

# Restrictions on Input

Algorithms for Nearest Neighbor Search: Lecture 4

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# Making Nearest Neighbors Easier

Tractable solution:  $poly(n)$  preprocessing,  $poly \log(n)$  search time

General case of nearest neighbors seems to be intractable

Any **assumption** that makes the problem easier?

## Two approaches:

- Define **intrinsic dimension** of search domain and assume it is small (usually constant or  $\mathcal{O}(\log \log n)$ )
- Fix some probability distribution over inputs and queries. Find an algorithm which is fast **with high probability over inputs/query**

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# Outline

- 1 Nearest Neighbors in Small Doubling Dimension
- 2 Disorder Method: A Combinatorial Solution of Nearest Neighbors
- 3 Probabilistic Analysis: Zipf Model
- 4 Open Problems

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# Chapter XI

## Nearest Neighbors in Small Doubling Dimension

### Mini-plan:

Notion of doubling dimension

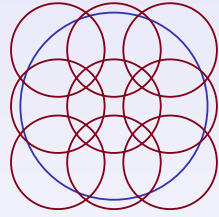
Solving 3-approximate nearest neighbors

From 3-approximation to  $(1 + \varepsilon)$ -approximation

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## Notion of Doubling Dimension

**Doubling constant**  $\lambda$  for search domain  $\mathbb{U}$ : minimal value such that for every  $r$  and every object  $p \in \mathbb{U}$  the ball  $B(p, 2r)$  has cover of at most  $\lambda$  balls of radius  $r$



**Doubling dimension:** logarithm of doubling constant  
 $\dim(\mathbb{U}) = \log \lambda$

**Exercise:** Prove that for Euclidean space  $\dim(\mathbb{R}^d) = \mathcal{O}(d)$

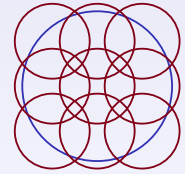
**Exercise:** Prove that  $\forall S \subset \mathbb{U} : \dim(S) \leq 2\dim(\mathbb{U})$

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## Doubling Dimension and $r$ -Nets

Set  $T \subset \mathbb{U}$  is an  $r$ -net for  $S \subset \mathbb{U}$  iff

- (1)  $\forall p, p' \in T : d(p, p') > r$
- (2)  $\forall s \in S \exists p \in T : d(s, p) < r$



### Lemma (Cover Lemma)

Every ball  $B(p, r)$  has  $\delta r$ -net of cardinality at most  $(\frac{1}{\delta})^{\mathcal{O}(\dim(\mathbb{U}))}$

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## Cover Lemma: Proof

### Greedy algorithm:

- 1 Start from empty  $T$
- 2 Find some object in  $S$  which is still  $\delta r$ -far from all objects in  $T$ , add it to  $T$
- 3 Stop when all objects in  $S$  are within  $\delta r$  from some point in  $T$

### Upper bound on size:

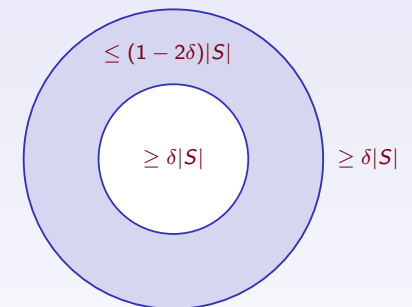
- Apply definition of doubling constant to  $B(p, r)$  recursively until getting  $\frac{\delta r}{3}$ -cover
- This cover has size  $(\frac{1}{\delta})^{\mathcal{O}(\dim(\mathbb{U}))}$
- Every element of this cover can contain at most one object from  $T$

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## Ring-Separator Lemma

Triple  $(p, r, 2r)$  is  $\delta$ -ring-separator for  $S$  iff

- 1  $|S \cap B(p, r)| \geq \delta|S|$
- 2  $|S/B(p, 2r)| \geq \delta|S|$



### Lemma (Ring-Separator Lemma)

For every  $S$  there is ring-separator with  $\delta \geq (\frac{1}{2})^{\mathcal{O}(\dim(S))}$

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## Ring-Separator Lemma: Proof

- Fix  $\delta = (\frac{1}{2})^{c \dim(S)}$  for some large  $c$
- For every  $p$  choose the maximal  $r_p$  such that  $|B(p, r_p)| < \delta |S|$
- Let  $p_0$  be the one having minimal  $r_{p_0}$
- If none of triples  $(p, r_p, 2r_p)$  is  $\delta$  ring-separator build an  $r_{p_0}$ -net for  $B(p_0, 2r_{p_0})$ :
  - Start from  $r_0$ , and set  $A := B(p_0, 2r_{p_0}) / B(p_0, r_{p_0})$
  - Iteratively add some point  $p$  from  $A$  to net, update  $A := A / B(p, r)$
- Since  $A$  decreased by at most  $2\delta |S|$  points each time there must be many points in cover. Since it is  $r_{p_0}$ -net for  $B(p_0, 2r_{p_0})$  there must be few points. Contradiction

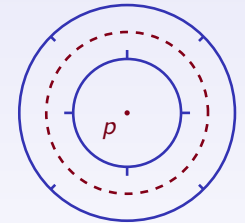
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## Ring-Separator Tree

Krauthgamer&Lee'05

### Preprocessing:

- 1 Find  $(\frac{1}{2})^{\mathcal{O}(\dim(S))}$  ring-separator  $(p, r, 2r)$  for  $S$
- 2 Put objects from  $B(p, 2r)$  to inner branch
- 3 Put objects from  $S / B(p, r)$  to outer branch
- 4 Recursively repeat



### Search:

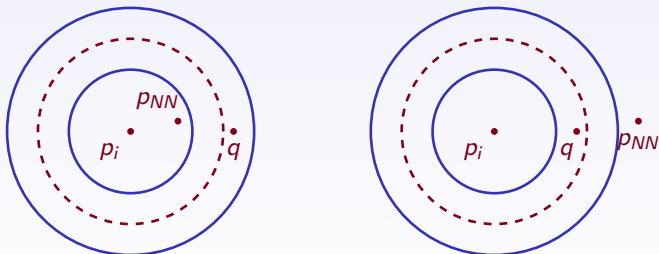
- 1 For every node  $(p, r, 2r)$ : if  $d(q, p) \leq 3r/2$  go only to inner branch otherwise go only to outer branch
- 2 Return the best object considered in search

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## 3-NN via Ring-Separator Tree

**Notation:**  $p_1, \dots, p_k$  are the centers of visited rings

- If  $p_{NN}(q) = p_k$  we are done
- If not, let us consider  $p_i$  where we miss the right branch. There are two cases:

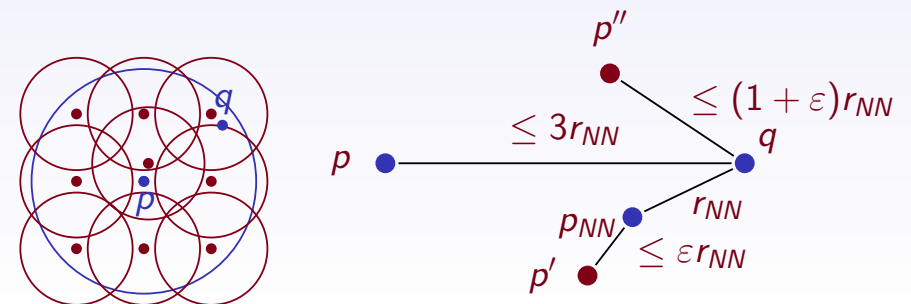


- Anyway,  $p_i$  at most 3 time worse than  $p_{NN}(q)$

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## From 3-NN to $r$ -NN: Reduction Algorithm

- 1 Find 3-approximate nearest neighbor  $p$  for  $q$
- 2 Quickly build a  $\varepsilon \frac{d(p, q)}{3}$  cover for  $B(p, 4 \frac{d(p, q)}{3})$ . See the next slide
- 3 Return an object in cover that is the closest to  $q$



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## From 3-NN to $r$ -NN: Net Construction

### Preprocessing:

- 1 For every  $i$  build  $2^i$ -net for  $S$  (every lower level contains all points from the higher level)
- 2 Compute **children pointers**: from every element  $p$  of  $2^i$ -net to all balls of  $2^{i-1}$ -net required to cover  $B(p, 2^i)$
- 3 Compute **brother pointers**: from every element  $p$  of  $2^i$ -net to all elements  $p'$  from  $2^i$ -net needed for covering  $B(p, 2^i)$
- 4 Compute **parent pointers**: from every element  $p$  of  $2^{i-1}$ -net to the element  $p'$  from  $2^i$ -net within  $2^i$  from it

### On-line net construction:

- 1 Go up by parent pointers until meeting ball big enough
- 2 Use brother pointer
- 3 Go by children pointers until getting cover small enough

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## Other Definitions of Intrinsic Dimension

- **Box dimension** is the minimal  $d$  that for every  $r$  our domain  $\mathbb{U}$  has  $r$ -net of size at most  $(1/r)^{d+o(1)}$
- **Karger-Ruhl dimension** of database  $S \subset \mathbb{U}$  is the minimal  $d$  that for every  $p \in S$  and every  $r$  the following inequality holds:  
 $|B(p, 2r) \cap S| \leq 2^d |B(p, r) \cap S|$
- **Measure-based dimensions**
- **Disorder dimension** (see next chapter)

**Exercise:** prove that

$$\forall S \subset \mathbb{U} : \dim_{\text{Doub}}(S) \leq 4 \dim_{\text{KR}}(S)$$

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## Chapter XII

### Disorder Method:

## A Combinatorial Solution of Nearest Neighbors

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## Concept of Disorder

Sort all objects in database  $S$  by their similarity to  $p$   
Let  $\text{rank}_p(s)$  be position of object  $s$  in this list

**Disorder inequality** for some constant  $D$ :

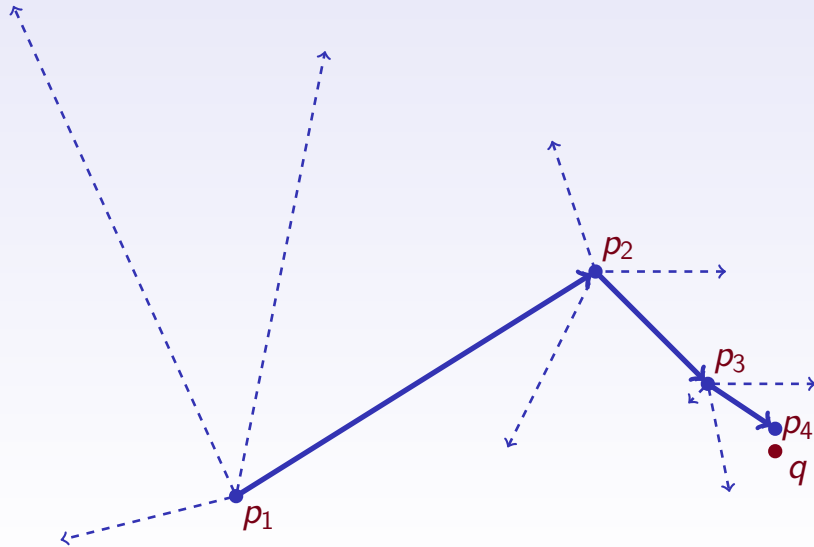
$$\forall p, r, s \in \{q\} \cup S : \text{rank}_r(s) \leq D \cdot (\text{rank}_p(r) + \text{rank}_p(s))$$

Minimal  $D$  providing disorder inequality is called **disorder constant** of a given set

For "regular" sets in  $d$ -dimensional Euclidean space  $D \approx 2^{d-1}$

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## Ranwalk Informally (1/2)



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## Ranwalk Informally (2/2)

### Hierarchical greedy navigation:

- 1 Start at random city  $p_1$
- 2 Among all **airlines** choose the one going most closely to  $q$ , move there (say, to  $p_2$ )
- 3 Among all **railway routes** from  $p_2$  choose the one going most closely to  $q$ , move there ( $p_3$ )
- 4 Among all **bus routes** from  $p_3$  choose the one going most closely to  $q$ , move there ( $p_4$ )
- 5 Repeat this  $\log n$  times and return the final city

**Transport system:** for level  $k$  choose  $c$  random arcs to  $\frac{n}{2^k}$  neighborhood

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## Ranwalk Algorithm

### Preprocessing:

- For every point  $p$  in database we sort all other points by their similarity to  $p$

Data structure:  $n$  lists of  $n - 1$  points each.

### Query processing:

- 1 Step 0: choose a random point  $p_0$  in the database.
- 2 From  $k = 1$  to  $k = \log n$  do Step  $k$ : Choose  $D' := 3D(\log \log n + 1)$  random points from  $\min(n, \frac{3Dn}{2^k})$ -neighborhood of  $p_{k-1}$ . Compute similarities of these points w.r.t.  $q$  and set  $p_k$  to be the most similar one.
- 3 If  $\text{rank}_{p_{\log n}}(q) > D$  go to step 0, otherwise search the whole  $D^2$ -neighborhood of  $p_{\log n}$  and return the point most similar to  $q$  as the final answer.

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## Analysis of Ranwalk

### Theorem (Goyal, YL, Schütze. 2007)

Assume that database points together with query point  $S \cup \{q\}$  satisfy disorder inequality with constant  $D$ :

$$\text{rank}_x(y) \leq D(\text{rank}_z(x) + \text{rank}_z(y)).$$

Then Ranwalk algorithm always answers nearest neighbor queries correctly. It uses the following resources:

Preprocessing space:  $\mathcal{O}(n^2)$ .

Preprocessing time:  $\mathcal{O}(n^2 \log n)$ .

Expected query time:  $\mathcal{O}(D \log n \log \log n + D^2)$ .

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## Arwalk Algorithm

### Preprocessing:

- For every point  $p$  in database we sort all other points by their similarity to  $p$ . For every level number  $k$  from 1 to  $\log n$  we store pointers to  $D' = 3D(\log \log n + \log 1/\delta)$  random points within  $\min(n, \frac{3Dn}{2^k})$  most similar to  $p$  points.

### Query processing:

- 1 Step 0: choose a random point  $p_0$  in the database.
- 2 From  $k = 1$  to  $k = \log n$  do Step  $k$ : go by  $p_{k-1}$  pointers of level  $k$ . Compute similarities of these  $D'$  points to  $q$  and set  $p_k$  to be the most similar one.
- 3 Return  $p_{\log n}$ .

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## Analysis of Algorithm

### Theorem (Goyal, YL, Schütze. 2007)

Assume that database points together with query point  $S \cup \{q\}$  satisfy disorder inequality with constant  $D$ :

$$\text{rank}_x(y) \leq D(\text{rank}_z(x) + \text{rank}_z(y)).$$

Then for any probability of error  $\delta$  Arwalk algorithm answers nearest neighbor query within the following constraints:

Preprocessing space:  $\mathcal{O}(nD \log n(\log \log n + \log 1/\delta))$ .

Preprocessing time:  $\mathcal{O}(n^2 \log n)$ .

Query time:  $\mathcal{O}(D \log n(\log \log n + \log 1/\delta))$ .

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## Chapter XIII

### Probabilistic Analysis: Zipf Model

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## Probabilistic Analysis in a Nutshell

- We define a probability distribution over databases
- We define probability distribution over query objects
- We construct a solution that is efficient/accurate with high probability over “random” input/query

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## Zipf Model

- Terms  $t_1, \dots, t_m$
- To generate a document we take every  $t_i$  with probability  $\frac{1}{i}$
- Database is  $n$  independently chosen documents
- Query document has exactly one term in every interval  $[e^i, e^{i+1}]$
- Similarity between documents is defined as the number of common terms

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## Magic Level Theorem

$$\text{Magic Level } q = \sqrt{2 \log_e n}$$

Theorem (Hoffmann, YL, Nowotka. CSR'07)

- 1 With very high probability there exists a document in database having  $q - \varepsilon$  **top** terms of query document
- 2 With very small probability there exists a document in database having **any**  $q + \varepsilon$  overlap with query document

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## Chapter XIV

### Future of Nearest Neighbors

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## Directions for Further Research (1/2)

- **Relational nearest neighbors**: using graph structure of underlying domain. Examples: co-occurrence similarity, recommendations via social network
- Nearest neighbors for **sparse vectors** in Euclidean space
- Low-distortion embeddings for social networks, **similarity visualization**
- Construct algorithms for **learning similarity function**

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## Directions for Further Research (2/2)

- **Probabilistic analysis** for specific domains: introduce reasonable input distributions and solve nearest neighbors for them
- Disorder method / Intrinsic dimension: fast algorithm for bounded **average dimension**
- Branch and bound techniques for **bichromatic nearest neighbors**
- New dynamic aspects: object descriptions are **changing in time**

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## OP1: NN for Sparse Vectors

**Database:**  $n$  vectors in  $\mathbb{R}^m$  each having at most  $k \ll m$  nonzero coordinates

**Query:** vector in  $\mathbb{R}^m$  also having at most  $k \ll m$  nonzero coordinates

**Similarity:** scalar product

Construct an algorithm for solving nearest neighbors on sparse vectors

**Constraints:**  $\text{poly}(n, m)$  preprocessing,  $\text{poly}(k, \log n)$  query

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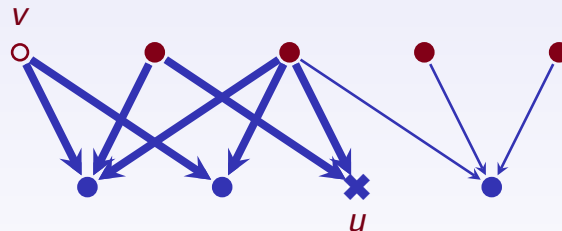
## OP2: 3-Step NN

**3-step similarity** between boy and girl in some bipartite boys-girls graph is equal to number of paths of length 3 between them

$n$  boys

boy degrees  $\leq k$

$m$  girls



Construct an algorithm for solving nearest neighbors in bipartite graphs with 3-step similarity

**Constraints:**  $\text{poly}(n, m)$  preprocessing,  $\text{poly}(k, \log n, \log m)$  query

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## Exercises

Prove that  $\dim_{\text{Doub}}(\mathbb{R}^d) = \mathcal{O}(d)$

Prove that  $\forall S \subset \mathbb{U} : \dim_{\text{Doub}}(S) \leq 2\dim_{\text{Doub}}(\mathbb{U})$

Prove that  $\forall S \subset \mathbb{U} : \dim_{\text{Doub}}(S) \leq 4\dim_{\text{KR}}(S)$

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## Highlights

- Doubling dimension: restriction on size of  $r$ -covers.  
Solution: ring-separator tree
- Disorder inequality: replacement of triangle inequality using rank values instead of actual similarity values
- Probabilistic analysis: Efficient algorithm for texts generated by Zipf model

Thanks for your attention! Questions?

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## References (1/2)

**Course homepage** <http://simsearch.yury.name/tutorial.html>



**Y. Lifshits**

The Homepage of Nearest Neighbors and Similarity Search

<http://simsearch.yury.name>



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