Datenbanksysteme II: Multidimensional Index Structures 2

Ulf Leser

Content of this Lecture

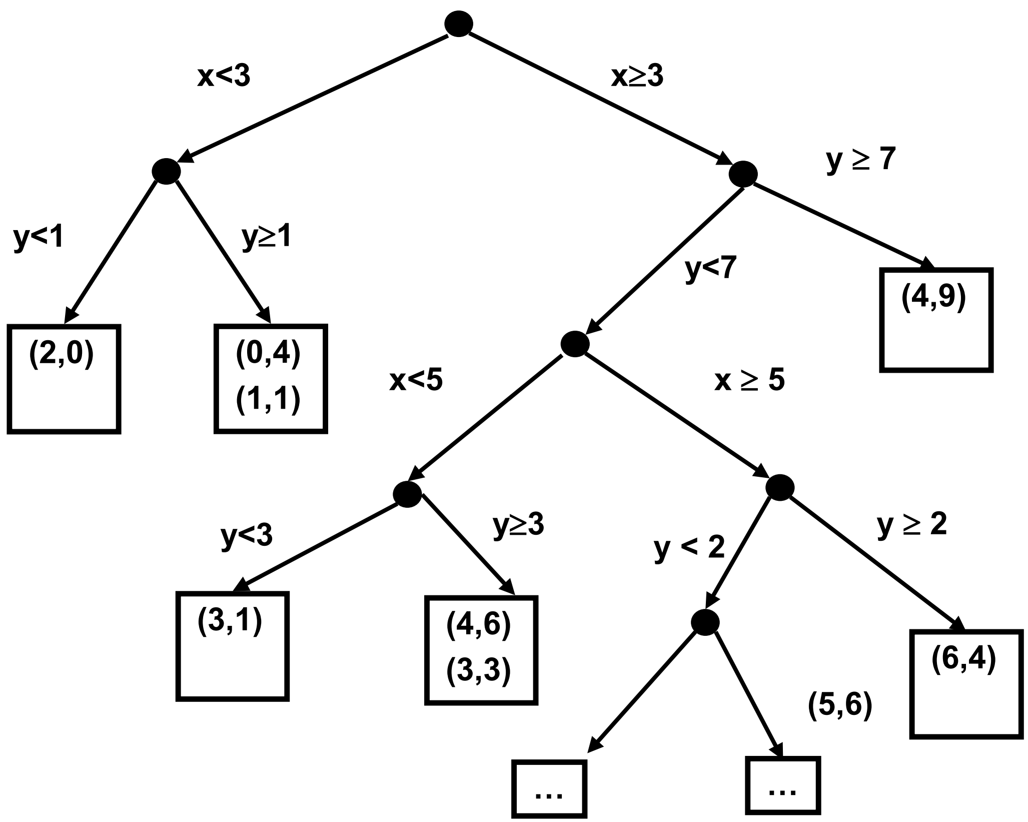
- Introduction
- Partitioned Hashing
- Grid Files
- kdb Trees
  - kd Tree
  - kdb Tree
- R Trees

kd Tree

- Grid file disadvantages
  - All hyperregions of the d-dimensional space are eventually split at the same scales (dimension/position)
  - First cell that overflows determines split
  - This choice is global and never undone
- kd Trees
  - Bentley: Multidimensional Binary Search Trees Used for Associative Searching. CACM, 1975.
  - Multidimensional variation of binary search trees
  - Hierarchical splitting of space into regions
  - Regions in different subtrees may use different split positions
  - Better adaptation to local clustering of data
  - Note: kd Tree originally is a main memory data structure

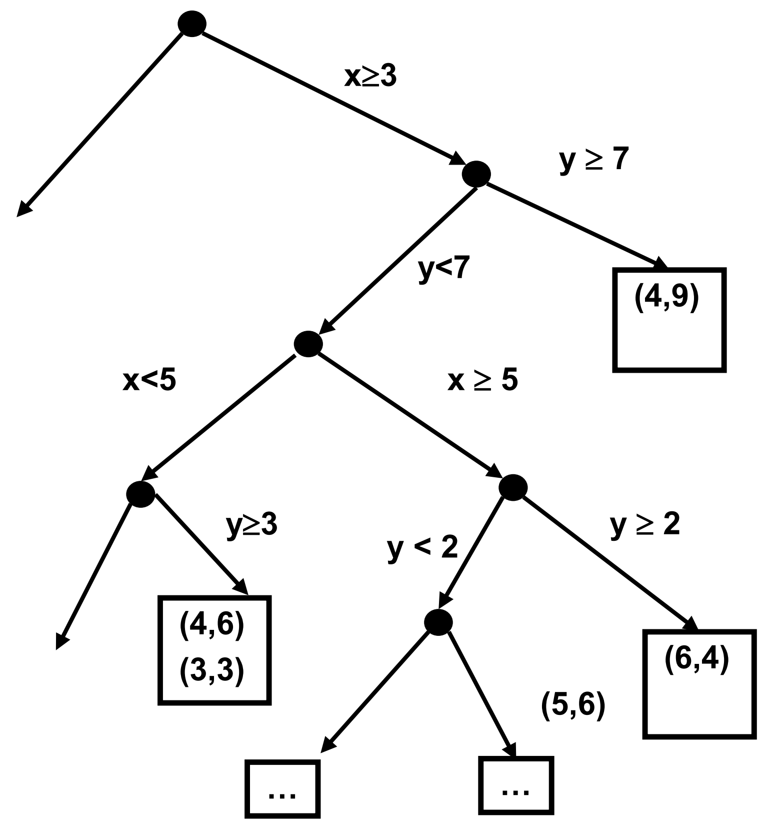
General Idea

- Binary, rooted tree
- Inner nodes define splits (dimension / value)
- Dimensions may be mixed in same level
- Leaves: Values + TIDs
- Each leaf represents d-dimensional convex hypercube with m border planes (m≤2d)
- No balancing
  - Bad WC search

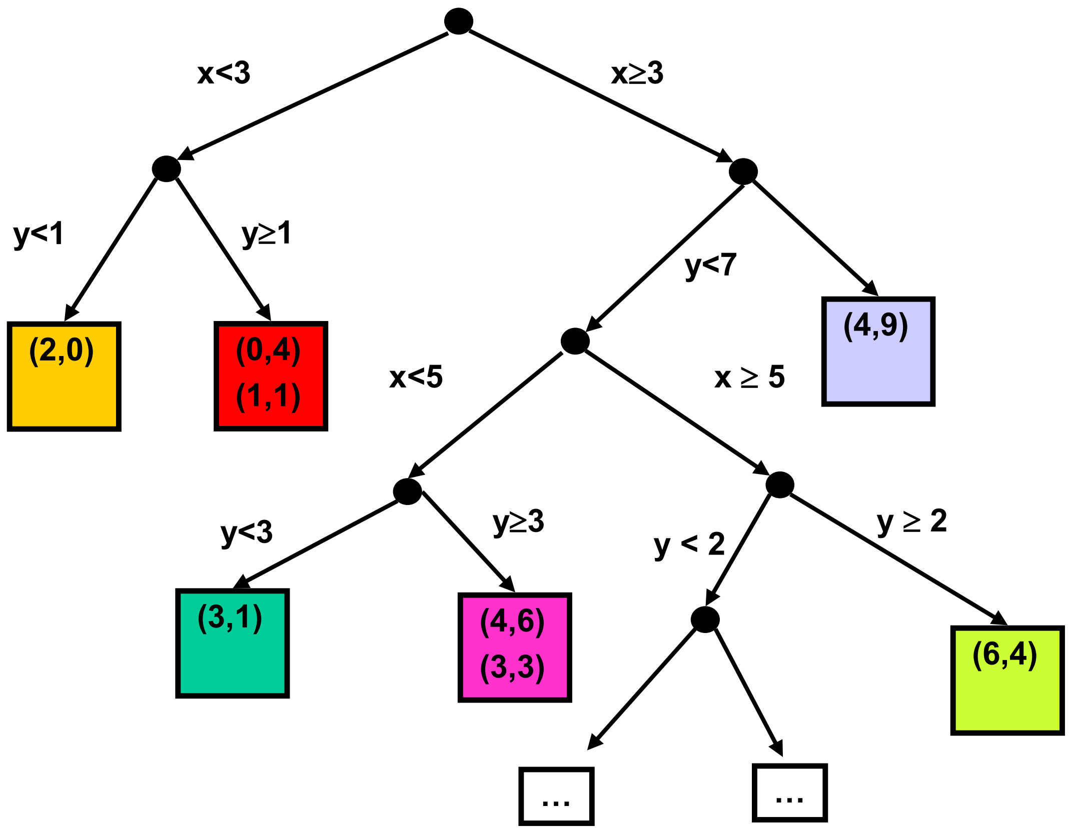


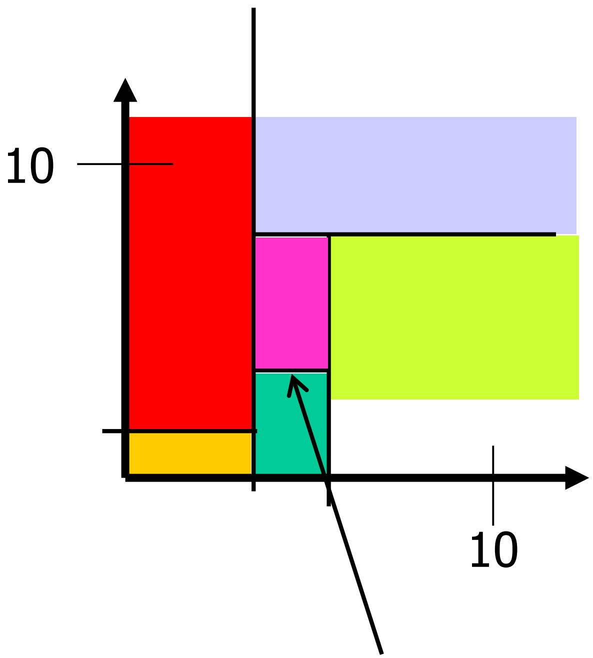
Blocks and Points

- Keep everything in memory
  - Leaves are singular points
  - Does not exploit caching / seq. reads
- Tree in mem and blocks on disk
  - Splits are delayed until block overflows
- Store everything on disk
  - k-DB Tree: Later
- On modern hardware
  - Random mem access in inner tree
  - Larger leaves create smaller trees
  - Parallel search? SIMD? Tree layout?
  - BB-Tree: Later



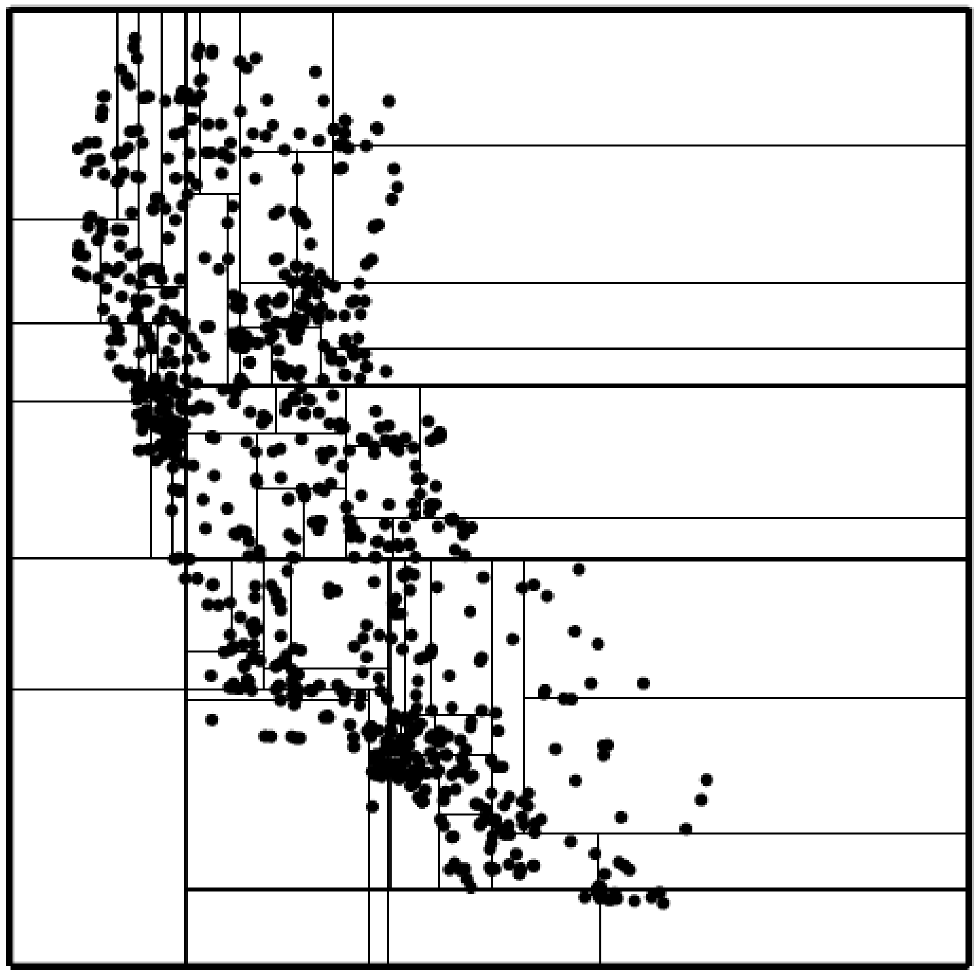
The Brick Wall





- Every split can be chosen freely within borders defined by parents
- Splits are local

Local Adaptation



Search Operations

- Exact point search
  - ?
- Partial match query
  - ?
- Range query
  - ?
- Nearest Neighborhood
  - ?

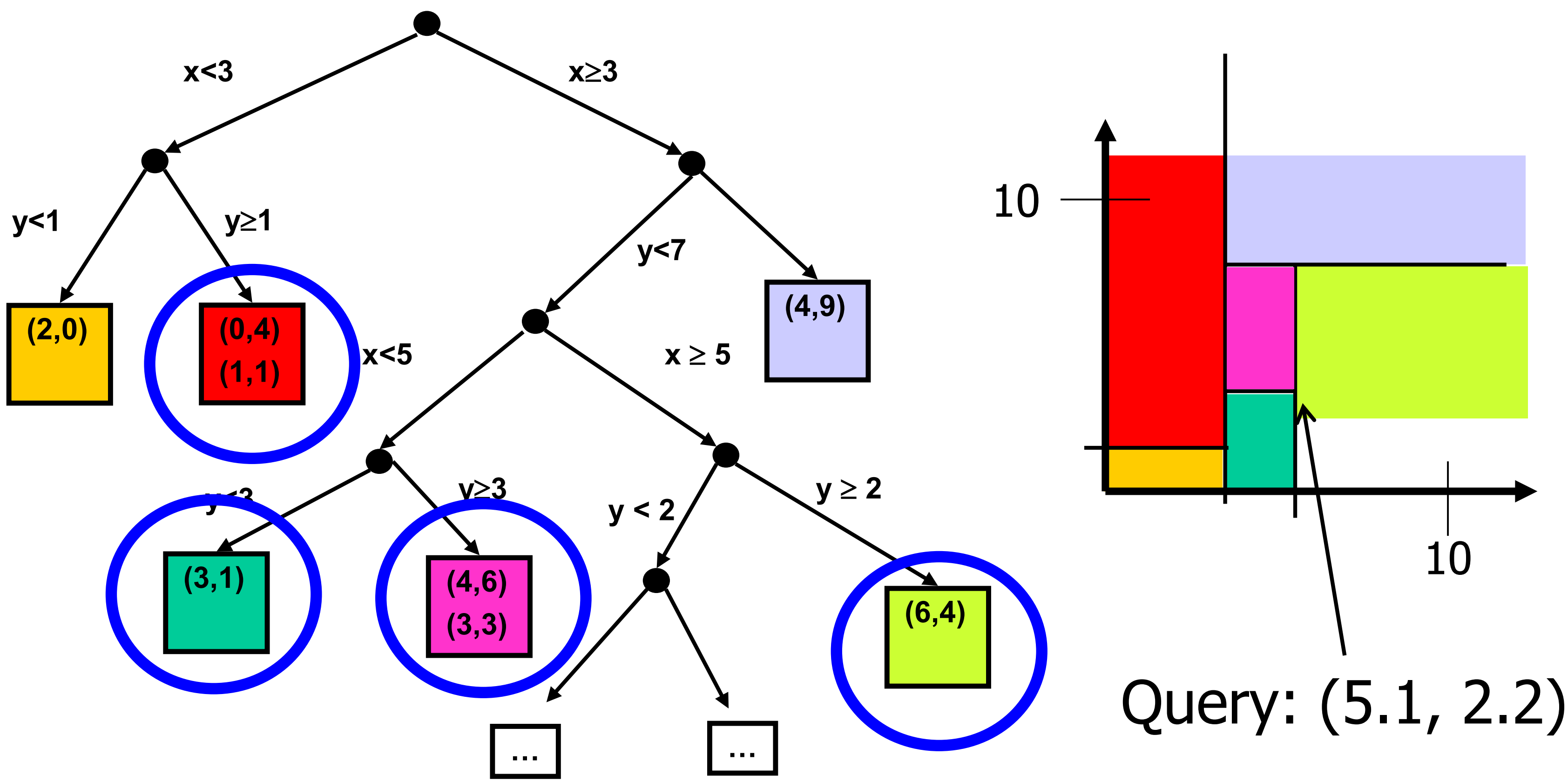
Search Operations

- Exact point search (result size 1)
  - In each inner node, decide upon direction based on split condition
  - Search inside leaf
  - Complexity = height of tree = O(n) in worst case
- Partial match query
  - If dimension of condition in inner node is part of the query – proceed as for exact match
  - Otherwise, follow all children (multiple search paths)
  - Worst case (no conditions) searchers entire tree
- Range query
  - Follow all children matching the range conditions (multiple paths)

Nearest Neighbor

- Search point
- Upon descending, build a priority queue of all directions not taken
  - Compute minimal distance between point and hyper-region not followed
  - Keep sorted by this minimal distance
- Once at a leaf, visit hyperregions in order of distance to query point
  - Jump to split point and follow closest path
  - Regions not visited are put into priority queue
  - Iterate until point found such that provably no closer point exists

Example



kd-Tree Insertion

- Search leaf block; if space available – done
  - The original kd-Tree has no blocks – we always split
- Otherwise, chose split (dimension + position) for this block
  - This is a local decision, valid for subtree of this node
  - Option 1: Use each dimension in turn and split region into two equally sized subspaces (expects uniform distribution)
  - Option 2: Consider current points in leaf and split in two sets of approximately equal size (expects temporally constant distribution)
    - But which dimension?
    - Considering all is expensive – use heuristics
  - Usual problem: We don't know the future points
  - Wrong decisions in early splits may lead to tree degradation
    - As for Grid-Files, there is no guarantee on fill degree

Deletion

- Search leaf block and delete point
- If block becomes (almost) empty
  - If empty: Remove; else: Do nothing – bad fill degree
  - Merge with neighbor leaf (if existing)
    - Two leaves and one parent node are replaces by one leaf
    - Not very clever if neighbor almost full
  - Balance with neighbor leaf (if existing)
    - Change split condition in parent such that children have equal size
    - Not very clever if neighbor almost empty
  - Consider larger neighborhood: Grant parents, grant-grant-par …
- kd trees have no guaranteed balance (~ depth)
- There is no guaranteed fill degree

Static kd Trees

- Assume the set of points to be indexed is static and known
- We can build worst-case optimal kd Trees
  - Rotate through dimensions
    - Typically in order of variance – wide spread dimensions first
  - Sort remaining points and choose median as split point
  - Guarantees tree depth of O(log(n)) for point queries
  - But clustering of points not considered – bad similarity queries
    - Nearby points are not nearby in the tree
- Variant (for sim-search): K-means trees
  - Iterative k-means clustering of points
  - K: Tree width (fanout)
  - Faster similarity queries, tree depth not guaranteed

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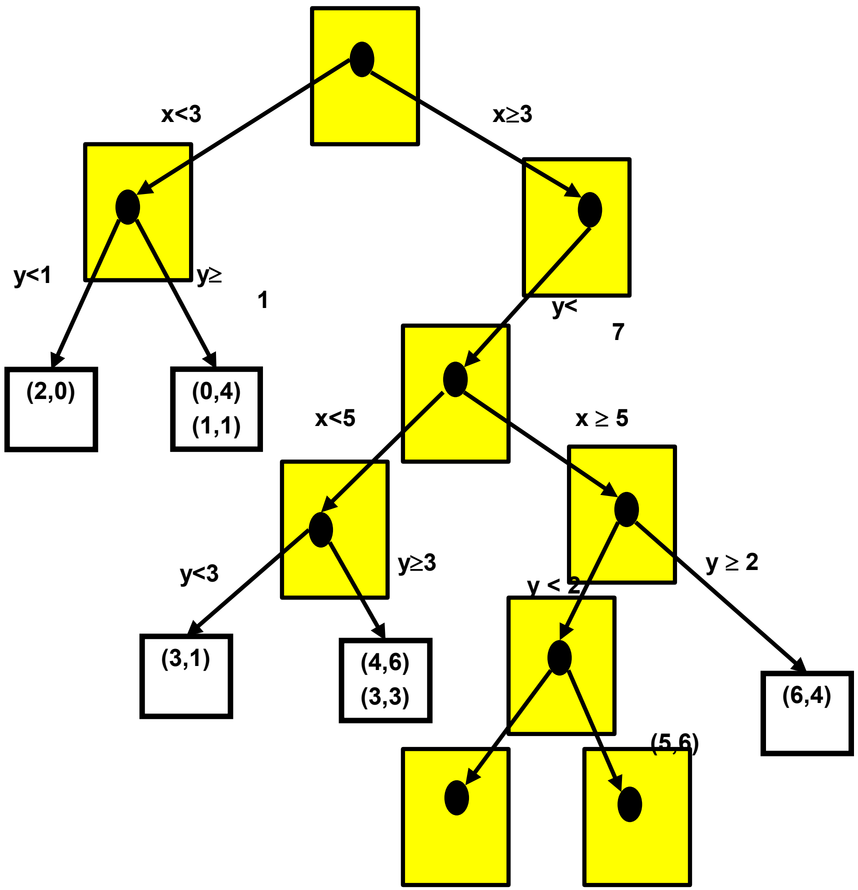
  - kd Tree
  - kdb Tree
- R Trees

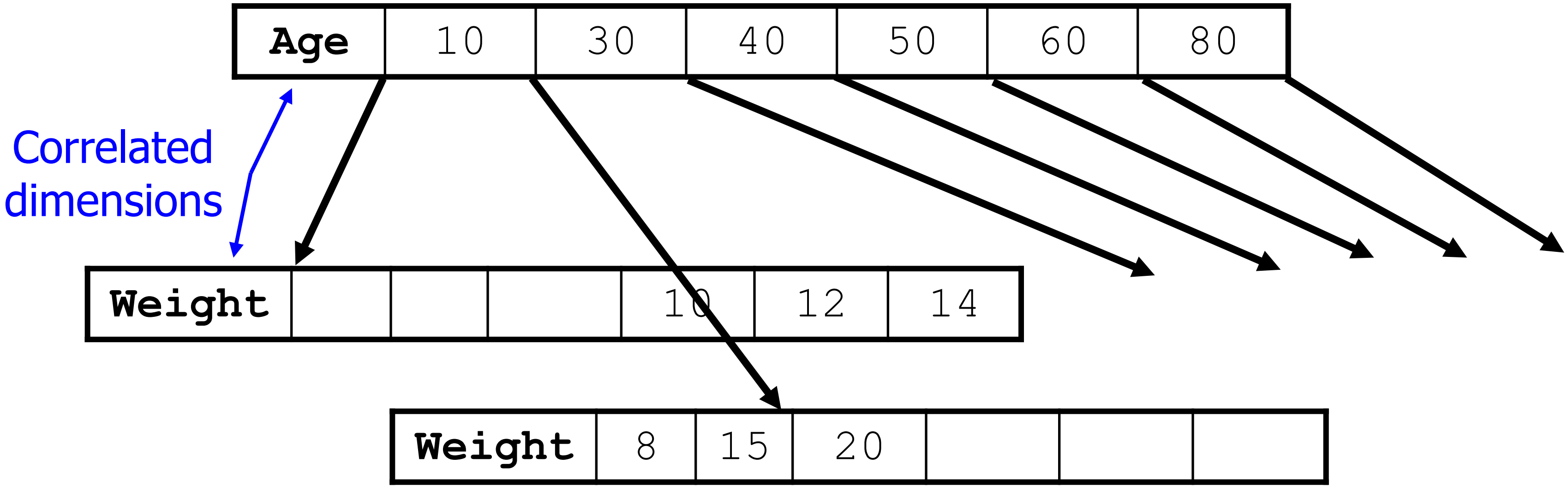
kd Trees on Secondary Storage – Naive Solution

- Store each inner node in one block
  - Inner blocks are essentially empty
  - Since tree is not balanced, worst case requires O(n) IO



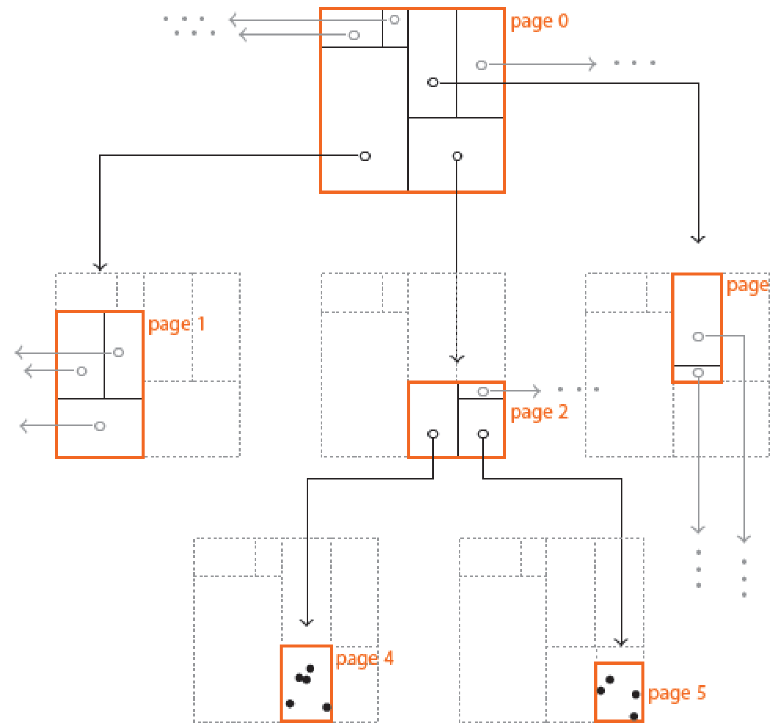
Better: Fill Inner Blocks

- Option 1: Build k-ary kd-Trees
  - Let inner nodes split one dimension at many values
  - When leaf overflows, insert new split into parent
  - When leaf underflows, merge and remove split from parent
  - Still not balanced, no guaranteed fill degree
    - With skewed data



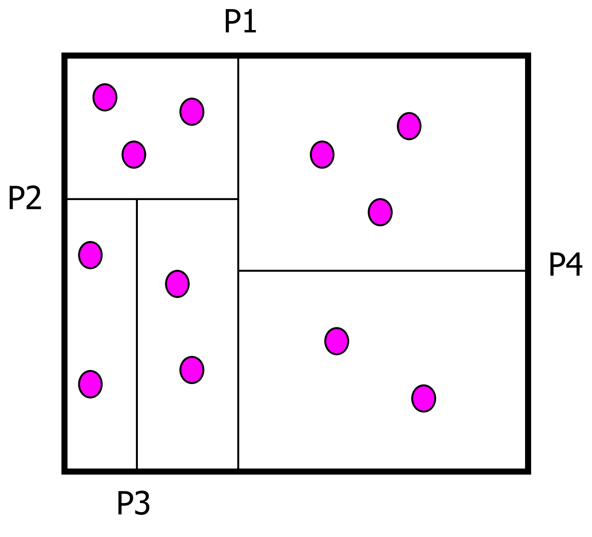
kdb trees

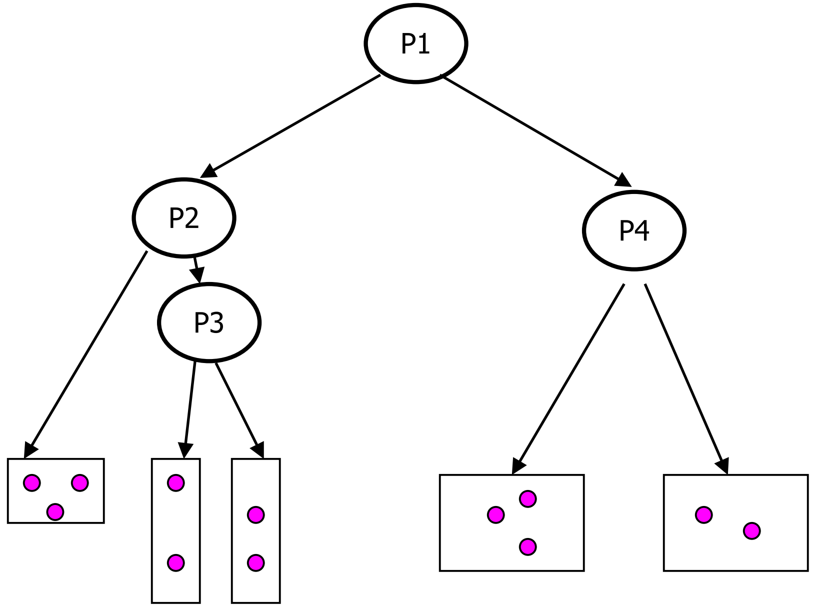
- Option 2: Map many inner nodes to a single blocks
  - Robinson: The K-D-B-Tree: A Search Structure for Large Multidimensional Dynamic Indexes. SIGMOD 1981.
  - Inner nodes have two children (mostly in the same block)
  - Each block holds many inner nodes
  - Inner blocks have many children
    - Roots of kd trees in other blocks
  - Can be balanced (later)
  - No guaranteed fill degree
- Operations
  - Searching: As with kd trees, but has guaranteed tree depth
  - Insertion/Deletion: Keep balance



Another View

- Inner blocks define bounding boxes on subtrees





Another View

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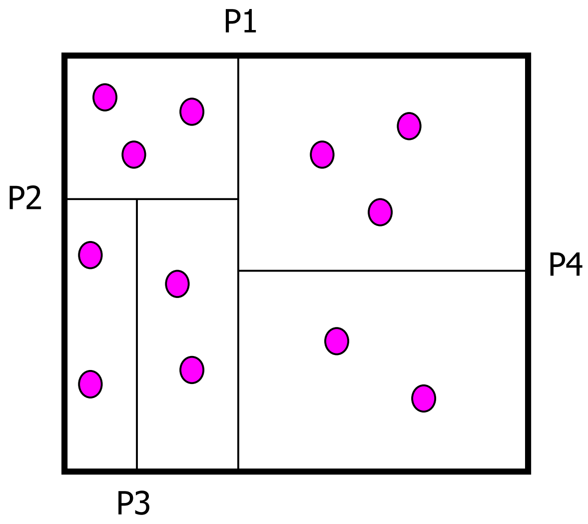
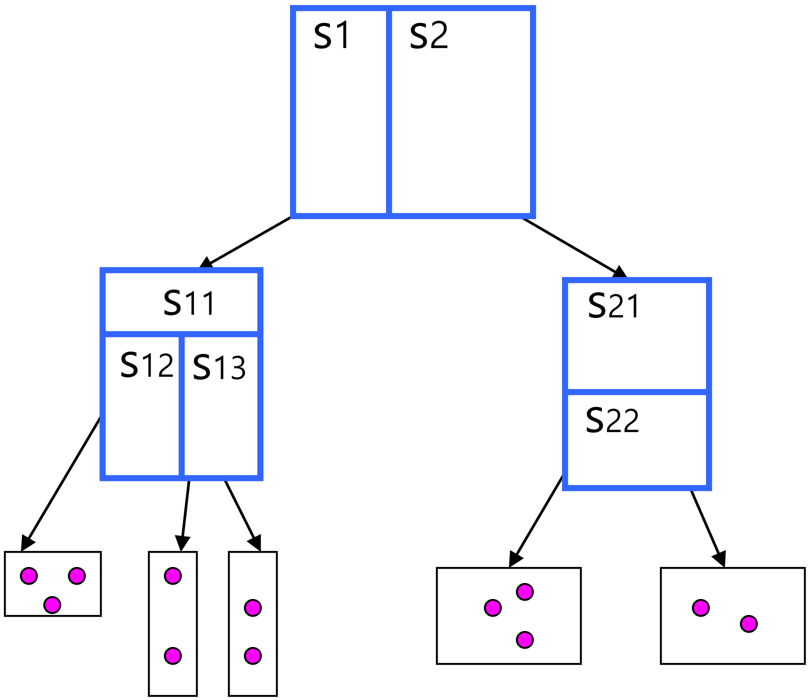
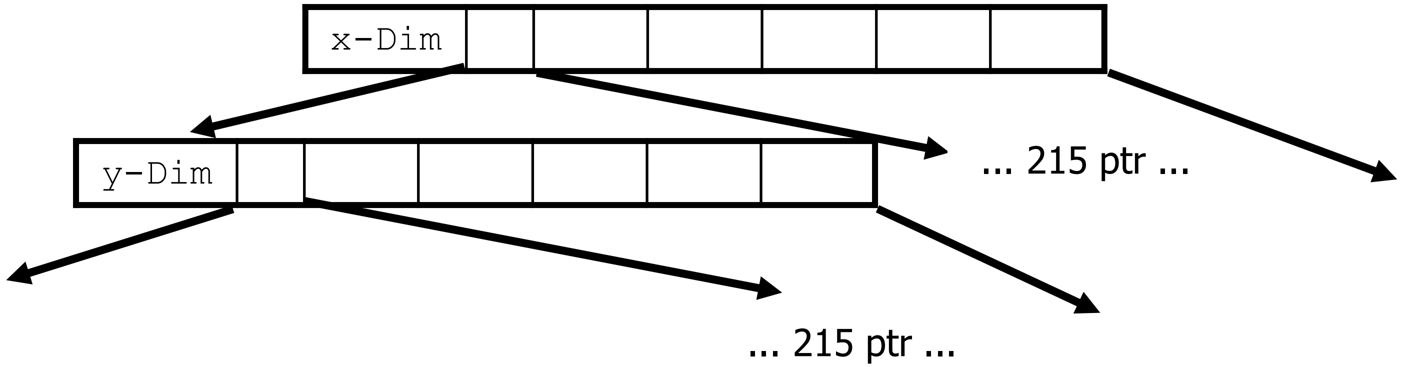




Example – Composite Index

- d=3, n=1E9, block size 4096, |point|=9, |b-ptr|=10
  - We need ~2.2M leaf blocks
- Composite B+ index
  - Inner blocks store 108-215 pointers; assume optimal density
  - We need 3 levels
    - 2nd level has 215 blocks and 46.000 pointers
    - 3rd level has 46K blocks and 10M pointers, 2.2M are needed
  - With uniform distribution, 1st level will mostly split on 1st dimension, 2nd level on 2nd dimension …
- Box query, 5% selectivity in each dimension
  - We read 5% of 2nd level blocks = 10 IO
  - For each, we read 5% of 3rd level blocks = 107 IO
  - For each, we read 5% of data blocks = 1150 IO
  - Altogether: ~1250 IO

Visualization



Example: Partial Box Query

- Box query on 2nd and 3rd dimensions only, asking for a 5% range in both dimensions
  - We need to scan all 215 2nd level blocks
    - Each 2nd level block contains the 5% range of 1^{st} dimension
  - For each, we read 5% of 3rd level blocks = 2300 blocks
  - For each, we read 5% of data blocks = ~25K data blocks
  - Altogether: 26.000 IO
- Note: 0.05 selectivity in two dimensions means 0.0025 selectivity altogether = 125K points
  - Only 270 blocks if optimally packed

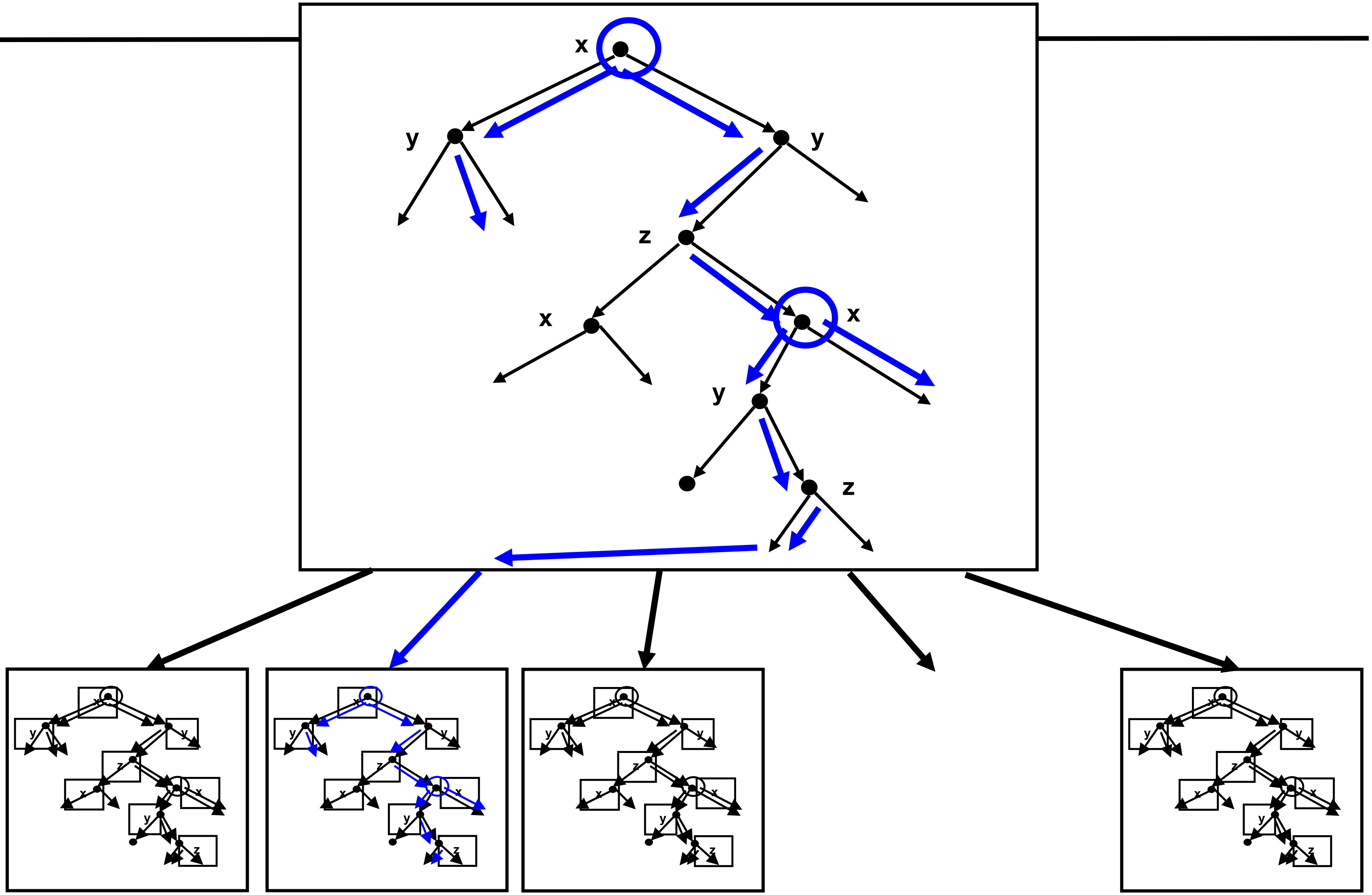
With Balanced kdb Tree

- Balanced kdb tree will have ~22 levels
  - ~455 points in one block (assume optimal packaging)
  - We need to address 1E9/455 ~2^{21} blocks
- Consider 128=2^7 inner nodes in one kdb-block
  - Rough estimate; we need to store 1 dim indicator, 1 split value, and 2 ptr for each inner node, but most ptr are just offsets into the same block
- kdb tree structure
  - 1st level block holds 128 inner nodes = levels 1-7 of kd tree
  - There are 128 2nd level blocks holding levels 8-14 of kd tree
  - There are ~16000 3rd level blocks , each addressing 128 data blocks

Space Covered

- 1st block splits space in 128 regions
- 2nd level block split space in ~16K regions, each region covering 0,00625% of the entire space
- Query selectivity is $(0.05)^3$ = 0,000125% of points and of space (given uniform distribution)
- Thus, we very likely find all results in 1 region of the 1st level and in 1 region of the second level
  - In the worst case, we overlap in all dimensions – 8 regions

Intuition



Box Query Continued

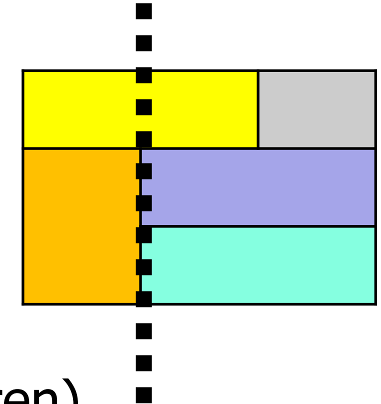
- Box query in all three coordinates, 5% selectivity in each dimension
  - We need to load the root block
  - Very likely, we need to look at only one 2nd level block
  - Very likely, we need to look at only one 3rd level block
  - Assume we need to load all therein addressed 128 data blocks
  - Altogether: 1+1+1+128 = 131 IO
    - That's almost optimal
      - But we made many favorable assumptions
      - kdb-Tree may reach almost optimal performance
    - Composite index had : ~1250 IO

Example - Partial Box Query with kdb Tree

- Box query on 2nd and 3rd dimensions only, asking for a 5% range in each dimension
  - In first block (7 levels), we have ~2 splits in each dimension
    - Two times 2 splits, one time three splits
    - Assume we miss the dimension with 3 splits
  - Hence, in ~4 of 7 splits we know where we need to go, in ~3 splits we need to follow both children
  - We need to check only 2^3=8 second-level blocks
    - Again – number gets higher when query range crosses split points
  - Same argument holds in 2nd level blocks = 8*8 data blocks
  - Same argument holds in 3nd level blocks = 8*8*8 data blocks
  - Altogether: 1+8+64+512 ~580 IO
    - Compare to 26.000 for composite index
    - But optimal would be only 270

Balancing upon Insertions

- Similar method as for B+ trees
  - Search appropriate leaf
  - If leaf overflows, split
    - Chose dimension and split value; re-distribute points into two blocks
    - Propagate to parent node
  - In parent node, a leaf must be replaced by an inner node
    - With two new blocks as children
  - This may make the parent overflow – propagate up the tree
- Splitting an inner node
  - Chose a dimension and split value
  - Distribute nodes to two new blocks
    - Split might have to be propagated downwards
    - "Default" split may lead to very bad fill degree
  - Propagate new pointers to parent (and their children)
  - Might lead to reorganization of entire tree



Conclusion

- kdb trees pro
  - Conceptually nice
  - May achieve optimal search performance
- Kdb contra
  - No guaranteed fill degree
    - Many insertions/deletions lead to almost empty leaves
  - Keeping balance requires sporadic tree reorganizations
    - Runtime of single operations become unpredictable
- Nice idea, difficult to implement, rarely used in practice

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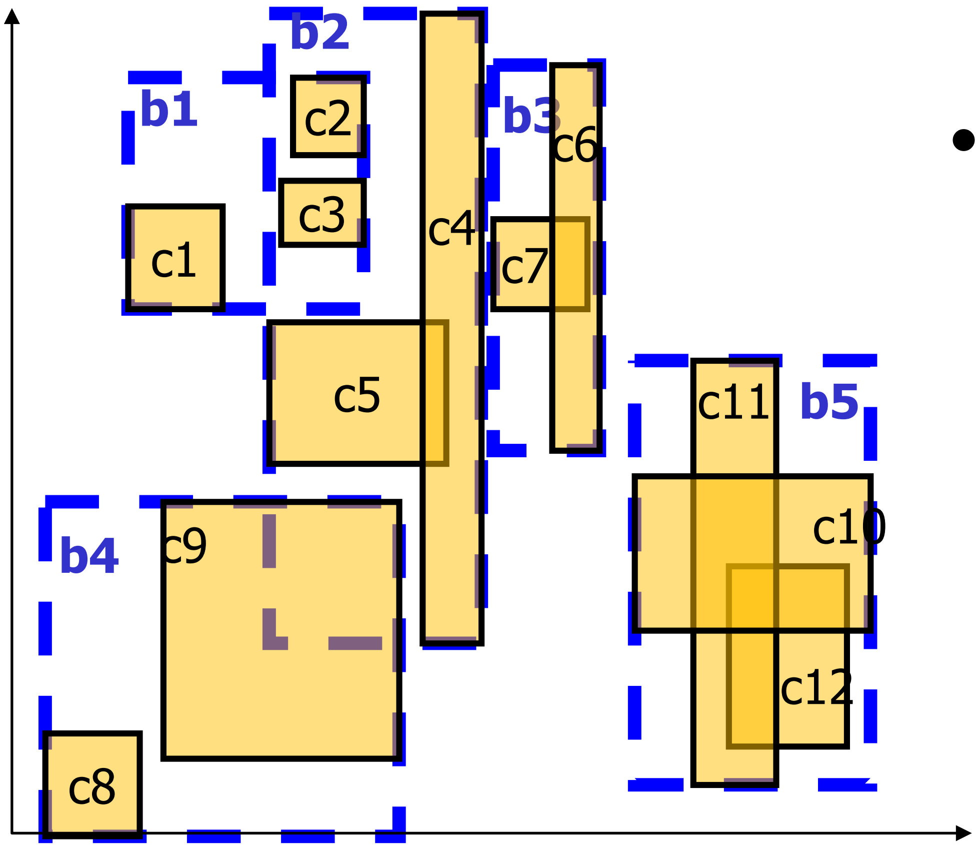
- Conclusions

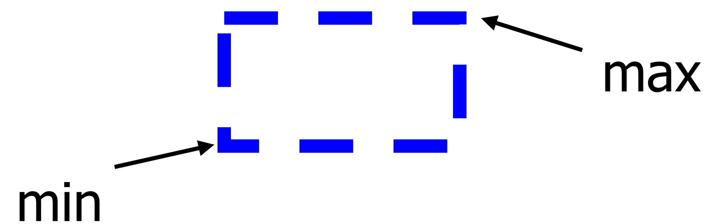
R-Trees

- Guttman. R-Trees: A Dynamic Index Structure for Spatial Searching. SIGMOD 1984.
- Can store geometric objects (with area) as well as points
  - Arbitrary geometric objects are represented by their minimal bounding box (MBB)
- Each object is stored in exactly one region on each level
- Since objects may overlap, regions may overlap
- Only regions containing data objects are represented
  - Allows for fast stop when searching in empty regions
- Tree is kept balanced (like B tree)
- Guaranteed fill degree (like B tree)
- Many variations (see literature)

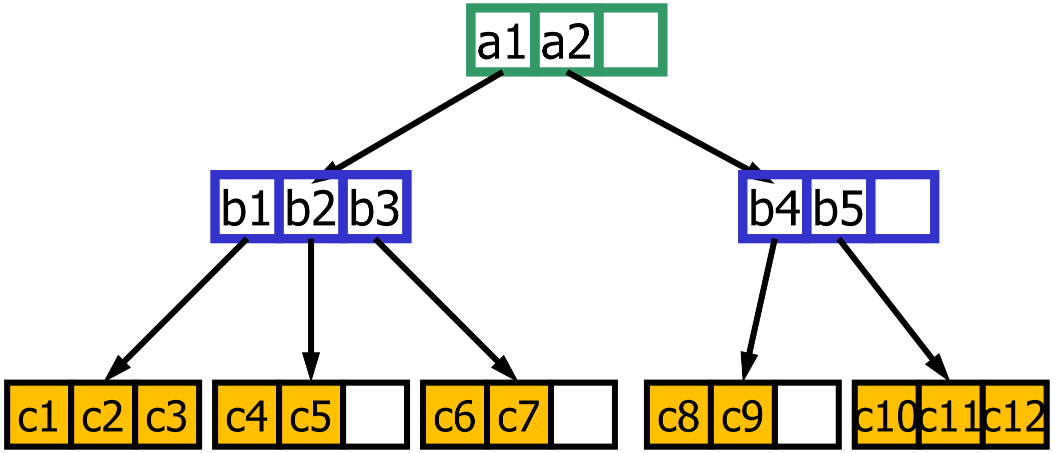
General Idea

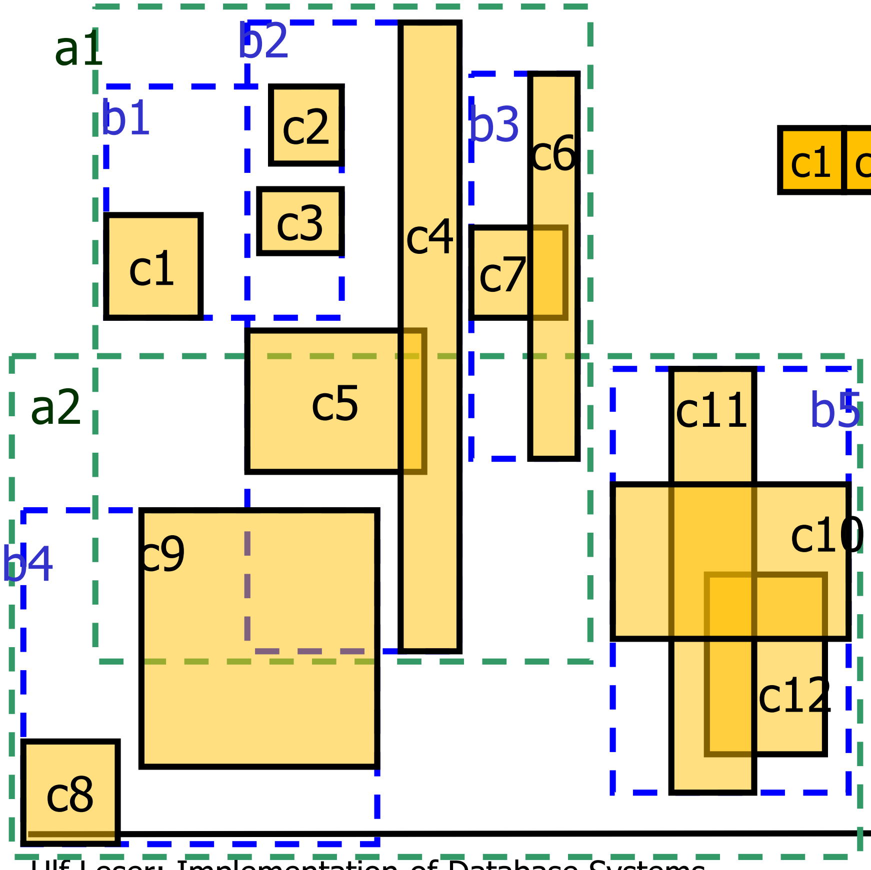
- We group clusters of spatial objects into minimal bounding box (MBB)
- Each MBB is represented by just two corner points





General Idea

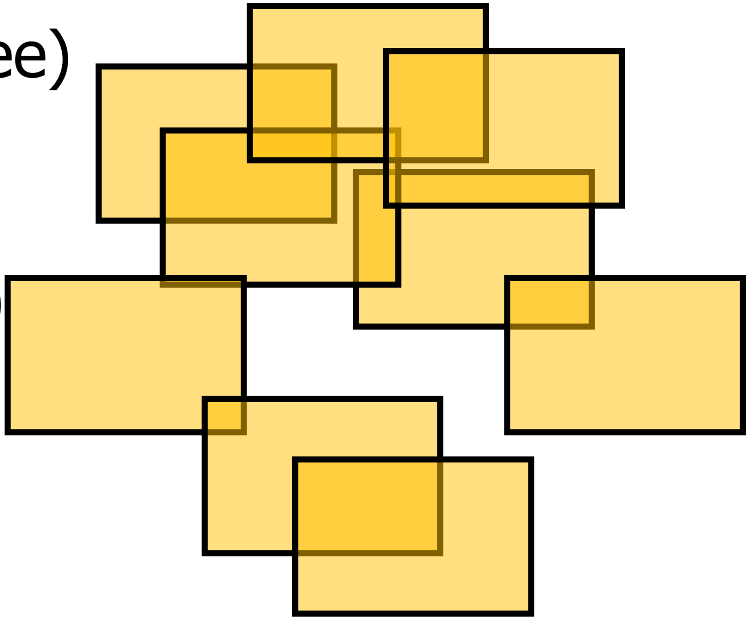




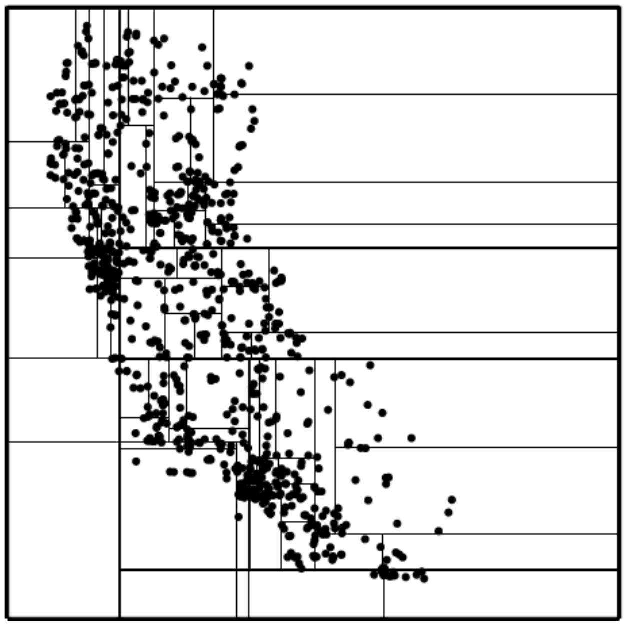
- Objects are stored only once in leaf nodes
- We group MBBs hierarchically into overlapping regions

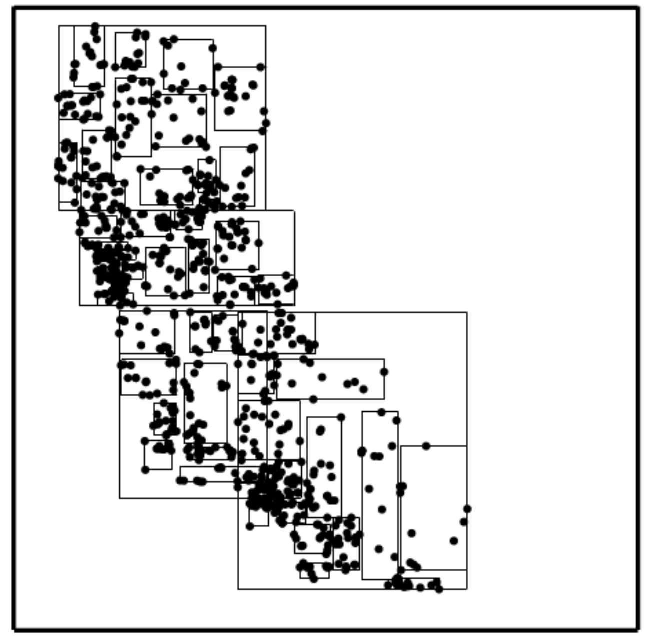
Motivation: Objects that are not points

- We need overlapping regions
  - For instance, if all MBBs overlap
  - No split possible which creates disjoints sets of objects
- Objects crossing a split
  - Stored in only one MBB (R-Tree)
    - Search must examine both
    - No redundant data
  - Stored in both MBB (R+-Tree)
    - Search may choose any one
    - Redundant data



R Tree versus kd Tree





Concepts

- Inner nodes consist of a set of d-dimensional regions
  - Every region is a (convex) hypercube - MBB
- Regions are hierarchically organized
- Each region of an inner node points to a subtree or a leaf
- The region border is the MBB of all objects in this subtree
  - Inner node: MBB of all child regions
  - Leaf blocks: All objects are contained in the respective region
- Regions in one level may overlap
- Regions of a level do not cover the space of its parent completely (as opposed to the KD-tree)

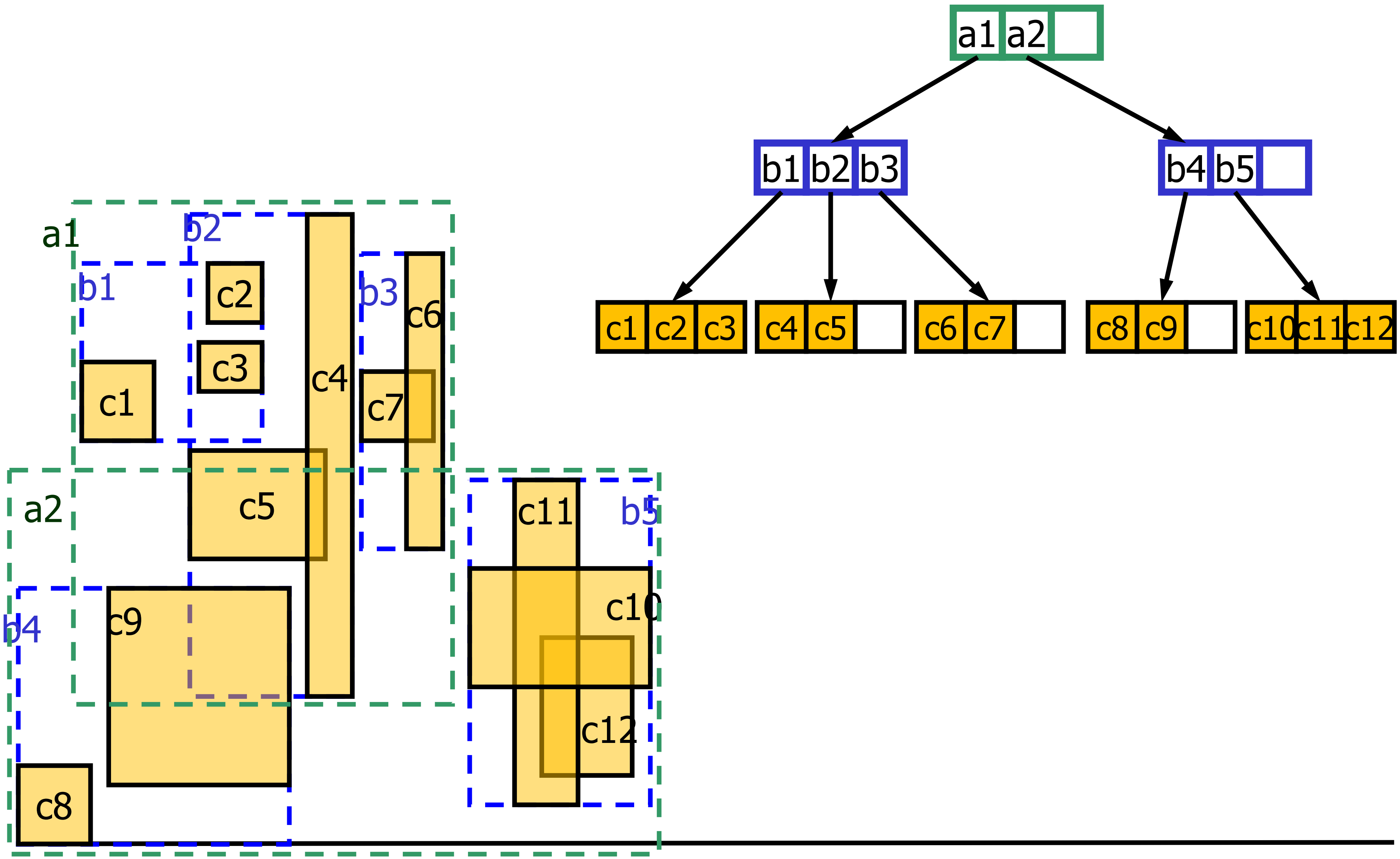
Concepts

- Guaranteed fill degree: The number of regions of a node (except for the root) is between m and M
  - M : the maximum number of entries in a node
  - $M = \lfloor size(P) / size(E) \rfloor$ P: disk page, E: entry
  - m: set to some fraction of M
- The root node has at least 2 entries
- Balanced: Leaf nodes are at the same level

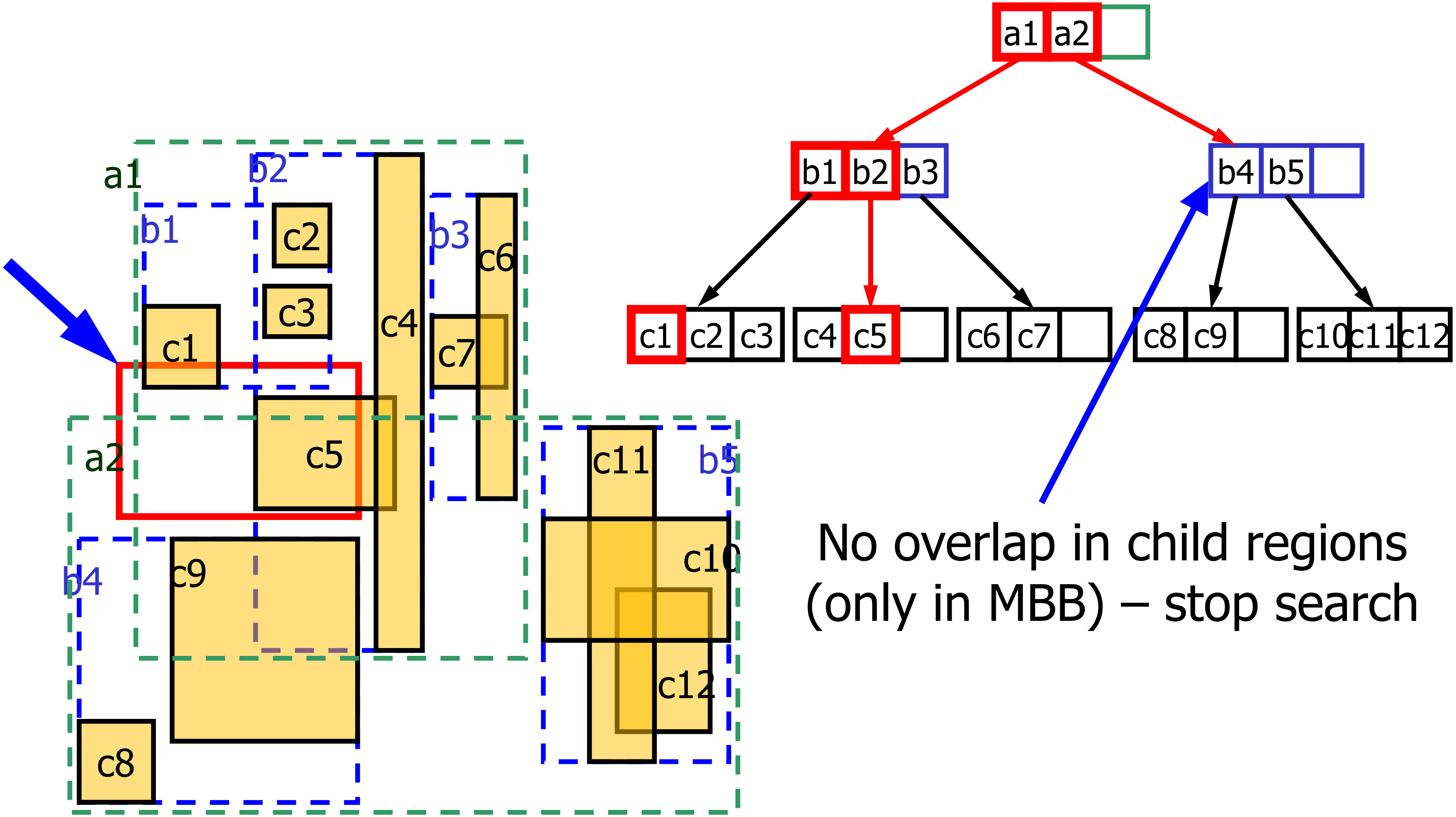
Searching

- All objects are contained within MBBs
- Thus, a query that does not intersect an MBB cannot intersect the contained objects
- Point query
  - At each inner node, find all regions containing the point
  - Multi-path: All those subtrees must be searched
- Range query: Find all objects (MBBs) overlapping with a given query range (MBB)
  - In each node, intersect query with all regions
  - More than one region might have non-empty overlap
  - All those subtrees must be searched

One State



Example: Searching



No overlap in child regions (only in MBB) – stop search

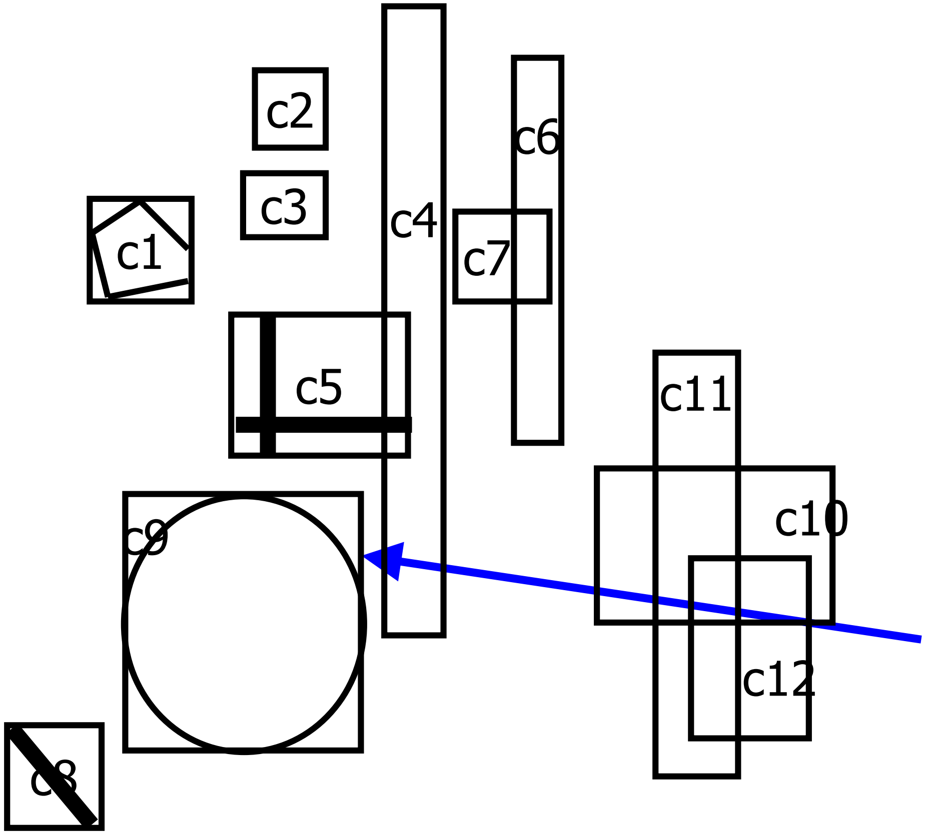
Inserting an Object

- Traverse the R-tree top-down, starting from the root
- In each node, find all candidate regions
  - Any region may overlap the object completely, partly, or not
  - Object may overlap none, one, or many regions – partly or completely
  - At least one region with complete overlap
    - Choose one (smallest?) and descend
  - None with complete, but at least one with partial overlap
    - Choose one (largest overlap?) and descend
  - No overlapping region at all
    - Choose one (closest?) and descend
- Eventually, we reach a leaf
  - We insert object in only one leaf

Continuation

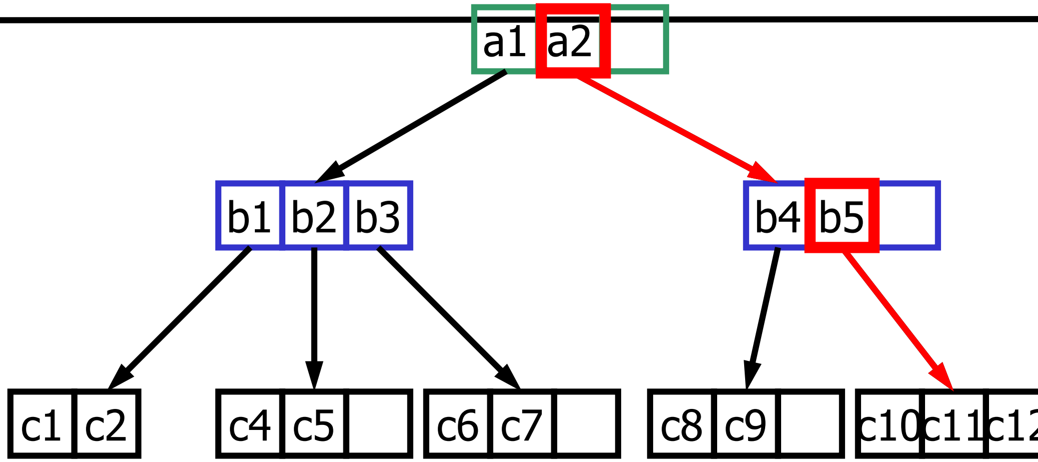
- If free space in leaf
  - Insert object and adapt MBB of leaf
  - Recursively adapt MBBs up the tree
  - This usually generates larger overlaps – search degrades
- If no free space in leaf
  - Split block in two regions
  - Compute MBBs
  - Adapt parent node: One more child, changed MBBs
  - May affect MBB of higher regions and/or incur overflows at high regions – ascend recursively

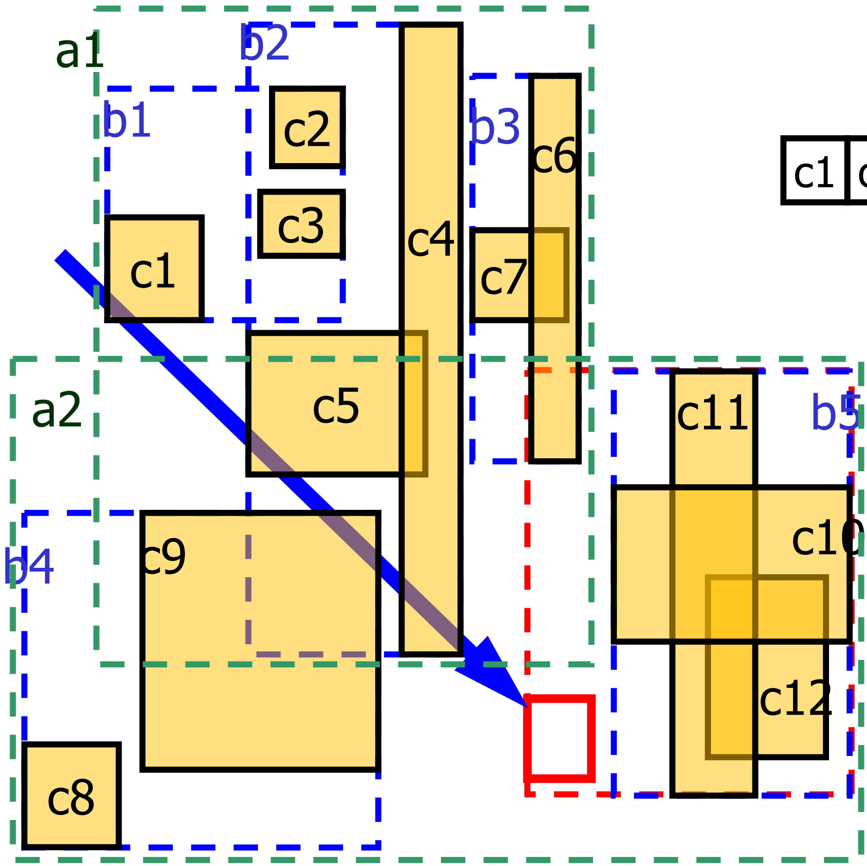
Example (from Donald Kossmann)



Compute MBBs for all non-rectangular objects

Example: Insertion, Search Phase

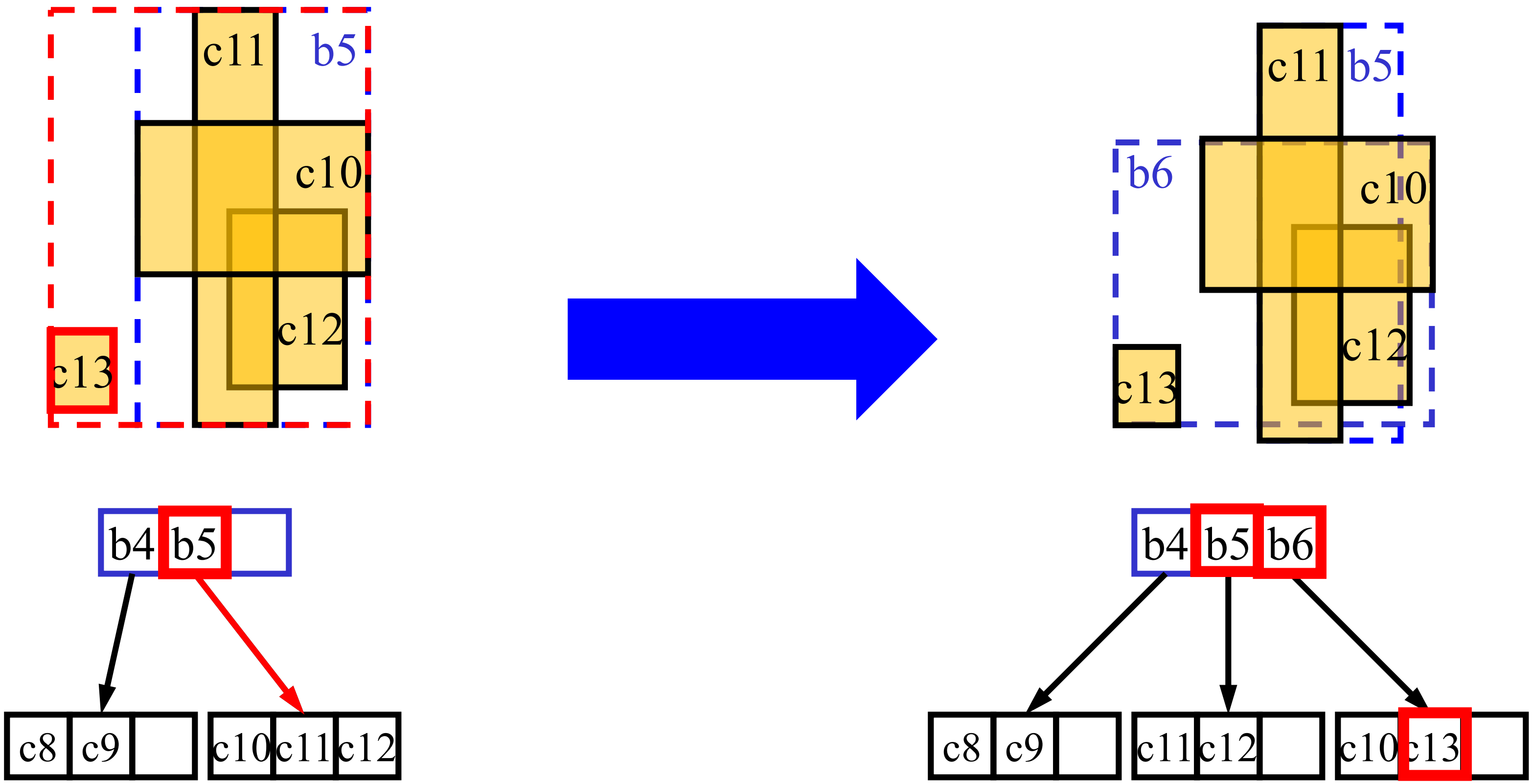




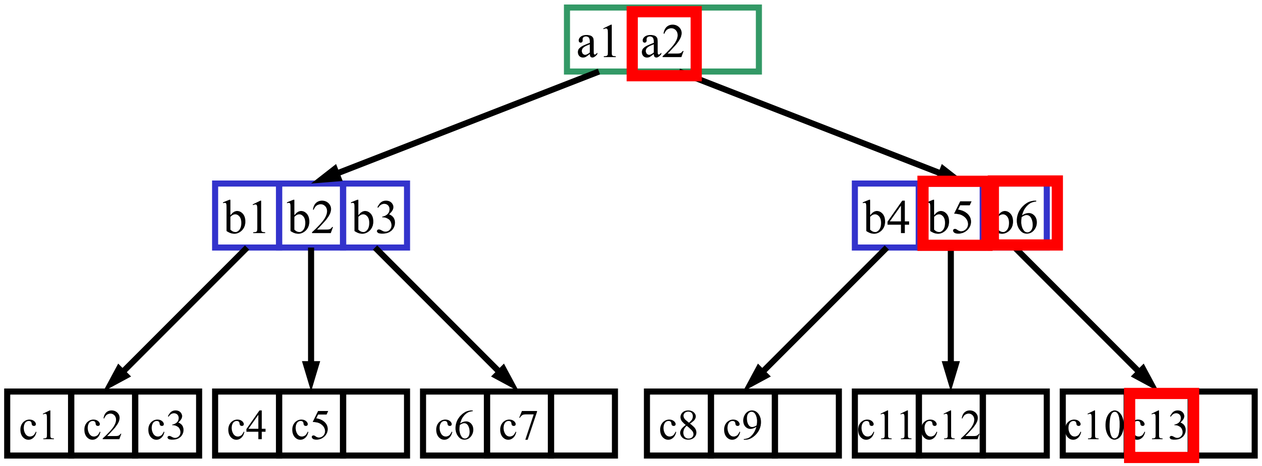
- Search regions whose MBB must be expanded the least
- Repeat on each level
- Here: Leaf overflow, split
  - Note: Choosing b4 would avoid split – but how can we know?

Example: Insertion, Split Phase

Several splits are possible



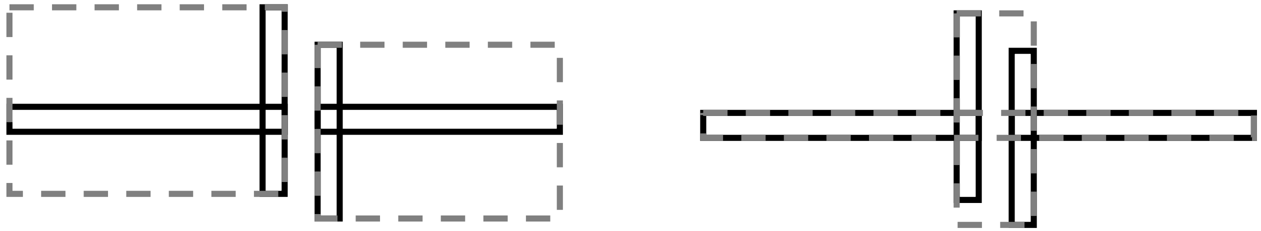
Example: Insertion, Adaptation Phase



- MBBs of all parent nodes must be adapted
- Block split might induce node splits in higher levels of the tree (not here)

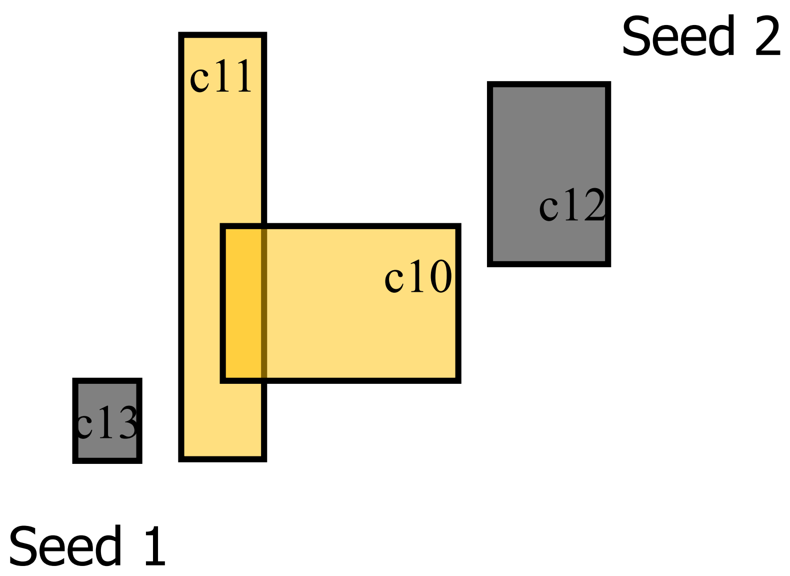
Where to Split

- Finding the best splitting strategy has seen ample research
- Option 1: Avoid overlaps
  - Compute split such that overlap is minimal (or even avoided)
  - Minimizes necessity to descend to different children during search
  - May create larger regions – more futile searches in “empty” regions
- Option 2: Minimize space coverage
  - Compute split such that total volume of all MBBs is minimal
  - Increases changes to descend on multiple paths during search
  - But: Unsuccessful searches can stop earlier



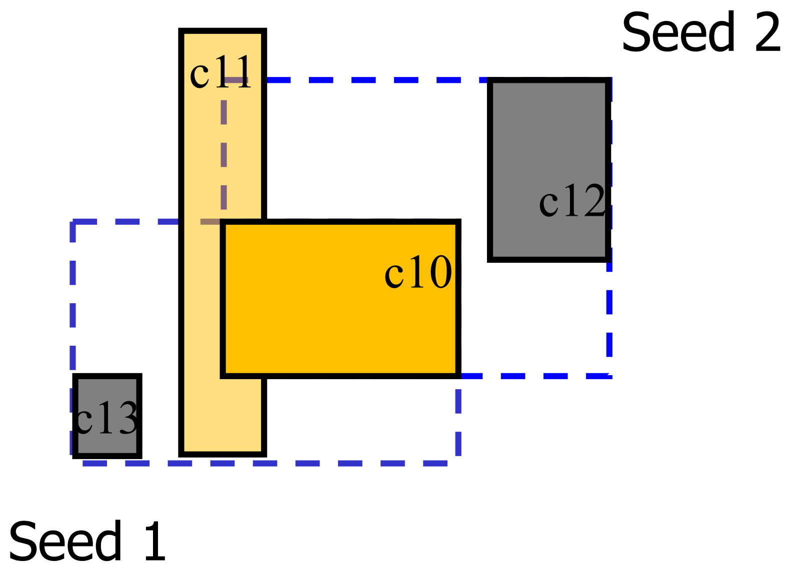
Split Strategies

- Rationale:
  - Pick two objects as seeds
  - Assign other objects to the closest seeds



Split Strategies

- Rationale:
  - Pick two objects as seeds
  - Assign other objects to the closest seeds
  - Closest: the total MBB volume minimally increases



Split Strategies

- Complexity
  - Consider a block with n objects
  - There are $2^n/2=2^n-2$ possibilities to partition this block into two
  - In multi-dimensional spaces, there is no simple sorting
  - Use heuristics instead of optimal solution
- Original Strategies (Minimizing Overlap)
  - Linear: Pick two pairs with greatest normalized separation. Greedily associate each other object to the region whose space is increased the least
  - Quadratic: Pick two pairs such that the two regions minimally overlap and are maximally large. Greedily associate each other object to the region whose space is increased the least
  - Exponential: Check all bipartitions and chose the one with minimal overlap

Linear Split

- In each dimension, find two objects with greatest separation
- Normalize the separation by the total extent in that dimension
- Put the two entries E1 and E2 with the greatest normalized separation into different groups

- Greedily associate each other of the M-1 objects to the region whose space is increased the least

Quadratic Split

- Pick the two seed entries E1 and E2 that would waste most area, if put together, that is to maximize:

  $$area(mbb(E1, E2) - area\,(E1) - area\,(e2)$$

- Complexity: $O\big((M+1)^2\big)$

- Greedily associate each other of the M-1 objects to the region whose space is increased the least

Deletions in the R Tree

- As usual: In case of underflow (<m% fill degree), the block is removed
- R Trees typically do not move objects to neighbor leafs
  - MBBs would have to be adopted
  - But relationship of MBBs may be quite arbitrary
  - May create very large overlaps, very large spaces covered
  - One could find optimal moves, but …
- Trick: Delete by Reinsertion
  - Re-Insert every objects that remained in the underflown block
  - Guarantees of the insert strategies will hold
  - No particular delete strategy required – focus on good insertions
  - But costly: A single delete may incur hundreds of inserts

R+ Tree

- Two effects leading to inefficiency during search
  - Overlapping MBBs lead to multiple search paths
  - A few large objects enforce large MBBs covering much dead space
- R+ Tree
  - Objects overlapping with two regions are stored in both (clipping)
  - MBBs in a node never overlap
- Much faster search, but
  - Search must perform duplicate removal as last steps
  - Insertion / deletion may have to walk multiple paths, incurring multiple adaptations
  - Worse space consumption due to redundancy,
  - Insertion may require down- and upward adaption
    - Like kdb Trees

Content of this Lecture

- Introduction
- Partitioned Hashing
- Grid Files
- kdb Trees
- R Trees
- Conclusions

Multidimensional Data Structures Wrap-Up

- Many more MDIS: X tree, VA-file, hb-tree, UB tree, …
  - Store objects more than once; other than rectangular shapes; map coordinates into integers; …
- All MDIS degrade with increasing number of dimensions (d>10) or very unusual skew
  - For neighborhood and range queries
  - Hierarchical MDIS degenerate to an expensive linear scan
- Trick: Find lower-dimensional representations with provable lower bounds on distance to prune space
  - Requires distance function-specific lower bounding techniques
- Alternative: Approximate MDIS (LSH, randomized kd Trees)
  - Find almost all neighbors, with/out given probability

Curse of Dimensionality – Consider a growing d

- Consider a typical rectangular partitioning method
- Some obvious problems
  - Points need more coordinates, less node capacity – fan-out decreases
  - Decreasing fan out – deeper trees
  - Just comparing two points becomes linearly more expensive
  - Intersecting two objects becomes more expensive
  - These operations are performed all the time when searching and inserting / deleting objects

Curse of Dimensionality – Consider a growing d

- Some less obvious mathematical facts
  - Weber, R., Scheck, H. and Blott, S. (1998). "A Quantitative Analysis and Performance Study for Similarity-Search Methods in High-Dimensional Spaces". VLDB
- If space is covered, #partitions grows exponentially
  - But usually there are not “exponentially many” points
  - Most partitions will be almost empty
- Average distances grows steadily
- Consider a 1-NN query
  - 1-NN queries search a hypersphere, but partitions are hypercubes
  - The larger d, the smaller the fraction of space a hypersphere of radius 0.5 fills within a hypercube of edge length 1
  - The larger d, the more partitions one has to search to find neighboring points – the space is empty, everything is far away