Systems Infrastructure for Data Science

Web Science Group
Uni Freiburg
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Lecture III: Multi-dimensional Indexing

Querying Multi-dimensional Data

```
SELECT *
  FROM CUSTOMERS
 WHERE ZIPCODE BETWEEN 8000 AND 8999
   AND REVENUE BETWEEN 3500 AND 6000
```

- This example query involves a **range predicate** in **two dimensions**.
- The general case: **spatial queries** over **spatial data**.

Spatial Data

- Spatial data is used to model multi-dimensional points, lines, rectangles, polygons, cubes, and other geometric objects that exist in space.

- Two main types:
  - **Point** Data
  - **Region** Data

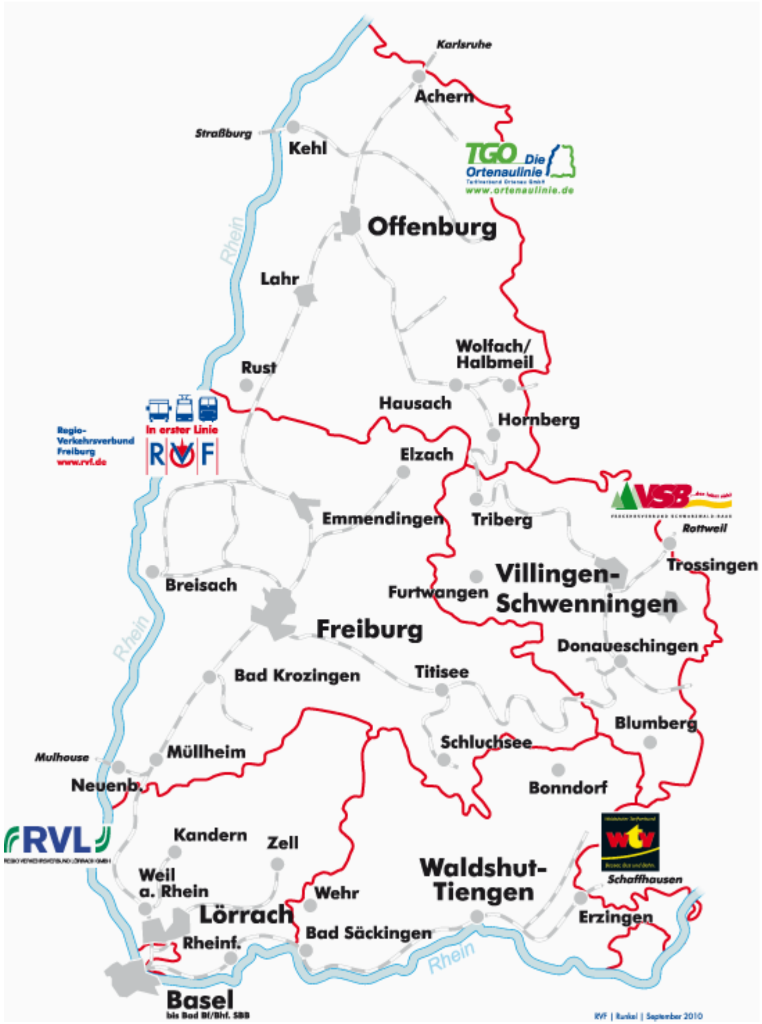
Point Data

- Points in a multi-dimensional space
- No area or volume
- Examples:
  - **Raster data** such as satellite imagery, where each pixel stores a directly measured value corresponding to a location in space (e.g., temperature, color)
  - **Feature vectors** extracted from images, text, signals such as time series, where the point data is obtained by transforming a data object

Region Data

- Objects have **spatial extent** (i.e., occupy a certain region of space) characterized by their location and boundary.
- DB typically stores geometric approximations for objects called "**vector data**", which is constructed using points, line segments, polygons, etc.
- Examples:
  - **Geographic applications** (roads and rivers represented as line segments; countries and lakes represented as polygons)
  - **Computer-Aided Design (CAD) applications** (airplane wing represented as polygons)

A Familiar Example for Spatial Data with Points, Lines, and Regions



Spatial Queries

- Spatial queries refer to queries on spatial data.
- Three main types:
  - **Spatial range** queries
  - **Nearest neighbor** queries
  - **Spatial join** queries

Spatial Range Queries

- A spatial range query has an associated region (i.e., location and boundary).
- The query should return all regions that overlap the specified range or all regions contained within the specified range.
- Examples: relational queries, GIS queries, CAD/CAM queries.
  - Find all employees with salaries between $50K and $60K, and ages between 40 and 50.
  - Find all cities within 100 kilometers of Freiburg.
  - Find all rivers in Baden-Württemberg.

Nearest Neighbor Queries

- A nearest neighbor query (*k*-NN) returns the *k* objects that have the smallest distance to a given reference object.
- Results must be ordered by proximity.
- Examples: GIS queries, similarity search in multi-media databases
  - Find the 10 cities nearest to Freiburg.
  - Find the 10 images that are the most similar to this picture of the criminal suspect (*using feature vector point data for images*).

Spatial Join Queries

- In a spatial join query, the **join condition involves regions and proximity**.
- These queries often times involve **self-join** operations and are expensive to evaluate.
- Example: Consider a relation with **points** representing a city or a mountain.
  - Find pairs of cities within 200 kilometers of each other.
  - Find all cities near a mountain.
- It gets more complex if we represent objects with **region** data instead of point data.

Spatial Applications Recap

- Traditional relations with *k* fields ~ collections of *k*-dimensional points
- Geographic Information Systems (GIS)
  - Geo-spatial information (2- and 3-dim datasets)
  - **All types** of spatial queries and data are common.
- Computer-Aided Design/Manufacturing (CAD/CAM)
  - Store spatial objects such as surface of airplane wing
  - Both **point and range** data.
  - **Range queries and spatial join queries** are the most common.
- Multi-media Databases
  - Images, audio, video, text, etc. stored and retrieved by content
  - First converted to **feature vector** form (high dimensionality)
  - **Nearest-neighbor queries** (for querying similarity) are the most common.

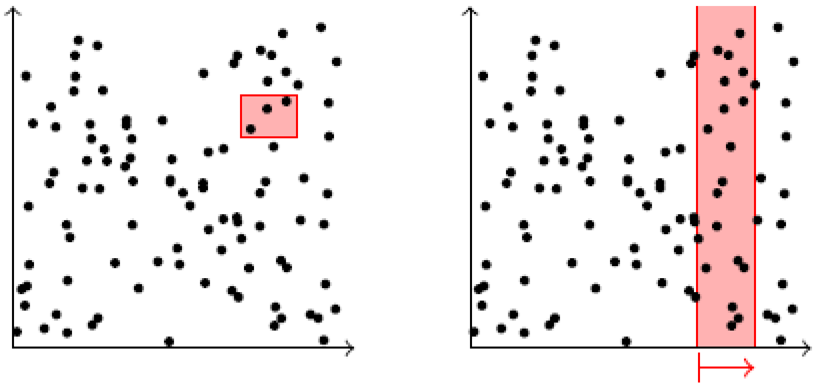
Many Solutions for Multi-dimensional Indexing

Quad Tree [Finkel 1974]
R-tree [Guttman 1984]
R+-tree [Sellis 1987]
R*-tree [Geckmann 1990]
Vp-tree [Chiueh 1994]
UB-tree [Bayer 1996]
SS-tree [White 1996]
M-tree [Ciaccia 1996]
Pyramid [Berchtold 1998]
DABS-tree [Bohm 1999]
Slim-tree [Faloutsos 2000]
P-Sphere-tree [Goldstein 2000]
K-D-B-Tree [Robinson 1981]
Grid File [Nievergelt 1984]
LSD-tree [Henrich 1989]
hB-tree [Lomet 1990]
TV-tree [Lin 1994]
hB--tree [Evangelidis 1995]
X-tree [Berchtold 1996]
SR-tree [Katayama 1997]
Hybrid-tree [Chakrabarti 1999]
IQ-tree [Bohm 2000]
landmark file [Bohm 2000]
A-tree [Sakurai 2000]

- Note that none of these is a “fits all” solution.

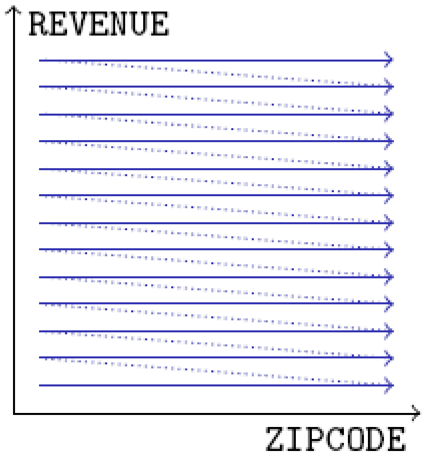
Can't we just use a B$^+$-tree?

- Maybe two B$^+$-trees, over ZIPCODE and REVENUE each?

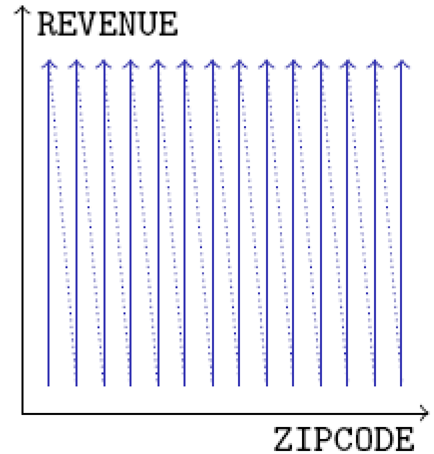


- Can only scan along either index at once, and both of them produce many **false hits**.
- If all you have are these two indexes, you can do **index intersection**:
  - Perform both scans in separation to obtain the *rids* of candidate tuples.
  - Then compute the (**expensive!**) intersection between the two *rid* lists (IBM DB2: IXAND – index AND'ing).

Maybe with a Composite Key?



⟨REVENUE, ZIPCODE⟩ index



⟨ZIPCODE, REVENUE⟩ index

- Exactly the same thing!
  - Indexes over composite keys are **not symmetric**: **The major attribute dominates** the organization of the B+-tree.
- Again, you can use the index if you really need to. Since the second argument is also stored in the index, you can discard non-qualifying tuples before fetching them from the data pages.

Single-dimensional Indexes

- B^+-trees are fundamentally single-dimensional indexes.
- When we create a **composite search key in B^+-tree**, e.g., an index on <*age, sal*>, we effectively **linearize** the 2-dimensional space, since we sort the data entries first by *age* and then by *sal*.
- Consider the following data entries:

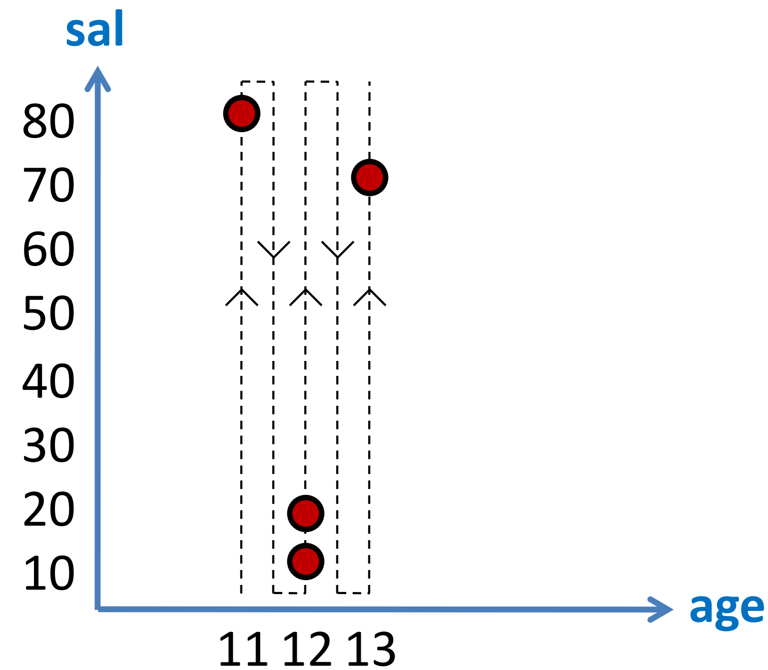
  <11, 80>

  <12, 10>

  <12, 20>

  <13, 70>

linear sort order in B^+-tree



Multi-dimensional Indexes

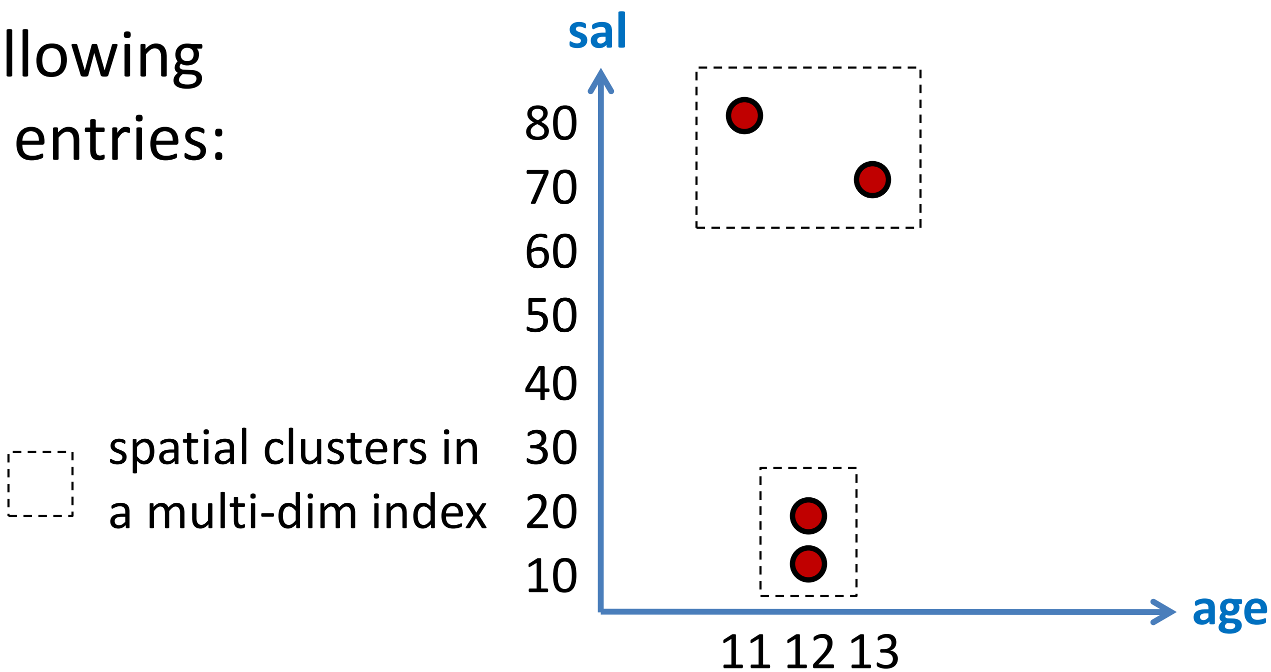
- A multi-dimensional index **clusters** entries so as to exploit "nearness" in multi-dimensional space.
- Keeping track of entries and maintaining a balanced index structure presents a challenge.
- Consider the following *<age, sal>* data entries:

  <11, 80>

  <12, 10>

  <12, 20>

  <13, 70>



Example Queries (B^+-tree vs. Multi-dim)

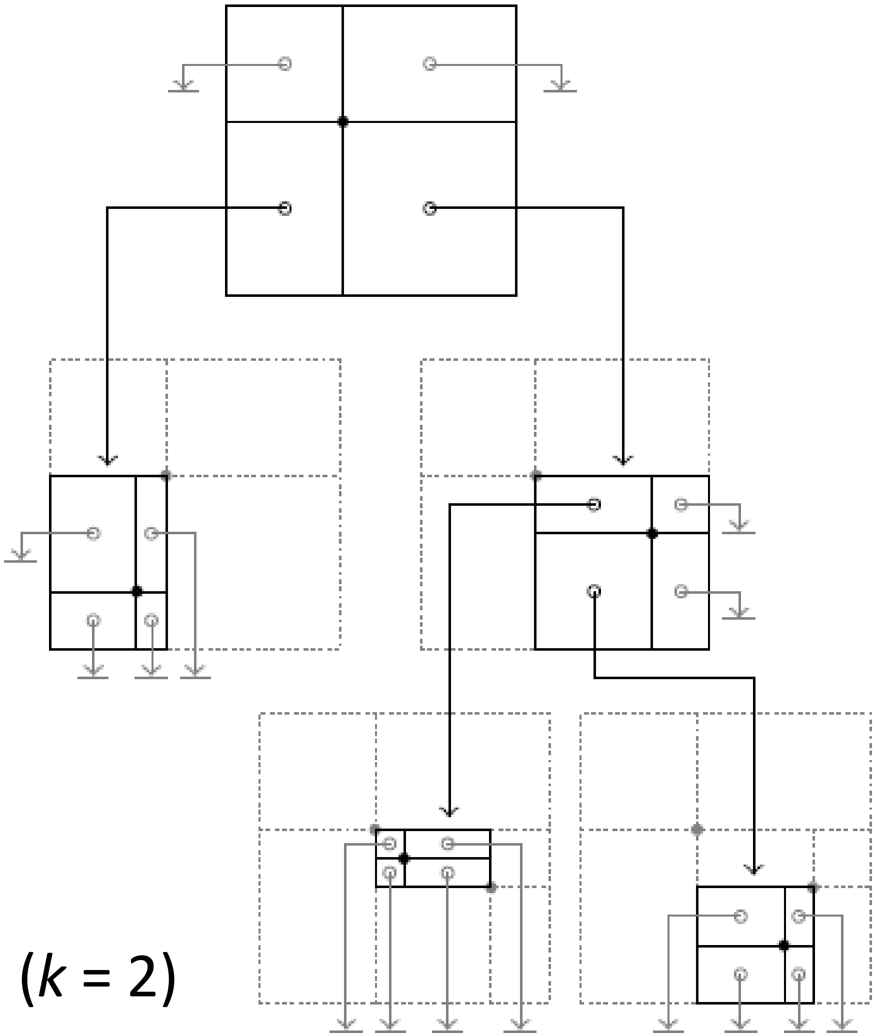
- *age < 12*
  - B^+-tree performs better than the multi-dim index.
- *sal < 20*
  - B^+-tree can not be used, since *age* is the first field in the search key.
- *age < 12 AND sal < 20*
  - B^+-tree effectively utilizes only the index on *age*, and performs badly if most tuples satisfy *age < 12*.

➢ If almost all data entries are to be retrieved in *age* order, then the multi-dim spatial index is likely to be slower than the B^+-tree index.

Multi-dimensional Indexes

- B^+-trees can answer one-dimensional queries only.
- We'd like to have a multi-dimensional index structure that
  - is **symmetric** in its dimensions,
  - **clusters** data in a space-aware fashion,
  - is **dynamic** with respect to updates, and
  - provides good support for **useful queries**.
- We'll start with data structures that have been designed for **in-memory** use, then tweak them into **disk-aware** database indexes.

Point Quad Trees

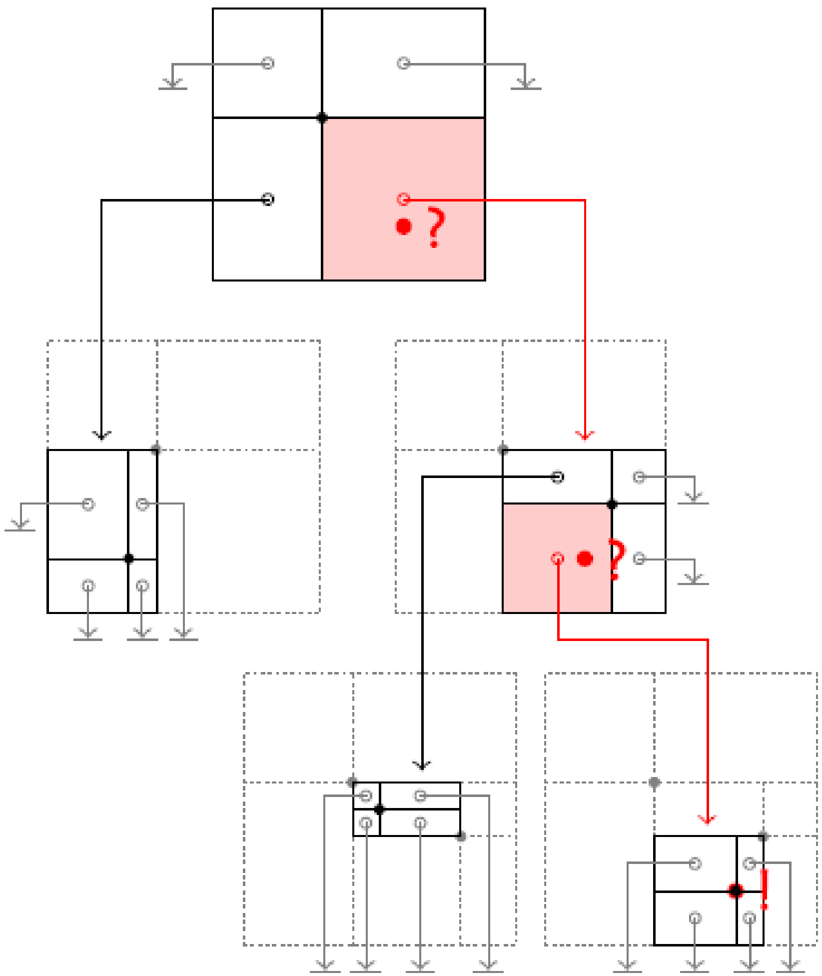


(*k* = 2)

- A binary tree in *k* dimensions
  => 2^k-ary tree
- Each data point **partitions** the data space into 2^k **disjoint regions**.
- In each node, a region points to another node (representing a **refined partitioning** for that region) or to a special **null value**.

➢ Finkel and Bentley, "Quad Trees: A Data Structure for Retrieval on Composite Keys", Acta Informatica, vol. 4, 1974.

Searching a Point Quad Tree

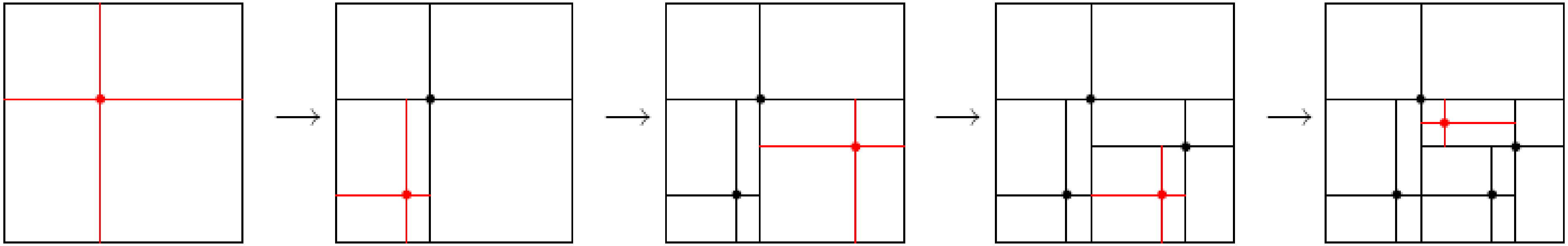


```
Function: p_search (q, node)
if q matches data point in node then
  return data point ;
else
  P ← partition containing q ;
  if P points to null then
    return not found ;
  else
    node′ ← node pointed to by P ;
    return p_search (q, node′) ;
```

```
Function: pointsearch (q)
return p_search (q, root) ;
```

Inserting into a Point Quad Tree

- Inserting a point q_{new} into a quad tree happens analogously to an insertion into a binary tree:
  - Traverse the tree just like during a search for q_{new} until you encounter a partition *P* with a null pointer.
  - Create a new node *n'* that spans the same area as *P* and is partitioned by q_{new}, with all partitions pointing to null.
  - Let *P* point to *n'*.
- Note that this procedure does **not** keep the tree **balanced**.



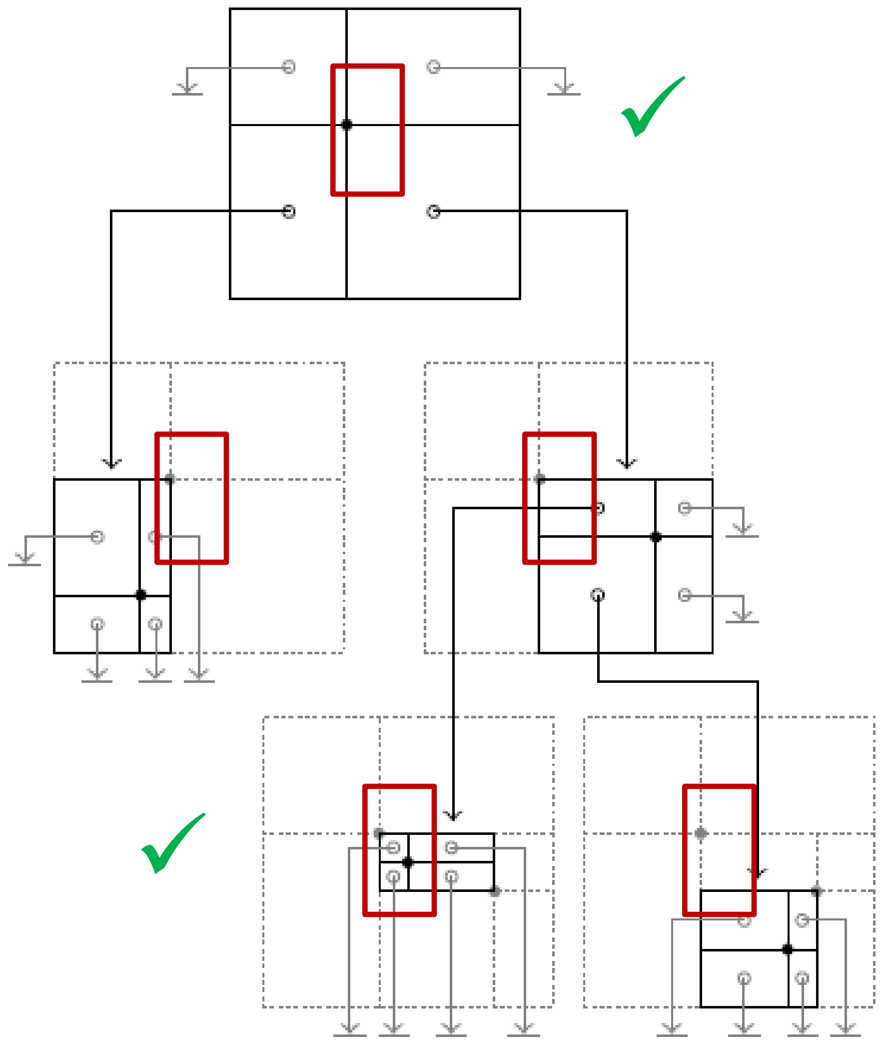
Evaluating Range Queries with a Point Quad Tree Index

- To evaluate a range query (i.e., rectangular regions), we may need to follow several children of a given quad tree node.

```
Function: r_search (Q, node)
if data point in node is in Q then
  append data point to result ;
foreach partition P in node that intersects with Q do
  node' ← node pointed to by P ;
  r_search (Q, node') ;
```

```
Function: regionsearch (Q)
return r_search (Q, root) ;
```

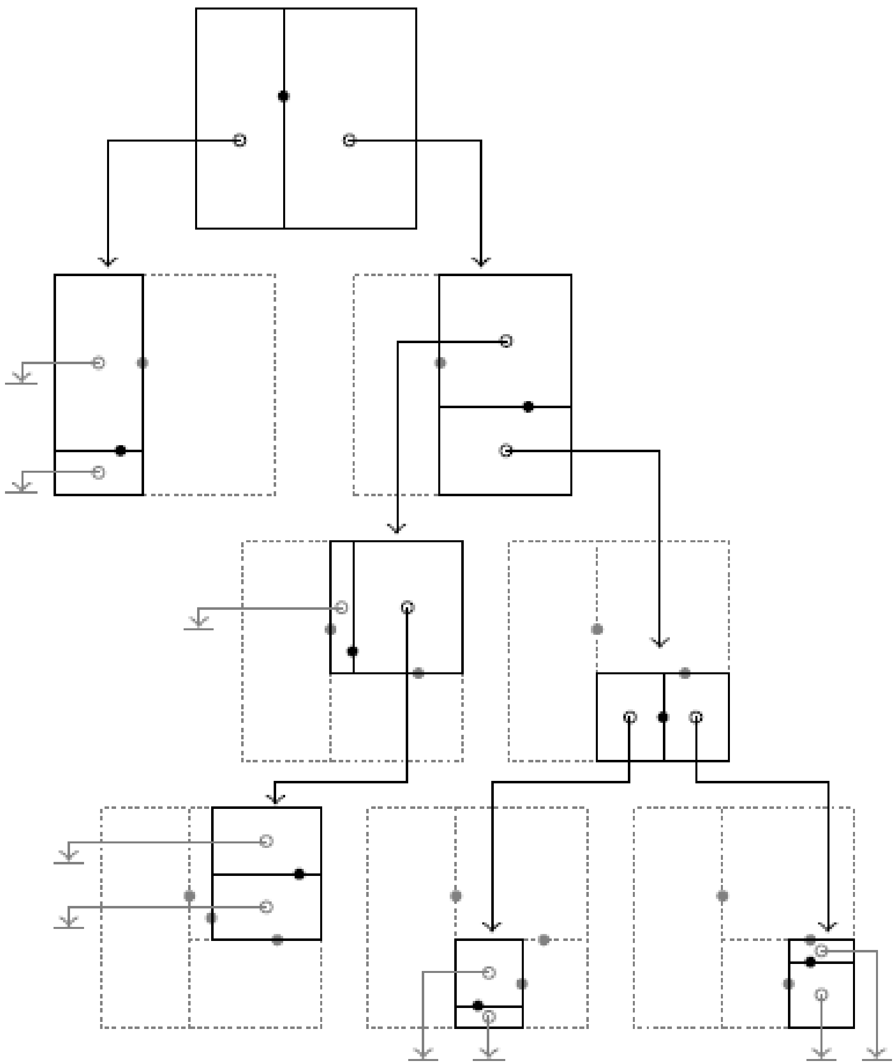
Range Query Example



Point Quad Trees

- Point Quad Trees
  - ✓ are **symmetric** with respect to all dimensions
  - ✓ can answer **point queries** and **region queries**
- However,
  - ✘ the shape of a quad tree depends on the **insertion order** of its content, in the worst case **degenerates** into a **linked list**
  - ✘ **null** pointers are **space inefficient** (particularly for large *k*)
  - ✘ they can only store **point data**
- Also, quad trees are designed for main memory.

k-d Trees



(*k* = 2)

- Index *k*-dimensional data, but keep the tree **binary**.
- For each tree level *l*, use a **different discriminator dimension** d_l along which to partition.
  - Typically: **round robin**

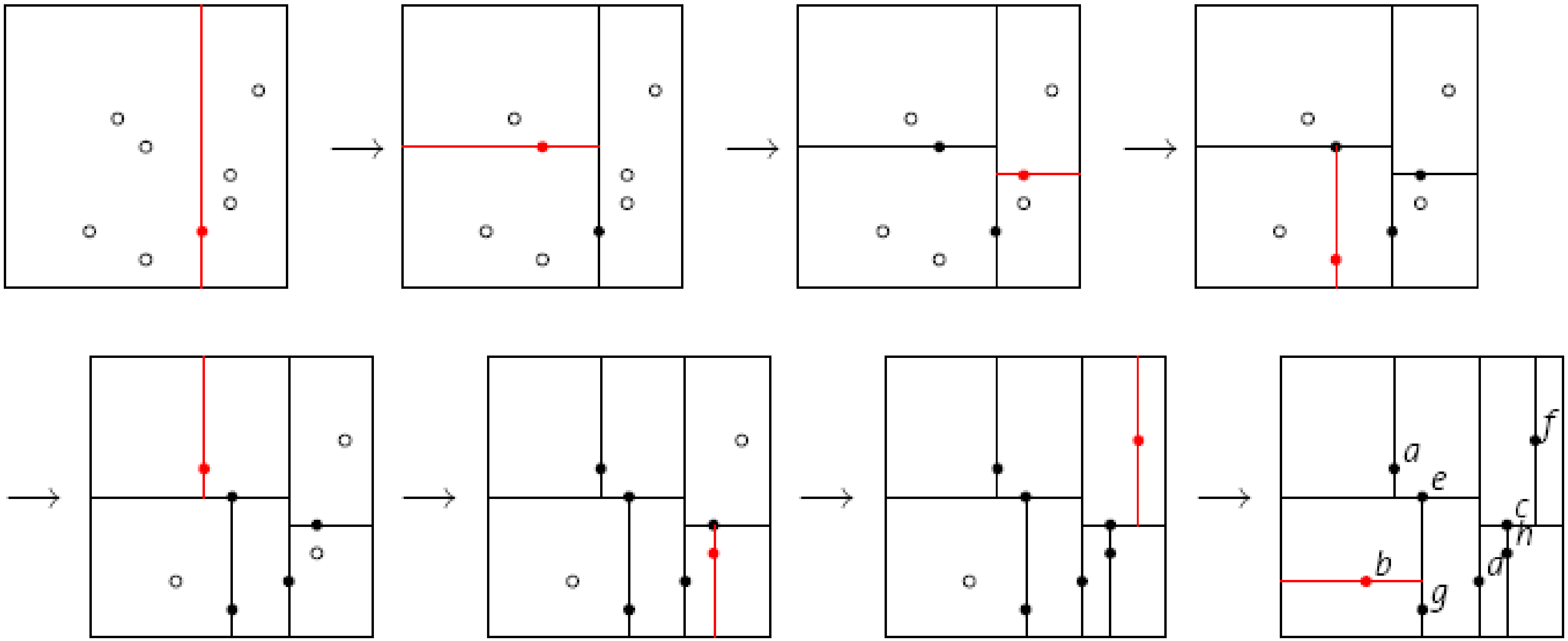
➢ Bentley, "Multidimensional Binary Search Trees Used for Associative Searching", Communications of the ACM, 18:9, 1975.

k-d Trees

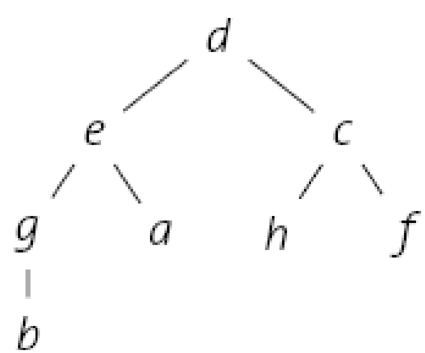
- k-d trees inherit the positive properties of the point quad trees, but improve on **space efficiency**.
- For a given point set, we can also construct a **balanced** k-d tree (v_i denotes coordinate i of point v):

```
Function: kdtree (pointset, level)
if pointset is empty then
    return null ;
else
    p ← median from pointset (along d_level) ;
    points_left ← {v ∈ pointset where v_{d_level} < p_{d_level}};
    points_right ← {v ∈ pointset where v_{d_level} ≥ p_{d_level}};
    n ← new k-d tree node, with data point p ;
    n.left ← kdtree (points_left, level + 1) ;
    n.right ← kdtree (points_right, level + 1) ;
    return n ;
```

Balanced k-d Tree Construction



Resulting tree shape:

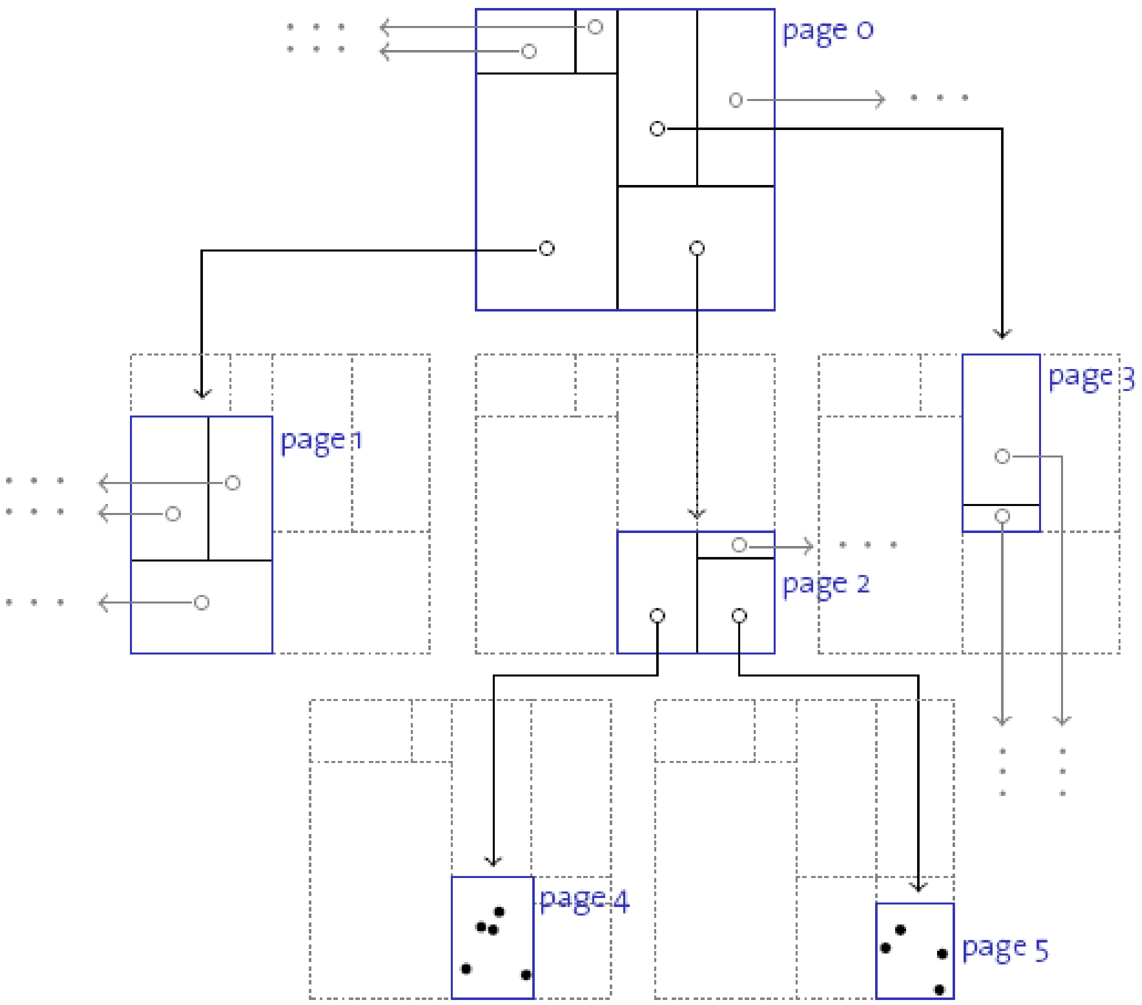


K-D-B Trees

- k-d trees improve on some of the deficiencies of point quad trees:
  - ✓ We can **balance** a k-d tree by **re-building** it. (For a limited number of points and in-memory processing, this may be sufficient.)
  - ✓ We are no longer wasting big amounts of **space**.
- It's time to bring k-d trees to the **disk**. The **K-D-B Tree**
  - – uses **page** as an organizational unit (e.g., each node in the K-D-B tree fills a page)
  - – uses a **k-d tree-like layout** to organize each page

➢ John T. Robinson, "The K-D-B Tree: A Search Structure for Large Multidimensional Dynamic Indexes", SIGMOD'81.

K-D-B Trees



region pages:

- contain entries $\langle region, pageID \rangle$
- no **null** pointers
- form a **balanced** tree
- all regions **disjoint** and **rectangular**

point pages:

- contain entries $\langle point, rid \rangle$
- $\rightsquigarrow$ B^+-tree leaf nodes

K-D-B Trees

- K-D-B Trees
  - ✓ are **symmetric** with respect to all dimensions
  - ✓ **cluster** data in a space-aware and page-oriented fashion
  - ✓ are **dynamic** with respect to updates
  - ✓ can answer **point queries** and **region queries**
- However,
  - ✘ we still don't have support for **region data** and
  - ✘ K-D-B Trees (like k-d trees) won't handle **deletes** dynamically.
- This is because we always partitioned the data space such that
  - every region is **rectangular**
  - regions never **intersect**

R-Trees

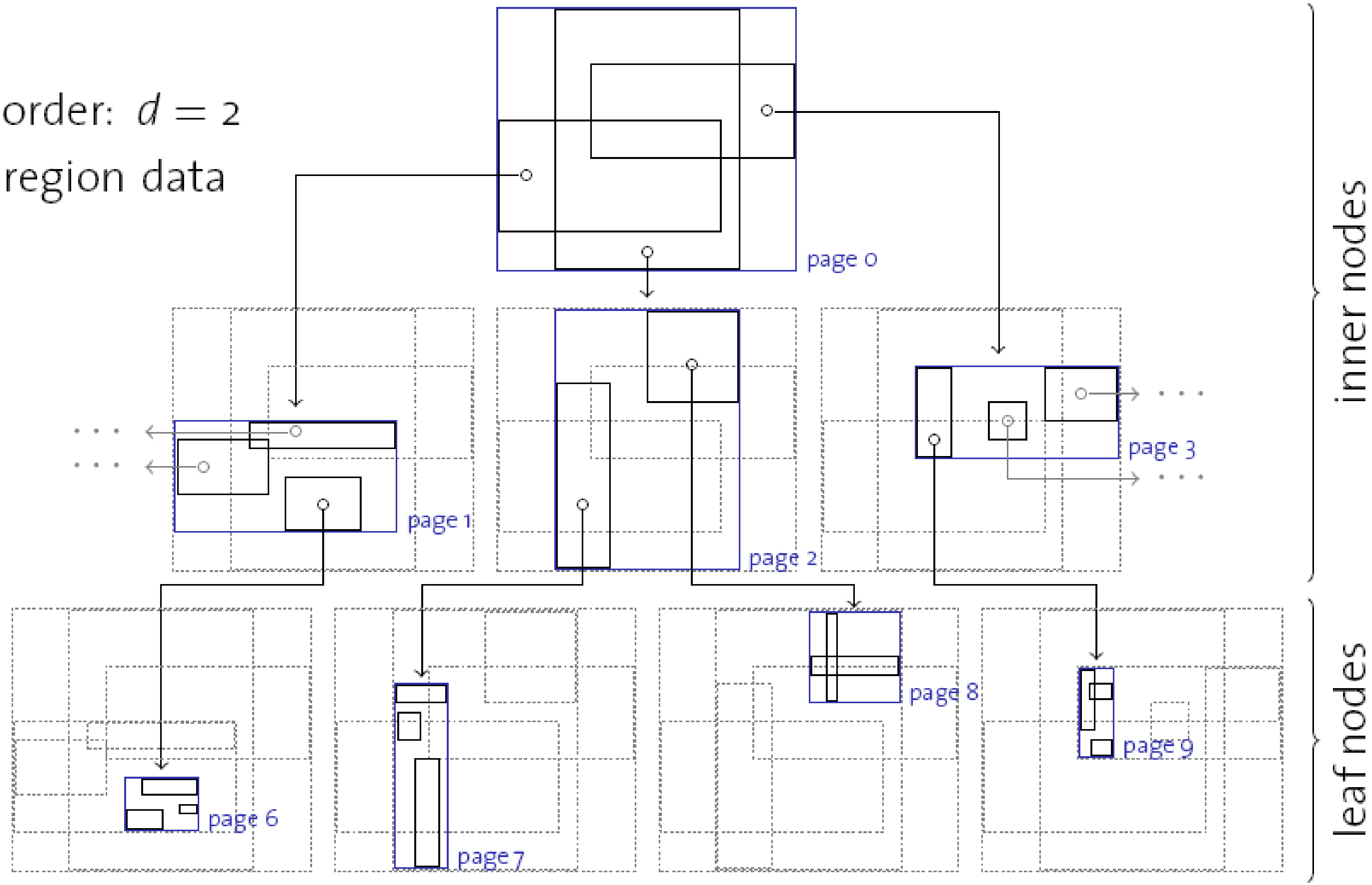
- R-trees do not have the disjointness requirement.
  - R-tree inner or leaf nodes contain *<region, pageID>* and *<region, rid>* entries, respectively. *region* is the **minimum bounding rectangle** that spans all data items reachable by the respective pointer.
  - Every node contains between *d* and *2d* entries except the root node (as in B^+-tree).
  - Insertion and deletion algorithms keep an R-tree **balanced at all times**.
- R-trees allow the storage of **point and region data**.

➢ Antonin Guttman, "R-Trees: A Dynamic Index Structure for Spatial Searching", SIGMOD'84.

R-Tree Example

order: $d = 2$

region data



Searching an R-Tree

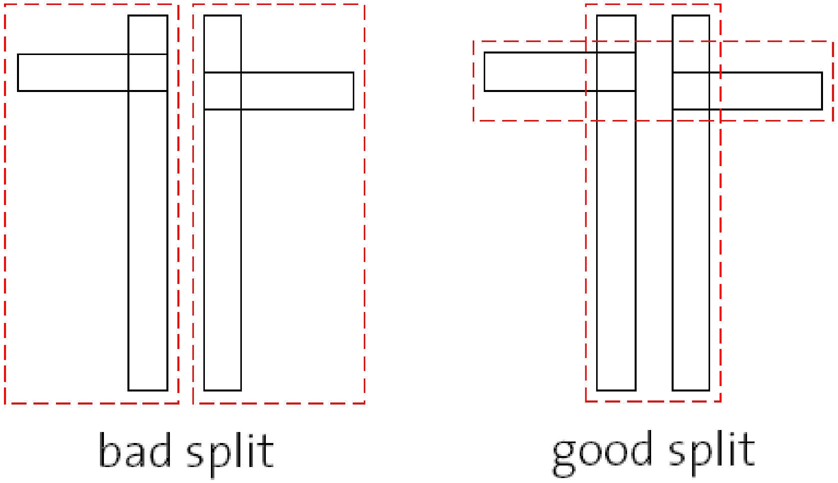
- Start at the root.
  - If current node is non-leaf, for each entry *<E, ptr>,* if region *E* overlaps *Q*, search subtree identified by *ptr*.
  - If current node is leaf, for each entry *<E, rid>,* if *E* overlaps *Q*, *rid* identifies an object that might overlap *Q*.
- While searching an R-tree, we may have to descend into more than one child node for point and region queries (in contrast, a B^+-tree equality search goes to just one leaf).

Inserting into an R-Tree

- Inserting into an R-tree very much resembles B^+-tree insertion:
  1. Choose a leaf node *n* to insert the new entry.
     - Try to minimize the necessary region enlargement(s).
  2. If *n* is full, split it (resulting in *n* and *n'*) and distribute old and new entries evenly across *n* and *n'*.
     - Splits may propagate bottom-up and eventually reach the root (as in B^+-tree).
  3. After the insertion, some regions in the ancestor nodes of *n* may need to be adjusted to cover the new entry.

Splitting an R-Tree Node

- To split an R-tree node, we have more than one alternative.



- Heuristic: Minimize the totally covered area.
  - Goal: To reduce the likelihood of both regions being searched on subsequent queries. Redistribute so as to minimize the total area.
  - Exhaustive search for the best split is infeasible. Guttman proposes two ways to approximate the search. Follow-up papers (e.g., the R*-tree paper) aim at improving the quality of node splits.

Deleting from an R-Tree

- All R-tree invariants are maintained during deletions.
  1. If an R-tree node *n* underflows (i.e., less than *d* entries are left after a deletion), the whole node is deleted.
  2. Then, all entries that existed in *n* are re-inserted into the R-tree, as discussed before.
- Note that Step 1 may lead to a recursive deletion of *n*'s parent.
  – Deletion, therefore, is a rather expensive task in an R-tree.

R-Tree Variants

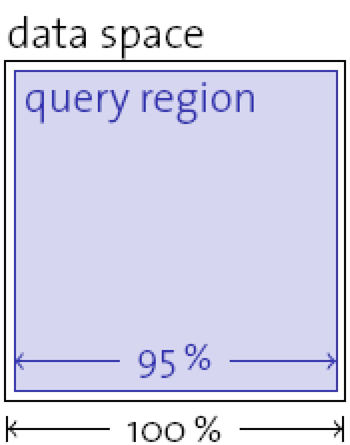
- The **R*-tree** uses the concept of **forced reinserts** to reduce overlap in tree nodes. When a node overflows, instead of splitting:
  - Remove some (say, 30% of the) entries and reinsert them into the tree.
  - Could result in all reinserted entries fitting on some existing pages, avoiding a split.
- R*-trees also use a different heuristic, minimizing **box perimeters** rather than box areas during insertion.
- Another variant, the **R$^+$-tree**, avoids overlap by inserting an object into **multiple leaves** if necessary.
  - Searches now take a single path to a leaf, at cost of redundancy.

Indexing High-dimensional Data

- Typically, high-dimensional datasets are collections of points, not regions.
  - Example: Feature vectors in multi-media applications
  - Very sparse
- Nearest neighbor queries are common.
  - R-tree becomes worse than sequential scan for most datasets with more than a dozen dimensions.
- As dimensionality increases, contrast (i.e., the ratio of distances between nearest and farthest points) usually decreases; “nearest neighbor” is not meaningful.
  - In any given data set, it is advisable to empirically test contrast.

High Dimensional Spaces

- For large *k*, all the techniques we discussed become ineffective:
  - Example: for *k = 100*, we'd get $2^{100} \sim 10^{30}$ partitions per node in a point quad tree. Even with billions of data points, almost all of these are empty.
  - Consider a really big search region, cube-sized covering 95% of the range along each dimension:



For $k = 100$, the probability of a point being in this region is still only $0.95^{100} \approx 0.59\,\%$.

  - We experience the **curse of dimensionality** here.

Summary

- **Point Quad Tree**
  - k-dimensional analogy to binary trees; main memory only.
- **k-d Tree, K-D-B Tree**
  - k-d tree: Partition space one dimension at a time (round-robin).
  - K-D-B Tree: B^+-tree-like organization with pages as nodes; nodes use a k-d-like structure internally.
- **R-Tree**
  - Regions within a node may overlap; fully dynamic; for point and region data.
- **Curse Of Dimensionality**
  - Most indexing structures become ineffective for large k; fall back to sequential scanning and approximation/compression.