# Similarity Search in High Dimensions II

Piotr Indyk MIT

#### Approximate Near(est) Neighbor

- c-Approximate Nearest Neighbor: build data structure which, for any query q
  - returns  $p' \in P$ ,  $||p-q|| \leq cr$ ,
  - where r is the distance to the nearest neighbor of q
- c-Approximate r-Near Neighbor: build data structure which, for any query q:
  - If there is a point  $p \in P$ ,  $||p-q|| \le r$
  - − it returns p' $\in$ P, ||p-q|| ≤ cr



 $\bigcirc$ 

# Algorithms for c-Approximate Near Neighbor

Space	Time	Comment	Norm	Ref
$dn+n^{O(1/\epsilon^2)}$	d * logn /ε²	c=1+ ε	Hamm, I <sub>2</sub>	[KOR'98, IM'98]
	(or 1)			
$n^{\Omega(1/\epsilon^2)}$	O(1)			[AIP'06]
dn+n <sup>1+p(c)</sup>	dn <sup>ρ(c)</sup>	ρ(c)=1/c	Hamm, I <sub>2</sub>	[IM'98], [GIM'98],[Cha'02]
		ρ(c)<1/c	l <sub>2</sub>	[DIIM'04]
dn * logs	dn <sup>σ(c)</sup>	$\sigma(c)=O(\log c/c)$	Hamm, I <sub>2</sub>	[Ind'01]
dn+n <sup>1+p(c)</sup>	dn <sup>ρ(c)</sup>	$\rho(c)=1/c^2 + o(1)$	l <sub>2</sub>	[Al'06]
		σ(c)=O(1/c)		[Pan'06]

#### Reductions

- c(1+γ)-Approx Nearest Neighbor reduces to c-Approx Near Neighbor
- Easy:
  - Space multiplied by  $(\log \Delta)/\gamma$ , where  $\Delta$  is the spread, i.e., all distances in P are in  $[1...\Delta]$
  - Query time multiplied by  $log((log \Delta)/\gamma)$
  - Probability of failure multiplied by  $(\log \Delta)/\gamma$
  - Idea:
    - Build data structures with r=  $\frac{1}{2}$ ,  $\frac{1}{2}(1+\gamma)$ ,  $\frac{1}{2}(1+\gamma)^2$ ,..., O( $\Delta$ )
    - To answer query, do binary search on values of r
- Hard: replace  $\log \Delta$  by  $\log n$

#### General reduction [Har Peled-Indyk-Motwani'11]

- Assume we have a data structure for dynamic c-Near Neighbor in under a metric D which, for parameters n,f has:
  - T(n,c,f) construction time
  - S(n,c,f) space bound
  - Q(n,c,f) query time
  - U(n,c,f) update time
- Then we get a data structure for  $c(1+O(\gamma))$ -Nearest Neighbor with:
  - $O(T(n,c,f)/\gamma \cdot \log^2 n + n\log n[Q(n,c,f)+U(n,c,f)])$  expected construction time
  - $O(S(n,c,f)/\gamma \cdot \log^2 n)$  space bound
  - Q(n,c,f) O(logn) query time
  - O(f logn) failure probability
- Generalizes, improves, simplifies and merges [Indyk-Motwani'98] and [Har Peled'01]

# Intro

- Basic idea: use different scales (i.e., radiuses r) for different clouds of points
  - At most n<sup>2</sup> total
  - Would like (log n)<sup>2</sup> per point, on the average
- We will see a simplified reduction:
  - From approximate nearest neighbor to exact near neighbor
  - Simplifying assumption
- Actual reduction a little more complex, but follows the same idea

()

 $\bigcirc$ 

### Example



### Notation

- $UB_{P}(r) = U_{p \in P}B(p, r)$
- CC<sub>P</sub>(r) is a partitioning of P induced by the connected components of UB<sub>P</sub>(r)
- r<sub>med</sub> is the smallest value of r such that UB<sub>P</sub>(r) has a component of size at least n/2 + 1
- $UB_{med} = UB_{P}(r_{med})$
- $CC_{med} = CC_{P}(r_{med})$
- Simplifying assumption: UB<sub>P</sub>(r<sub>med</sub>) has a component of size exactly

n/2+1



### A simplified reduction

- Set  $r_{top} = \Theta(nr_{med} \log(n)/\gamma)$
- Exact near neighbor data structures NN:
  - For i=0...log<sub>1+ $\gamma$ </sub> (2r<sub>top</sub>/r<sub>med</sub>), create NN(P, r<sub>med</sub>(1+ $\gamma$ )<sup>i</sup>/2)
  - For each component C∈CC<sub>med</sub>
    recurse on C
  - Recurse on P'⊂P that contains one point per each component
    C∈CC<sub>med</sub> (at most n/2 points)
- Note that the recursion has depth O(log n)



Inner radius  $=r_{med}/2$ Outer radius  $=r_{top}$ 

### Search

- 1. Use NN(P,  $r_{med}/2$ ) to check whether  $D(q,P) < r_{med}/2$ 
  - If yes, recurse on the component C containing q
- 2. Else use NN(P,  $r_{top}$ ) to check whether  $D(q,P)>r_{top}$ 
  - If yes, recurse on P'
- 3. Else perform binary search on NN(P,  $r_{med}(1+\gamma)^{i/2}$ )
- Correctness for Cases 1 and 3 follows from the procedure
- Case 2 need a little work:
  - Each "contraction" introduces an additive error up to n  $r_{med}$
  - But the distance to nearest neighbor lower-bounded by  $r_{top} = \Theta(nr_{med} \log(n)/\gamma)$
  - Accumulated relative error at most  $(1+n r_{med}/r_{top})^{O(\log n)} = (1+\gamma/\log(n))^{O(\log n)}$



### Space

 Let B(n) be the maximum number of points stored by the data structure

 $-\operatorname{Space} = O(B(n) \log_{1+\gamma} (r_{top}/r_{med}))$ 

• We have

 $B(n) = \max_{k,n1+n2+\ldots+nk=n} \Sigma_i B(n_i) + B(k) + n$ subject to k < n/2 , 1 < n < n/2

This solves to O(n log n)

### **Construction time**

- Estimating r<sub>med</sub>
  - Selects a point p uniformly at random from P
  - Return  $r^*$  =median of the set D(p,p') over  $p' \in P$
  - We have

 $r_{med} \le r^* \le (n - 1)r_{med}$ with probability >1/2

- Approximating CC<sub>P</sub>(r\*)
  - n queries and updates to NN with r\*



# Algorithms for c-Approximate Near Neighbor

	Space	Time	Comment	Norm	Ref
	$dn+n^{O(1/\epsilon^2)}$	d * logn /ε²	c=1+ ε	Hamm, I <sub>2</sub>	[KOR'98, IM'98]
		(or 1)			
	$n^{\Omega(1/\epsilon^2)}$	O(1)			[AIP'06]
→	dn+n <sup>1+ρ(c)</sup>	dn <sup>ρ(c)</sup>	ρ(c)=1/c	Hamm, I <sub>2</sub>	[IM'98], [GIM'98],[Cha'02]
			ρ(c)<1/c	I <sub>2</sub>	[DIIM'04]
	dn * logs	dn <sup>σ(c)</sup>	σ(c)=O(log c/c)	Hamm, I <sub>2</sub>	[Ind'01]
	dn+n <sup>1+ρ(c)</sup>	dn <sup>ρ(c)</sup>	$\rho(c)=1/c^2 + o(1)$	l <sub>2</sub>	[Al'06]
			σ(c)=O(1/c)	I <sub>2</sub>	[Pan'06]

# Locality-Sensitive Hashing

#### [Indyk-Motwani'98]

- Idea: construct hash functions
  g: R<sup>d</sup> → U such that for any points p,q:
  - If ||p-q|| ≤ r, then Pr[g(p)=g(q)] is "high" "not-so-small"
  - If ||p-q|| >cr, then Pr[g(p)=g(q)] is "small"
- Then we can solve the problem by hashing
- Related work: [Paturi-Rajasekaran-Reif'95, Greene-Parnas-Yao'94, Karp-Waarts-Zweig'95, Califano-Rigoutsos'93, Broder'97]







# LSH

- A family H of functions h: R<sup>d</sup> → U is called (P<sub>1</sub>,P<sub>2</sub>,r,cr)-sensitive, if for any p,q:
   – if ||p-q|| <r then Pr[ h(p)=h(q) ] > P<sub>1</sub>
  - if ||p-q|| > cr then  $Pr[h(p)=h(q)] < P_2$
- Example: Hamming distance
  - KOR'98:  $h(p) = \sum_{i \in S} p_i u_i \mod 2$
  - IM'98:  $h(p)=p_i$ , i.e., the i-th bit of p
    - Probabilities: Pr[ h(p)=h(q) ] = 1-H(p,q)/d

p=10010010 q=11010110

# Algorithm

- We use functions of the form  $g(p) = \langle h_1(p), h_2(p), \dots, h_k(p) \rangle$
- Preprocessing:
  - Select  $g_1 \dots g_L$
  - For all  $p \in P$ , hash p to buckets  $g_1(p) \dots g_L(p)$
- Query:
  - Retrieve the points from buckets  $g_1(q), g_2(q), ..., until$ 
    - Either the points from all L buckets have been retrieved, or
    - Total number of points retrieved exceeds 3L
  - Answer the query based on the retrieved points
  - Total time: O(dL)

#### Analysis [IM'98, Gionis-Indyk-Motwani'99]

- Lemma1: the algorithm solves capproximate NN with:
  - Number of hash functions:

L=n<sup>ρ</sup>, ρ=log(1/P1)/log(1/P2)

Constant success probability per query q

- Lemma 2: for Hamming LSH functions, we have  $\rho\text{=}1\text{/}c$ 

### Proof of Lemma 1 by picture

- Points in {0,1}<sup>d</sup>
- Collision prob. for k=1..3, L=1..3 (recall: L=#indices, k=#h's)
- Distance ranges from 0 to d=10

