Approximate Nearest Neighbor Search in High Dimensions

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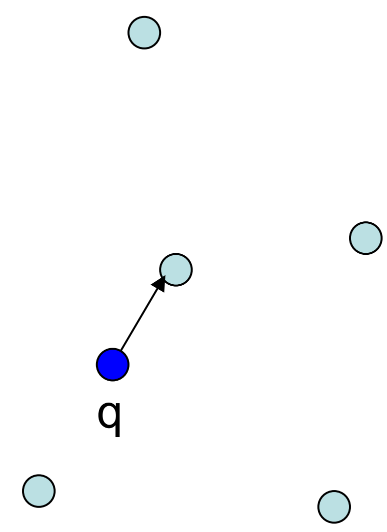
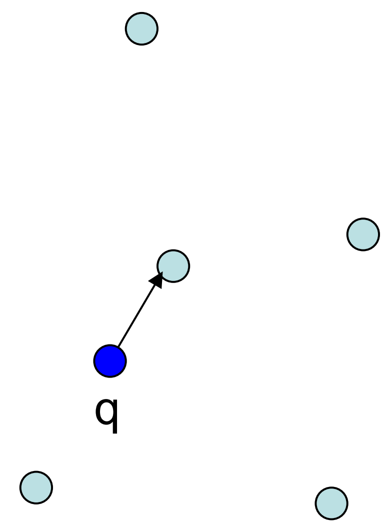
Nearest Neighbor Search

- **Given:** a set P of n distinct points in a d-dimensional space R^d under some norm $||.||$
- **Goal:** build a data structure which, given any query $q \in R^d$ returns a point $p \in P$ minimizing $||p-q||$
- What is a data structure ?
  - A data structure of size M is an **array** $D[1 \ldots M]$ of numbers ("the memory"), together with an associated **algorithm** A that, given a point q, returns a point in P as specified above
  - Example in a moment
  - See [Fefferman-Klartag'09] for an exposition
- Want:
  - Fast running time of the algorithm A
  - Small data structure size M



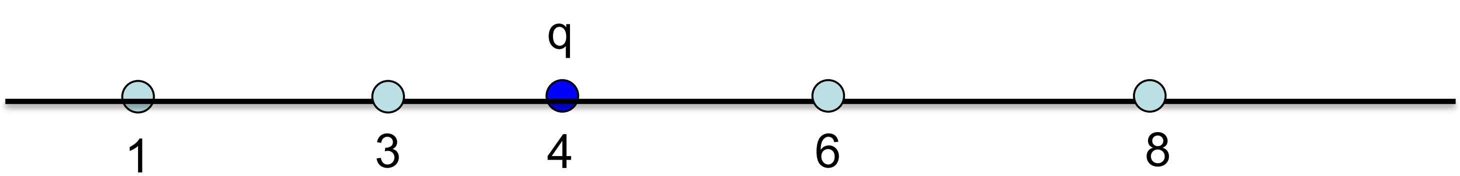
Nearest Neighbor Search

- Best match problem [Minsky-Papert'69], Post office problem [Knuth'73]
- Broad applications in computer science, machine learning etc
  - E.g., searching for similar audio files, images, videos, etc
  - Google "wiki" "nearest neighbor search"
  - Think $n \gg 10^6$, $d > 50$
- Many connections to geometric functional analysis, discrete metric spaces, etc.



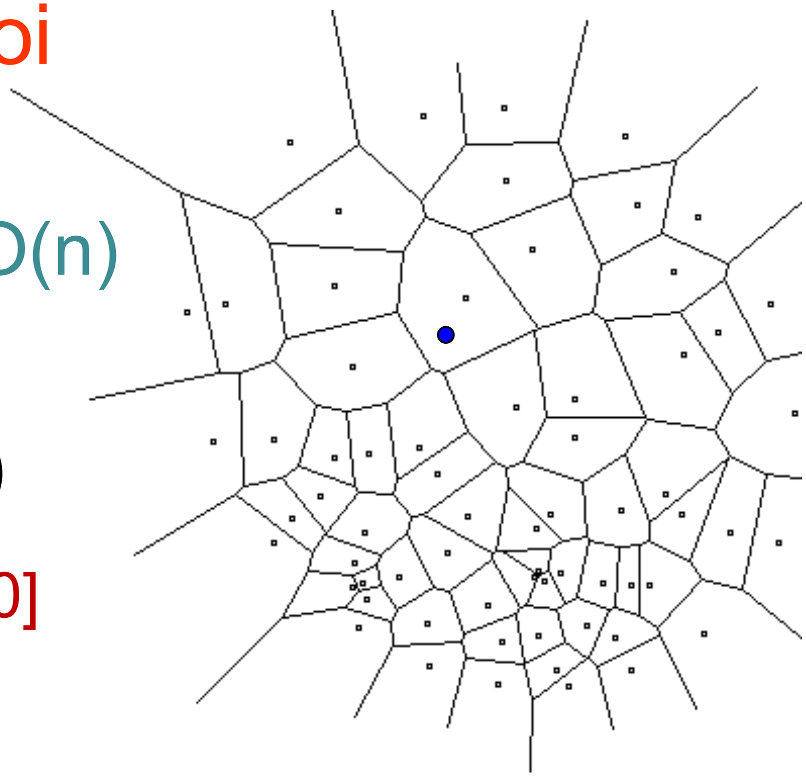
Example: d=1

- Pointset P: $x_1 < x_2 \ldots < x_n$, $x_i \in R$
- Query: $q \in R$
- Nearest neighbor: equivalent to finding smallest x_i greater than q ("successor" of q)
- Performance:
  - Query time: $O(\log n)$ (binary search)
  - Space: $O(n)$ (suffices to store sorted input)



Example: d=2

- Space partitioning: Voronoi diagram
  – Combinatorial complexity O(n)
- Given q, find the cell q belongs to (point location)
- Performance [Lipton-Tarjan'80]
  – Query time: O(log n)
  – Space: O(n)



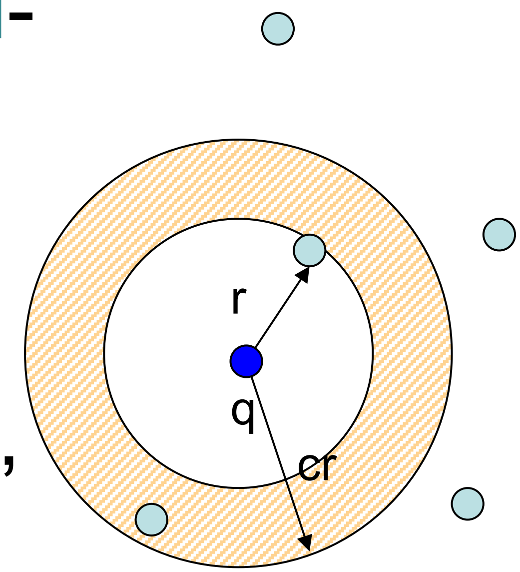
The case of d>2

- Voronoi diagram has size $n^{\lceil d/2 \rceil}$
  - $n^{O(d)}$ space, $(d+\log n)^{O(1)}$ time [Dobkin-Lipton'78,Meiser'93,Clarkson'88]
- We can also perform a linear scan: $O(dn)$ space, $O(dn)$ time
  - Can speedup the scan time by roughly $O(n^{1/d})$
- These are pretty much the only known **general** solutions !
- In fact, exact algorithm with $n^{1-\beta}$ query time for some $\beta>0$ and poly(n) preprocessing would violate certain complexity-theoretic conjecture (SETH)
  - See next lecture by V. V. Williams

Approximate Nearest Neighbor

- **Given:** a set P of n points in a d-dimensional space R^d under some norm $||.||$, parameter $c>1$
- **Goal:** data structure which, given any query q returns $p' \in P$, where

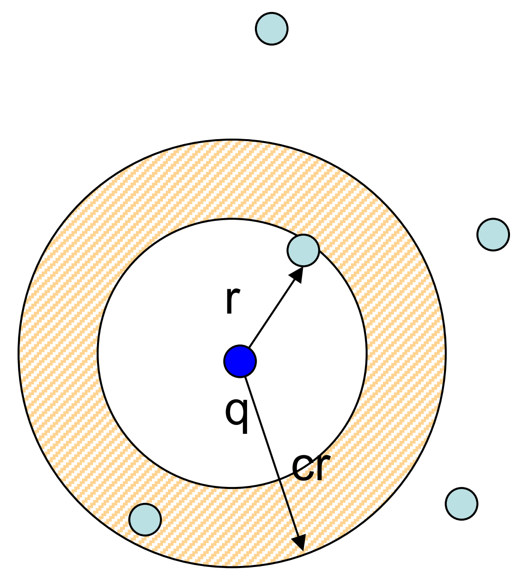
$$||p'-q|| \leq c \min_{p \in P} ||p-q||$$



(c,r)-Approximate Near Neighbor

- **Given:** a set P of n points in a d-dimensional space R^d under some norm $||.||$, parameters $c>1$ and $r>0$
- **Goal:** build a data structure D which, for any query q:
  - If there is $p \in P$ s.t. $||q-p|| \leq r$,
  - Then return $p' \in P$ s.t $||q-p'|| \leq cr$
- Decision version of approximate nearest neighbor
  - Equivalent up to $(\log n)^{O(1)}$ factors in space and query time
- Randomized version (c,r,δ)-ANN: for any query q

$$\Pr_D[D \text{ answers } q \text{ as above}] > 1-\delta$$



Approximate Near(est) Neighbor Algorithms

- Space/time exponential in d [Arya-Mount'93],[Clarkson'94], [Arya-Mount-Netanyahu-Silverman-Wu'98] [Kleinberg'97], [Har-Peled'02], ….
- Space/time polynomial in d [Indyk-Motwani'98], [Kushilevitz-Ostrovsky-Rabani'98], [Indyk'98], [Gionis-Indyk-Motwani'99], [Charikar'02], [Datar-Immorlica-Indyk-Mirrokni'04], [Chakrabarti-Regev'04], [Panigrahy'06], [Ailon-Chazelle'06], [Andoni-Indyk'06],…., [Andoni-Indyk-Nguyen-Razenshteyn'14], [Andoni-Razenshteyn'15] [Andoni-Indyk-Laarhoven-Razenshteyn-Schmidt'15], [Andoni-Nguyen-Nikolov-Razenshteyn-Waingarten'17], [Andoni-Naor-Nikolov-Razenshteyn-Waingarten'18], …

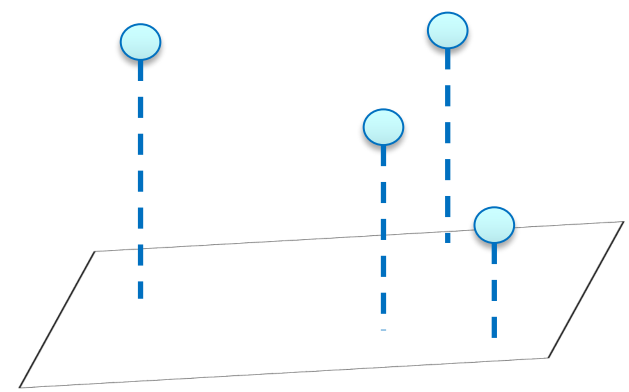
Plan

- Non-adaptive approach: l_1, l_2 and friends
  - Dimensionality reduction
  - Randomized space partitions (a.k.a. Locality-Sensitive Hashing)
- Adaptive approach: faster, more general

Non-adaptive data structures

Dimensionality reduction

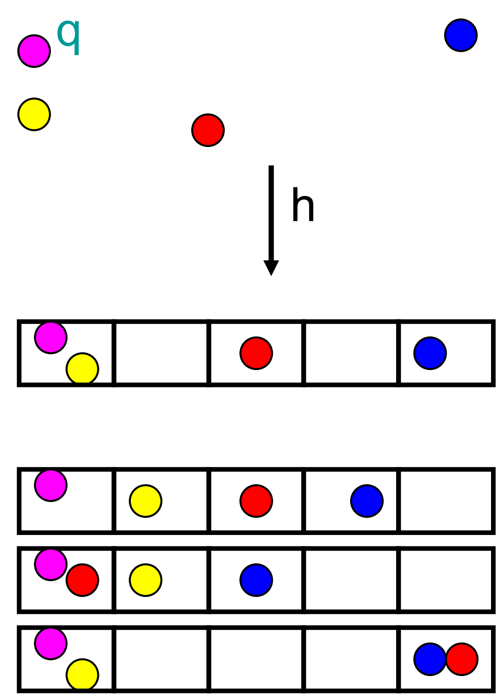
- Consider approximation c=1+$\varepsilon \leq 2$
- Two steps:
  - Design a data structure with
    - Space: $(1/\varepsilon)^{O(d)}$
    - Query time: O(d)
  - Use random projection [Johnson-Lindenstrauss'84]
    - Dimension: d → $O(\log(n)/\varepsilon^2)$
    - All distances preserved up to $1\pm\varepsilon$ (in l_2)
- Yields space $n^{O(1/\varepsilon^2)}$ and query time $O(d \log(n)/\varepsilon^2)$ [Ostrovski-Rabani'98]
- Space too large to be practical



Locality-Sensitive Hashing (LSH)

Locality-Sensitive Hashing

- A family H of functions $h: R^d \rightarrow U$ is called (P_1,P_2,r,cr)-sensitive for $||.||$, if for any pair of points p,q:
  - If $||p-q|| \leq r$ then $Pr_{h \in H}[\ h(p)=h(q)\ ] \geq P_1$
  - If $||p-q|| \geq cr$ then $Pr_{h \in H}[\ h(p)=h(q)\ ] \leq P_2$
- Theorem [Indyk-Motwani'98]: Suppose there is an H as above. Then there is a $(c,r,0.1)$-ANN data structure with space $O(dn+nL)$ and time $O(dL)$ where $L=n^{\rho}/P_1$, $\rho=\log(P_1)/\log(P_2)$
- Non-adaptive: the memory cells accessed to answer queries depend on query q but not on data set P

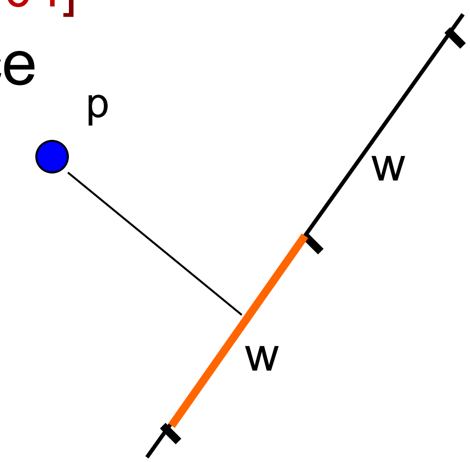


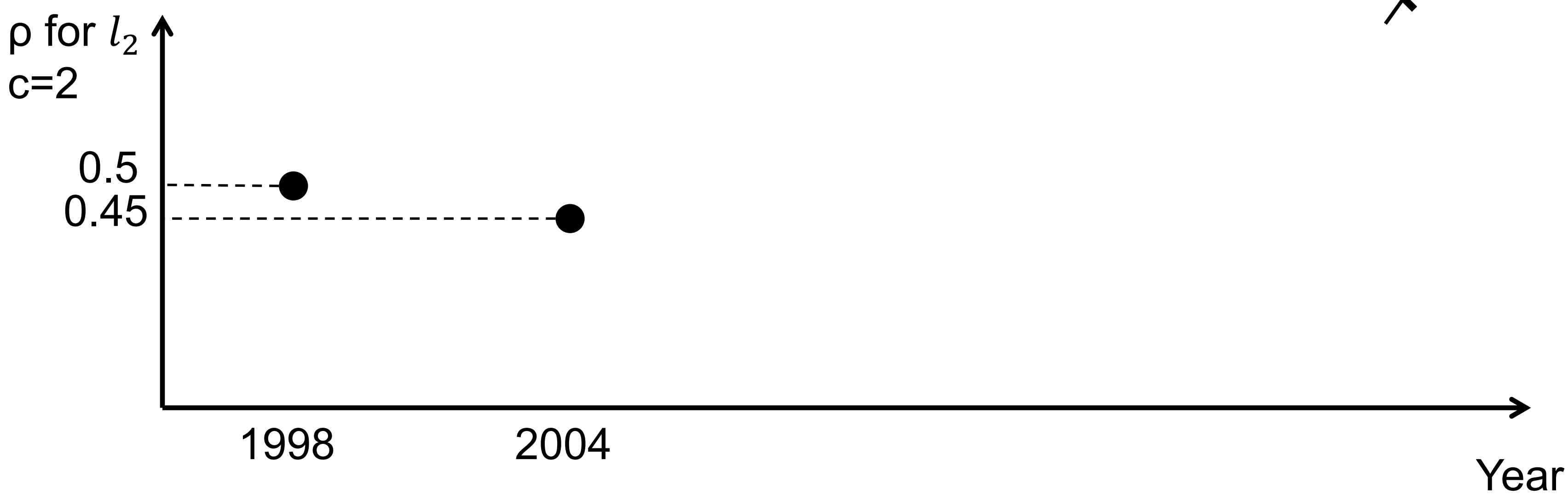
LSH: examples

- $\{0,1\}^d$ under $||.||_1$:
  - $H=\{h_i : h_i(p)=p_i , i=1..d\}$
  - $Pr_{h\in H} [h_i(p)=h_i(q)]=1- ||p-q||_1 /d$
  - Yields exponent $\rho=1/c$
- Works for R^d under $||. ||_p$, $p\in[1,2]$

LSH: examples

- R^d under $||.||_2$ [Datar-Indyk-Immorlica-Mirrokni'04]
  - Project on a random 1-dimensional space and round
  - Yields exponent $\rho<1/c$

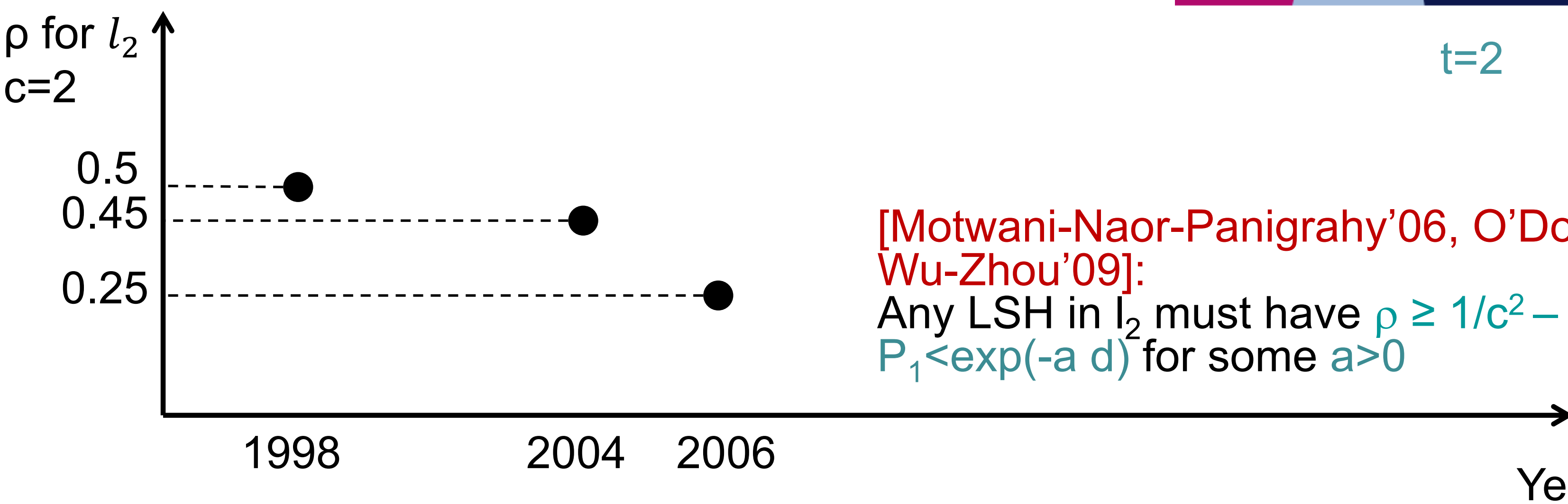




LSH: examples

- R^d under $||.||_2$
- Project (on a t-space) and round [Charikar et al'98, Andoni-Indyk'06]
  - Intervals → lattice of balls
  - Can hit empty space, so hash until a ball is hit
  - Yields exponent $\rho \to 1/c^2$ as $t \to \infty$

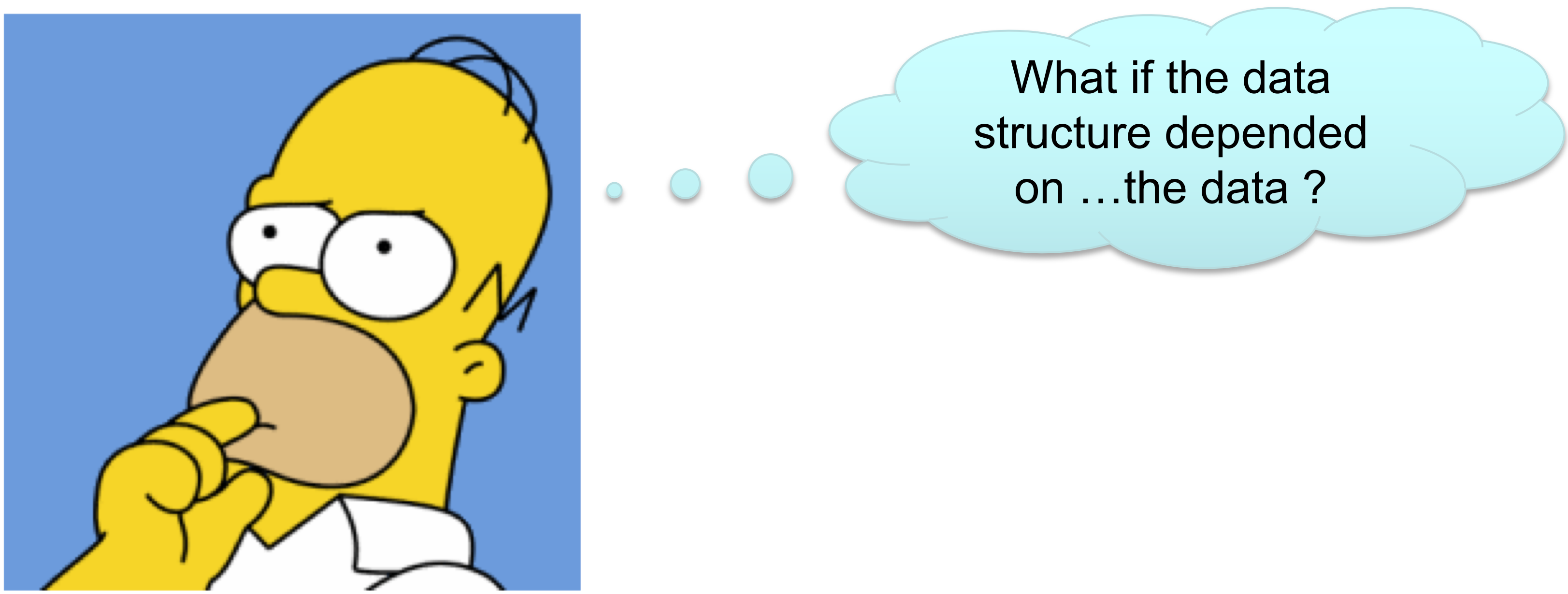
t=2



[Motwani-Naor-Panigrahy'06, O'Donnell-Wu-Zhou'09]:
Any LSH in l_2 must have $\rho \geq 1/c^2 - o(1)$ or $P_1 < \exp(-a\ d)$ for some $a > 0$

Adaptive data structures

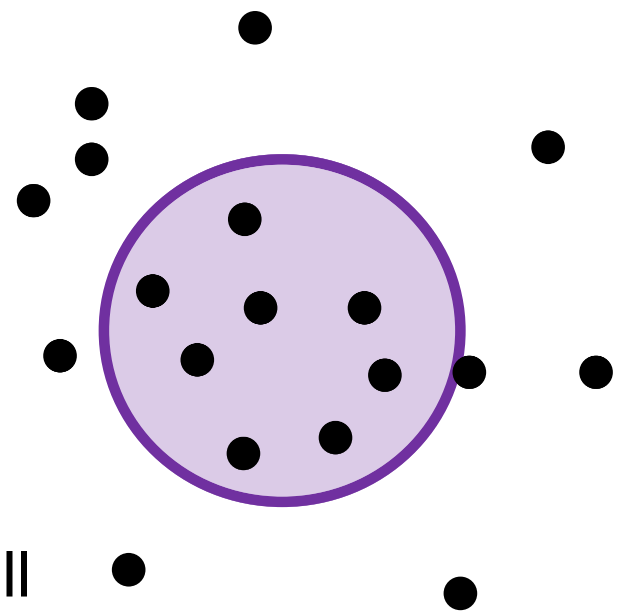
The “idea”



- Why is the answer not obvious ?
- It is often possible to get a data structure that works well when the data *has some structure* (clusters, low-dimensional subspace, i.i.d. from some distribution,etc)
- The tricky part is what to do when the data *does not have* that structure, or any structure in particular

The actual idea

- Every point-set has some structure that can be exploited algorithmically
- Details depend on the context/problem, but at a high level:
  - Either there is dense cluster of small radius, or
  - Points are “spread” out
- Applications:
  - Faster algorithms for l_1 , l_2
  - Algorithms for general norms



Faster Algorithms

Basic Data Adaptive Method

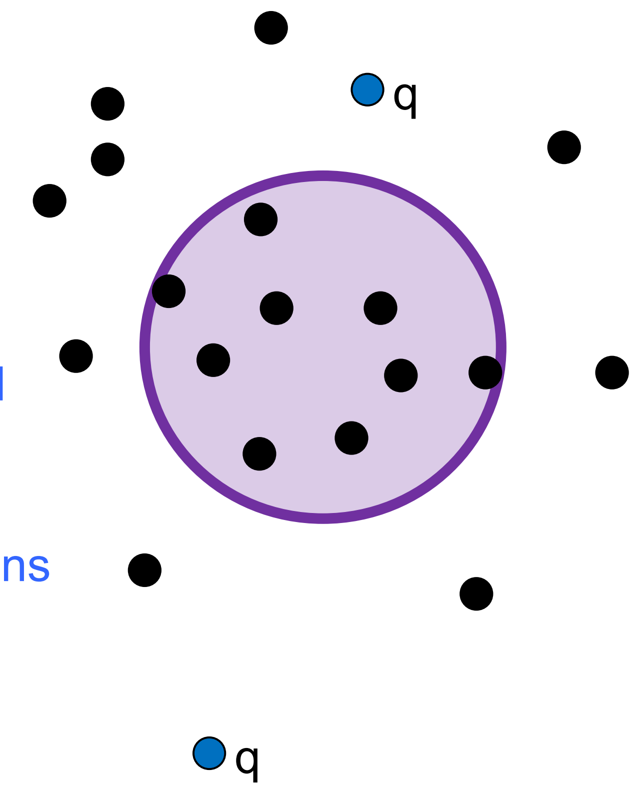
P=input pointset, r=radius, c=approximation

Preprocessing:

1. As long as there is a ball B_i of radius $O(cr)$ containing T points in P
   - $P=P-B_i$
   - $i=i+1$
2. Build LSH data structure on P

   No dense clusters – most points are >>cr from q
3. For each ball B_i build a specialized data structure for $B_i \cap P$

   Diameter bounded by O(cr) – better LSH functions



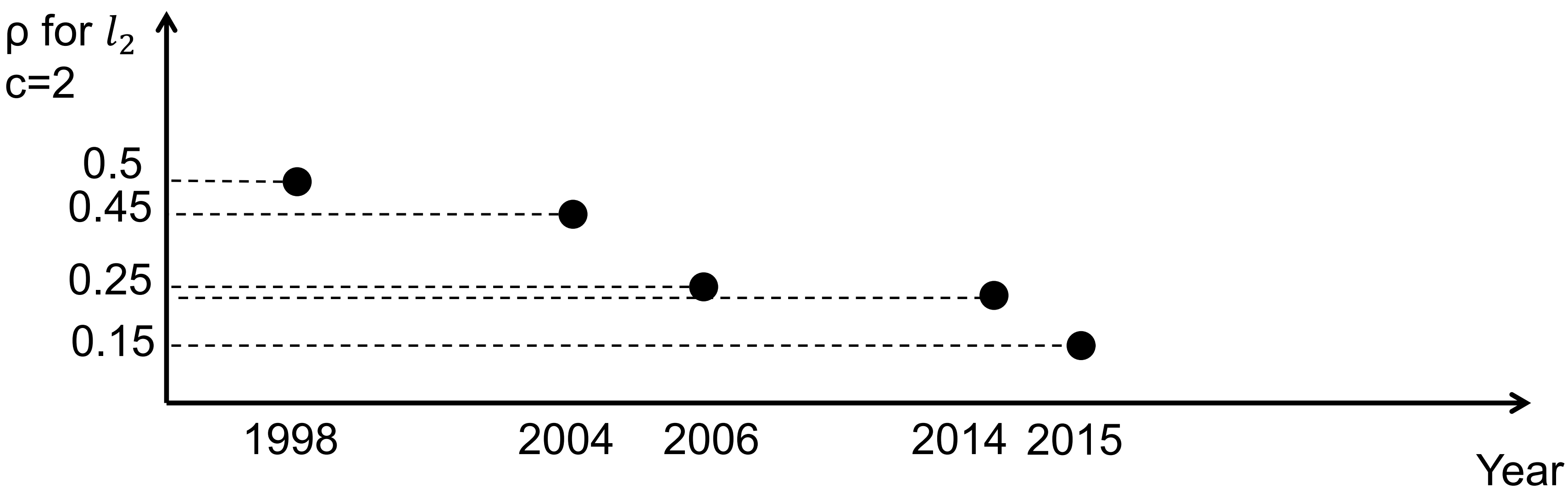
Query procedure:

1. Query the main data structure
2. Query all data structures for balls that are "close" to the query

Results (for l_2)

- For c-approximation:

Algorithm	**Query Time**	**Index Space**
Non-adaptive LSH	dn^{1/c^2}	n^{1+1/c^2}
Andoni, Indyk, Nguyen, Razenshteyn'14	$dn^{0.87/c^2+O(1)/c^3}$	$n^{1+0.87/c^2+O(1)/c^3}$
Andoni-Razenshteyn'15	$dn^{1/(2c^2-1)}$	$n^{1+1/(2c^2-1)}$



More general algorithms

Generality

- Non-adaptive methods:
  - Dimensionality reduction: mostly l_2
    - No dimensionality reduction in l_1 [Brinkman-Charikar'03, Lee-Naor'04]
    - Any space supporting dimensionality reduction with low distortion is "very close" to l_2 [Johnson-Naor'09]
  - Locality-sensitive hashing: l_p for $p \in [1,2]$, Jaccard coefficient, Angular distance etc
    - Does not work e.g., for l_∞
  - Reductions:
    - Small powers of the above
    - Low-distortion embeddings into the above (edit distance, Ulam metric, transportation norm,..)
- What about general norms ?

General norms

- Every d-dimensional normed space is within $\sqrt{d}$ from ℓ_2^d (after a linear transformation) [John'48]
  - Yields approximation factor of O($\sqrt{d}$) – pretty large
- Low-distortion embedding of any symmetric norm [Andoni-Nguyen-Nikolov-Razenshteyn-Waingarten'17]
  - Embedding into $\oplus_{\ell_\infty} \oplus_{\ell_1} \ell_\infty$
  - Yields approximation factor of $\mathrm{poly}(\log\log n)$
- Algorithms for any norm via cutting modulus [Andoni-Naor-Nikolov-Razenshteyn-Waingarten'18]
  - Yields approximation factor of O(log d)
  - The algorithm operates in the "cell-probe" model (counts only memory accesses, not computation)
  - Can be converted into an "actual" algorithm for specific norms or with a weaker guarantee

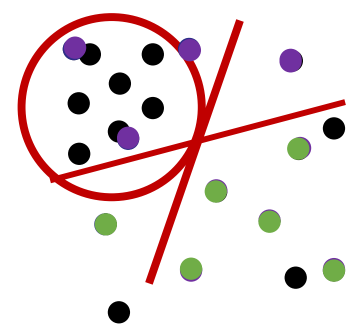
Cutting modulus

- Parameter $\Xi(M, \alpha)$ defined for any metric space $M = (X, D)$ and "error parameter" α>0
- It is at most $O(\log(d)/\alpha^2)$ for any normed space $||.||$ over R^d [Naor'17]
- Related to non-linear spectral gaps
  – See the talk by Assaf Naor next week

The core partitioning procedure

- Theorem:
  - Let $M = (X, D)$ with $|X| = N$ and take $\alpha, r > 0$
  - There is a “small” collection $\mathcal{F} \subset 2^X$ s.t. for every n-point dataset $P \subset X$:
    - Either there exists a ball of radius $\lesssim \Xi(M, \alpha) \cdot r$ with $\Omega(n)$ points
    - Or there is a distribution $\mathcal{D}$ over “few” sets from $\mathcal{F}$ that partition P (approximately) evenly and, for every $x_1, x_2 \in X$ with $D(x_1, x_2) \leq r$:

$$\Pr_{A \sim \mathcal{D}}[A \text{ separates } x_1 \text{ and } x_2] \lesssim \alpha$$



- ANN data structure can be constructed using divide and conquer approach

Conclusions + Open Problems

- Approximate Nearest Neighbor Search
  - Non-adaptive approach: l_1 , l_2 and friends
  - Adaptive approach: faster, more general
- Connections to geometric and metric functional analysis
- Open questions:
  - Deterministic algorithms ? Very little known
  - Better data structure for edit distance ?
    - No poly(n) space, $n^{1-\beta}$ query time, poly(log(d))-approx. known
  - Same for transportation norm, but replace poly(log(d)) with poly(loglog(d))
- Software: google "FALCONN"

THANK YOU!