

Approximate Nearest Neighbor Problem: Improving Query Time

CS468, 10/9/2006

Outline

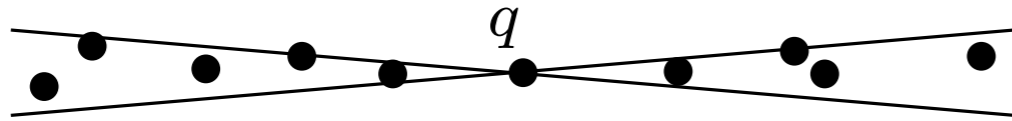
- Reducing the "constant" from $O(\epsilon^{-d})$ to $O(\epsilon^{-(d-1)/2})$ in query time
- Need to know ϵ ahead of time
 - Preprocessing time and storage feature $O(\epsilon^{-d})$, $O(\epsilon^{-(d-1)/2})$ etc.

Outline

- Reducing the "constant" from $O(\epsilon^{-d})$ to $O(\epsilon^{-(d-1)/2})$ in query time
- Need to know ϵ ahead of time
 - Preprocessing time and storage feature $O(\epsilon^{-d})$, $O(\epsilon^{-(d-1)/2})$ etc.
- Timothy M. Chan. *Approximate Nearest Neighbor Queries Revisited*. Discrete and Computational Geometry 1998.
 - Decomposition of space into cones
 - BBD-tree for range searching in \mathbb{R}^{d-k} + point location in \mathbb{R}^k
- Kenneth Clarkson. *An Algorithm for Approximate Closest-point Queries*. SoCG 1994.
 - Additional $\log(\rho/\epsilon)$ in space complexity
 - Polytope approximation in \mathbb{R}^{d+1}

Chen's Algorithm: Motivation

$(1 + \epsilon)$ -ANN among (sorted) points in a narrow cone

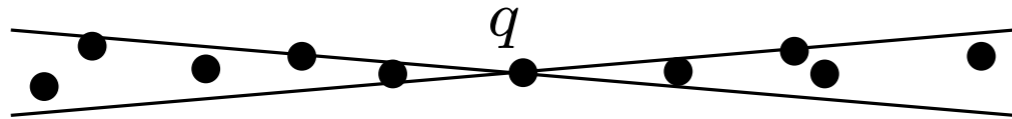


$O(\log n)$ by binary search

Need a data structure that returns a sorted points given q and a cone direction

Chen's Algorithm: Motivation

$(1 + \epsilon)$ -ANN among (sorted) points in a narrow cone



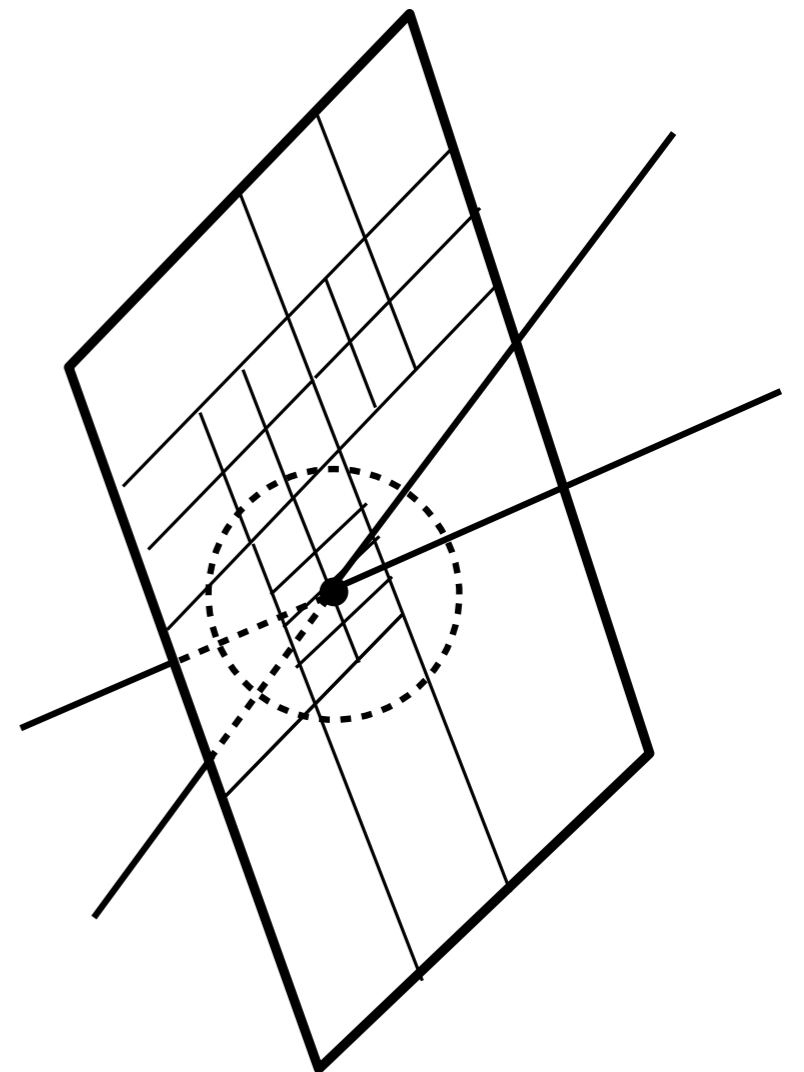
$O(\log n)$ by binary search

Need a data structure that returns a sorted points given q and a cone direction

Uses the BBD-tree data structure

Given a **query point** $q \in \mathbb{R}^d$ and a **radius** r
one can find $O(\log n)$ cells of the BBD-tree
which **contain** $B(q, r)$
and **are contained in** $B(q, 2r)$.
This takes $O(\log n)$ time

Use for approximate range searching in \mathbb{R}^{d-1}



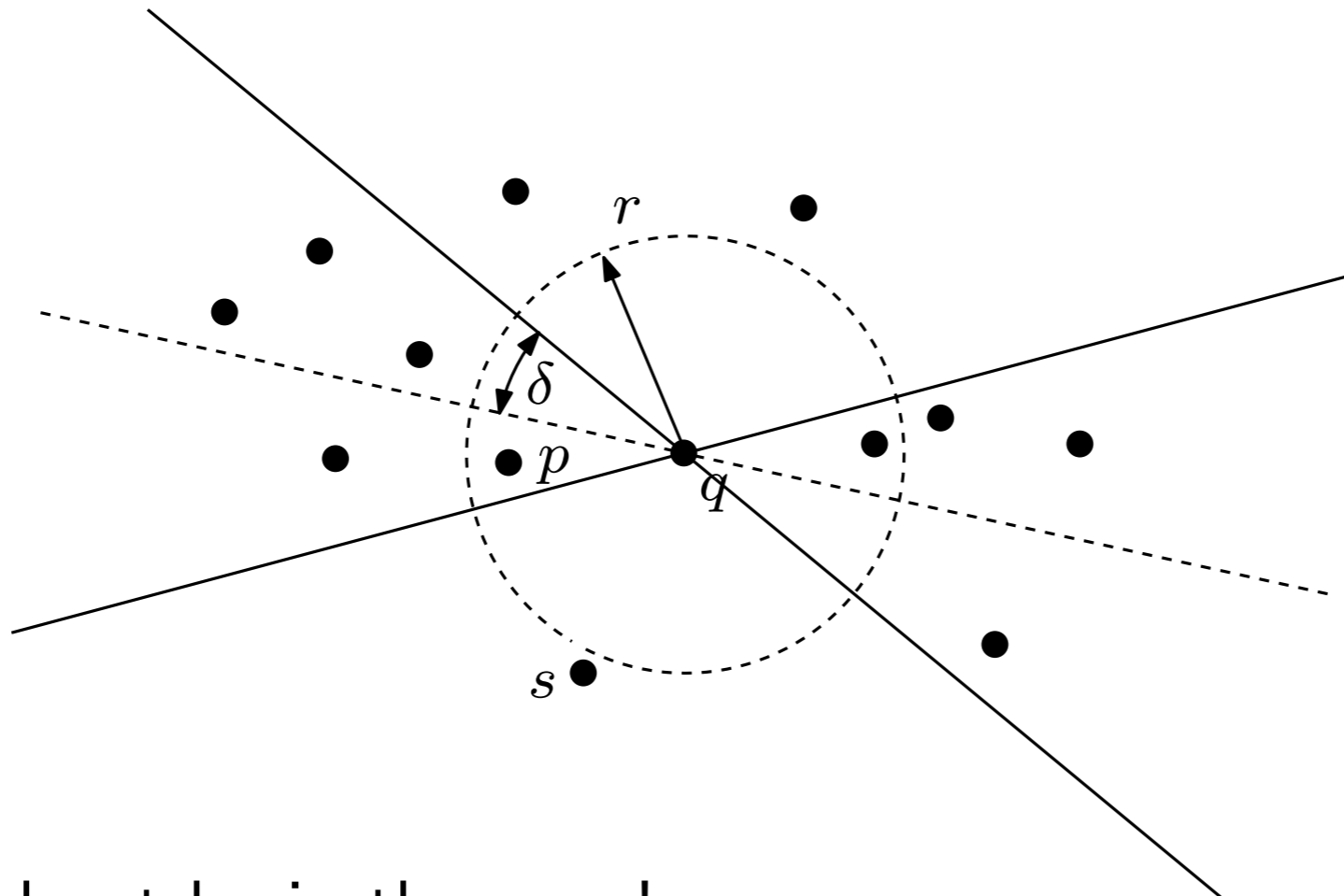
Conic ANN (with a Hint)

Input: Query point q and a 2-approximation r to the NN distance

Output: A points s such that

$$\|q - s\| \leq (1 + \epsilon)\|q - p\|$$

where p is the NN inside a cone with apex q and angle $\delta = \sqrt{\epsilon/16}$



Note: s need not be in the cone!

Note: The cone is fixed (not a part of input, mod. translation to q)

Main $(1 + \epsilon)$ -ANN Algorithm

Uses the "conic-ANN with a hint" as a subroutine

Query (given only q)

- Obtain r by [Arya and Mount 1998]
- Get one point per data structure, return the one closest to q


Main $(1 + \epsilon)$ -ANN Algorithm

Uses the "conic-ANN with a hint" as a subroutine

Query (given only q)

- Obtain r by [Arya and Mount 1998]
- Get one point per data structure, return the one closest to q

Preprocessing

- "Tile" \mathbb{R}^d with $O(\epsilon^{-(d-1)/2})$ cones of angle $\delta = \Theta(\sqrt{\epsilon})$

- Build a "conic-ANN" data structure for each cone

Main $(1 + \epsilon)$ -ANN Algorithm

Uses the "conic-ANN with a hint" as a subroutine

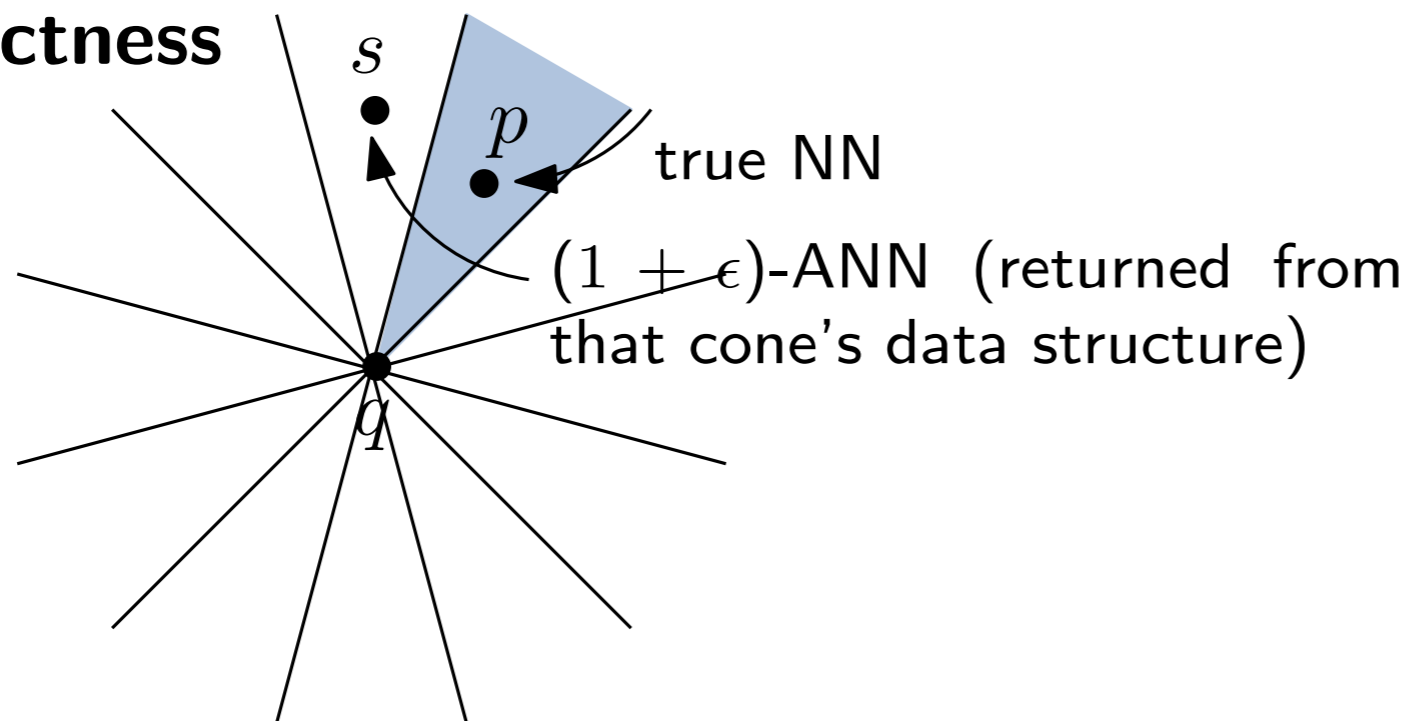
Query (given only q)

- Obtain r by [Arya and Mount 1998]
- Get one point per data structure, return the one closest to q

Preprocessing

- "Tile" \mathbb{R}^d with $O(\epsilon^{-(d-1)/2})$ cones of angle $\delta = \Theta(\sqrt{\epsilon})$
- Build a "conic-ANN" data structure for each cone

Correctness



Main $(1 + \epsilon)$ -ANN Algorithm

Uses the "conic-ANN with a hint" as a subroutine

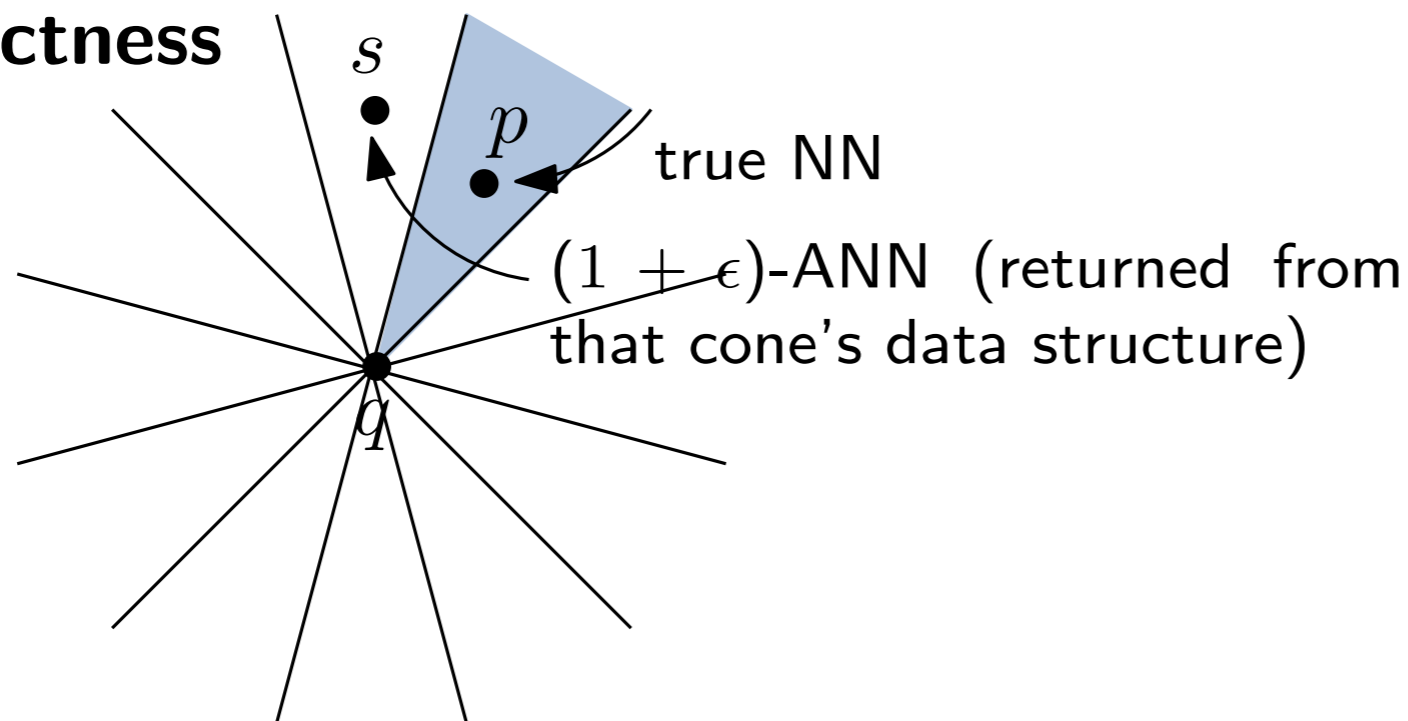
Query (given only q)

- Obtain r by [Arya and Mount 1998]
- Get one point per data structure, return the one closest to q

Preprocessing

- "Tile" \mathbb{R}^d with $O(\epsilon^{-(d-1)/2})$ cones of angle $\delta = \Theta(\sqrt{\epsilon})$
- Build a "conic-ANN" data structure for each cone

Correctness



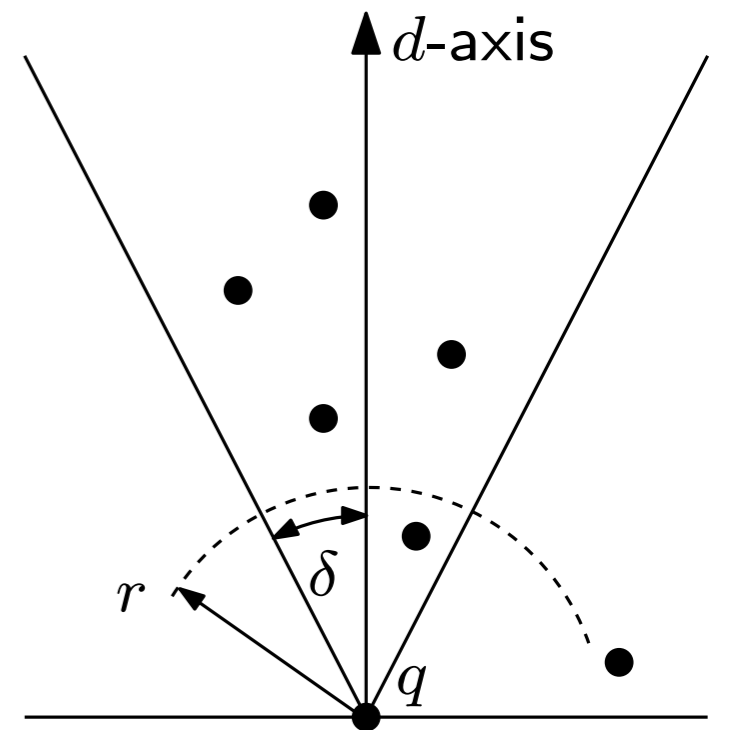
Query time

$$O(\epsilon^{-(d-1)/2} \log n)$$

[# of cones] [conic query]

Conic-ANN Data Structure

For preprocessing given only direction of the cone (wlog: d -axis) and angle δ



Conic-ANN Data Structure

For preprocessing given only direction of the cone (wlog: d -axis) and angle δ

Query Algorithm (given q and r)

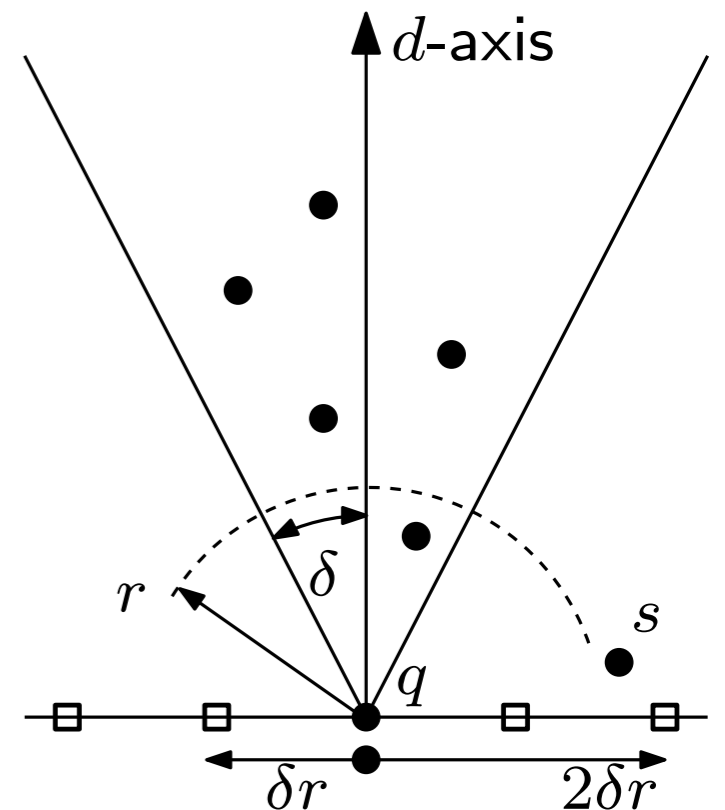
Approximate range query on the set of projections

$\{p' = [p_1 \ p_2 \ \cdots \ p_{d-1}]^T, p \in P\}$ with $B(q, \delta r)$

- returns $O(\log n)$ BBD-nodes (cells) in $O(\log n)$ time

$O(\log n)$ binary searches

Return the point s such that $|s_d - q_d|$ is min



Conic-ANN Data Structure

For preprocessing given only direction of the cone (wlog: d -axis) and angle δ

Query Algorithm (given q and r)

Approximate range query on the set of projections

$\{p' = [p_1 \ p_2 \ \cdots \ p_{d-1}]^T, p \in P\}$ with $B(q, \delta r)$

- returns $O(\log n)$ BBD-nodes (cells) in $O(\log n)$ time

$O(\log n)$ binary searches

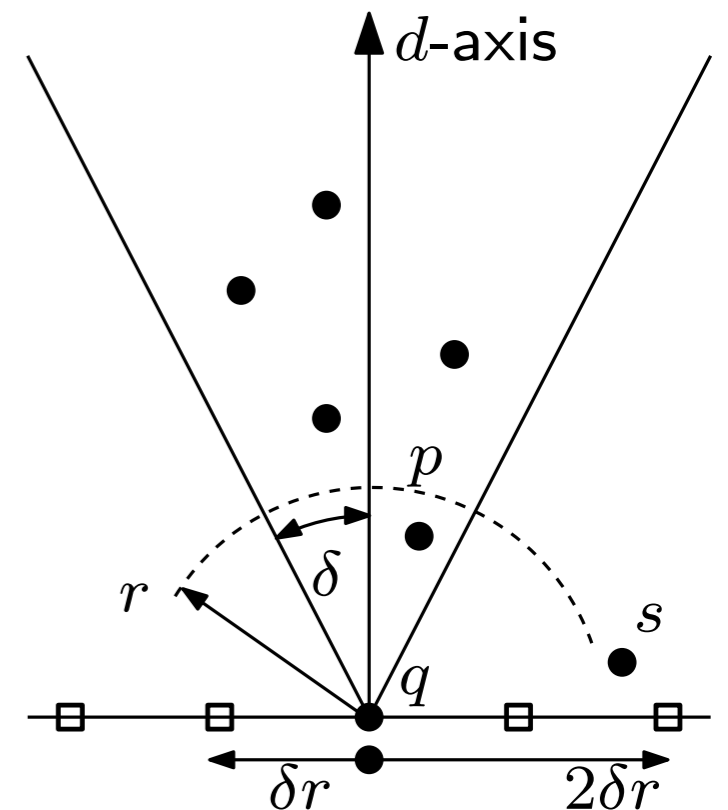
Return the point s such that $|s_d - q_d|$ is min

Correctness (proof for $\|q - s\| \leq (1 + \epsilon)\|q - p\|$)

$$|s_d - q_d| \leq |p_d - q_d| \leq \|p - q\|$$

$$|s' - q'| \leq 2\delta r \leq 4\delta \|p - q\|$$

$$\|s - q\| \leq \sqrt{1 + 16\delta^2} \|p - q\| = (1 + \epsilon) \|p - q\|$$



Conic-ANN Data Structure

For preprocessing given only direction of the cone (wlog: d -axis) and angle δ

Query Algorithm (given q and r)

Approximate range query on the set of projections

$\{p' = [p_1 \ p_2 \ \cdots \ p_{d-1}]^T, p \in P\}$ with $B(q, \delta r)$

- returns $O(\log n)$ BBD-nodes (cells) in $O(\log n)$ time

$O(\log n)$ binary searches

Return the point s such that $|s_d - q_d|$ is min

Correctness (proof for $\|q - s\| \leq (1 + \epsilon)\|q - p\|$)

$$|s_d - q_d| \leq |p_d - q_d| \leq \|p - q\|$$

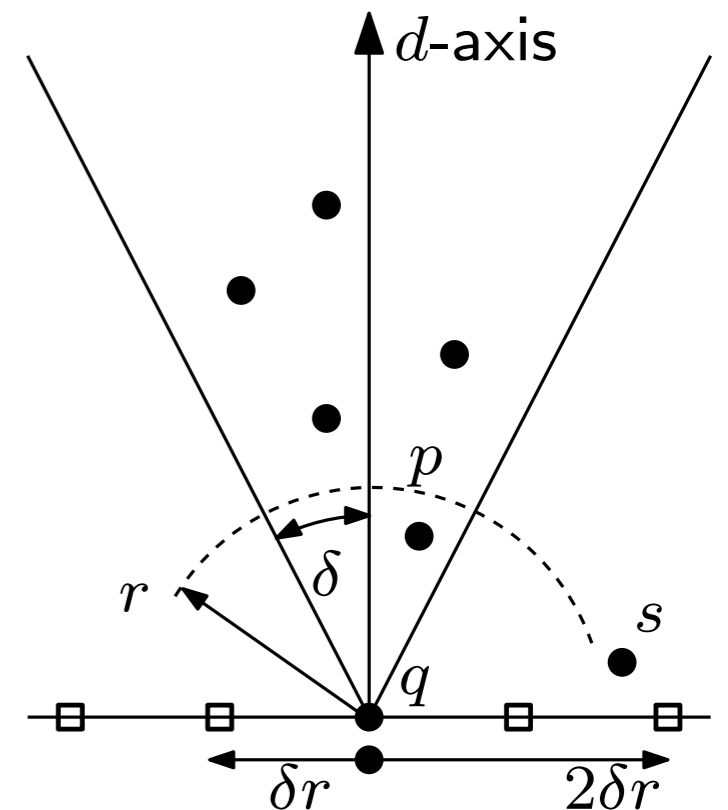
$$|s' - q'| \leq 2\delta r \leq 4\delta \|p - q\|$$

$$\|s - q\| \leq \sqrt{1 + 16\delta^2} \|p - q\| = (1 + \epsilon) \|p - q\|$$

Data structure

BBD-tree on the projection set

For every tree node v the associated list of points is sorted in the d coordinate



Conic-ANN Analysis

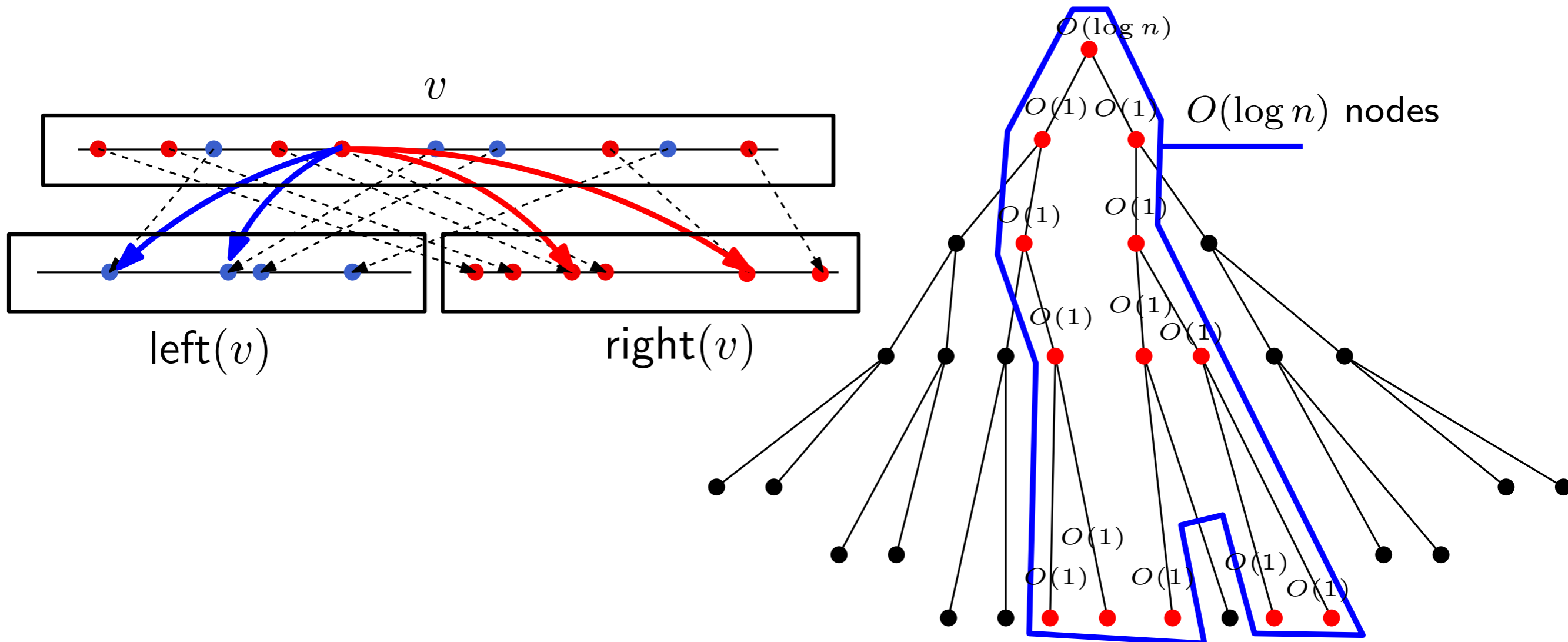
Construction (preprocessing)

BBD-tree $O(n \log n)$ + sorting $O(n \log n) = O(n \log n)$

Query

Approximate range query $O(\log n)$ + bin. searches $O(\log^2 n) = O(\log^2 n)$

Improving query time by exploiting correlation [Lueker and Willard]



Summary and Remarks

Variant with projecting to $d - 2$ dimensions

- BBD tree + planar point location

Rough ($\approx d^{3/2}$) approximation algorithms

- Polynomial dependence on d

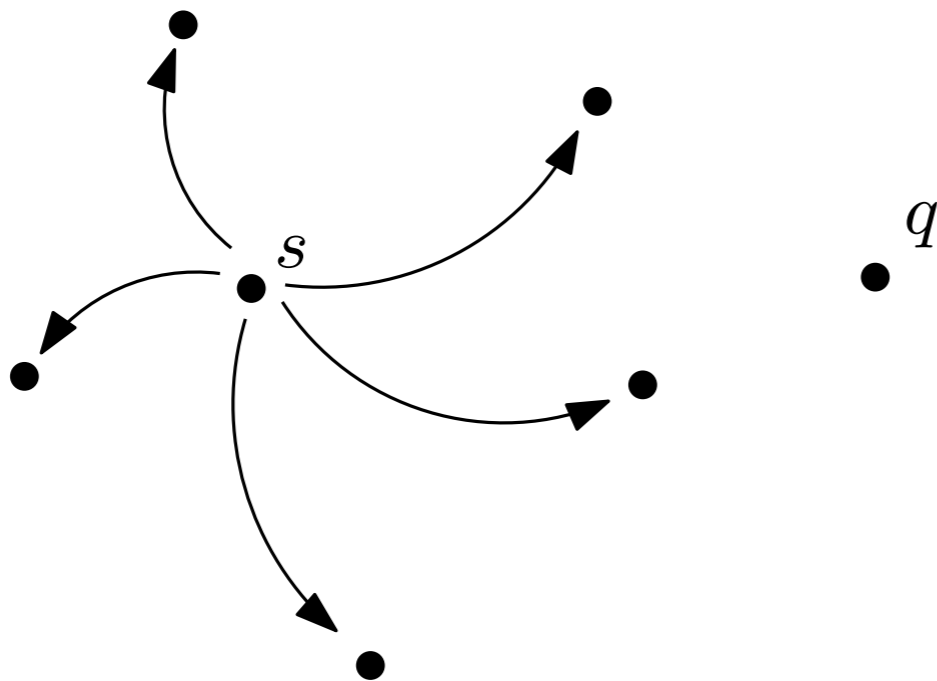
Clarkson's Algorithm: Iterative Improvement

Exact nearest neighbor problem

Data structure For each site s , a (small) list L_s of other sites such that

for **any** query point q

if s is not the nearest neighbor of q , then L_s contains a site closer to q



Clarkson's Algorithm: Iterative Improvement

Exact nearest neighbor problem

Data structure For each site s , a (small) list L_s of other sites such that

for **any** query point q

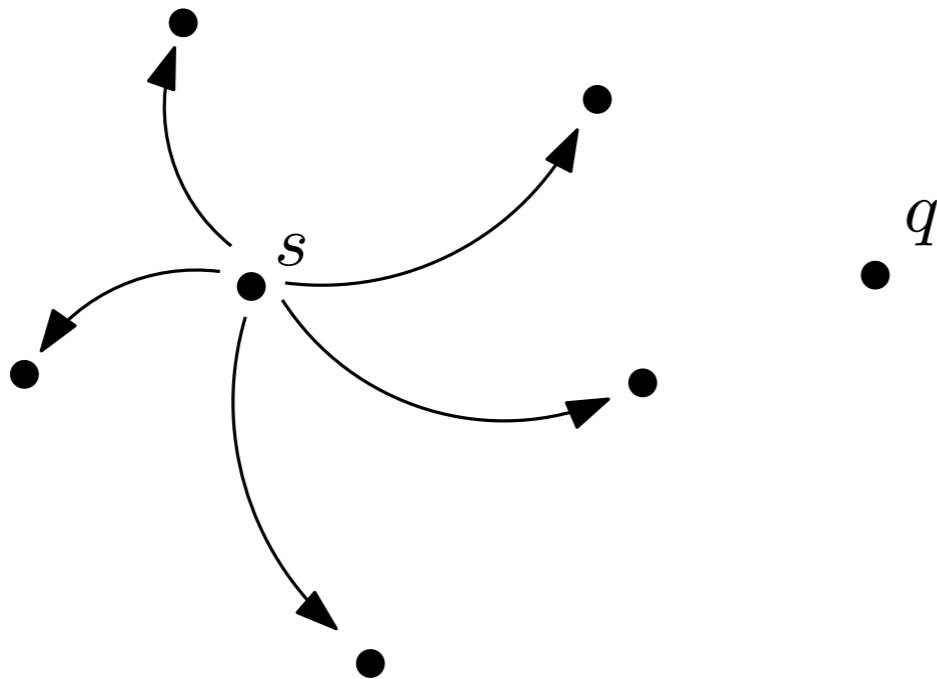
if s is not the nearest neighbor of q , then L_s contains a site closer to q

Algorithm

$s \leftarrow$ arbitrary site

while $\exists t \in L_s : \|t - q\| < \|s - q\|$ do $s \leftarrow t$

return s



Clarkson's Algorithm: Iterative Improvement

Exact nearest neighbor problem

Data structure For each site s , a (small) list L_s of other sites such that

for **any** query point q

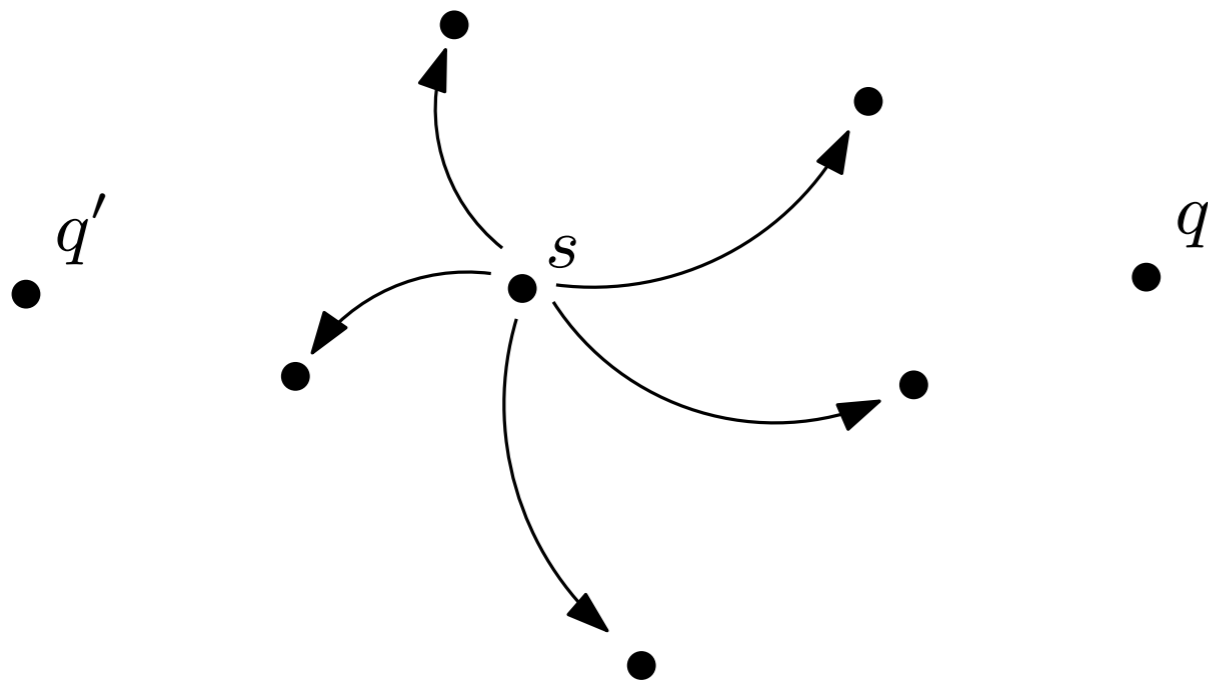
if s is not the nearest neighbor of q , then L_s contains a site closer to q

Algorithm

$s \leftarrow$ arbitrary site

while $\exists t \in L_s : \|t - q\| < \|s - q\|$ do $s \leftarrow t$

return s



Note

The same L_s valid for all q !

Not Useful for Exact NN

Reason 1: space complexity $\Omega(n^2)$

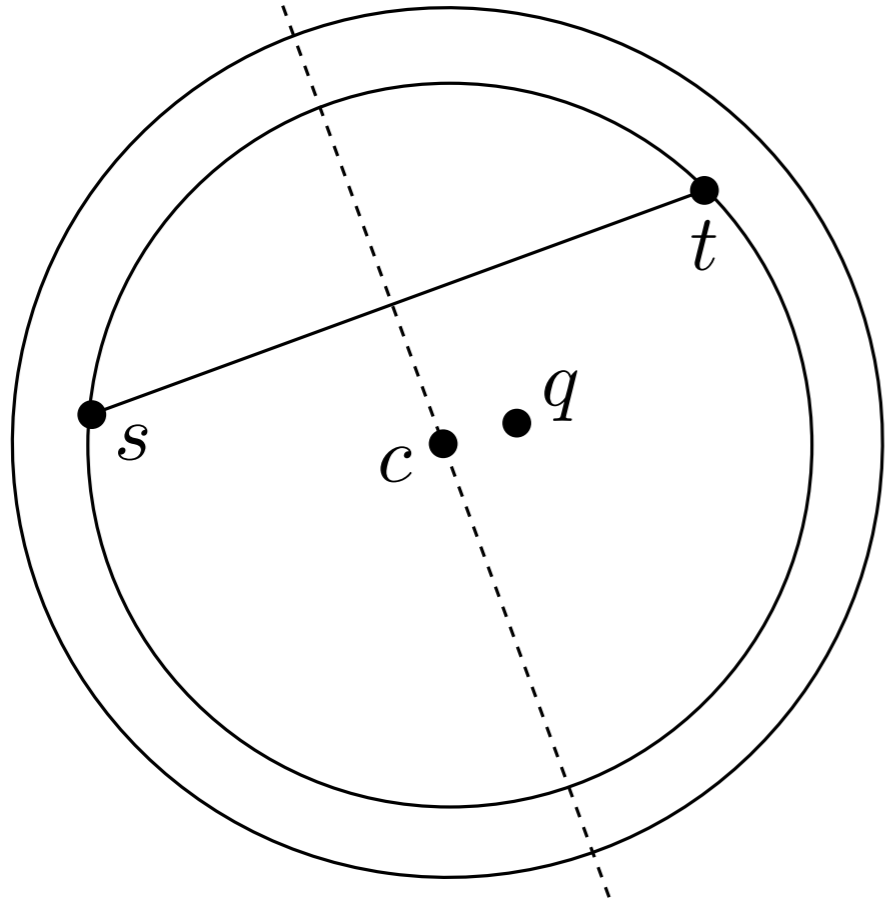
For all s , L_s has to include all Delaunay neighbors of s

For $d > 2$, Delaunay triangulation may have $\Omega(n^2)$ edges

Not Useful for Exact NN

Reason 1: space complexity $\Omega(n^2)$

For all s , L_s has to include all Delaunay neighbors of s



For $d > 2$, Delaunay triangulation may have $\Omega(n^2)$ edges

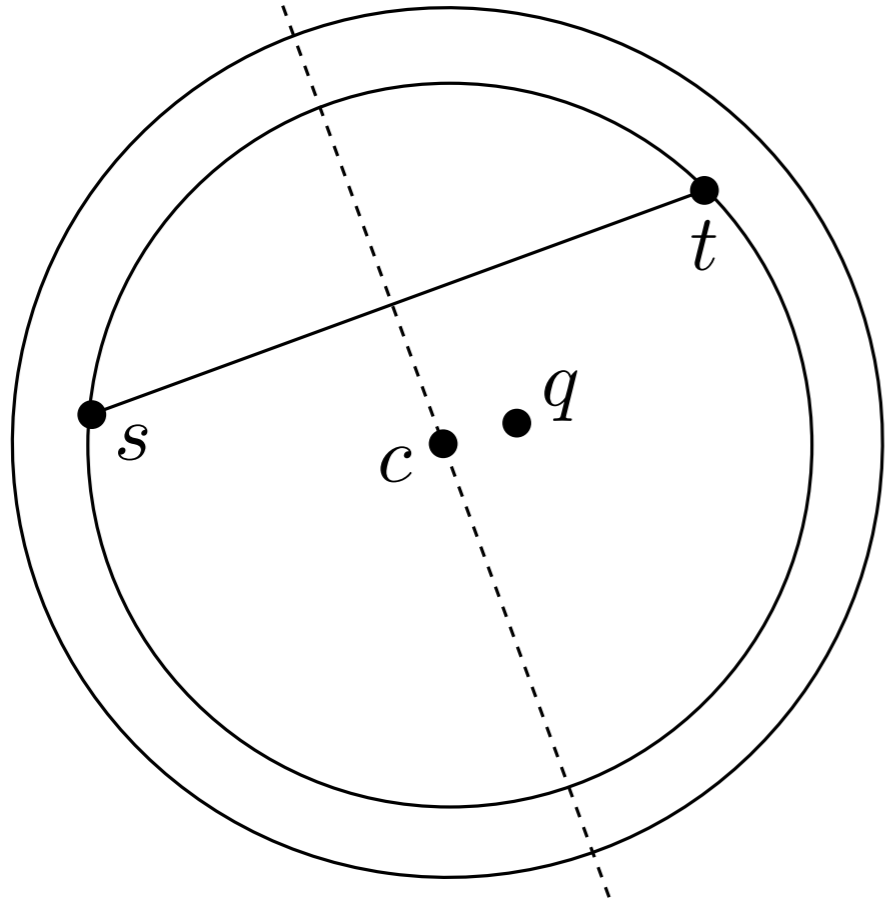
Proof:

t Delaunay neighbor of s , but $t \notin L_s$
 t is the only site closer to q than s

Not Useful for Exact NN

Reason 1: space complexity $\Omega(n^2)$

For all s , L_s has to include all Delaunay neighbors of s



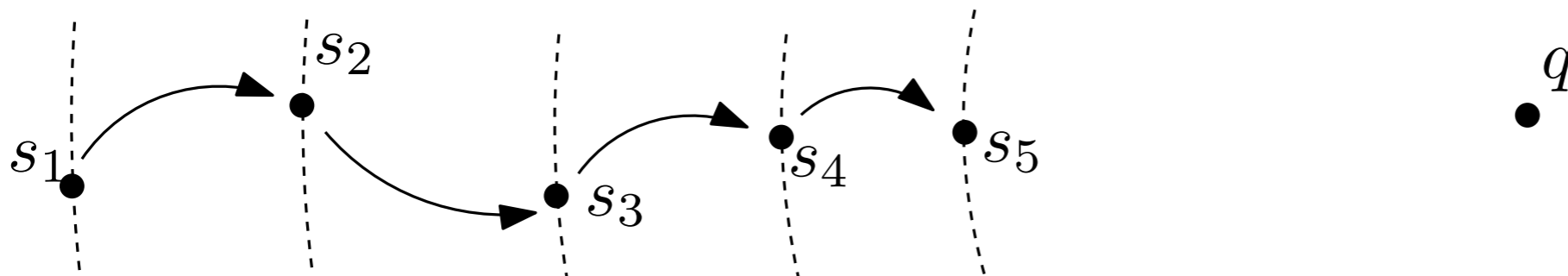
For $d > 2$, Delaunay triangulation may have $\Omega(n^2)$ edges

Proof:

t Delaunay neighbor of s , but $t \notin L_s$
 t is the only site closer to q than s

Reason 2: query time $\Omega(n)$

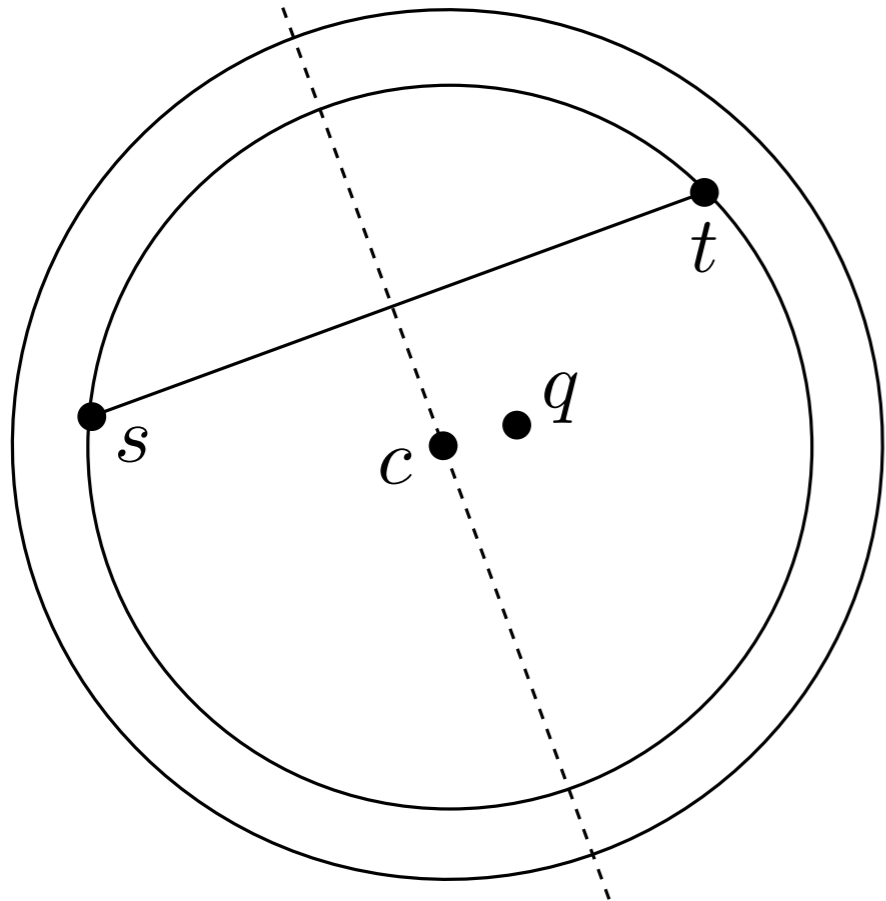
No "sufficient progress" guarantee, may have to visit all sites



Not Useful for Exact NN

Reason 1: space complexity $\Omega(n^2)$

For all s , L_s has to include all Delaunay neighbors of s



For $d > 2$, Delaunay triangulation may have $\Omega(n^2)$ edges

Proof:

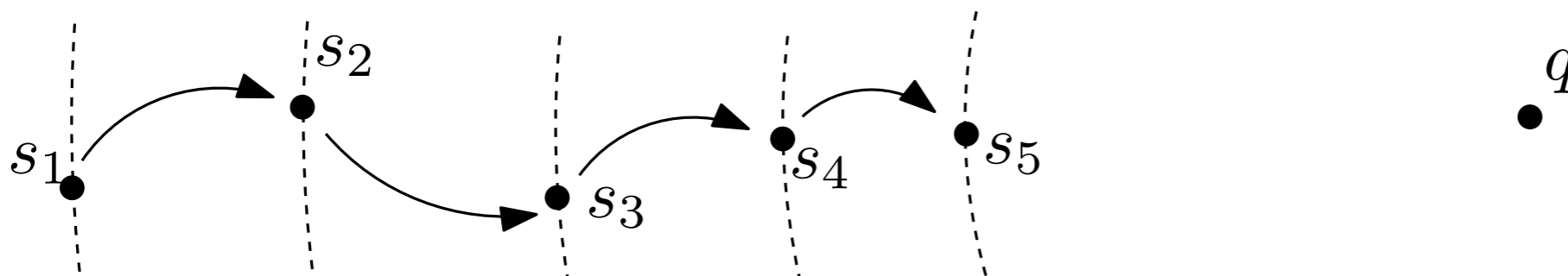
t Delaunay neighbor of s , but $t \notin L_s$
 t is the only site closer to q than s

Conclusion

No improvement over the trivial algorithm!

Reason 2: query time $\Omega(n)$

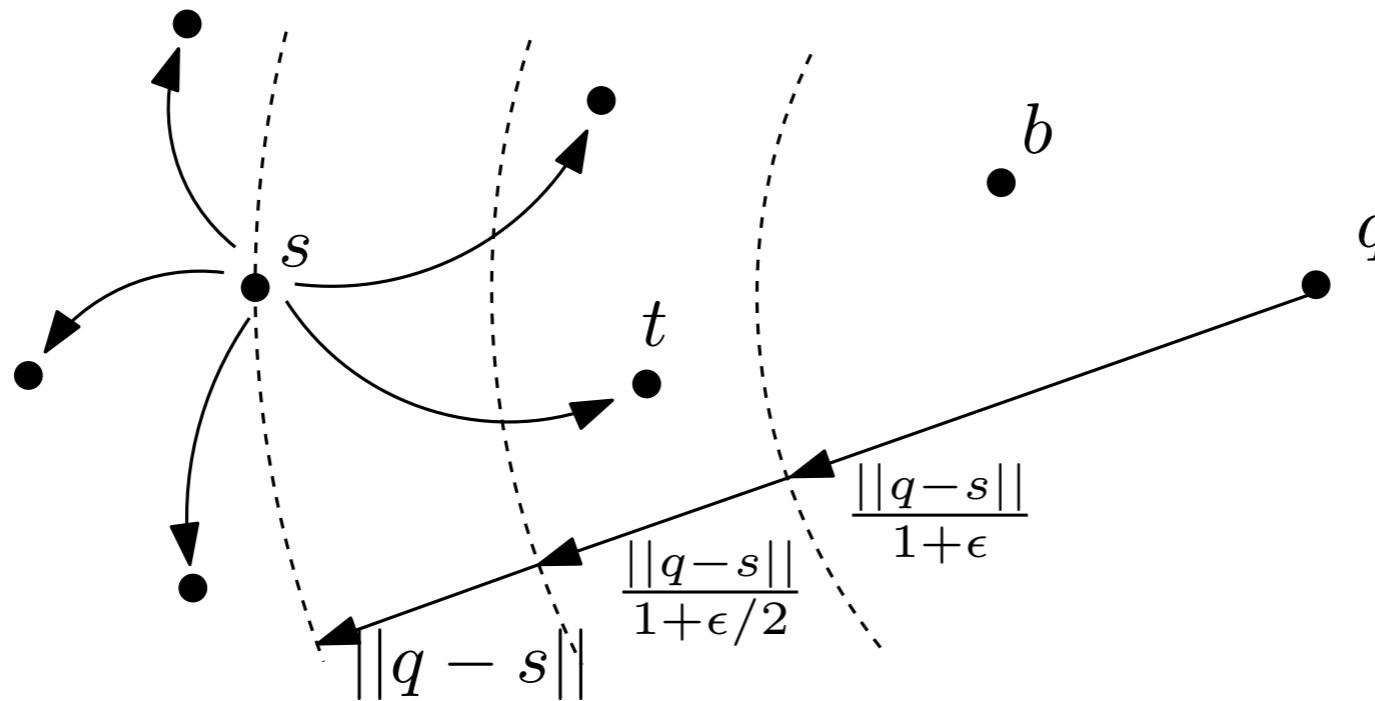
No "sufficient progress" guarantee, may have to visit all sites



Modification for ANN

Data structure For each site s , a (small) list L_s of other sites such that for **any** query point q

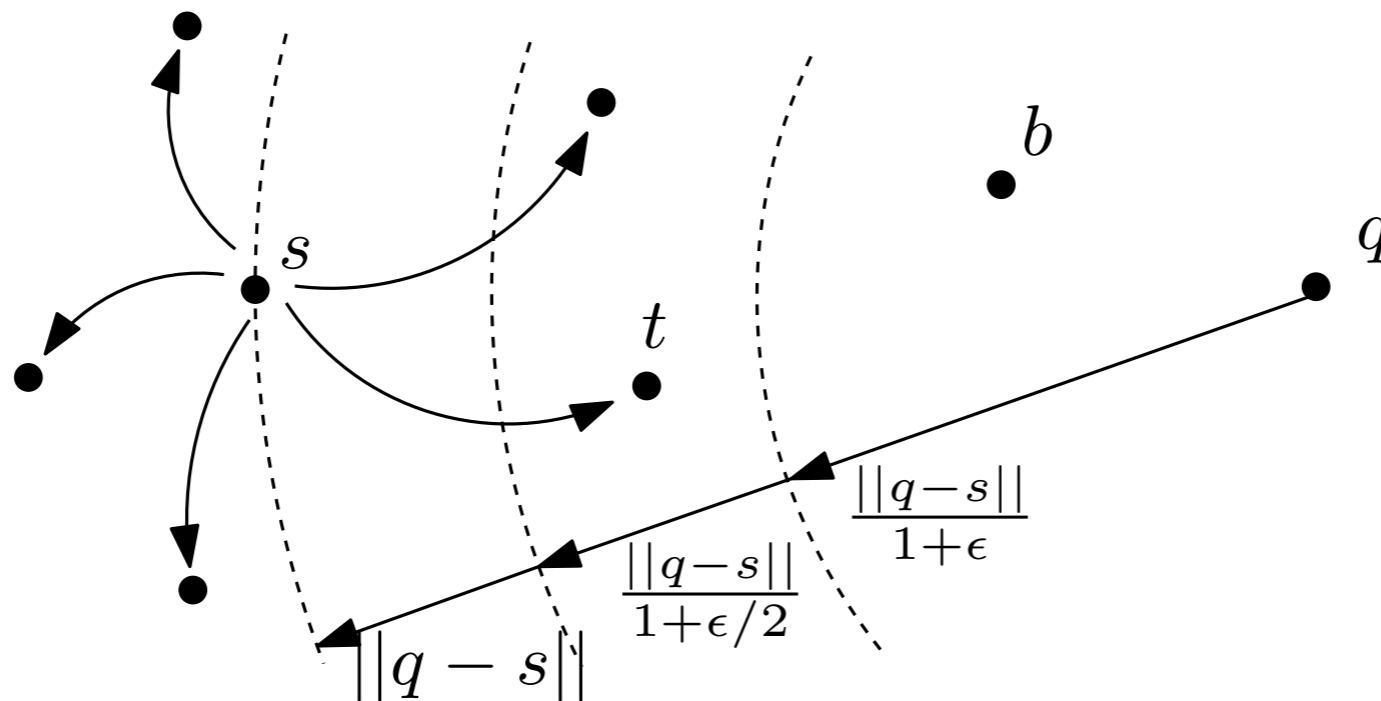
if s is not a $(1 + \epsilon)$ -ANN of q ,
then L_s contains a site $(1 + \epsilon/2)$ -closer to q



Modification for ANN

Data structure For each site s , a (small) list L_s of other sites such that for any query point q

if s is not a $(1 + \epsilon)$ -ANN of q ,
then L_s contains a site $(1 + \epsilon/2)$ -closer to q



Algorithm (simple version)

$s \leftarrow$ arbitrary site

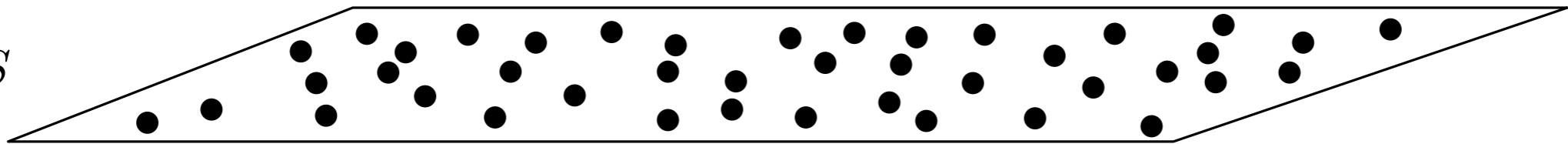
while $\exists t \in L_s : \|q-t\| \leq \frac{\|q-s\|}{1+\epsilon/2}$ do $s \leftarrow t$

return s

Query Algorithm

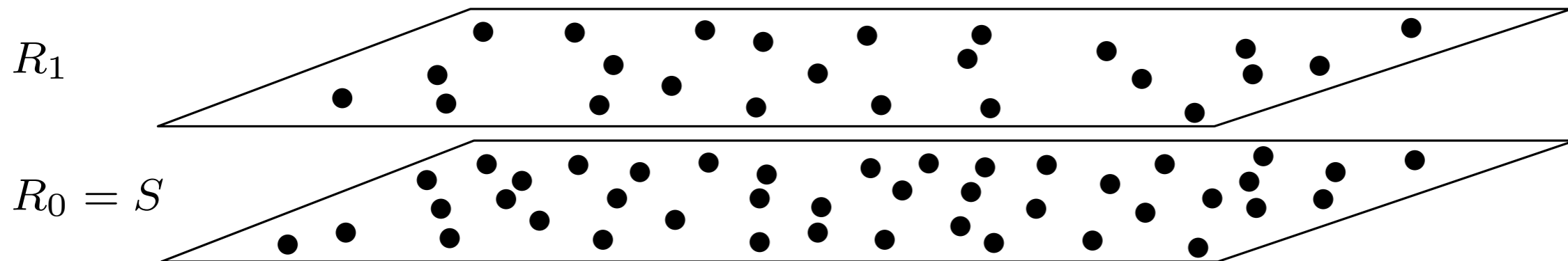
Skip list approach [Arya and Mount 1993]

$R_0 = S$



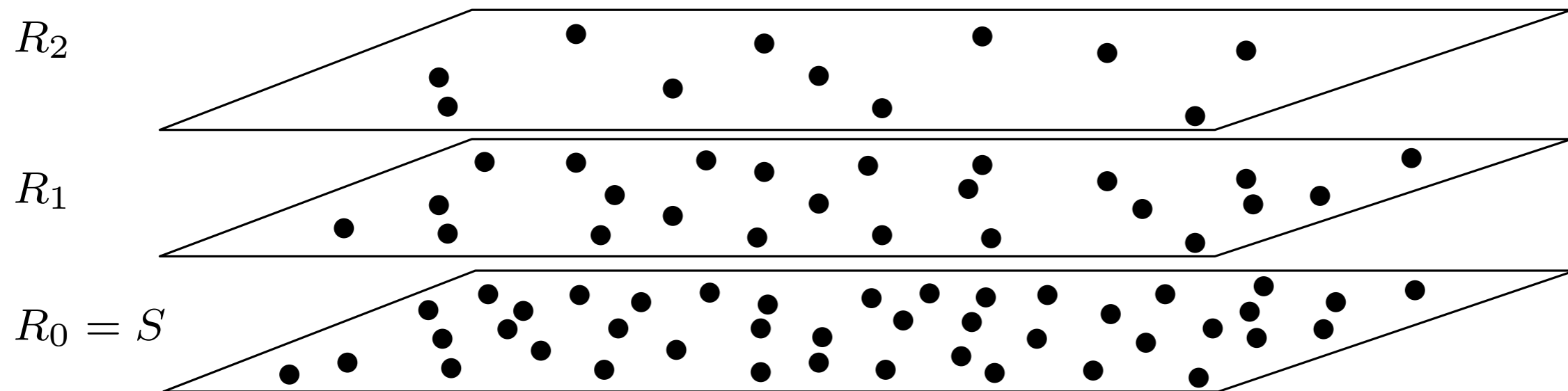
Query Algorithm

Skip list approach [Arya and Mount 1993]



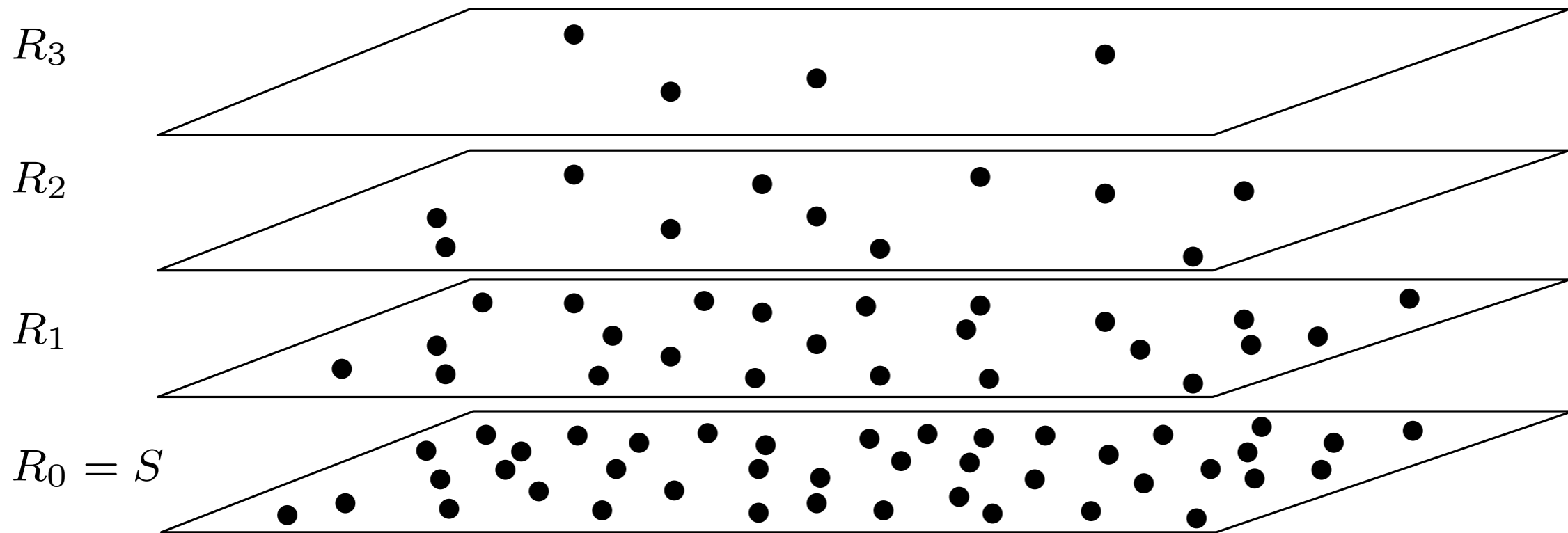
Query Algorithm

Skip list approach [Arya and Mount 1993]



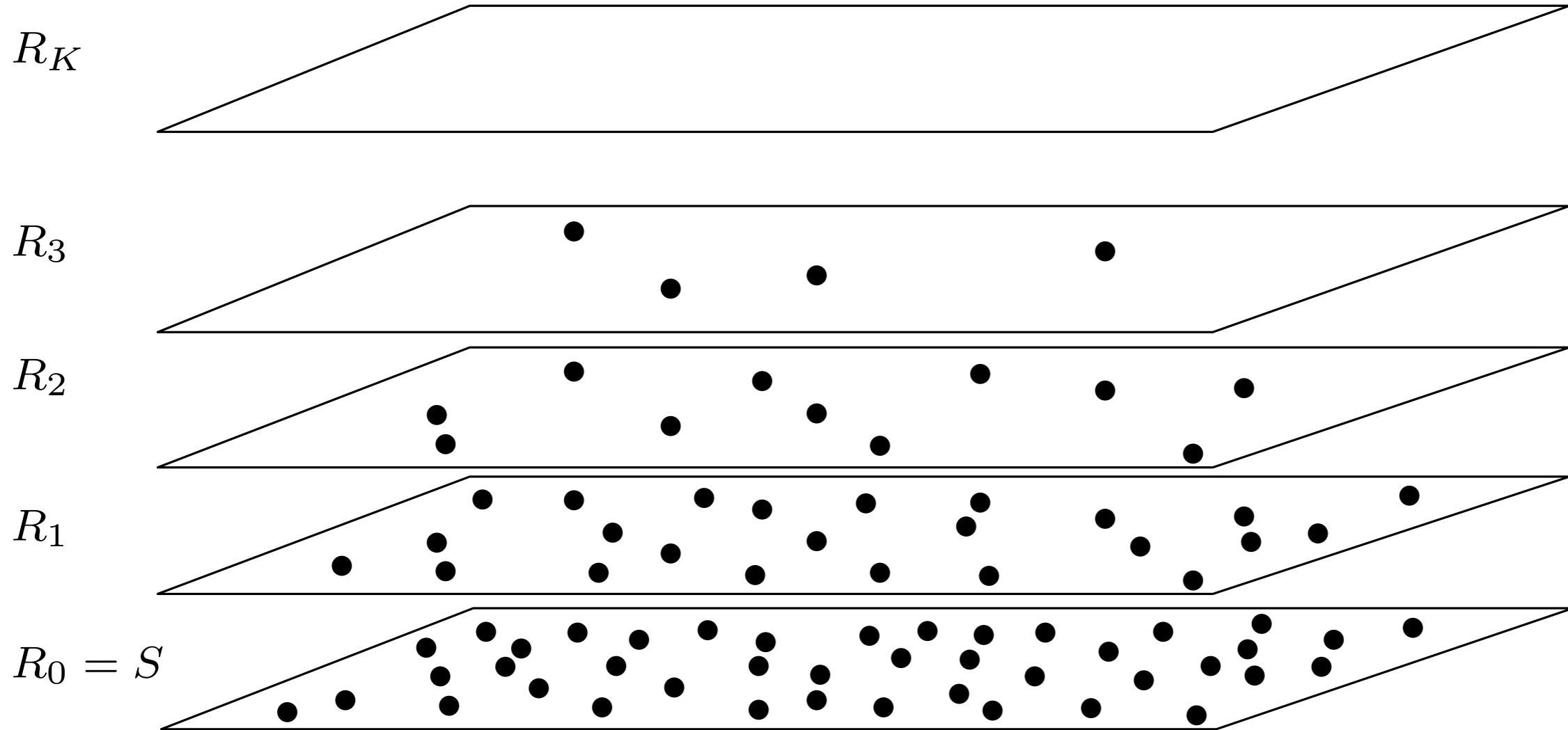
Query Algorithm

Skip list approach [Arya and Mount 1993]



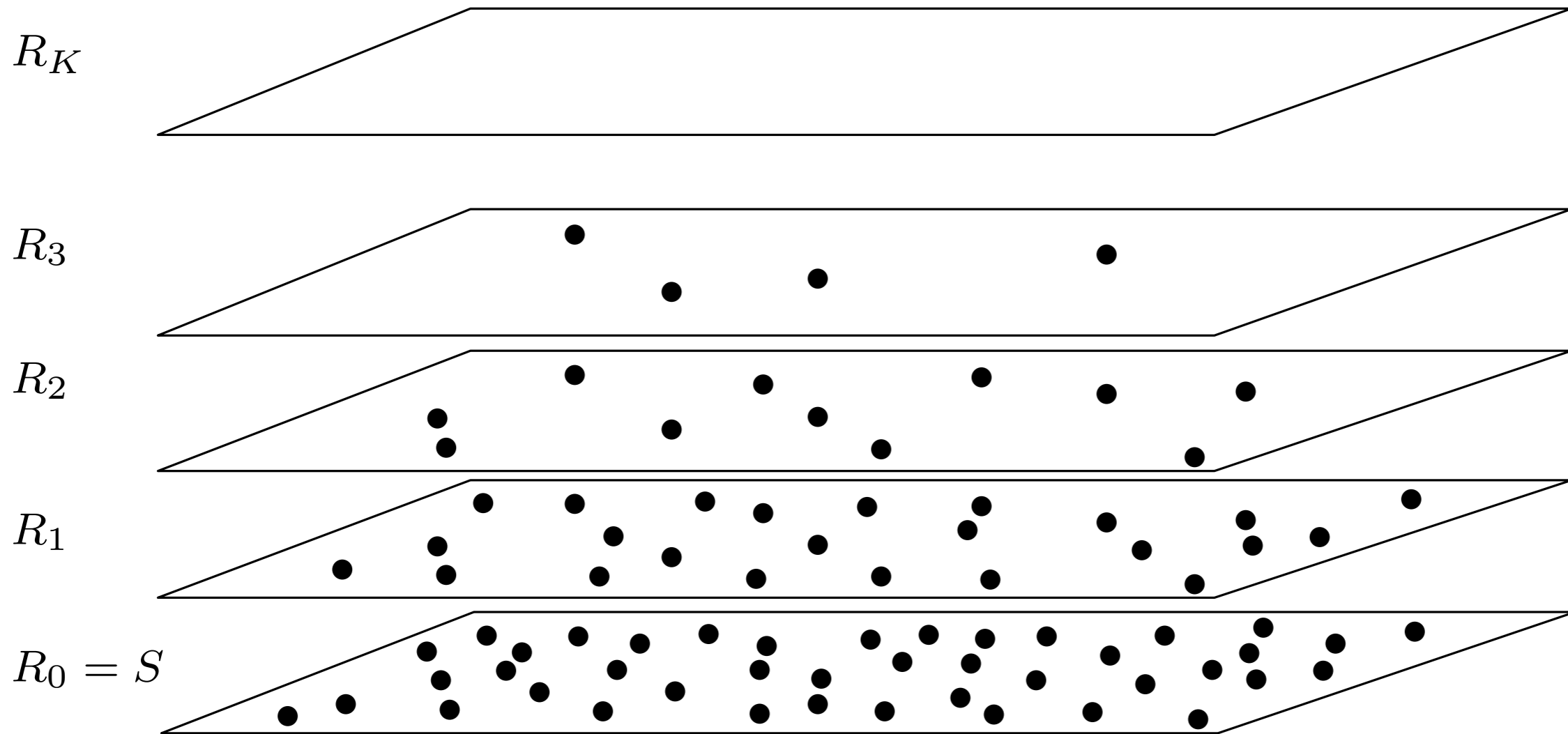
Query Algorithm

Skip list approach [Arya and Mount 1993]



Query Algorithm

Skip list approach [Arya and Mount 1993]



Algorithm

- start with any $t_{K-1} \in R_{K-1}$
 - for $j = K - 2, K - 3, \dots, 0$
 - find $t_j = (1 + \epsilon)$ -ANN of q in R_j starting from t_{j+1}
 - return t_0
- [using naive algorithm]
-

Query Time Analysis

Suppose that any node's list size is at most c

Observation: Query time = $c \cdot$ number of visited nodes

Compare with a [regular path](#)

- Visit nodes [in the order of proximity to \$q\$](#) , then go to the lower level

Query Time Analysis

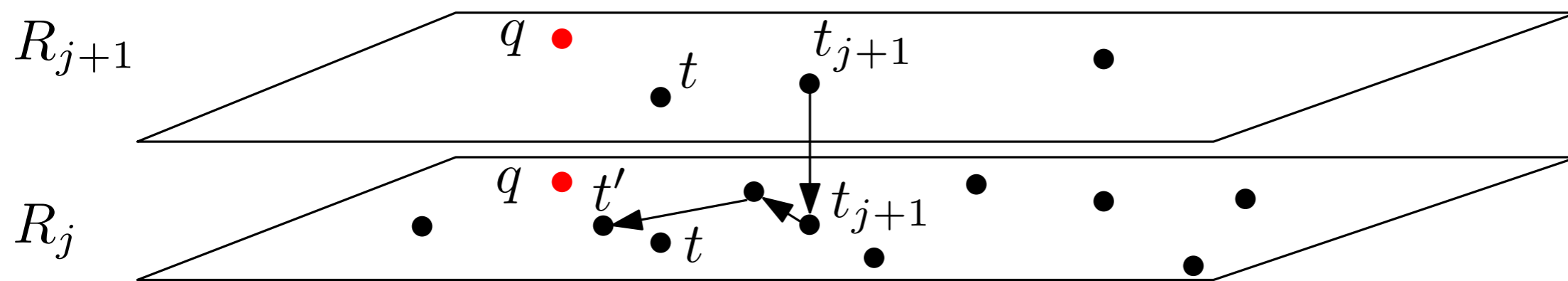
Suppose that any node's list size is at most c

Observation: Query time = $c \cdot$ number of visited nodes

Compare with a **regular path**

- Visit nodes **in the order of proximity to q** , then go to the lower level

Claim: Our path visits at most $2K$ nodes more



$$(1 + \epsilon/2)^2 \geq 1 + \epsilon \quad \Rightarrow \quad \|q - t'\| \leq \|q - t\|$$

Query Time Analysis

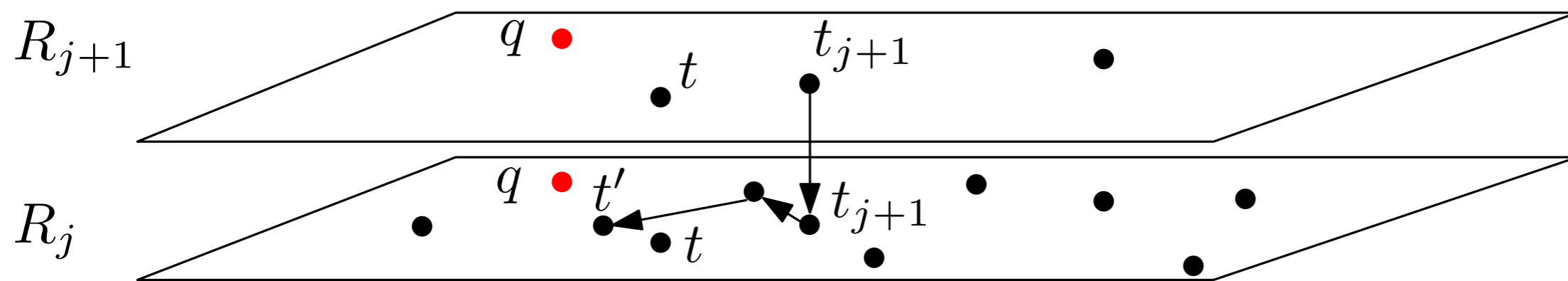
Suppose that any node's list size is at most c

Observation: Query time = $c \cdot$ number of visited nodes

Compare with a **regular path**

- Visit nodes **in the order of proximity to q** , then go to the lower level

Claim: Our path visits at most $2K$ nodes more



$$(1 + \epsilon/2)^2 \geq 1 + \epsilon \quad \Rightarrow \quad \|q - t'\| \leq \|q - t\|$$

$$\Pr[\text{regular path length} \geq C \log n] \leq O(n^{-C})$$

[distribution of points across levels]
[starting search point]

Query Time Analysis

What about *any* q ?

Skip list

n possible search targets

Probability of failure $n \cdot O(n^{-C}) = O(n^{-(C-1)})$

Query Time Analysis

What about *any* q ?

Skip list

n possible search targets

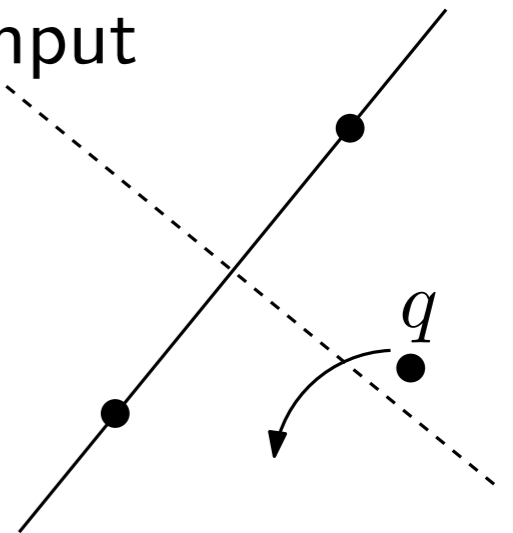
Probability of failure $n \cdot O(n^{-C}) = O(n^{-(C-1)})$

Only $n^{O(d)}$ "combinatorially distinct" regular paths

- If q_1 and q_2 include the same distance ordering on the input sites, their regular paths are the same
- Arrangement of $\binom{n}{2}$ bisecting hyperplanes has

$$\binom{\binom{n}{2}}{d} \leq (n^2)^d = n^{2d}$$

d -dimensional cells



Query Time Analysis

What about *any* q ?

Skip list

n possible search targets

Probability of failure $n \cdot O(n^{-C}) = O(n^{-(C-1)})$

Only $n^{O(d)}$ "combinatorially distinct" regular paths

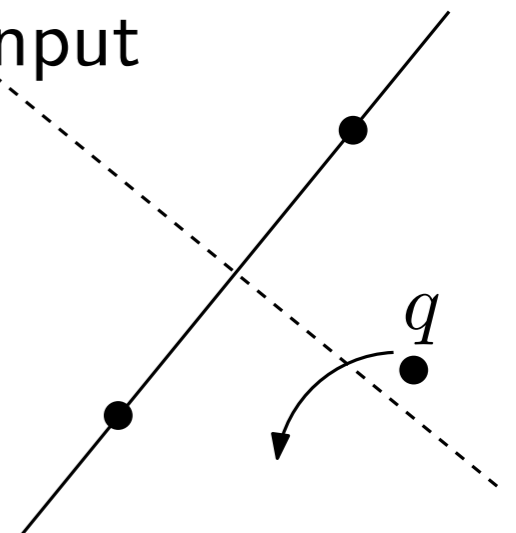
- If q_1 and q_2 include the same distance ordering on the input sites, their regular paths are the same
- Arrangement of $\binom{n}{2}$ bisecting hyperplanes has

$$\binom{\binom{n}{2}}{d} \leq (n^2)^d = n^{2d}$$

d -dimensional cells

Setting $C = 2d + C'$

$$\Pr[\text{regular path length} \leq O(d) \log n] = O(n^{-C'})$$



Weighted Voronoi Diagrams

Goal For each site s , compute L_s such that

$$\forall q \in \mathbb{R}^d$$

$$\forall b \in S : \|q - b\| \geq \frac{\|q - s\|}{1 + \epsilon}$$

[s is an $(1 + \epsilon)$ -ANN of q]

\Leftrightarrow

$$\forall t \in L_s : \|q - t\| \geq \frac{\|q - s\|}{1 + \epsilon/2}$$

[no "improvement" in L_s]

Weighted Voronoi Diagrams

Goal For each site s , compute L_s such that

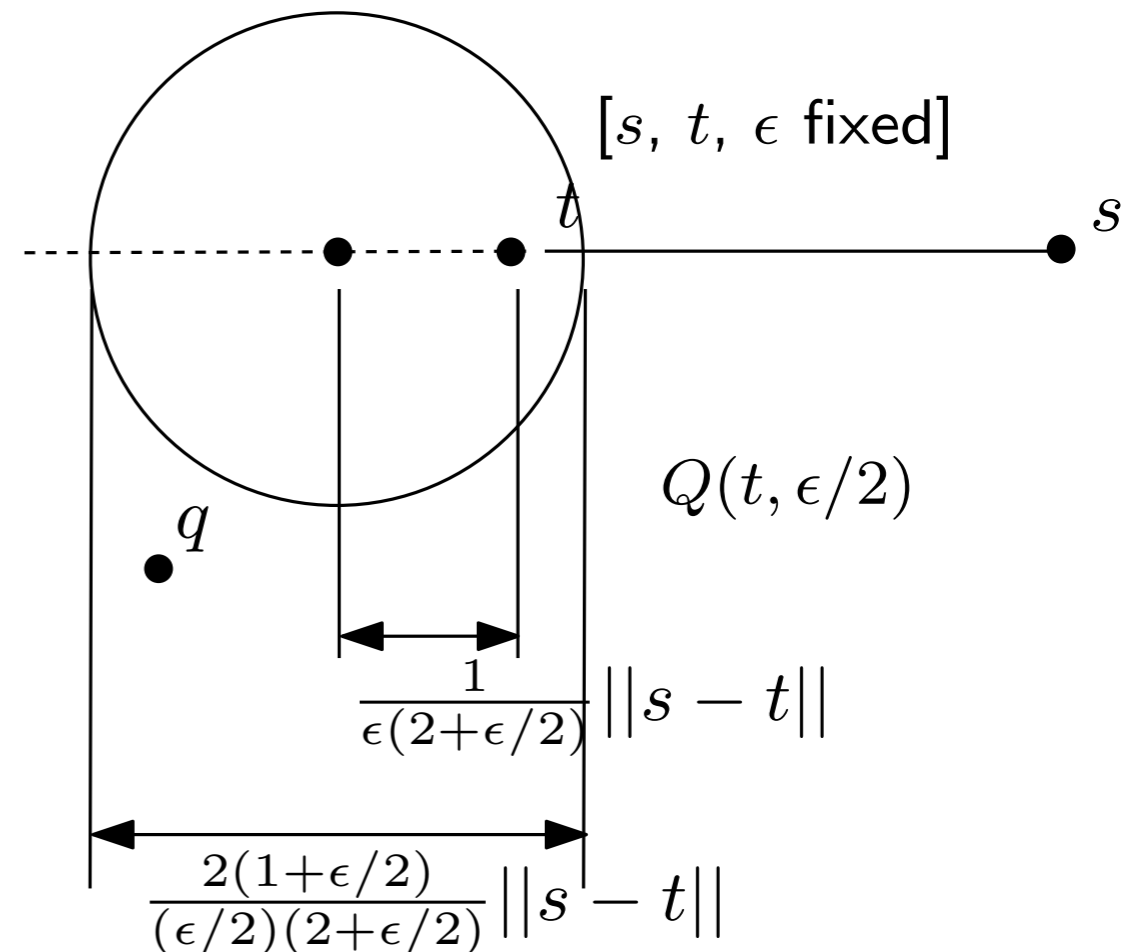
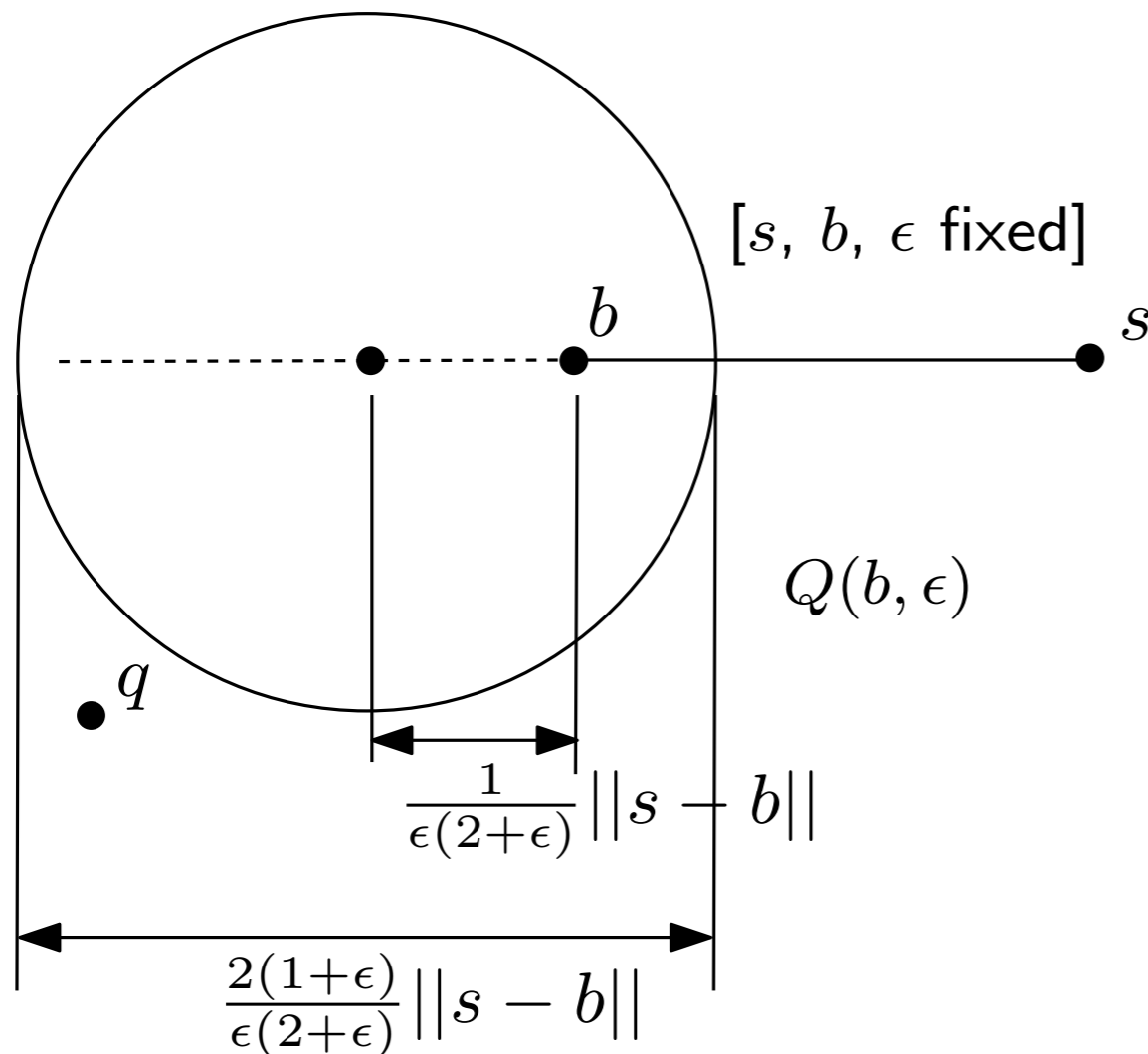
$$\forall q \in \mathbb{R}^d$$

$$\forall b \in S : \|q - b\| \geq \frac{\|q - s\|}{1 + \epsilon} \quad \Leftrightarrow$$

[s is an $(1 + \epsilon)$ -ANN of q]

$$\forall t \in L_s : \|q - t\| \geq \frac{\|q - s\|}{1 + \epsilon/2}$$

[no "improvement" in L_s]



Weighted Voronoi Diagrams

Goal For each site s , compute L_s such that

$$\forall q \in \mathbb{R}^d$$

$$\forall b \in S : \|q - b\| \geq \frac{\|q - s\|}{1 + \epsilon} \quad \Leftrightarrow$$

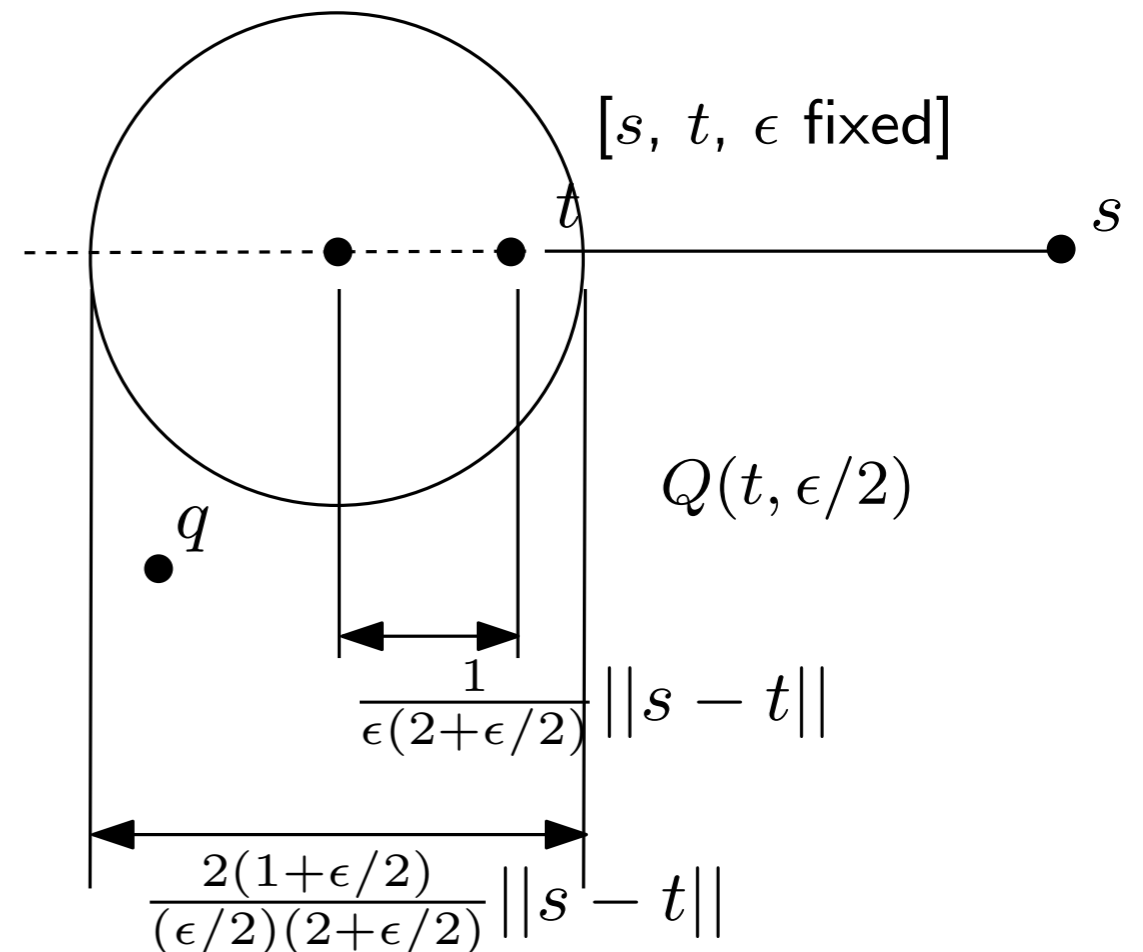
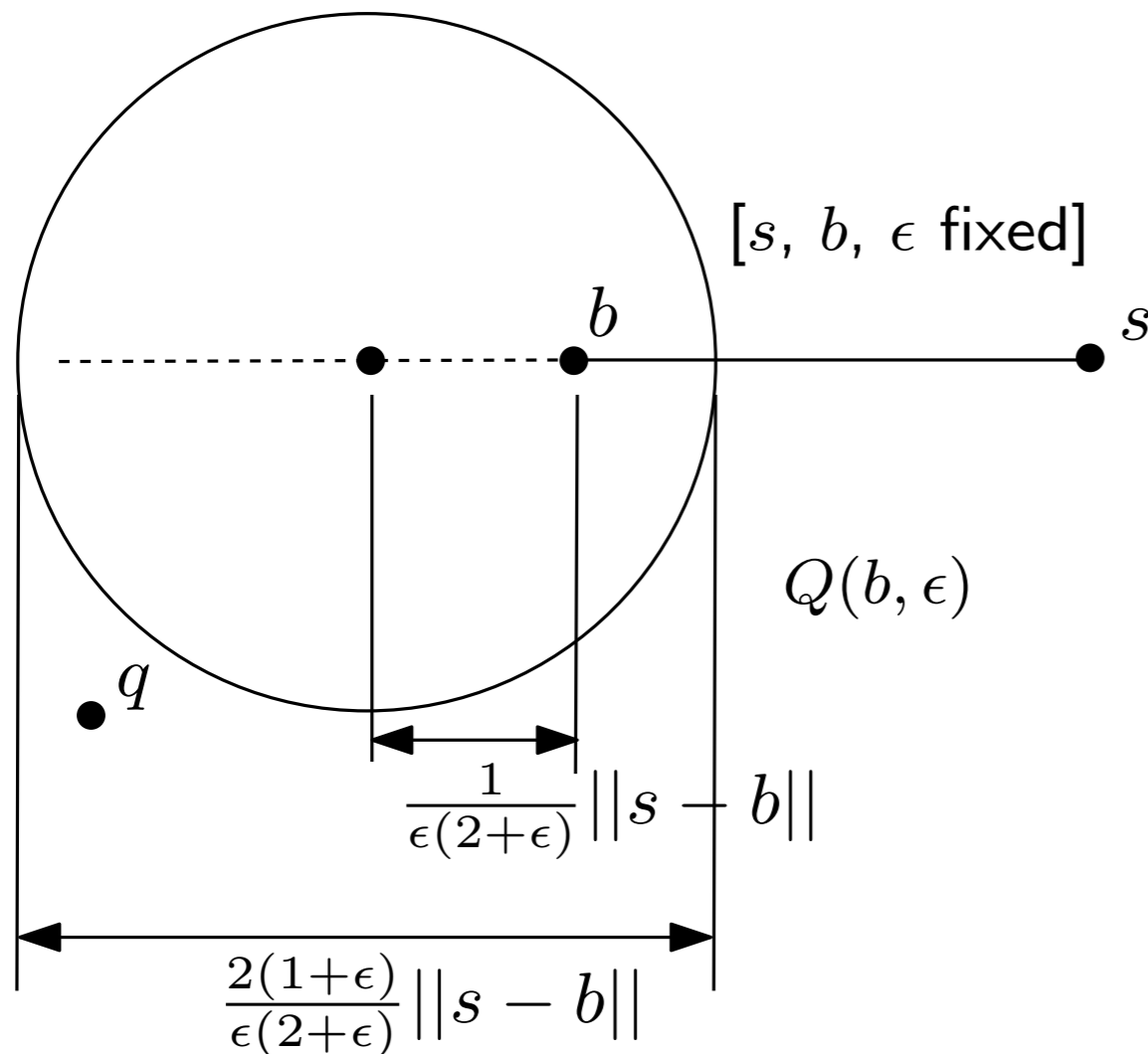
[s is an $(1 + \epsilon)$ -ANN of q]

$$\forall b \in S : q \in Q(b, \epsilon) \quad \Leftrightarrow$$

$$\forall t \in L_s : \|q - t\| \geq \frac{\|q - s\|}{1 + \epsilon/2}$$

[no "improvement" in L_s]

$$\forall t \in L_s : q \in Q(t, \epsilon/2)$$



Weighted Voronoi Diagrams

Goal For each site s , compute L_s such that

$$\forall q \in \mathbb{R}^d$$

$$\forall b \in S : \|q - b\| \geq \frac{\|q - s\|}{1 + \epsilon} \quad \Leftrightarrow$$

[s is an $(1 + \epsilon)$ -ANN of q]

$$\forall b \in S : q \in Q(b, \epsilon) \quad \Leftrightarrow$$

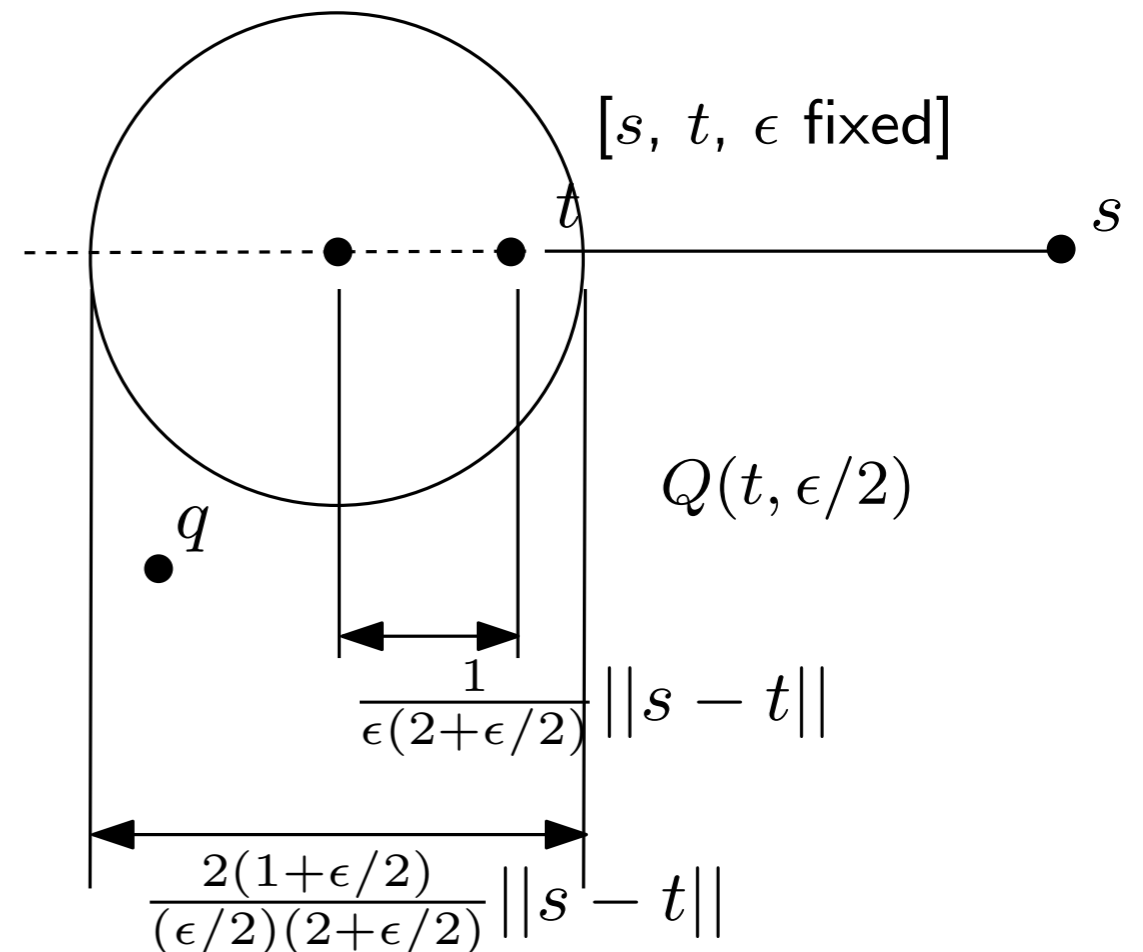
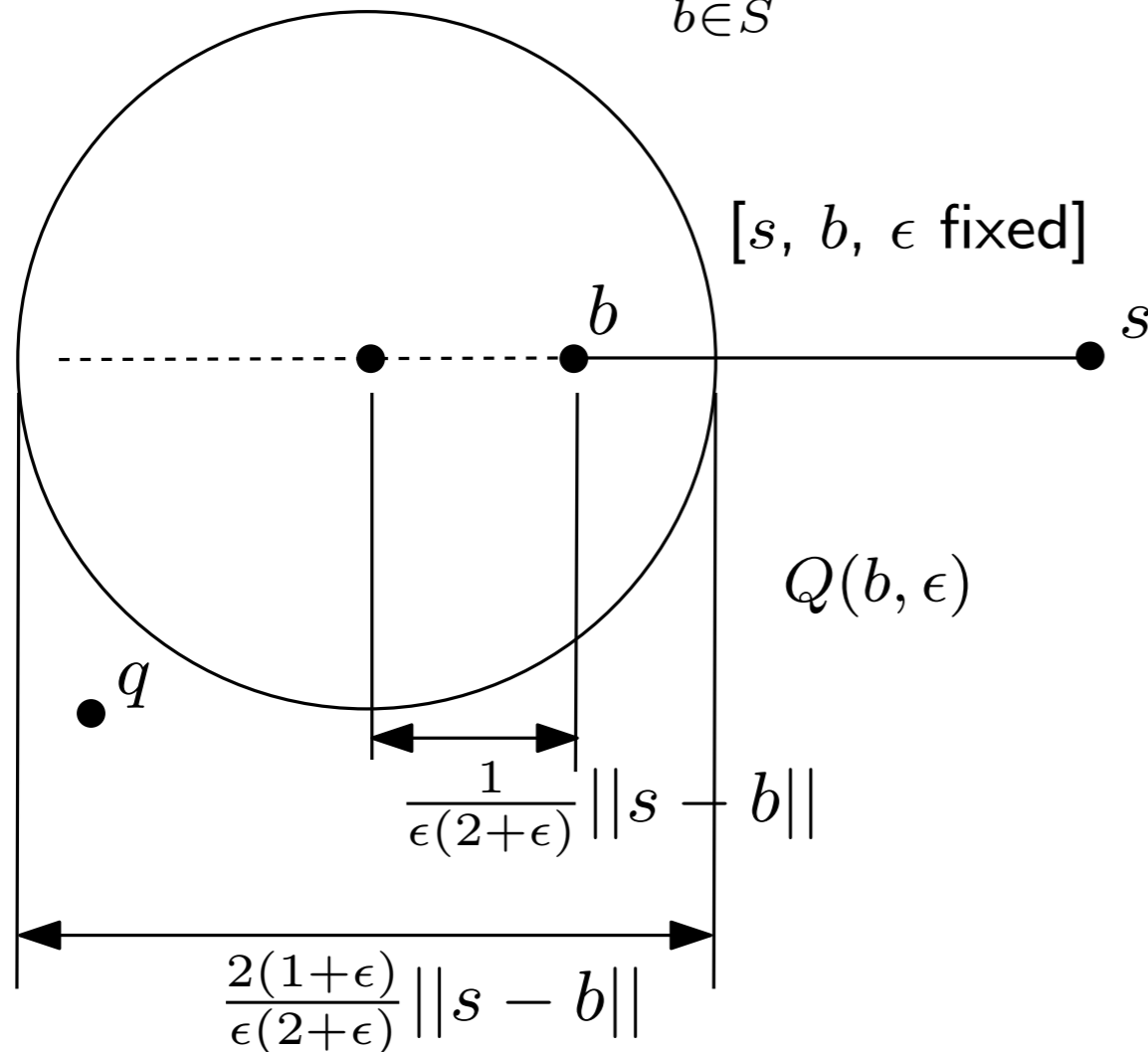
$$\bigcap_{b \in S} Q(b, \epsilon) \quad \supseteq$$

$$\forall t \in L_s : \|q - t\| \geq \frac{\|q - s\|}{1 + \epsilon/2}$$

[no "improvement" in L_s]

$$\forall t \in L_s : q \in Q(t, \epsilon/2)$$

$$\bigcap_{t \in L_s} Q(t, \epsilon/2)$$



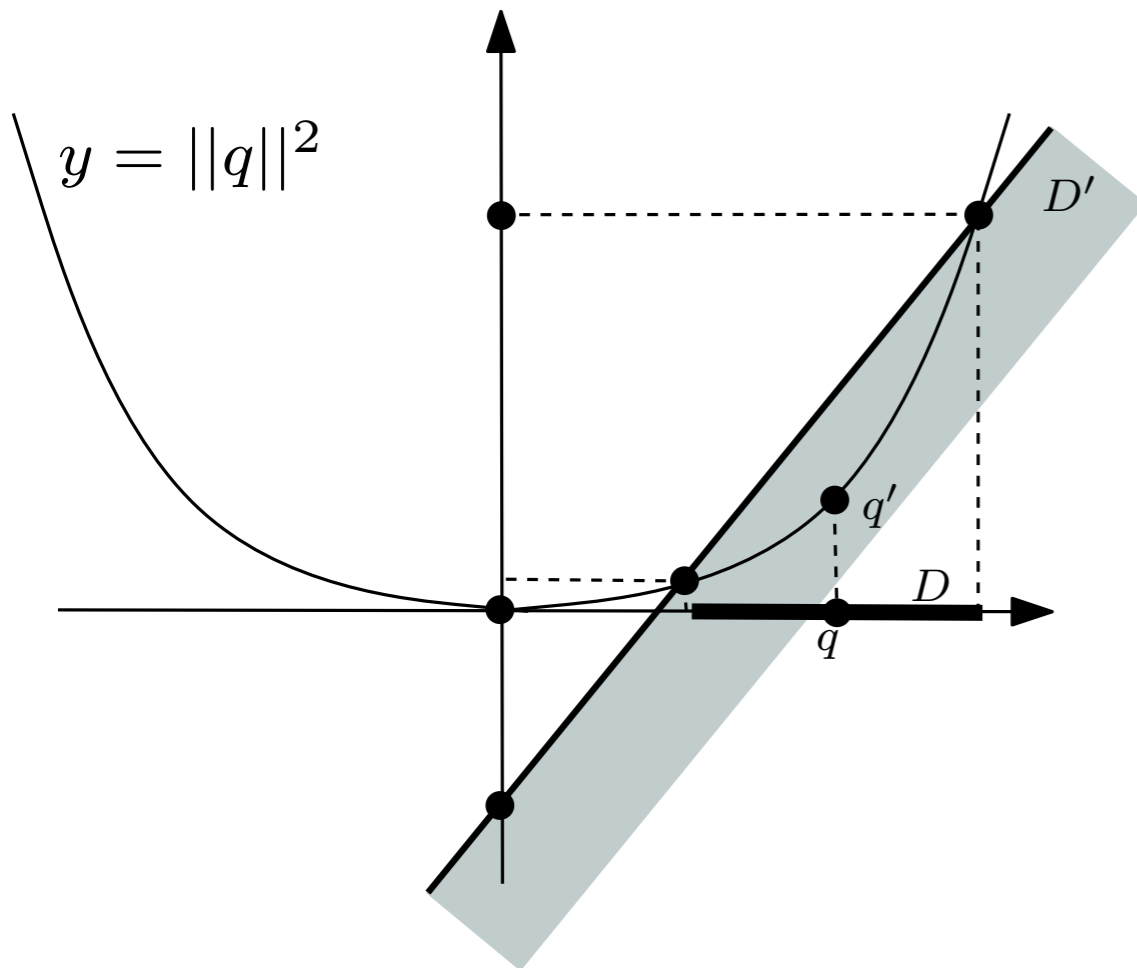
Linearization ("Lifting")

A point **inside/outside** a sphere in \mathbb{R}^d ?



A point **above/below** a hyperplane in \mathbb{R}^{d+1} ?

Example for $d=1$



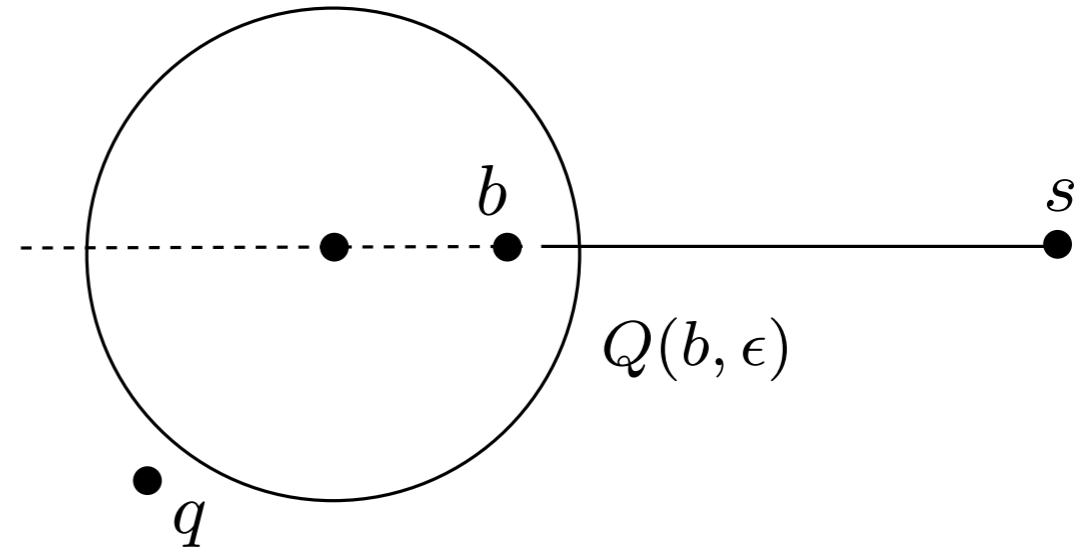
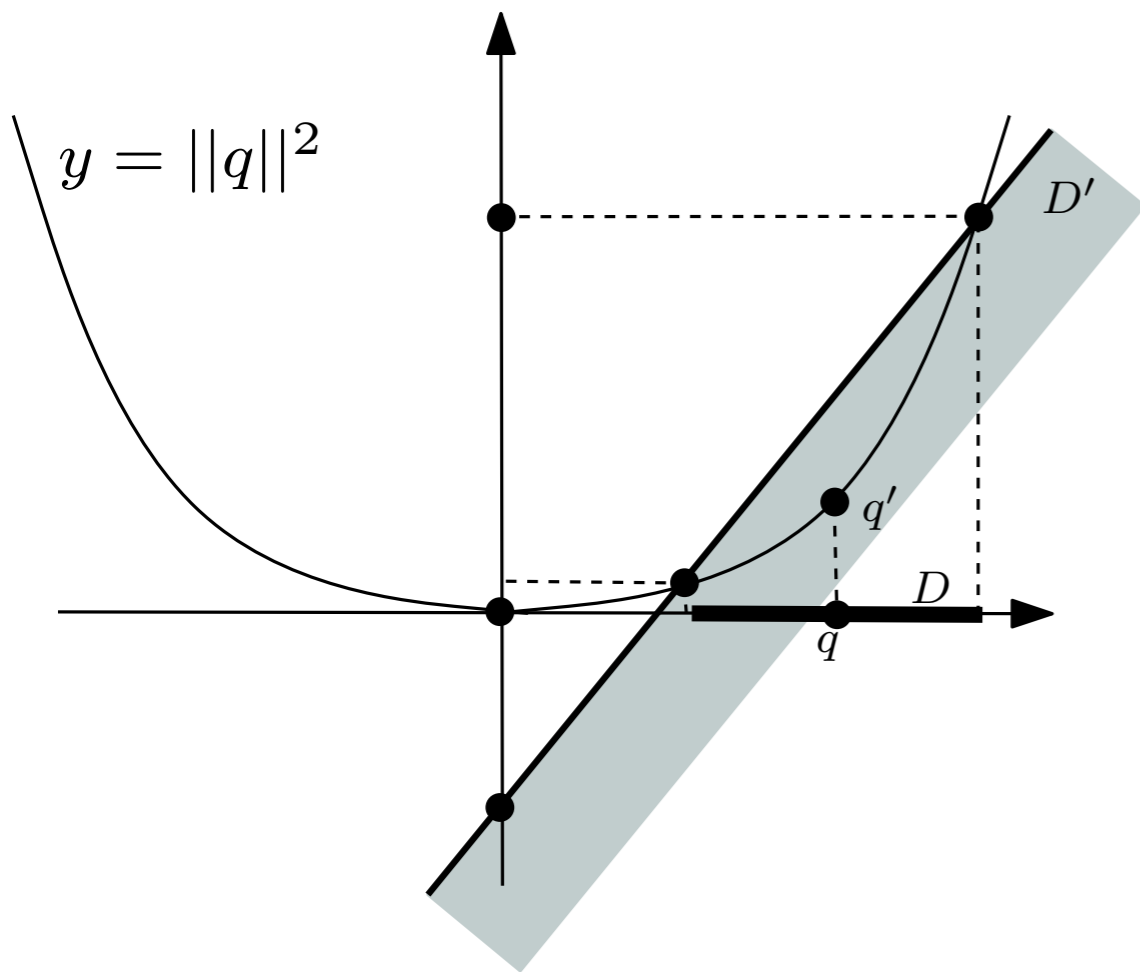
Linearization ("Lifting")

A point **inside/outside** a sphere in \mathbb{R}^d ?



A point **above/below** a hyperplane in \mathbb{R}^{d+1} ?

Example for $d=1$



$$Q(b, \epsilon) = \{q \in \mathbb{R}^d : \|q - s\| \leq (1 + \epsilon)\|q - b\|\}$$

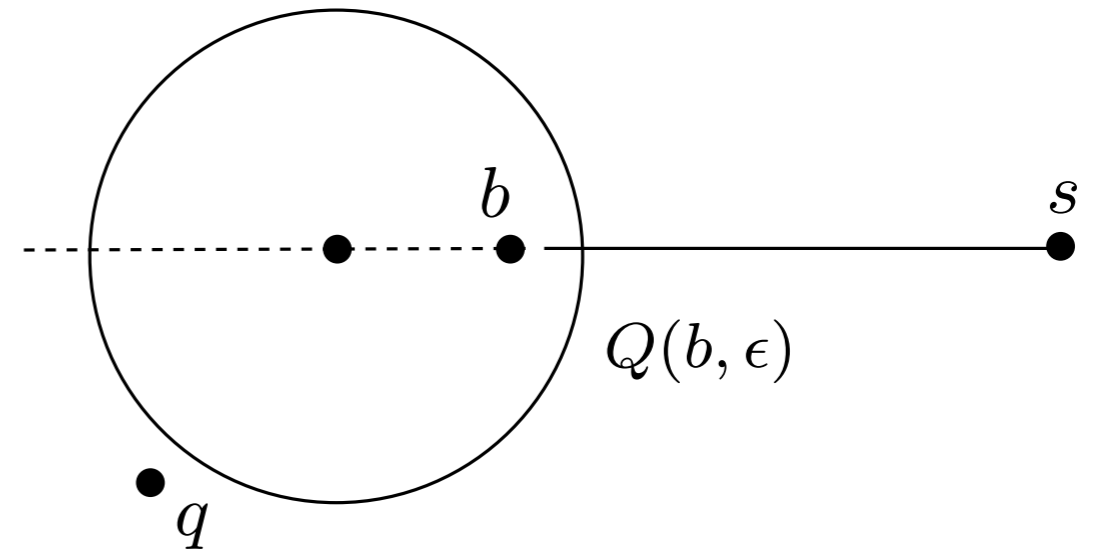
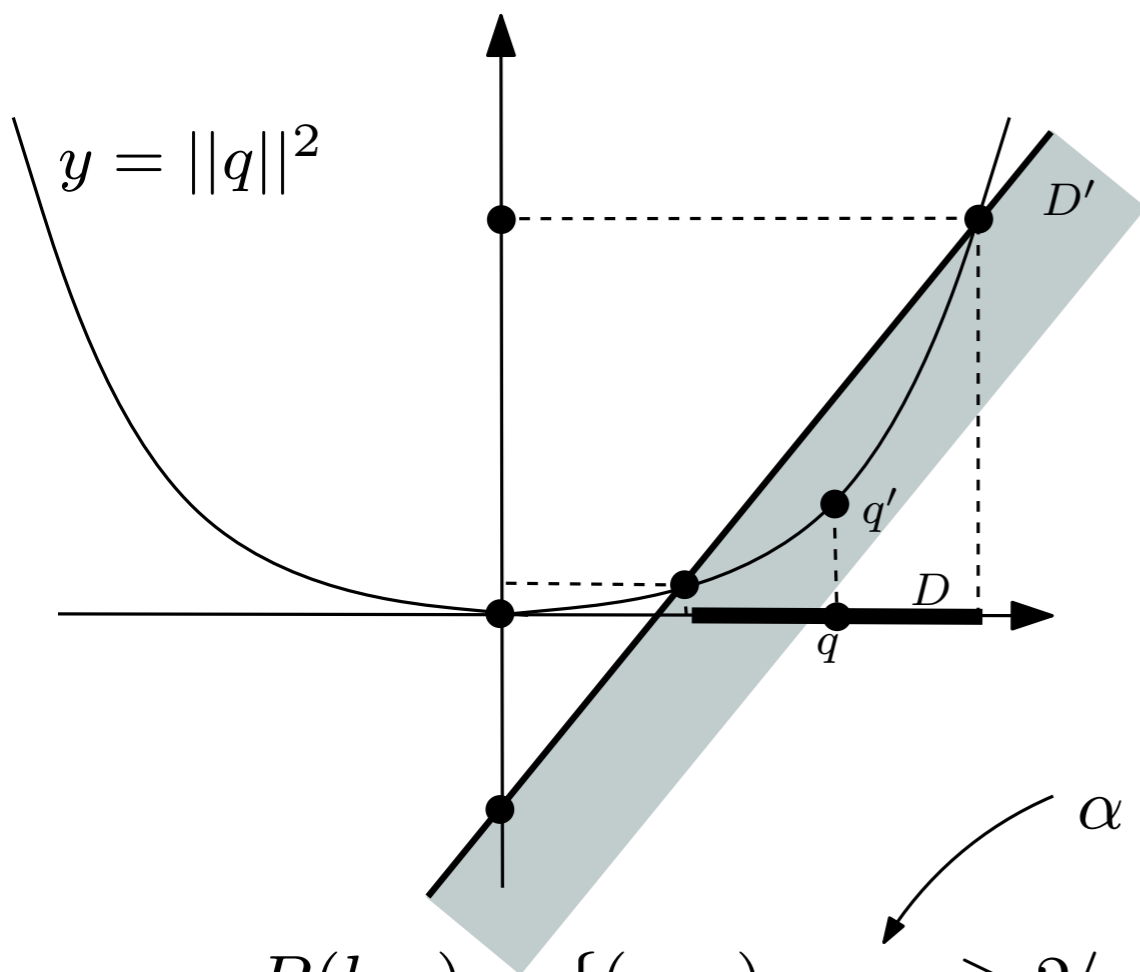
Linearization ("Lifting")

A point **inside/outside** a sphere in \mathbb{R}^d ?



A point **above/below** a hyperplane in \mathbb{R}^{d+1} ?

Example for $d=1$



$$Q(b, \epsilon) = \{q \in \mathbb{R}^d : \|q - s\| \leq (1 + \epsilon)\|q - b\|\}$$

$$\alpha \approx 2\epsilon$$

$$P(b, \epsilon) = \{(q, y) : \alpha y \geq 2\langle q, b \rangle - \|b\|^2\} \cap \{(q, y) : y = \|q\|^2\}$$

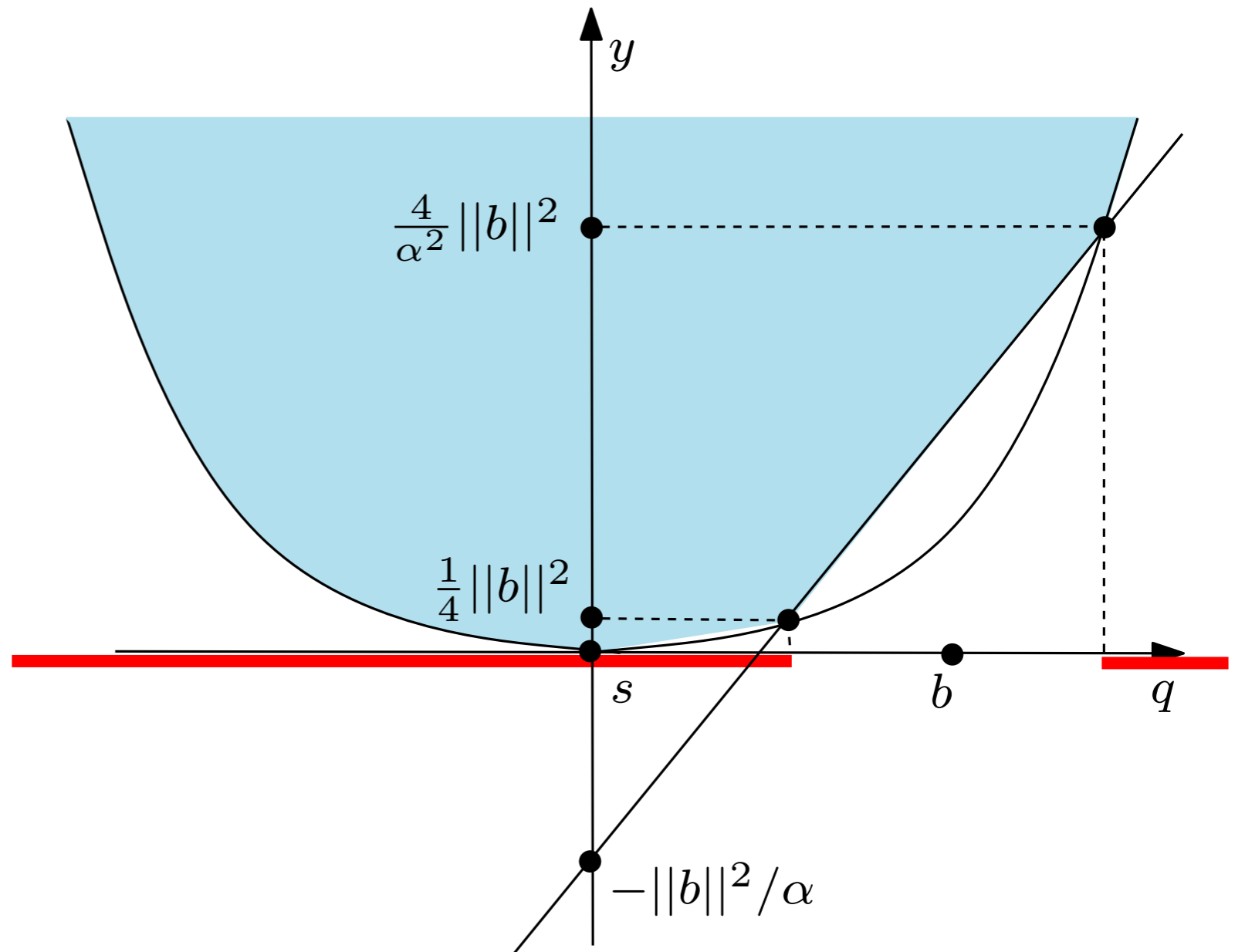
$H(b, \epsilon)$, halfspace in \mathbb{R}^{d+1}
(note: contains the origin)

Ψ , standard paraboloid in \mathbb{R}^{d+1}
(note: independent of b, ϵ)

Final Formulation

Paraboloid

$$\Psi = \{(q, y) : y = \|q\|^2\}$$



Final Formulation

Paraboloid

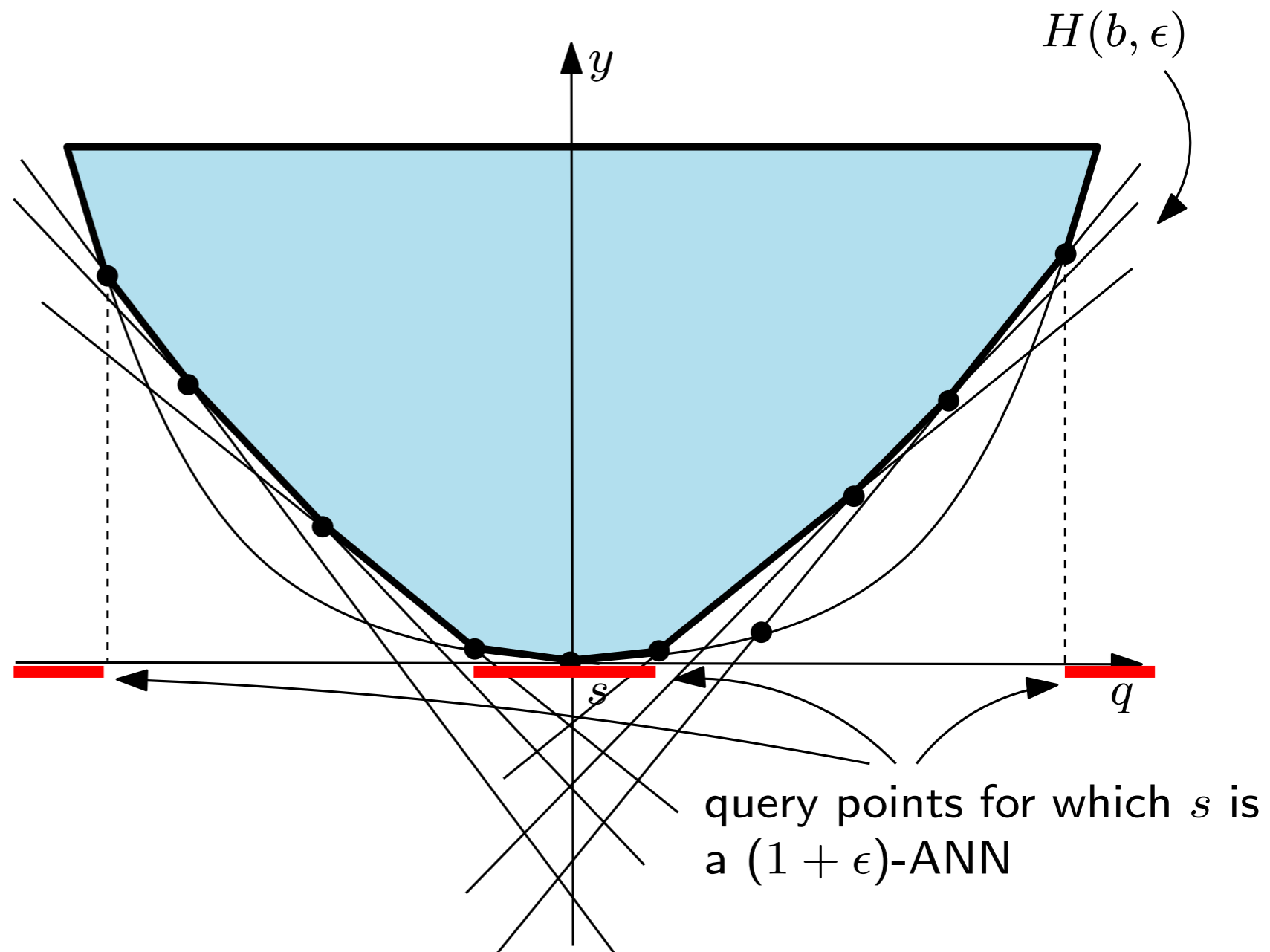
$$\Psi = \{(q, y) : y = \|q\|^2\}$$

Halfspaces

$$H(b, \epsilon) = \{(q, y) : \alpha y \geq 2\langle b, q \rangle - \|b\|^2\}$$

for all $b \in S$

) [can compute using S and ϵ]



Final Formulation

Paraboloid

$$\Psi = \{(q, y) : y = \|q\|^2\}$$

Halfspaces

$$H(b, \epsilon) = \{(q, y) : \alpha y \geq 2\langle b, q \rangle - \|b\|^2\}$$

for all $b \in S$

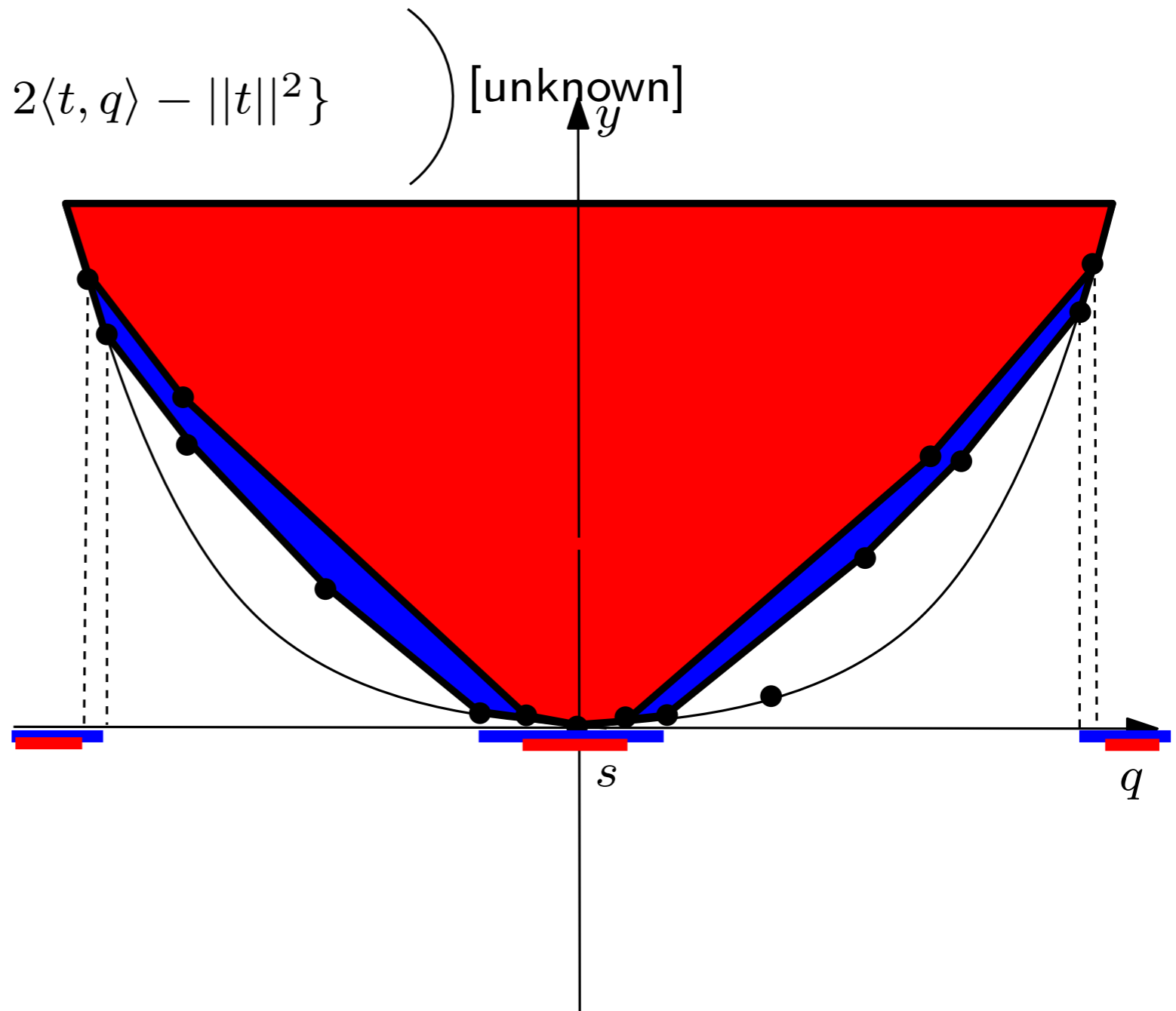
) [can compute using S and ϵ]

Halfspaces

$$G(t, \epsilon' = \epsilon/2) = \{(q, y) : \alpha' y \geq 2\langle t, q \rangle - \|t\|^2\}$$

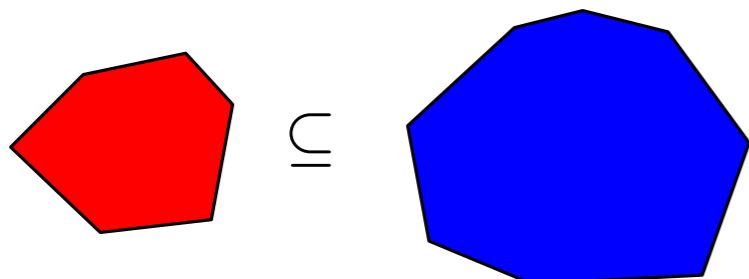
for all $t \in L_s$

) [unknown]



Goal

It suffices to make sure that



Preprocessing

initialize the weight of all sites to 1

repeat

pick a (weighted) random sample $R \subseteq S$ of size $C_1 cd \log c$

if $\bigcap_{t \in R} G(t, \epsilon/2) \cap \Psi \subseteq \bigcap_{b \in S} H(b, \epsilon)$

return R

else

$v =$ a violating vertex of $\bigcap_{t \in R} G(t, \epsilon/2) \cap \Psi$

double the weight of $V = \{t \in S \setminus R : v \notin G(t, \epsilon/2)\}$

The sample size depends on c , the **optimal** size of L_S

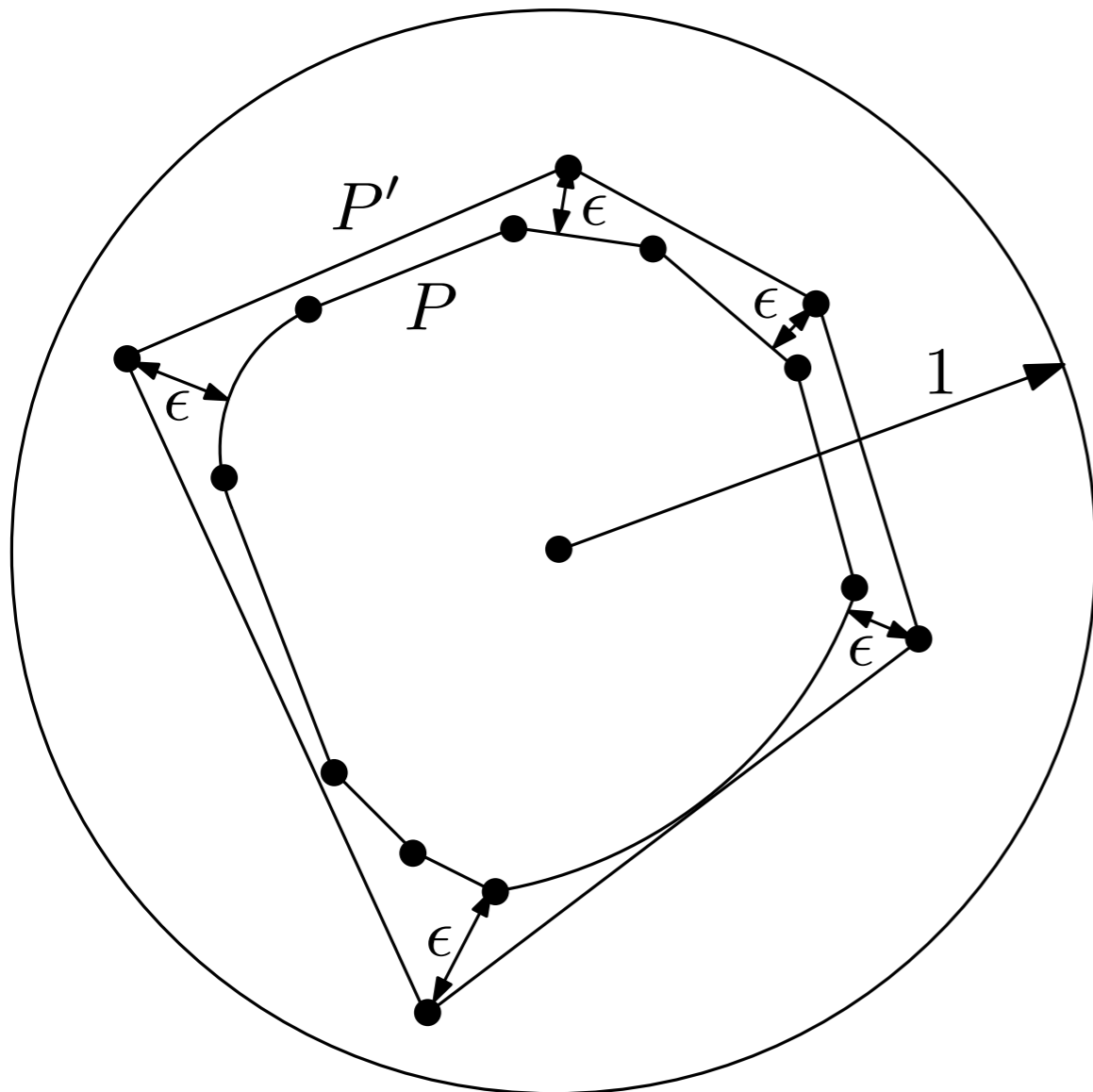
Next we bound c using polytope approximation

Size of L_S

Exhibit a list of size $O\left(\epsilon^{-(d-1)/2} \log \frac{\rho}{\epsilon}\right)$, where $\rho = \frac{\max_{s,t \in S} \|s-t\|}{\min_{s,t \in S} \|s-t\|}$

Lemma For any convex and compact set $P \subset \mathbb{R}^d$ contained in the unit sphere and any $\epsilon \in (0, 1)$, there is a polytope $P' \supset P$ with at most $O(\epsilon^{(d-1)/2})$ facets which is in the ϵ -neighborhood of P .

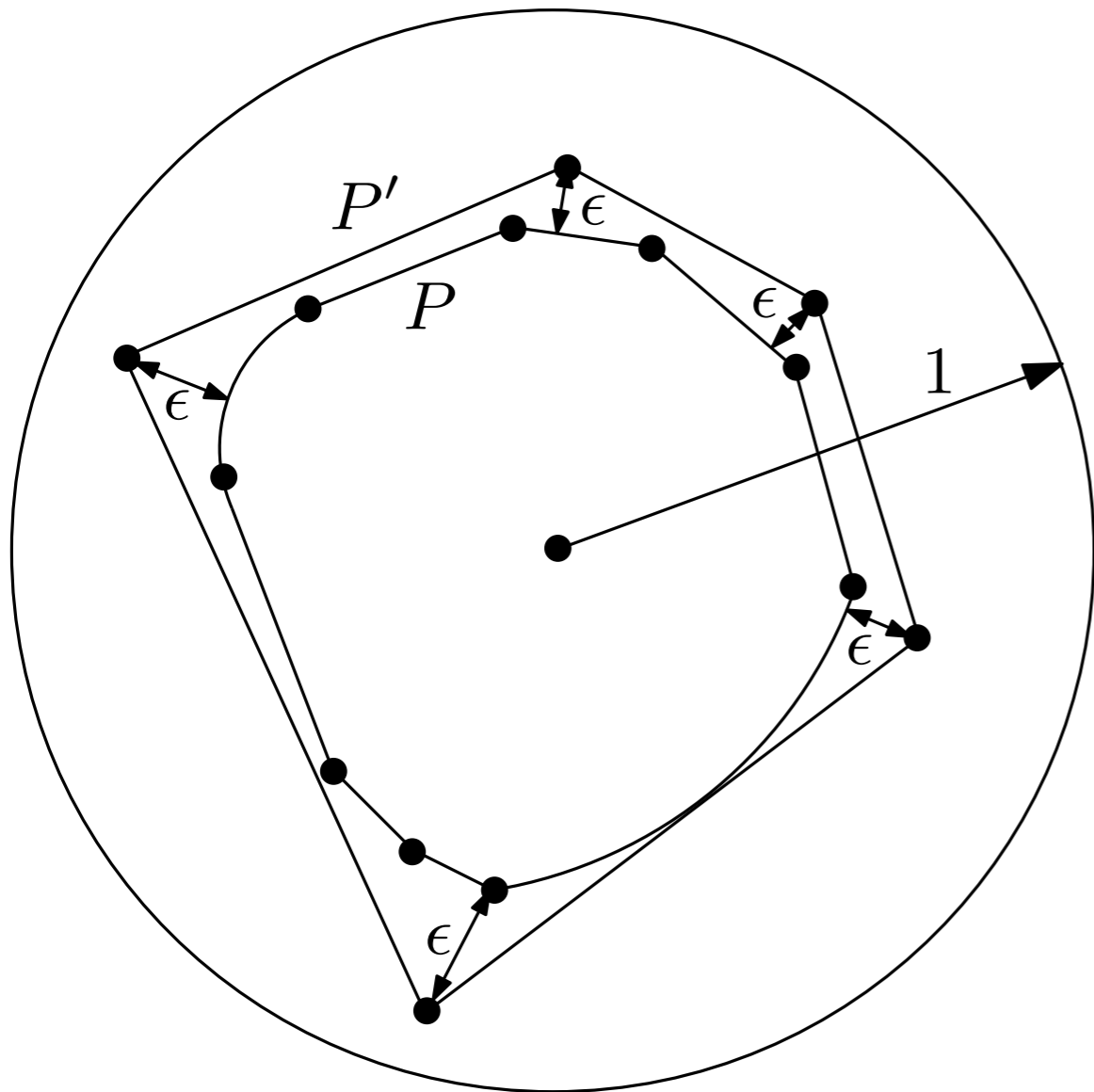
Note Always "outer" approximation



Size of L_S

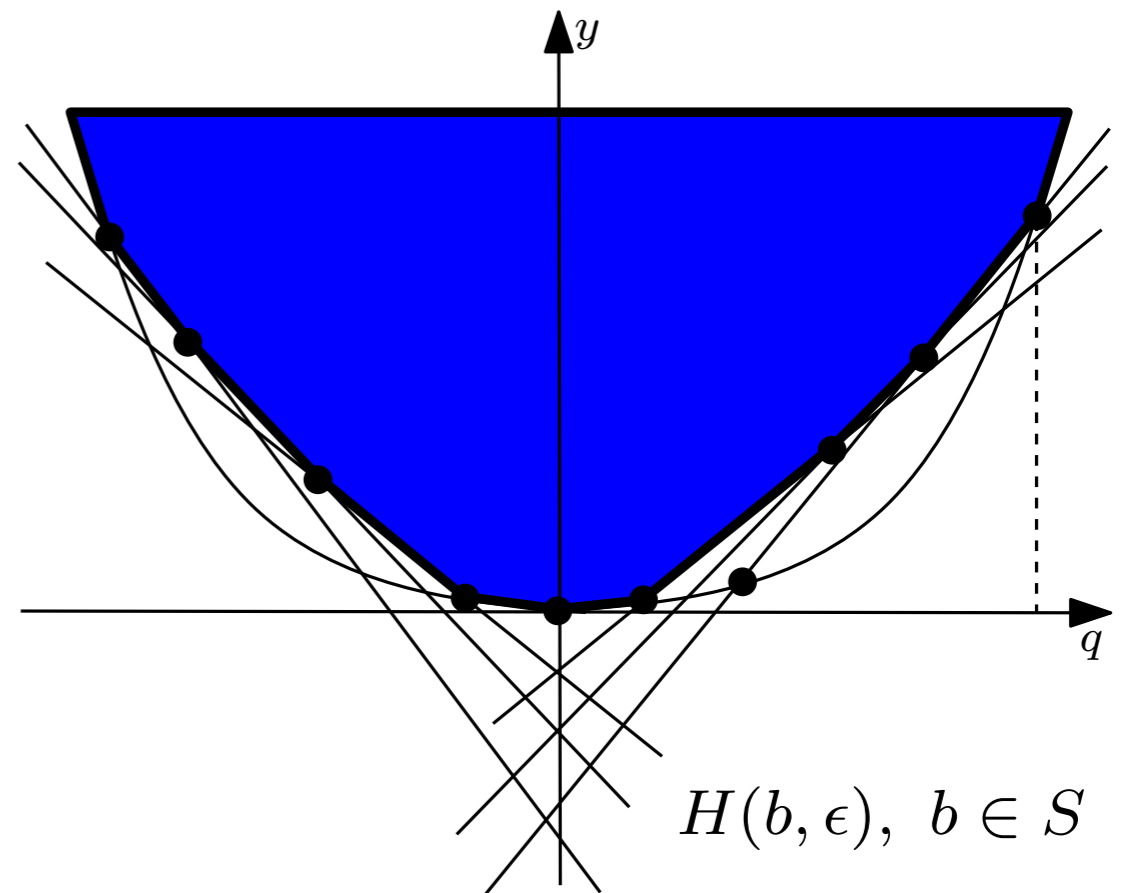
Exhibit a list of size $O\left(\epsilon^{-(d-1)/2} \log \frac{\rho}{\epsilon}\right)$, where $\rho = \frac{\max_{s,t \in S} \|s-t\|}{\min_{s,t \in S} \|s-t\|}$

Lemma For any convex and compact set $P \subset \mathbb{R}^d$ contained in the unit sphere and any $\epsilon \in (0, 1)$, there is a polytope $P' \supset P$ with at most $O(\epsilon^{(d-1)/2})$ facets which is in the ϵ -neighborhood of P .



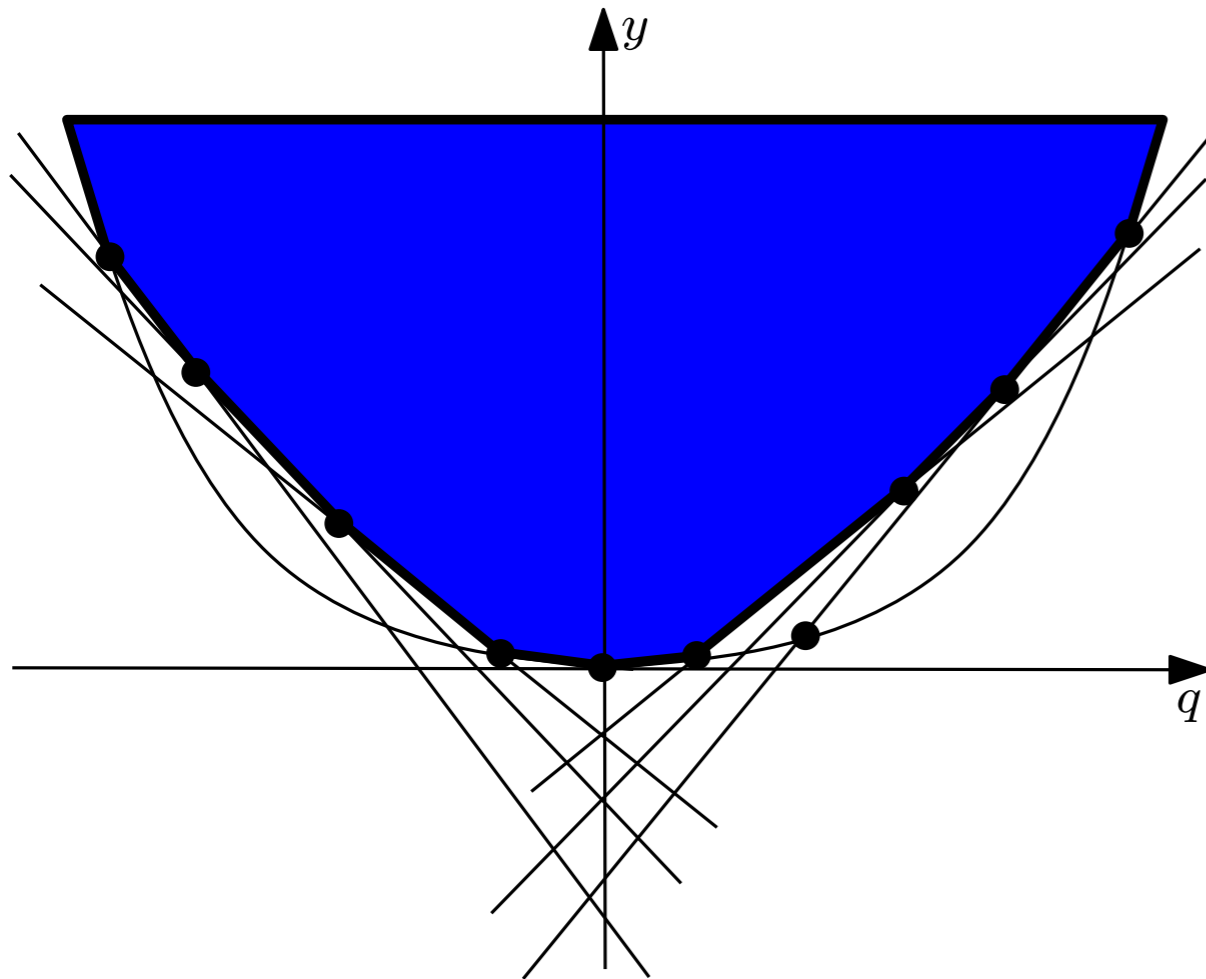
Note Always "outer" approximation

Recall We need an "inner" approximation of this



Size of L_s

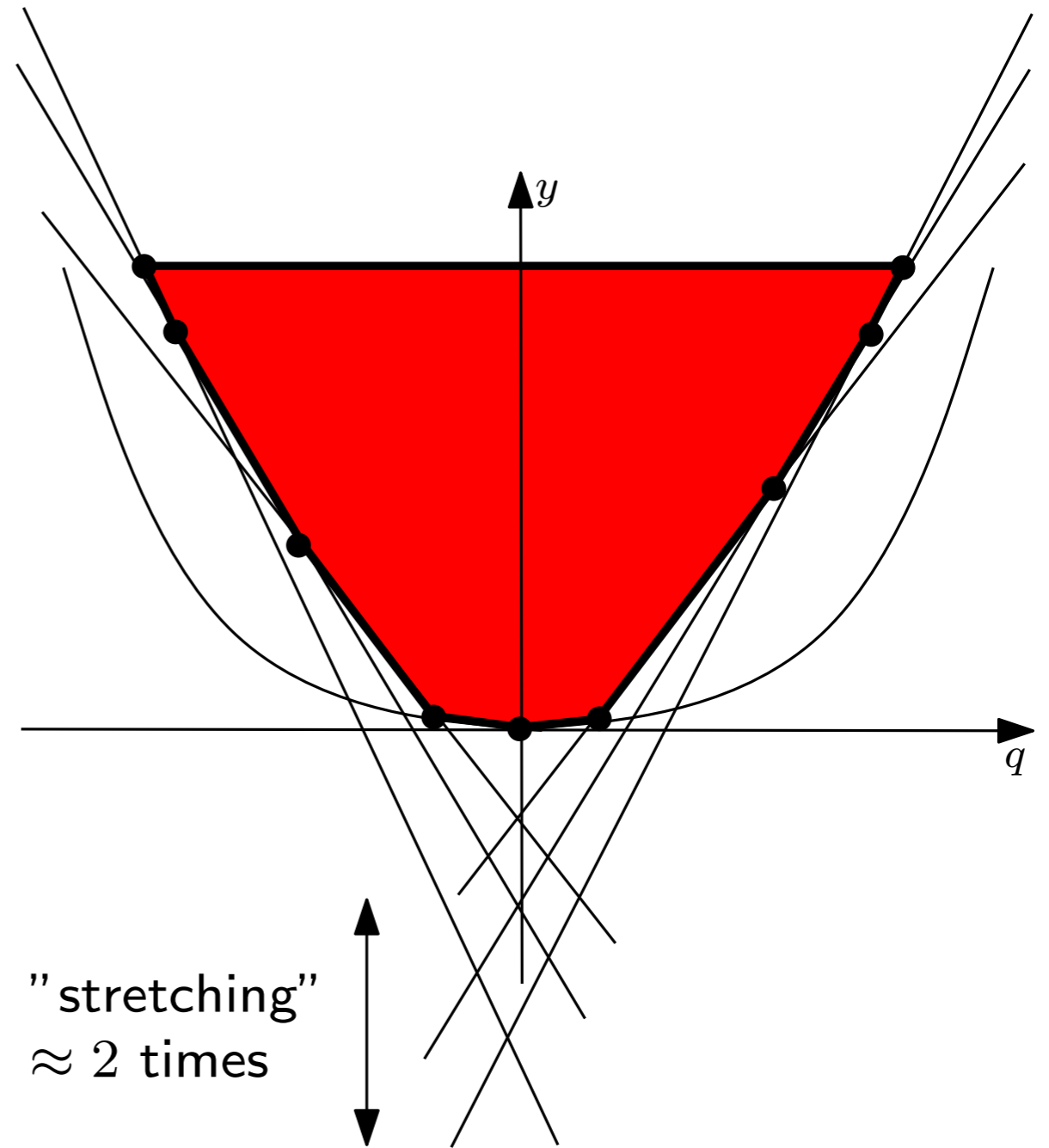
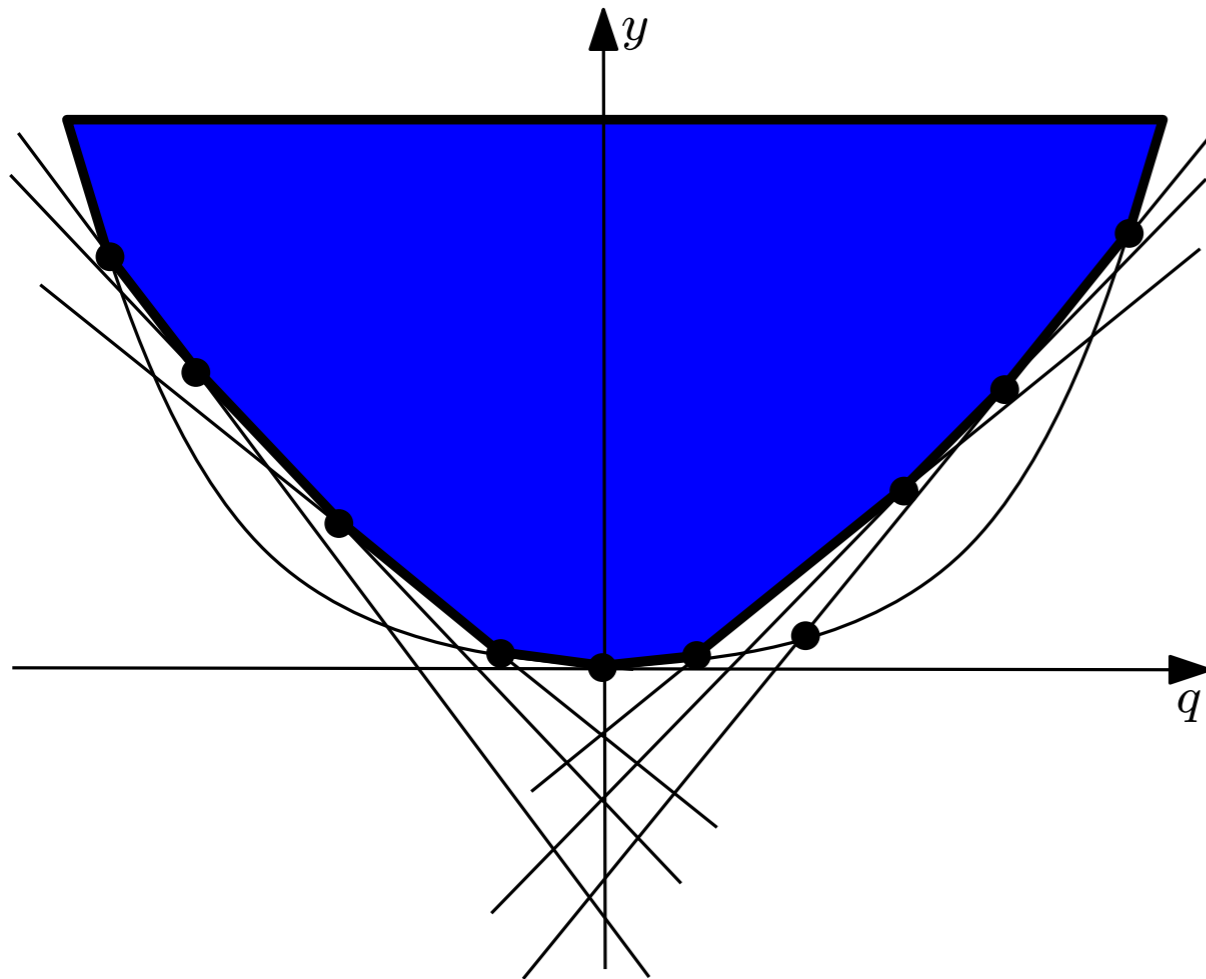
Want an "inner" approximation of this



Size of L_s

Want an "inner" approximation of this

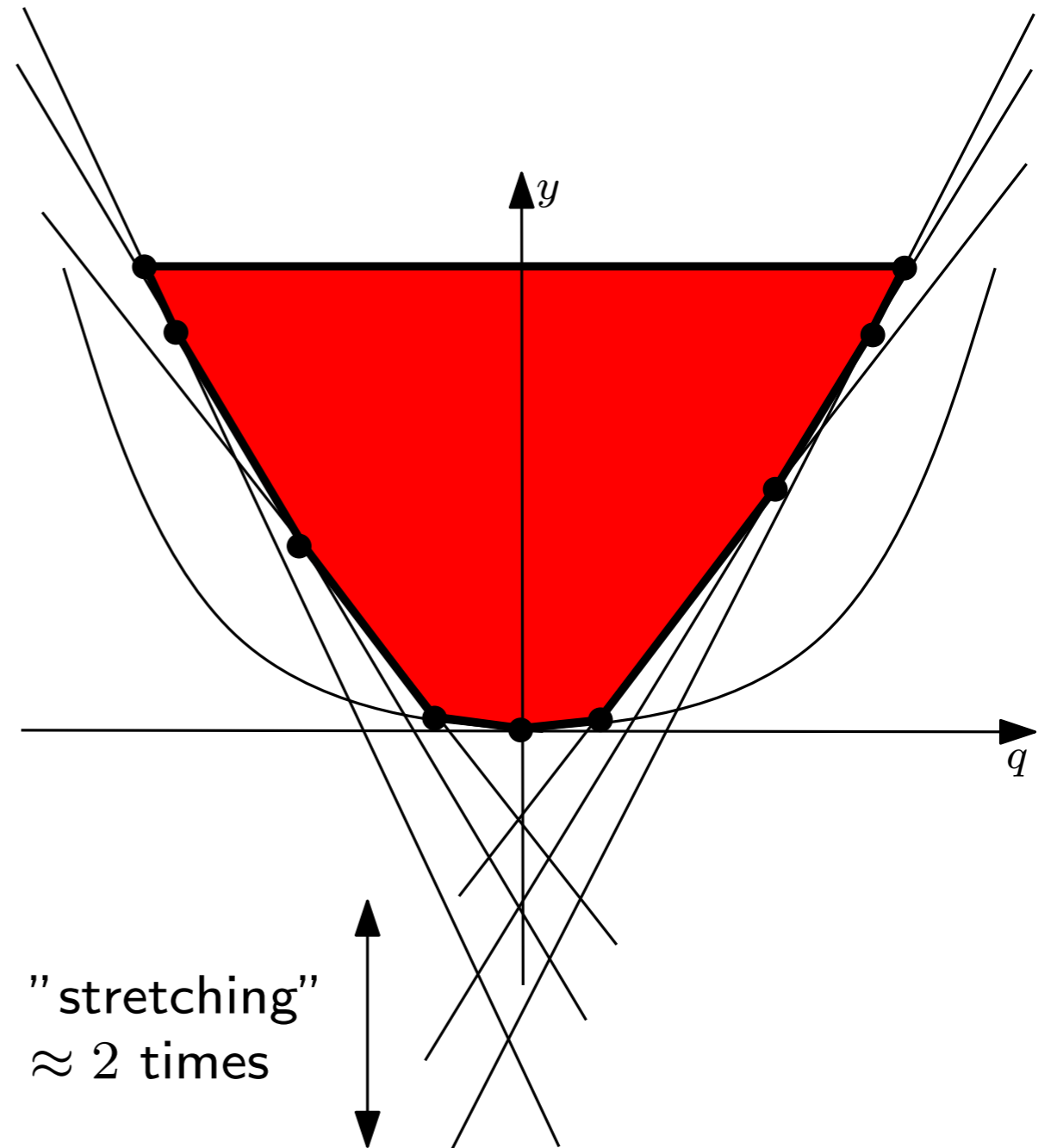
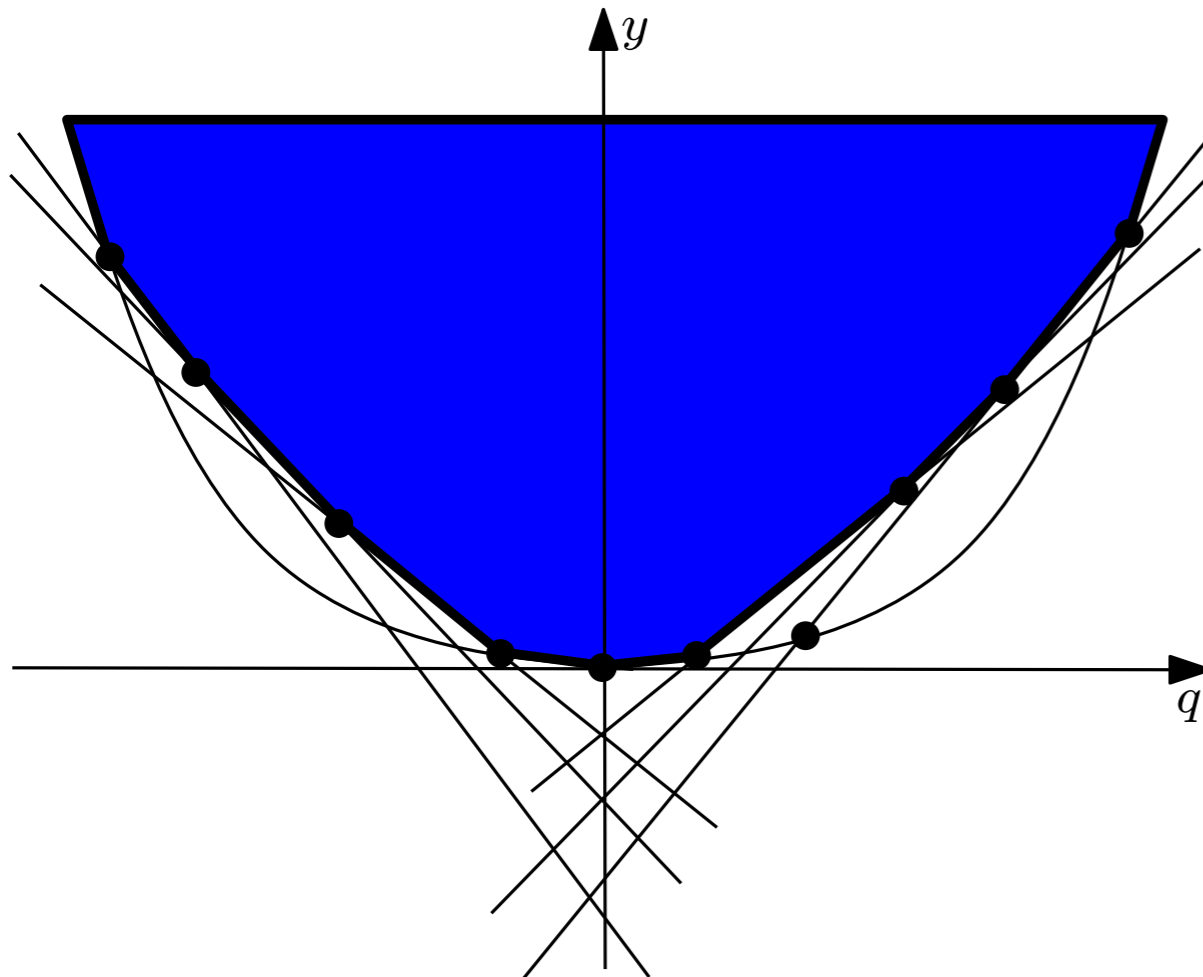
using only these hyperplanes as potential facets



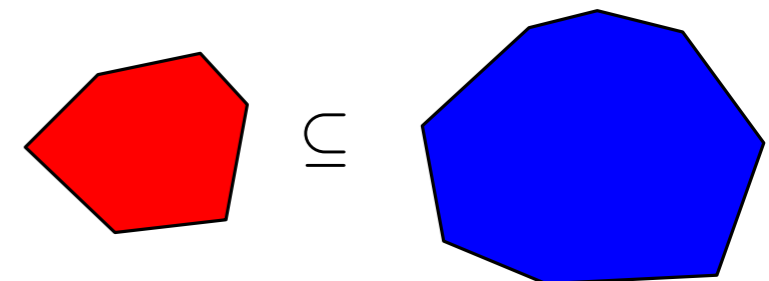
Size of L_S

Want an "inner" approximation of this

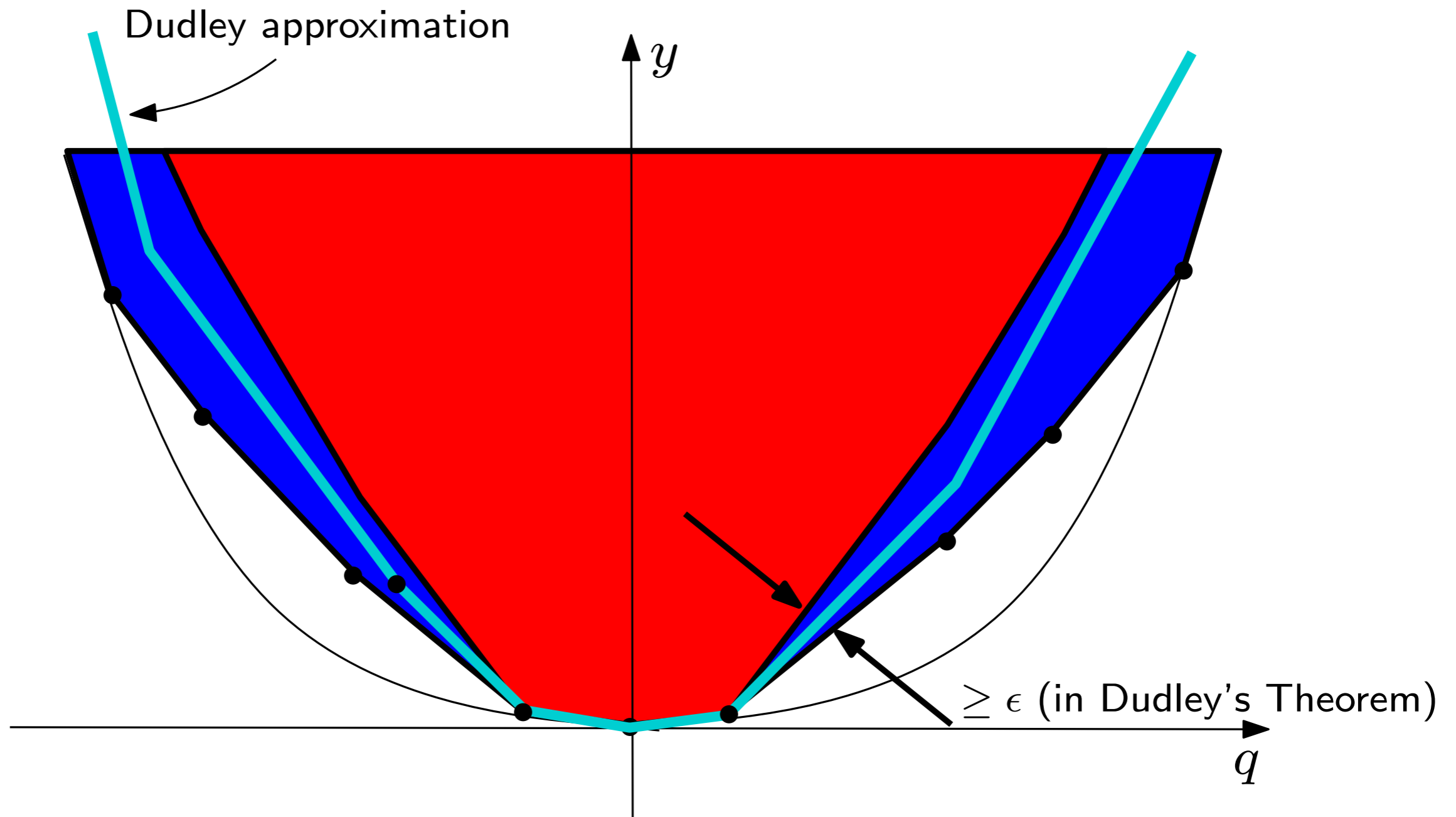
using only these hyperplanes as potential facets



Goal: Subsample (as much as possible) the hyperplanes on the right so that



Size of L_s

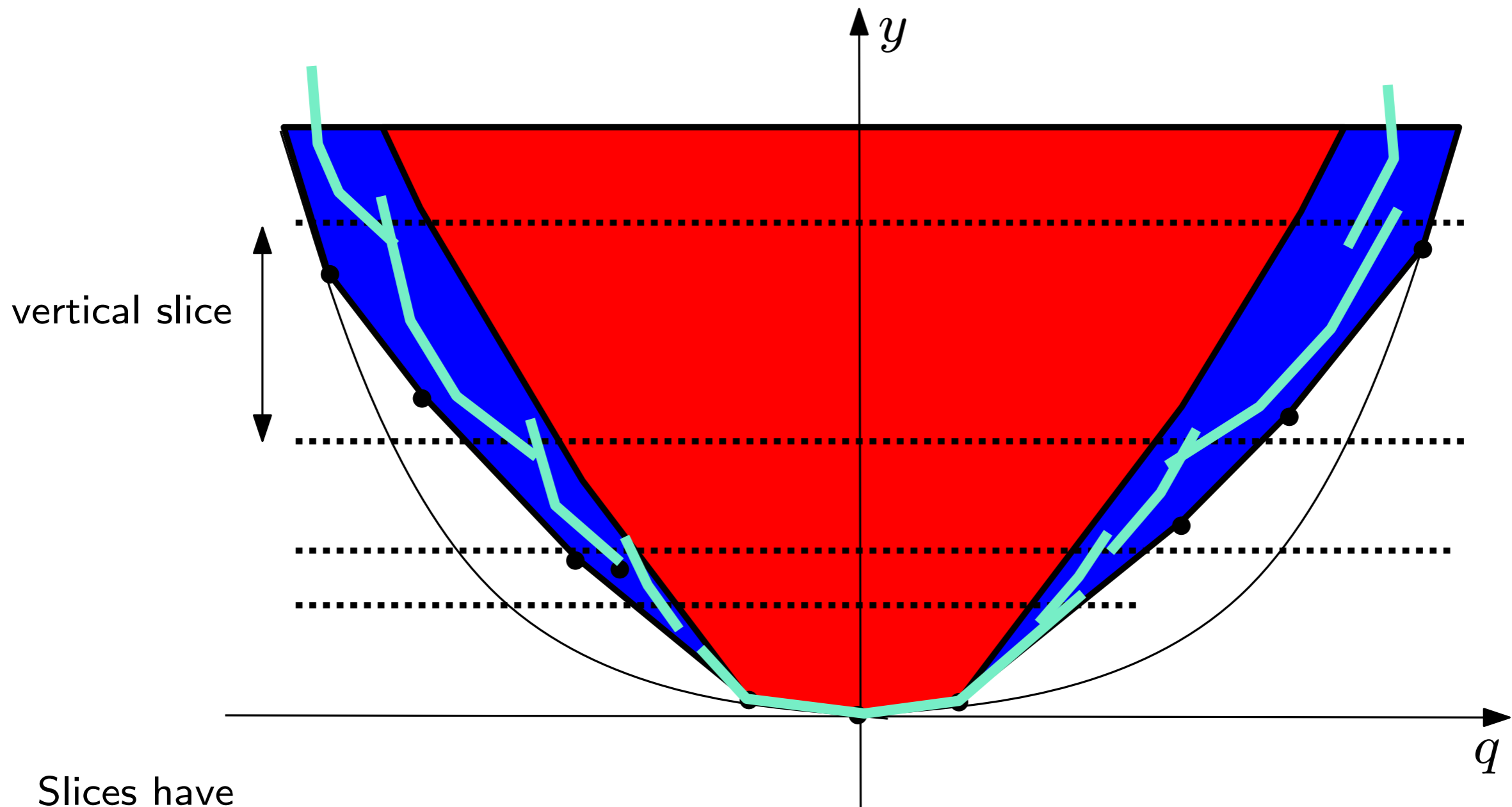


Straightforward application of Dudley's Theorem does not work!

The value of ϵ dictated by the smallest scale

Size of L_s

Solution: height-dependent slicing, per-slice Dudley approximations



Slices have

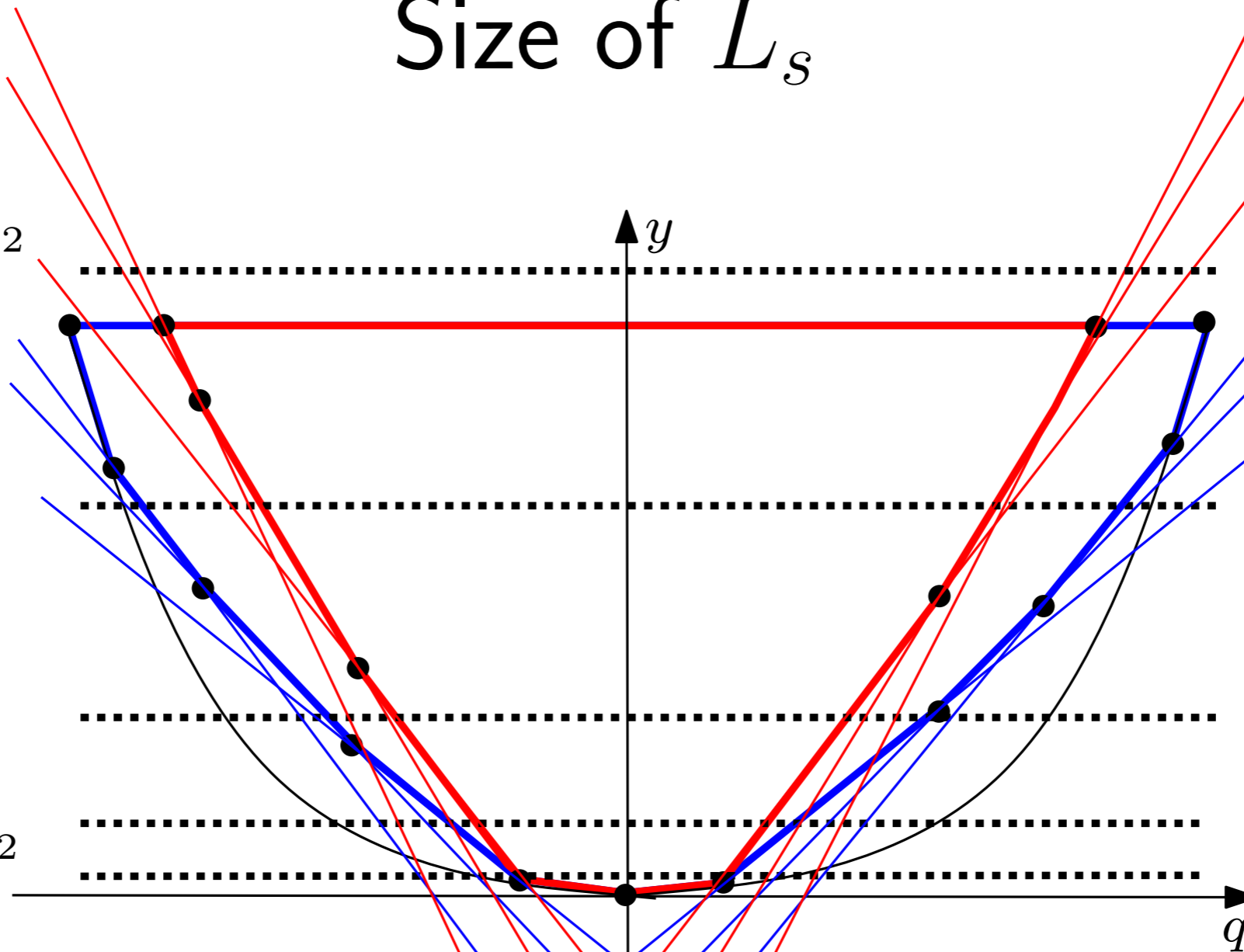
- geometrically increasing height
- "constant" gap

Size of L_S

$$d_m > \frac{4}{\alpha^2} \max_{b \in S} \|b\|^2$$

$$d_i = \frac{3}{2} d_{i-1}$$

$$d_0 = \frac{1}{4} \min_{b \in S} \|b\|^2$$



Number of slices
 $m = O(\log(\rho/\alpha))$

Recall: ρ – spread

Complexity (number of facets) of approximation $O(\epsilon^{-(d-1)/2})$ per slice

Key fact

Red and blue projections into the q -hyperplane **within one slice** are at least a factor of $1 + \epsilon$ apart, so the same ϵ can be used in all approximations

Clarkson's Algorithm: Summary

- Improved query time at the expense of specifying ϵ in advance
- $O(\epsilon^{-(d-1)/2})$ instead of $O(\epsilon^{-d})$
- Express the condition on L_s in the form of $P(S, \epsilon) \supseteq Q(L_s, \epsilon/2)$
- Preprocessing by iterative random sampling from S and checking the containment condition
- Query procedure using
 - top-down search on a skip list
 - iterative improvement algorithm within one level