A Unified Approach to Proximity Search Through Delone Sets

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Proximity Searching: Applications

Proximity searching:

A set of related geometric retrieval problems that involve finding the objects close to a given query object.

- Pattern recognition and classification
- Object recognition in images
- Content-based retrieval:
  - Shape matching
  - Image/Document retrieval
  - Biometric identification (face/fingerprint/voice recognition)
- Clustering and phylogeny
- Data compression (vector quantization)
- Physical simulation (collision detection and response)
- Computer graphics: photon mapping and point-based modeling

. . . and many more

Nearest Neighbor Searching

Nearest Neighbor Searching

Preprocess a point set $P \subset \mathbb{R}^d$, so that given any query point $q \in \mathbb{R}^d$, can efficiently find its closest point in P.

Assumptions:

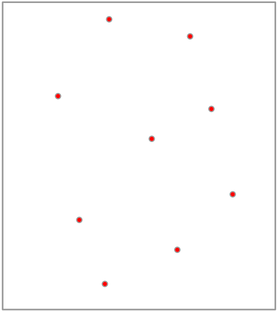
- Real d-dimensional space
- Assume Euclidean distance
- Dimension is a constant (e.g., $d \leq 20$)

Nearest Neighbor Searching - Exact?

Ideal: $O(n)$ space and $O(\log n)$ query time

Voronoi Diagrams

- Subdivide space into regions according to which point is closest
- Apply point location to answer queries



- In $\mathbb{R}^2$: $O(n)$ space and $O(\log n)$ time
- No good solutions higher dimensions
- Curse of dimensionality

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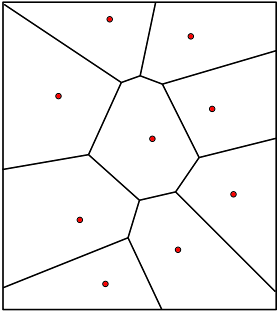

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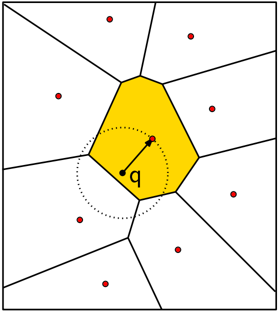

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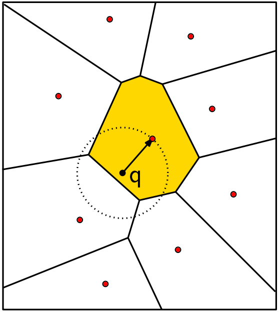

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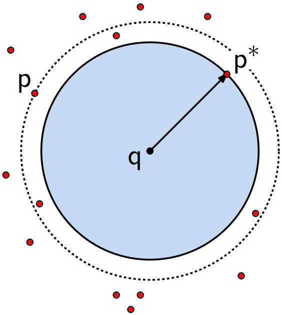
Nearest Neighbor Searching - Approximate ..

Approximate Nearest Neighbor (ANN)

Given a query point q, whose true nearest neighbor is p^*, return any point $p \in P$, such that

$$\mathrm{dist}(q, p) \;\leq\; (1 + \varepsilon) \cdot \mathrm{dist}(q, p^*)$$



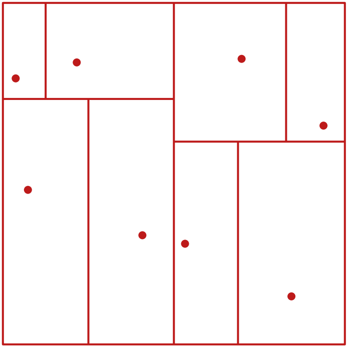
Brief Survey

- Logarithmic query times, exponential dependencies on d
  - Trees (e.g., k-d trees, BBD, AVD)
  - Grids (e.g., bucketing, shifted/rotated, DVD)
  - Algebraic (Chebyshev polymonials)
- Sublinear query times, near-linear storage, polymonial dependencies on d
  - Locality-sensitive Hashing (LSH)
- And many more
  - Neighborhood graphs
  - Spectral methods (PCA)
  - Dynamic Continuous Indexing (DCI)
  - Offline (e.g., one-shot, batch queries)
  - Other metric spaces (e.g., doubling-dimension, Bregman distances)
  - Other variants: moving points, uncertainty, ...

ANN Search with kd-Trees

ANN Searching with kd-trees

- Preprocessing: $O(n \log n)$ time, $O(n)$ space
- Query Processing:
  - Locate the cell containing q
  - Establish initial search radius
  - Visit cells in increasing order of distance
  - Stop when: cell-dist $>$ NN-dist$/(1+\varepsilon)$
- Query time: $O(\log n + (1/\varepsilon)^d)$
- Works well in practice



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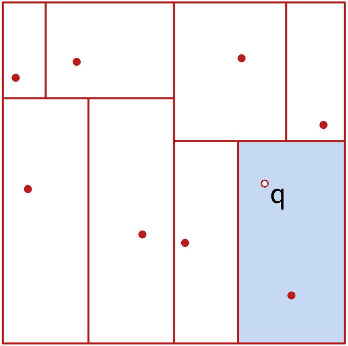

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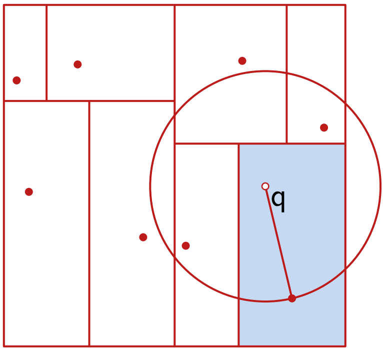

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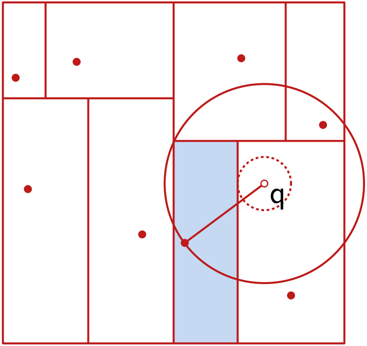

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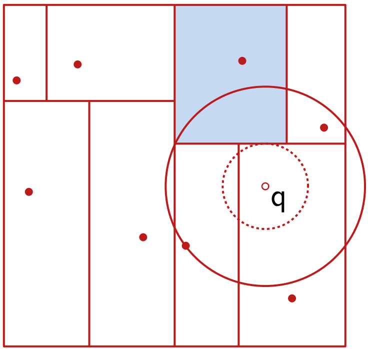

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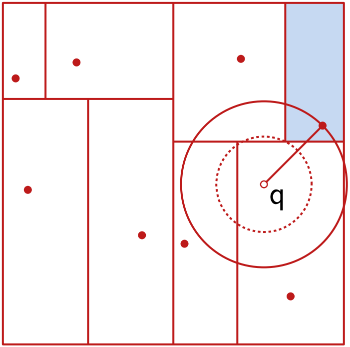

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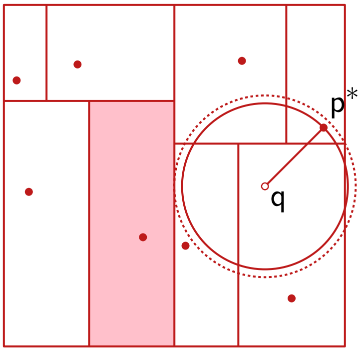

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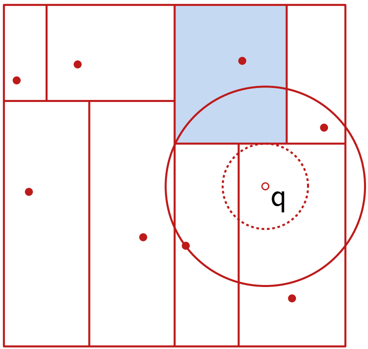

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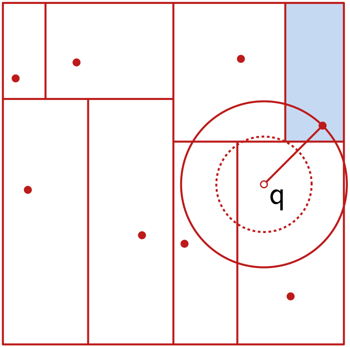

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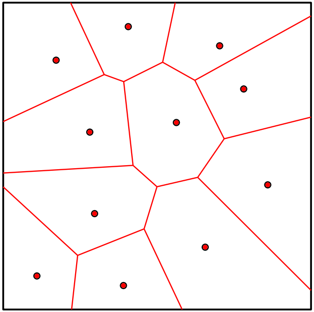
Approximate Voronoi Diagrams

Trade-offs: More space but lower query times?

Approximate Voronoi Diagram (AVD)

- Quadtree subdivision into cells
- Each cell stores a representative, $r \in P$, such that r is an ε-ANN of any point q in the cell



Har-Peled (2001):
Given a set of n points in $\mathbb{R}^d$, ε-approximate nearest neighbor queries can be answered in space $\widetilde{O}(n/\varepsilon^{d-1})$ and in time $O(\log(n/\varepsilon))$

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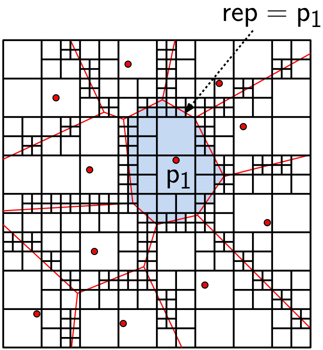

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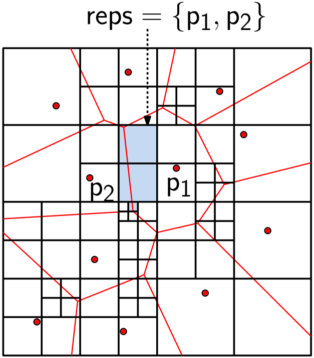
Space-Time Tradeoffs

Multi-Rep AVDs [Arya, Malamatos (2002)]

- Quadtree subdivision into cells
- Each cell stores up to t representatives, $\{r_1, \ldots, r_t\} \in P$
- Given any point q in the cell, at least one rep is an ε-ANN of q

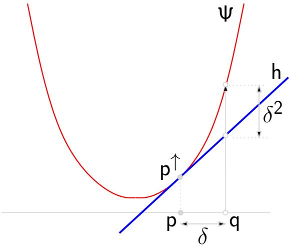


- Increase $t \Rightarrow$ decrease space, increase query time
- Theoretical bounds are strong [Arya, et al. 2009, 2017]
- Storage can be prohibitive in practice

ANN Searching and Polytope Approximation

Lifting and Distances

- Project a point p vertically to $p^{\uparrow}$ on a paraboloid Ψ
- Let h be the tangent hyperplane at $p^{\uparrow}$
- For any point q at distance δ from p, the vertical distance between Ψ and h is δ^2



Lifting and Voronoi Diagrams

- Lift the points of P vertically to Ψ
- Intersect their tangent upper halfspaces
- The projected skeleton of the resulting polytope is the Voronoi diagram of P

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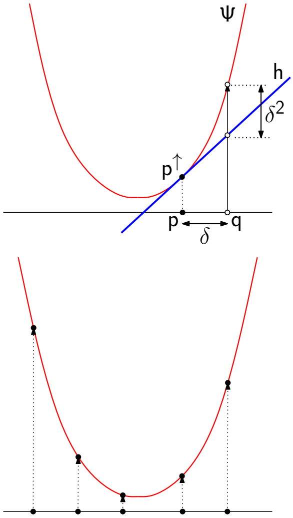

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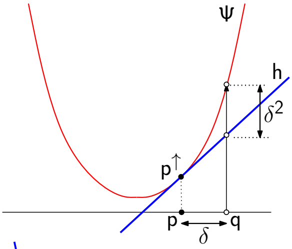

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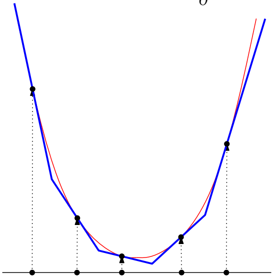

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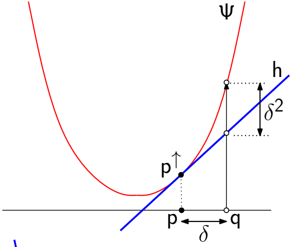
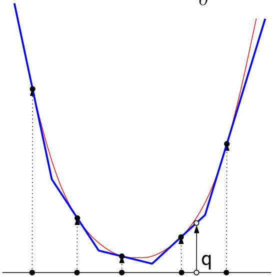
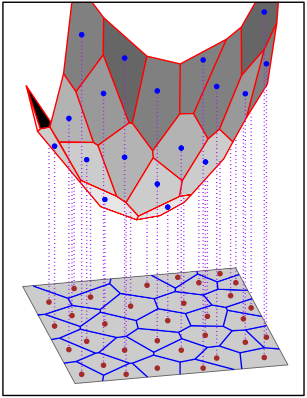




ANN Searching and Polytope Approximation

Lifting and Voronoi Diagrams

Lift the points of P to Ψ, take the upper envelope of the tangent hyperplanes, and project the skeleton back onto the plane. The result is the Voronoi diagram of P.



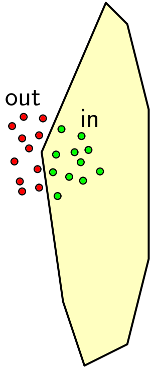
Intuition: Improved representations of polytopes lead to improvements for ANN

Polytope Membership Queries

Polytope Membership Queries

Given a polytope K in $\mathbb{R}^d$, preprocess K to answer membership queries:

Given a point $q \in \mathbb{R}^d$, is $q \in K$?



Assumptions:

- Dimension d is a constant
- K given as intersection of n halfspaces

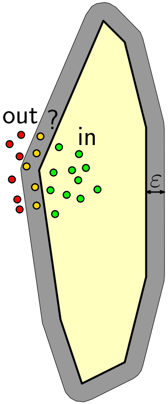
Dual: Halfspace emptiness searching [Matoušek (1992)]

- $d \leq 3 \;\Rightarrow$ Space: $O(n)$, Query time: $O(\log n)$
- $d \geq 4 \;\Rightarrow$ Space: $O(n^{\lfloor d/2 \rfloor})$, Query time: $O(\log n)$

Approximate Polytope Membership Queries

ε-APM Queries:

- Given an approximation parameter $\varepsilon > 0$ (at preprocessing time)
- Assume the polytope scaled to unit diameter
- If the query point's distance from K:
  - $0 \Rightarrow$ Inside
  - $> \varepsilon \Rightarrow$ Outside
  - Otherwise: Either answer is acceptable



Arya, da Fonesca, Mount [SODA 2017]

Query time: $O(\log \frac{1}{\varepsilon})$ $\leftarrow$ optimal

Storage: $O(1/\varepsilon^{(d-1)/2})$ $\leftarrow$ optimal

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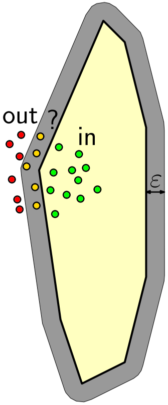

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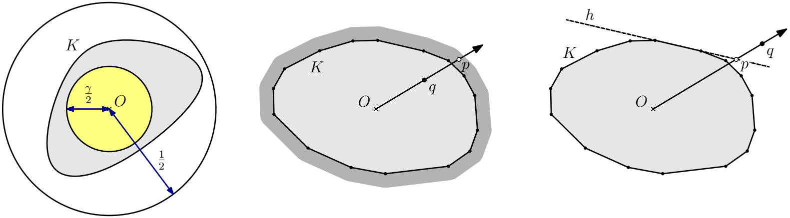
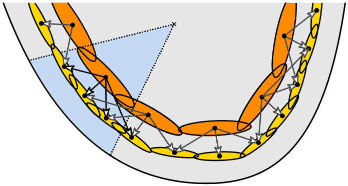
Polytope Approximation and Ray Shooting Queries



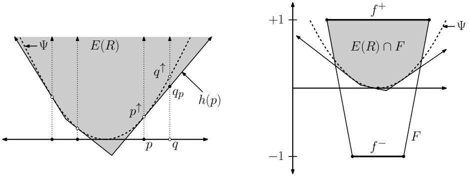
Ray shooting preliminaries

Polytope Approximation and Ray Shooting Queries (2)

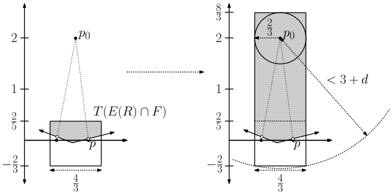


Data structure for APM based on ray shooting

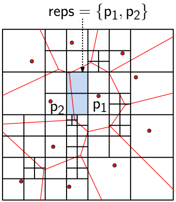
Polytope Approximation and Ray Shooting Queries (3)

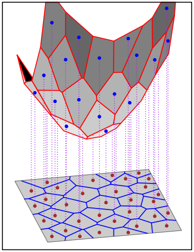


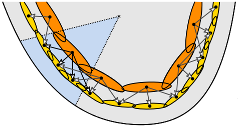
Projective transformation for vertical ray shooting

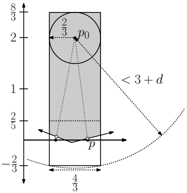


State-of-the-art in ANN









Nearly two decades of work on this problem

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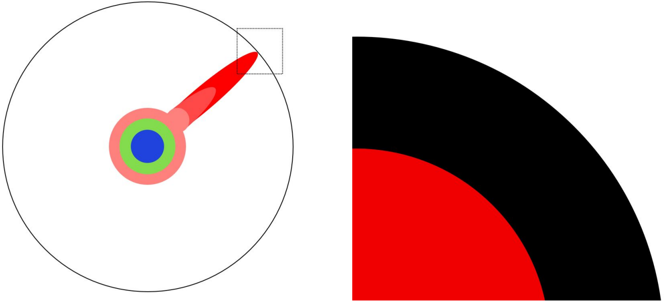
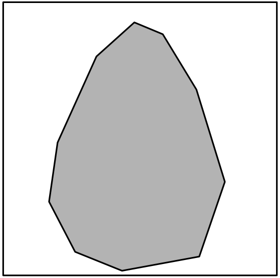


Matt Might, The Illustrated Guide to a Ph.D.
http://matt.might.net/articles/phd-school-in-pictures/

Intuition - Quadtree Search

Quadtree-based query approach:

- Preprocessing: Build a quadtree, subdividing each node that cannot be resolved as being inside or outside
- Stop at diameter ε
- Query: Find the leaf node containing q and return its label



Analysis:

Query time: $O(\log \frac{1}{\varepsilon})$ (Quadtree descent)
Storage: $O(1/\varepsilon^{d-1})$ (Number of leaves)

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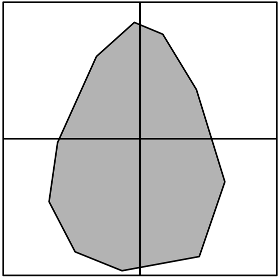

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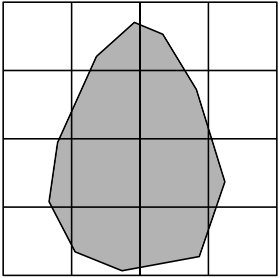

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Intuition - Quadtree Search

Quadtree-based query approach:

- Preprocessing: Build a quadtree, subdividing each node that cannot be resolved as being inside or outside
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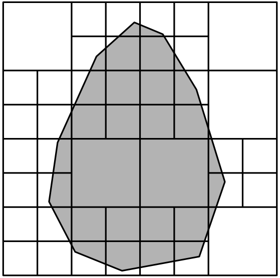

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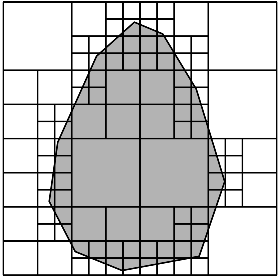

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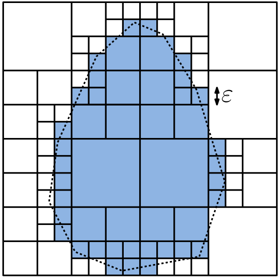

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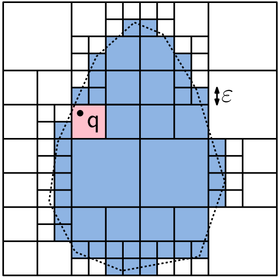

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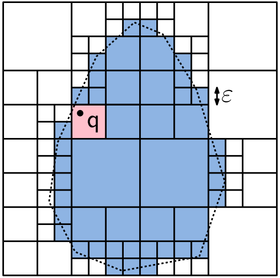

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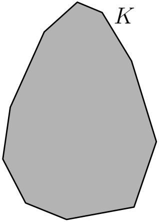

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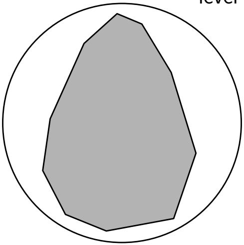

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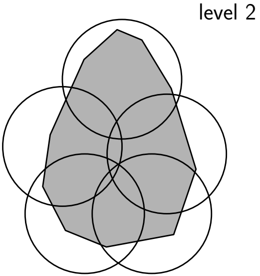

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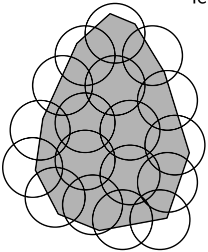

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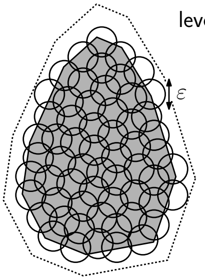

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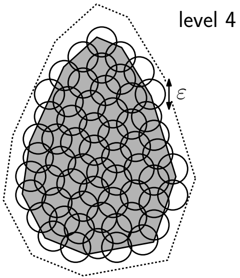

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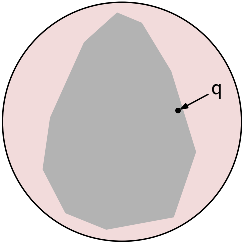

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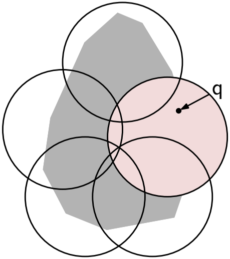

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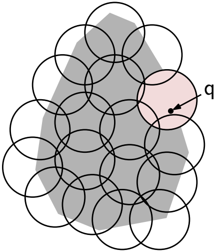

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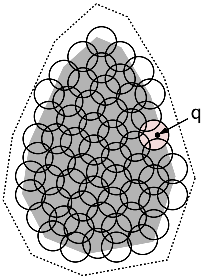

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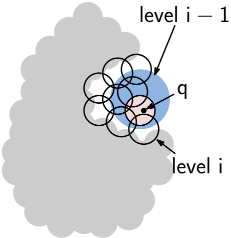

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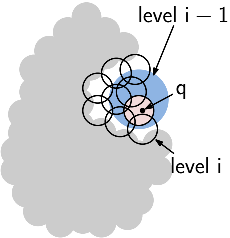

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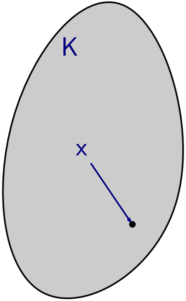
Macbeath Regions

Want cells that conform to K's shape



Macbeath Region [Macbeath (1952)]

Given convex body K, $x \in K$, and $\lambda > 0$:

- $M_K^\lambda(x) = x + \lambda((K - x) \cap (x - K))$
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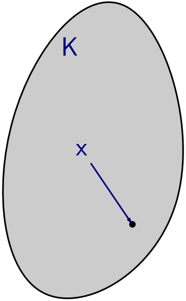

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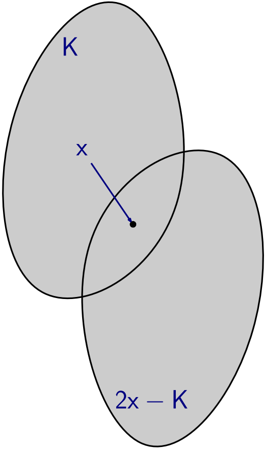

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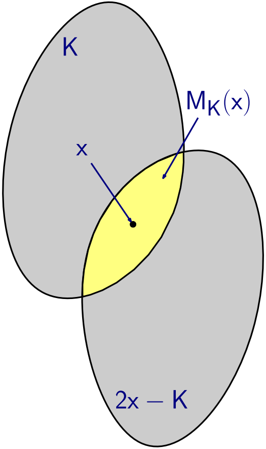

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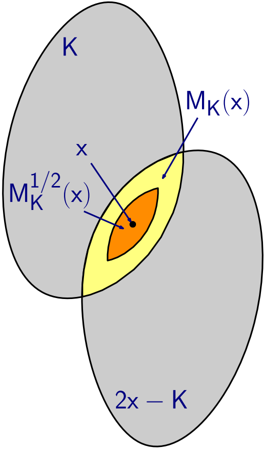

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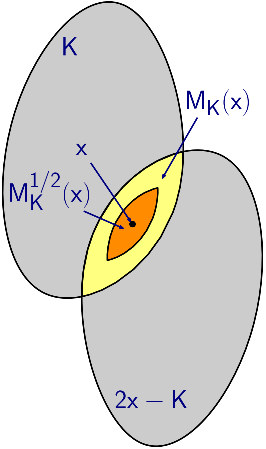


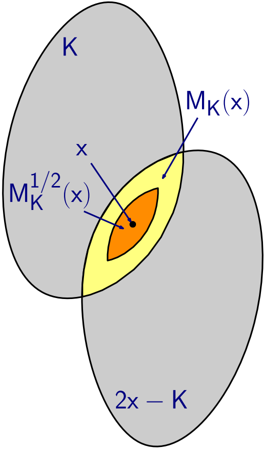
Properties of Macbeath Regions

Properties:

- Symmetry: $M^\lambda(x)$ is convex and centrally symmetric about x
- Expansion-Containment: [Ewald et al (1970)] If for $\lambda < 1$, $M^\lambda(x)$ and $M^\lambda(y)$ intersect, then

$$M^\lambda(y) \subseteq M^{c\lambda}(x), \quad \text{where } c = \frac{3+\lambda}{1-\lambda}.$$

Upshot: By expansion-containment, shrunken Macbeath regions behave "like" Euclidean balls, but they conform locally to K's boundary ... metric balls?



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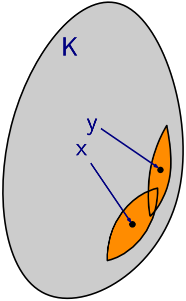

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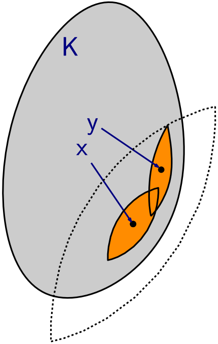

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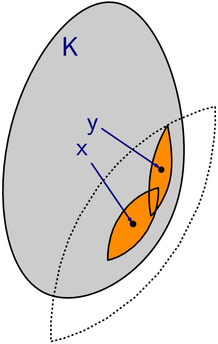

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Metric Spaces

Metric Space: A set $\mathbb{X}$ and distance measure $f : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ that satisfies:

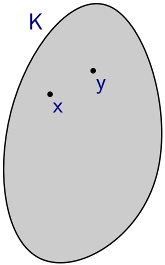
- Nonnegativity: $f(x, y) \geq 0$, and $f(x, y) = 0$ if and only if $x = y$
- Symmetry: $f(x, y) = f(y, x)$
- Triangle Inequality: $f(x, z) \leq f(x, y) + f(y, z)$

Macbeath Regions and the Hilbert Geometry

- Hilbert Metric: Given $x, y \in K$, let x' and y' be the intersection of $\overleftrightarrow{xy}$ with ∂K. Define

$$f_K(x, y) = \frac{1}{2} \ln \left(\frac{\|x' - y\|}{\|x' - x\|} \frac{\|x - y'\|}{\|y - y'\|} \right)$$

- Hilbert Ball: $B_H(x, \delta) = \{y \in K : f_K(x, y) \leq \delta\}$



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e.g. $B_H(x, 0.091) \subseteq M^{0.2}(x) \subseteq B_H(x, 0.203), \forall x \in K.$

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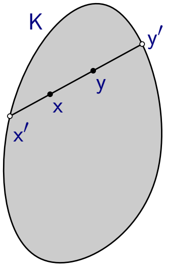

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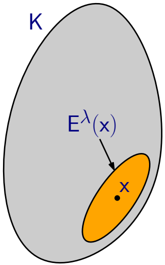
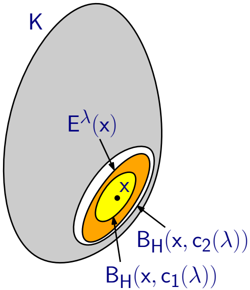


Macbeath Regions and the Hilbert Geometry

- Hilbert Metric: Given $x, y \in K$, let x' and y' be the intersection of $\overleftrightarrow{xy}$ with ∂K. Define

$$f_K(x,y) = \frac{1}{2} \ln \left(\frac{\|x'-y\|}{\|x'-x\|} \frac{\|x-y'\|}{\|y-y'\|} \right)$$

- Hilbert Ball: $B_H(x,\delta) = \{y \in K : f_K(x,y) \le \delta\}$



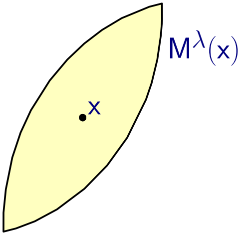
[Vernicos and Walsh (2016)]

For all $x \in K$ and $0 \le \lambda < 1$:

$$B_H\left(x, \frac{1}{2}\ln(1+\lambda)\right) \subseteq M^\lambda(x) \subseteq B_H\left(x, \frac{1}{2}\ln\frac{1+\lambda}{1-\lambda}\right)$$

e.g. $B_H(x, 0.091) \subseteq M^{0.2}(x) \subseteq B_H(x, 0.203), \forall x \in K$.

Macbeath Ellipsoids



Macbeath regions can be combinatorially complex. Want a coarse approximation of low-complexity.

John ellipsoid [John (1948)]

Given a centrally symmetric convex body M in $\mathbb{R}^d$, there exist ellipsoids E_1, E_2 such that $E_1 \subseteq M \subseteq E_2$ and E_2 is a $\sqrt{d}$-scaling of E_1

Macbeath ellipsoid:

- $E(x)$: maximum volume ellipsoid in $M(x)$
- $E^\lambda(x)$: scaling by factor λ
- $E^\lambda(x) \subseteq M^\lambda(x) \subseteq E^{\lambda\sqrt{d}}(x)$

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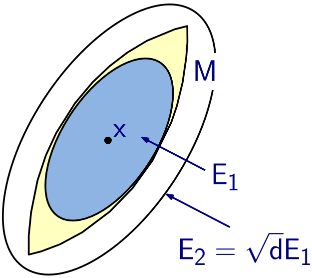

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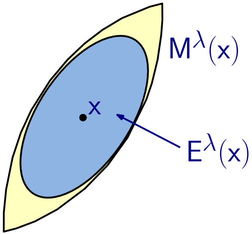

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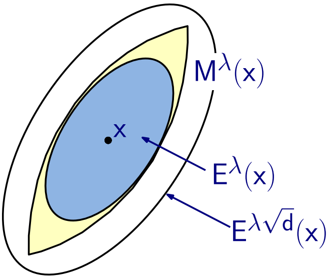

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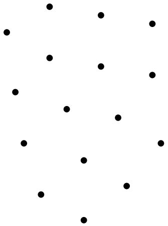
Delone Sets



A subset $X \subseteq \mathbb{X}$ is an:

- ε-packing: If the balls of radius $\varepsilon/2$ centered at every point of X are disjoint
- ε-covering: If every point of $\mathbb{X}$ is within distance ε of some point of X
- $(\varepsilon_p, \varepsilon_c)$-Delone Set: If X is an ε_p-packing and an ε_c-covering

We seek economical Delone sets for K, that fit within K's δ-expansion for $\delta = 1, \frac{1}{2}, \frac{1}{4}, \ldots, \varepsilon$

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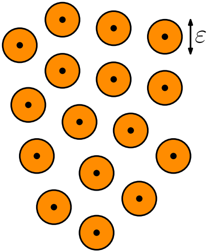

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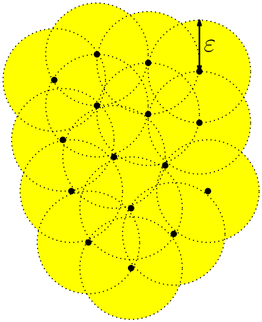

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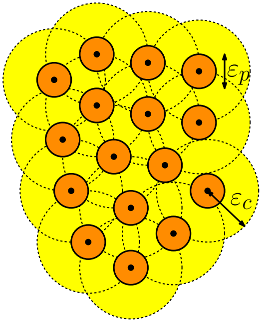

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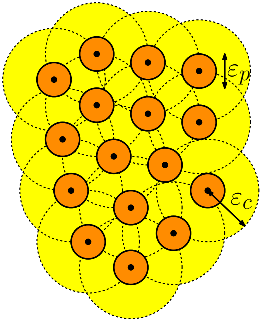

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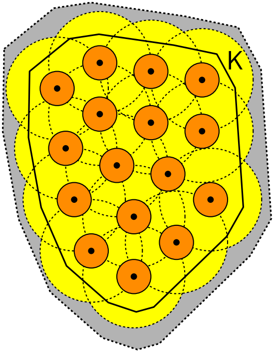

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Macbeath Ellipsoids and Delone Sets

Delone sets from Macbeath ellipsoids:

- For $\delta > 0$, let K_δ be an expansion of K by distance δ
- Let λ_0 be a small constant $(1/(4\sqrt{d}+1))$
- Let $X_\delta \subset K$ be a maximal set of points such that $E^{\lambda_0}(x)$ are disjoint for all $x \in X_\delta$
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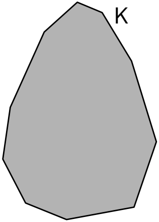

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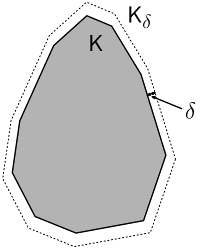

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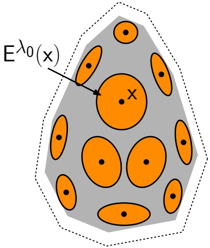

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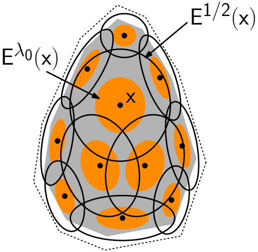

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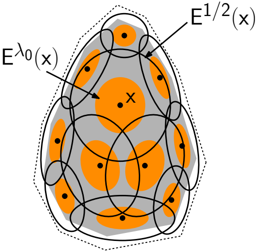

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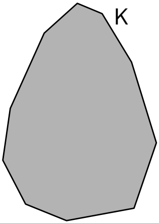

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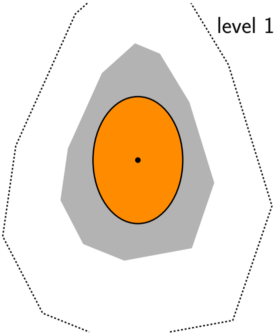

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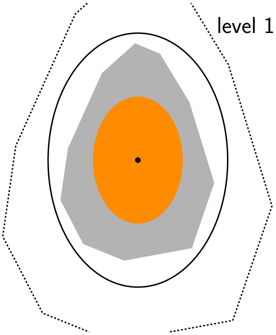

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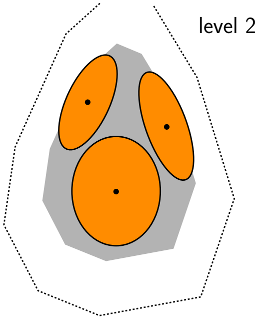

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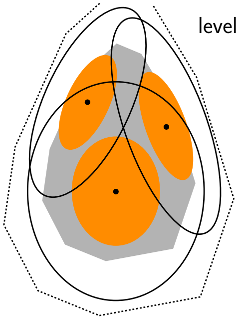

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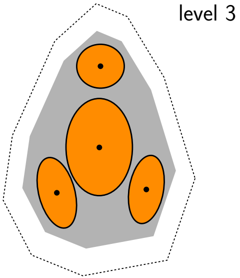

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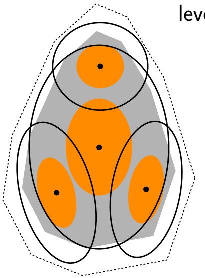

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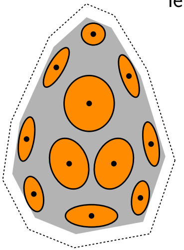

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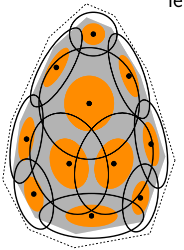

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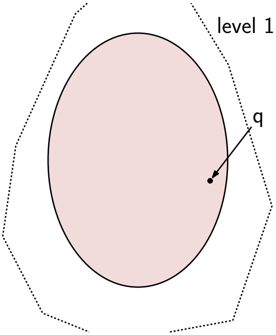

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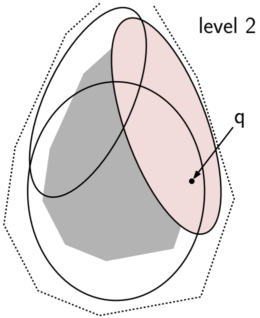

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- Descend the DAG from root (level ℓ) until:
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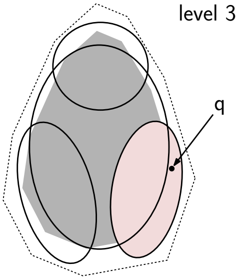
  - Reach leaf $u \Rightarrow$ "inside"



APM Data Structure

Preprocessing:

- Input: K and $\varepsilon > 0$
- For $i = 0, 1, \ldots$
  - $\delta_i \leftarrow 2^i \varepsilon$
  - $X_i \leftarrow$ Macbeath Delone set for K_{δ_i}
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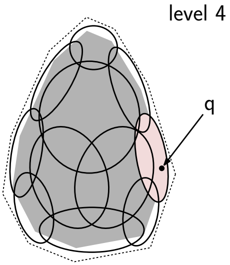

Analysis

- Total Query time: $O(\log \frac{1}{\varepsilon})$
  - Out-degree: $O(1)$ (By expansion-containment)
  - Query time per level: $O(1)$
  - Number of levels: $O(\log \frac{1}{\varepsilon})$ (From ε to $O(1)$)
- Total storage: $O(1/\varepsilon^{(d-1)/2})$
  - Economical cap cover [AFM (2016)]: Number of Macbeath regions needed to cover K_{δ_i} is $O(1/\delta^{(d-1)/2})$
  - Storage for bottom level: $O(1/\varepsilon^{(d-1)/2})$
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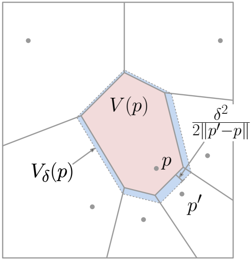
Bypassing the Lifting Transform

Implications of approximating the upper envelope

δ-expanded Voronoi Cell

$$V_\delta(p) = \{x \in \mathbb{R}^d : \|p-x\|^2 \leq \|p'-x\|^2 + \delta^2, \forall p' \in P\}$$



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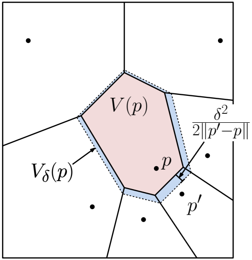

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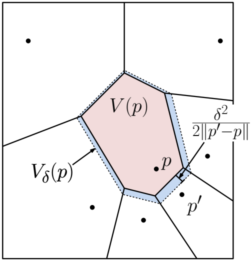
Lemma

$V_\delta(p)$ can be expressed as $\bigcap_{p' \in P \setminus \{p\}} H_{p',\delta}$ where

$$H_{p',\delta} = \{x \in \mathbb{R}^d : \langle x, v_{p'} \rangle \leq a_{p'} + \delta^2\},$$

with $v_{p'} = 2(p'-p)$ and $a_{p'} = \|p'\|^2 - \|p\|^2$.



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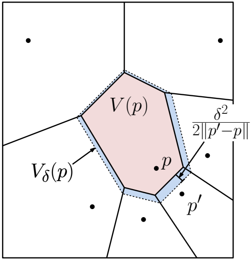
Lemma

$\forall q \in V_\delta(p)$, if $\delta^2 \leq \|p - q\|^2 \cdot \min(\varepsilon, 1/2)$ then p is an ε-ANN of q.

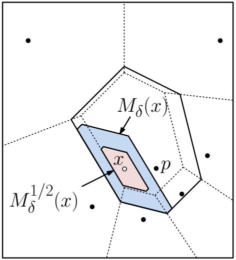


Working with Expanded Voronoi Cells

- Macbeath regions w.r.t. expanded Voronoi cells
- Points from different cells ...

Lemma - Expansion-Containment

If $x, y \in \mathbb{R}^d$ such that $M_\delta^\lambda(x) \cap M_\delta^\lambda(y) \neq \emptyset$, then for any $\alpha \geq 0$ and $\beta = \frac{2+\alpha(1+\lambda)}{1-\lambda}$, $M^{\alpha\lambda}(y) \subseteq M^{2\beta\lambda}(x)$.



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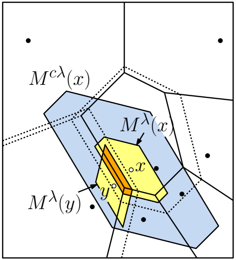

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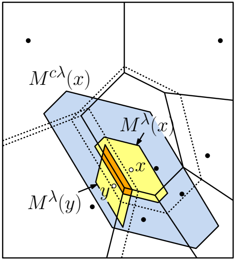

New Data Structure for ANN

$(r_{\min}, r_{\max})$-restricted ε-ANN queries:

- If $d(q, P) > r_{max}$ $\Rightarrow$ Outside
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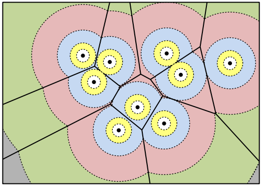

Layers

Setting $\gamma_0 = r_{min}$, $\gamma_i = 2^i \gamma_0$ and $\widehat{\gamma}_i = \min(\gamma_i, r_{\max})$

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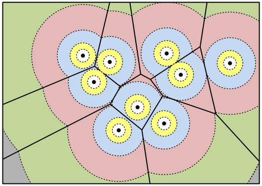

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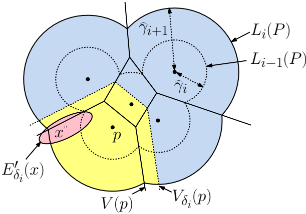
Set $r_{\min} = \delta_{\min}/2$, $r_{\max} = \delta_{\max}/\varepsilon$ and $\Phi(P) = \delta_{max}/\delta_{min}$.

Theorem

Given an n-element point set $P \subset \mathbb{R}^d$ and $\varepsilon > 0$, there exists a DAG structure of height $\ell = O\left(\log \frac{\Phi(P)}{\varepsilon}\right)$ that can answer ε-ANN queries in time $O(\ell)$ space $O(\ell n/\varepsilon^{(d-1)/2})$.



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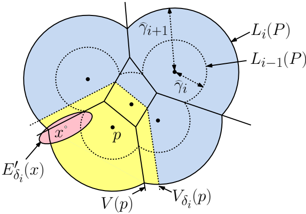

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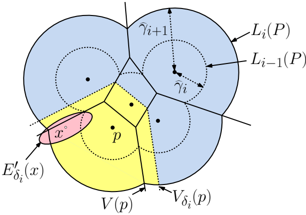

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