MPRI – Computation Geometry and Topology

Nearest Neighbor Search

Steve Oudot

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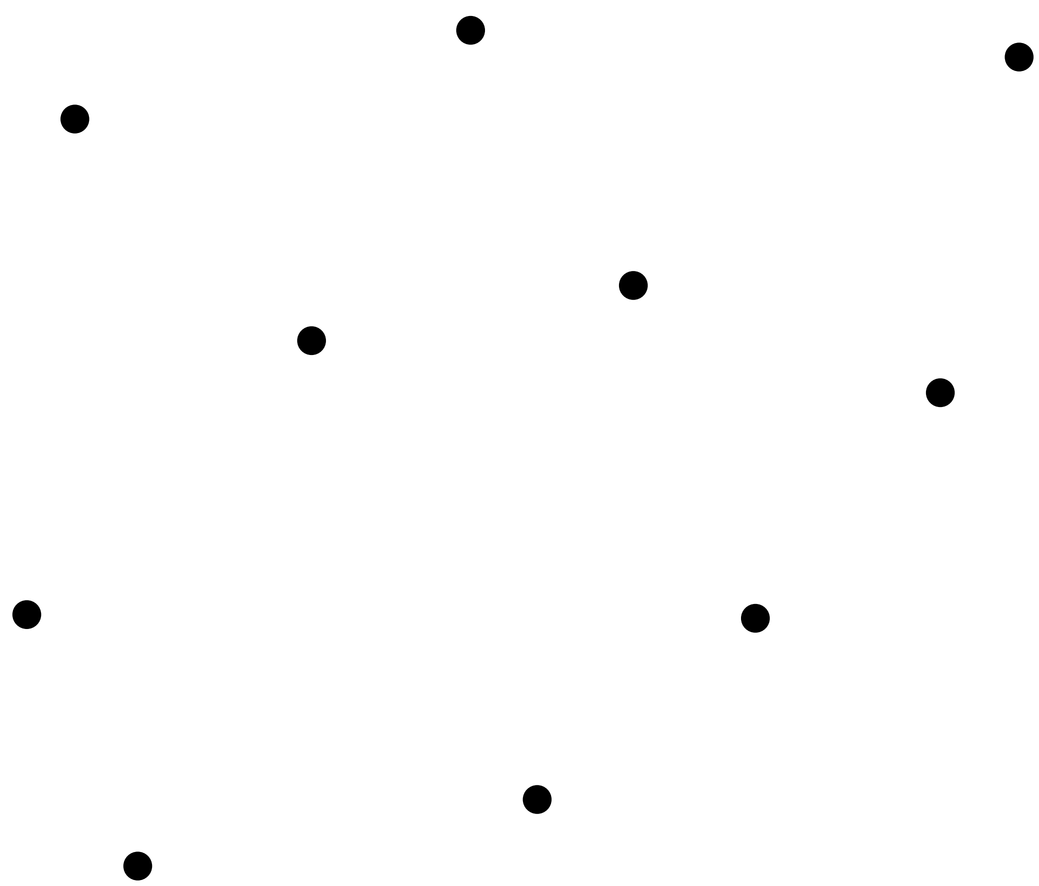
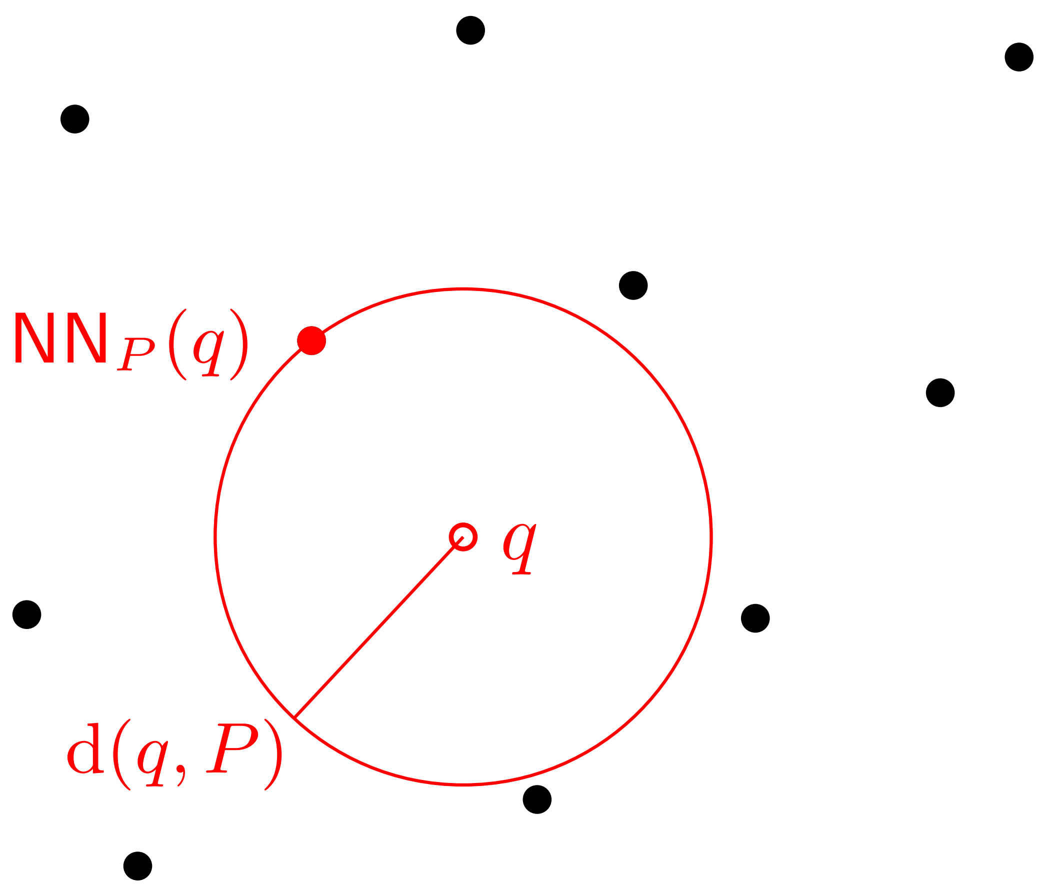
Nearest-Neighbor problem

pre-processing input: P



Nearest-Neighbor problem



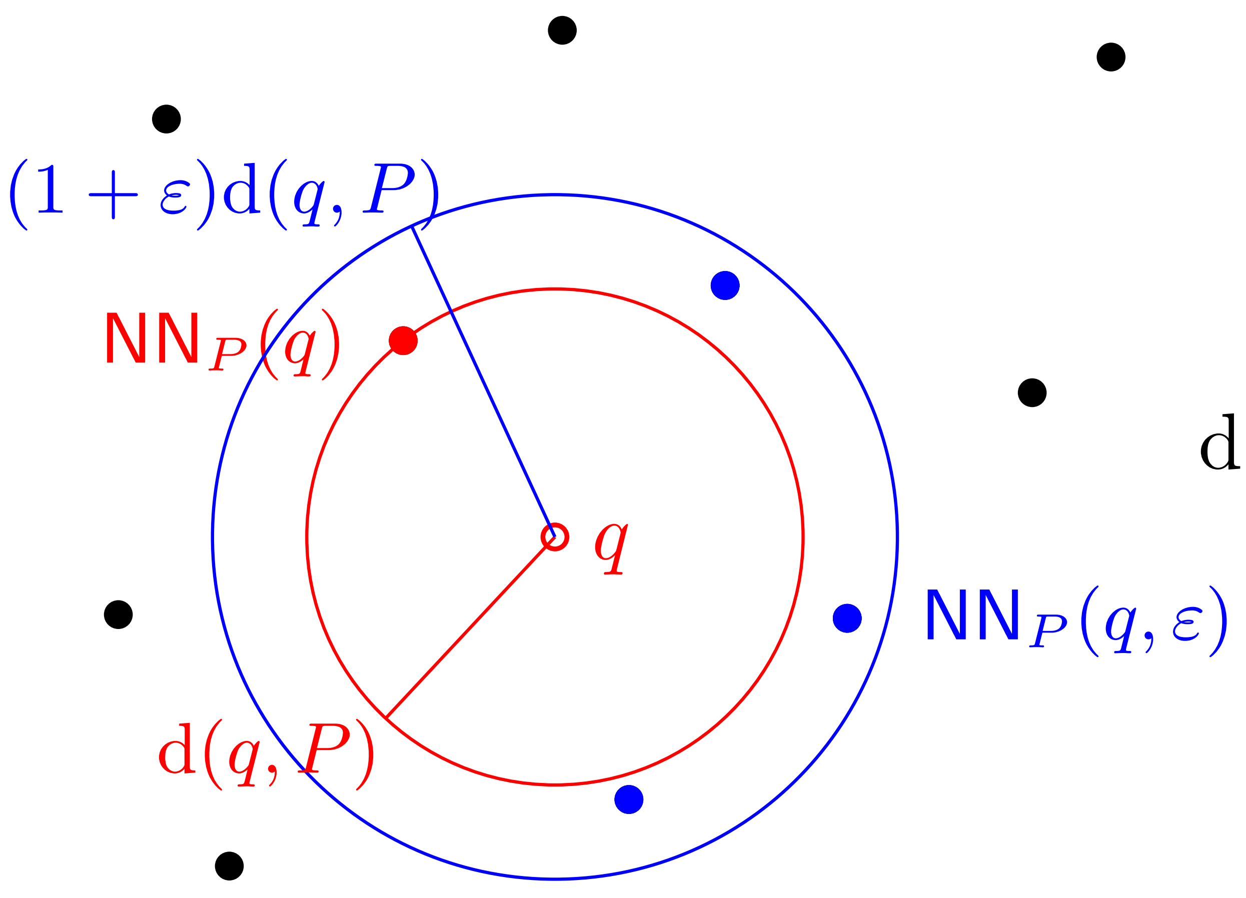
pre-processing input: P

query input: q

goal: find $p \in \mathrm{NN}_P(q)$

$\mathrm{d}(q,p) = \min_{p' \in P} \mathrm{d}(q,p')$

ε-Nearest-Neighbor problem



pre-processing input: P, ε

query input: q

goal: find $p \in \mathrm{NN}_P(q,\varepsilon)$

$$\mathrm{d}(q,p) \leq (1+\varepsilon)\ \min_{p' \in P} \mathrm{d}(q,p')$$

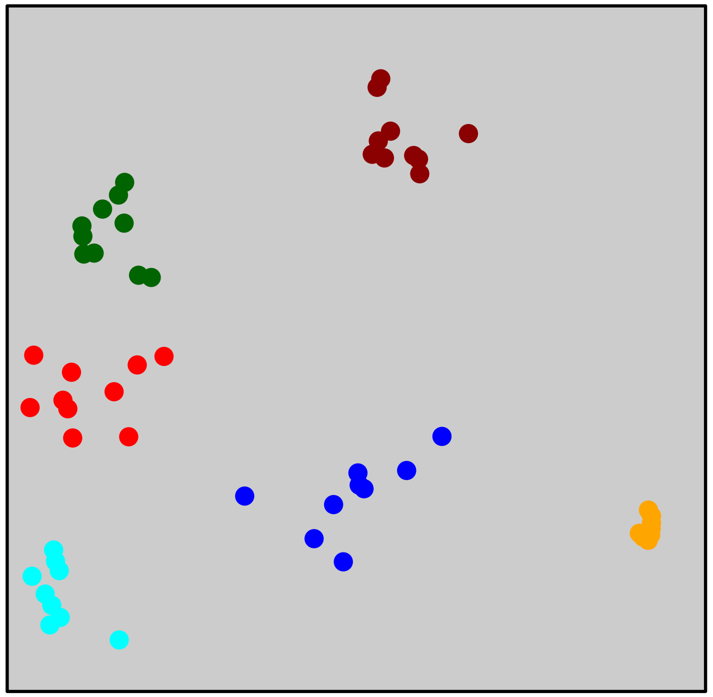
Nearest-Neighbor problem

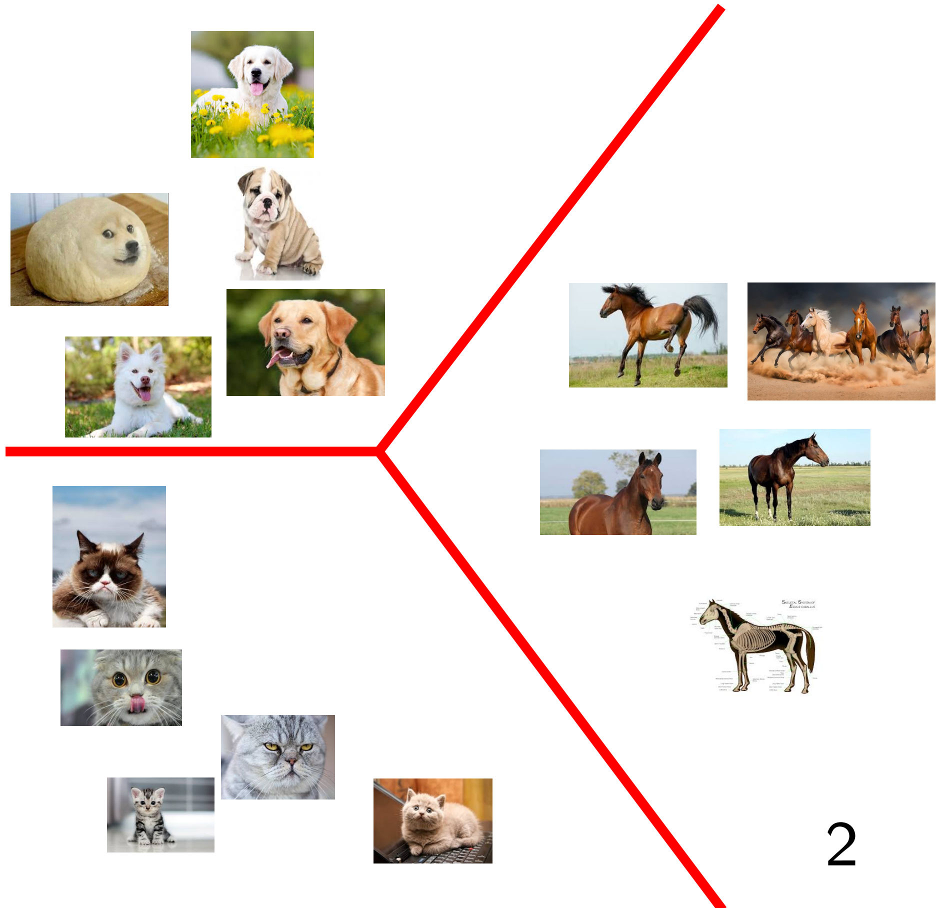
Variants:

- k-nearest neighbors: find the k points closest to q in P
- r-nearest neighbor: find a point $p \in P$ such that $\mathrm{d}(q, p) \leq r$
- metrics:
    - ℓ_2, ℓ_p, ℓ_∞
    - strings: Hamming distance
    - images: optimal transport distances
    - point clouds: (Gromov-)Hausdorff distances
    - proteins: RMSD distances
    - $\cdots$

Applications

- clustering, e.g. k-means, mean-shift
- information retrieval in databases
- information theory, e.g. vector quantization
- supervised learning, e.g. NN-classifiers
- . . .





Linear scan

Input: $P = \{p_1, \cdots, p_n\} \subset \mathbb{R}^d$, $q \in \mathbb{R}^d$

$\mathrm{d_{min}} := \infty$ (dist. to nearest neighbor among the pts viewed so far)

for $i = 1$ to n do:

$\quad \mathrm{d_{min}} := \min\{\mathrm{d_{min}}, \mathrm{d}(q, p_i)\}$

return $\mathrm{d_{min}}$ or index i that achieves $\mathrm{d_{min}}$

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Complexity:

space: $O(d\,n)$ — n points, d coordinates each

time: $O(d\,n)$ — n iterations, 1 distance computation each

Strategy and Challenges

Strategy:

- preprocess the n point of P in $\mathbb{R}^d$ into some data structure DS for fast nearest-neighbor queries answers

Ideal wish list:

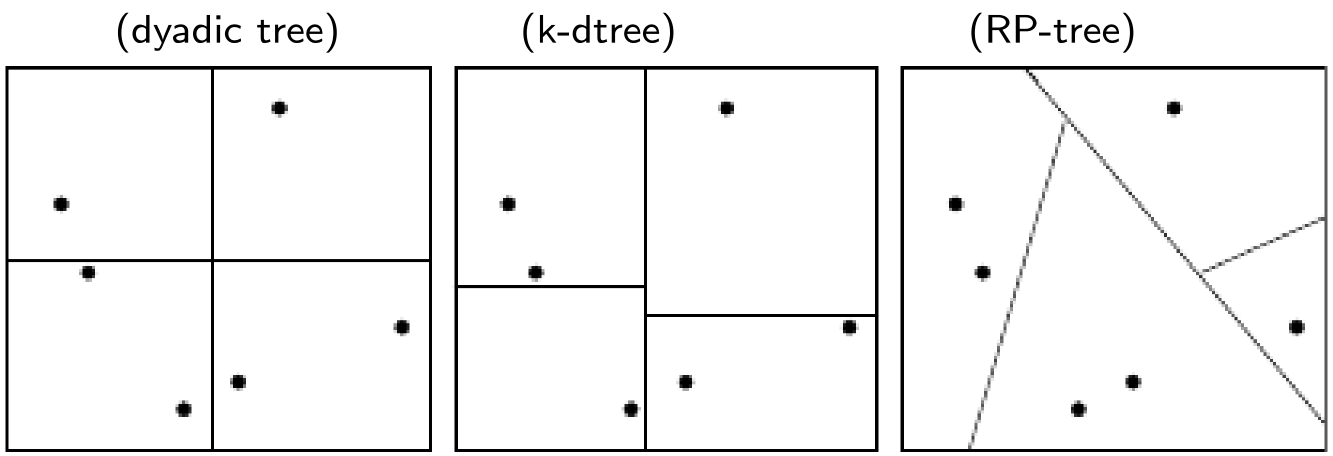
- DS should have linear size in n and polynomial size in d
- a query should take sublinear time in n and polynomial time in d

  e.g. binary search trees in $d = 1$: linear size, $O(\log n)$ time

Core difficulties:

- *Curse of dimensionality*: hard to outperform linear scan in high d
- Interpretation: meaningfulness of distances in high d (concentration)

Approaches



exact NN search

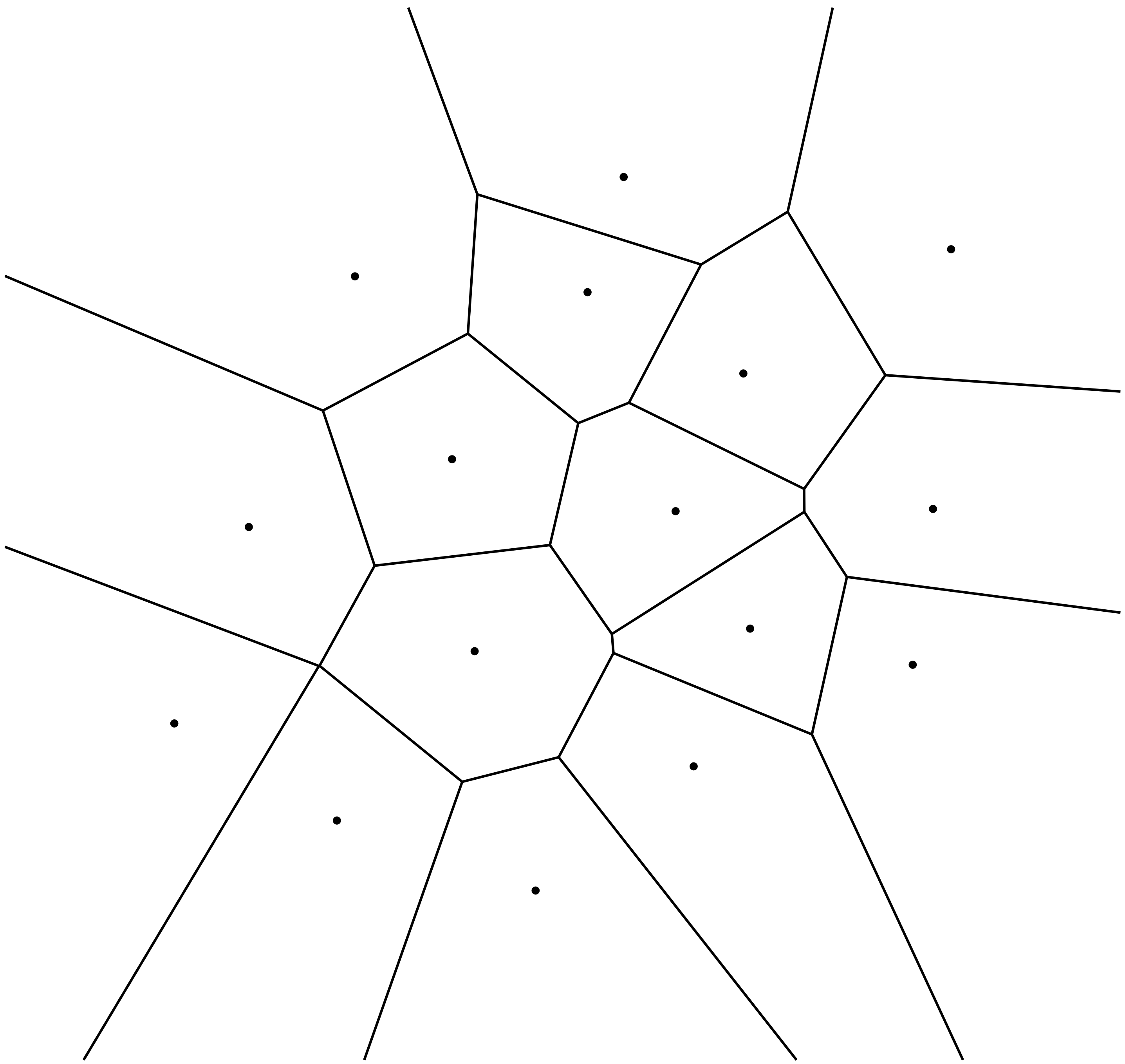
- Linear scan
- Voronoi diagrams
- Tree-like data structures
  - quadtrees (split at midpoint in all coordinates)
  - tries / dyadic trees (split at mean, cycle around coordinates)
  - kd-trees (split at median, cycle around coordinates)
  - Random Projection trees (split at median along random coordinates)
  - PCA trees (split at median along 1st eigenvector of covariance matrix)
  - $\cdots$

approx. NN search

- Locality Sensitive Hashing

Voronoi diagrams

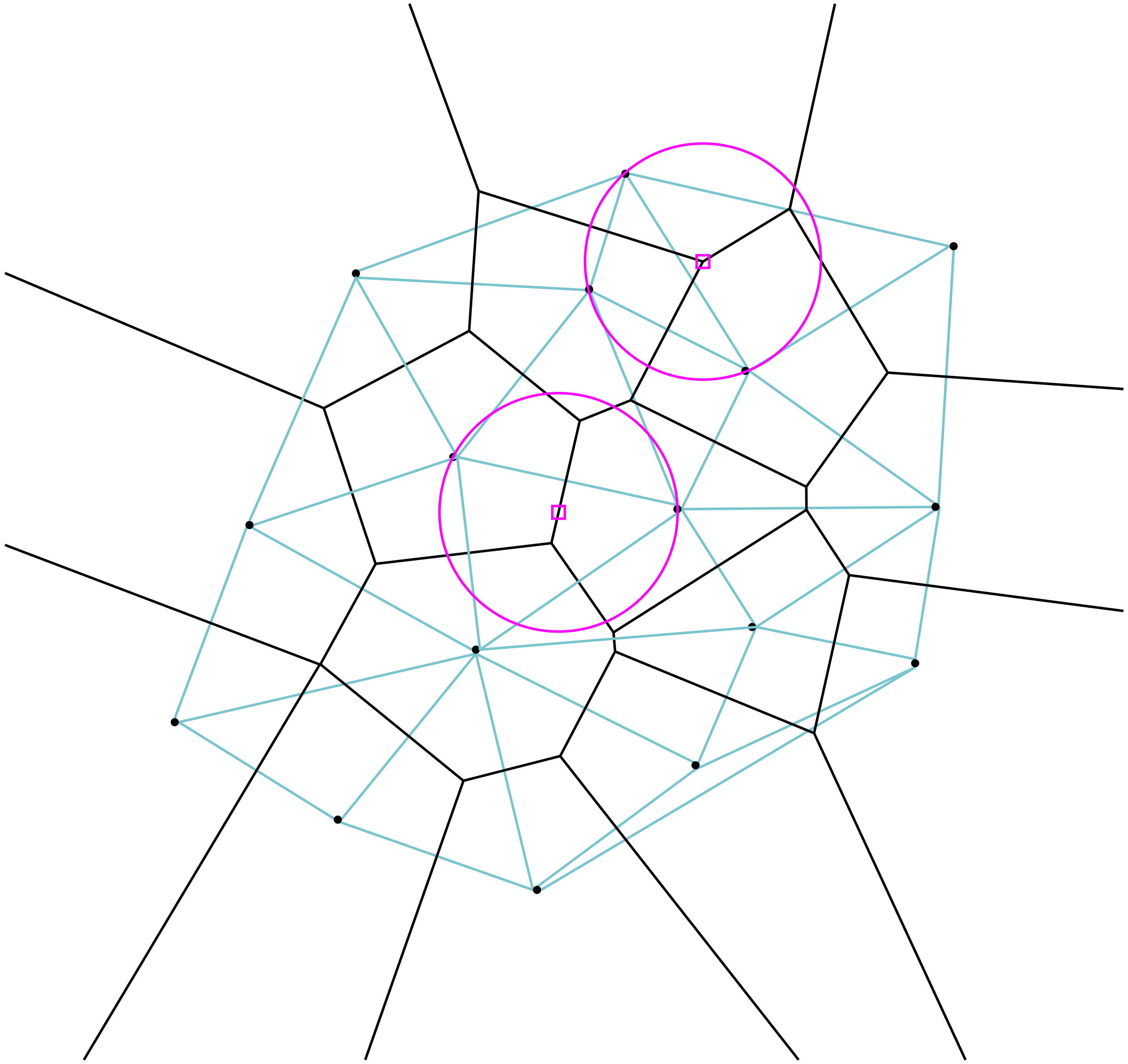
Definition



$$V(p) := \{q \in \mathbb{R}^d \mid p \in \mathrm{NN}_P(q)\}$$

affine diagram

Definition



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affine diagram

computed/stored via dual

(Delaunay triangulation)

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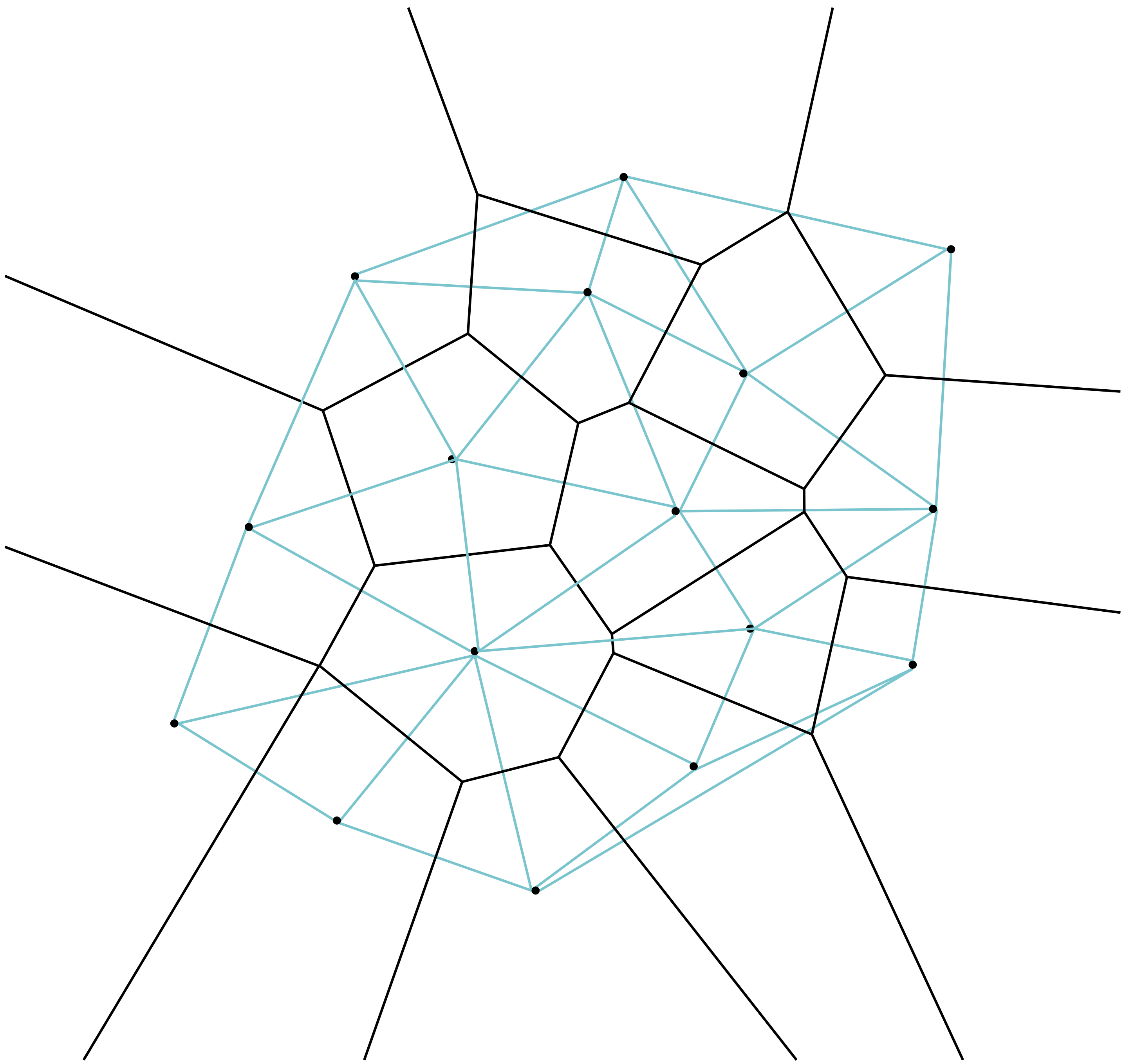

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affine diagram

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(Delaunay triangulation)

size:

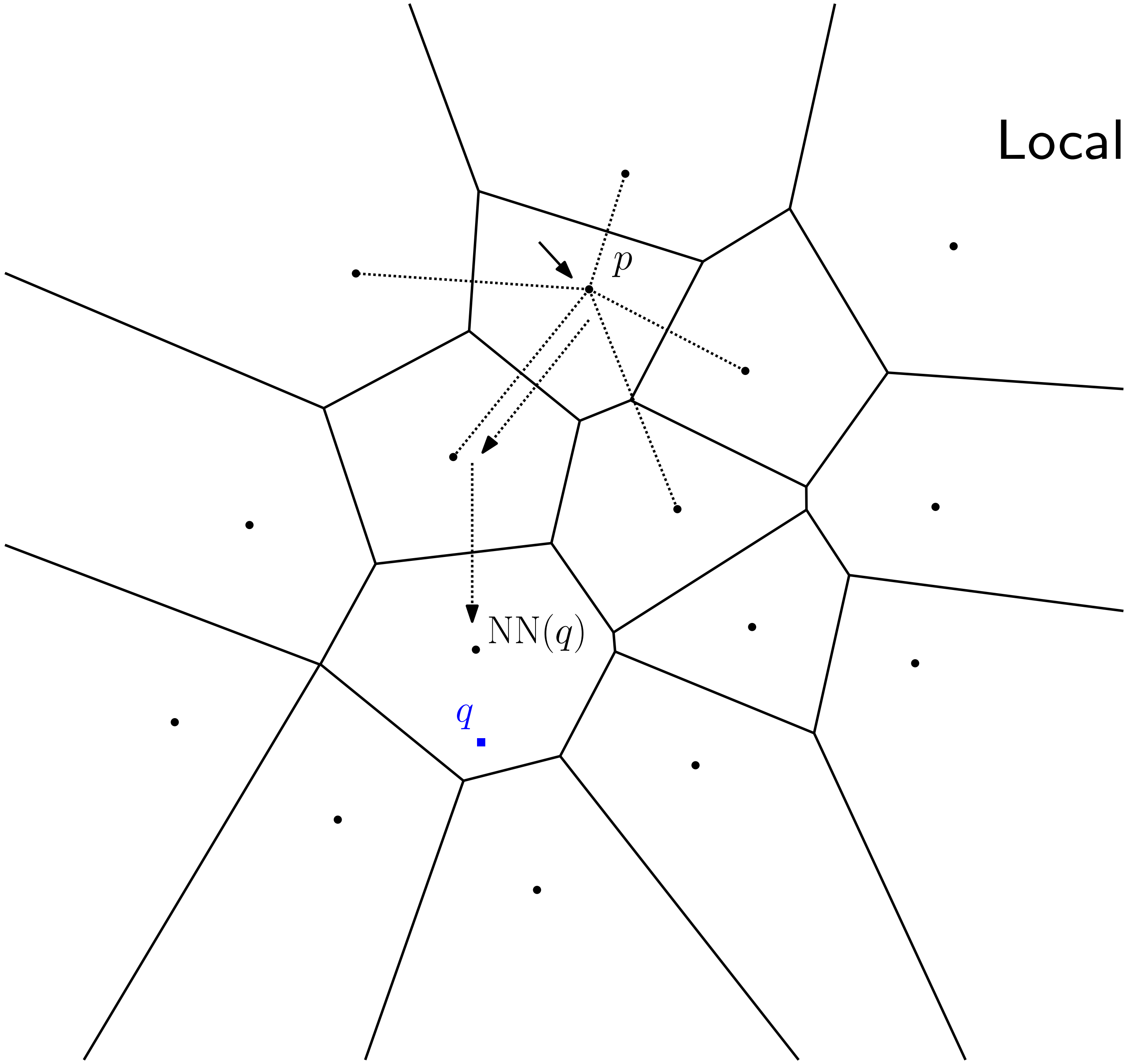
- worst case: $\Theta\left(n^{\lceil d/2 \rceil}\right)$

  Upper Bound Thm [McMullen'70]

- average case (unif. distrib.):

  $2^{O(d \log d)} n$

Usage for NN-search



Localizing by **walk**:

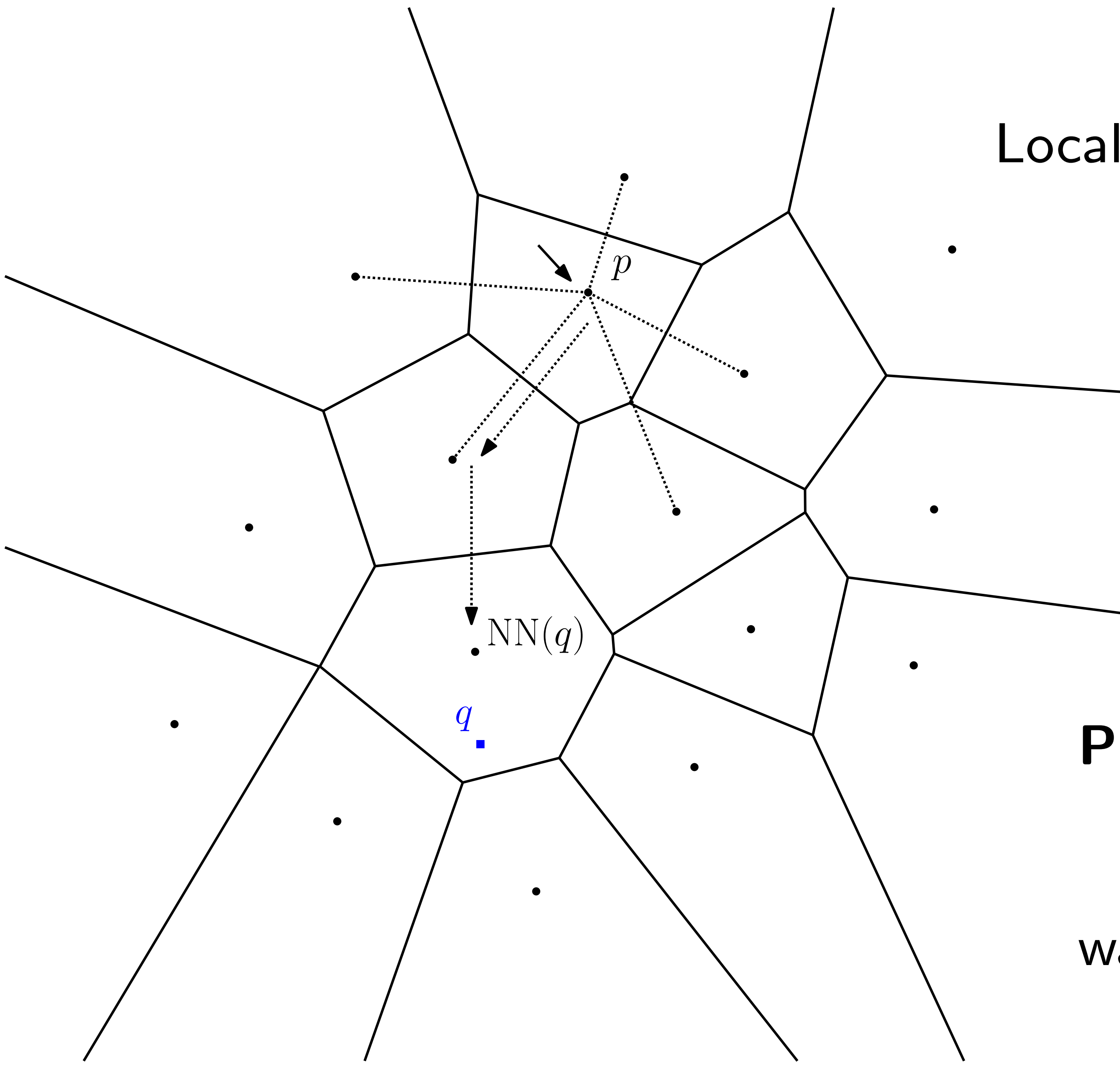
start from $p \in P$ random

while $\exists\ p'$ neighb. of p in Del.

s.t. $\mathrm{d}(q, p') < \mathrm{d}(q, p)$:

update $p := p'$

Usage for NN-search



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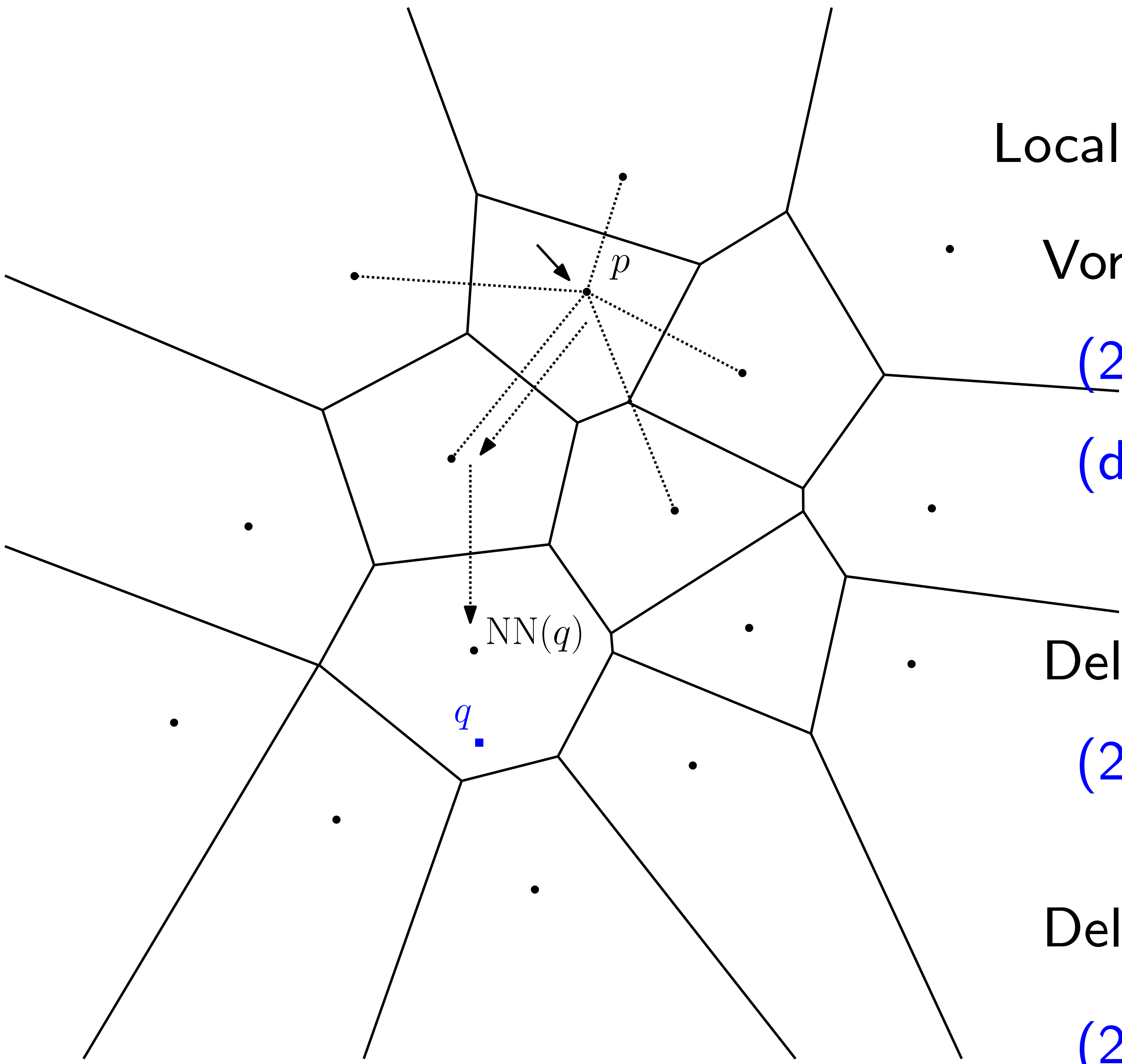
Prop: Del. neighborhood is complete

walk time:

worst case: $O(|\text{Del}(P)|)$

avg. case (2d): $O(\sqrt{n})$

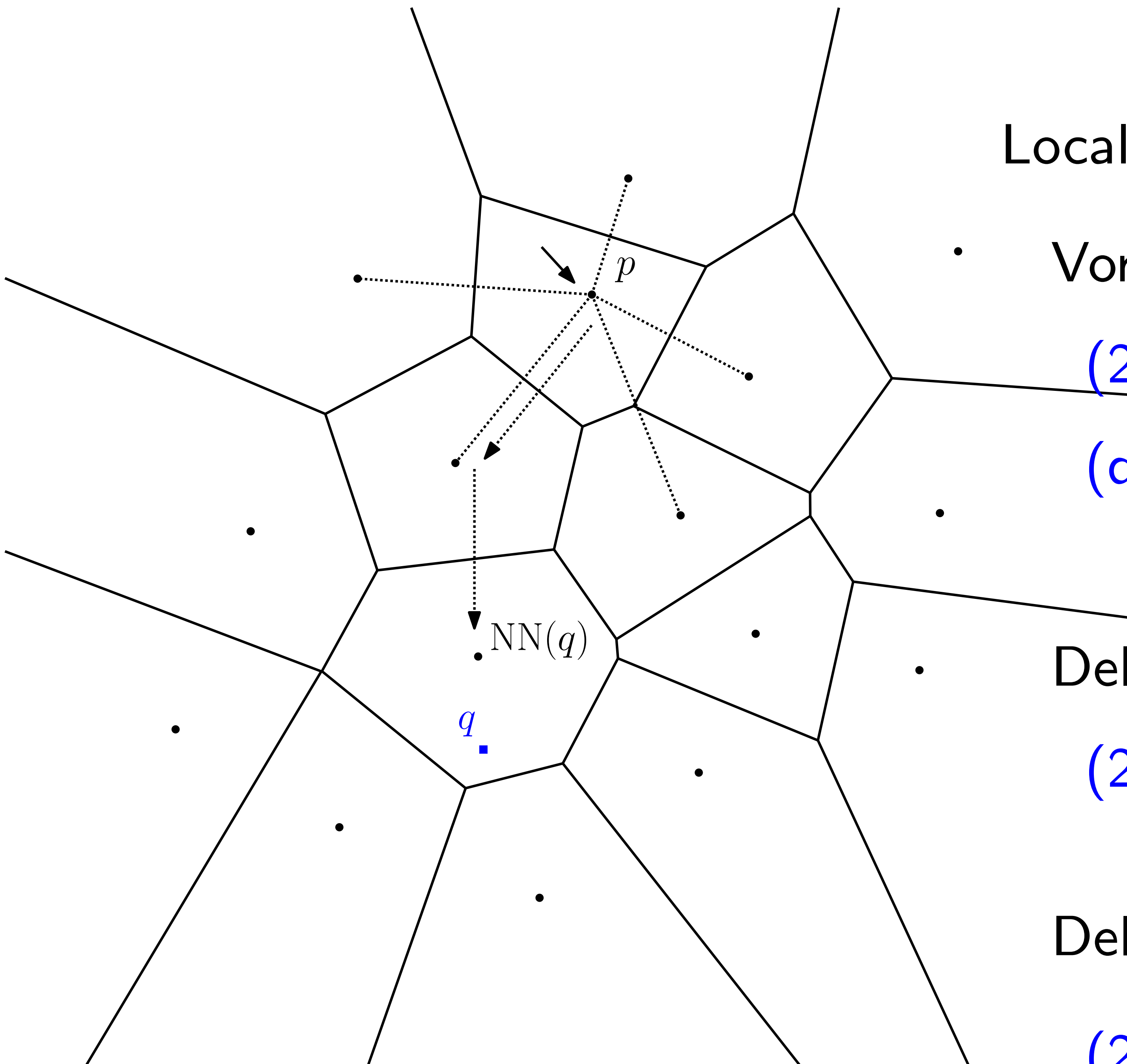
Usage for NN-search



Localizing by **hierarchy**:

- Voronoi subdivision [Kirk.'83, Meiser'93]:
  - (2D) $O(n)$ space, $O(\log n)$ time
  - (dD) $\Theta(n^d)$ space, $O(d^5 \log n)$ time
- Delaunay tree [Mulmuley'91]:
  - (2D) $O(n \log n)$ space, $O(\log n)$ time
- Delaunay tree + walk [Devillers'02]:
  - (2D) $O(n \log n)$ space, $O(\log n)$ time
  - (dD) $O(n^{\lceil \frac{d}{2} \rceil})$ space, $O(n^{\lceil \frac{d-2}{2} \rceil})$ time

Usage for NN-search



For small dimensions (2 or 3) only!

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k-d trees

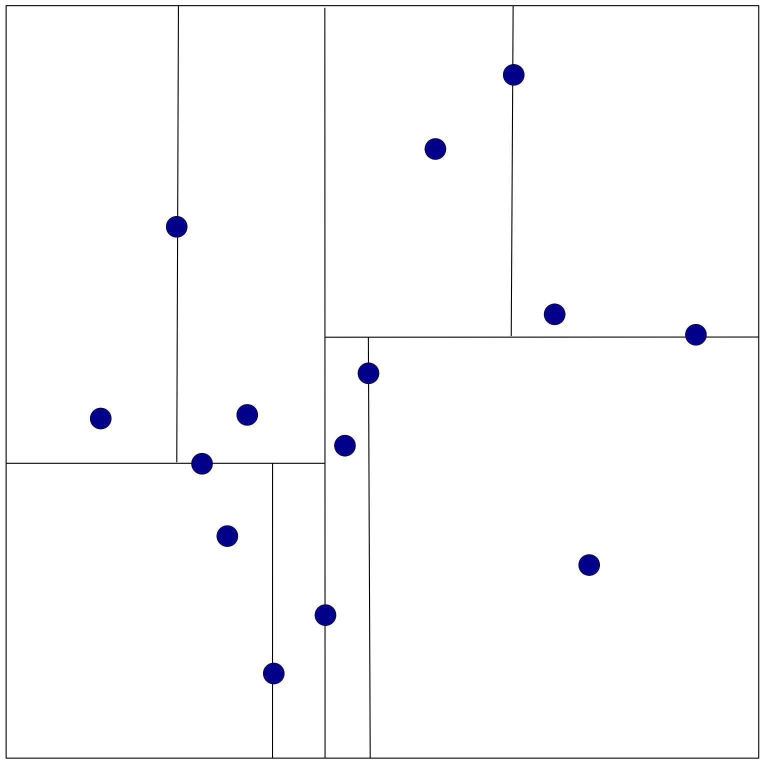
Definition

- a binary tree

- each internal node implements a spatial partition induced by a hyperplane H, splitting the point cloud into two equal subsets
  - ▶ right subtree: all points lying on one side of H
  - ▶ left subtree: remaining points

- subdivision stops whenever fewer than n_0 remain

  $\rightsquigarrow$ size: $O(dn)$



$(n_0 = 1)$

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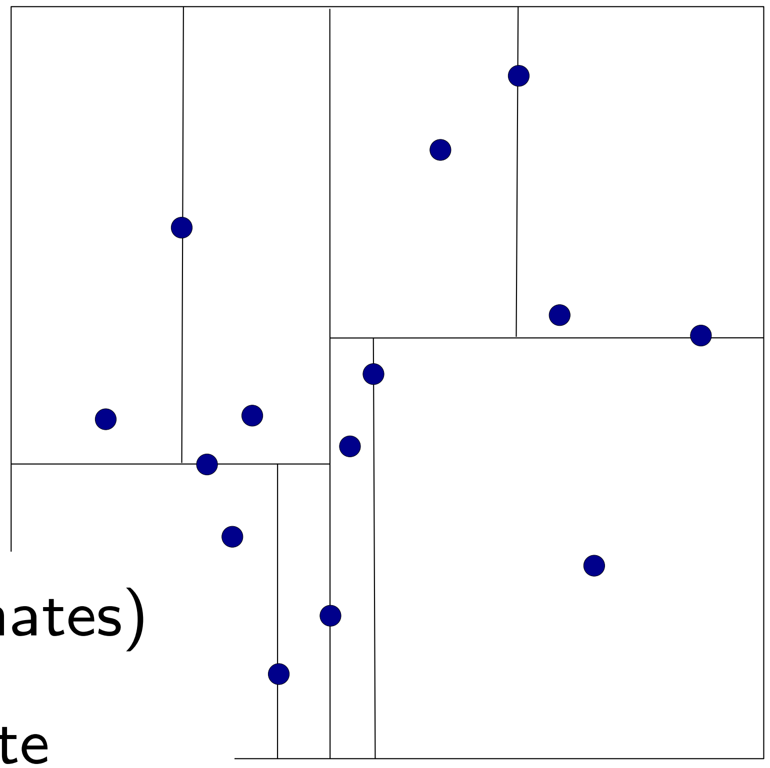
kd-tree specifics:

H orthogonal to coordinate axis (cycle through coordinates)

H goes through the median in the considered coordinate



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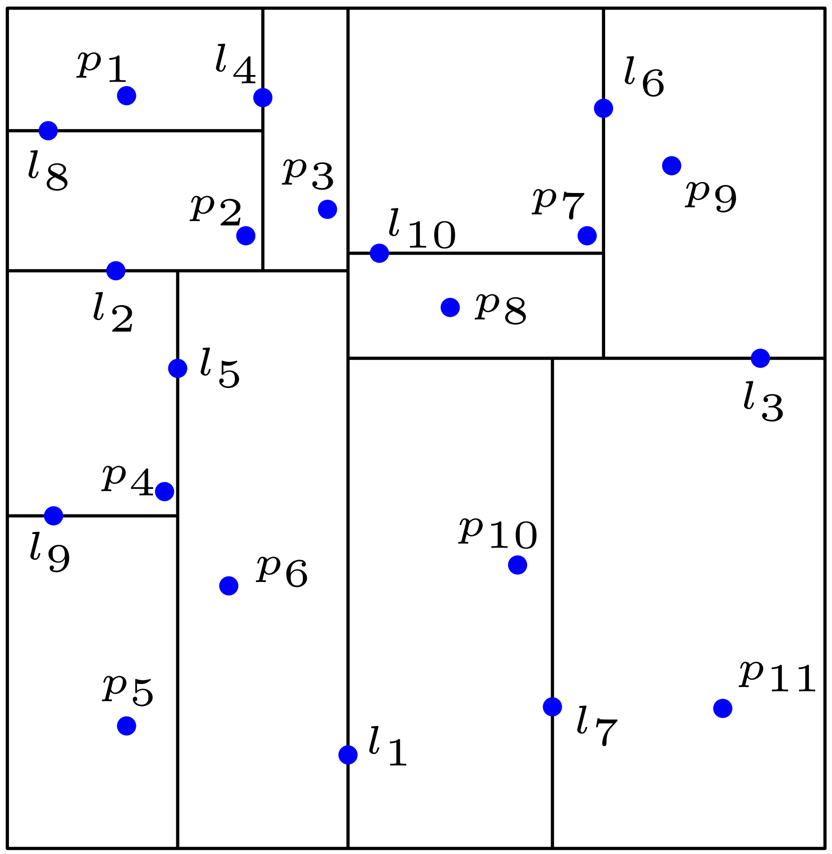
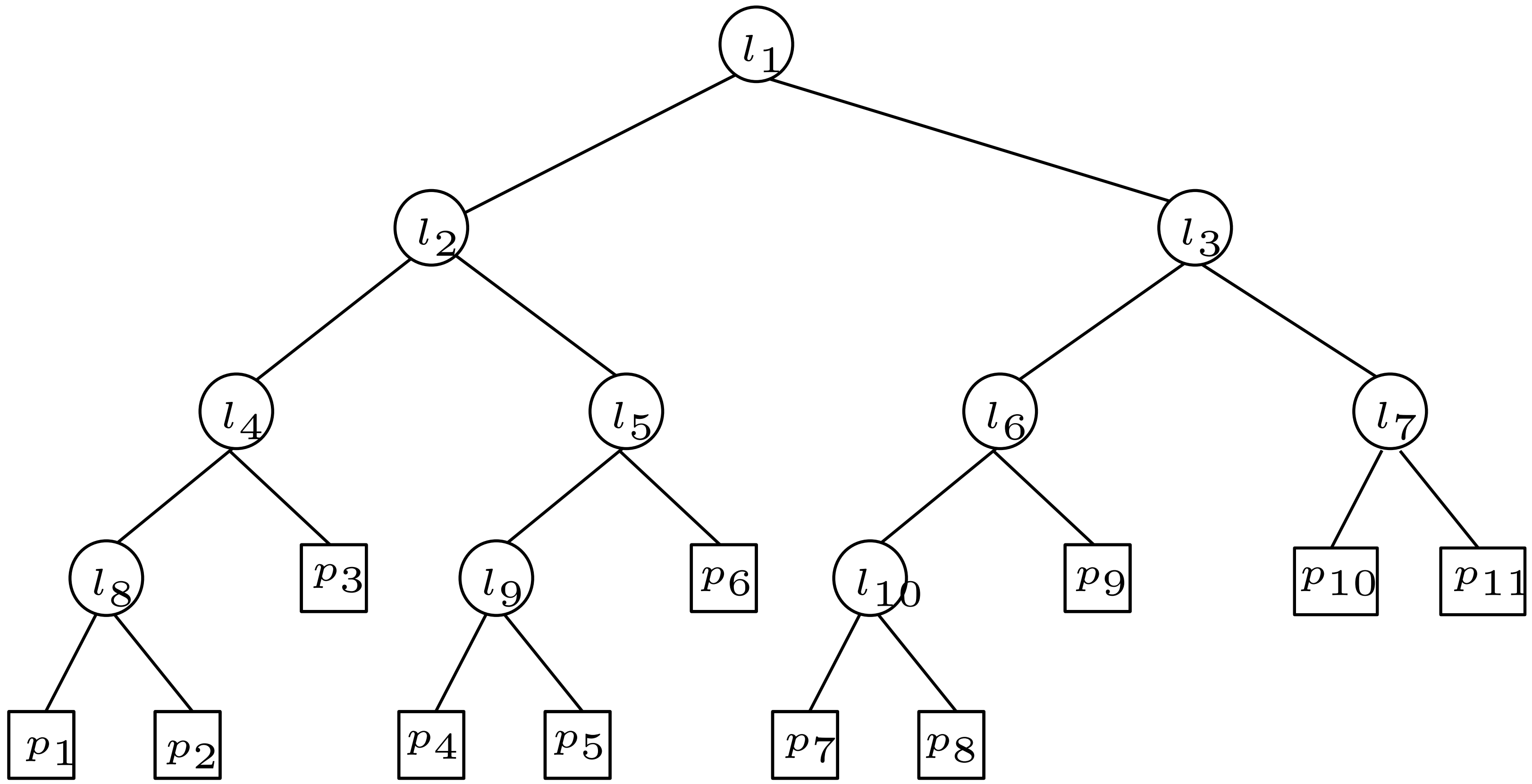
Example





l_i: data at internal node

p_i: data at leaf node

$n_0 = 1$

(note: left-right labels are arbitrary)

Usage for NN search

Strategy 1: defeatist search

$\mathrm{d}_{\min} := \infty$ (dist. to pts viewed so far)

search ($node$): ($node = root$ initially)

if $node = leaf$:

$\mathrm{d}_{\min} := \min\{\mathrm{d}_{min},\ \min_{p \in node.batch} \mathrm{d}(q,p)\}$

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if q on "left" side of $node.H$

recurse on $node.left$

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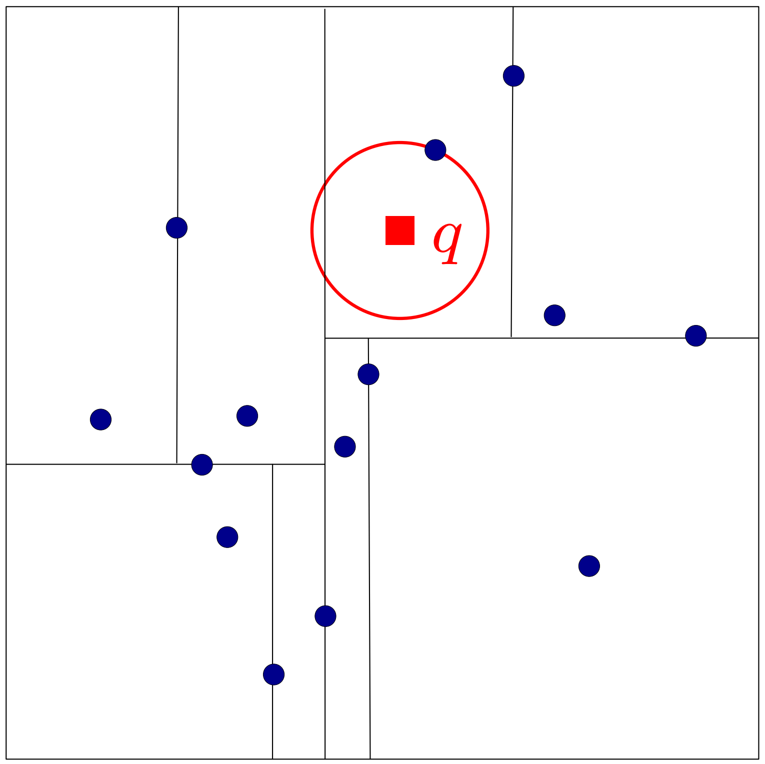

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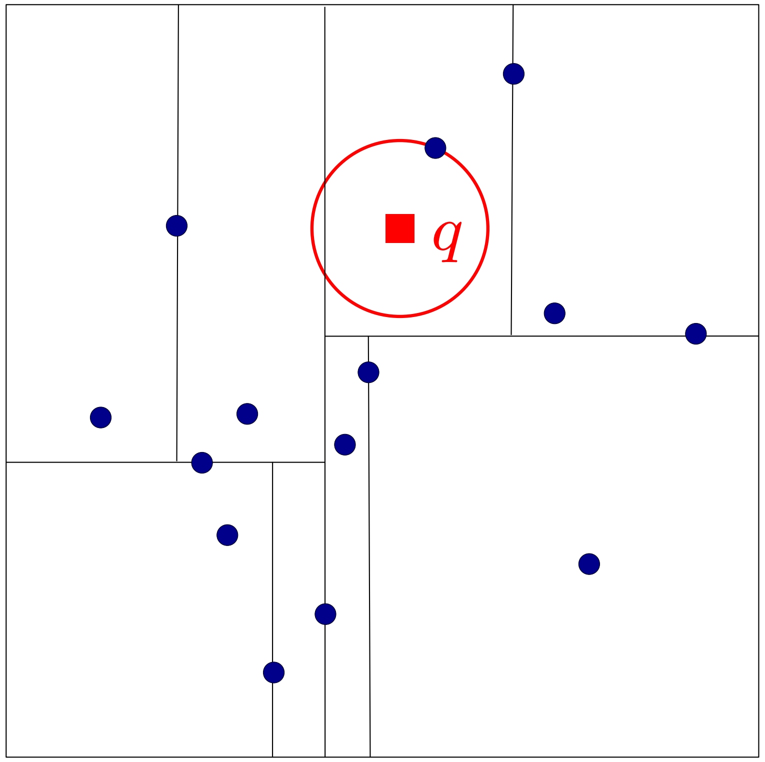

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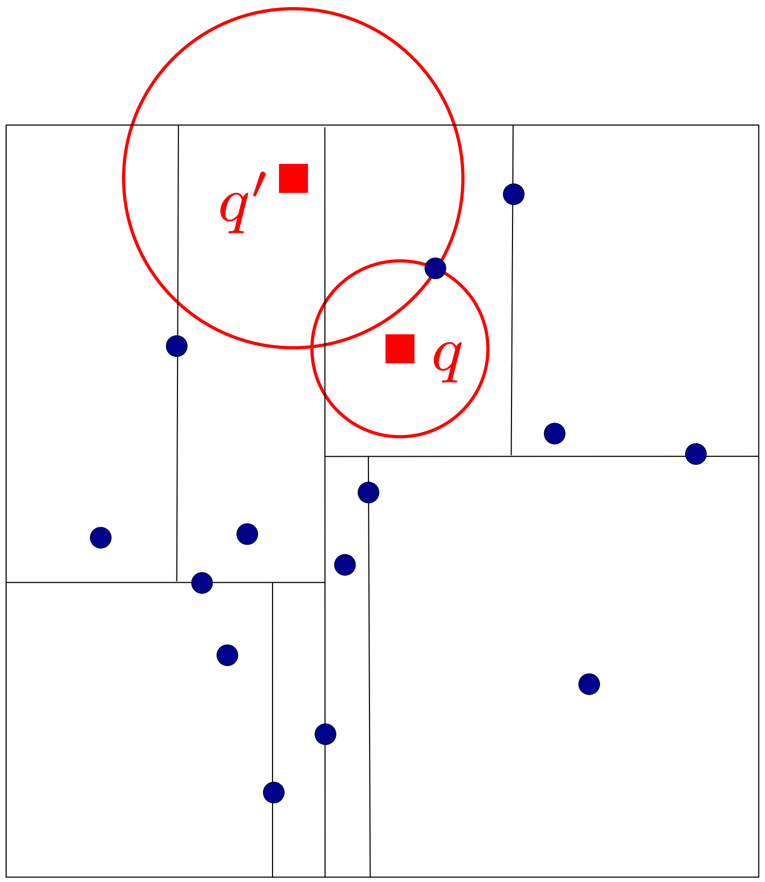
May fail!



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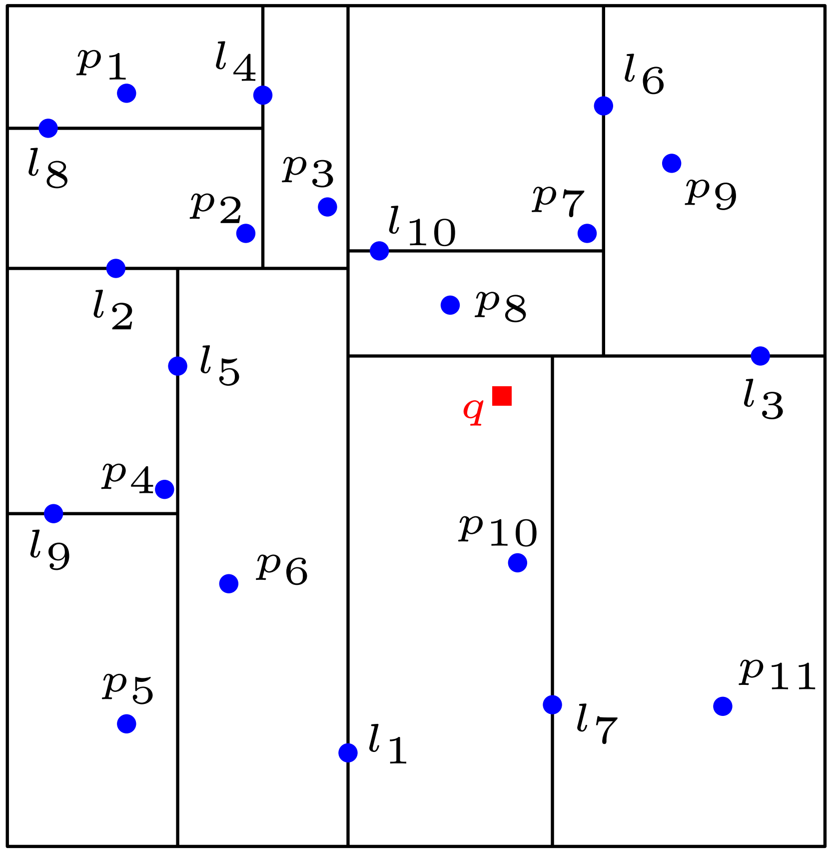

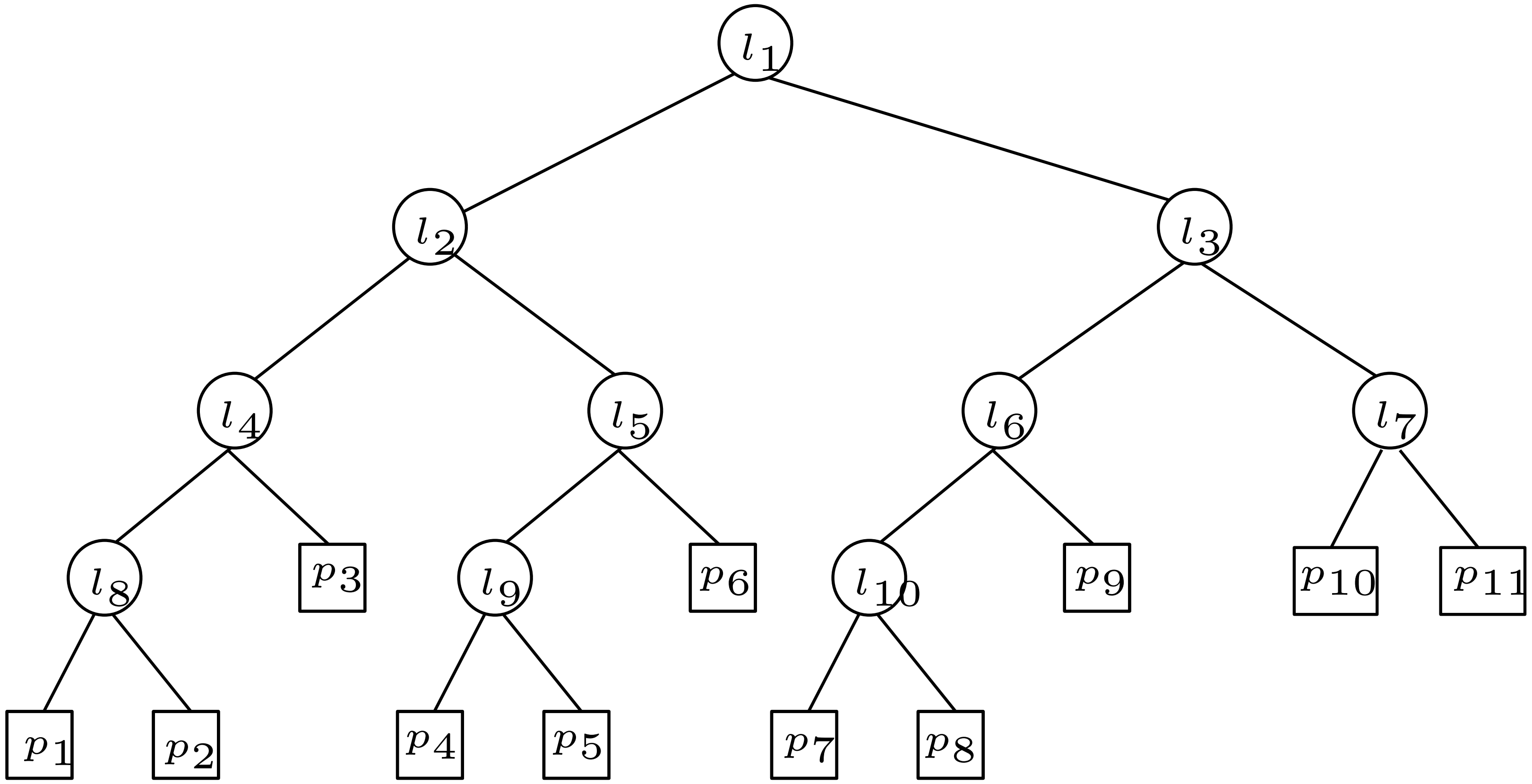

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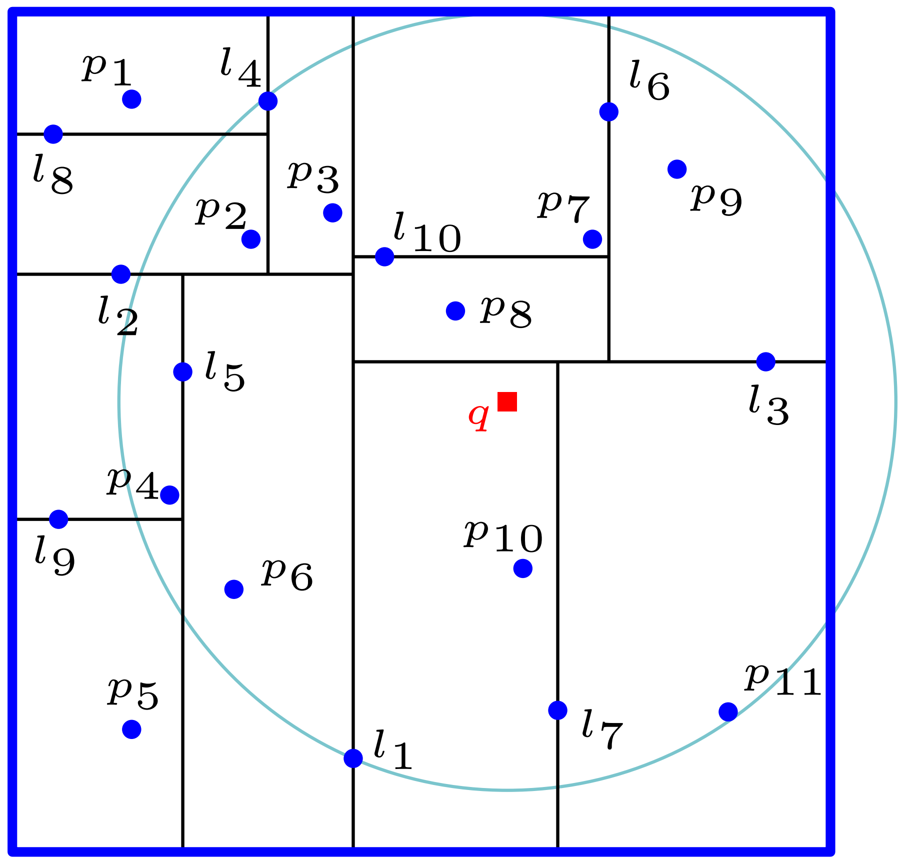

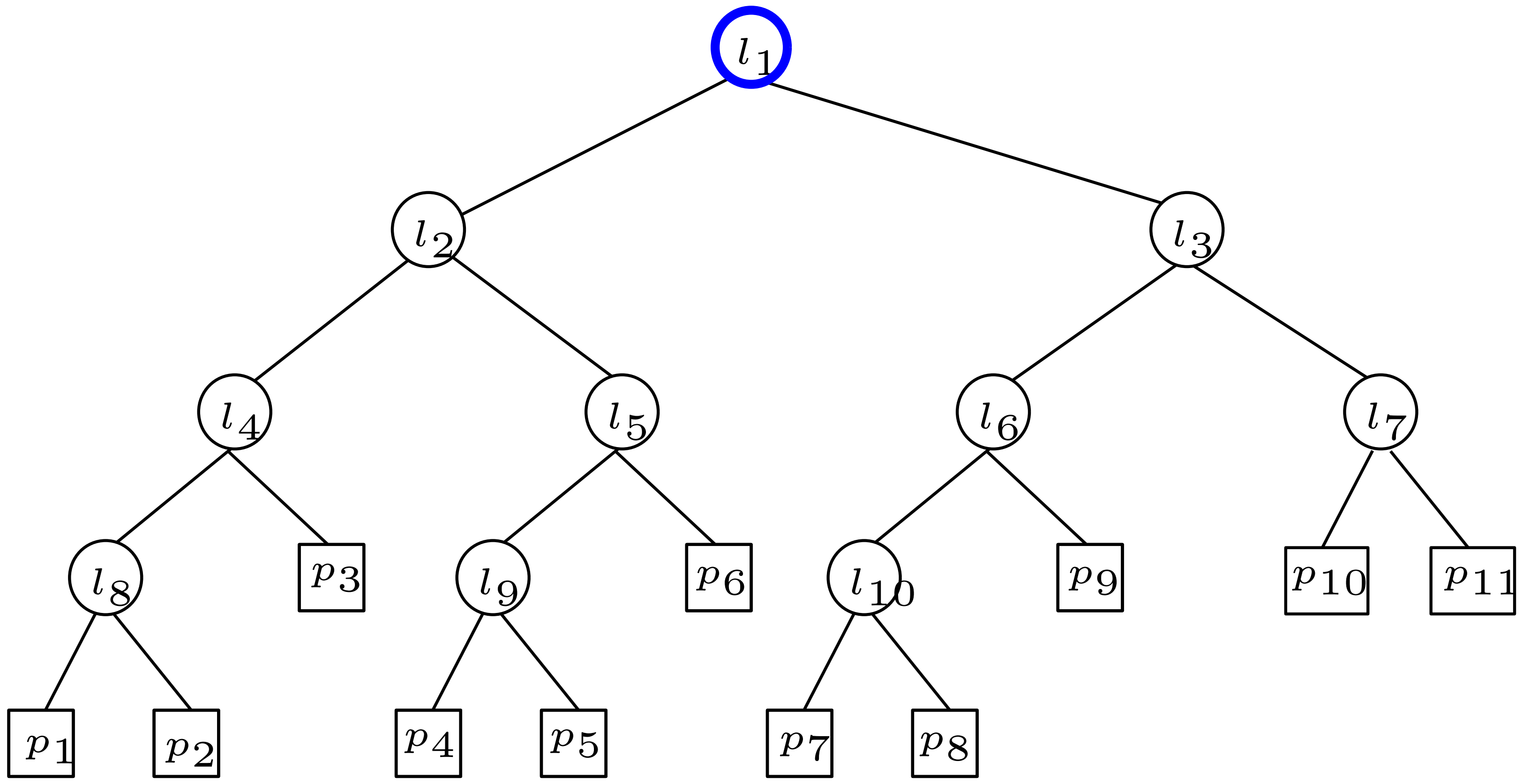

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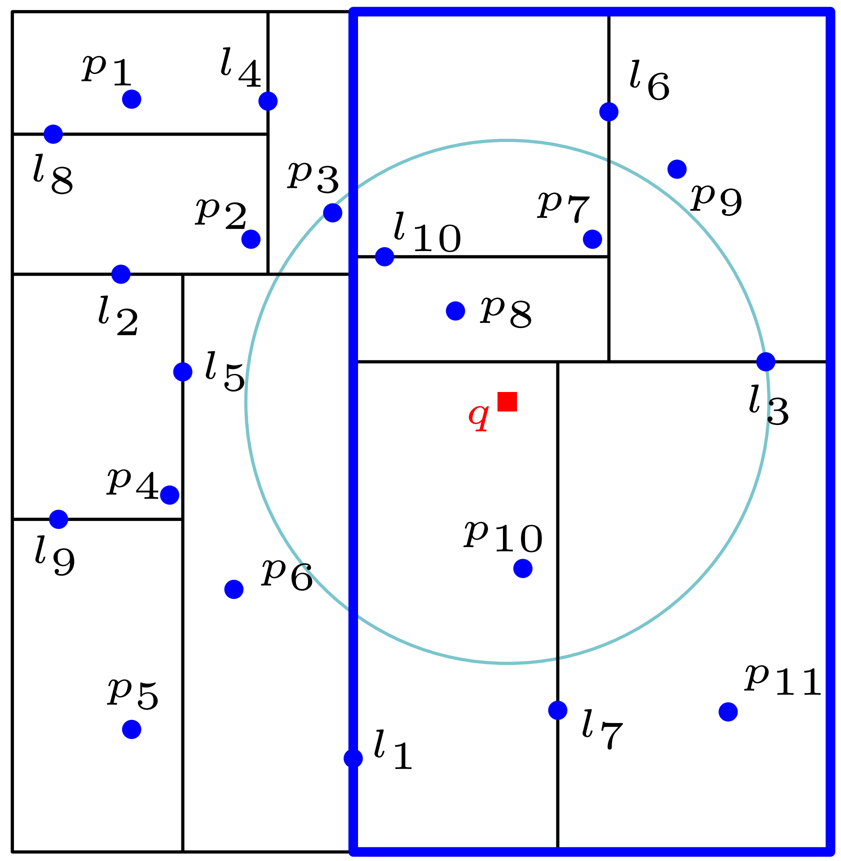

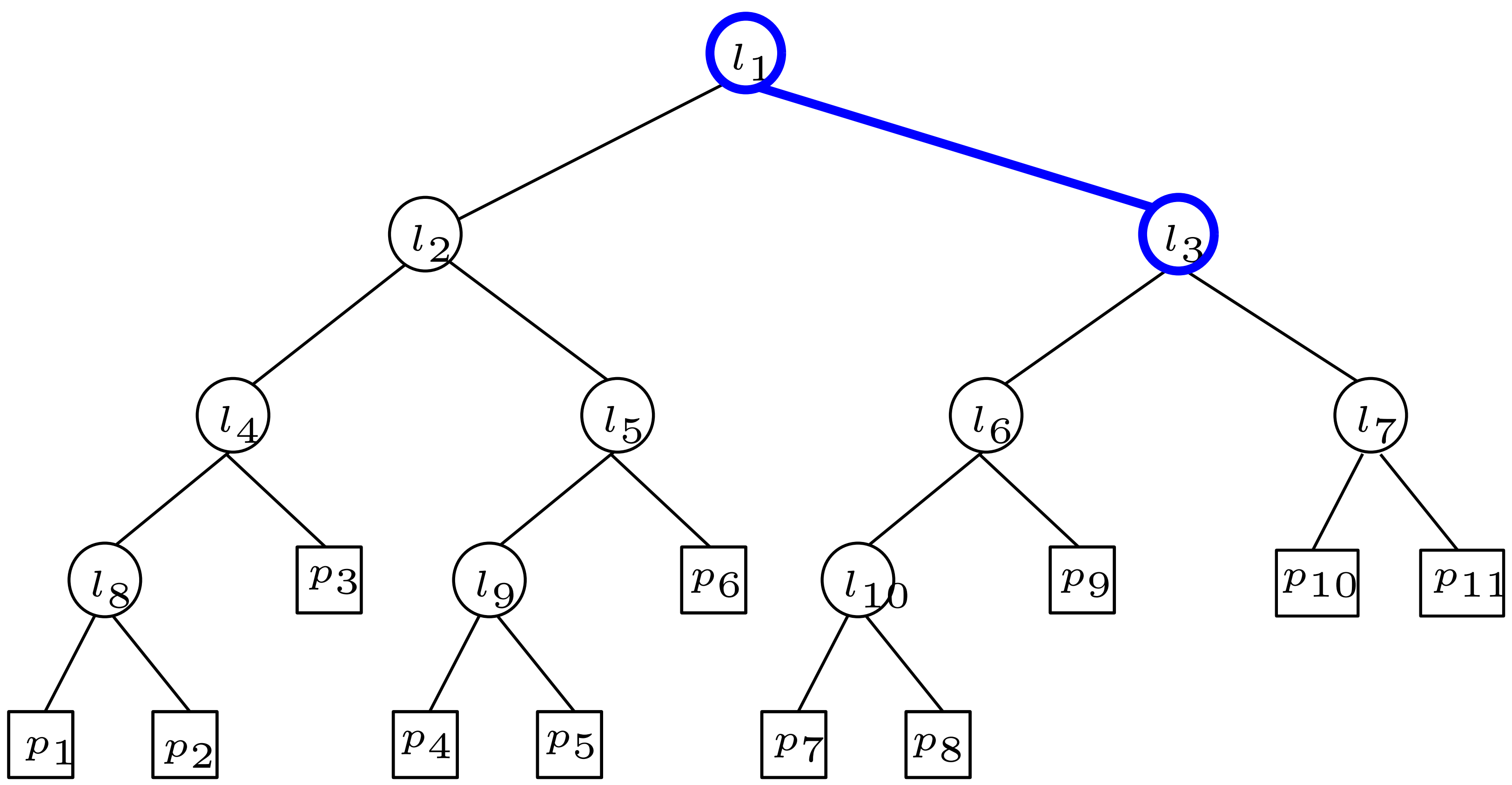

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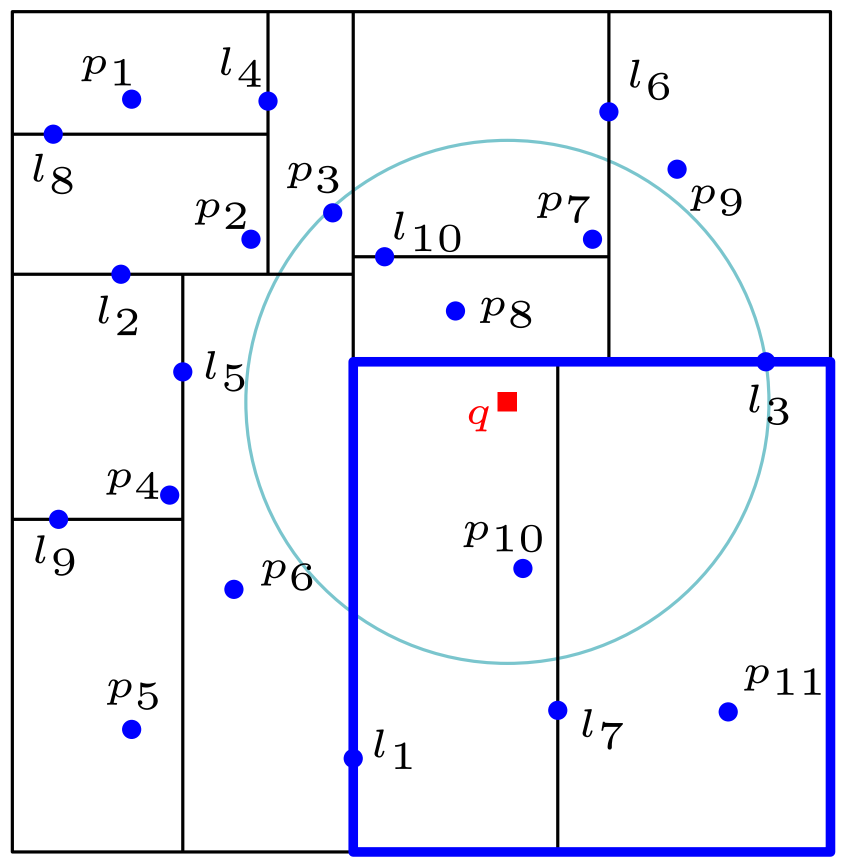

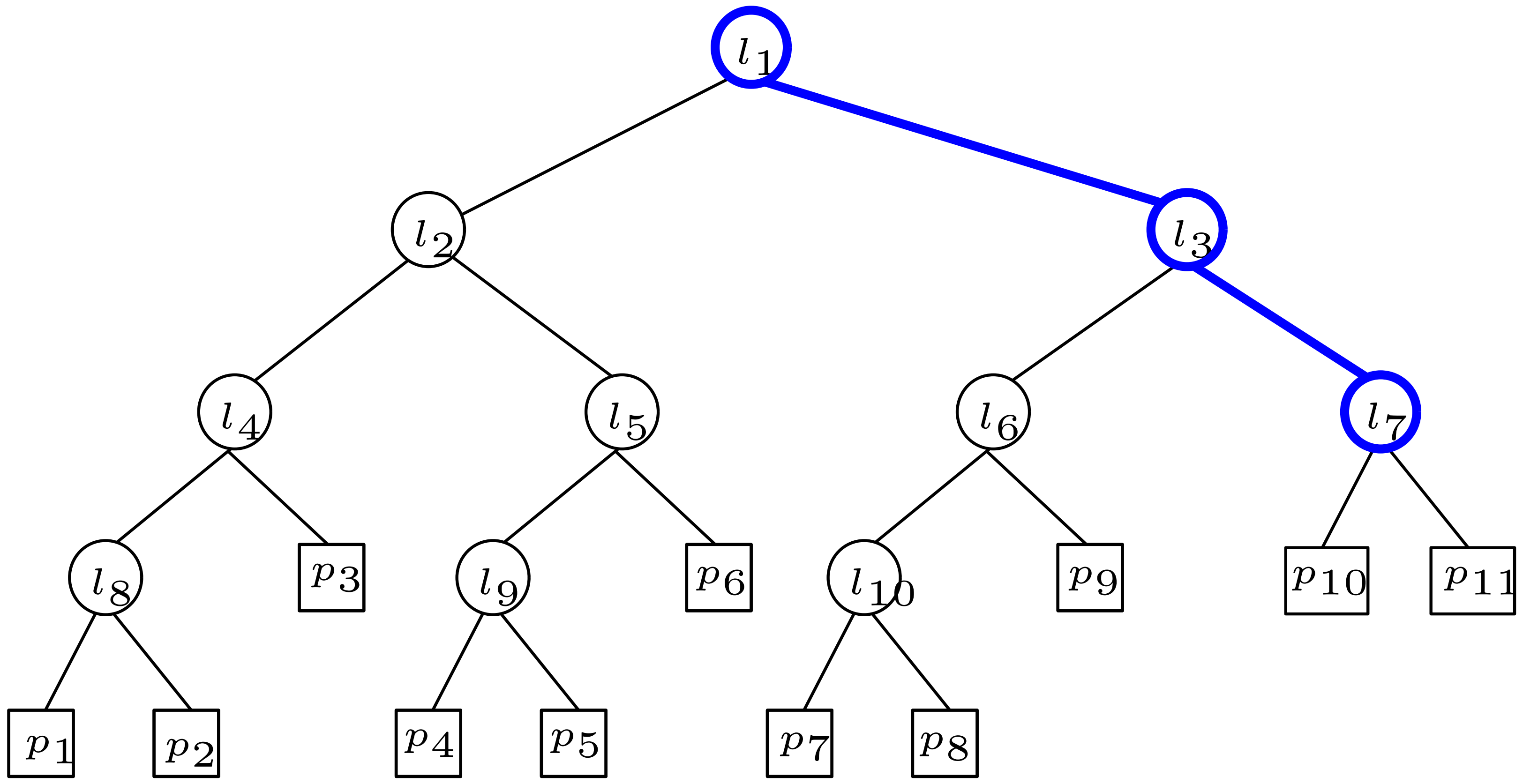

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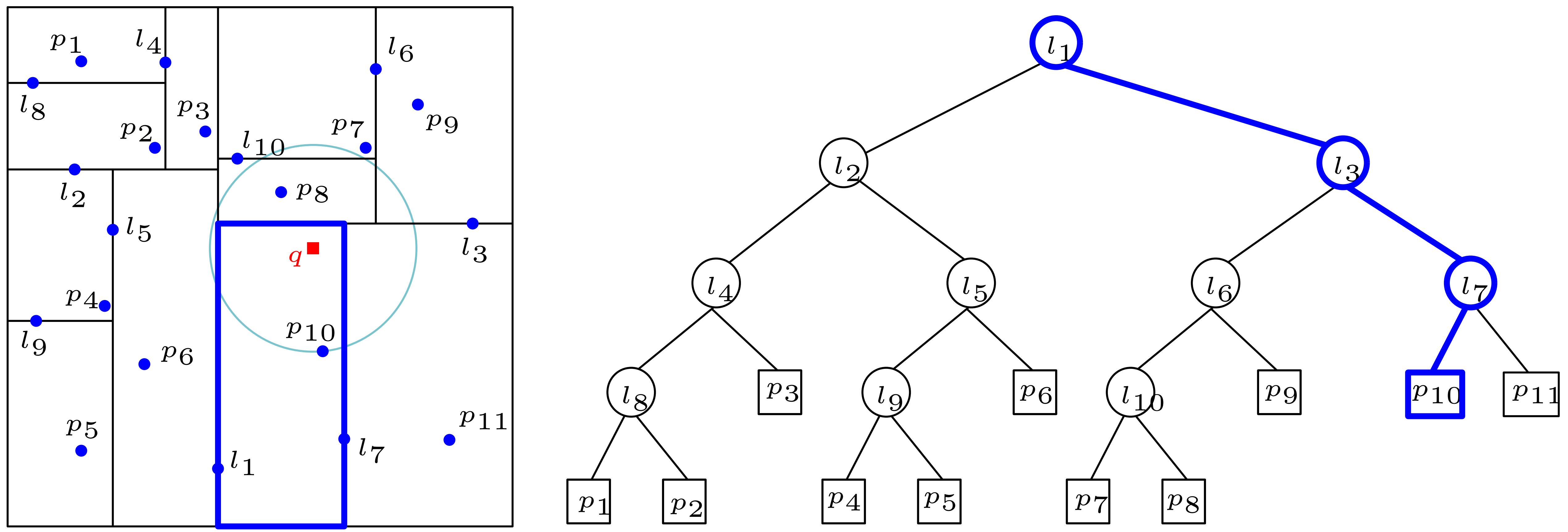

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Usage for NN search

Strategy 2: backtracking search

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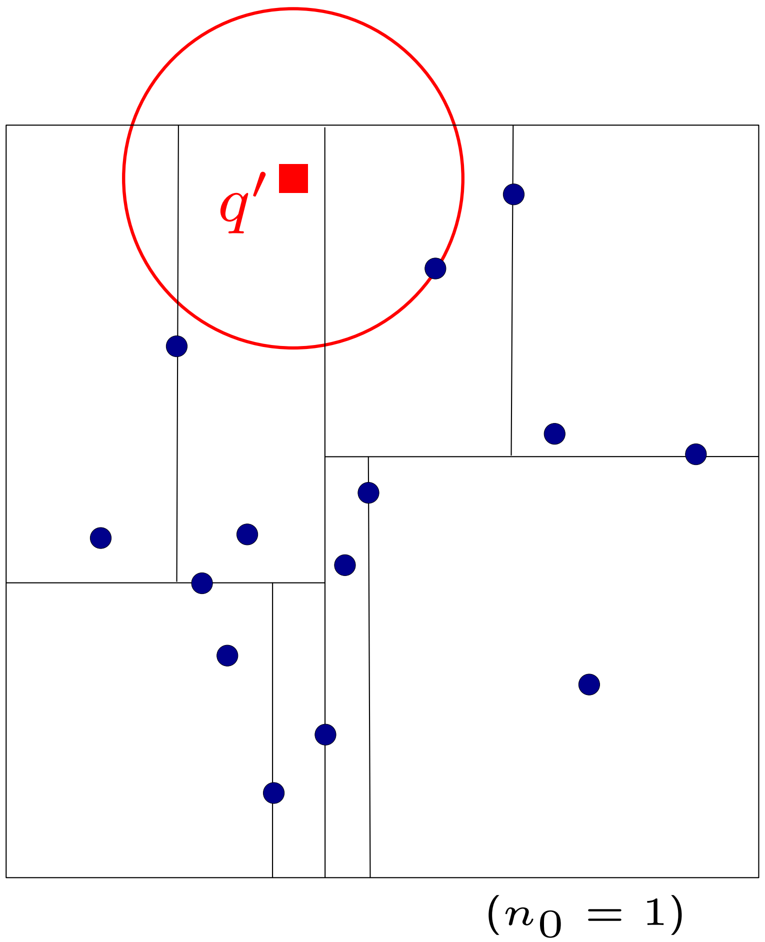

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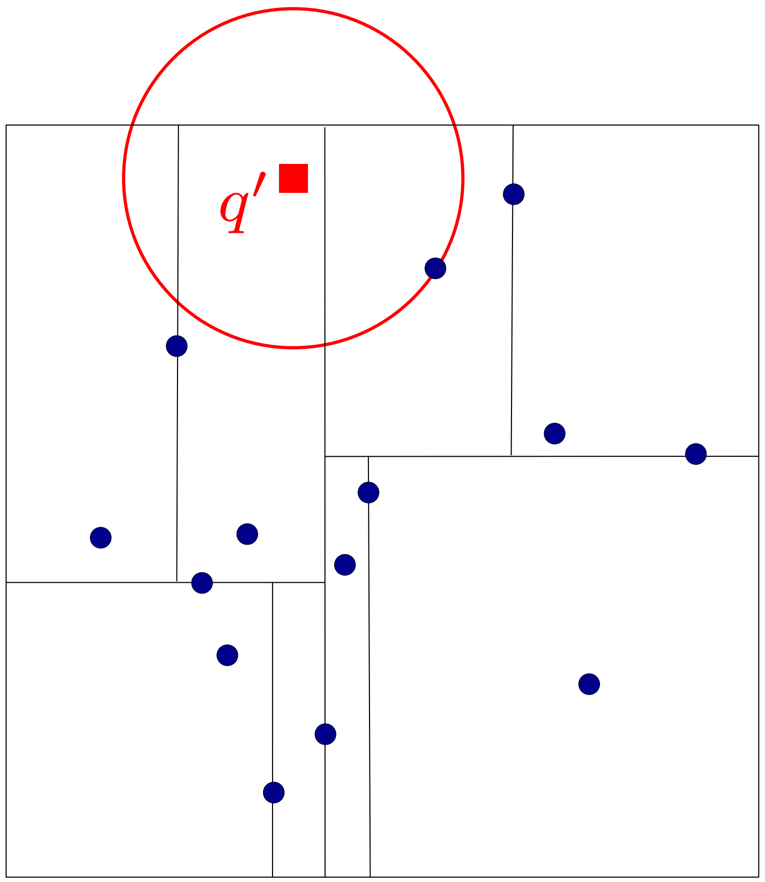
Always succeeds

$\mathrm{d}_{\min} \geq \mathrm{d}(q, \mathrm{NN}(q)) \Rightarrow B(q, \mathrm{d}_{\min})$ intersects all cells containing $\mathrm{NN}(q)$ in subdivision throughout search



$(n_0 = 1)$

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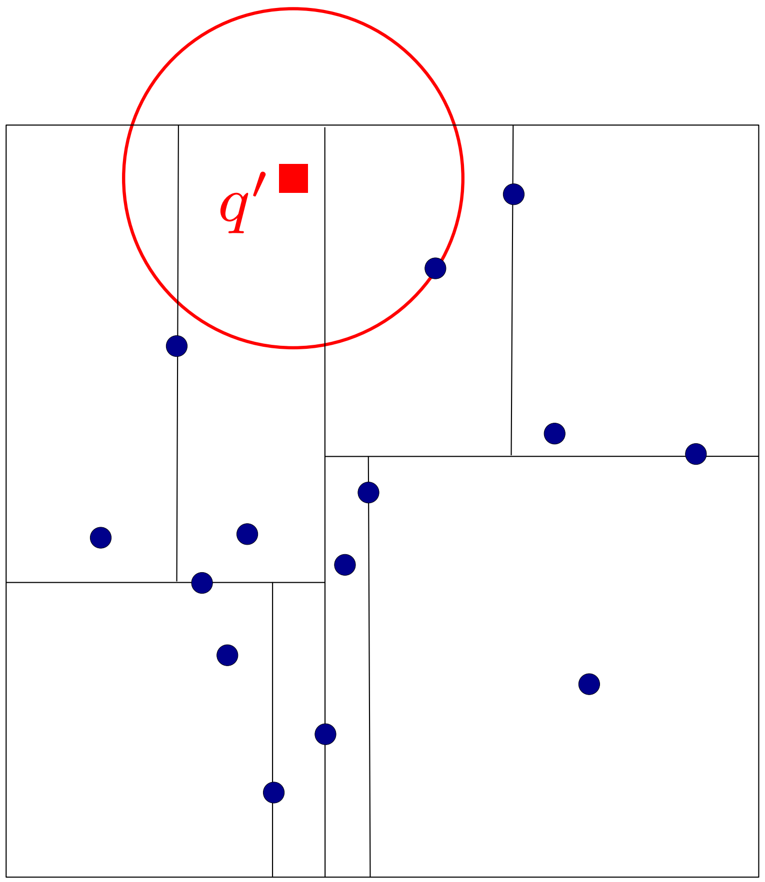
Always succeeds

Query time may be up to linear

(all cells visited)



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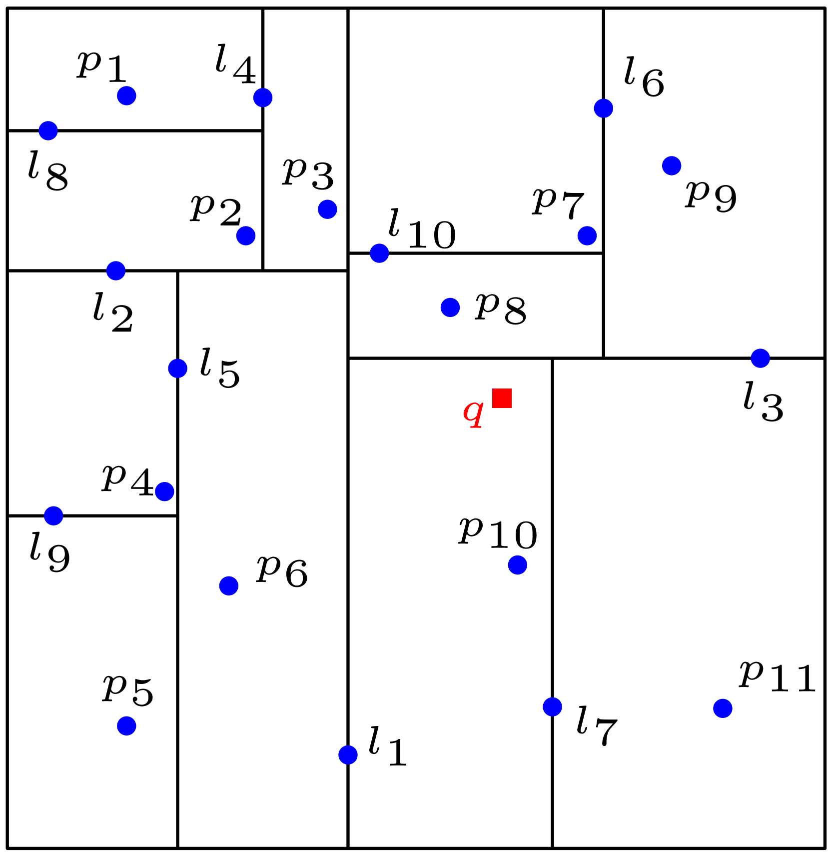

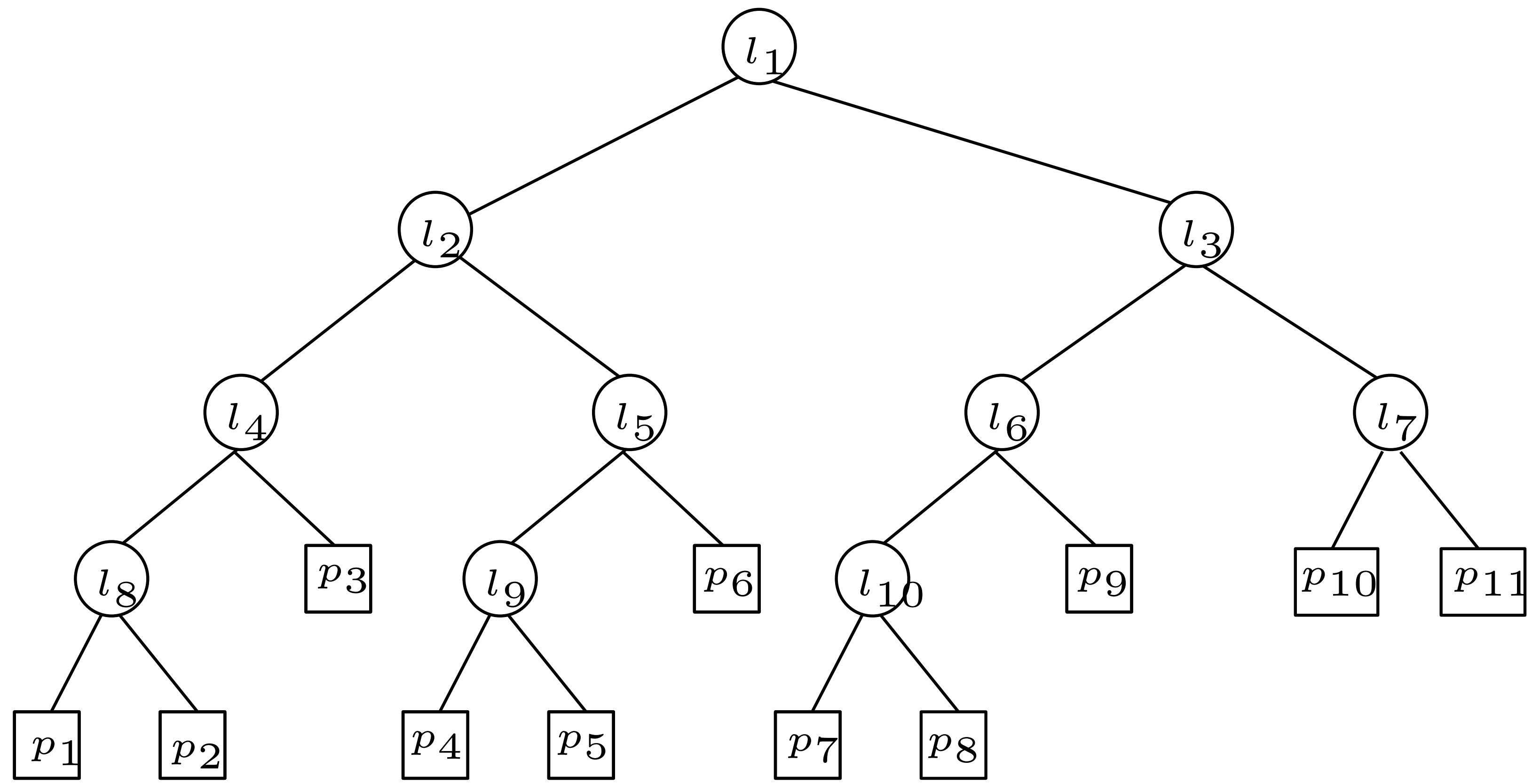

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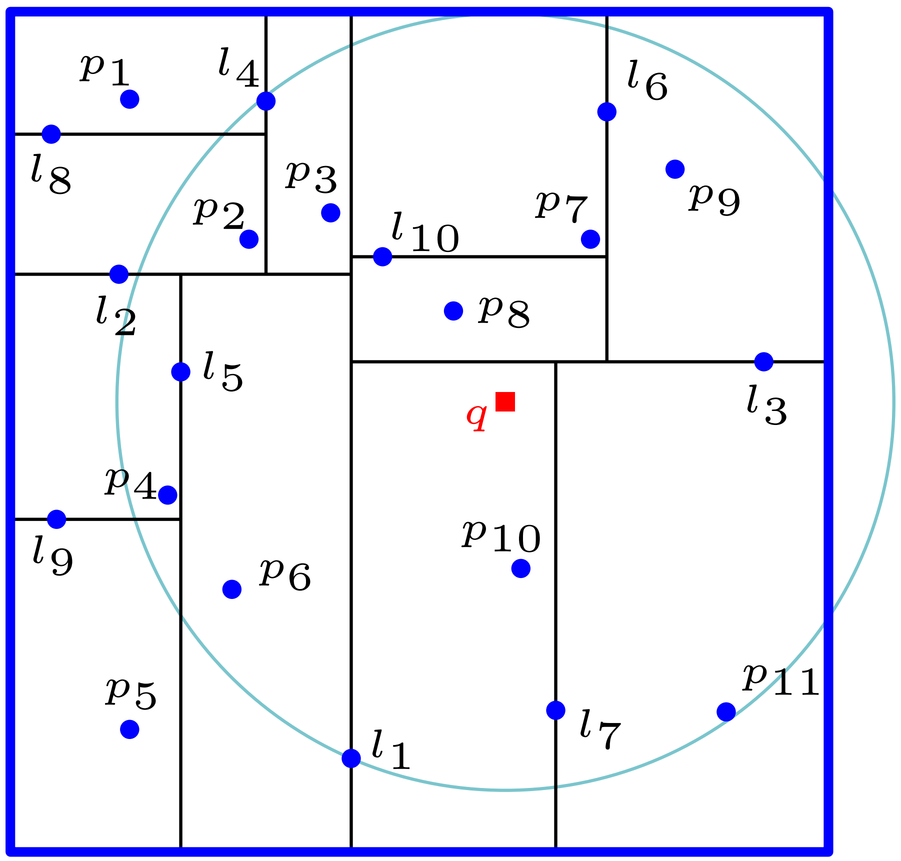

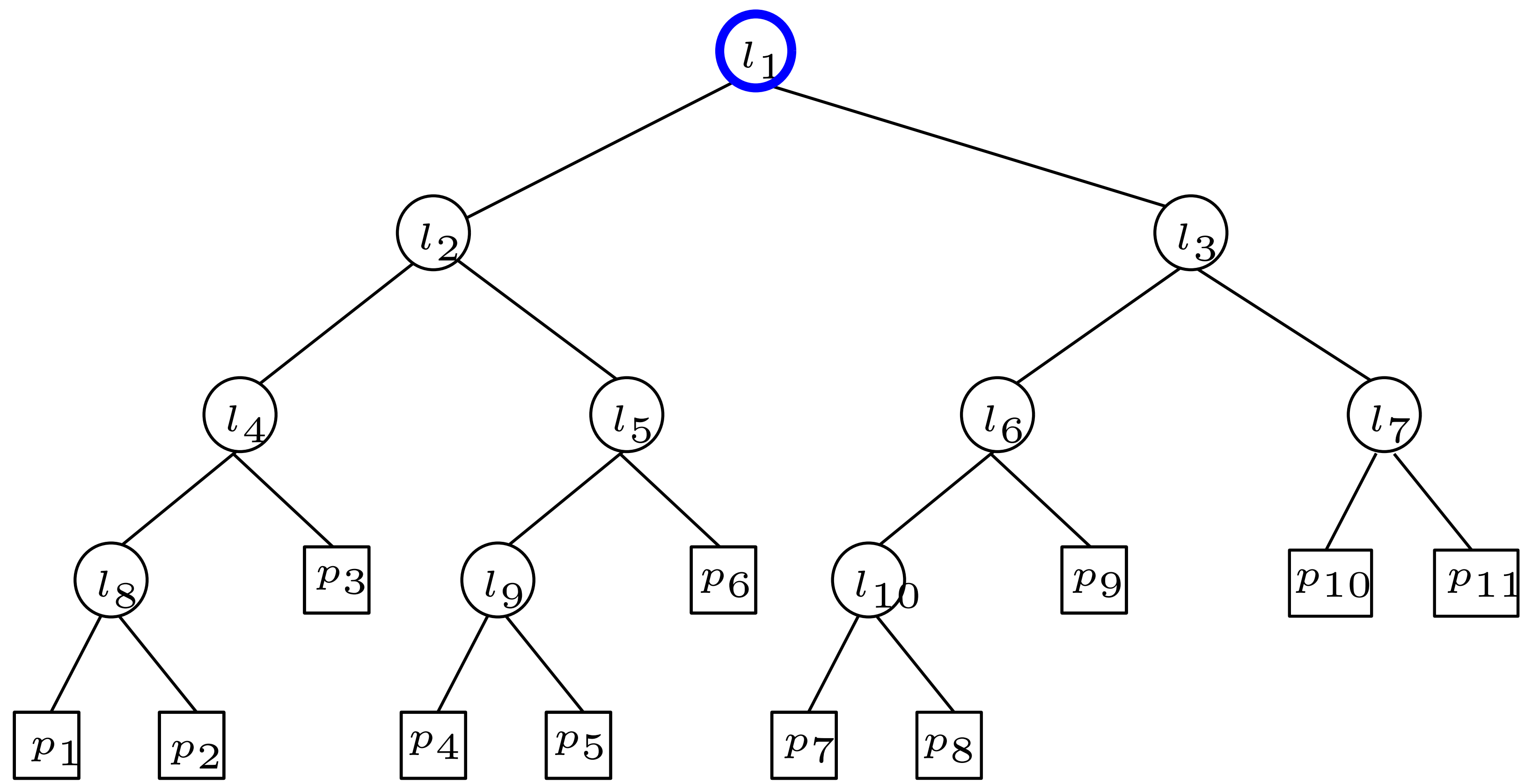

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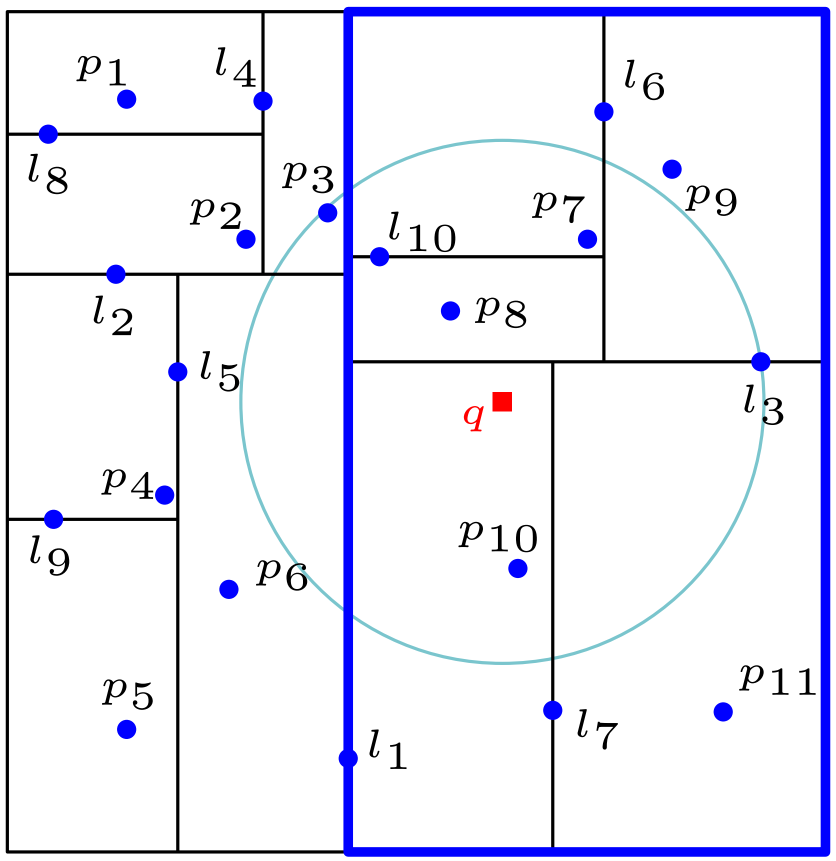

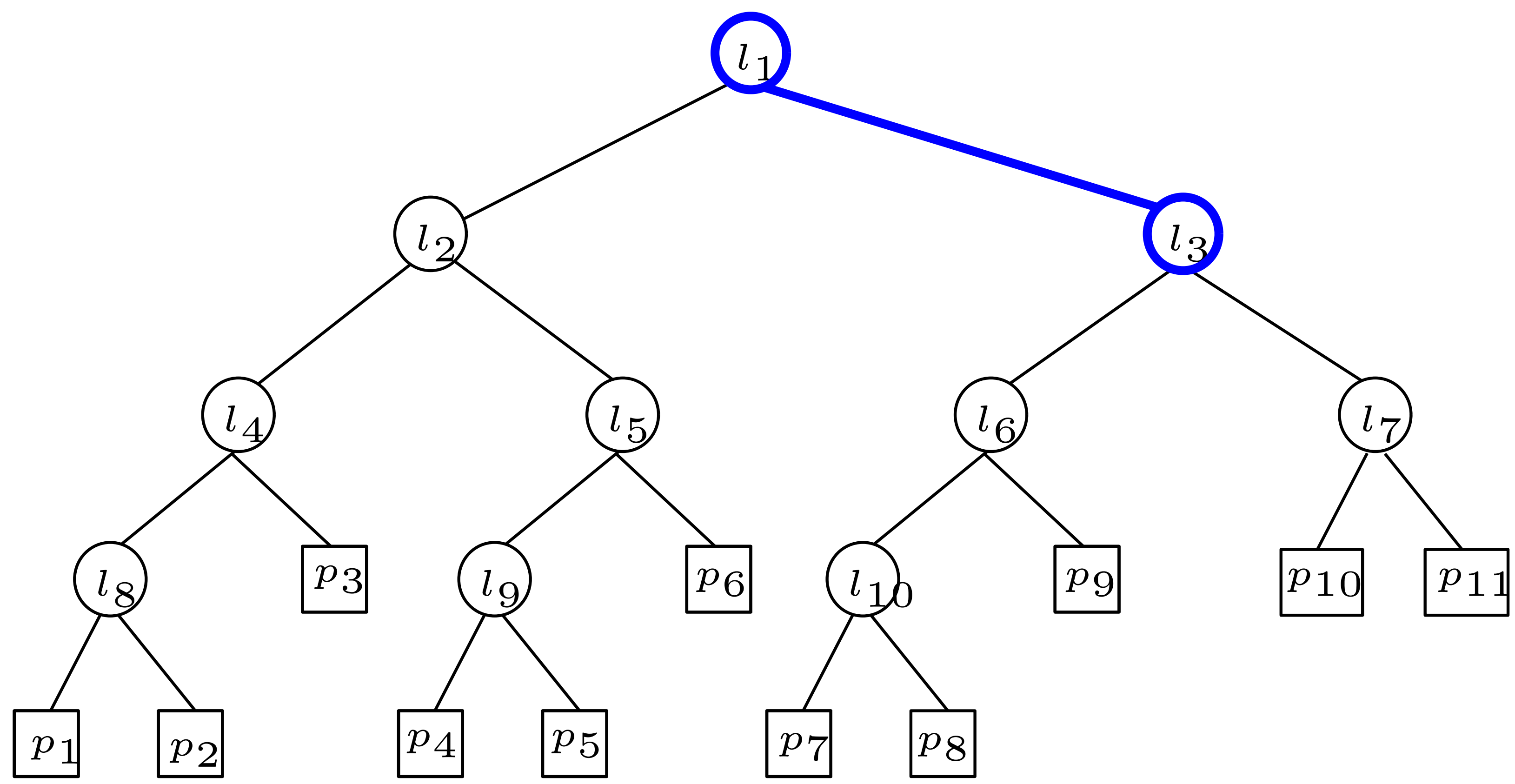

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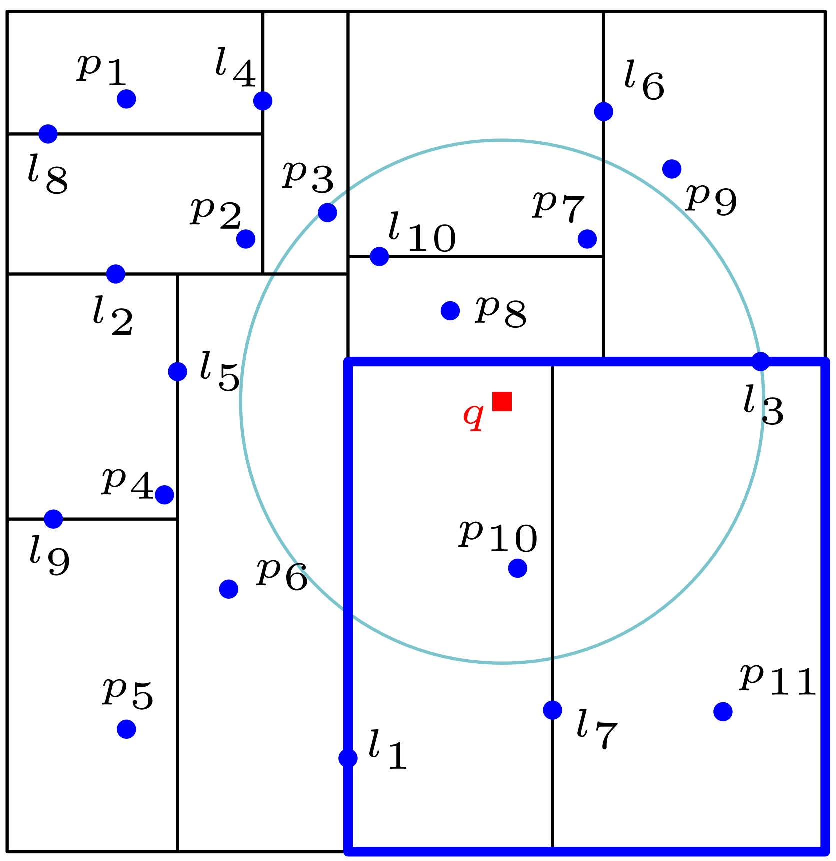

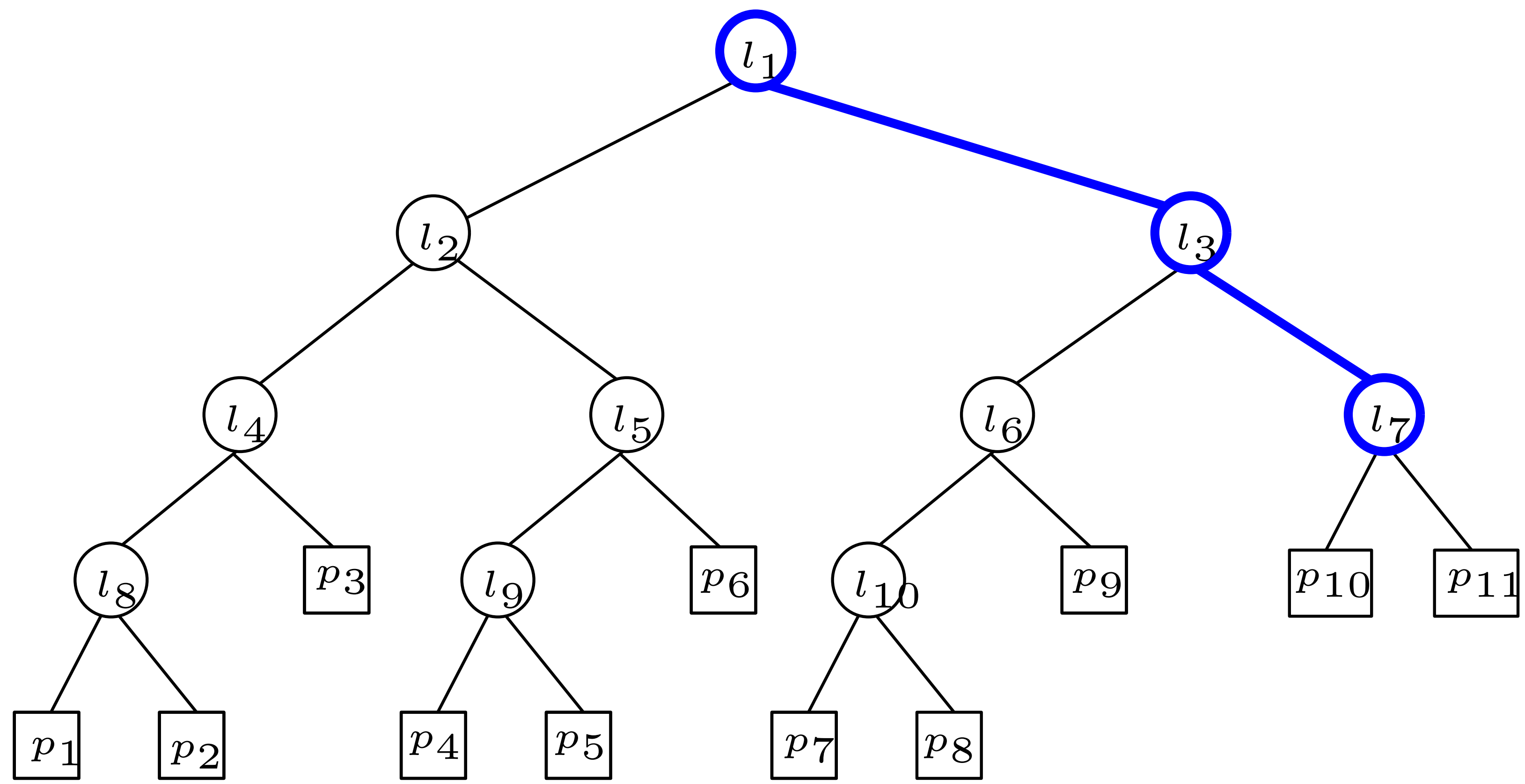

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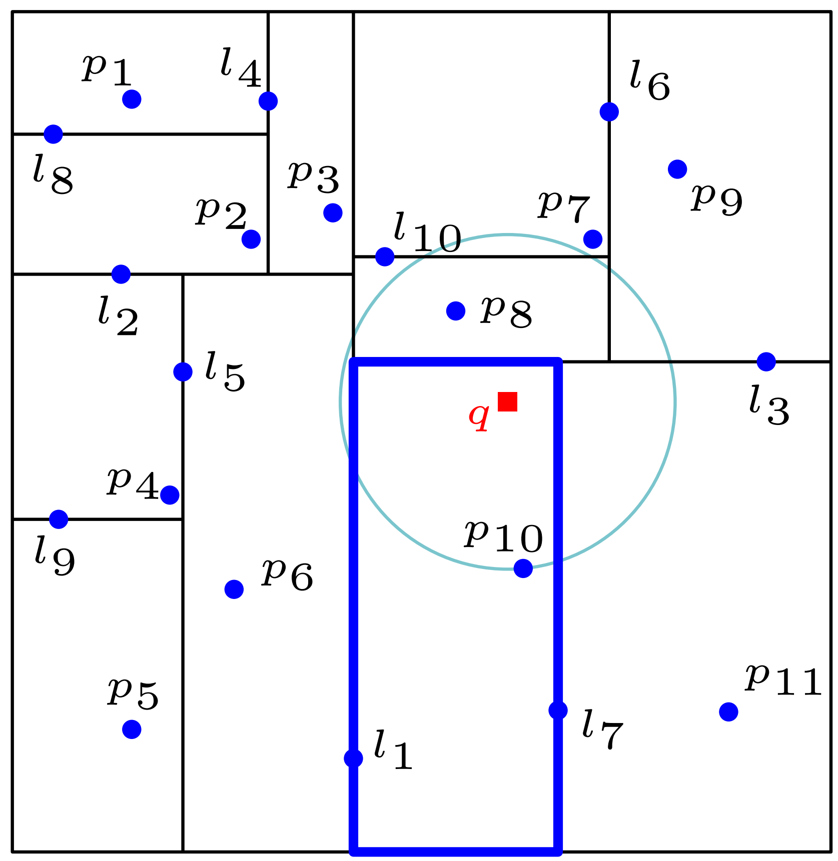
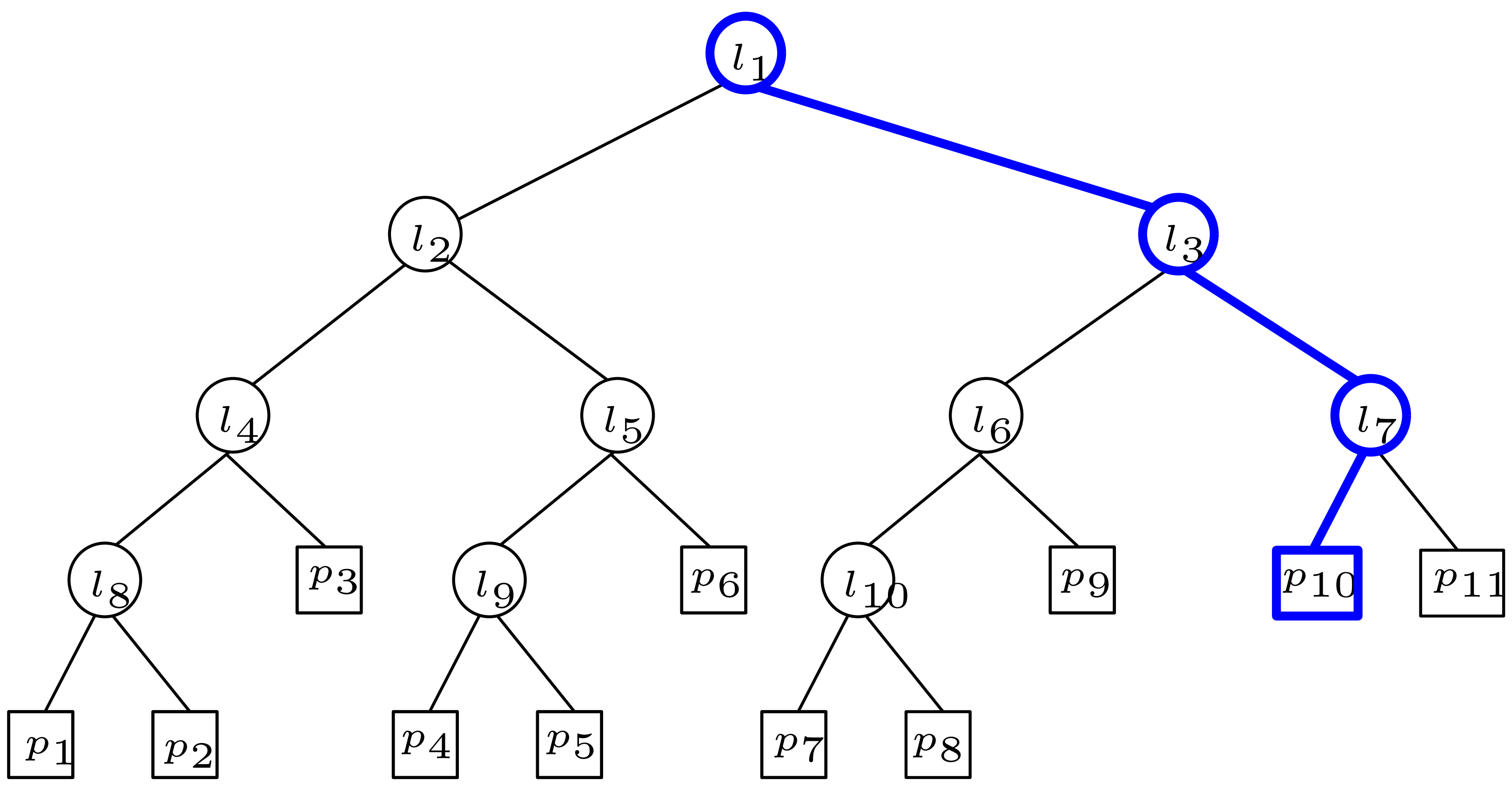


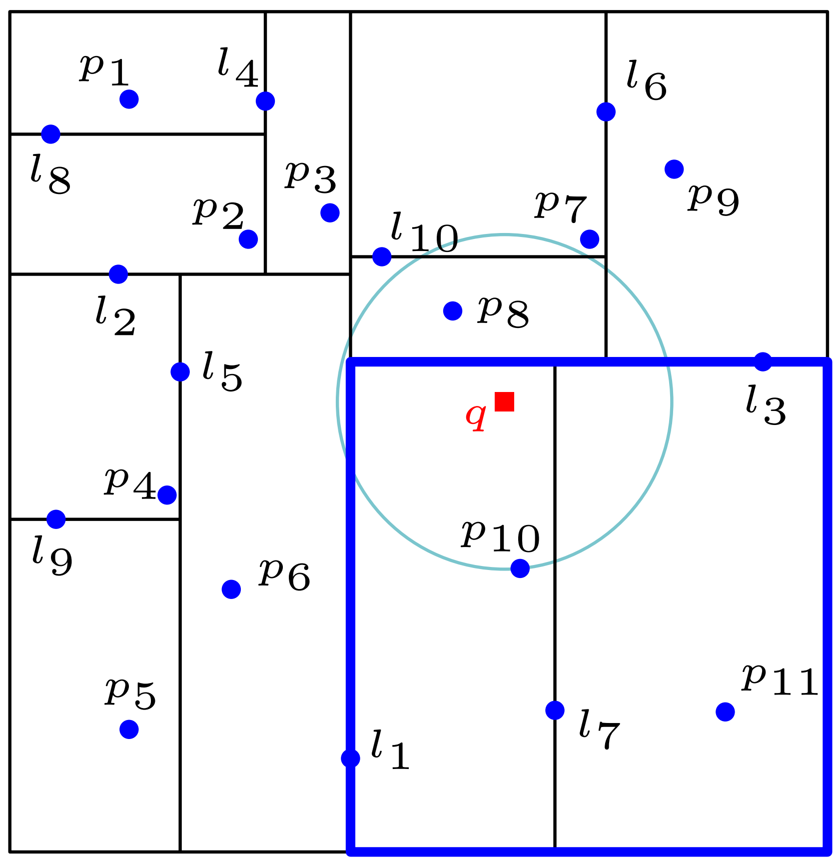


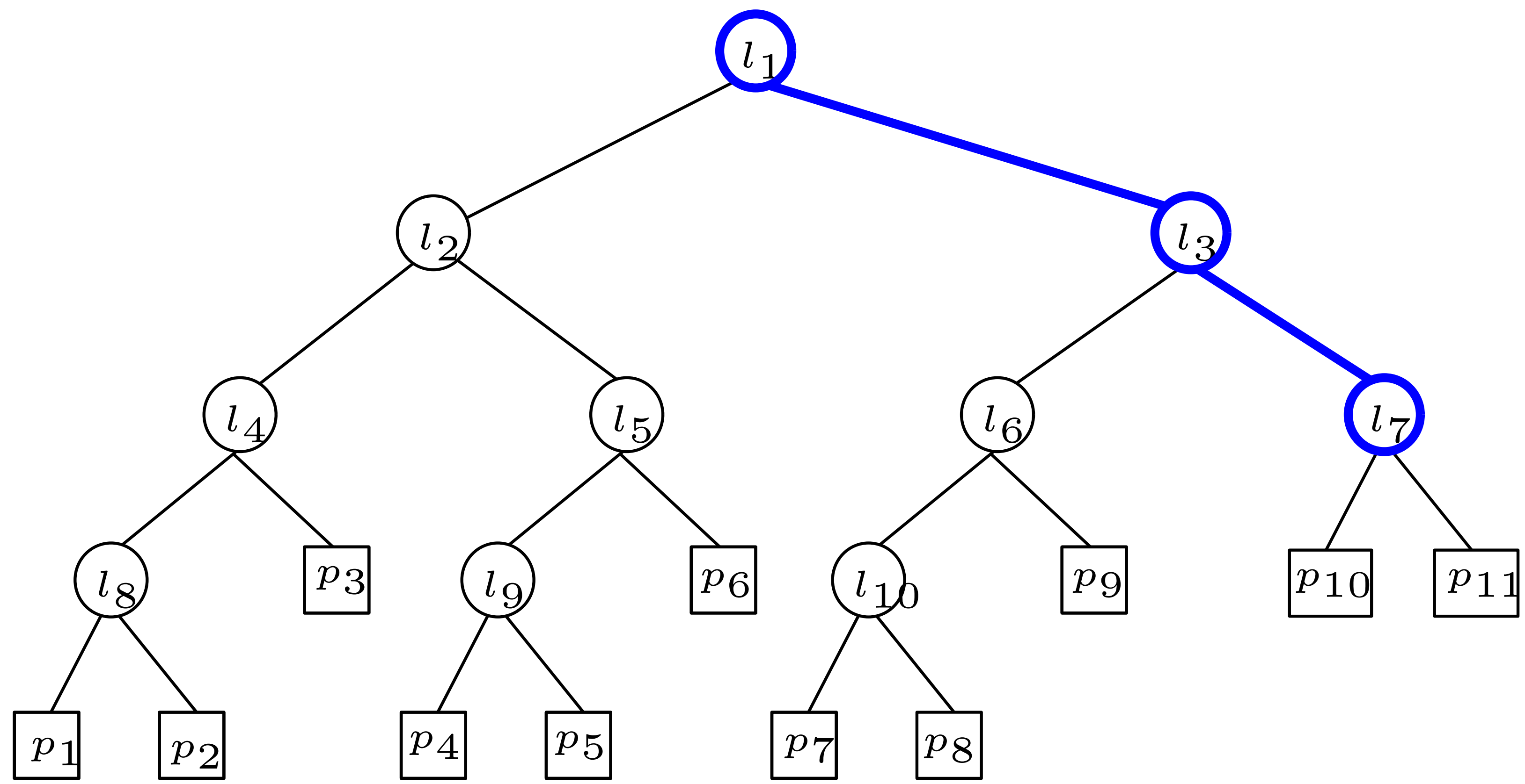
l_i: data at internal node

p_i: data at leaf node

(note: left-right labels are arbitrary)

Example





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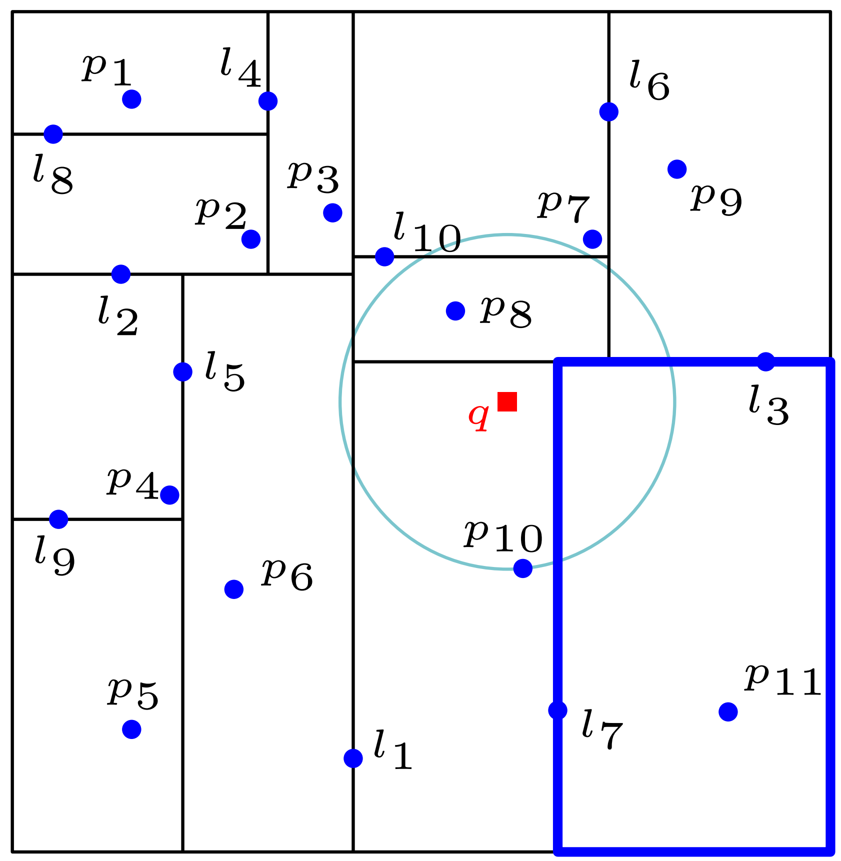

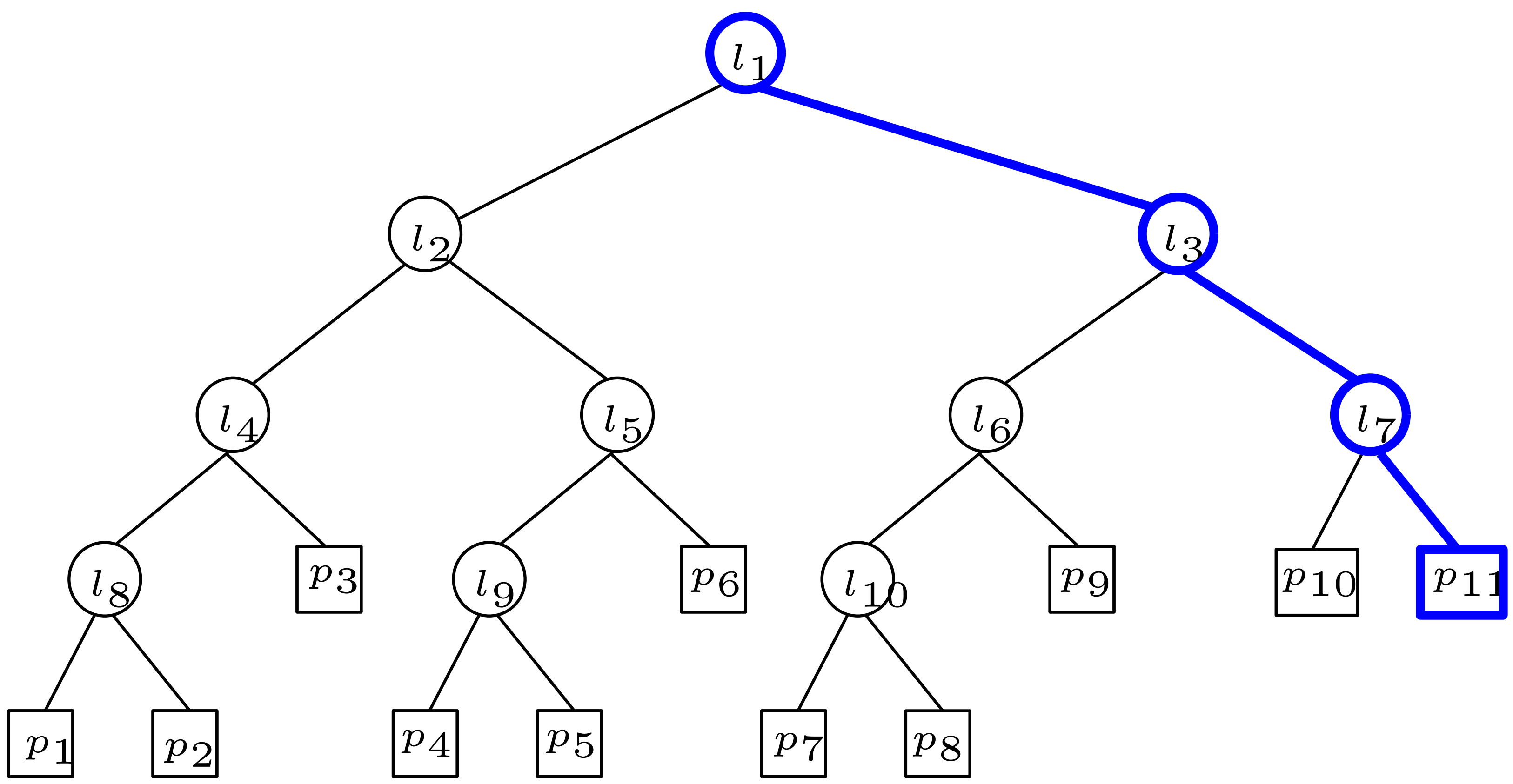

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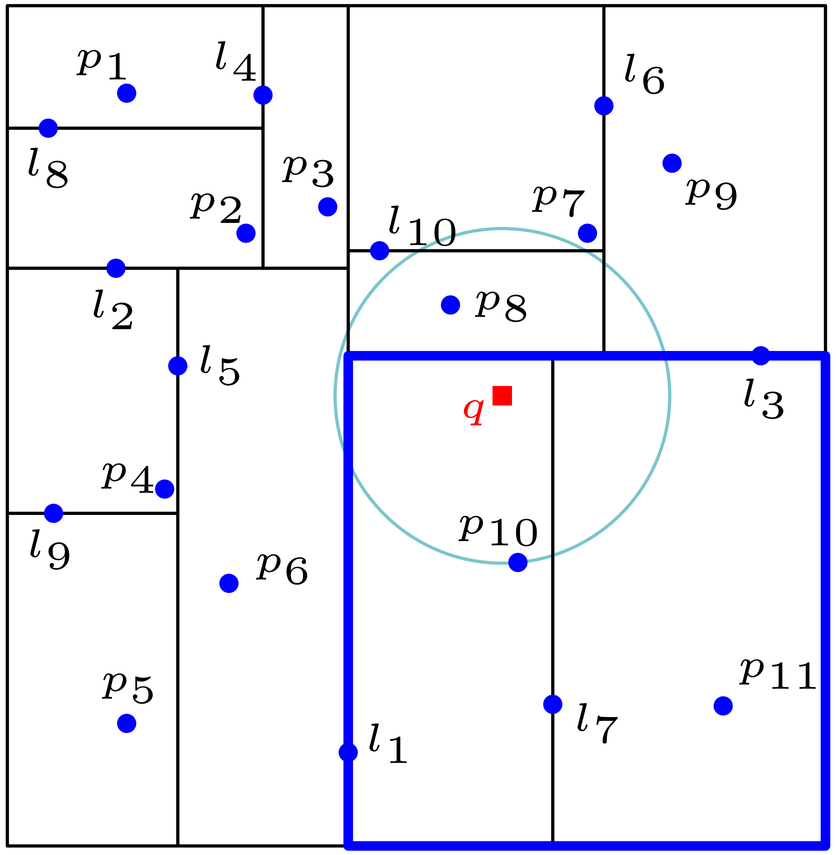

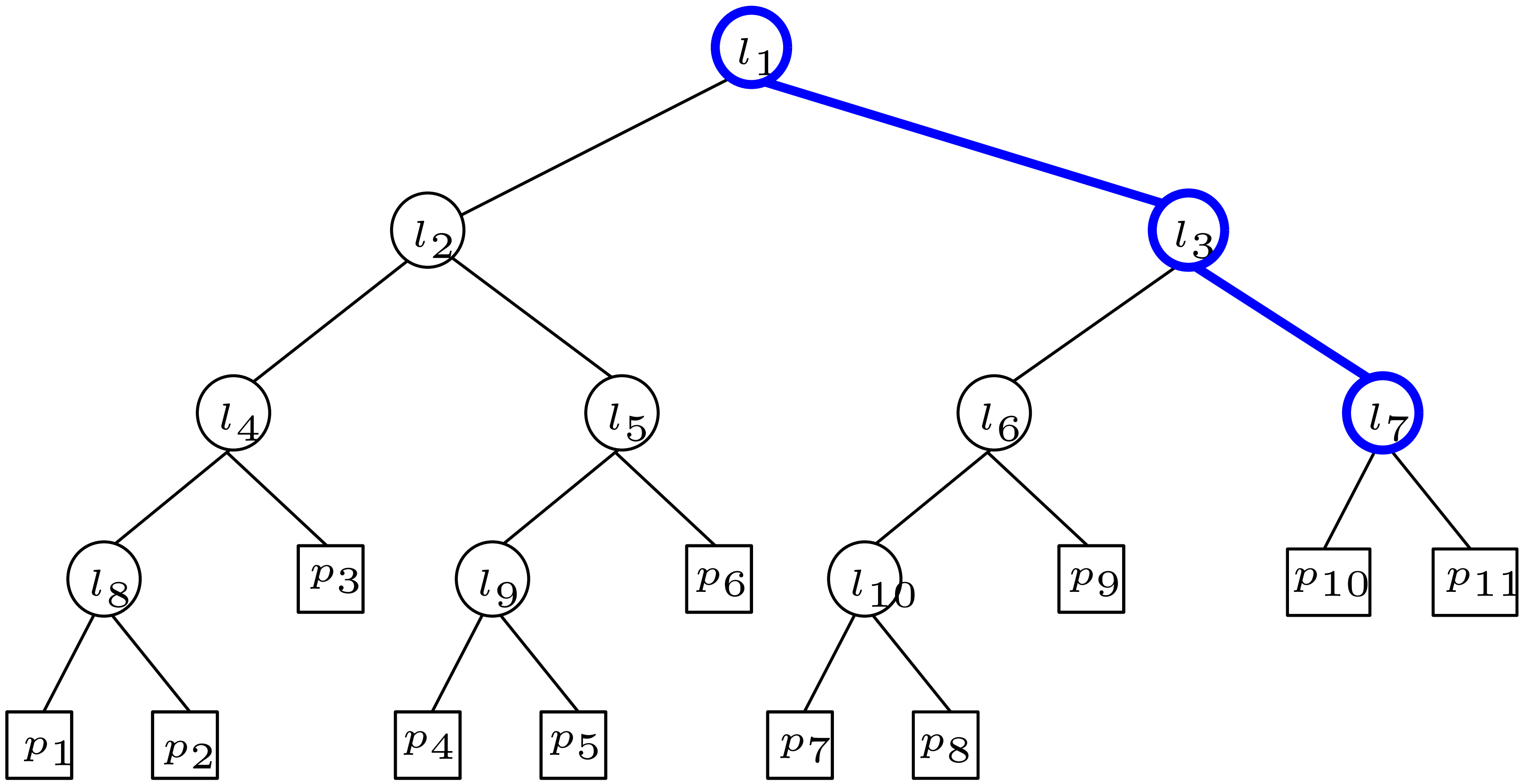

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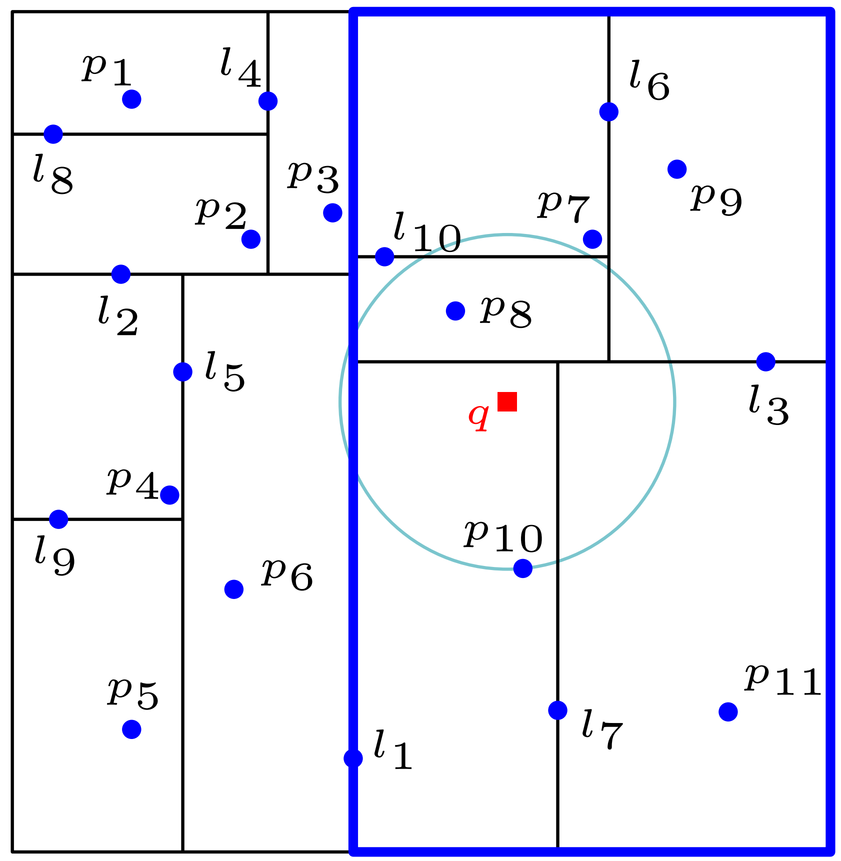

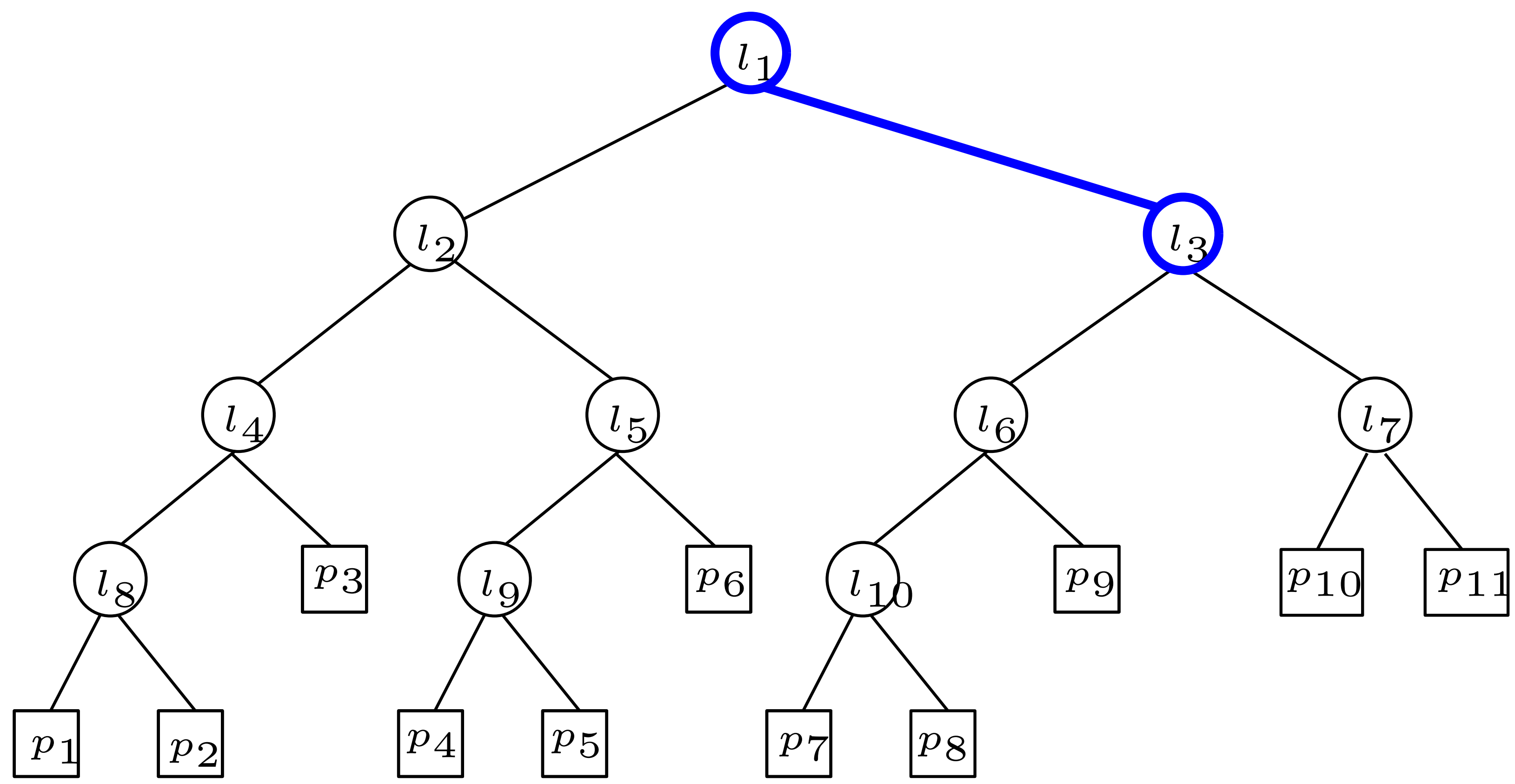

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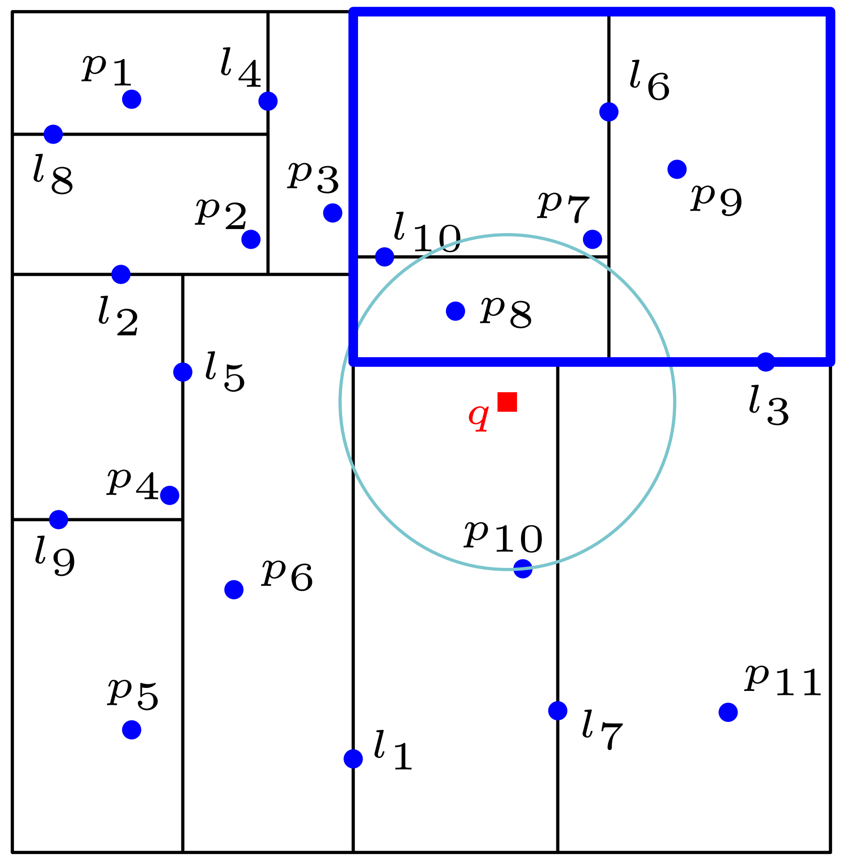

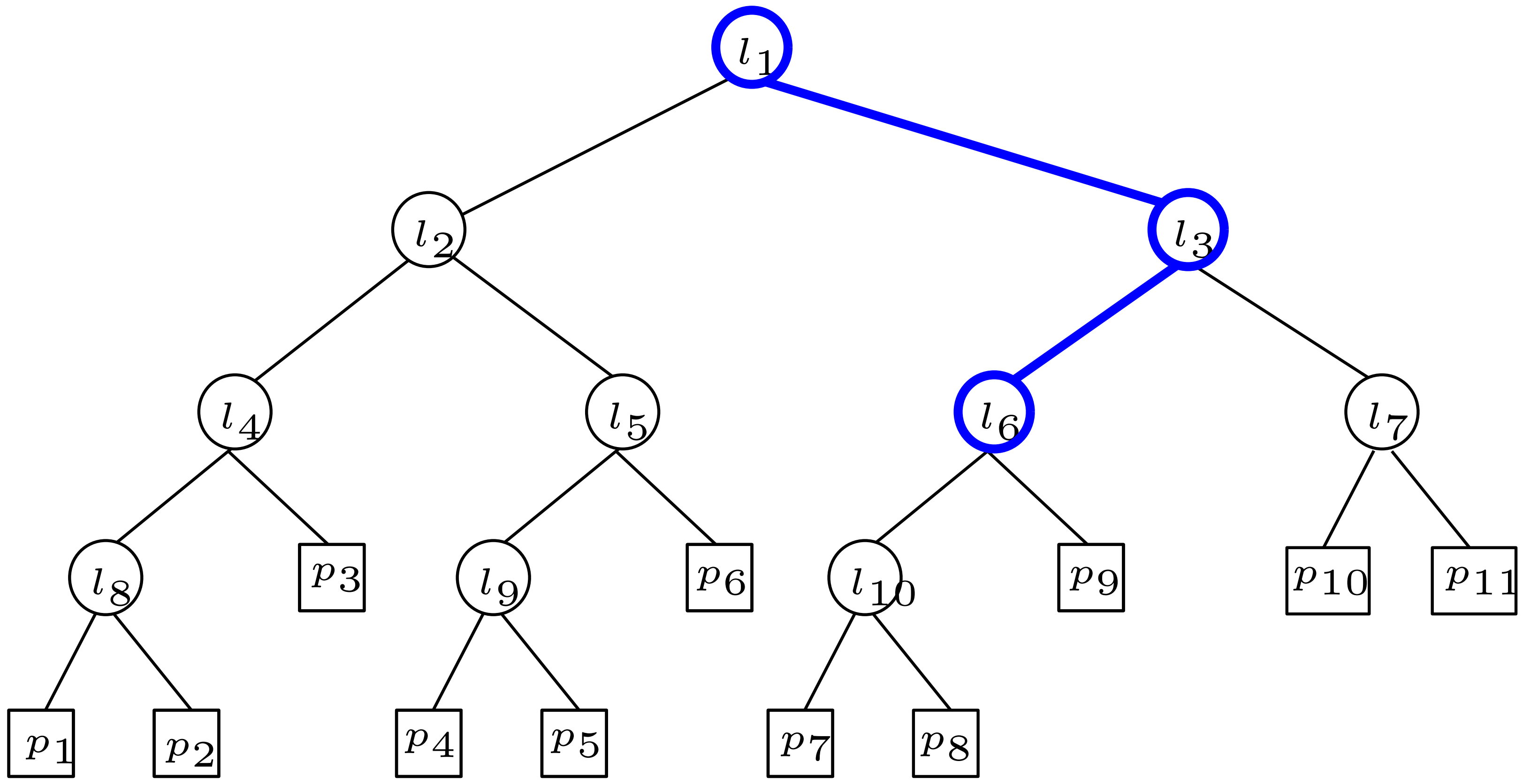

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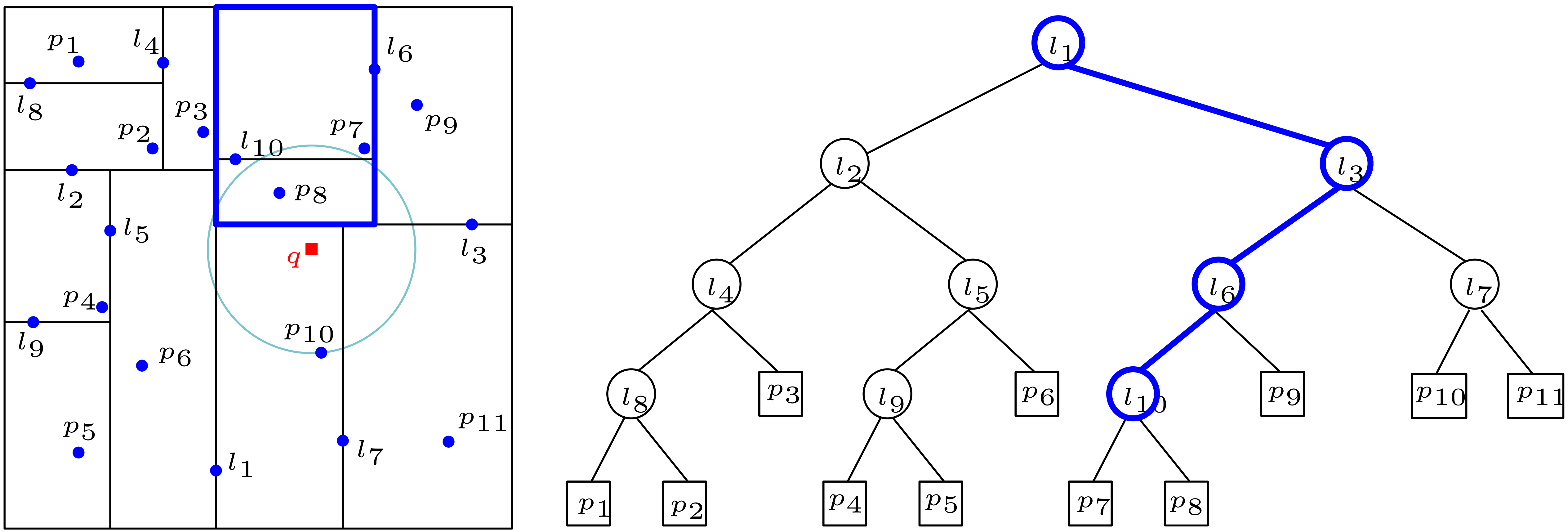

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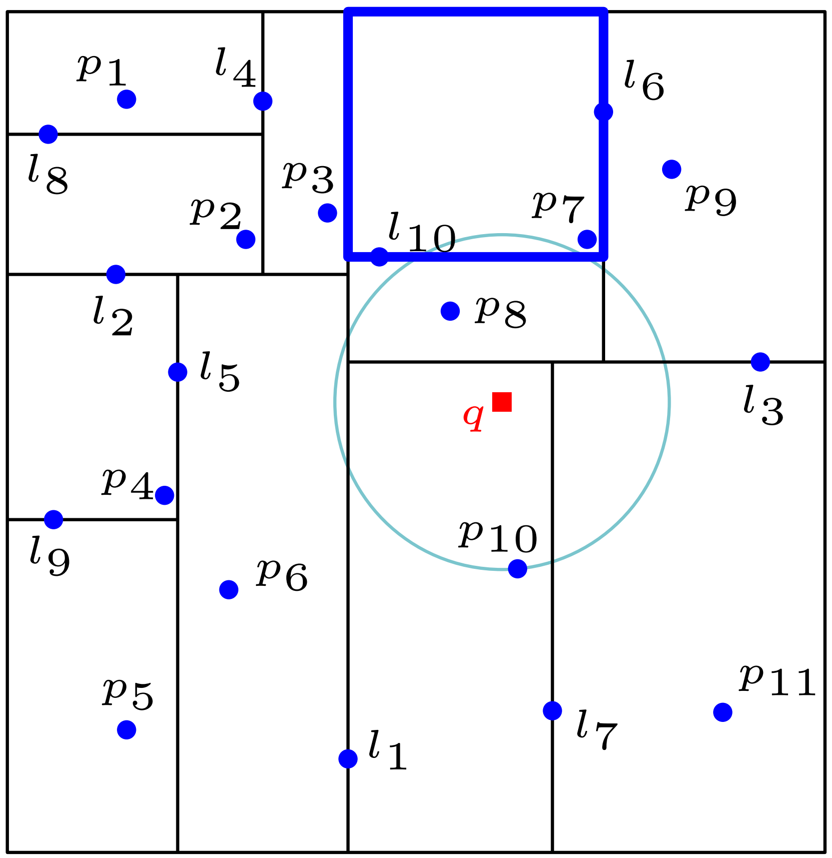

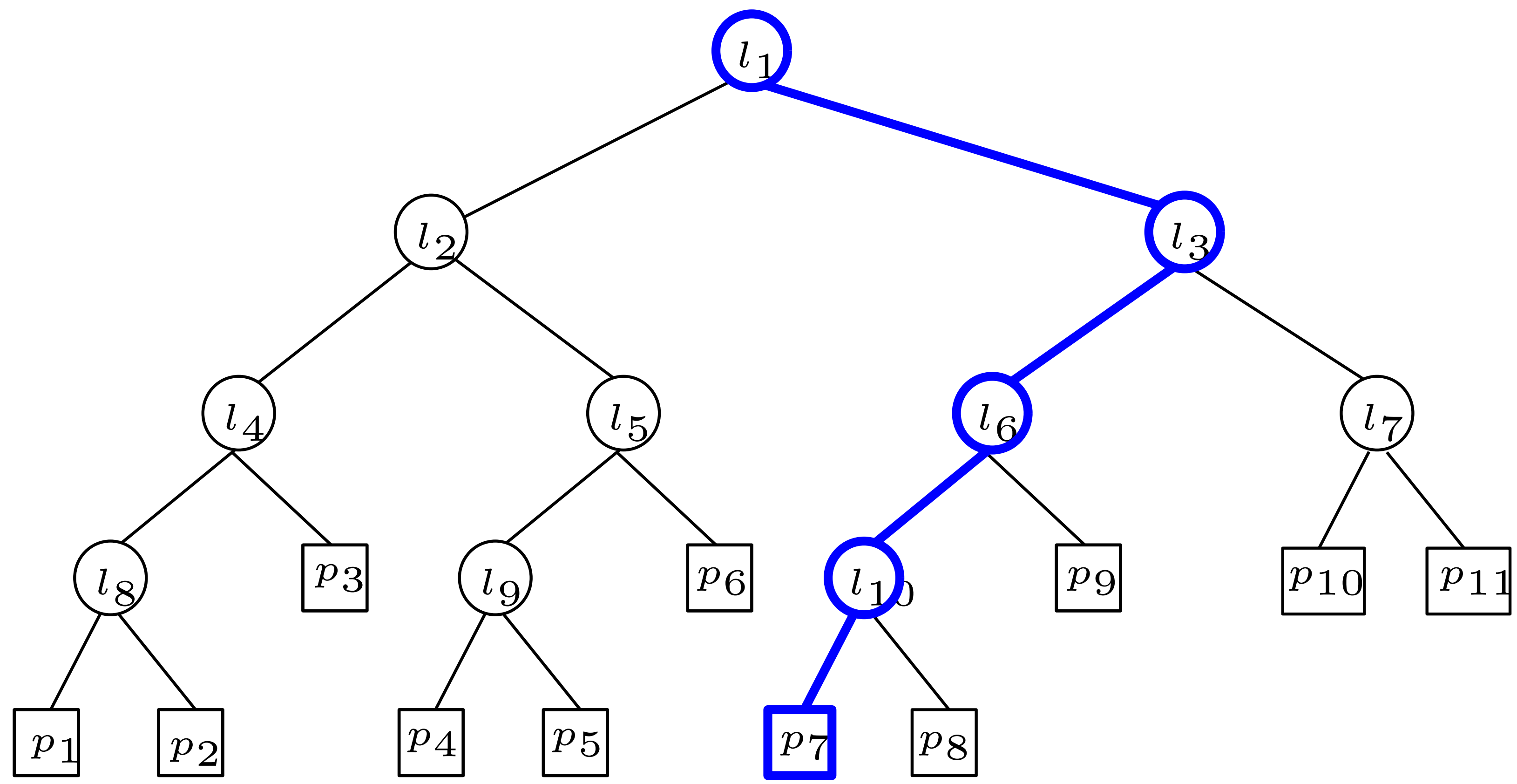

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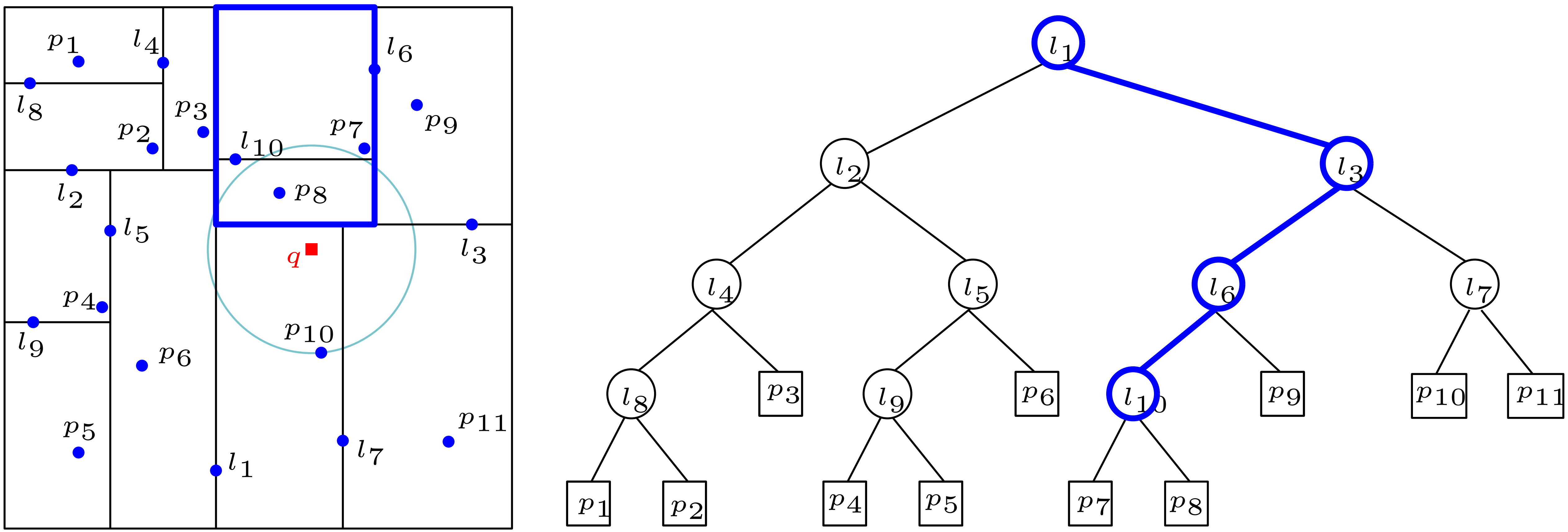

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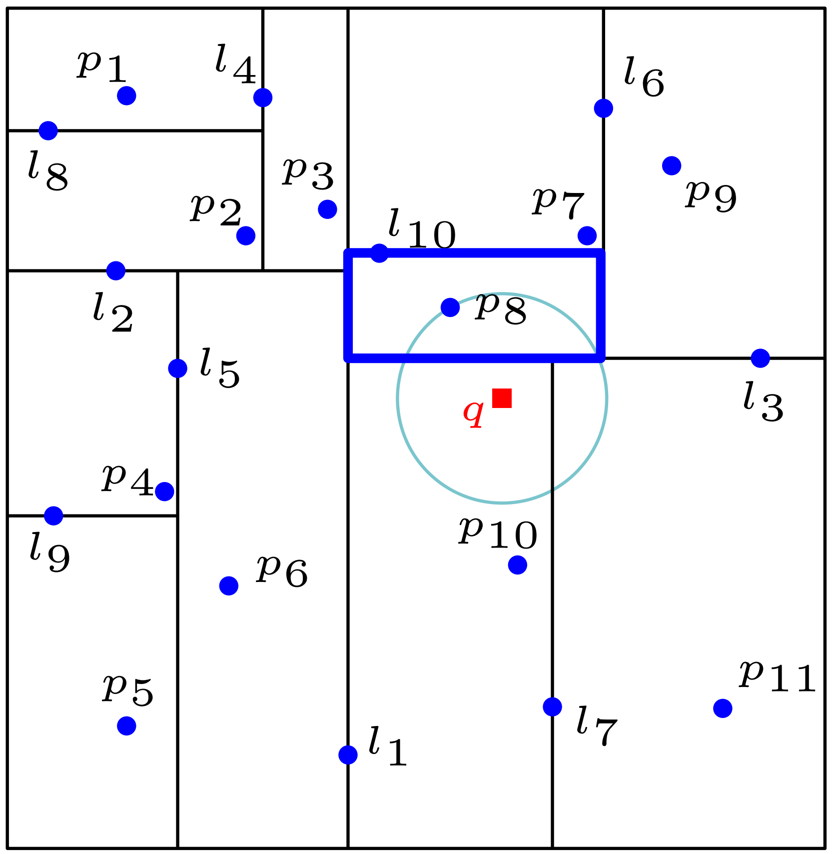

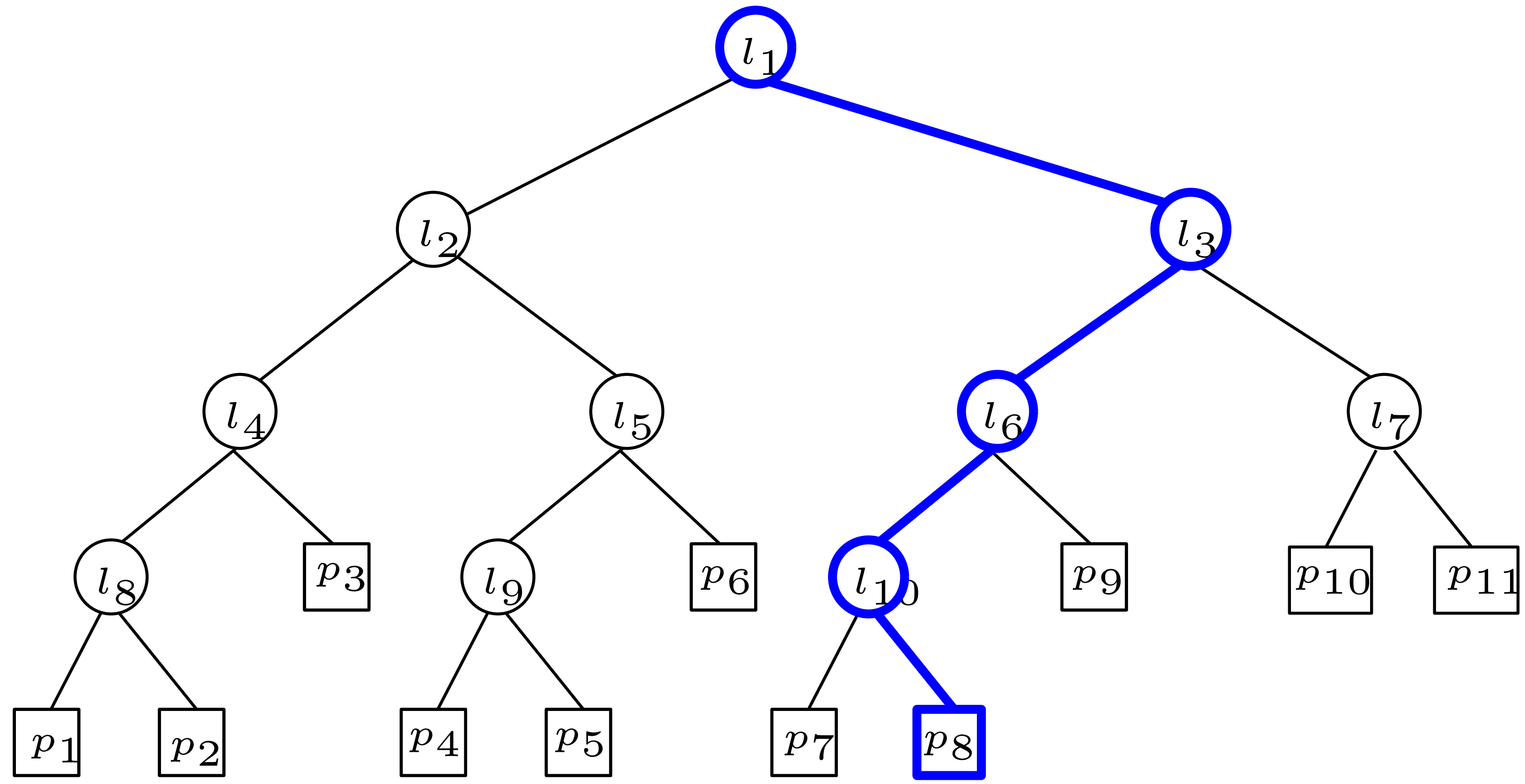

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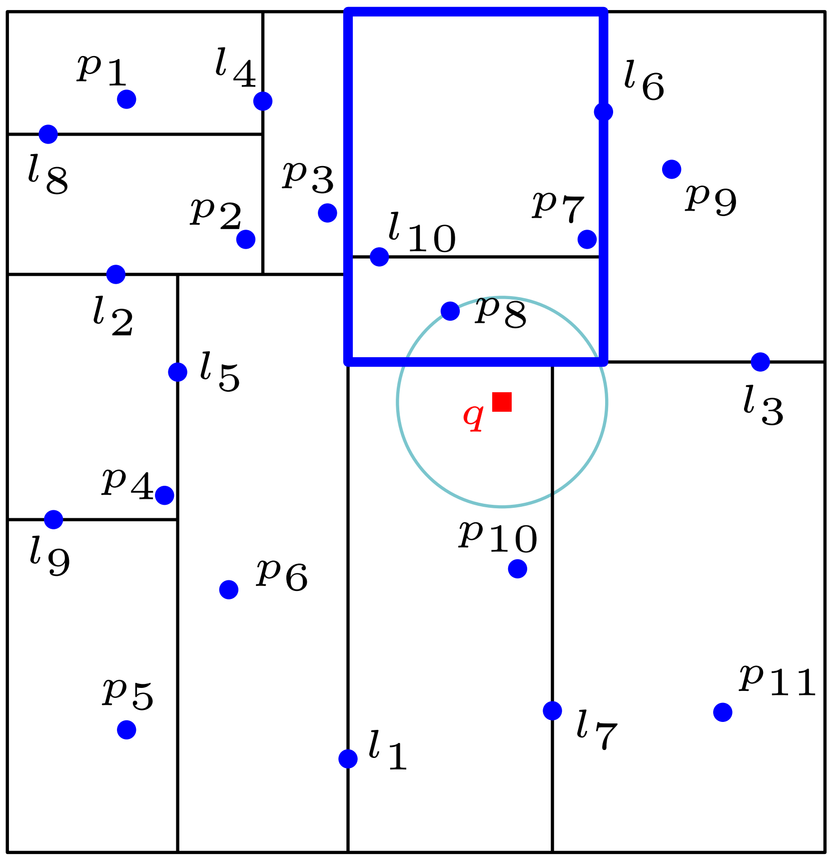

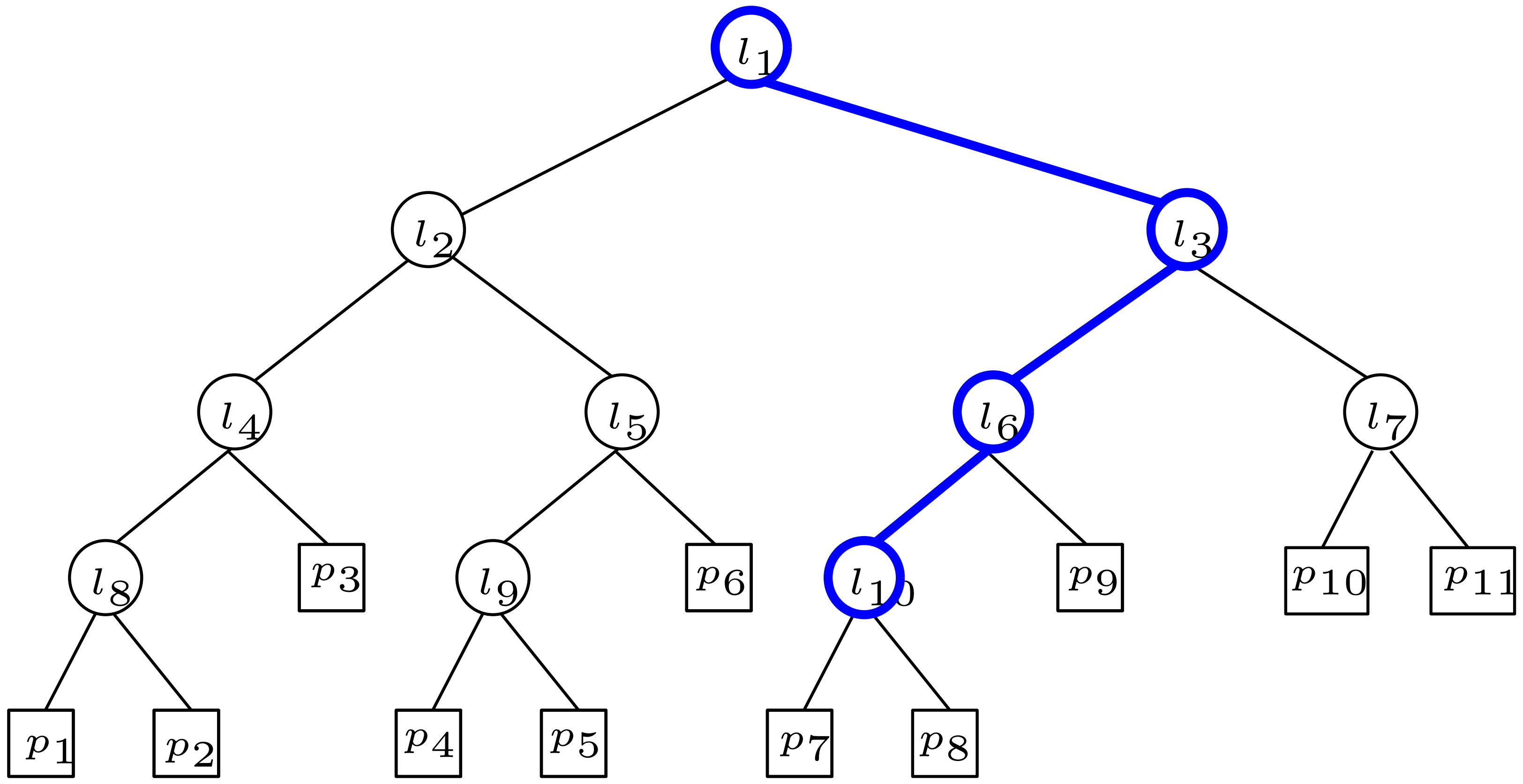

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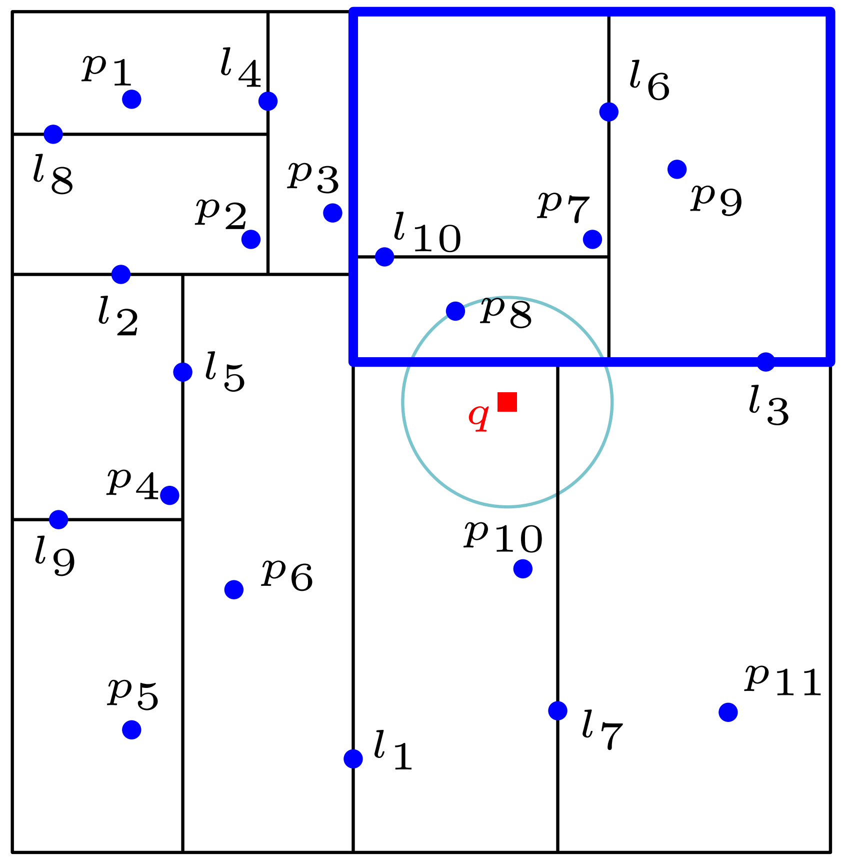

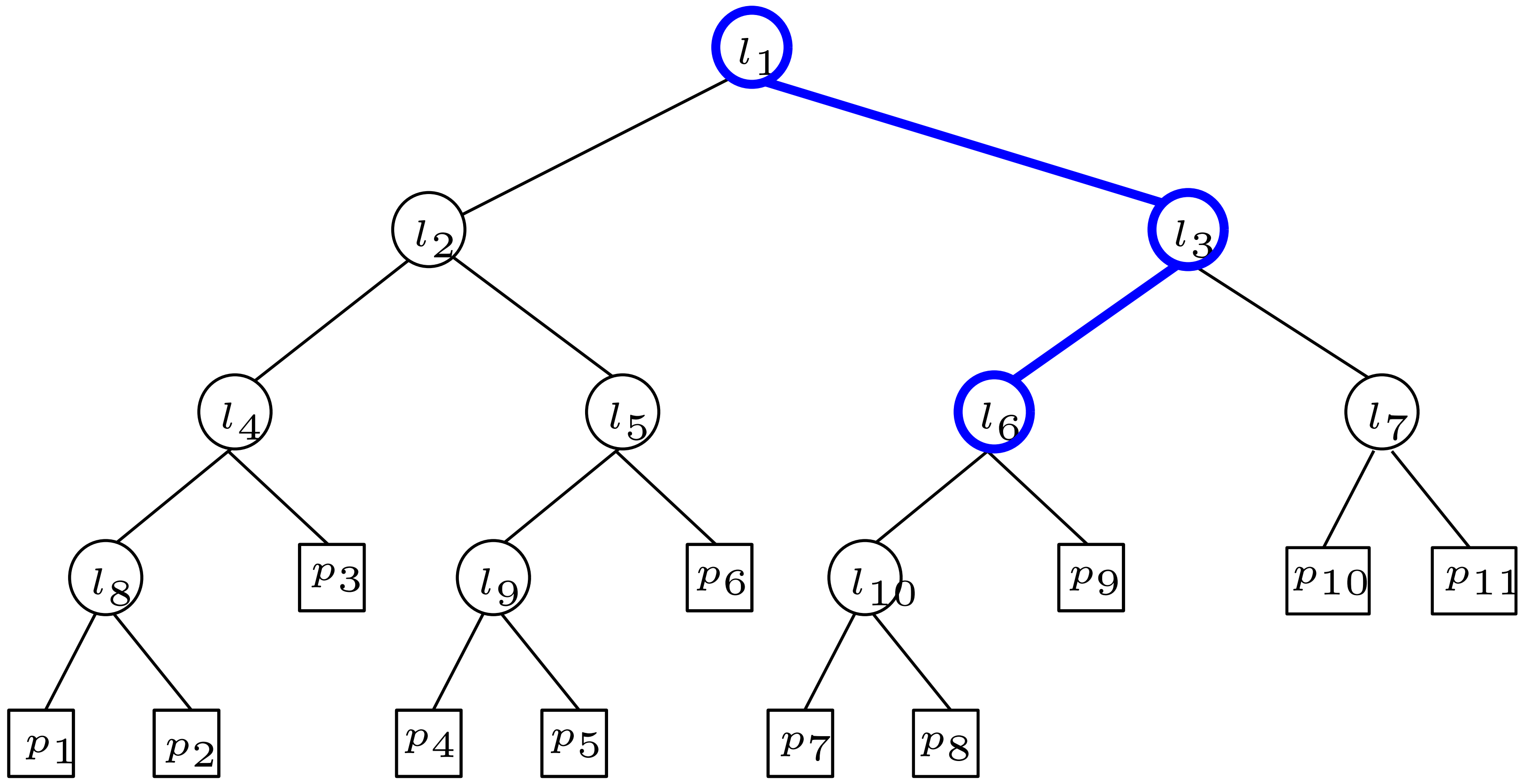

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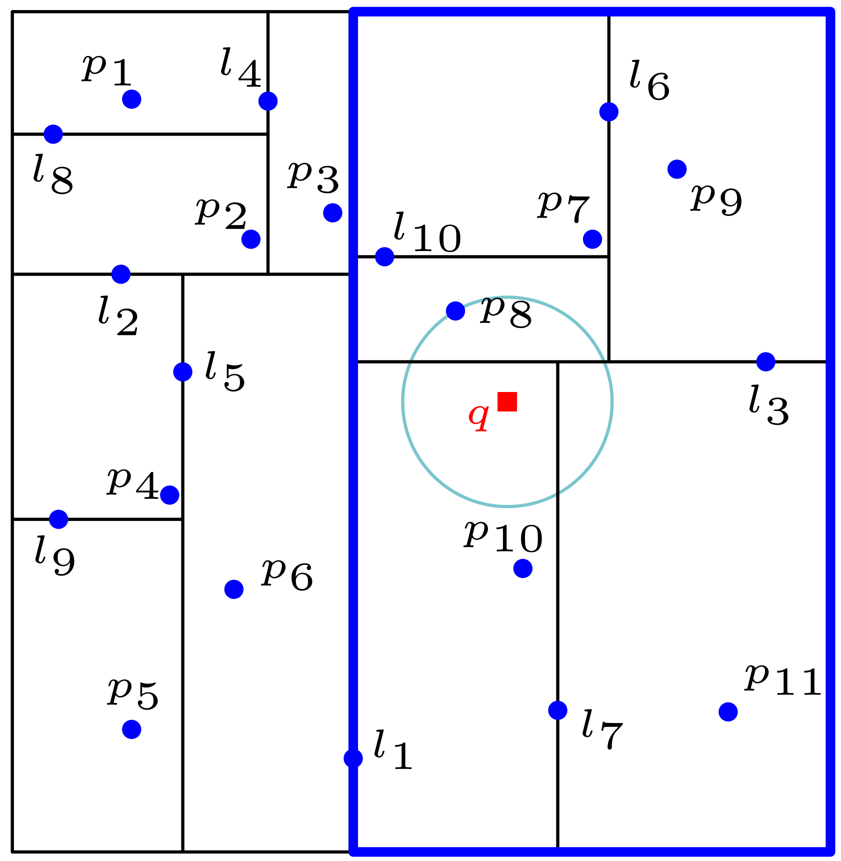

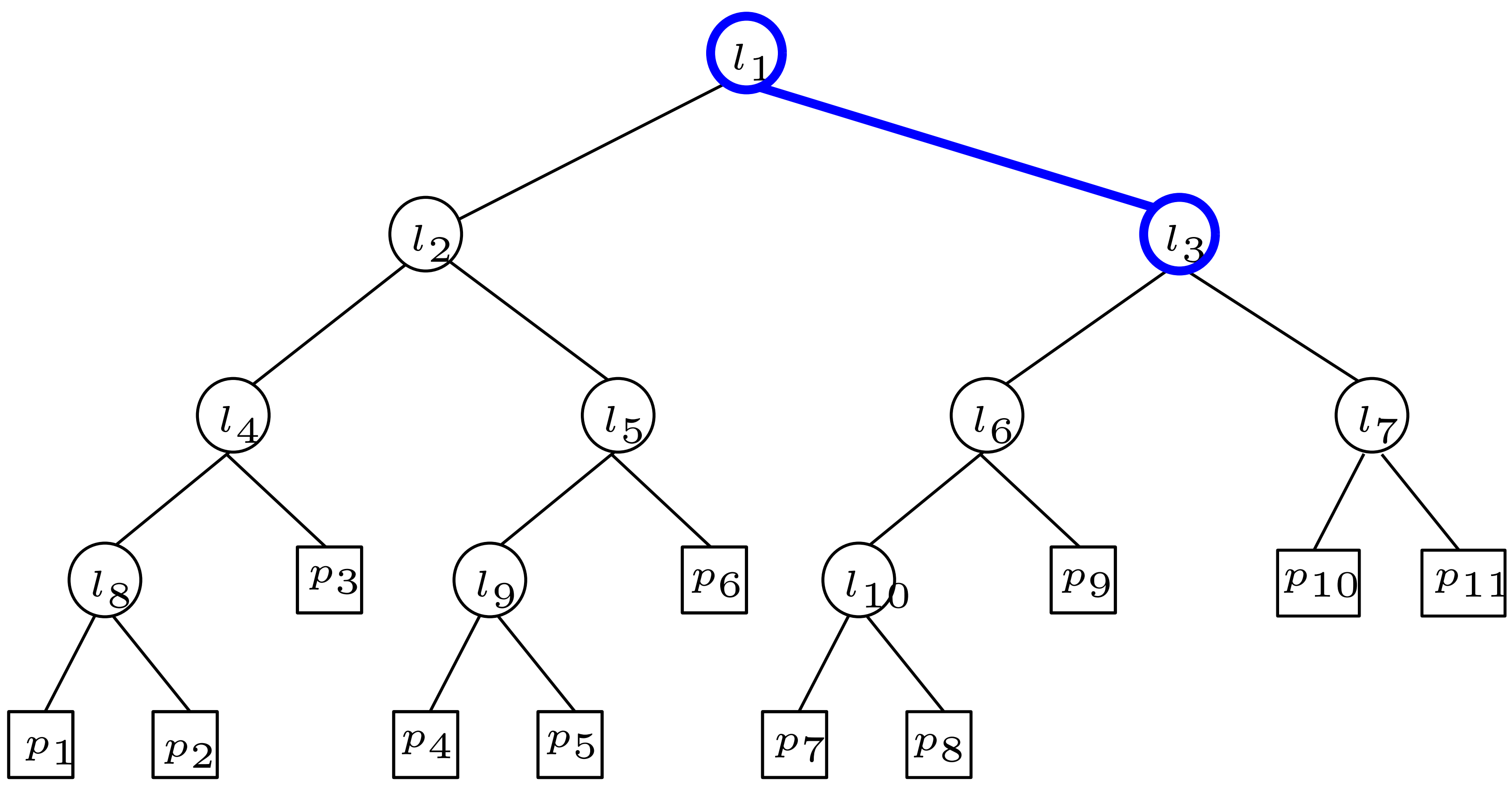

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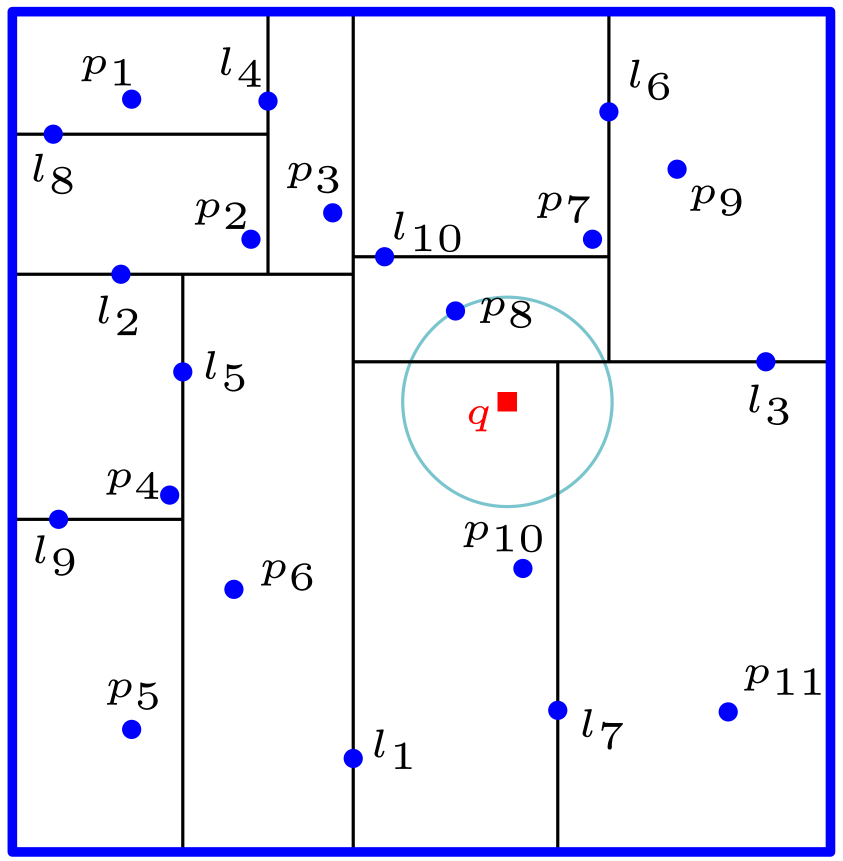

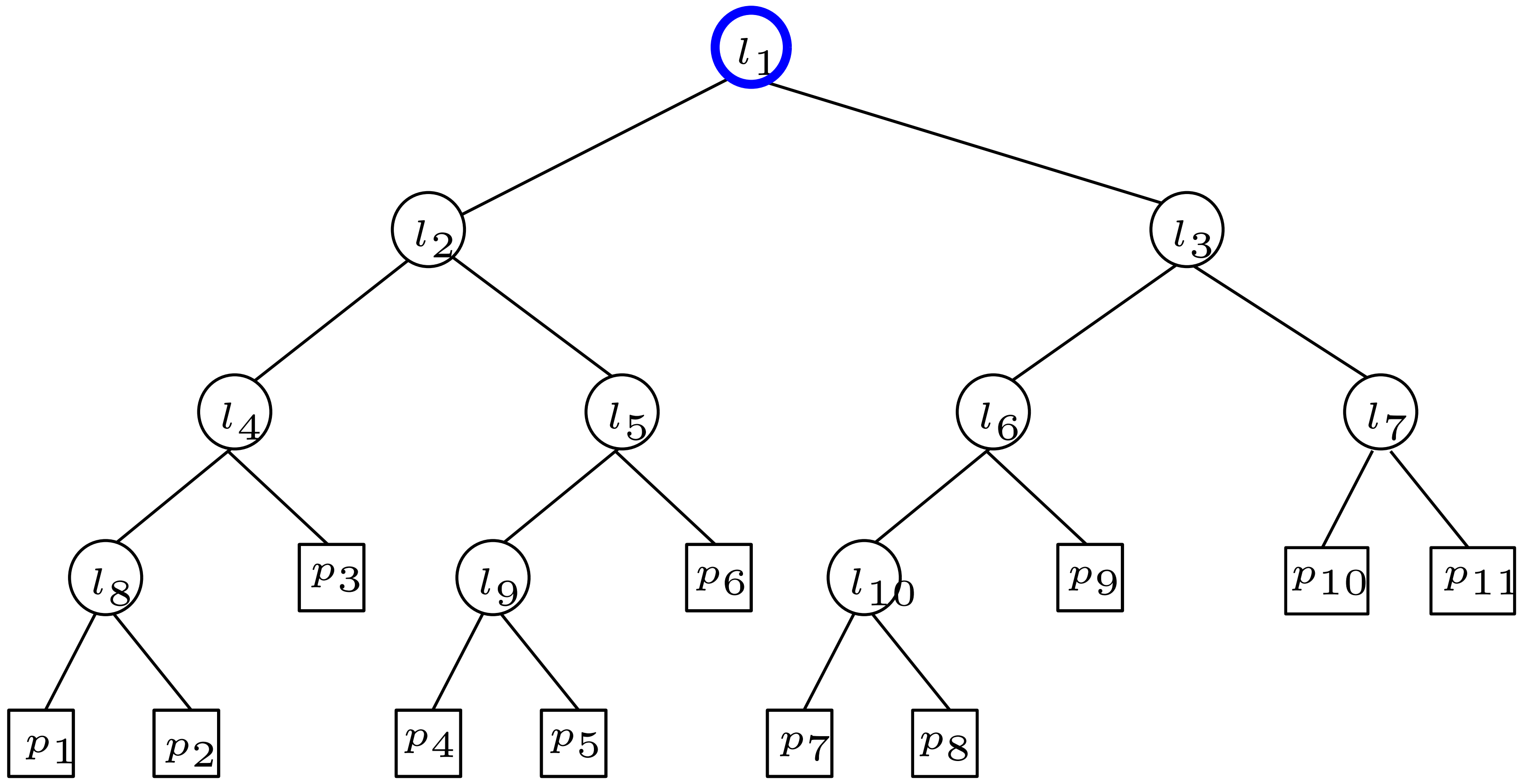

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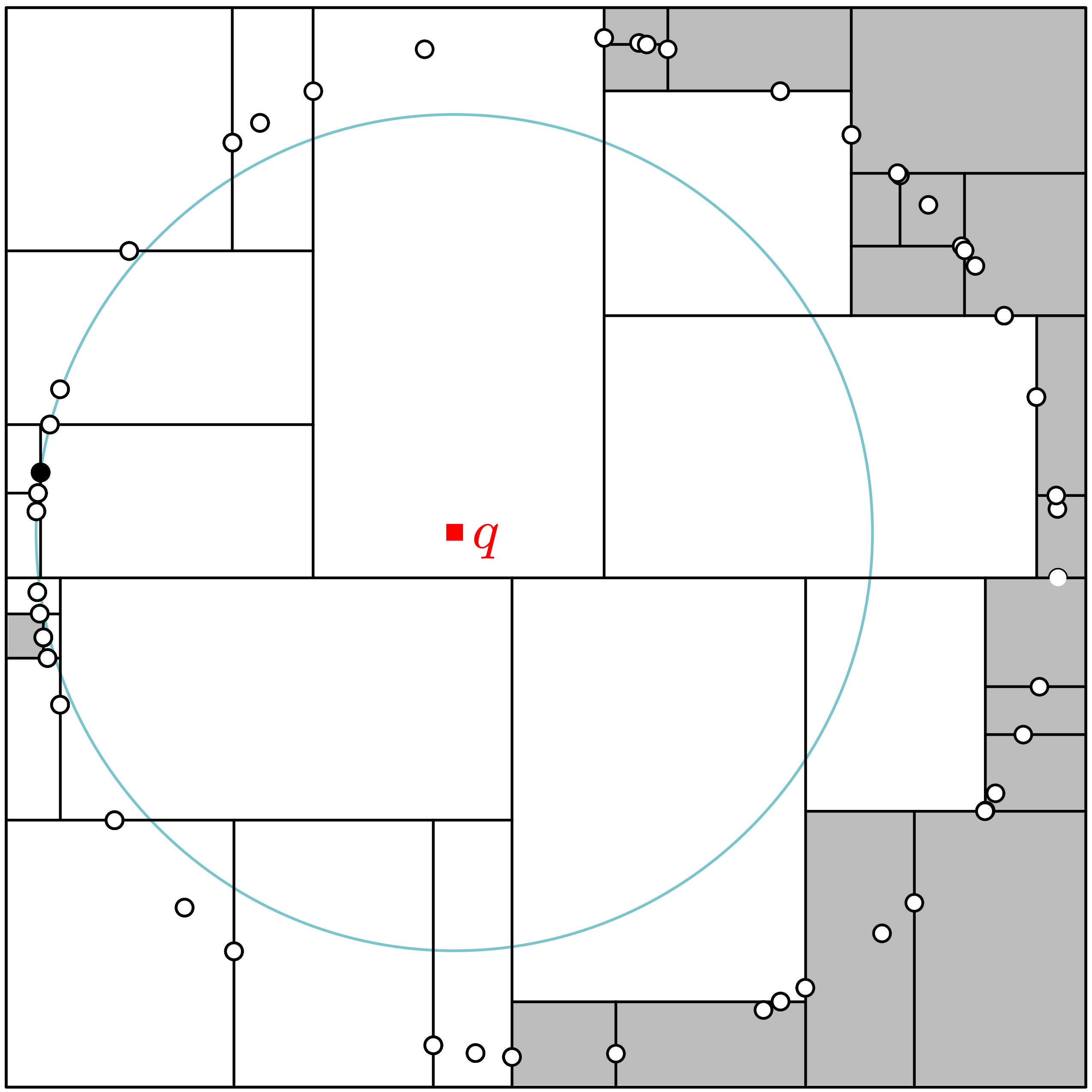


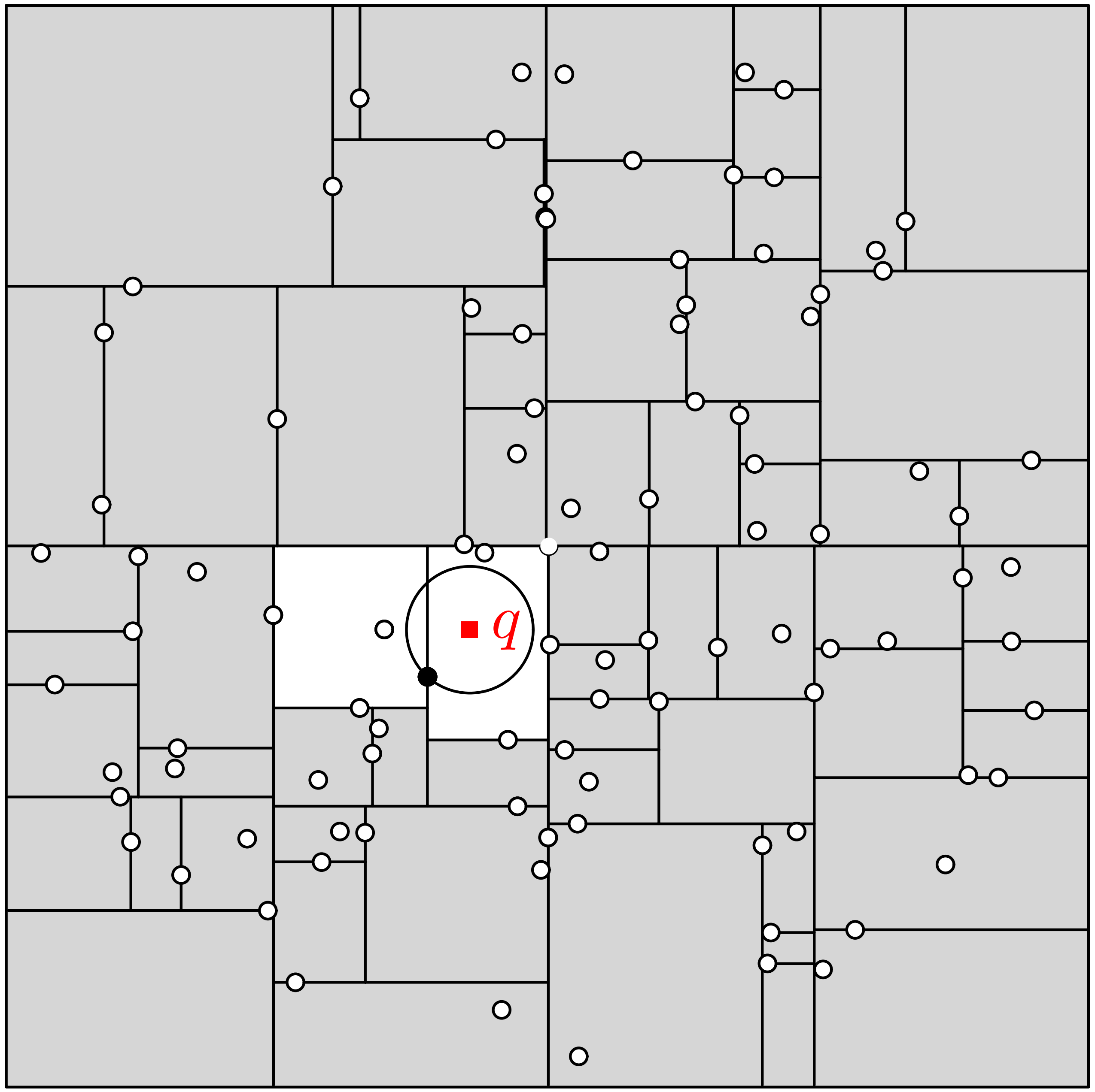
worst-case input (non-unif. distrib.):

long skinny cells

$\Downarrow$

query time $= \Omega(dn)$

Example



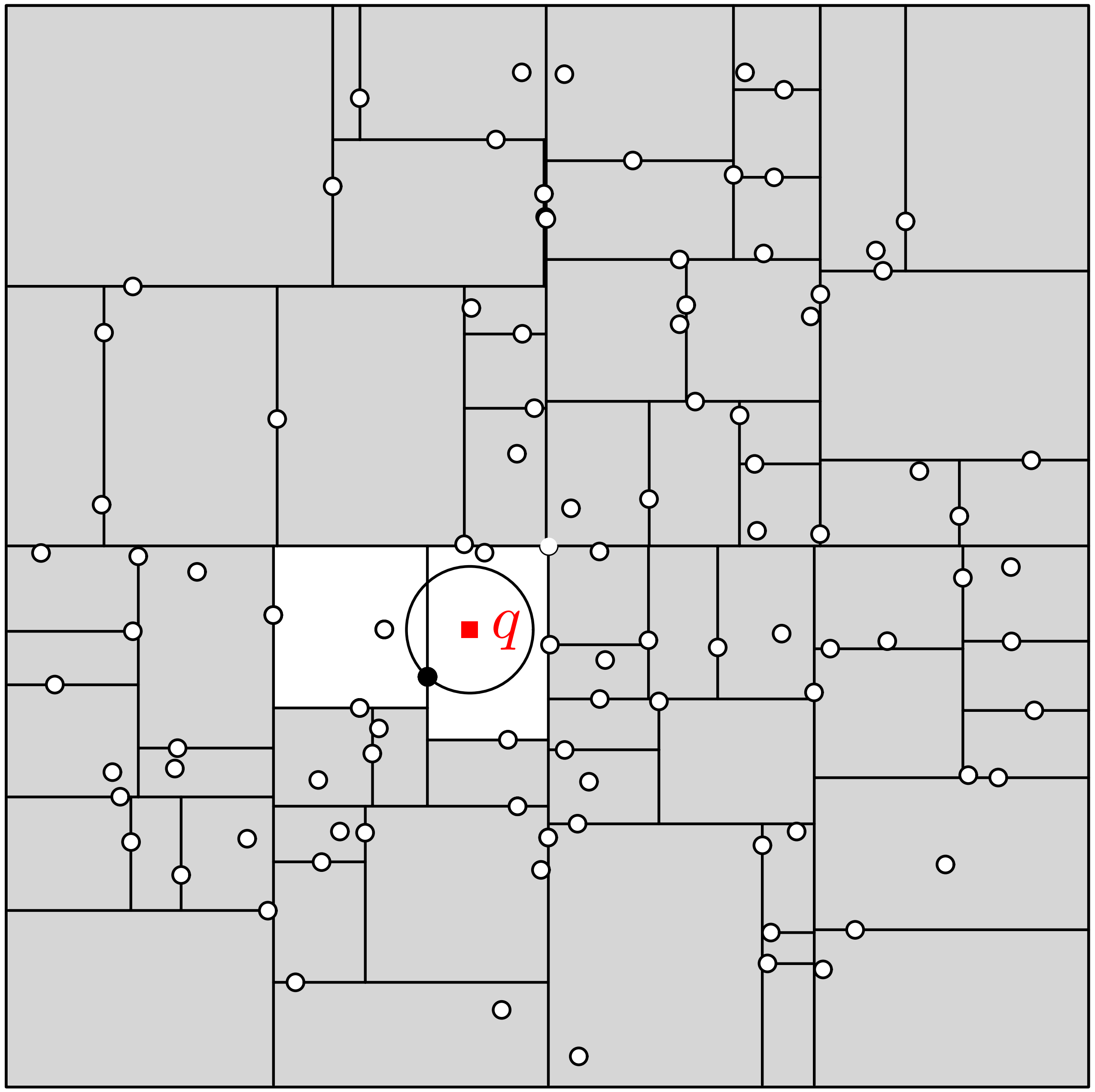
best-case input (unif. distrib.):

small fat cells

$$\Downarrow$$

query time $= O(c_d \log n)$

Example



best-case input (unif. distrib.):

small fat cells

$\Downarrow$

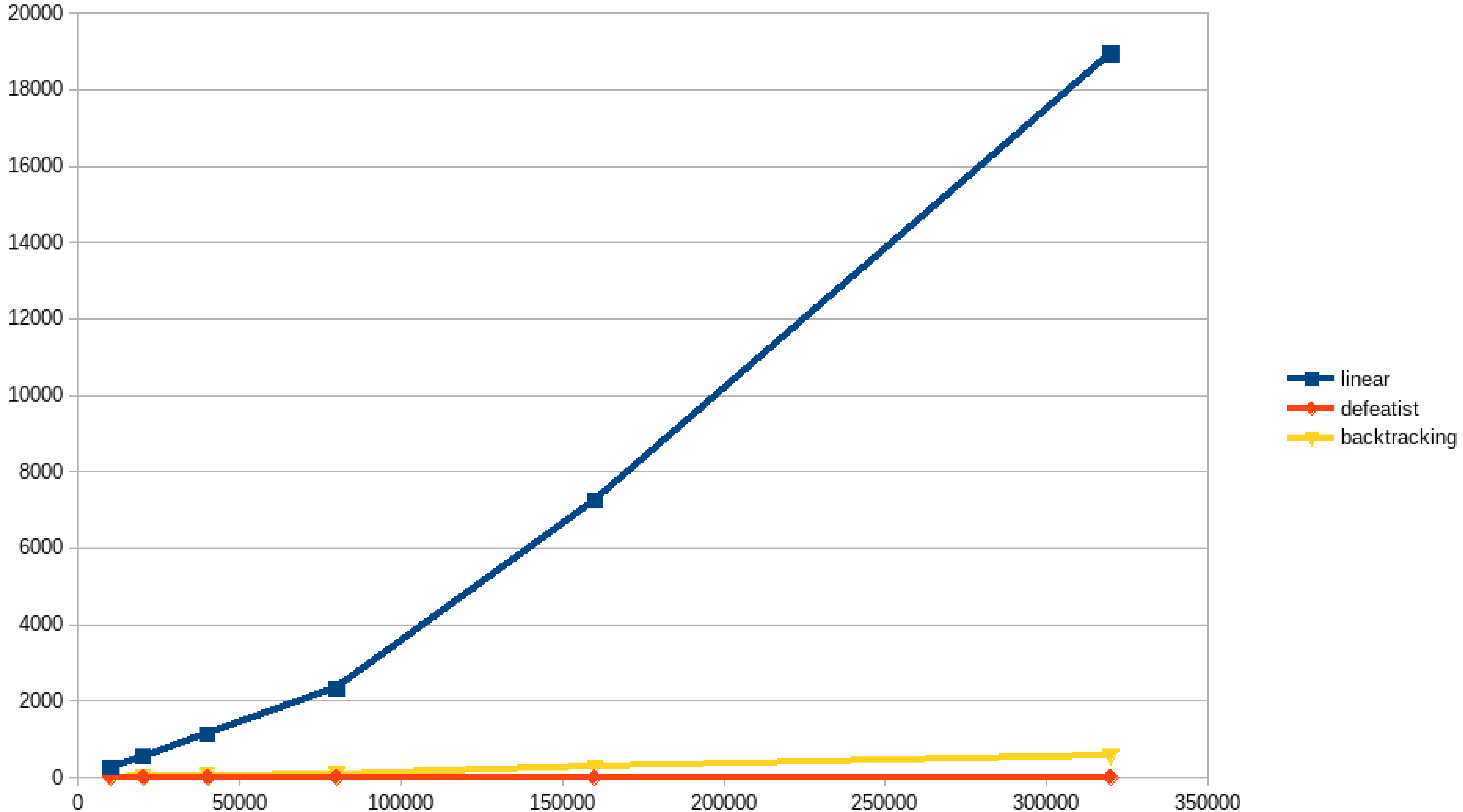
query time $= O(c_d \log n)$

Randomness should help!

(many variants: priority search, early backtracking, random cutting hyperplanes, etc.)

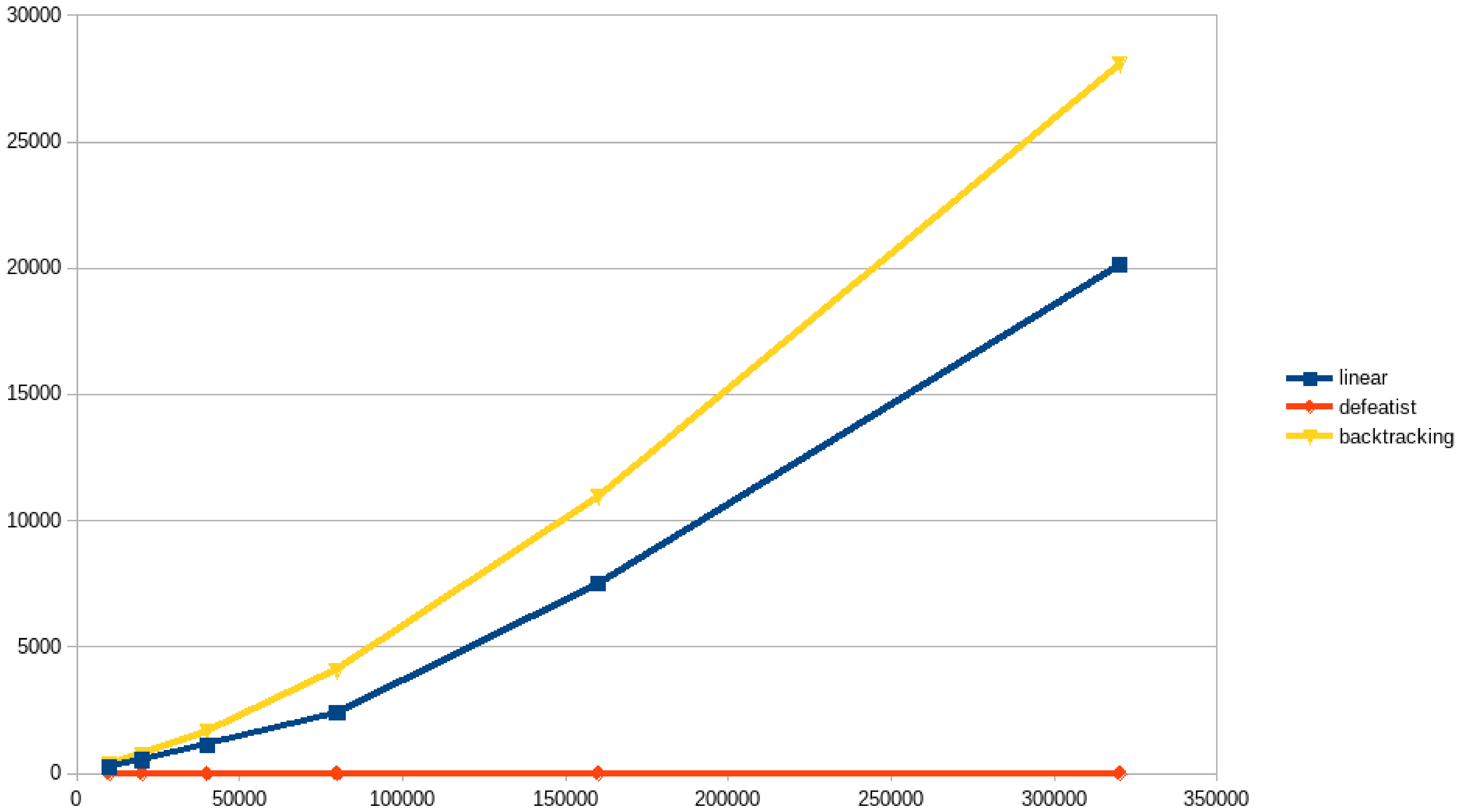
Benchmarks

avg. query time (μs) vs. # data points: (uniform measure in unit square in 2d)

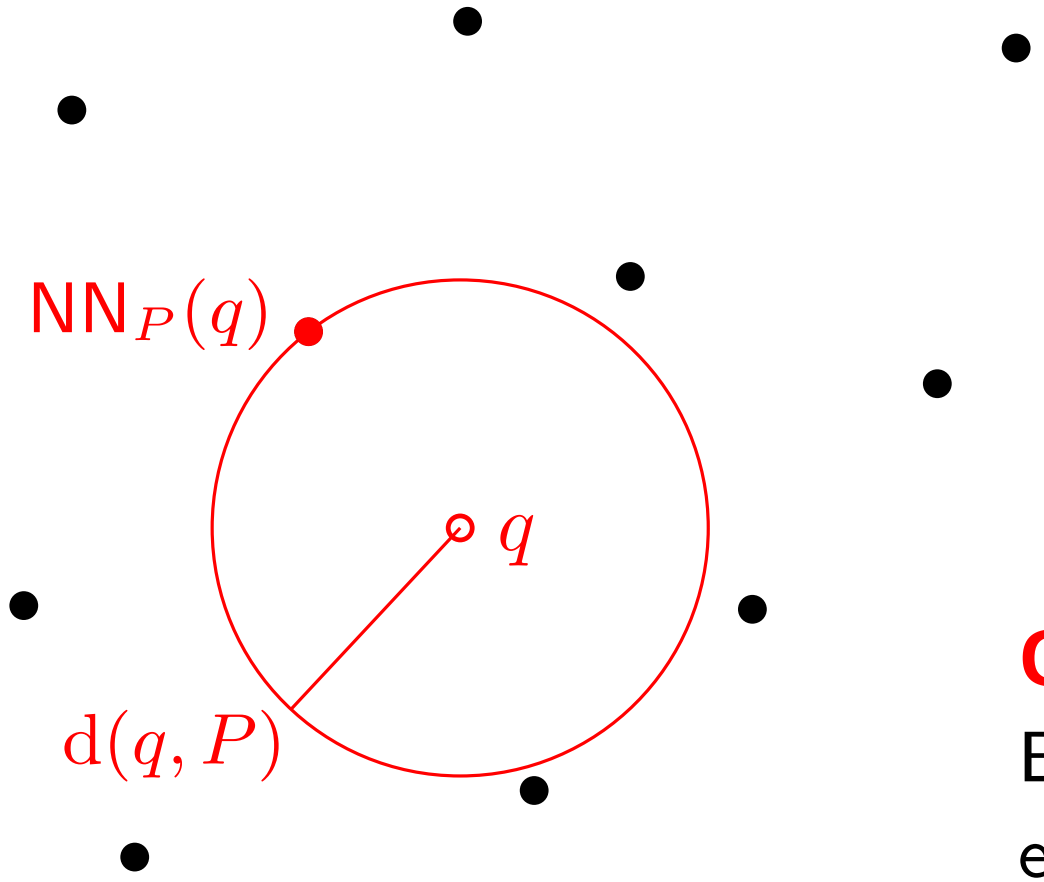


Benchmarks

avg. query time (μs) vs. # data points: (uniform measure on unit circle in 2d)



High dimensions



pre-processing input: $P \subset \mathbb{R}^d$

query input: q

goal: find $p \in \mathrm{NN}_P(q)$

Curse of Dimensionality:
Every data structure for NN-search has either exponential size or exponential query time (in d) in the worst case.

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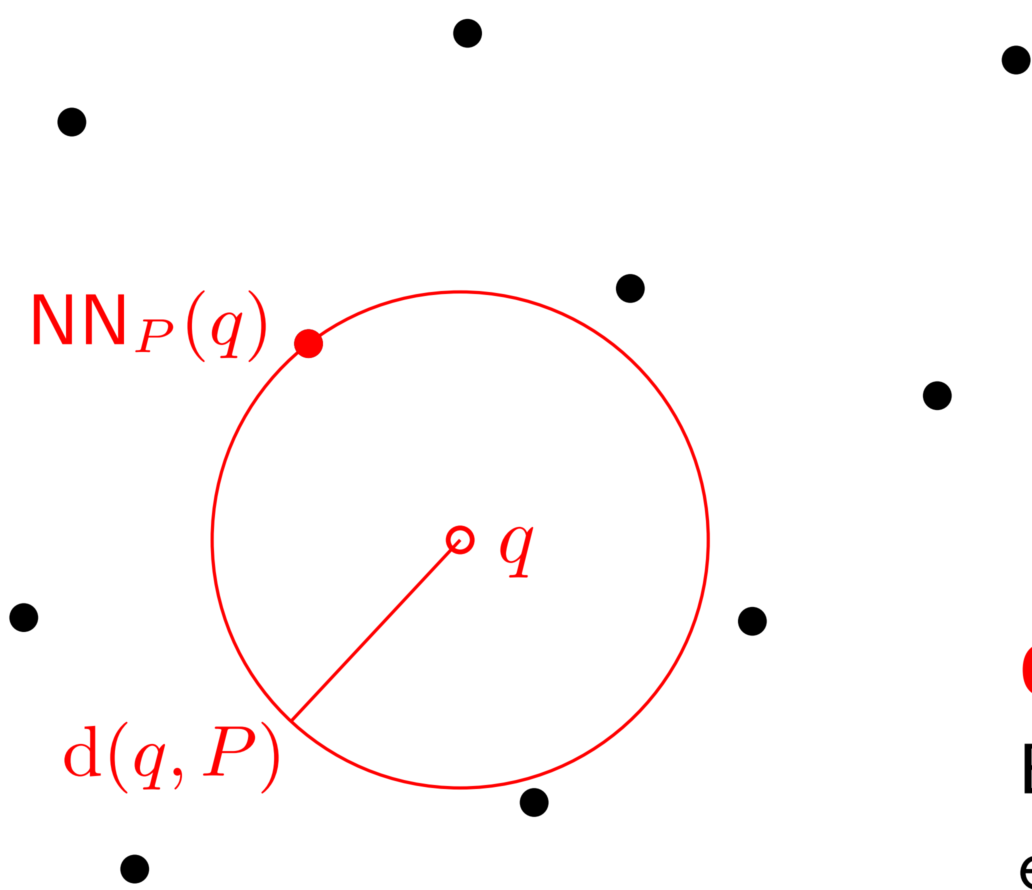

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$\rightarrow$ **holds both in theory and in practice** [Weber et al. '98] [Arya et al. '98]

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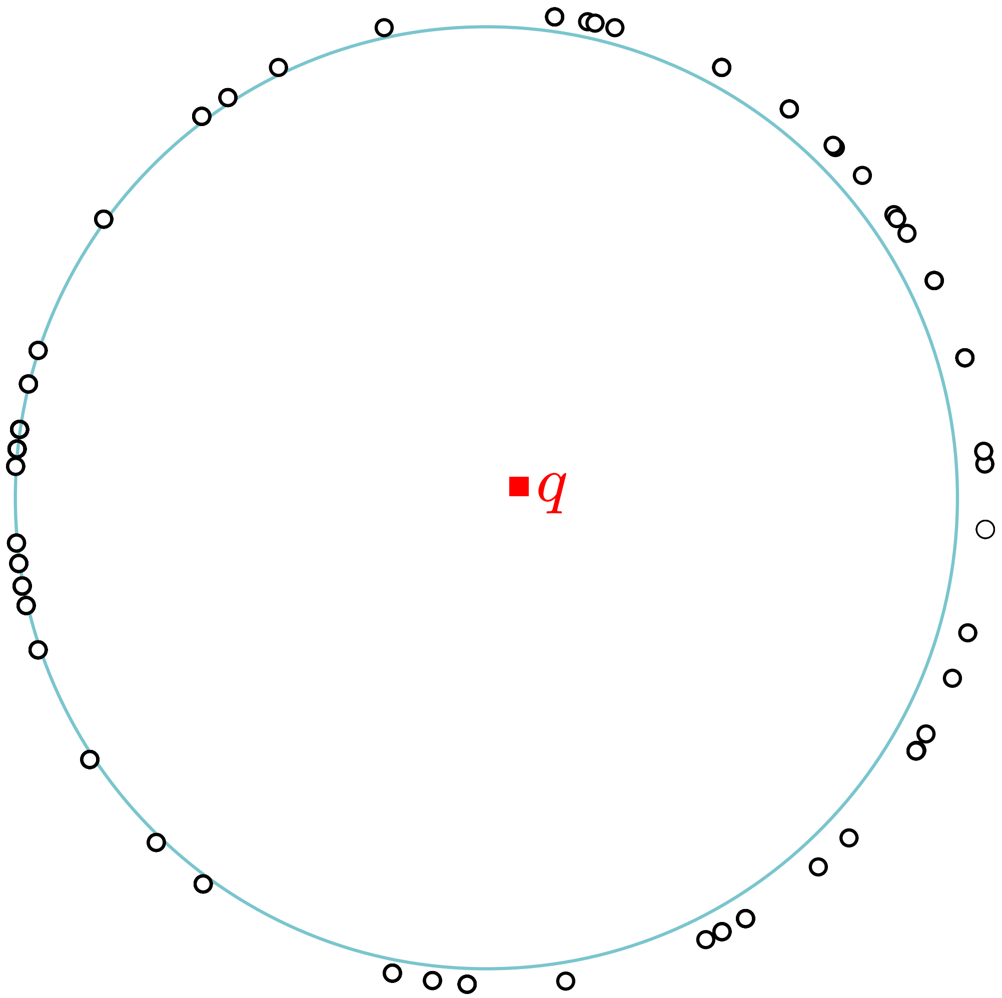

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→ **holds both in theory and in practice** [Weber et al. '98] [Arya et al. '98]

→ underlying phenomenon: **concentration of measure**

(distances concentrate around mean) [Demartinez '94]

Random Projection/Partition Trees

Exploiting randomness: RP-trees

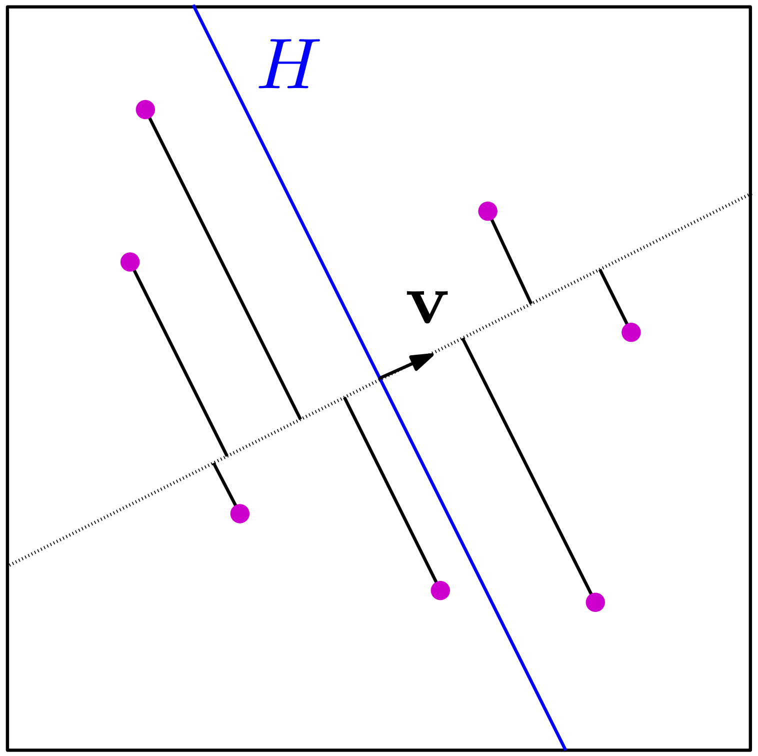
Random Projection/Partition tree:

at each internal node (corresponding to a cell C):

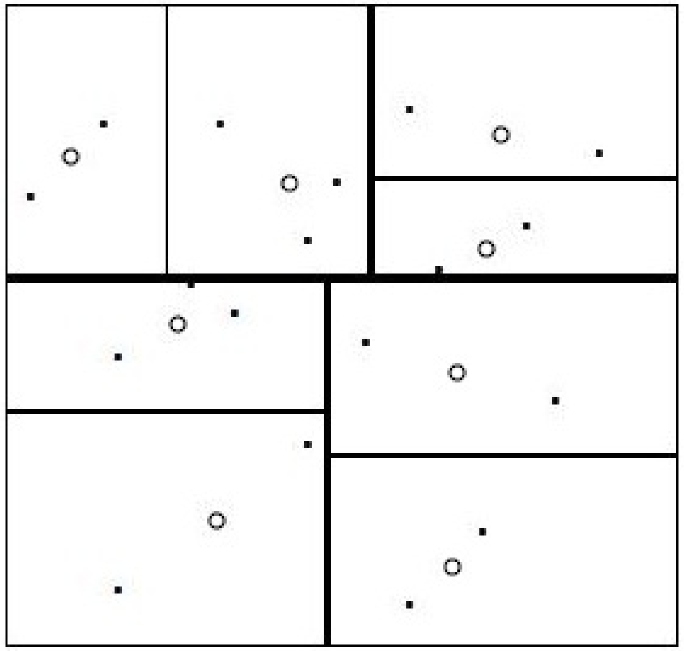
- choose $\mathbf{v} \sim \text{unif}(\mathbb{S}^{d-1})$ and $\beta \sim \text{unif}([\frac{1}{4}, \frac{3}{4}])$

- let $H = \mathbf{v}^{\perp} + \text{median}_{\beta}\{(P \cap C) \cdot \mathbf{v}\}\, \mathbf{v}$

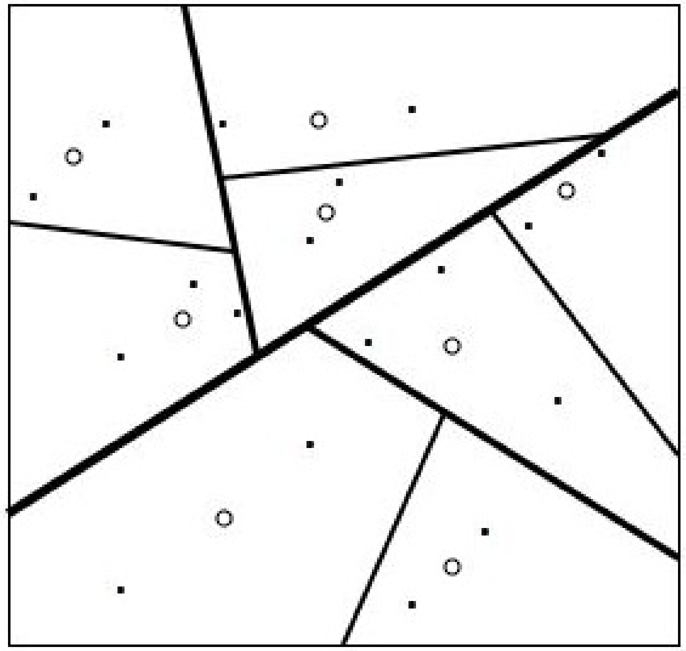
- partition $P \cap C$ by H (as in kd-tree)



at each leaf node, store at most n_0 points



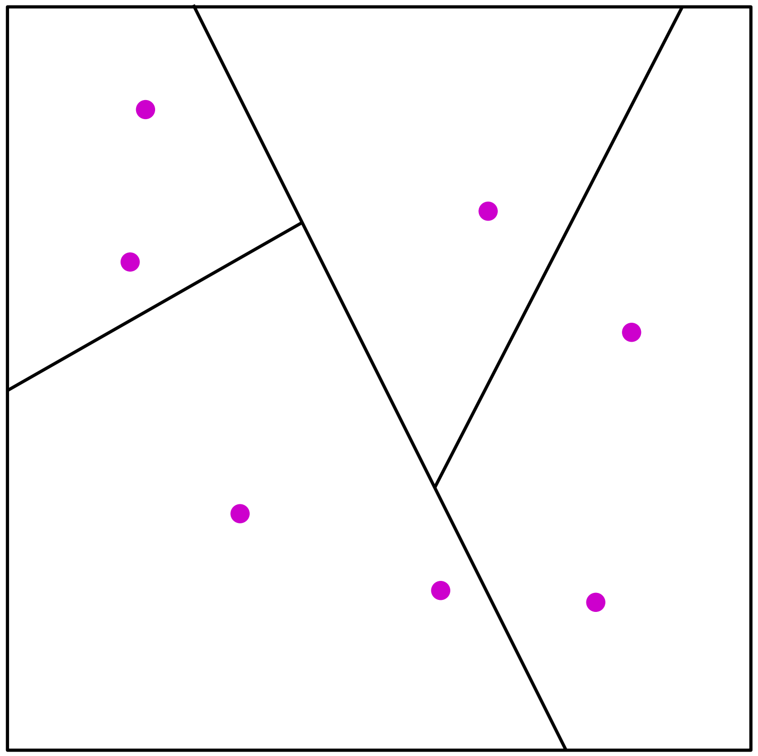
kd-tree



RP-tree

Exploiting randomness: RP-trees

Prop: [Dasgupta, Freund'08]
There is a constant $c > 0$ such that, for any cell C in a RP-tree built on $P \in \mathbb{R}^d$, with probability at least $1/2$ (over the choice of $\mathbf{v}, \beta$) all the cells lying at least $c\,k\log k$ levels below C in the tree have at most half the radius of C, where $k = \dim_2(P \cap C)$.



doubling dimension of $S \subseteq \mathbb{R}^d$: smallest $k \in \mathbb{N}$ such that, for every Euclidean ball B, $B \cap S$ can be covered by 2^k Euclidean balls of half radius.

radius of $S \subseteq \mathbb{R}^d$: smallest $r > 0$ such that $\exists x \in C$ with $B(x, r) \supseteq S$.

Exploiting randomness: RP-trees

Thm: [Dasgupta, Sinha'13]
Suppose $p_1, \cdots, p_n \overset{\text{iid}}{\sim} \mu$ continuous probability measure in $\mathbb{R}^d$ with doubling dimension $k \geq 2$. Then $\exists c_0 > 0$ s.t. for any $q \in \mathbb{R}^d$ and $\delta < 1/e$, with proba. $\geq 1 - 3\delta$ over the choice of the p_i's:

$$\mathbb{P}_{\mathbf{v},\beta}\left[\text{defeatist search does not return } \mathrm{NN}_P(q)\right] \leq c_0(k+\ln n_0)\left(\frac{8\,\ln 1/\delta}{n_0}\right)^{1/k}$$

doubling dimension of μ: smallest $k \in \mathbb{N}$ such that, for every $x \in \mathbb{R}^d$ and every $r > 0$: $\mu(B(x, 2r)) \leq 2^k\,\mu(B(x,r))$.

Exploiting randomness: RP-trees

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$\rightarrow$ take $n_0 \propto (k \ln k)^k \ln 1/\delta$ to make $\mathbb{P}_{\mathbf{v},\beta}[\cdots]$ an arbitrarily small constant

$\rightarrow$ query time: $O(d((k \ln k)^k + \log n))$ $\longleftarrow$ sensitive to intrinsic dimension k; requires to know k

Exploiting randomness: RP-trees

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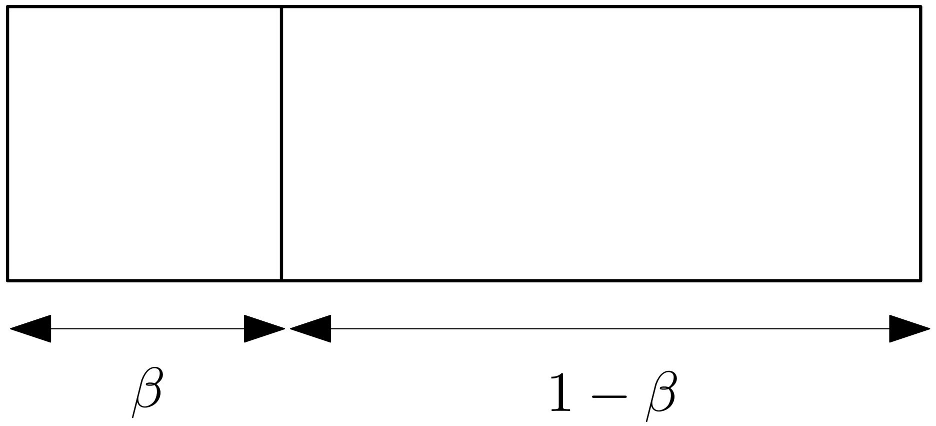
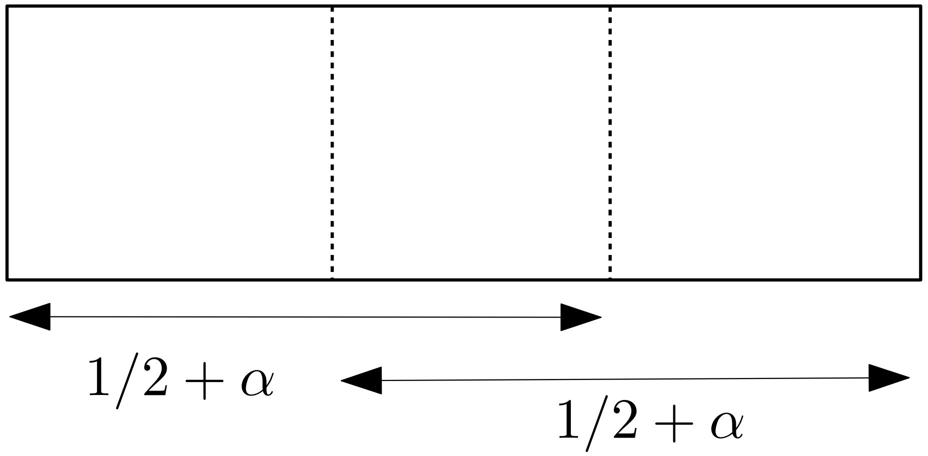
Variant: **spill-trees** (overlapping splits)



(RP-tree)



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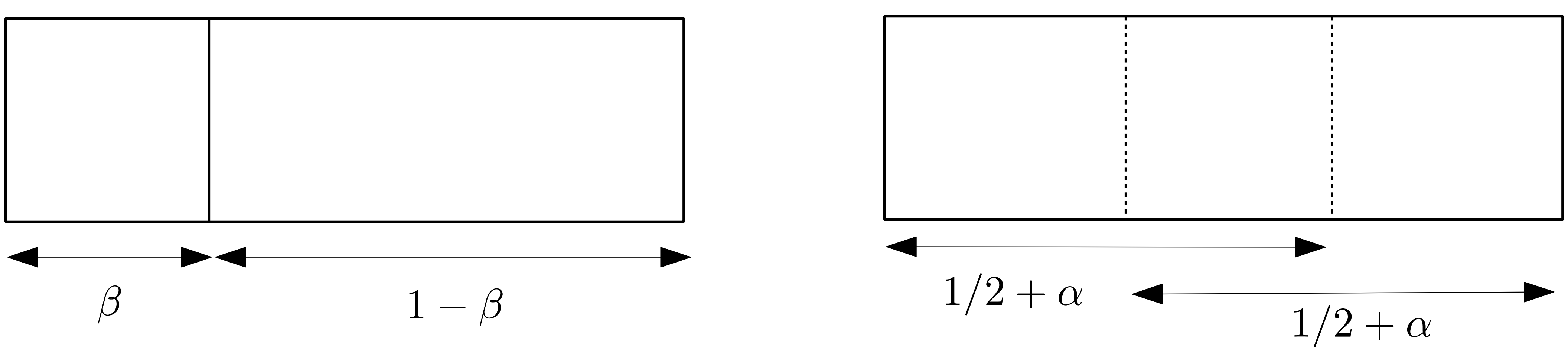
Variant: **spill-trees** (overlapping splits)

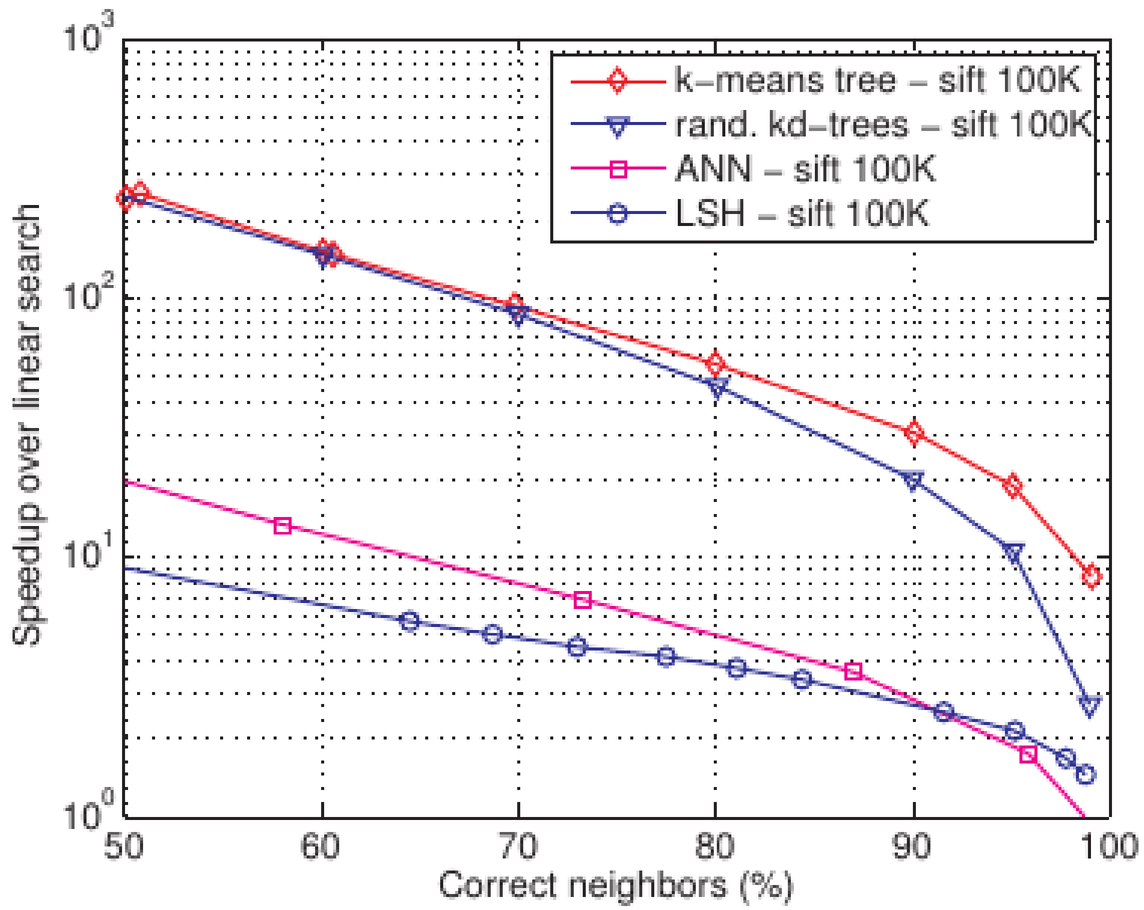
similar behavior



(RP-tree) (spill-tree)

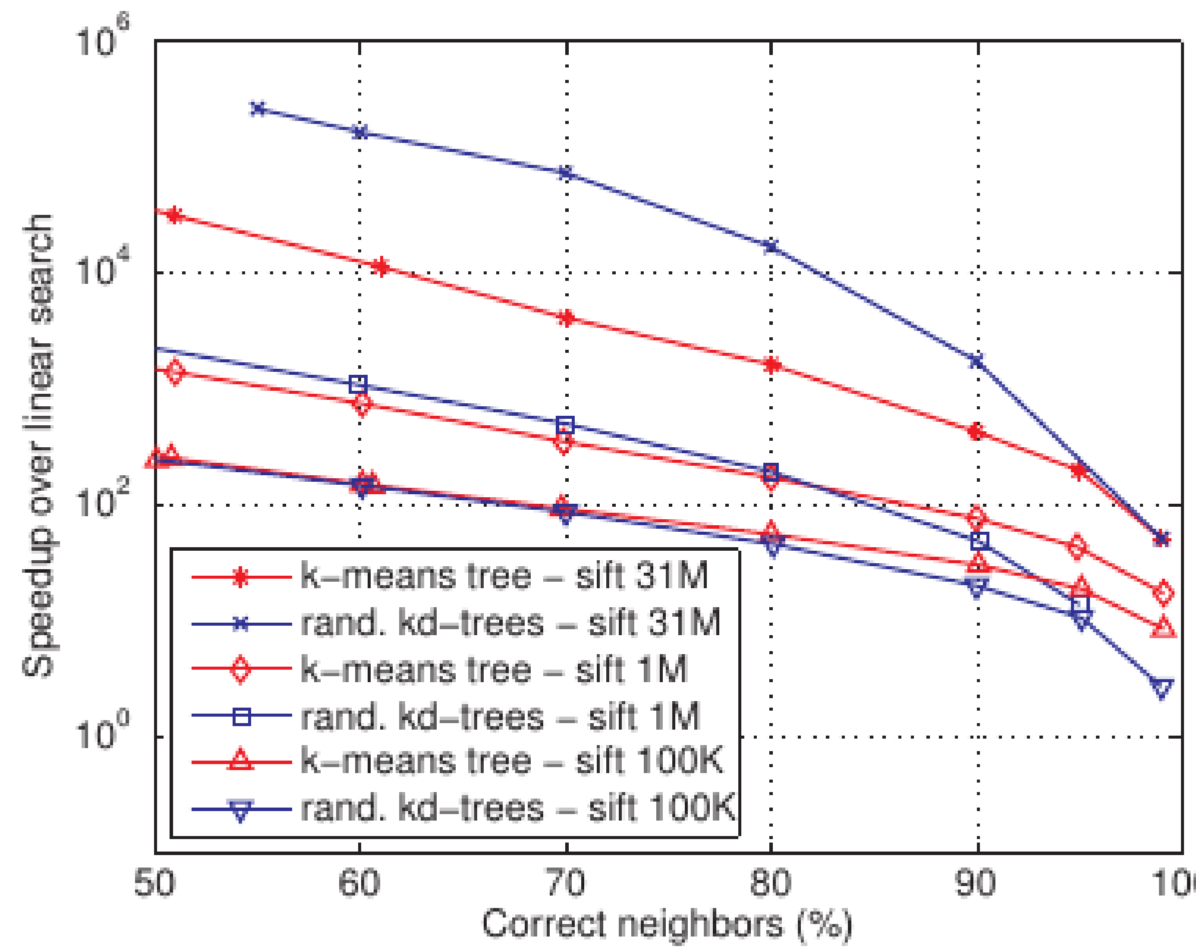
Benchmarking

contenders



(a)

effect of size on winners

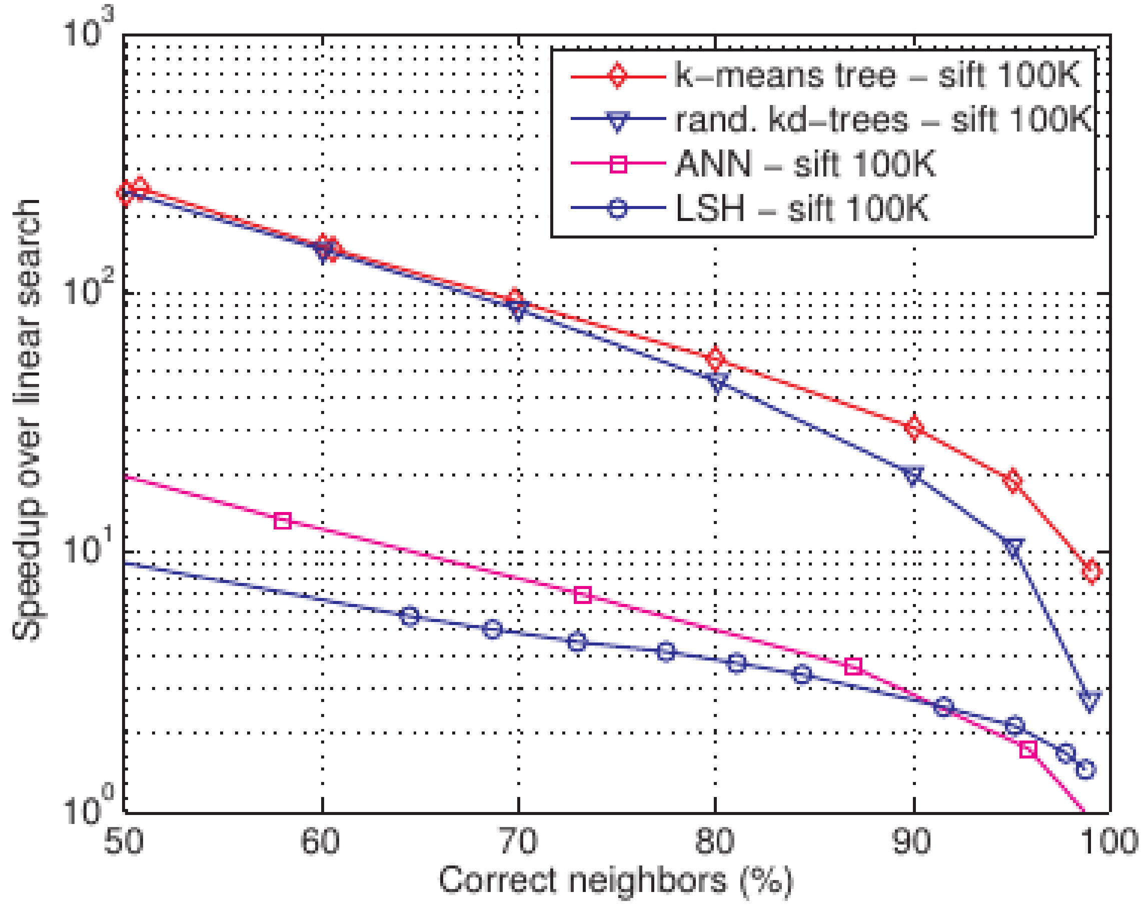


(b)

RP-trees vs. other methods on data sets of 100k, 1M and 31M features

Benchmarking

contenders



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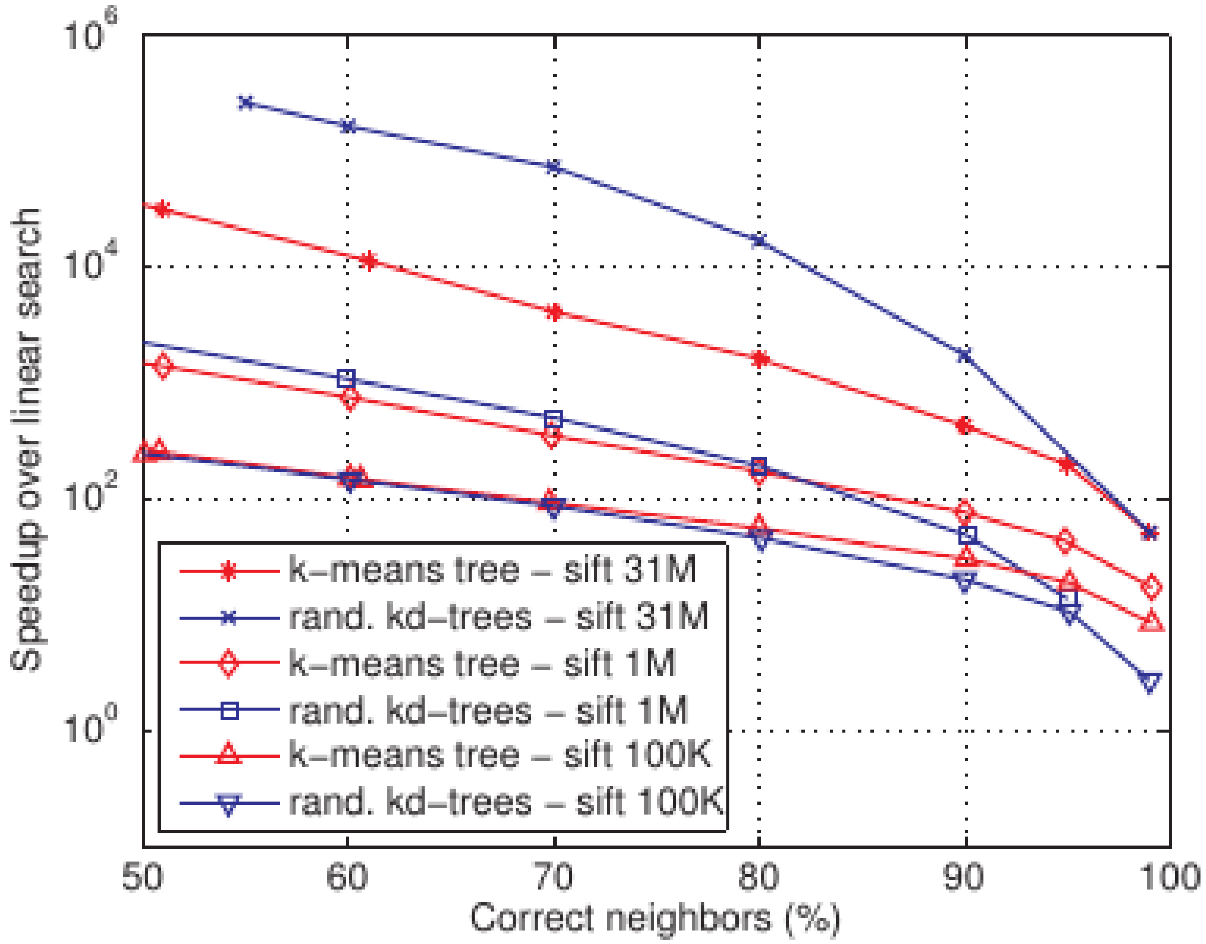
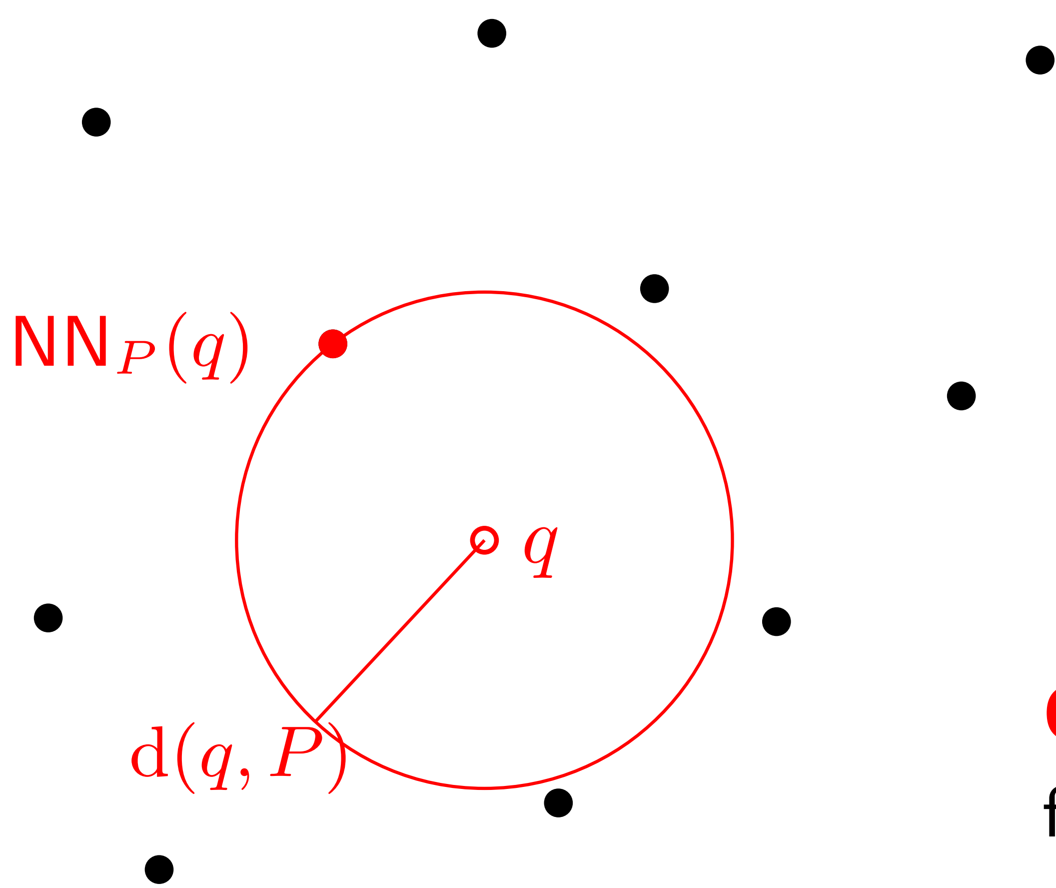


(b)

Random kd-trees (RP-trees, spill-trees) are fast, scalable and reliable on **data with low-dimensional intrinsic structure**

Locality-Sensitive Hashing

Back to the NN problem



pre-processing input: P

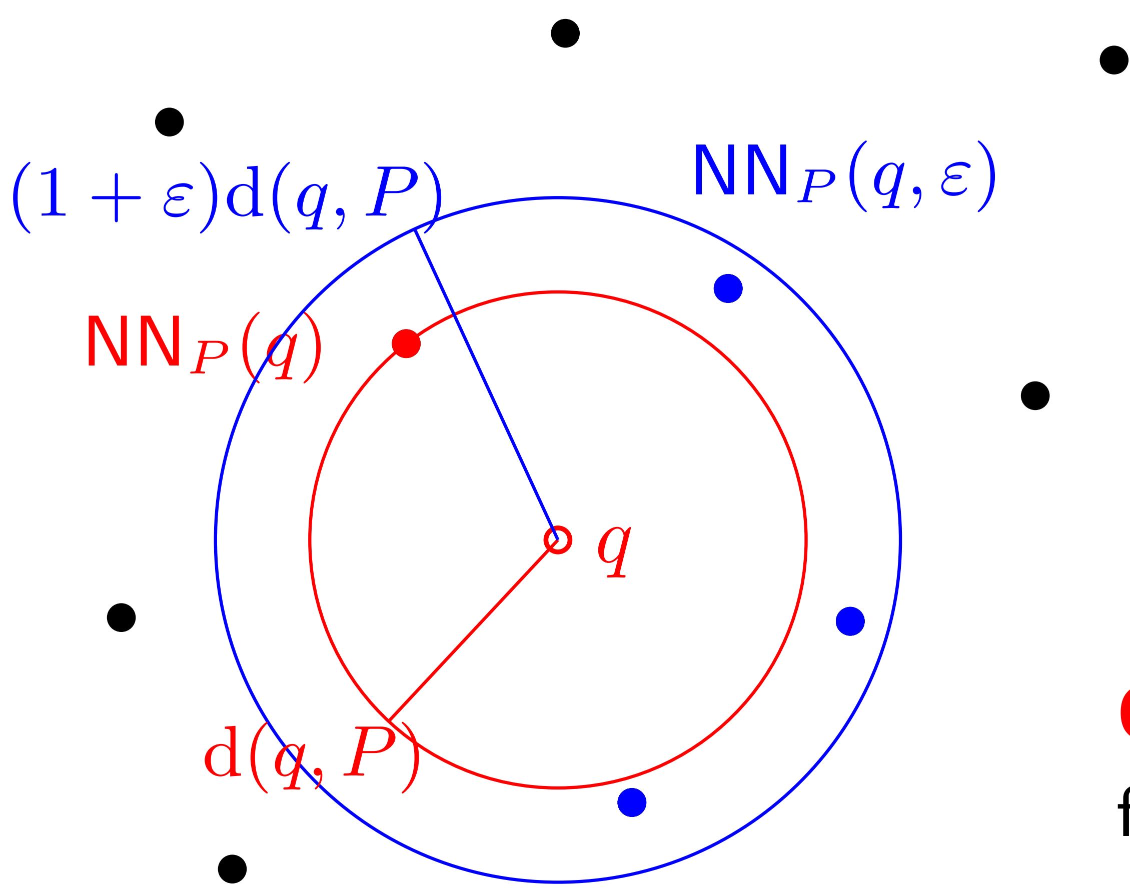
query input: q

goal: find $p \in \mathrm{NN}_P(q)$

Curse of Dimensionality: every DS for NN-search has either exponential size or exponential query time (in d) in the worst case.

$\rightarrow$ holds in theory and in practice for exact NN queries [Weber et al. '98]

Back to the ε-NN problem



pre-processing input: P, ε

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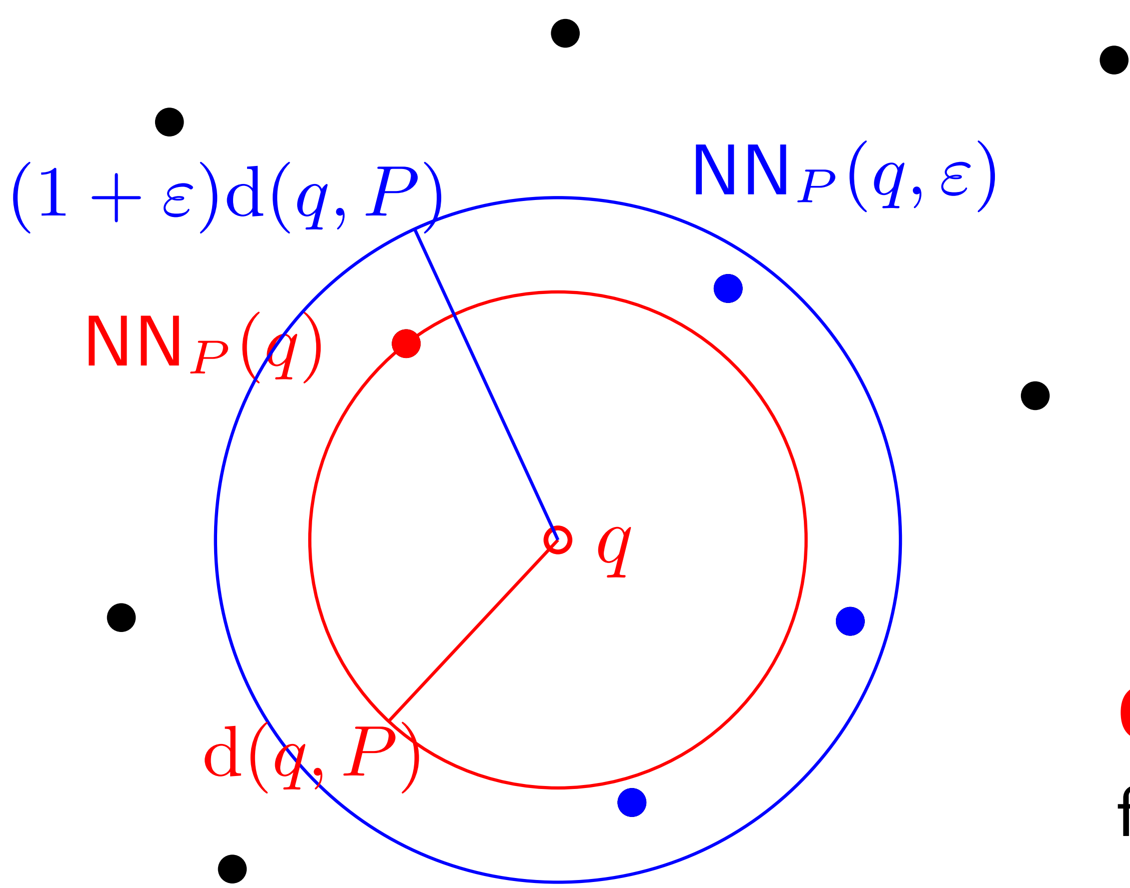

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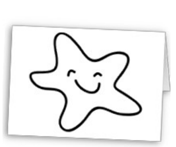


$\rightarrow$ no longer true in Real-RAM model thanks to LSH [Indyk, Motwani '98]

Locality-Sensitive Hashing

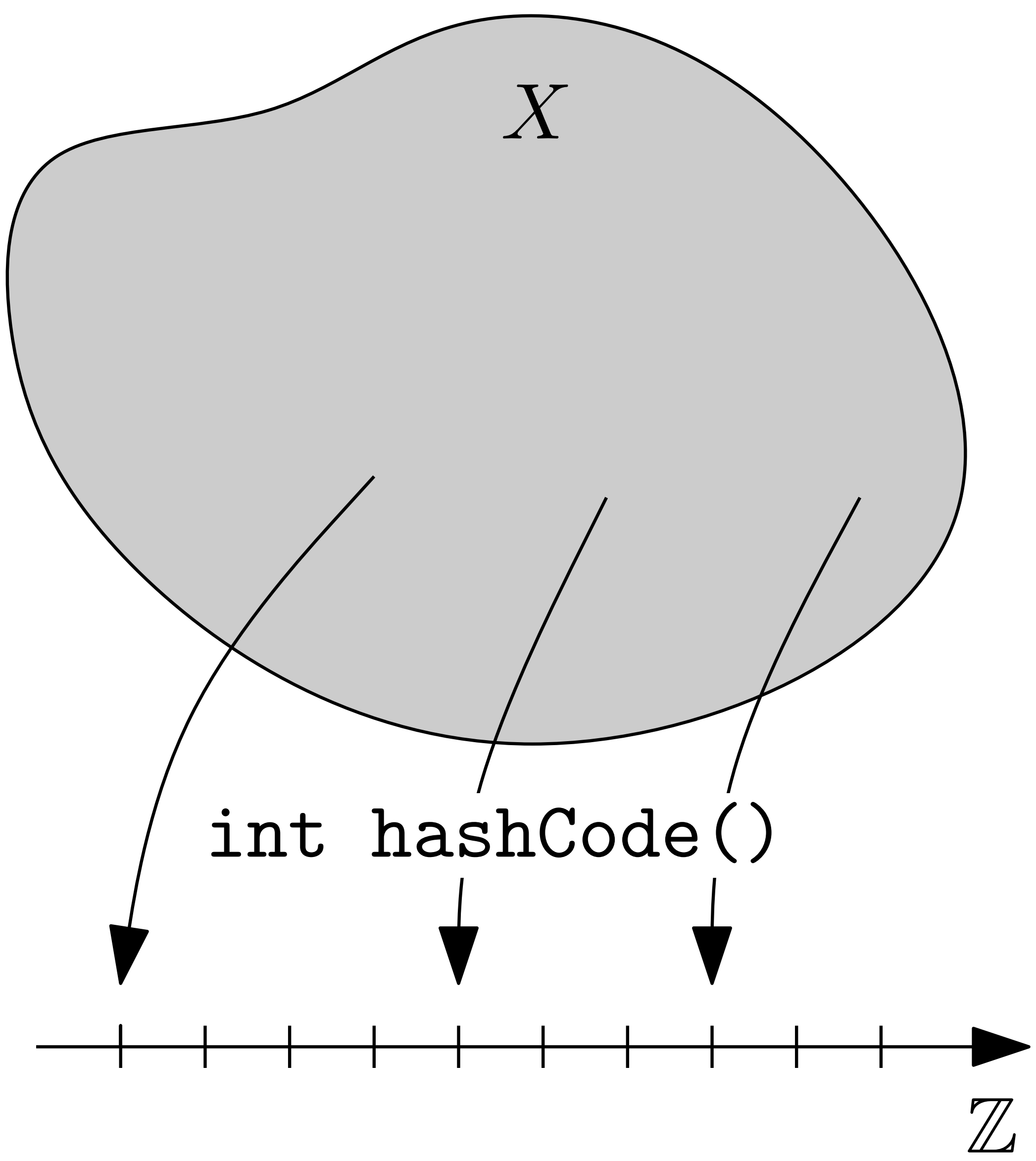
Comparing elements via hashing:

$\texttt{hashCode} : X \to \mathbb{Z}$

$x = y \Rightarrow \texttt{hashCode}(x) = \texttt{hashCode}(y)$

$x \neq y \Rightarrow \texttt{hashCode}(x) \neq \texttt{hashCode}(y)$

(no collisions hypothesis)



Locality-Sensitive Hashing

Comparing elements via hashing:

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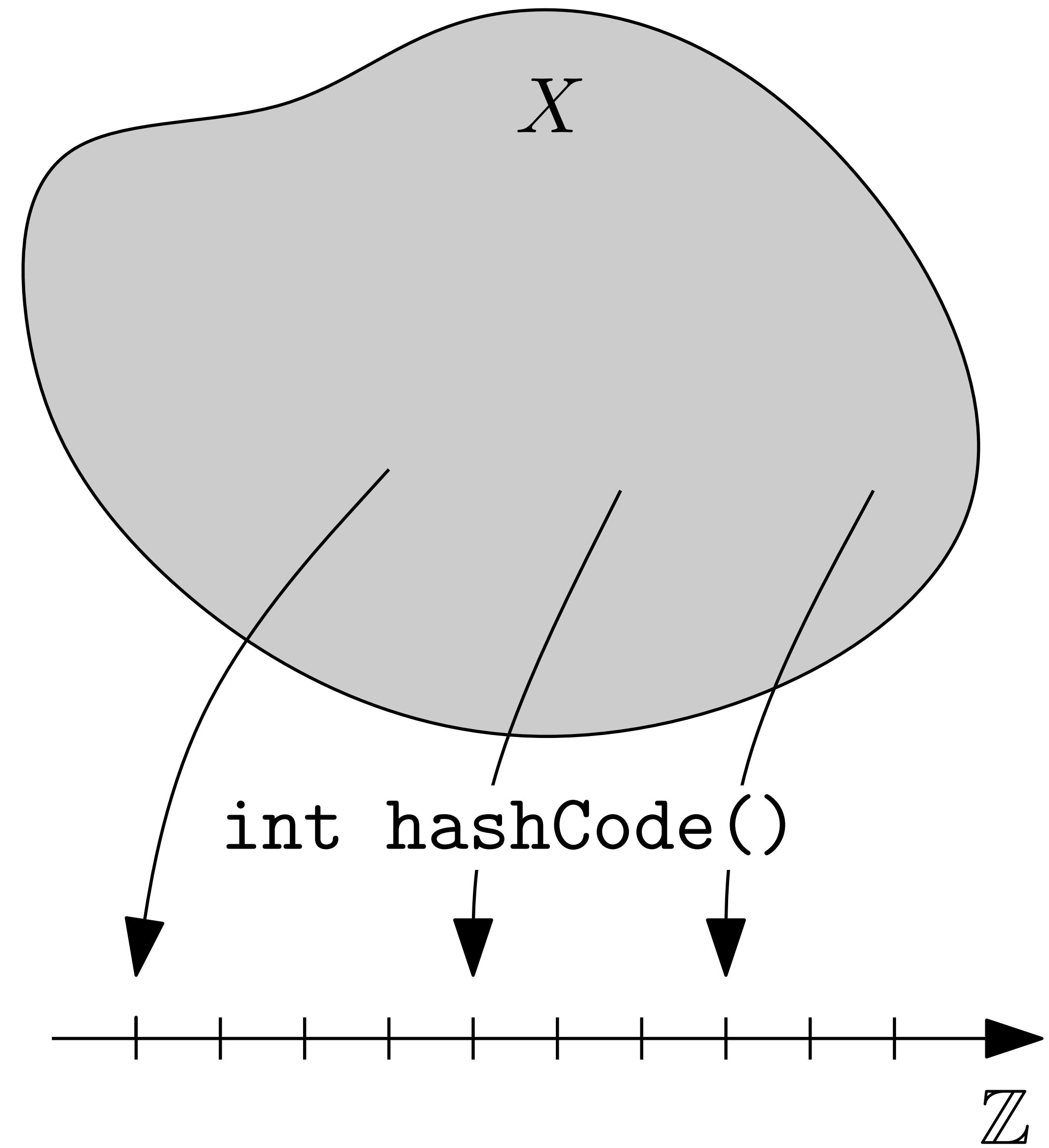

Metric case (X, d): given $r > 0$,

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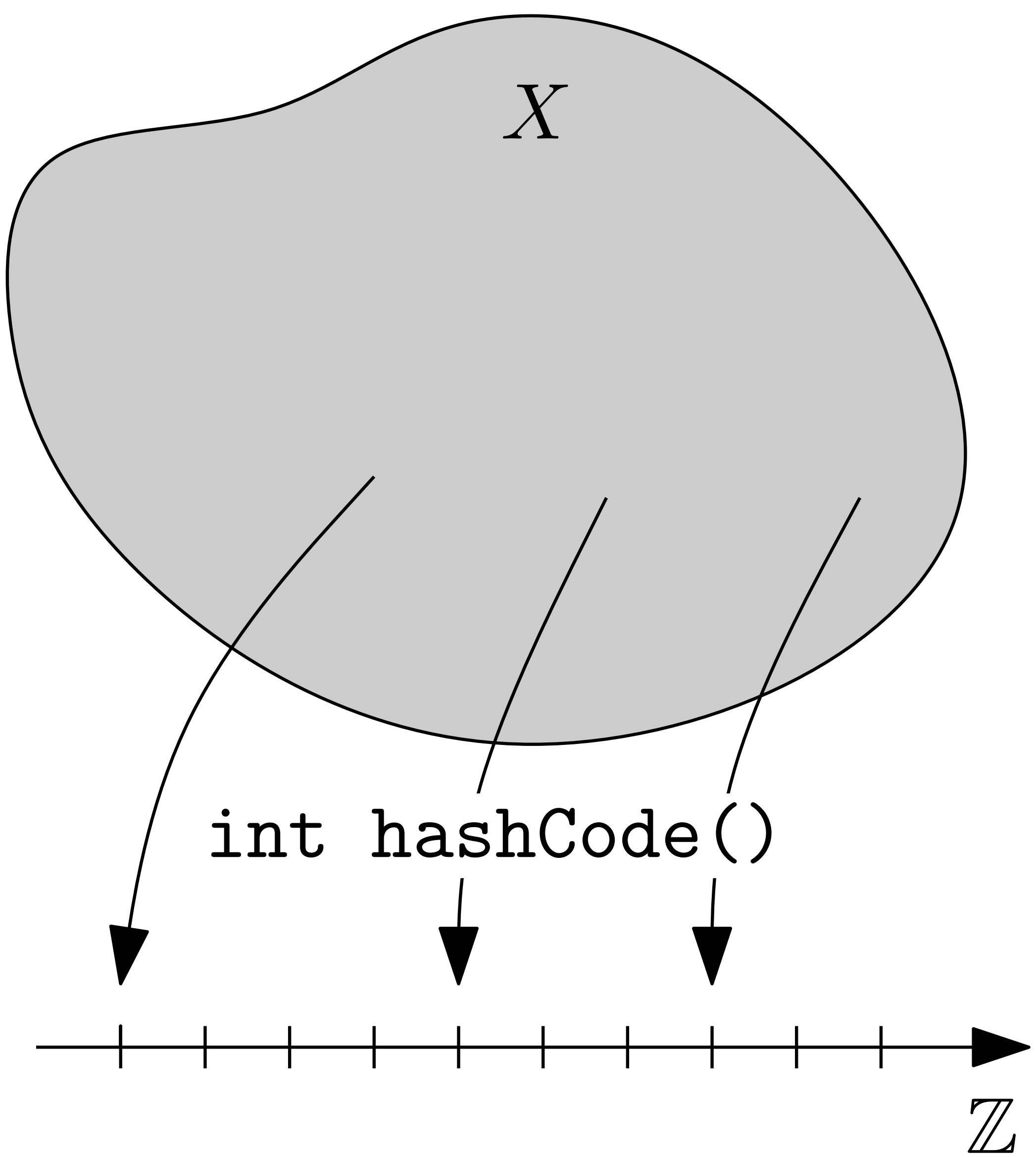

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too good to be true $\to$ allow for some slack

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Def: Given $r_1 < r_2$, $p_1 > p_2$ and $\mathcal{U} \subset \mathbb{N}$, a family $\mathcal{F}$ of hash functions $f : (X, \mathrm{d}) \to \mathcal{U}$ is (r_1, r_2, p_1, p_2)-**sensitive** if $\forall x, y \in X$,

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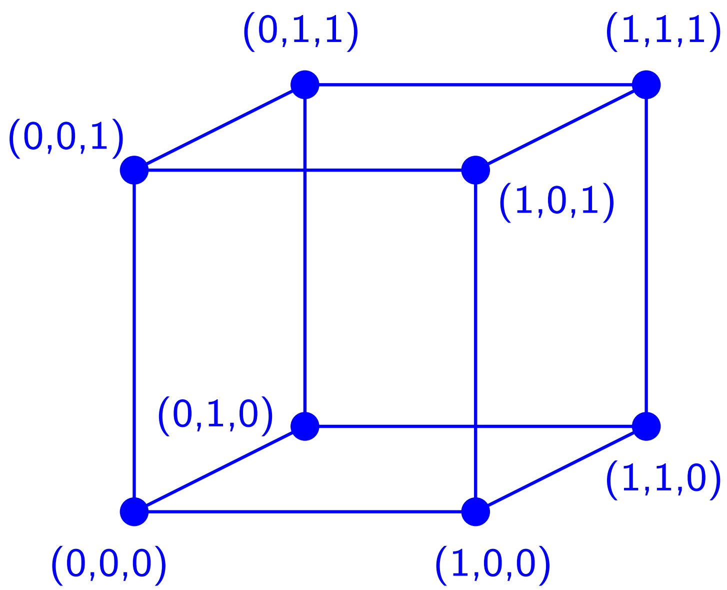

Example 1: $(X, \mathrm{d}) = (\{0,1\}^d, \mathrm{d}_{\mathcal{H}})$

$\to$ take $\mathcal{F} = \{f_i\}_{i=1}^d$ where $f_i(b_1 \cdots b_d) = b_i$ | unif. proba. on $\mathcal{F}$

$\to$ $\mathcal{F}$ is $(r, r(1+\varepsilon), 1 - \frac{r}{d}, 1 - \frac{r(1+\varepsilon)}{d})$-sensitive for all $r \geq 1$ and $\varepsilon \geq 0$.

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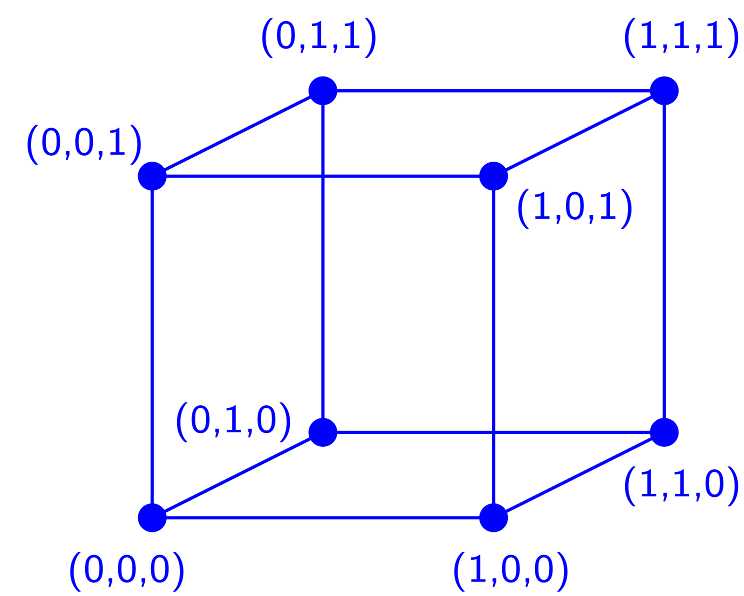

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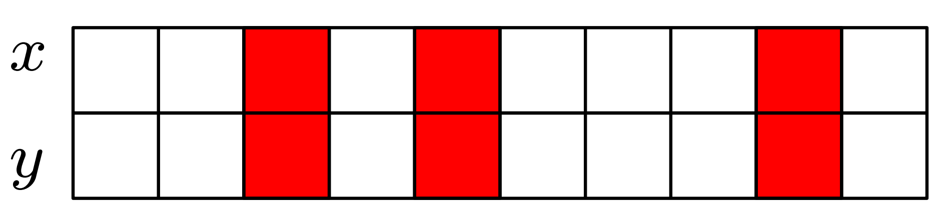
proof: $\forall x, y$, $\mathbb{P}_f[f(x) = f(y)] = \frac{d - \mathrm{d}_{\mathcal{H}}(x,y)}{d} = 1 - \frac{\mathrm{d}_{\mathcal{H}}(x,y)}{d}$



$\mathrm{d}_{\mathcal{H}}(x, y)$ bits differ $\Rightarrow$ $d - \mathrm{d}_{\mathcal{H}}(x, y)$ functions make x and y collide

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Example 2: $(X, \mathrm{d}) = (\mathbb{R}^d, \|\cdot\|_2)$

$\to$ take $\mathcal{F} = \{f_{\mathbf{v},b}\}_{\mathbf{v}\in\mathbb{R}^d}^{b\in[0,r]}$ where $f_{\mathbf{v},b}(x) = \lfloor \frac{x\cdot\mathbf{v}+b}{r} \rfloor$

$\to$ choose $\mathbf{v} = (v_1, \cdots, v_d)$ with $v_i \sim \mathcal{N}(0, 1)$, and b uniformly in $[0, r]$

$\to$ $\mathcal{F}$ is $(r, r(1+\varepsilon), p_1, p_2)$ sensitive for $p_1 = g(1)$ and $p_2 = g(1+\varepsilon)$,

where $g(\kappa) = 1 - 2\mathrm{cdf}(-r/\kappa) - \frac{2}{\sqrt{2\pi}r/\kappa}(1 - e^{-r^2/2\kappa^2})$

cumulative density func. of normal distrib.

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Lemma [Johnson, Lindenstrauss 84]:

For any dimensions $0 < k < d$ there is a probability distribution μ over the projections $\mathbb{R}^d \to \mathbb{R}^k$ such that, given any set P of n points in $\mathbb{R}^d$ and any $\varepsilon \in (0, 1)$ with $k > 10 \ln n / \varepsilon^2$, a projection $\pi : \mathbb{R}^d \to \mathbb{R}^k$ sampled at random from μ satisfies w.h.p.

$$\forall p, q \in P,\ (1 - \varepsilon)\|p - q\| \leq \|\pi(p) - \pi(q)\| \leq (1 + \varepsilon)\|p - q\|$$

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$\to$ **General idea:**

- choose k-dimensional vector of random functions $(f_1, \cdots, f_k) \in \mathcal{F}^k$
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- given $q \in X$, hash q and choose collision with smallest distance

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Technical detail: family works only for fixed r_1, r_2

$\rightarrow$ fix $r_1 = r$ and $r_2 = r(1 + \varepsilon)$, and solve (r, ε)-NN query

The (r, ε)-NN problem (PLEB)

Goal: pre-process P such that, for any query point q,

- if $\mathrm{d}(q, P) \leq r$ then answer YES and return some $p \in \mathrm{NN}_P(q, r, \varepsilon)$,
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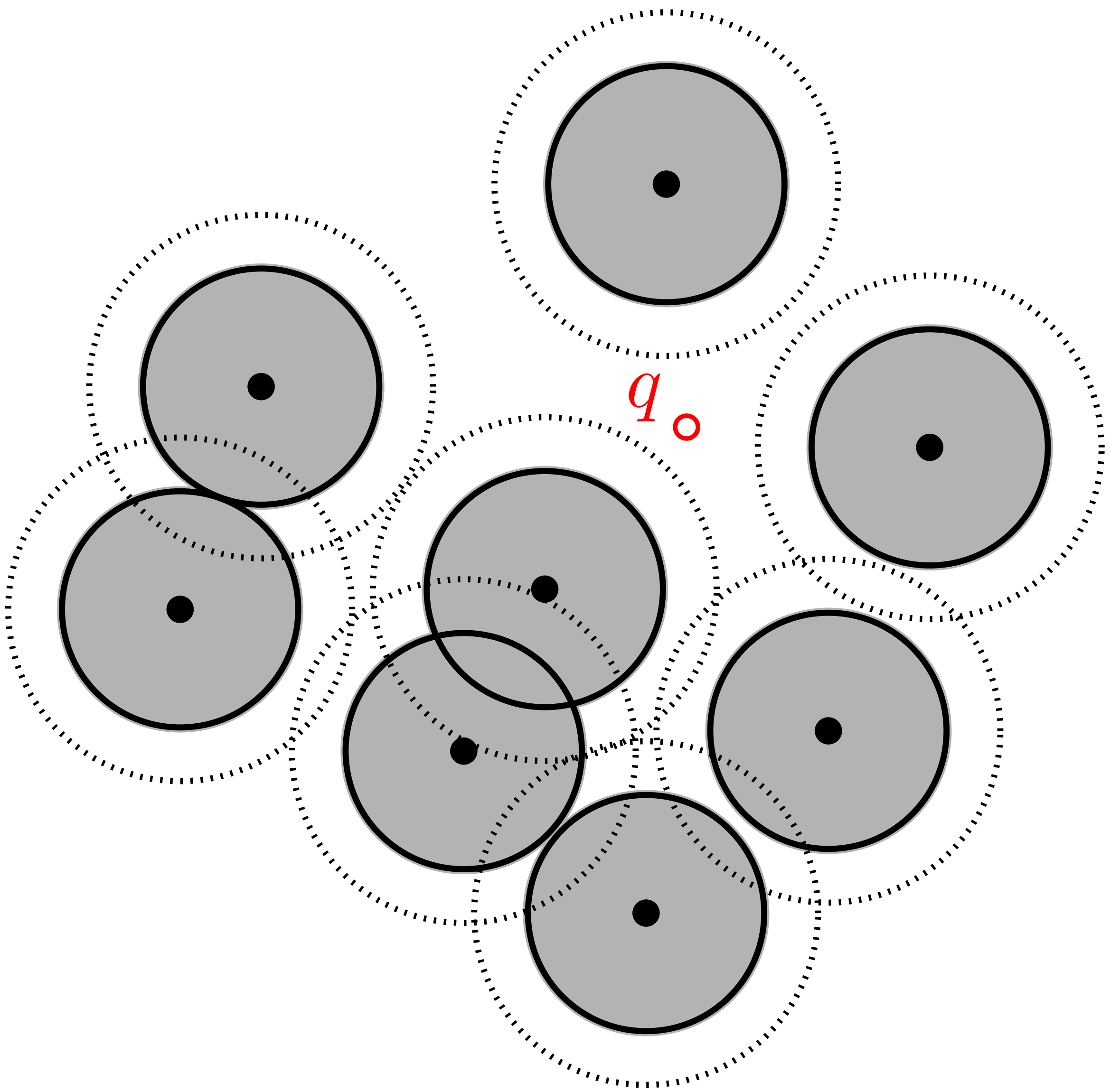

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Step 1: boost the sensitivity of the hash family

$\mathcal{G} = \{g = (f_1, \cdots, f_k) \in \mathcal{F}^k \mid f_1, \cdots, f_k$ chosen randomly in $\mathcal{F}\}$

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$\rightarrow \forall x, y$, $\mathrm{d}(x, y) \leq r \Rightarrow \mathbb{P}[g(x) = g(y)] \geq p_1^k$ (coords. are independent)

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Step 2: pre-process the data points

- choose τ random functions $g_1, \cdots, g_\tau$ from boosted hash family $\mathcal{G}$,

- initialise τ hash tables $H_1, \cdots, H_\tau$

- $\forall i = 1, \cdots, \tau$, hash every point $p \in P$ into H_i using $g_i(p)$ as the key

- use chaining to store the points in the same entry of H_i

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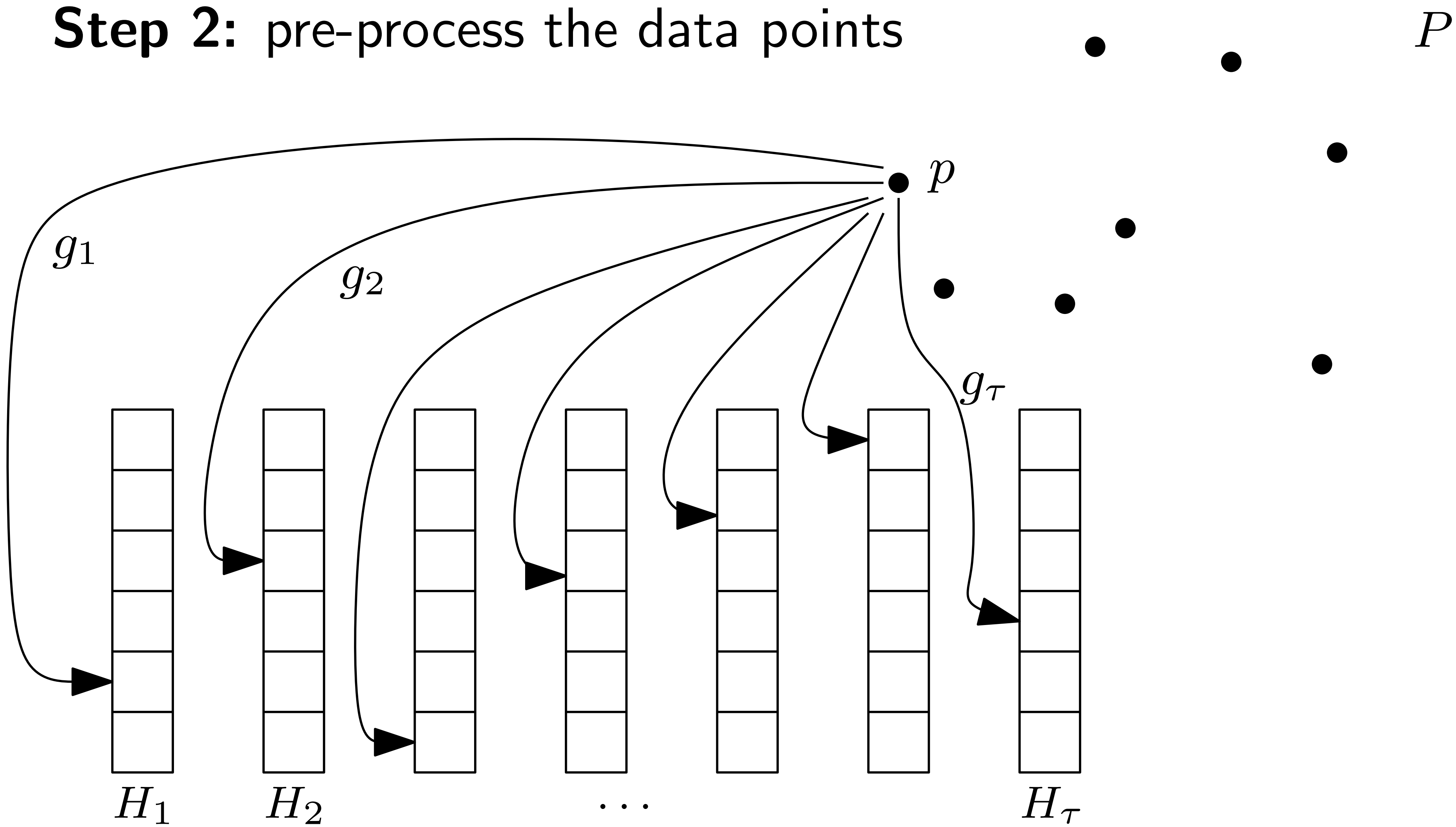

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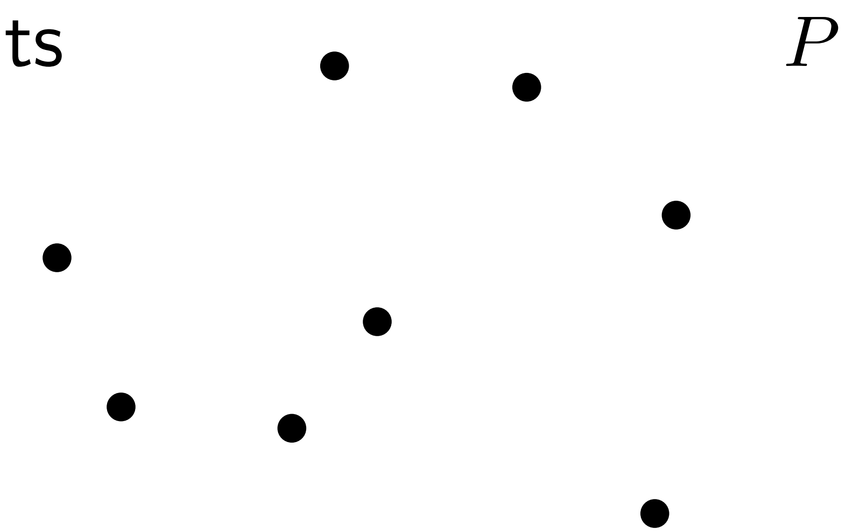

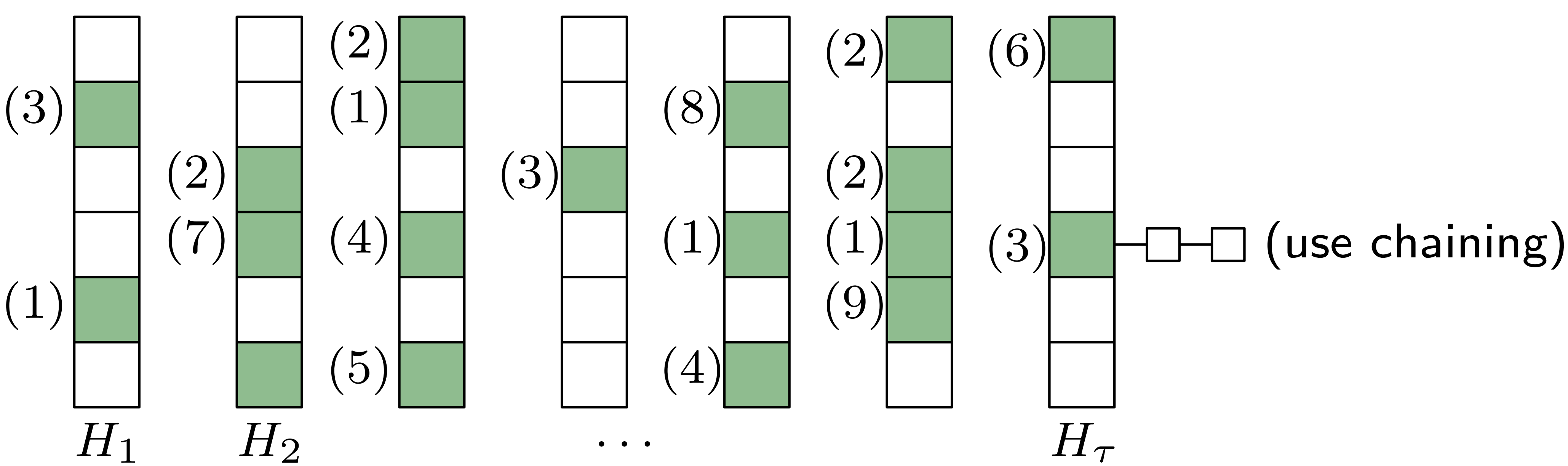

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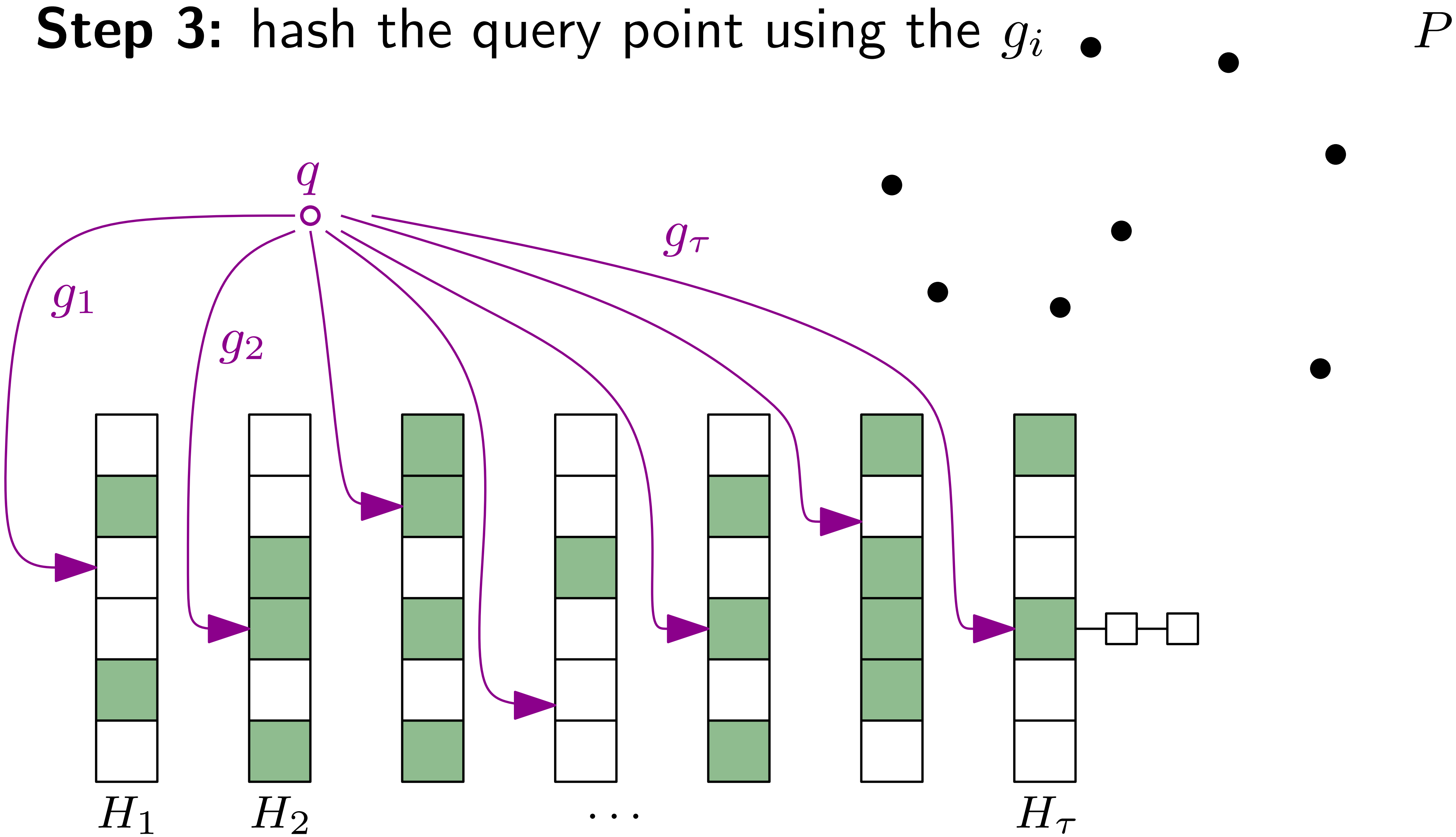

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if there are more than 2τ collisions **then** return NO

else let $p_1, \cdots, p_l$ be the collisions ($l \leq 2\tau$):

  if some p_j is such that $\mathrm{d}(p_j, q) \leq r(1+\varepsilon)$ **then** return YES and p_j

  else return NO

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    $\Rightarrow \mathbb{P}[p$ collides with q in H_i for at least one $i] \geq 1 - \left(1 - p_1^k\right)^\tau$

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▶ in Hamming cube: let $k := \log_{1/p_2} n \leq \frac{d}{1+\varepsilon} \ln n$ and $\tau := n^{\ln p_1 / \ln p_2} \leq n^{1/1+\varepsilon}$:

Pr[success] $\geq \frac{1}{2} - \frac{1}{e}$

query time in $O(\tau(k+d)) \subseteq O\left(\frac{d}{1+\varepsilon} n^{1/1+\varepsilon} \ln n\right)$

$\Rightarrow\;$ $\mathbb{P}$[answer is YES] $\geq 1 - \left(1 - p_1^k\right)^\tau - \frac{n p_2^k}{2}$ (union bound)

From (r, ε)-NN to ε-NN

- Hamming cube $(X, \mathrm{d}) = (\{0,1\}^d, \mathrm{d}_{\mathcal{H}})$

  Observation: inter-point distances lie within $\{0, 1, 2, \cdots, d\}$

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$\rightarrow$ solve case $\mathrm{d}_{\mathcal{H}}(q, P) = 0$ independently (use lexicographical sorting)

$\rightarrow$ take geometric sequence $r_0 = 1$, $r_1 = 1 + \varepsilon$, $\cdots$, $r_j = (1+\varepsilon)^j$, $\cdots$

$\rightarrow$ for $j = 0$ to $\lceil \log_{1+\varepsilon} d \rceil = O(\frac{1}{\varepsilon} \log d)$, solve (r_j, r_{j+1})-NN query

$\rightarrow$ let j_l be the lowest j s.t. the answer to (r_j, r_{j+1})-MM query is YES

$\rightarrow$ return r_{j_l} and the output point of the (r_{j_l}, r_{j_l+1})-NN query

$\rightarrow$ if no YES answer, return d and any point of P

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  Observation: deterministically, $r_{j_l} \geq \mathrm{d}_{\mathcal{H}}(q,P)/(1+\varepsilon)$

  $\Rightarrow$ output $\in NN_P(q, \varepsilon(2+\varepsilon))$ iff LSH data structure works for $j = j_l$

  $\Rightarrow \mathbb{P}[\textit{success}] \geq \frac{1}{2} - \frac{1}{e}$

From (r, ε)-NN to ε-NN

- General case: use **hierarchical clustering tree** [Har-Peled'01]
  - consider geometric sequences of scales as before
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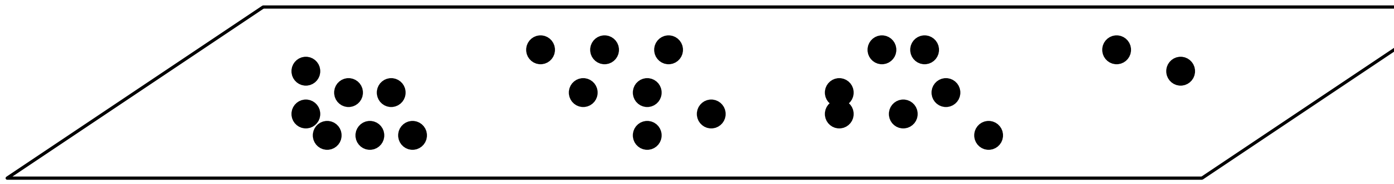

From (r, ε)-NN to ε-NN

- General case: use **hierarchical clustering tree** [Har-Peled'01]
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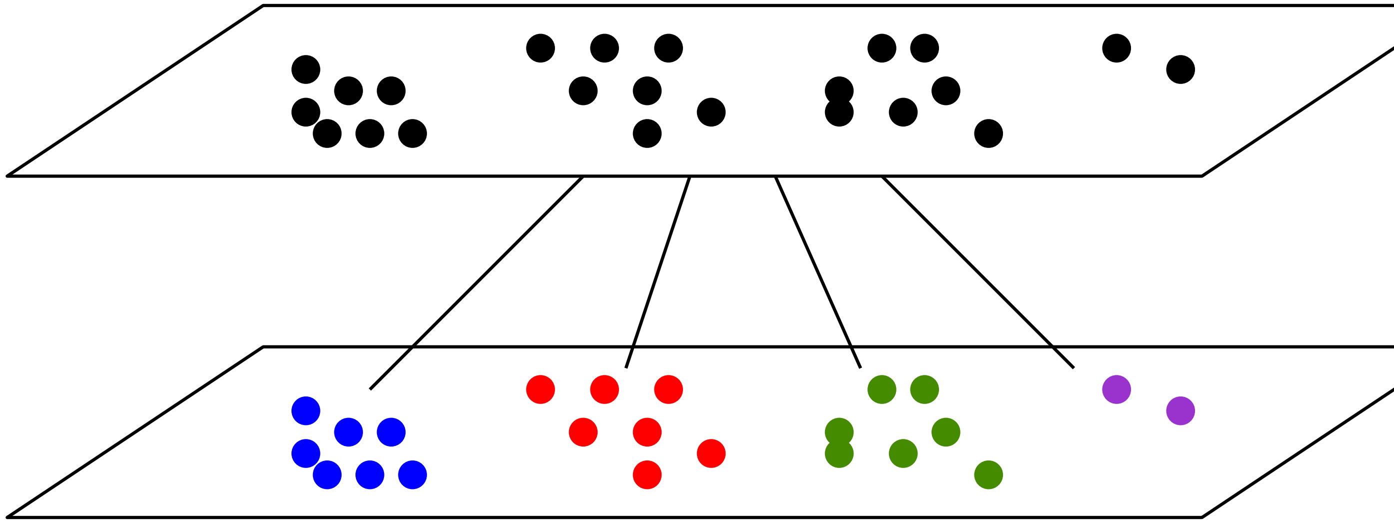

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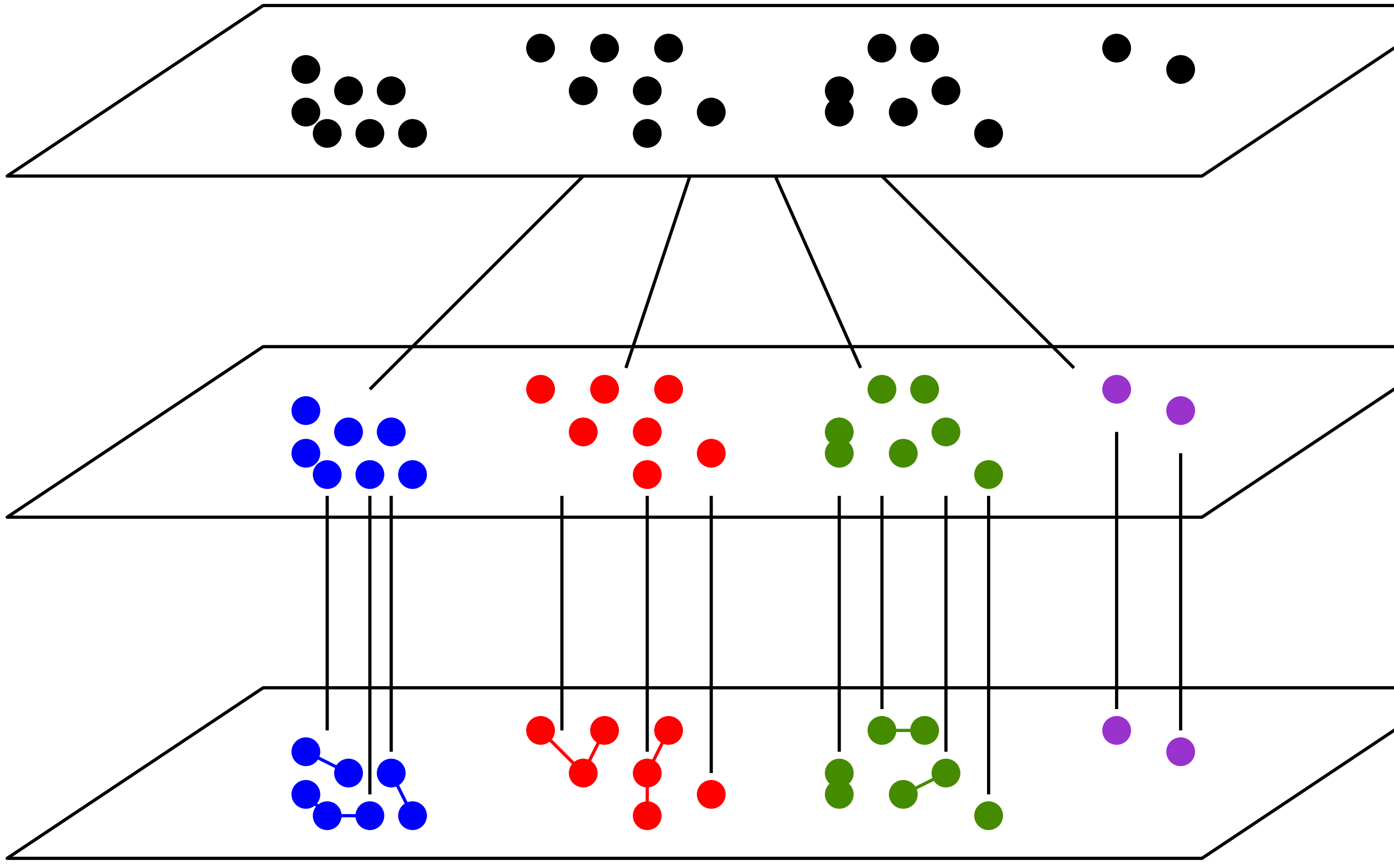
Assign $P_v \subseteq P$ and $[r_v, R_v]$ to each node v



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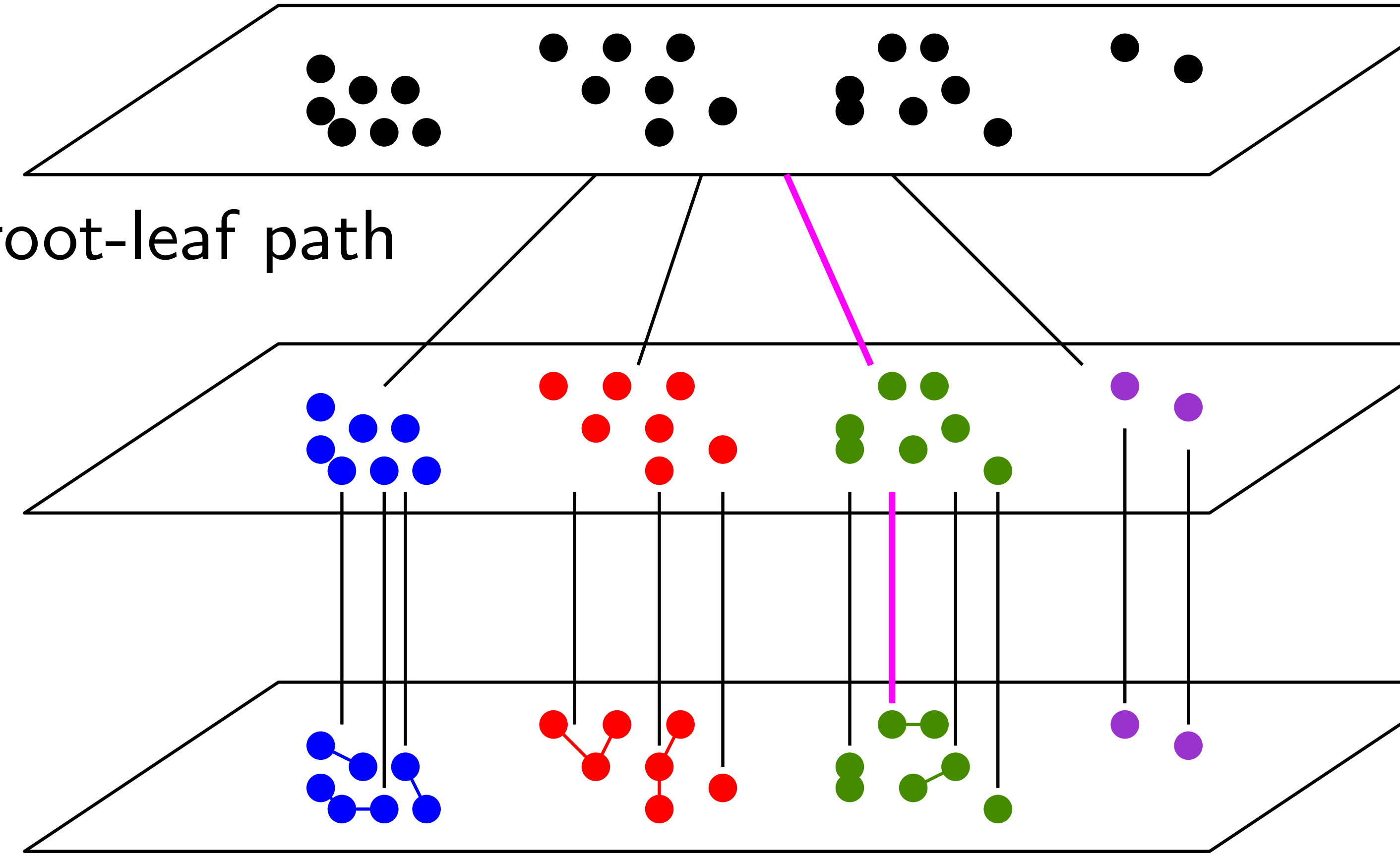
- traverse down the tree along one root-leaf path



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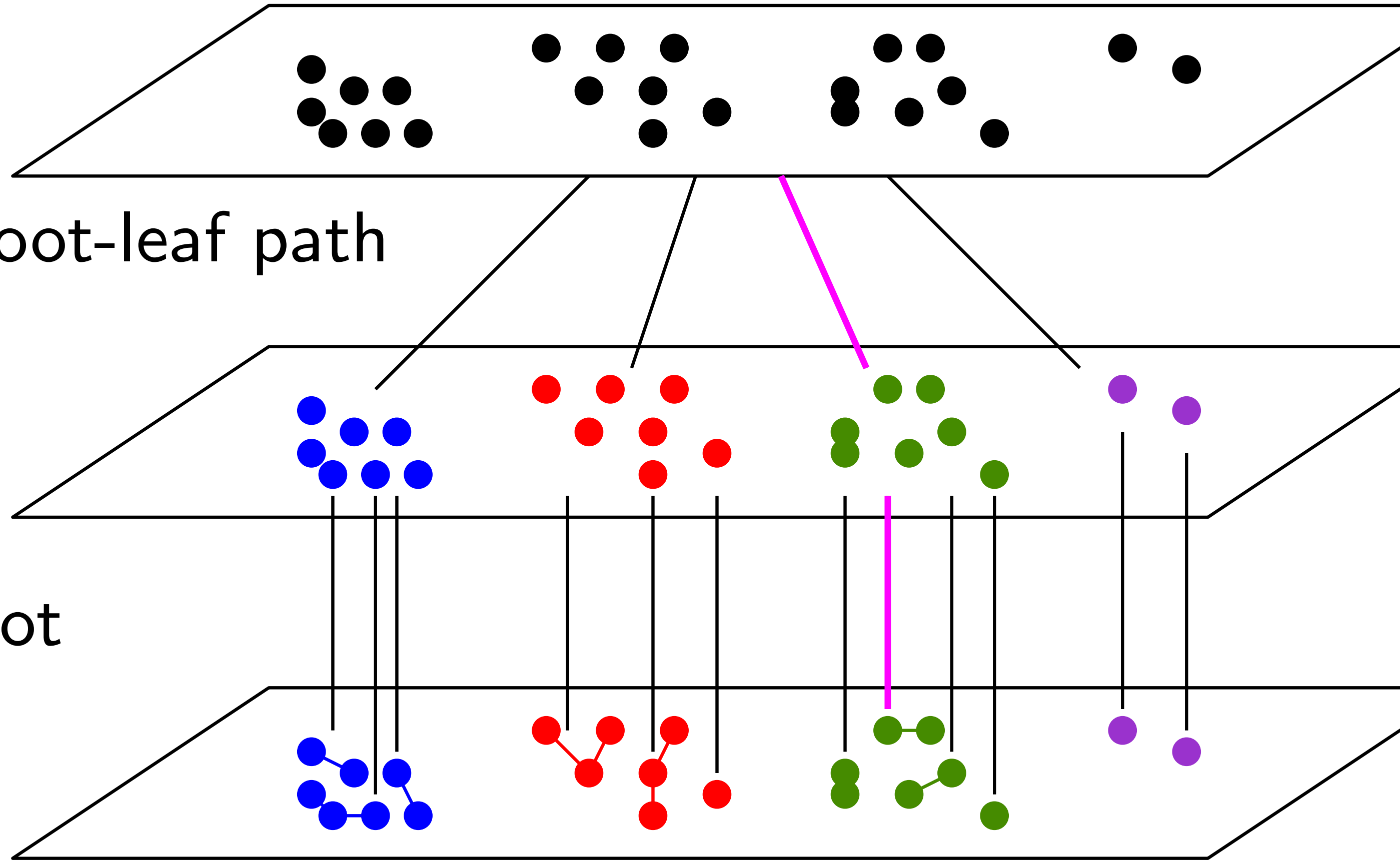
ε-NN query:

- traverse down the tree along one root-leaf path
- at each visited node v, perform

  (r_v, ε)-NN and (R_v, ε)-NN queries

  $\rightarrow$ decide if $\mathrm{d}(q, P) \in [r_v, R_v]$ or not



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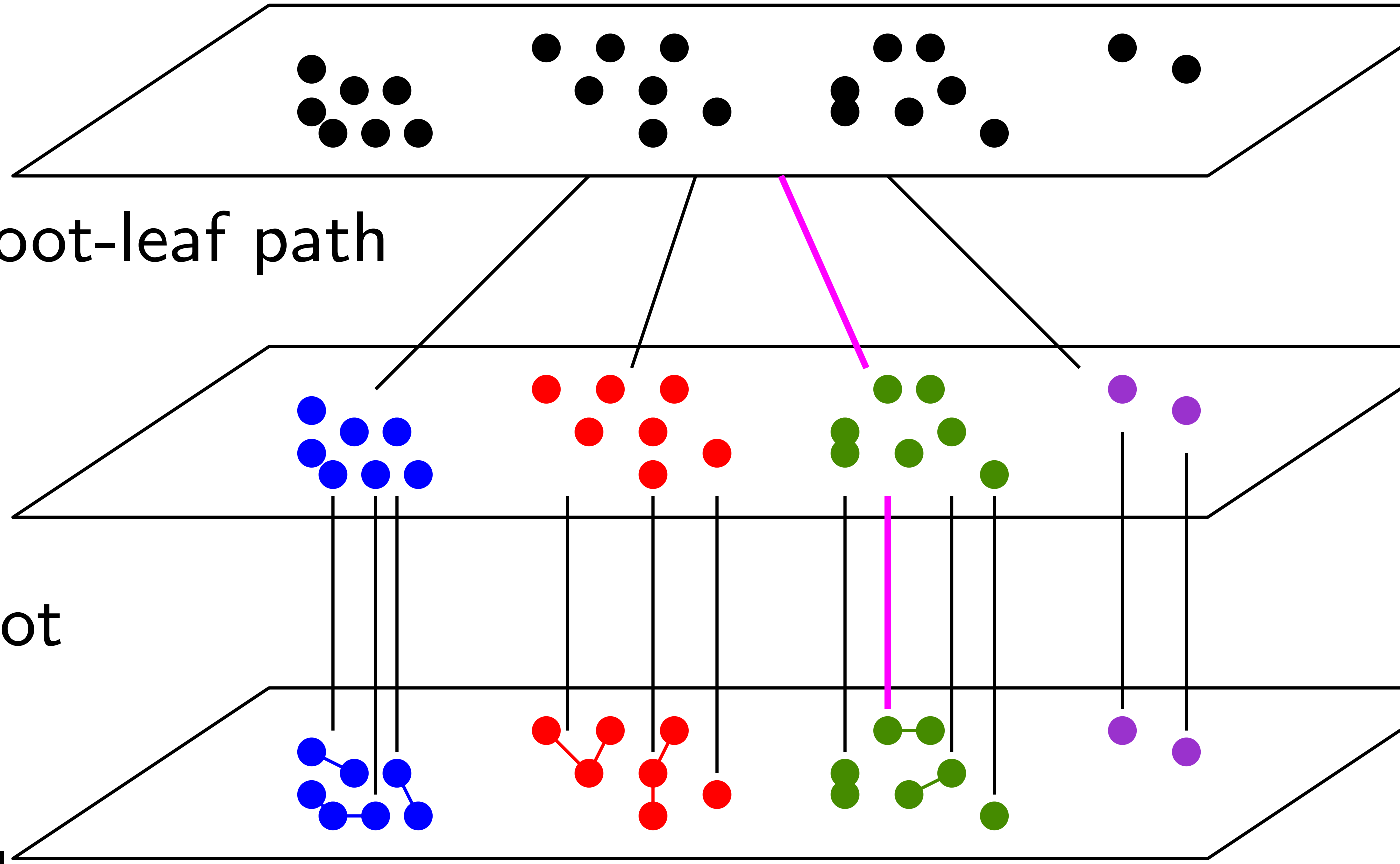
  $\rightarrow$ decide if $\mathrm{d}(q, P) \in [r_v, R_v]$ or not
  $\rightarrow$ if so, locate $\mathrm{d}(q, P)$ in $[r_v, R_v]$
  $\rightarrow$ if not, recurse into one child only



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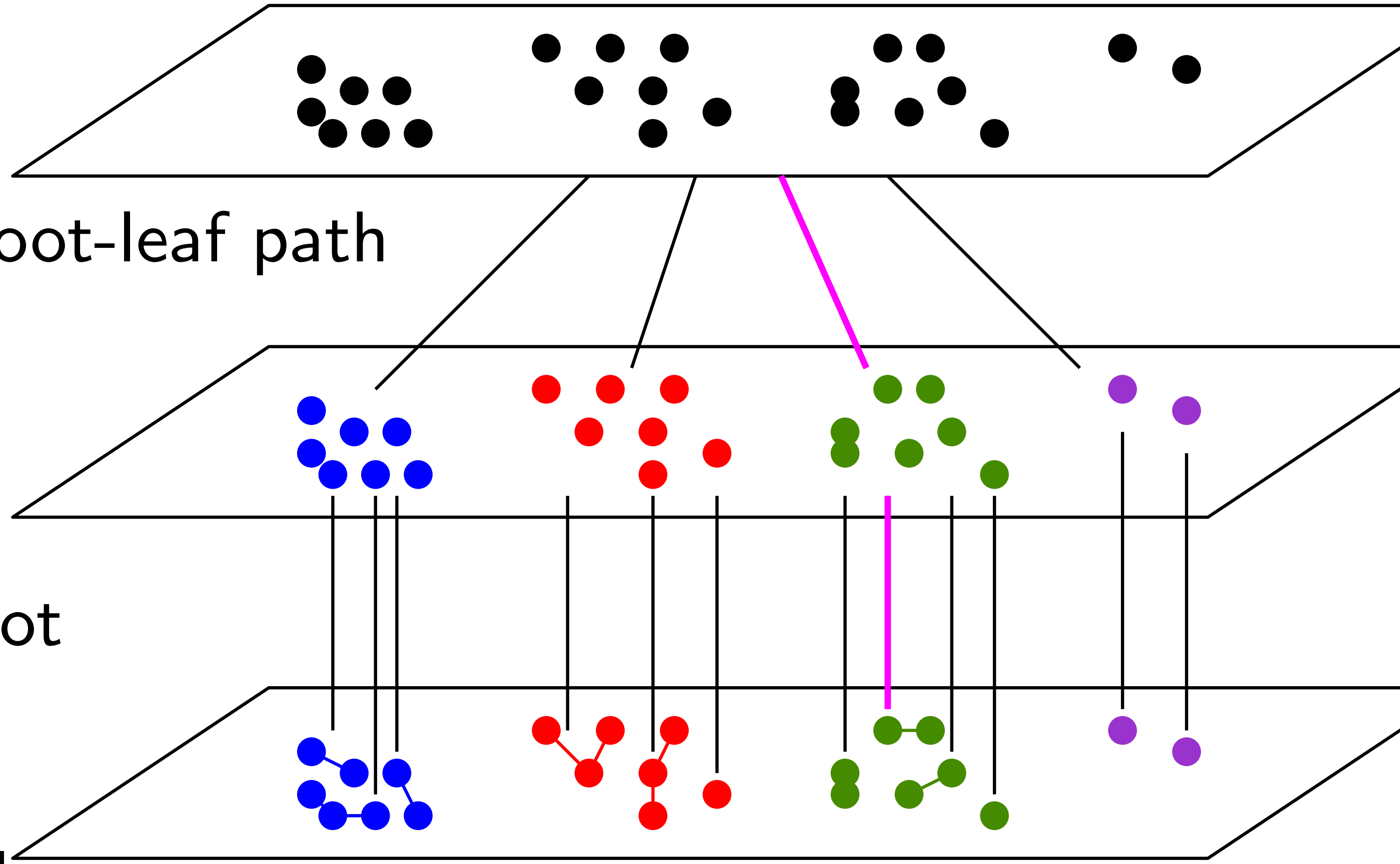

$O(\frac{1}{\varepsilon} \log \frac{n}{\varepsilon})$ (r, ε)-NN queries per ε-NN query

Take-Home Messages

- (Approximate) NN search requires an exponential amount of resources (space/time) in the algebraic comparison tree model [Arya et al. 98].

- Using random hashing allows to beat the *curse of dimensionality*.

- The price to pay is that algorithms become almost linear
$\rightarrow$ in practice, a trade-off must be found.

- The complexity of the exact NN search problem is not fully understood.

$\rightarrow$ what about *reverse* NN search? [Cheong et al. 09], [Arthur, O. 10], ...