



# Plan of activities

- In the following we will go through 3 distinct topics, all of them being related by the common objective to provide efficient support to the execution of MM similarity queries
  - We will first complete the description of the R-tree, by detailing how insertions and splitting of nodes can be carried out
  - 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
  - Finally, we will try to shed some light on the phenomenon of dimensionality curse, and then present some index structures that have been designed to overcome such problem

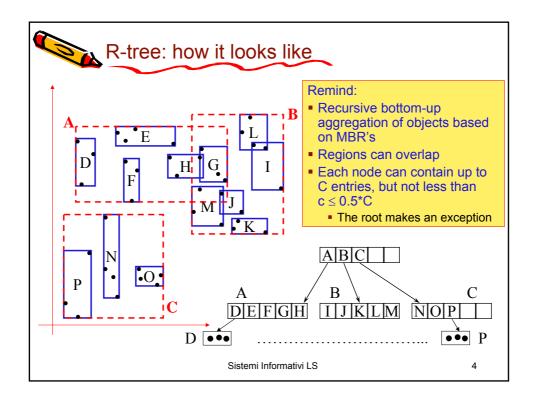
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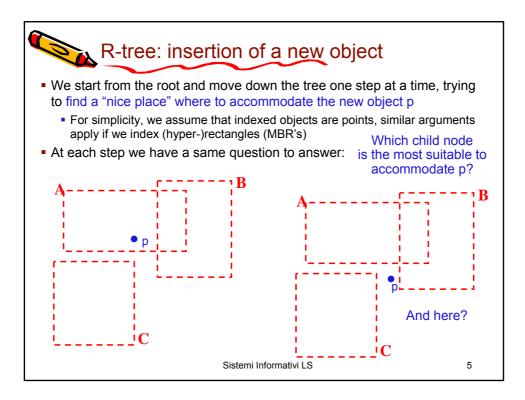


### Back to the R-tree (Guttman, 1984)

- Remind what said some weeks ago:
  - 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!
- 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

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# 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):

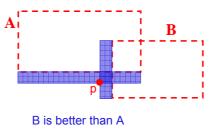
- If N is a leaf then: return N // we are done
- 3. { choose among the entries Ec in N
  - the one, Ec\*, for which Penalty(Ep,Ec\*) is minimum;
- return ChooseSubtree(Ep,Ec\*.ptr) } // recursive call 4.
- 5. end.
- We invoke the method on the index root
- The specific criterion used to decide "how bad" 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

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### 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



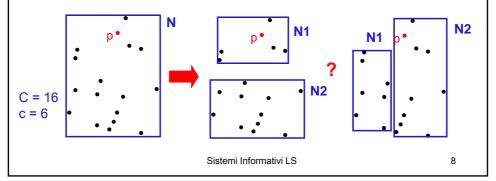
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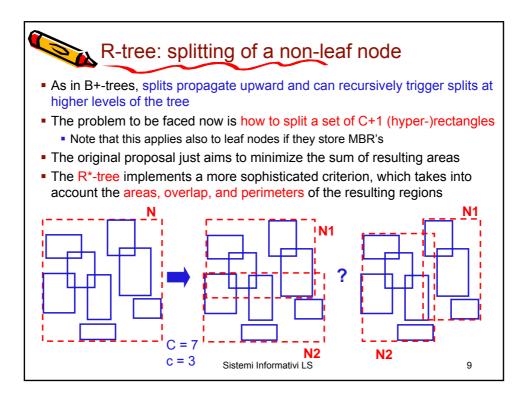
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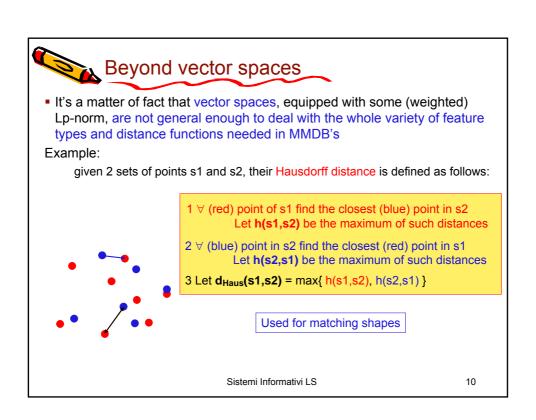


# R-tree: splitting of a leaf node

- 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









### Another example: set similarity

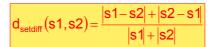
• We have logs of WWW accesses, where each log entry has format like:

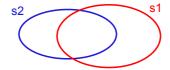
www-db.deis.unibo.it pciaccia [11/Jan/1999:10:41:37 +0100]
 "GET /~mpatella/ HTTP/1.0" 200 1573

Log entries are grouped into sessions (= sets of visited pages):

S = <ip\_address, user\_id, [url<sub>1</sub>,...,url<sub>k</sub>]>

and we want to compare "similar sessions" (i.e., similar sets), using:





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## 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 to be inserted, deleted, or substituted so as to transform a string s1 into another string s2

 $d_{edit}('ball','bull') = 1$ 

d<sub>edit</sub>('balls','bell') = 2

d<sub>edit</sub>('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

dedit('gatctggtgg', 'agcaaatcag') = 7

	g	а	t	С	t	g	g	t	g	1	g
Г	1	=	2	Ш	3	4	5	=	6	7	=
Г	-	а	g	С	а	а	а	t	С	а	g

The edit distance can be computed using a dynamic programming procedure, similar to the one seen for the DTW

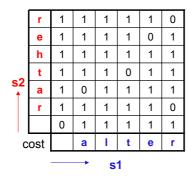
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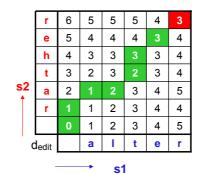


## Computing the Edit Distance

 The cost matrix is used to incrementally build the new matrix dedit, whose elements are recursively defined as:

$$\textbf{d}_{\mathsf{edit};_{i,j}} = \mathsf{cost}_{i,j} + \mathsf{min}\{\textbf{d}_{\mathsf{edit};_{i-1,j}}, \textbf{d}_{\mathsf{edit};_{i,j-1}}, \textbf{d}_{\mathsf{edit};_{i-1,j-1}}\}$$





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## 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:

> $d(x,y) \ge 0$ ,  $d(x,y) = 0 \Leftrightarrow x = y$ (positivity)

d(x,y) = d(y,x)(symmetry) (triangle inequality)

 $d(x,y) \le d(x,z) + d(z,y)$ 

- All the distance functions seen in the previous examples are metrics, and so are the (weighted) Lp-norms
- The only distance we have seen so far that does not fit the metric framework is the DTW

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

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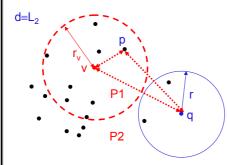
### Principles of metric indexing (1)

• Given a "metric dataset"  $P \subseteq U$ , 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 : 
$$d(p,v) \le r_v$$
} 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  $\{p: d(p,q) \le r\}$  If  $d(q,v) > r_v + r$  we can conclude that no point in P1 belongs to the result **Proof**:

```
 \begin{tabular}{ll} \begin{tabular}{ll} 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) \\ $\geq r$ \\ \end{tabular}
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Similar arguments can be applied to P2

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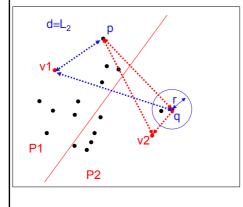


## Principles of metric indexing (2)

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 = 
$$\{p : d(p,v1) \le d(p,v2)\}$$

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



Consider a range query  $\{p: d(p,q) \le r\}$  If  $d(q,v1) - d(q,v2) > 2^*r$  we can conclude that no point in P1 belongs to the result **Proof**:

 $\label{eq:continuous_problem} \begin{array}{ll} \text{we show that } d(p,q) > r \text{ holds } \forall p \in P1. \\ d(q,v1) - d(p,q) \leq d(p,v1) & \text{(triangle ineq.)} \\ d(p,v1) \leq d(p,v2) & \text{(def. of P1)} \\ d(p,v2) \leq d(p,q) + d(q,v2) & \text{(triangle ineq.)} \\ \end{array}$ 

#### Then:

$$\begin{aligned} d(q,v1) - d(p,q) &\leq d(p,q) + d(q,v2) \\ d(p,q) &\geq (d(q,v1) - d(q,v2))/2 \\ &> r \end{aligned}$$
 (by hyp.)

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

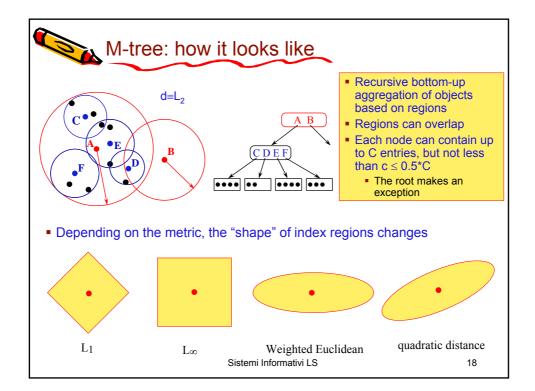
- The M-tree has been the first dynamic, paged, and balanced metric index
- Intuitively, it generalizes "R-tree principles" to arbitrary metric spaces
  - The M-tree treats the distance function as a "black box"
- Since 1997 [CPZ97] it has been used by several research groups for:
  - Image retrieval, 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 <a href="http://www-db.deis.unibo.it/Mtree/">http://www-db.deis.unibo.it/Mtree/</a>



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

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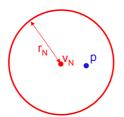


### The M-tree regions

■ Each node N of the tree has an associated region, Reg(N), defined as  $Reg(N) = \{p: p \in U , d(p,v_N) \le r_N\}$ 

#### where:

- V<sub>N</sub> (the "center") is also called a routing object, and
- r<sub>N</sub> 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<sub>N</sub>) ≤ r<sub>N</sub>



 This immediately makes it possible to apply the pruning principle:

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

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# Entries of leaf and internal nodes

Each node N stores a variable number of entries

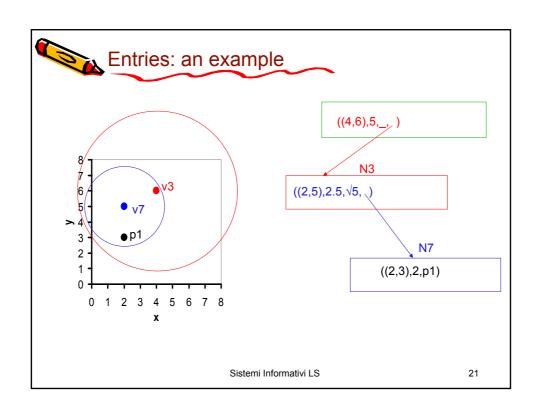
#### Leaf node:

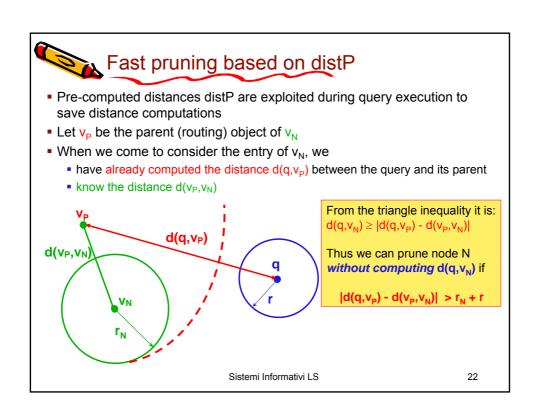
- An entry E has the form E=(ObjFeatures,distP,TID), where
  - ObjFeatures are the feature values of the indexed object
  - distP is the distance between the object and its parent routing object (i.e, the routing object of node N)

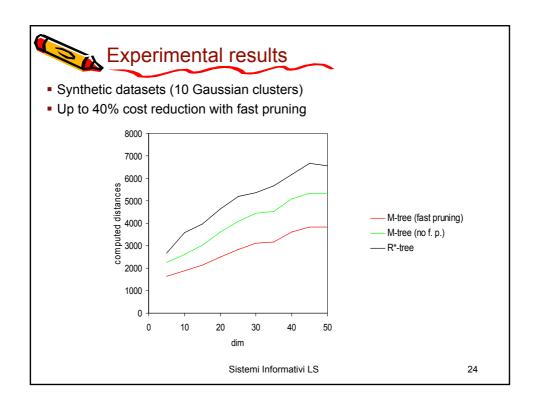
#### Internal node:

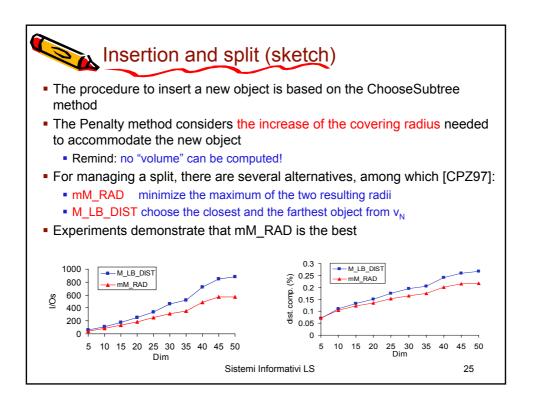
- An entry E has the form E=(RoutingObjFeatures,CoveringRadius,distP,PID), where
  - RoutingObjFeatures are the feature values of the routing object
  - CoveringRadius is the radius of the region
  - distP is the distance between the routing object and its parent routing object (this is undefined for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

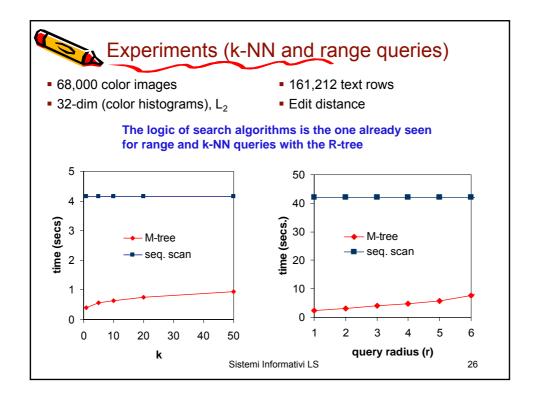
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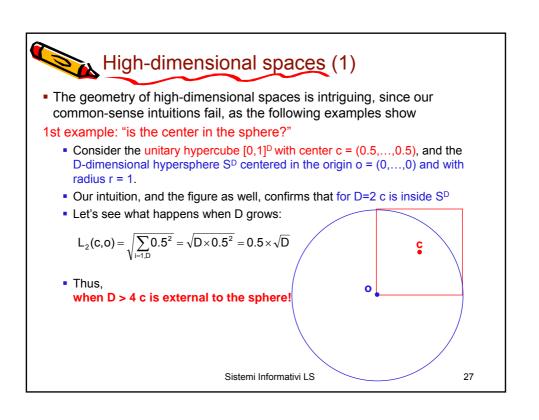














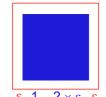
## High-dimensional spaces (2)

#### 2nd example: "where are the points?"

- Consider again the unitary hypercube [0,1]<sup>D</sup>
- Now, take a hypercube B of side  $1 2 \times \epsilon$  and center c = (0.5,...,0.5)
- The volume of B grows like

$$Vol(B) = (1-2\times\epsilon)^D$$

• As the table shows, even for (very) small ε values, Vol(B) sharply reduces



ε \ D	2	50	100	500	1000
0.1	0.64	1.43E-05	2.04E-10	3.51E-49	1.23E-97
0.05	0.81	0.01	2.66E-05	1.32E-23	1.75E-46
0.01	0.96	0.36	0.13	4.10E-05	1.68E-09

- If we have N points uniformly distributed over [0,1]<sup>D</sup>, then only a fraction equal to Vol(B) will be contained, on the average, in B
- Thus, all points are close to the surface of [0,1]<sup>D</sup>!

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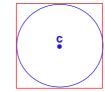


# High-dimensional spaces (3)

#### 3rd example: "How big a sphere is?"

- Consider the unitary hypercube [0,1]<sup>D</sup> and the D-dimensional hypersphere S<sup>D</sup> centered in c = (0.5,...,0.5) and with radius r = 0.5
- The volume of  $S^D$  can be computed as (D even):  $Vol(S^D) =$
- The following table (from [WSB98]) shows, for various values of D and assuming that points are uniformly distributed over [0,1]D:
  - The volume of S<sup>D</sup>, Vol(S<sup>D</sup>)
  - The number of points N needed to have, on the average, at least 1 point in SD (this is just 1/ Vol(SD))

D	Vol(SD)	N
2	0.785	1.27
4	0.308	3.24
10	0.002	401.50
20	2.46E-08	40631627
40	3.28E-21	3.05E+20
100	1.87E-70	5.35E+69



 Thus, the number of points should grow exponentially to have at least 1 point in Sd!

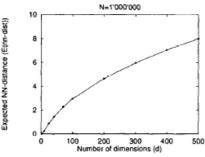
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# High-dimensional spaces (4)

#### 4th example: "How far is the nearest neighbor?"

- Continuing with the previous example, we can compute the expected (Euclidean) distance of the nearest neighbor of the center c = (0.5,...,0.5) of S<sup>D</sup>
- The following graph (from [WSB98]) shows how the NN distance grows with D when N = 10<sup>6</sup>



Thus, the closest point is far away!

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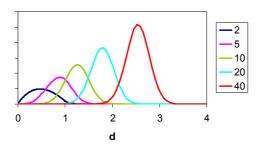
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# High-dimensional spaces (5)

#### 5th example: "How far are the other points?"

- We now plot the distance distribution of the dataset, for various values of D
- The distance distribution shows, for a given value of d, which is the percentage of points whose distance is d



- It can be observed that when D grows, the variance of distances decreases
- Thus, in high-dimensional spaces all the points tend to have the same distance from the query!

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### Basic facts about high-dim. spaces (1)

- The analysis in [WSB98] demonstrates that, no matter how smart you are in designing a new index structure, there always exists a value of D such that the index performance will deteriorate, and sequential scan will become the best alternative!
- However, the analysis applies to uniformly distributed datasets and Euclidean distance...
- If your data are not uniformly distributed (as it always happens!), then the authors argue that their analysis still applies, provided one considers the "intrinsic dimensionality" of the dataset
- The concept of "intrinsic dimensionality" is not precisely definable, intuitively it is the "true dimensionality" of our data
  - E.g.: a line has intrinsic dimensionality 1, regardless of D
- Some attempts to characterize the intrinsic dimensionality of a dataset have been based on the concept of fractals (e.g., see [FK94])

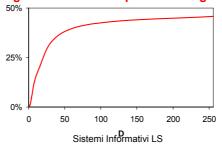
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## χ Basic facts about high-dim. spaces (2)

- From a more pragmatical point of view, experimental results obtained with both spatial and metric indexes confirm that high-dimensional datasets are often a nightmare!
- This is the so-called "dimensionality curse"!
- For the structures we have seen (R-tree and M-tree), what is observed is an incredible amount of overlap between the regions of index nodes
  - The graph shows the percentage of M-tree regions that enclose a query point q, i.e., those regions for which d<sub>MIN</sub>(q,Reg(N)) = 0
  - Thus, all such regions can never be pruned during a k-NN search!





### Note: Partitioning without overlap

- If we partition the [0,1]<sup>D</sup> space into non-overlapping regions, similar problems arise
- For instance, consider a uniform distribution of points, and assume we split a dimension in the mid-point 0.5 (thus, each time we double the number of regions). We can split at most D' = \[ \log\_2 \nabla \right] \] dimensions
- Consider the region: Reg =  $[0,0.5] \times ... \times [0,0.5] \times [0,1] \times ... \times [0,1]$ whose farthest point is q = (1,...,1)
- The Euclidean distance of q from Reg is:

$$L_2(Reg,q) = \sqrt{\sum_{i=1,D'} (1-0.5)^2} = \sqrt{D' \times 0.5^2} = 0.5 \times \sqrt{D'} = 0.5 \times \sqrt{\lceil log_2 N \rceil}$$

- With N = 10<sup>6</sup> we have D'=20 and L<sub>2</sub>(Reg,q)=2.236
- Since this is independent of D, whereas the expected NN distance grows with D, for values of D large enough (D ≥ 80) Reg will be accessed, and this holds for any other region!

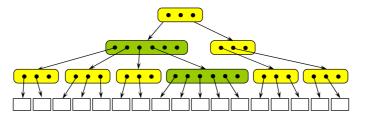
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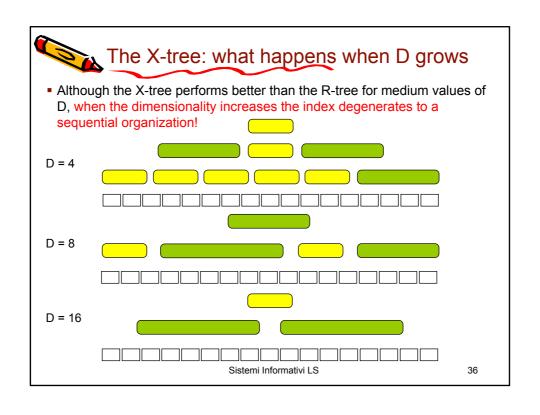


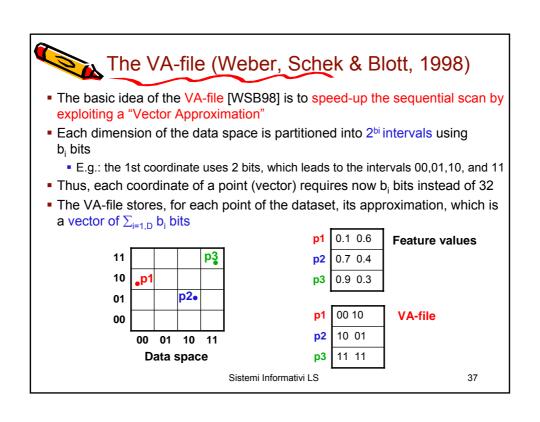
## The X-tree [BKK96]: basic idea

- The X-tree is an evolution of the R-tree, aiming to deal with the "overlap problem"
- When a node has to be split, if an overlap-free split is possible then it is performed as usual, otherwise a new, larger, super-node, is allocated
  - Thus, now we have nodes of variable size
- The price to be paid is that searching within a super-node is more costly than searching within nodes



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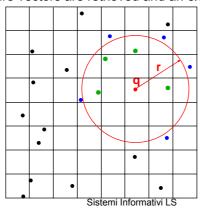


## The VA-file: query processing

- Query processing with the VA-file is based on a filter & refine approach
- For simplicity, consider a range query

Filter: the VA file is accessed and only the points in the regions that intersect the query region are kept

Refine: the feature vectors are retrieved and an exact check is made



actual results false drops excluded points

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# Conclusions (?)

- The issue of efficiently indexing complex datasets is far from having been solved
- Starting from the end of 90's, many solutions have been proposed, and new ideas have emerged
- Unfortunately, the absence of a well-defined and accepted benchmark makes it almost impossible to compare all such solutions
- The basic lesson to be learned is that, no matter how a structure has been cleverly designed, ultimately it has to be contrasted with the sequential scan!
- Thus, be skeptical if someone claims to have designed an index showing "superior performance" w.r.t. the others: always look if sequential scan has been taken as a competitor!

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