] is (somewhat) an extension of the B+-tree to multi-dimensional spaces, in that:
- The B+-tree organizes objects into
  - a set of (non-overlapping) 1-D intervals,
  - and then applies recursively this basic principle up to the root,
- the R-tree does the same but now using
  - a set of (possibly overlapping) m-D intervals, i.e., (hyper-)rectangles!,
  - and then applies recursively this basic principle up to the root

- The R-tree is also available in some commercial DBMS's, such as Oracle9i
- In the following we just present the aspects relevant to query processing, and postpone the discussion on R-tree management (insertion and split)

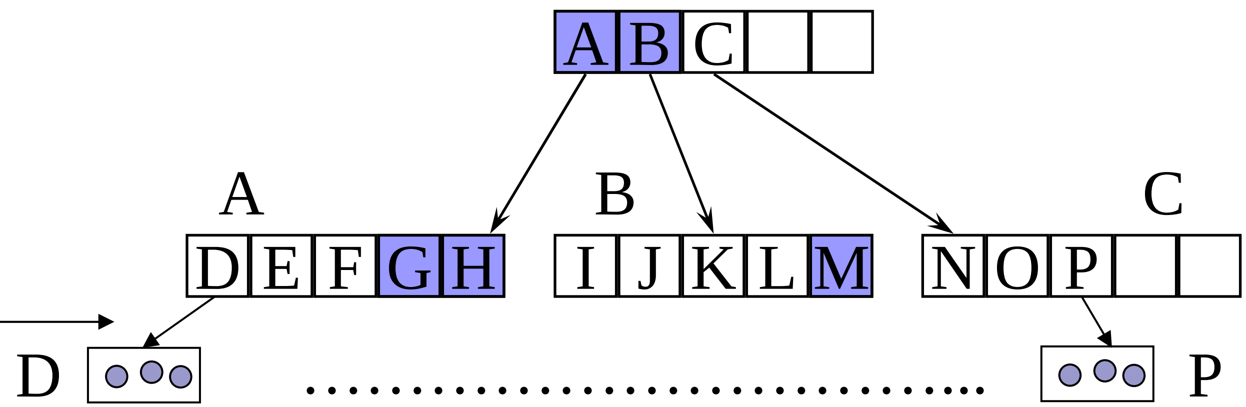
➡ Be sure to understand what the index looks like and how it is used to answer queries; for the moment don't be concerned on how an R-tree with a given structure can be built!

R-tree: the intuition



- Recursive bottom-up aggregation of objects based on MBR's
- Regions can overlap

- This is a 2-D *range query* using L2, other queries and distance functions can be supported as well



R-tree basic properties (i)

- The R-tree is a dynamic, height-balanced, and paged tree
- Each node stores a variable number of *entries*

Leaf node:

- An entry E has the form E=(tuple-key,TID), where tuple-key is the "spatial key" (position) of the tuple whose address is TID (remind: TID is a pointer)

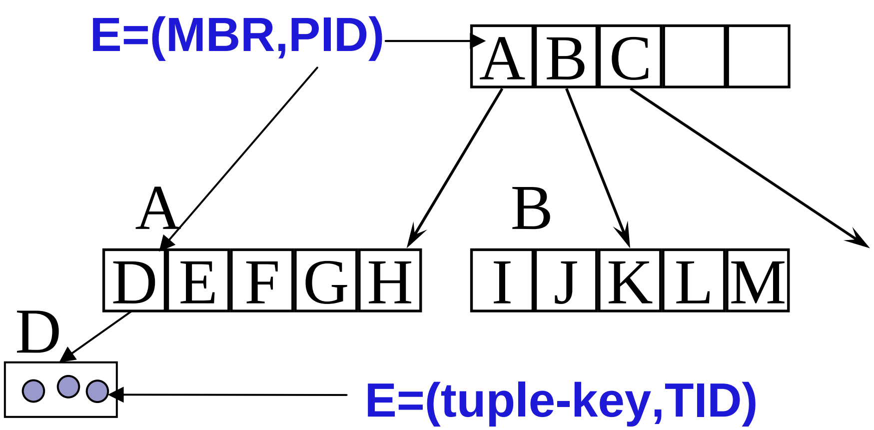
Internal node:

- An entry E has the form E=(MBR,PID), where MBR is the "Minimum Bounding Rectangle" (with sides parallel to the coordinate axes) of all the points reachable from ("under") the child node whose address is PID (PID = page identifier)

- We can uniform things by saying that each entry has the format

  E=(key,ptr)

- If N is the node pointed by E.ptr, then E.key is the "spatial key" of N

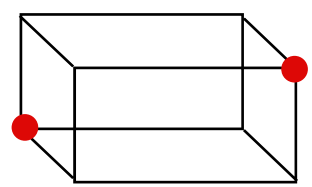


R-tree basic properties (ii)

- The number of entries varies between c and C, with $c \leq 0.5*C$ being a design parameter of the R-tree and C being determined by the node size and the size of an entry (in turn this depends on the space dimensionality)

- The root (if not a leaf) makes an exception, since it can have as low as 2 children

- Note that a (hyper-)rectangle of $\Re^D$ with sides parallel to the coordinate axes can be represented using only 2*D floats that encode the coordinate values of 2 opposite vertices



Search: range query (i)

- We start with a query type simpler than k-NN queries, namely the

> **Range Query**
> - Given a point q, a relation R, a search radius $r \geq 0$, and a distance function d,
> - Determine all the objects t in R such that $d(t,q) \leq r$

- The region of $\Re^D$ defined as $Reg(q) = \{p: p \in \Re^D, d(p,q) \leq r\}$ is also called the query region (thus, the result is always contained in the query region)
  - For simplicity, both d and r are understood in the notation Reg(q)

- In the literature there are several variants of range queries, such as:
  - Point query: when r = 0 (i.e., it looks for a perfect (exact) match)
  - Window query: when the query region is a (hyper-)rectangle (a window)

Search: range query (ii)

- The algorithm for processing a range query is extremely simple:
  - We start from the root and, for each entry E in the root node, we check if E.key intersects Reg(q):

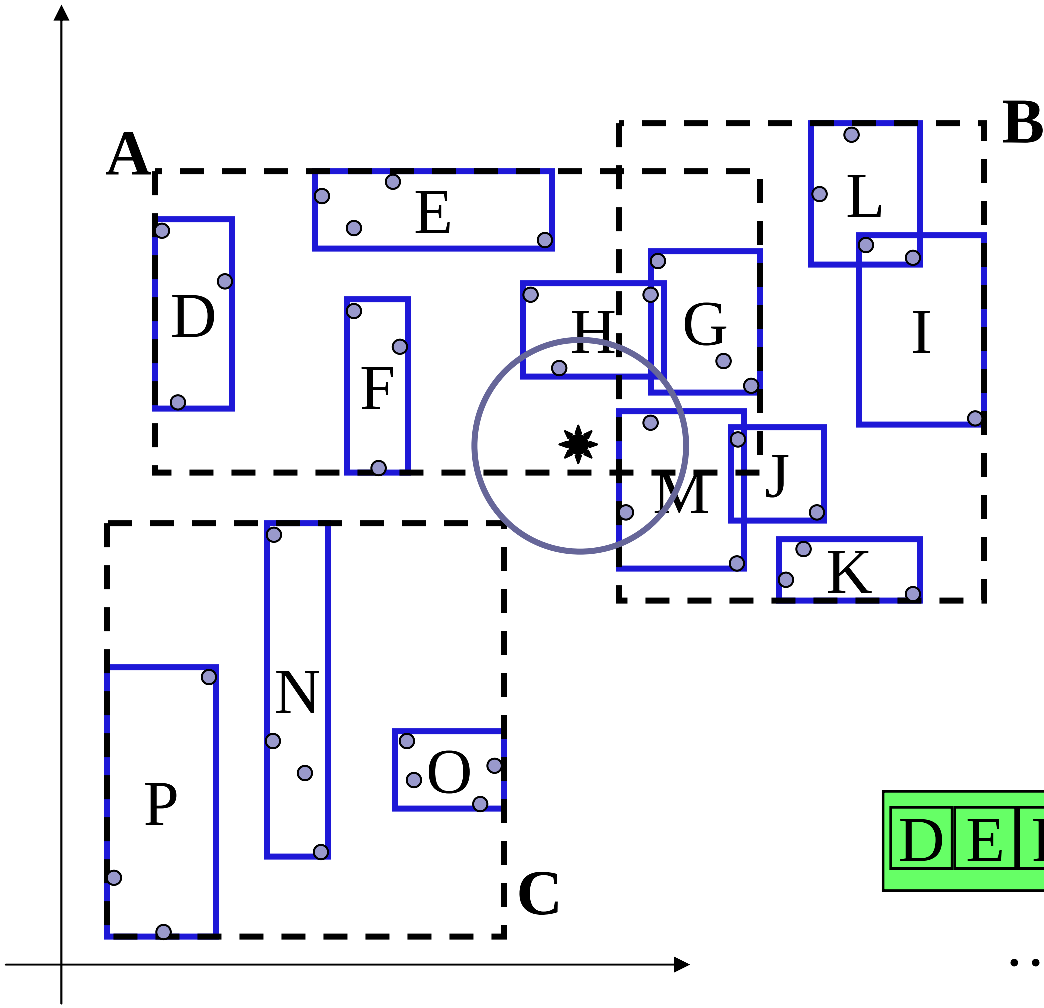
    Req(q) $\cap$ E.key $\neq \emptyset$: we access the child node N referenced by E.ptr

    Req(q) $\cap$ E.key $= \emptyset$: we can discard node N from the search
  - When we arrive at a leaf node we just check for each entry E if E.key $\in$ Reg(q), that is, if d(E.key,q) $\leq$ r.
    - If this is the case we can add E to the result of the index search

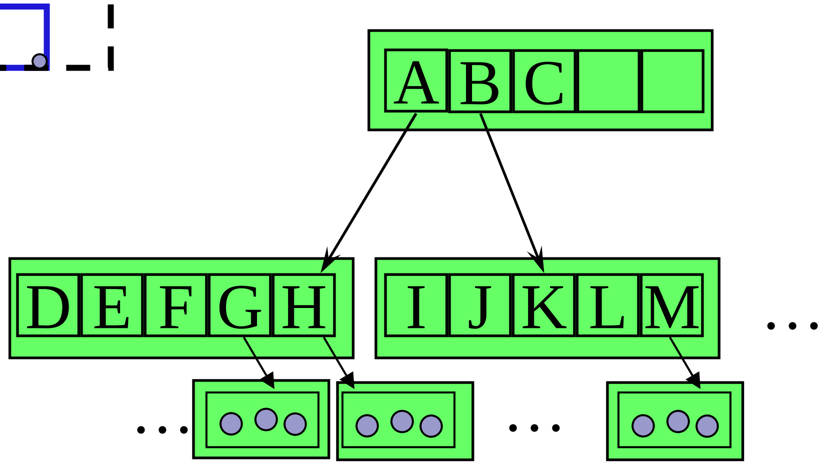
RangeQuery(q,r,N)
{ if N is a leaf then: for each E in N:
if d(E.key,q) $\leq$ r then add E to the result
else: for each E in N:
if Req(q) $\cap$ E.key $\neq \emptyset$ then RangeQuery(q,r,*(E.ptr) }

- The recursion starts from the root of the R-tree
  - The notation N = *(E.ptr) means "N is the node pointed by E.ptr"
  - Sometimes we also write ptr(N) in place of E.ptr

Range queries in action



- The navigation follows a depth-first pattern
- This ensures that, at each time step, the maximum number of nodes in memory is h=height of the R-tree
- Such nodes are managed using a stack



Search: k-NN query (i)

- With the aim to better understand the logic of k-NN search, let us define for a node N = *(E.ptr) of the R-tree its region as

  Reg(*(E.ptr)) = Reg(N) = {p: p $\in \Re^D$, p $\in$ E.key=E.MBR}

- Thus, we access node N if and only if (iff) Req(q) $\cap$ Reg(N) $\neq \emptyset$
- Let us now define d_{MIN}(q,Reg(N)) = $\inf_p$\{d(q,p) | p $\in$ Reg(N)\}, that is, the minimum possible distance between q and a point in Reg(N)

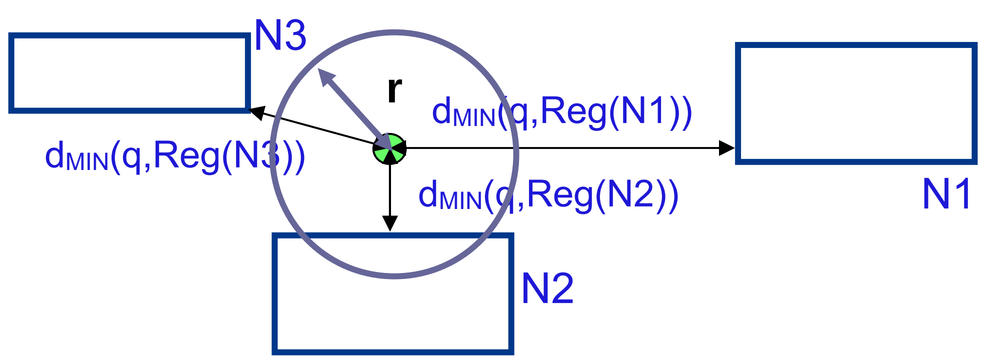
  - The "MinDist" d_{MIN}(q,Reg(N)) is a lower bound on the distances from q to any indexed point reachable from N

- We can make the following basic observation:

  Req(q) $\cap$ Reg(N) $\neq \emptyset$

  $\Leftrightarrow$

  d_{MIN}(q,Reg(N)) $\leq$ r



Search: k-NN query (ii)

- We now present an algorithm, called kNNOptimal [BBK+97], for solving k-NN queries with an R-tree
  - The algorithm also applies to other index structures (e.g., the M-tree) that we will see in this course
- For simplicity, consider the basic case k=1
- For a given query point q, let $t_{NN}(q)$ be the 1st nearest neighbor (1-NN = NN) of q in R, and denote with $r_{NN} = d(q, t_{NN}(q))$ its distance from q
  - Clearly, r_{NN} is only known when the algorithm terminates

Theorem:

- Any algorithm for 1-NN queries must visit at least all the nodes N whose MinDist is less than r_{NN}

Proof: Assume that an algorithm ALG stops by reporting as NN of q a point t and that ALG does not read a node N such that (s.t.) $d_{MIN}(q,Reg(N)) < d(q,t)$; then Reg(N) might contain a point t' s.t. $d(q,t') < d(q,t)$, thus contradicting the hypothesis that t is the NN of q ■

The logic of the kNNOptimal Algorithm

- The kNNOptimal algorithm uses a priority queue PQ, whose elements are pairs [ptr(N), d_{MIN}(q,Reg(N))]
- PQ is ordered by *increasing values* of d_{MIN}(q,Reg(N))
  - DEQUEUE(PQ) extracts from PQ the pair with minimal MinDist
  - ENQUEUE(PQ, [ptr(N), d_{MIN}(q,Reg(N))]) performs an ordered insertion of the pair in the queue
- Pruning of the nodes is based on the following observation:

> - If, at a certain point of the execution of the algorithm, we have found a point t s.t. d(q,t) = r,
> - Then, all the nodes N with $d_{MIN}(q,Reg(N)) \geq r$ can be excluded from the search, since they cannot lead to an improvement of the result

  - In the description of the algorithm, the pruning of pairs of PQ based on the above criterion is concisely denoted as UPDATE(PQ)
  - With a slight abuse of terminology, we also say that “the node N is in PQ” meaning that the corresponding pair [ptr(N), d_{MIN}(q,Reg(N))] is in PQ
- Intuitively, kNNOptimal performs a “*range search with a variable (shrinking) search radius*” until no improvement is possible anymore

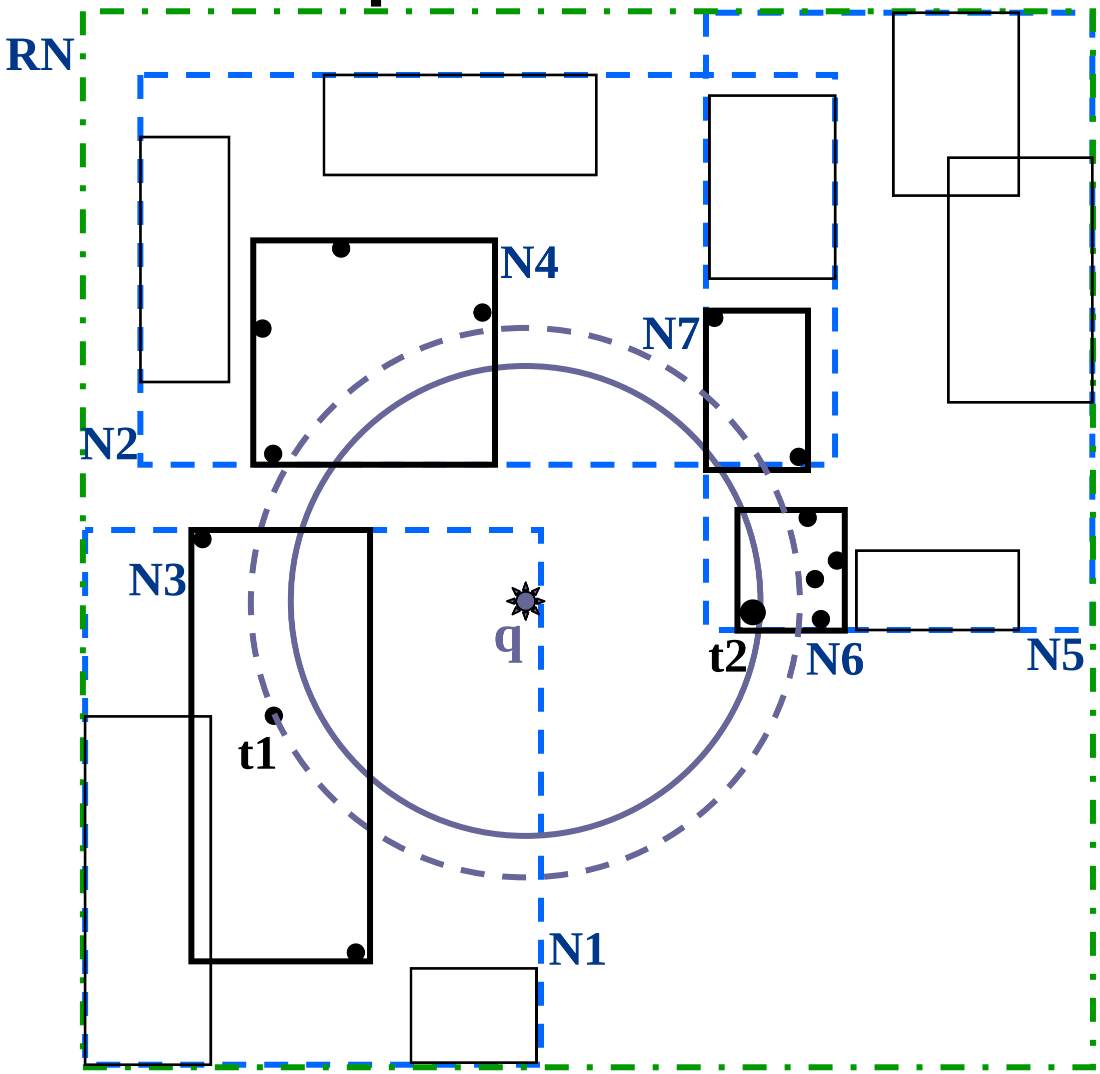
The kNNOptimal Algorithm (case k=1)

Input: query point q, index tree with root node RN

Output: $t_{NN}(q)$, the nearest neighbor of q, and $r_{NN} = d(q, t_{NN}(q))$

```
Initialize PQ with [ptr(RN),0];     // starts from the root node
r_NN := ∞;                          // this is the initial "search radius"
while PQ ≠ ∅:                                          // until the queue is not empty…
    [ptr(N), d_MIN(q,Reg(N))] := DEQUEUE(PQ);          // … get the closest pair…
    Read(N);                                           // … and reads the node
    if N is a leaf then: for each point t in N:
                    if d(q,t) < r_NN then: {t_NN(q) := t; r_NN := d(q,t); UPDATE(PQ)}
                          // reduces the search radius and prunes nodes
              else: for each child node Nc of N:
                    if d_MIN(q,Reg(Nc)) < r_NN then:
                          ENQUEUE(PQ,[ptr(Nc), d_MIN(q,Reg(Nc))]);
return t_NN(q) and r_NN;
end.
```

kNNOptimal in action



- Nodes are numbered following the order in which they are accessed
- Objects are numbered as they are found to improve (reduce) the search radius
- The accessed leaf nodes are shown in red

Correctness and Optimality of kNNOptimal

- The kNNOptimal algorithm is clearly correct
- To show that it is also optimal, that is, it reads the minimum number of nodes, it is sufficient to prove that

it never reads a node N s.t. $d_{MIN}(q,Reg(N)) > r_{NN}$

Proof:

- Indeed, N is read only if, at a certain execution step, it becomes the 1st element in the priority queue PQ
- Let N1 be the node containing $t_{NN}(q)$, N2 its parent node, N3 the parent node of N2, and so on, up to Nh = RN (h = height of the tree)
- Now observe that, by definition of MinDist, it is:

$$r_{NN} \geq d_{MIN}(q,Reg(N1)) \geq d_{MIN}(q,Reg(N2)) \geq \ldots \geq d_{MIN}(q,Reg(Nh))$$

- At each time step before we find $t_{NN}(q)$, one (and only one) of the nodes N1,N2,…,Nh is in the priority queue
- It follows that N can never become the 1st element of PQ ■

The general case (k ≥ 1)

- The algorithm is easily extended to the case k ≥ 1 by using:
  - a data structure, which we call ResultList, where we maintain the k closest objects found so far, together with their distances from q
  - as "current search radius" the distance, $r_{k\text{-}NN}$, of the current k-th NN of q, that is, the k-th element of ResultList

ResultList

ObjectID	distance
t15	4
t24	8
t18	9
t4	12
t2	**15**

k = 5

- No node with distance ≥ 15 needs to be read

- The rest of the algorithm remains unchanged

The kNNOptimal Algorithm (case k $\geq$ 1)

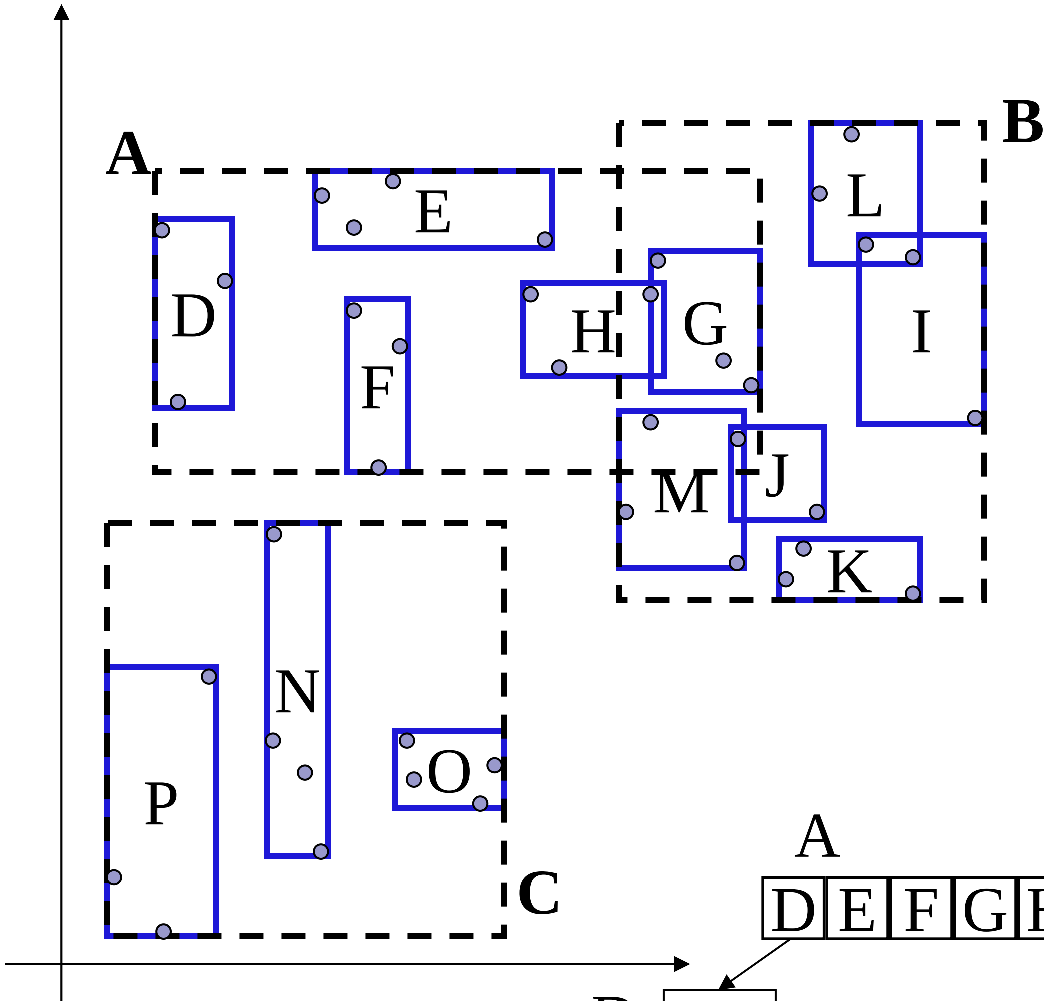
Input: query point q, integer k $\geq$ 1, index tree with root node RN
Output: the k nearest neighbors of q, together with their distances

Initialize PQ with [ptr(RN),0];
for i=1 to k: ResultList(i) := [null,∞]; $r_{k\text{-}NN}$:= ResultList(k).dist;
while PQ $\neq \emptyset$:
    [ptr(N), d_{MIN}(q,Reg(N))] := DEQUEUE(PQ);
    Read(N);
    if N is a leaf then: for each point t in N:
        if d(q,t) < $r_{k\text{-}NN}$ then: { remove the element in ResultList(k);
            insert [t,d(q,t)] in ResultList;
            $r_{k\text{-}NN}$:= ResultList(k).dist; UPDATE(PQ)}
    else: for each child node Nc of N:
        if d_{MIN}(q,Reg(Nc)) < $r_{k\text{-}NN}$ then:
            ENQUEUE(PQ,[ptr(Nc), d_{MIN}(q,Reg(Nc))]);
return ResultList;
end.

Back to the R-tree

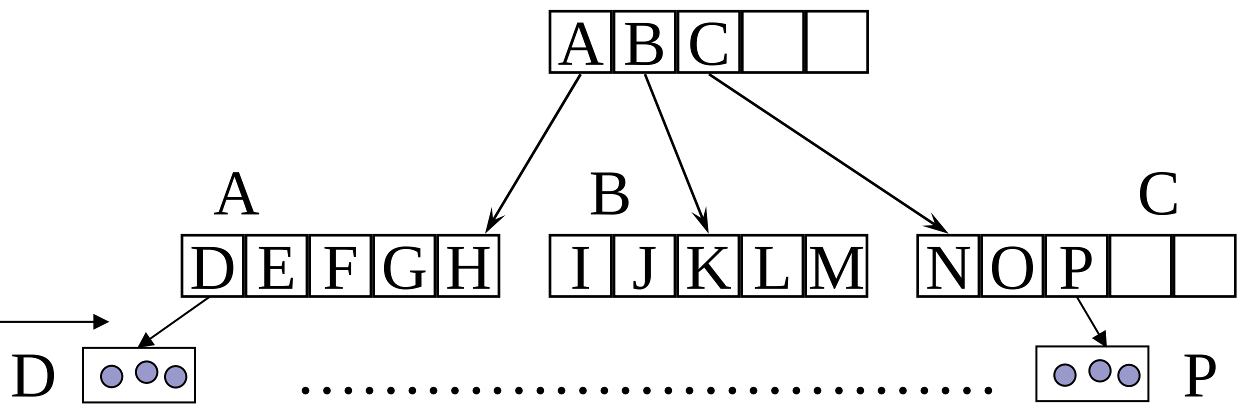
- It's now time to discuss how an R-tree can be effectively built
- It has to be considered that many "*R-tree variants*" exist, and it's not our intention to go through their details
- It just suffices to say that one of such variants leads to what is known as the R*-tree [BKS+90], which is the commonest version in use
- With respect to the original proposal [Gut84], the R*-tree adds smarter insertion and split heuristics, plus a so-called "forced reinsert" technique that we do not consider here

R-tree: how it looks like



Remind:

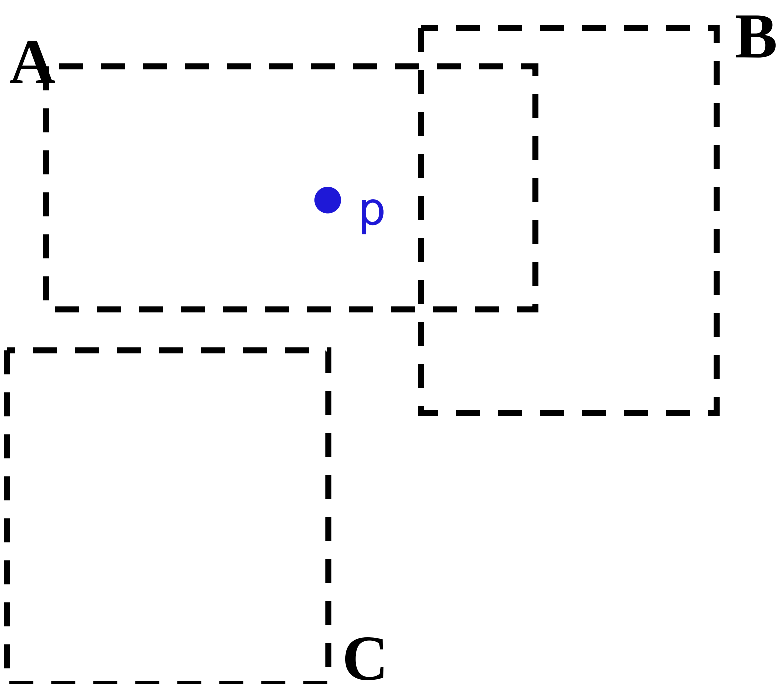
- Recursive bottom-up aggregation of objects based on MBR's
- Regions can overlap
- Each node can contain up to C entries, but not less than c ≤ 0.5*C
  - The root makes an exception

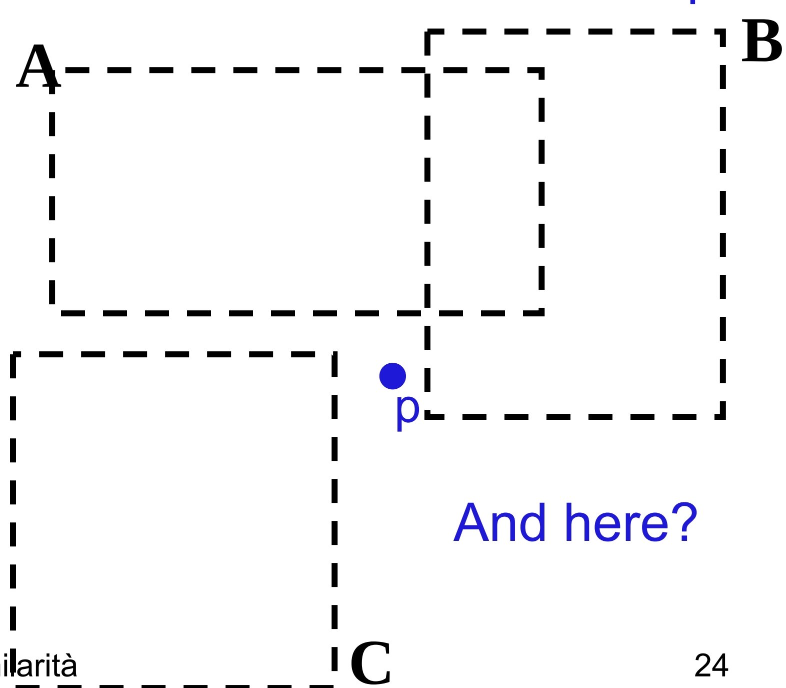


R-tree: insertion of a new object

- We start from the root and move down the tree one step at a time, trying to find a “nice place” where to accommodate the new object p
  - For simplicity, we assume that indexed objects are points, similar arguments apply if we index (hyper-)rectangles (MBR’s)
- At each step we have a same question to answer:

Which child node is the most suitable to accommodate p?





And here?

R-tree: the ChooseSubtree method

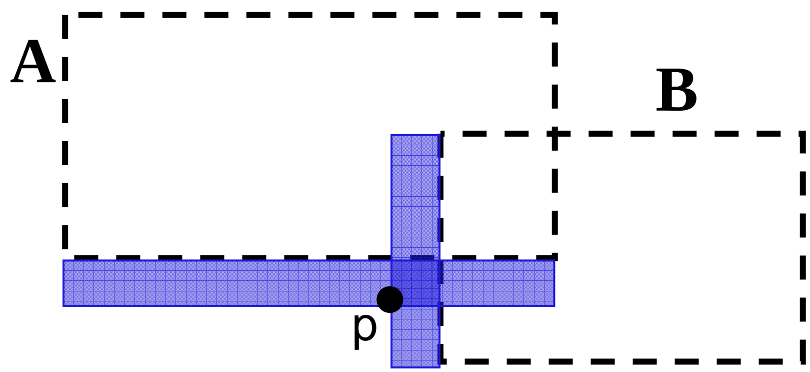
- The recursive algorithm that descends the tree to insert a new object p, together with its TID, is called ChooseSubtree

```
ChooseSubtree(Ep=(p,TID),ptr(N))
Read(N);
If N is a leaf    then:    return N                                  // we are done
                  else:    { choose among the entries Ec in N
                                 the one, Ec*, for which Penalty(Ep,Ec*) is minimum;
                             return ChooseSubtree(Ep,Ec*.ptr) }      // recursive call
end.
```

- We invoke the method on the index root
- The specific criterion used to decide "how bad" an entry is, should we choose it to insert p, is encapsulated in the Penalty method
  - Variants of the R-tree differ in how they implement Penalty
- This insertion algorithm is the one used by most multi-dimensional and metric trees

R-tree: the Penalty method

- If point p is inside the region of an entry Ec, then the penalty is 0
- Otherwise, Penalty can be computed as the increment of volume (area) of the MBR
  - However, if Ec points to a leaf node, then [BKS+90] shows that it's better to consider the increment of overlap with the other entries
- Both criteria aim to obtain trees with better performance:
  - Large area: increases the number of nodes to be visited by a query
  - Large overlap: also degrades performance

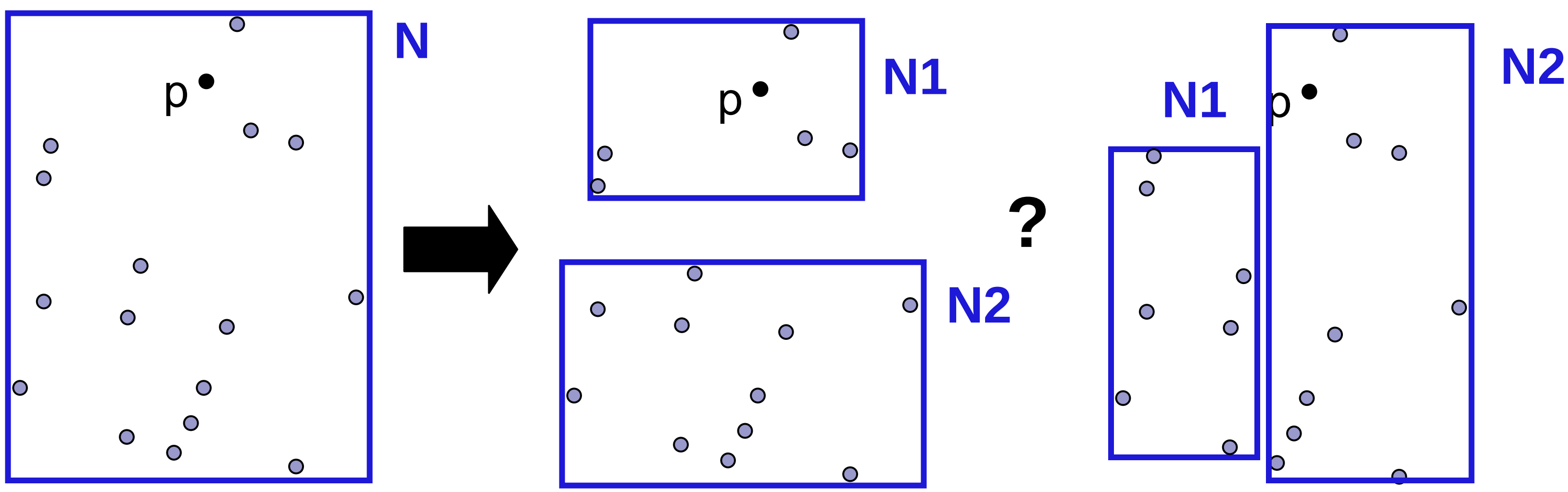


B is better than A

R-tree: splitting of a leaf node

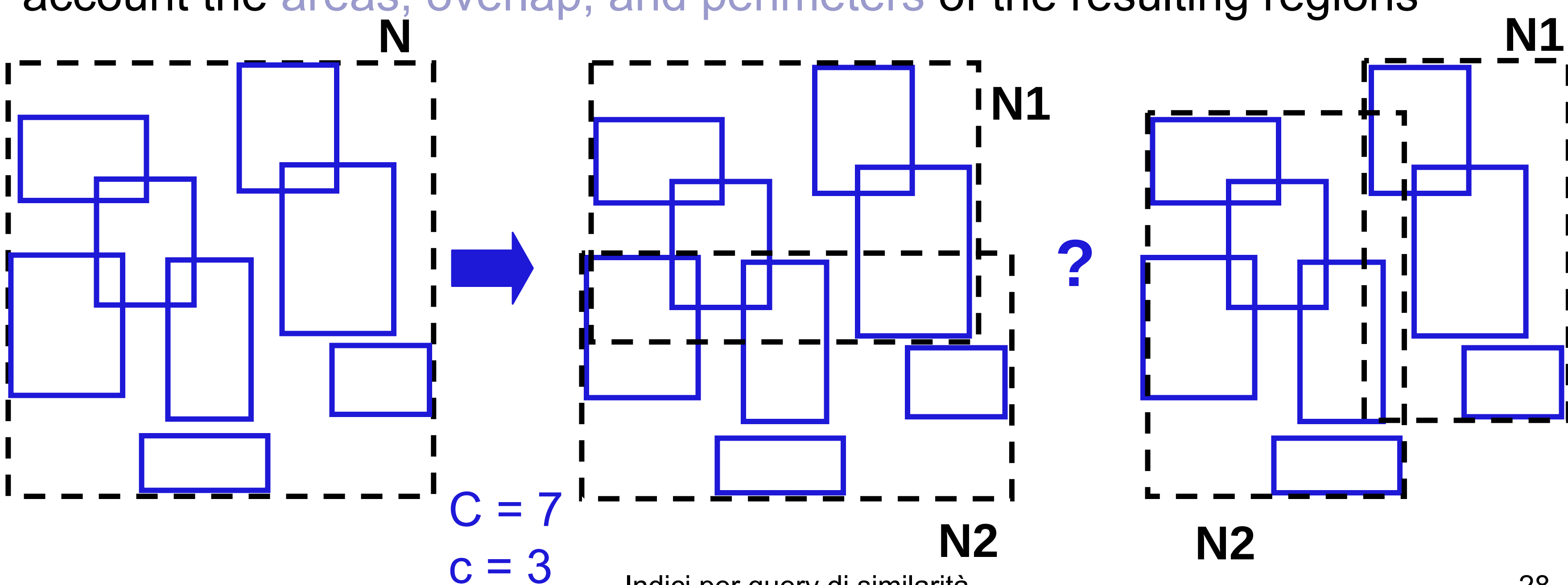
- When p has to be inserted into a leaf node that already contains C entries, an overflow occurs, and N has to be split
- For leaf nodes whose entries are points the solution aims to split the set of C+1 points into 2 subsets, each with at least c and at most C points
- Among the several possibilities, one could consider the choice that leads to have a minimum overall area
  - However, this is an NP-Hard problem, thus heuristics have to be applied

C = 16
c = 6



R-tree: splitting of a non-leaf node

- As in B+-trees, splits propagate upward and can recursively trigger splits at higher levels of the tree
- The problem to be faced now is how to split a set of C+1 (hyper-)rectangles
  - Note that this applies also to leaf nodes if they store MBR's
- The original proposal just aims to minimize the sum of resulting areas
- The R*-tree implements a more sophisticated criterion, which takes into account the areas, overlap, and perimeters of the resulting regions

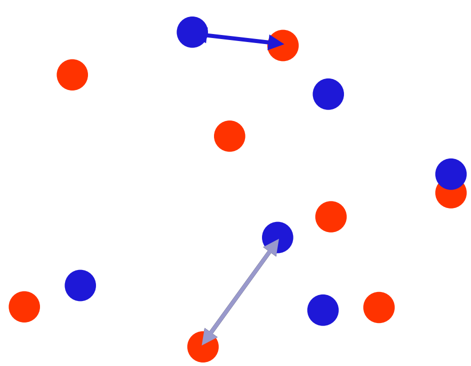


Beyond vector spaces

- It's a matter of fact that vector spaces, equipped with some (weighted) Lp-norm, are not general enough to deal with the whole variety of feature types and distance functions needed in MMDB's

Example:

given 2 sets of points s1 and s2, their Hausdorff distance is defined as follows:



1 ∀ (red) point of s1 find the closest (blue) point in s2
Let **h(s1,s2)** be the maximum of such distances

2 ∀ (blue) point in s2 find the closest (red) point in s1
Let **h(s2,s1)** be the maximum of such distances

3 Let $\mathbf{d_{Haus}(s1,s2)}$ = max{ h(s1,s2), h(s2,s1) }

Used for matching shapes

Another example: edit distance

- A common distance measure for *strings* is the so-called edit distance, defined as the minimum number of characters that have be inserted, deleted, or substituted so as to transform a string s1 into another string s2

d_{edit}('ball','bull') = 1 d_{edit}('balls','bell') = 2 d_{edit}('rather','alter') = 3

- The edit distance is also commonly used in *genomic* DB's to compare DNA sequences. Each DNA sequence is a string over the 4-letters alphabet of bases:

  a: adenine
  c: cytosine
  g: guanine
  t: thymine

d_{edit}('gatctggtgg','agcaaatcag') = 7

g	a	t	c	t	g	g	t	g	-	g
1	=	2	=	3	4	5	=	6	7	=
-	a	g	c	a	a	a	t	c	a	g

The edit distance can be computed using a dynamic programming procedure

Metric spaces

- A metric space M = (U,d) is a pair, where
  U is a domain ("universe") of values, and
  d is a distance function that, $\forall$ x,y,z $\in$ U, satisfies the metric axioms:

$d(x,y) \geq 0$, $d(x,y) = 0 \Leftrightarrow x = y$	**(positivity)**
$d(x,y) = d(y,x)$	**(symmetry)**
$d(x,y) \leq d(x,z) + d(z,y)$	**(triangle inequality)**

  - All the distance functions seen in the previous examples are metrics, and so are the (weighted) Lp-norms

Metric indexes only use the metric axioms
to organize objects, and exploit
the triangle inequality to prune the search space

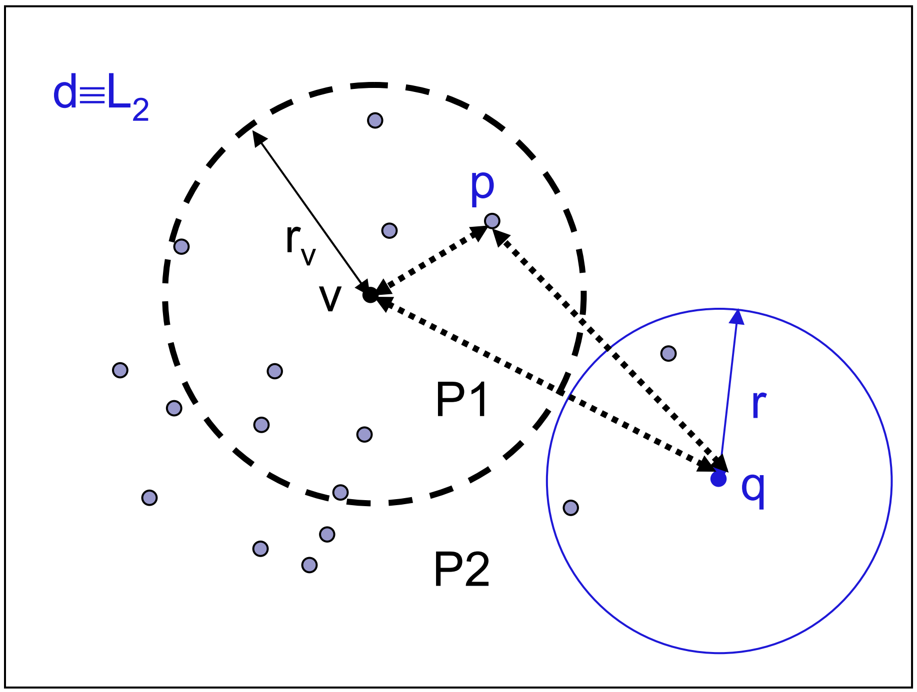
Principles of metric indexing (i)

- Given a "metric dataset" $P \subseteq \mathbf{U}$, one of the two following principles can be applied to partition it into two subsets

Ball decomposition: take a point v ("vantage point"), compute the distances of all other points p w.r.t. v, d(p,v), and define

$P1 = \{p : d(p,v) \leq r_v \}$ $P2 = \{p : d(p,v) > r_v \}$

If r_v is chosen so that $|P1| \approx |P2| \approx |P|/2$ we obtain a balanced partition



Consider a range query $\{p: d(p,q) \leq r\}$
If $\mathbf{d(q,v) > r_v + r}$ we can conclude that no point in P1 belongs to the result
Proof:
we show that $d(p,q) > r$ holds $\forall p \in P1$.

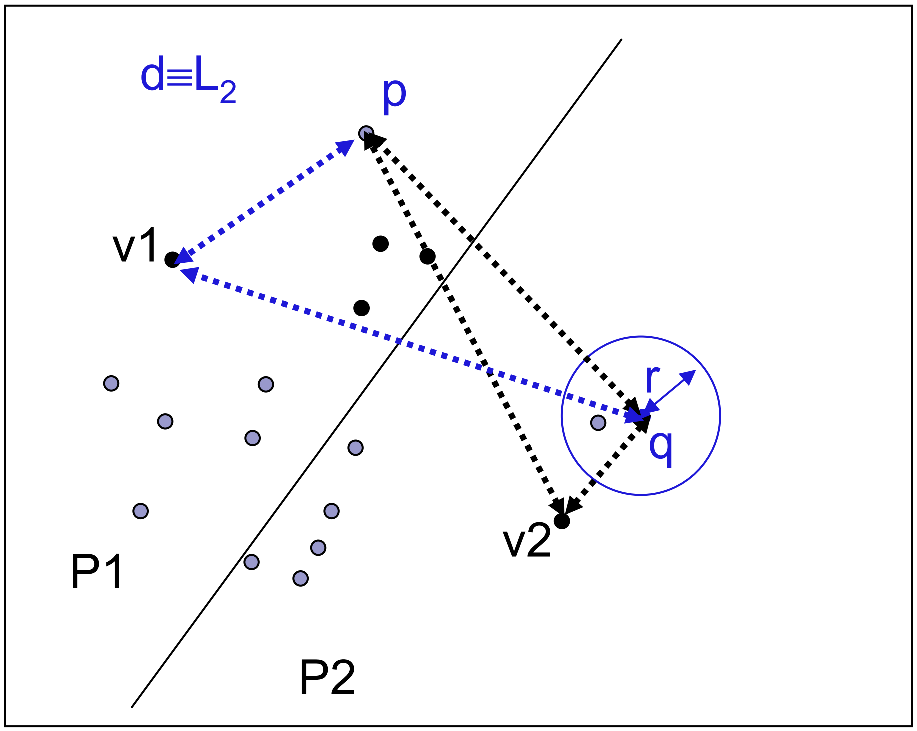
$d(p,q) \geq d(q,v) - d(p,v)$ (triangle ineq.)
$> r_v + r - d(p,v)$ (by hyp.)
$\geq r_v + r - r_v$ (by def. of P1)
$\geq r$ ■

Similar arguments can be applied to P2

Principles of metric indexing (ii)

Generalized Hyperplane: take two points v1 and v2, compute the distances of all other points p w.r.t. v1 and v2, and define

$P1 = \{p : d(p,v1) \leq d(p,v2)\}$ $P2 = \{p : d(p,v2) < d(p,v1) \}$



Consider a range query $\{p: d(p,q) \leq r\}$
If **d(q,v1) – d(q,v2) > 2*r** we can conclude that no point in P1 belongs to the result
Proof:
we show that $d(p,q) > r$ holds $\forall p \in P1$.

$d(q,v1) - d(p,q) \leq d(p,v1)$	(triangle ineq.)
$d(p,v1) \leq d(p,v2)$	(def. of P1)
$d(p,v2) \leq d(p,q) + d(q,v2)$	(triangle ineq.)

Then:

$d(q,v1) - d(p,q) \leq d(p,q) + d(q,v2)$

$d(p,q) \geq (d(q,v1) - d(q,v2))/2$

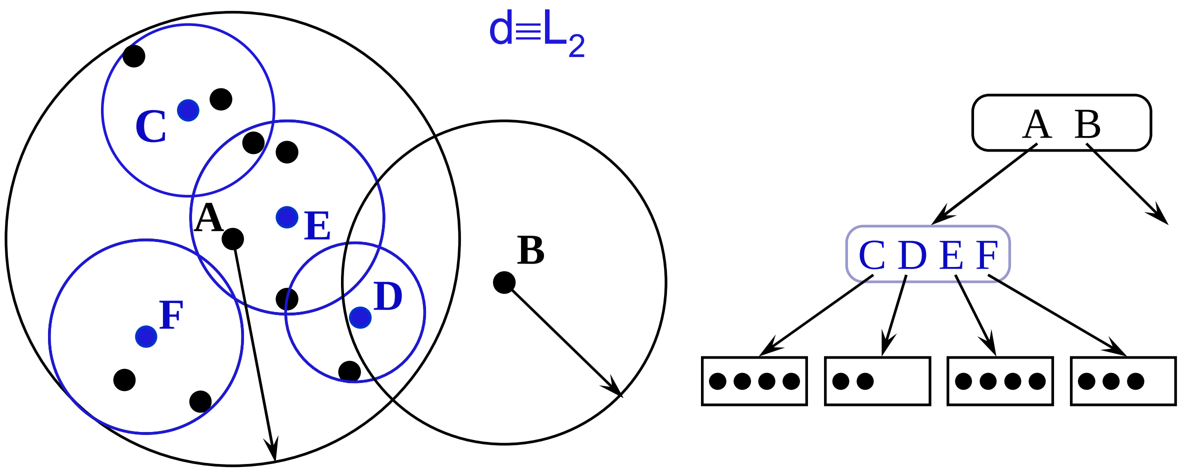
$> r$ (by hyp.) ■

The M-tree (Ciaccia, Patella, Zezula, 1997)

- The M-tree has been the first dynamic, paged, and balanced metric index
- Intuitively, it generalizes "R-tree principles" to arbitrary metric spaces
  - The M-tree treats the distance function as a "black box"
- Since 1997 [CPZ97] it has been used by several research groups for:
  - Image retrieval, text indexing, shape matching, clustering algorithms (including the WWW log example), fingerprint matching, DNA DB's, etc.
  - [CNB+01] and [HS03] are both excellent surveys on searching in metric spaces
- C++ source code freely available at http://www-db.deis.unibo.it/Mtree/

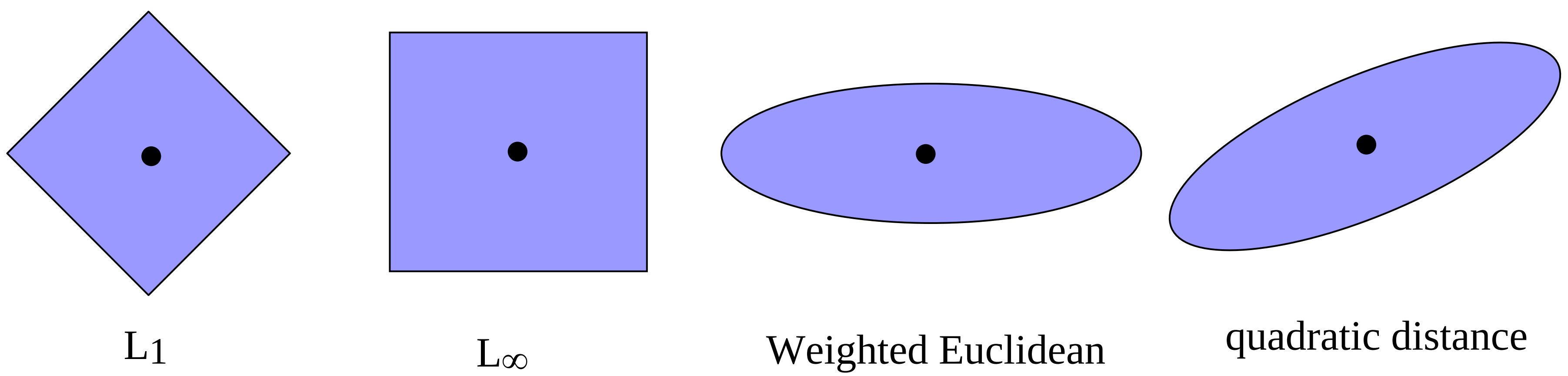
- Remind: at a first sight, the M-tree "looks like" an R-tree.
  However, remember that the M-tree only "knows" about distance values, thus it ignores coordinate values and does not rely on any "geometric" (coordinate-based) reasoning

M-tree: how it looks like



- Recursive bottom-up aggregation of objects based on regions
- Regions can overlap
- Each node can contain up to C entries, but not less than $c \leq 0.5*C$
  - The root makes an exception

- Depending on the metric, the "shape" of index regions changes



The M-tree regions

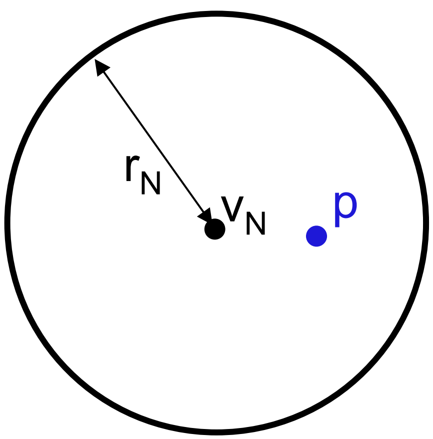
- Each node N of the tree has an associated region, Reg(N), defined as

$$\mathbf{Reg(N) = \{p: p \in U , d(p,v_N) \leq r_N\}}$$

where:

- $\mathbf{v_N}$ (the "center") is also called a *routing object*, and
- $\mathbf{r_N}$ is called the *(covering) radius* of the region

- The set of indexed points p that are reachable from node N are guaranteed to have $d(p,v_N) \leq r_N$



- This immediately makes it possible to apply the pruning principle:

If $d(q,v_N) > r_N + r$ then prune node N:

Entries of leaf and internal nodes

- Each node N stores a variable number of *entries*

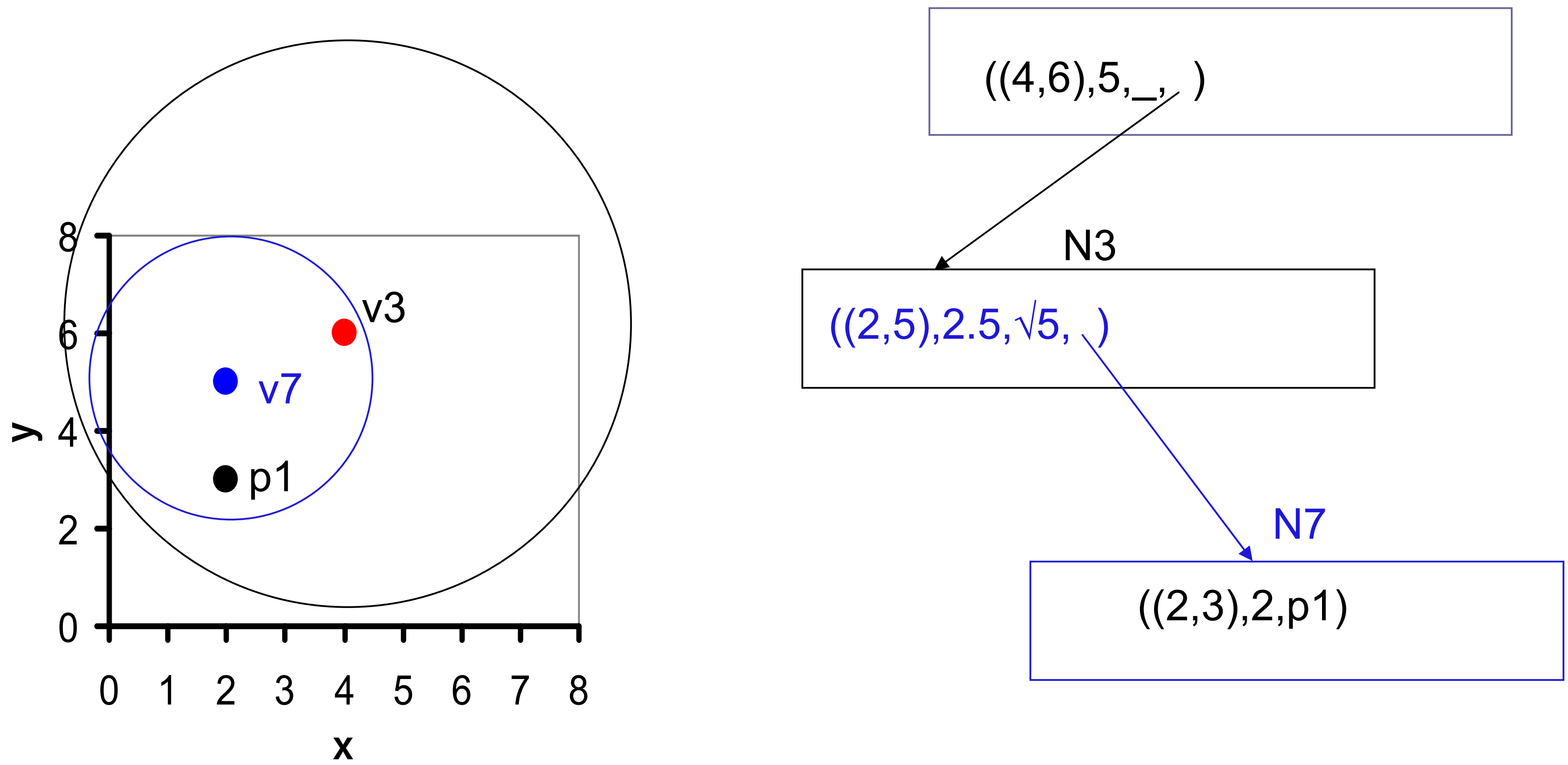
Leaf node:

- An entry E has the form E=(ObjFeatures,distP,TID), where
  - ObjFeatures are the feature values of the indexed object
  - distP is the distance between the object and its parent routing object (i.e, the routing object of node N)

Internal node:

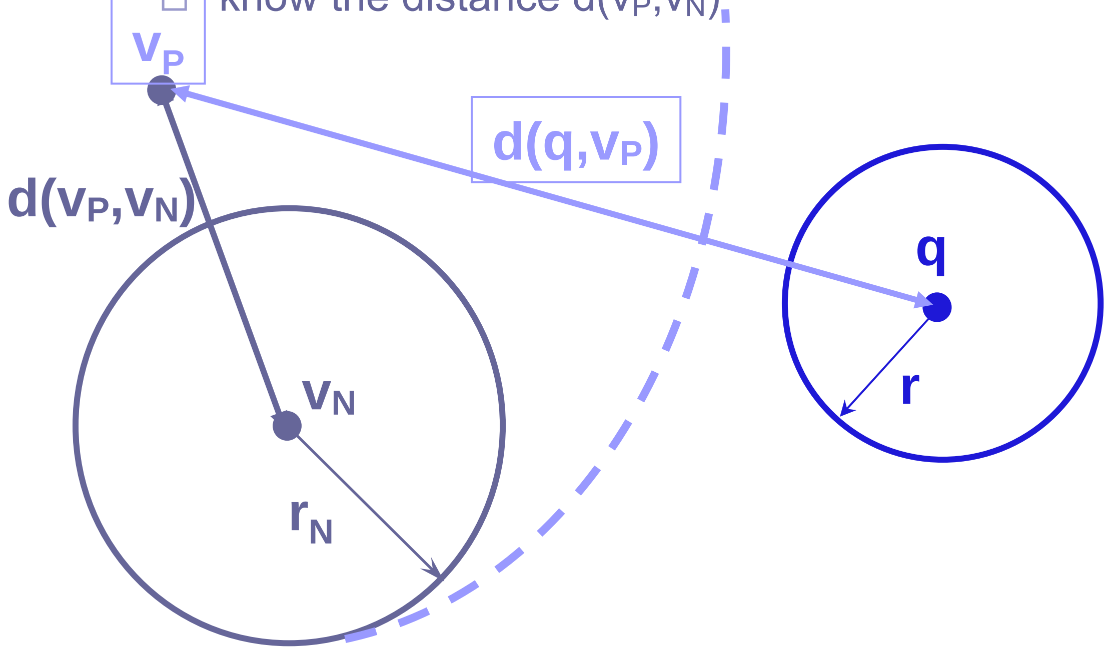
- An entry E has the form E=(RoutingObjFeatures,CoveringRadius,distP,PID), where
  - RoutingObjFeatures are the feature values of the routing object
  - CoveringRadius is the radius of the region
  - distP is the distance between the routing object and its parent routing object (this is undefined for entries in the root node)

Entries: an example



Fast pruning based on distP

- Pre-computed distances distP are exploited during query execution to save distance computations
- Let v_P be the parent (routing) object of v_N
- When we come to consider the entry of v_N, we
  - have already computed the distance $d(q,v_P)$ between the query and its parent
  - know the distance $d(v_P,v_N)$



From the triangle inequality it is:
$d(q,v_N) \geq |d(q,v_P) - d(v_P,v_N)|$

Thus we can prune node N ***without computing*** **$d(q,v_N)$** if

$$|d(q,v_P) - d(v_P,v_N)| > r_N + r$$

Example (edit distance)

query = "spire", r = 1

d("spire", "shakespeare") =
= 3 ≤ 5 +1

| d("spire", "spare") –
d("parse", "spare") | =
= | 1 – 4 | = 3 ≤ 1 +1