Combinatorial Approach to Data Mining

Yury Lifshits

Caltech

http://yury.name

MIT, 29 November 2007

Based on joint work with Navin Goyal, Benjamin Hoffmann, Dirk Nowotka, Hinrich Schütze and Shengyu Zhang

Nearest neighbors

Preprocess a set S such that given any q
the closest point in S to q can be found quickly

Near-duplicates

Find all pairs of objects with distance
below some threshold in subquadratic time

Navigability design

Construct a graph such that local routing
is leading to target in logarithmic number of steps

Clustering

Split a set to k parts minimizing in-cluster distances

Nearest neighbors

Preprocess a set S such that given any q
the closest point in S to q can be found quickly

Near-duplicates

Find all pairs of objects with distance
below some threshold in subquadratic time

Navigability design

Construct a graph such that local routing
is leading to target in logarithmic number of steps

Clustering

Split a set to k parts minimizing in-cluster distances

Today: distances are not given,
triangle inequality is not satisfied

Outline

1. Combinatorial Framework
2. Results: New Algorithms
3. One Proof: Visibility Graph
4. Open Problems

1

Combinatorial Framework

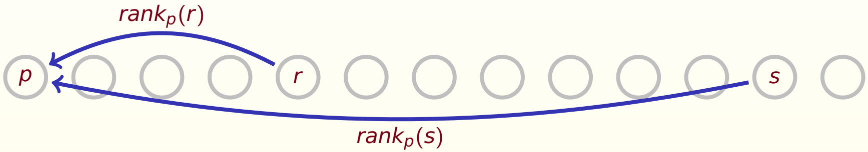
Comparison Oracle

- Dataset $p_1, \ldots, p_n$
- Objects and distance (or similarity) function are NOT given
- Instead, there is a comparison oracle answering queries of the form:

Who is closer to A: B or C?

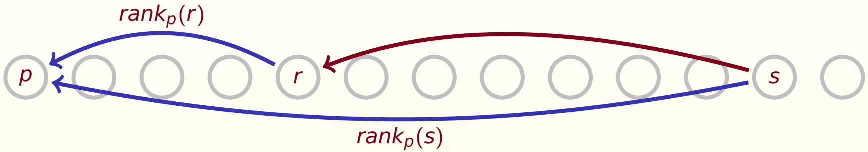
Disorder Inequality

Sort all objects by their similarity to p:

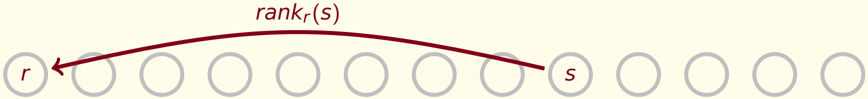


Disorder Inequality

Sort all objects by their similarity to p:

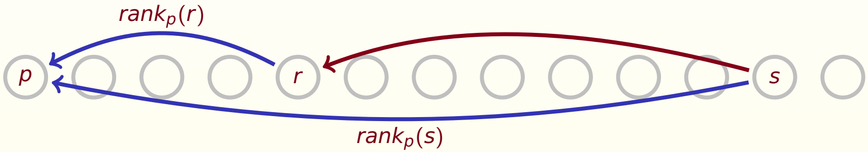


Then by similarity to r:

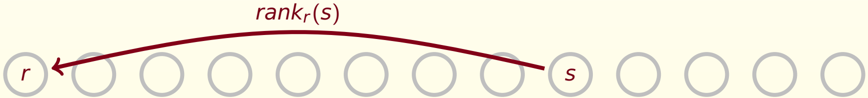


Disorder Inequality

Sort all objects by their similarity to p:



Then by similarity to r:



Dataset has **disorder** D if

$$\forall p, r, s: \quad rank_r(s) \leq D(rank_p(r) + rank_p(s))$$

Combinatorial Framework

$$=$$

Comparison oracle

Who is closer to A: B or C?

$$+$$

Disorder inequality

$$rank_r(s) \leq D(rank_p(r) + rank_p(s))$$

Combinatorial Framework: Pro & Contra

Advantages:

- Does not require triangle inequality for distances
- Applicable to any data model and any similarity function
- Require only comparative training information
- Sensitive to “local density” of a dataset

Combinatorial Framework: Pro & Contra

Advantages:

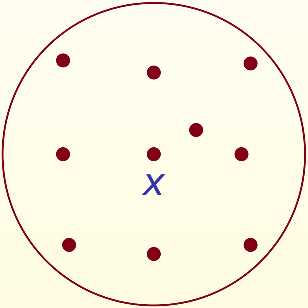
- Does not require triangle inequality for distances
- Applicable to any data model and any similarity function
- Require only comparative training information
- Sensitive to “local density” of a dataset

Limitation: worst-case form of disorder inequality

Combinatorial Ball

$$B(x, r) = \{y : \mathrm{rank}_x(y) < r\}$$

In other words, it is a subset of dataset S: the object x itself and $r - 1$ its nearest neighbors



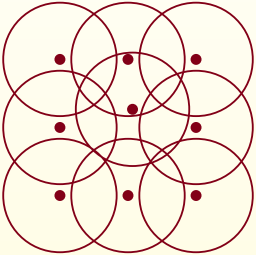
$B(x, 10)$

Combinatorial Net

A subset $R \subseteq S$ is called a **combinatorial r-net** iff the following two properties holds:

Covering: $\forall y \in S, \exists x \in R,$ s.t. $\text{rank}_x(y) < r$.

Separation: $\forall x_i, x_j \in R,$ $\text{rank}_{x_i}(x_j) \geq r$ OR $\text{rank}_{x_j}(x_i) \geq r$

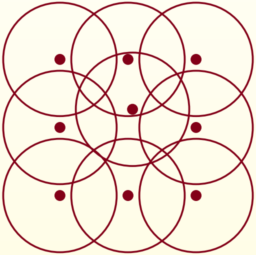


Combinatorial Net

A subset $R \subseteq S$ is called a **combinatorial r-net** iff the following two properties holds:

Covering: $\forall y \in S, \exists x \in R,$ s.t. $\text{rank}_x(y) < r$.

Separation: $\forall x_i, x_j \in R,$ $\text{rank}_{x_i}(x_j) \geq r$ OR $\text{rank}_{x_j}(x_i) \geq r$



How to construct a combinatorial net?
What upper bound on its size can we guarantee?

Disorder vs. Others

- If expansion rate is c, disorder constant is at most c^2
- Doubling dimension and disorder dimension are incomparable
- Disorder inequality implies combinatorial form of “doubling effect”

2

Results:
Combinatorial Algorithms

Basic Data Structure

Combinatorial nets:

For every $0 \le i \le \log n$, construct a $\frac{n}{2^i}$-net

Basic Data Structure

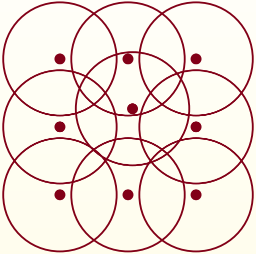
Combinatorial nets:

For every $0 \leq i \leq \log n$, construct a $\frac{n}{2^i}$-net

Pointers, pointers, pointers:

- Direct & inverted indices: links between centers and members of their balls
- Cousin links: for every center keep pointers to close centers on the same level
- Navigation links: for every center keep pointers to close centers on the next level

Fast Net Construction



Theorem

Combinatorial nets can be constructed in $\mathcal{O}(D^7 n \log^2 n)$ time

Nearest Neighbor Search

Assume $S \cup \{q\}$ has disorder constant D

Theorem

There is a deterministic and exact algorithm for nearest neighbor search:

- *Preprocessing:* $\mathcal{O}(D^7 n \log^2 n)$
- *Search:* $\mathcal{O}(D^4 \log n)$

Nearest Neighbor Search

Assume $S \cup \{q\}$ has disorder constant D

Theorem

There is a deterministic and exact algorithm for nearest neighbor search:

- *Preprocessing:* $\mathcal{O}(D^7 n \log^2 n)$
- *Search:* $\mathcal{O}(D^4 \log n)$

Variations:

- $\mathcal{O}(n)$ size of data structure, still $poly(D) \log n$ search
- Randomized algorithm, $\mathcal{O}(D \log n)$ search

Navigability Design

Local routing in a graph:

Given target description
and the current node p
a message is forwarded
via one of the out-going edges from p

Navigability Design

Local routing in a graph:

Given target description
and the current node p
a message is forwarded
via one of the out-going edges from p

Design task:

Given a collection of points $S = \{p_1, \ldots, p_n\}$
construct a low-degree graph
and rules for local decisions
such that given a start $p \in S$ and a target q
the nearest neighbor of q in S
can be reached in a small number of steps

Visibility Graph

Theorem

Any dataset S has a **visibility graph***:*

- $poly(D) n \log^2 n$ *construction time*
- $\mathcal{O}(D^4 \log n)$ *out-degrees*
- *Naïve greedy routing deterministically reaches exact nearest neighbor of q in at most $\log n$ steps*

Near-Duplicates

Assume, comparison oracle can also tell us whether $\sigma(x, y) > T$ for some similarity threshold T

Theorem

All pairs with over-T similarity can be found deterministically in time

$$poly(D)(n \log^2 n + |Output|)$$

Clustering

Combinatorial objective function for k-clustering:

$$\text{Minimize} \quad \sum_{i \in [k]} \sum_{x,y \in C_i} rank_x(y)$$

Clustering

Combinatorial objective function for k-clustering:

$$\text{Minimize} \quad \sum_{i \in [k]} \sum_{x,y \in C_i} rank_x(y)$$

Theorem

A $32D^3$-approximate clustering can be constructed in time $poly(D) n \log^2 n$

3

One Proof: Visibility Graph

Problem Statement

Input:

Dataset $S = \{p_1, \ldots, p_n\}$
Represented by comparison oracle
Having disorder constant D

Problem Statement

Input:

Dataset $S = \{p_1, \ldots, p_n\}$
Represented by comparison oracle
Having disorder constant D

Design Task:

Connect every object with few others
Set local rules for routing

Problem Statement

Input:

Dataset $S = \{p_1, \ldots, p_n\}$
Represented by comparison oracle
Having disorder constant D

Design Task:

Connect every object with few others
Set local rules for routing

Routing Requirement: Given a target point q and a starting point $p \in S$ the nearest neighbor of q in S should be reached by a few steps in the graph

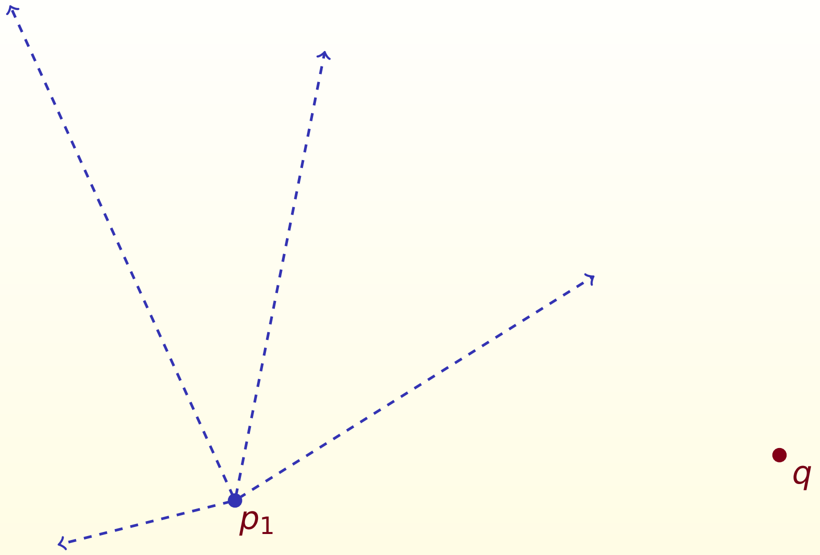
Greedy Routing

1. Use oracle to compare distances to q from current point p and from all its neighbors in the graph
2. If p is not the closet one, move to the one which is the closest
3. Otherwise, STOP and return p

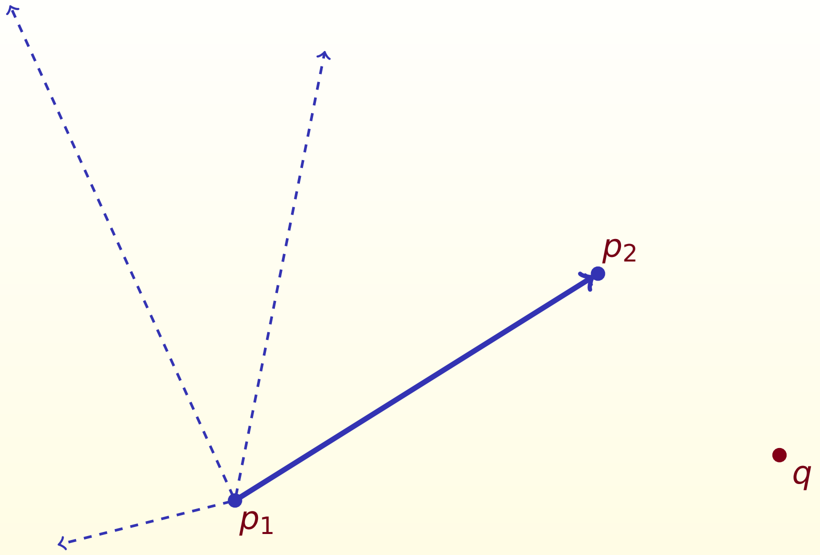
Greedy Routing

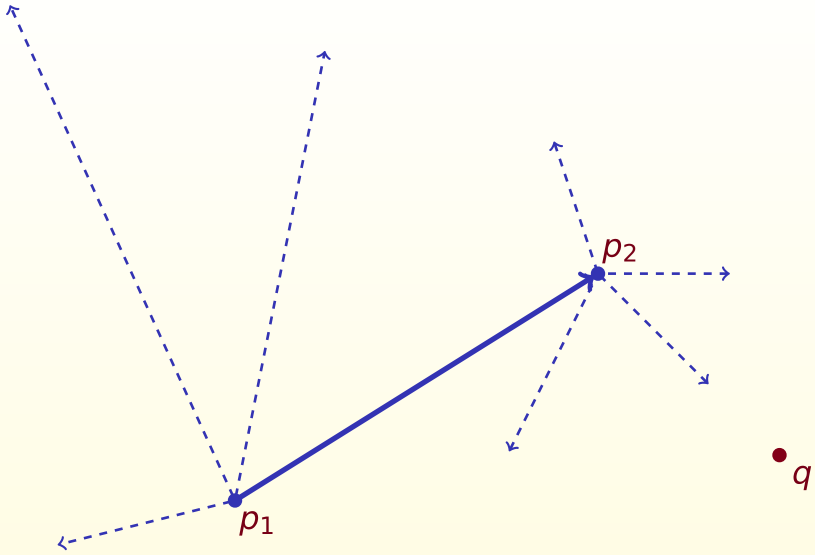
1. Use oracle to compare distances to q from current point p and from all its neighbors in the graph
2. If p is not the closet one, move to the one which is the closest
3. Otherwise, STOP and return p

Also known as local search, hill climbing etc.

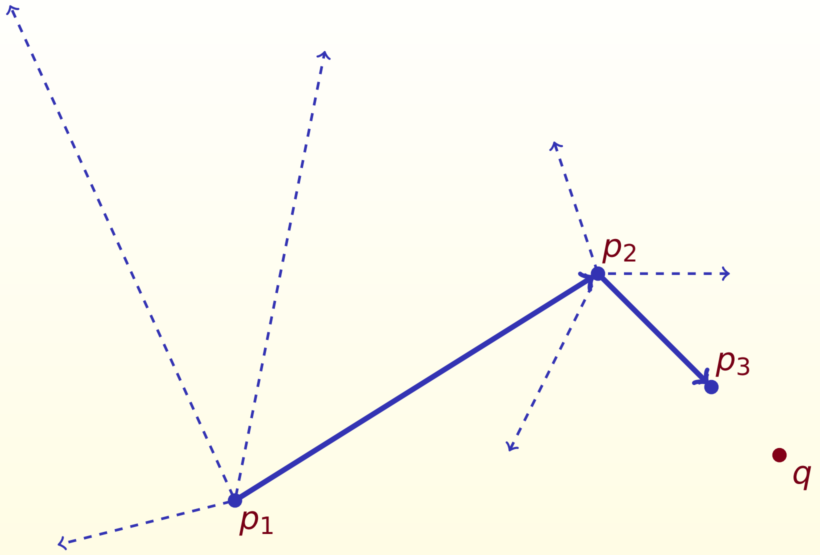


p_1
q

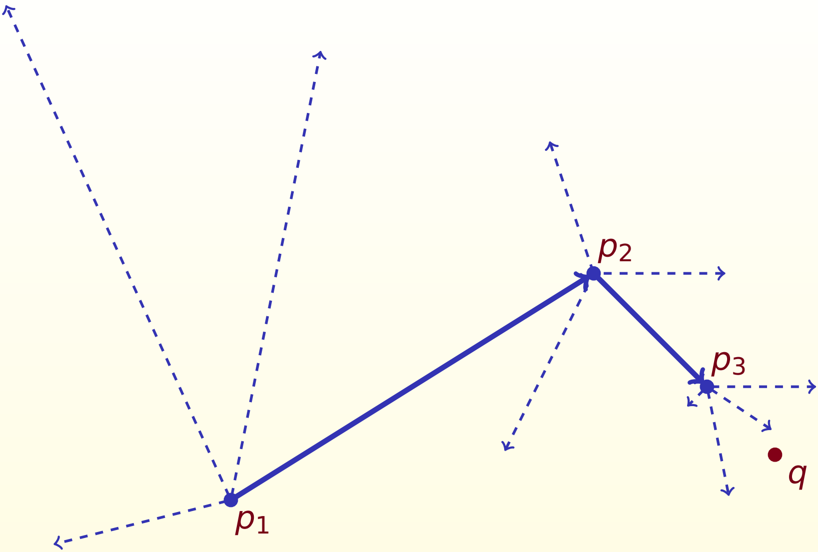

p_2
q
p_1



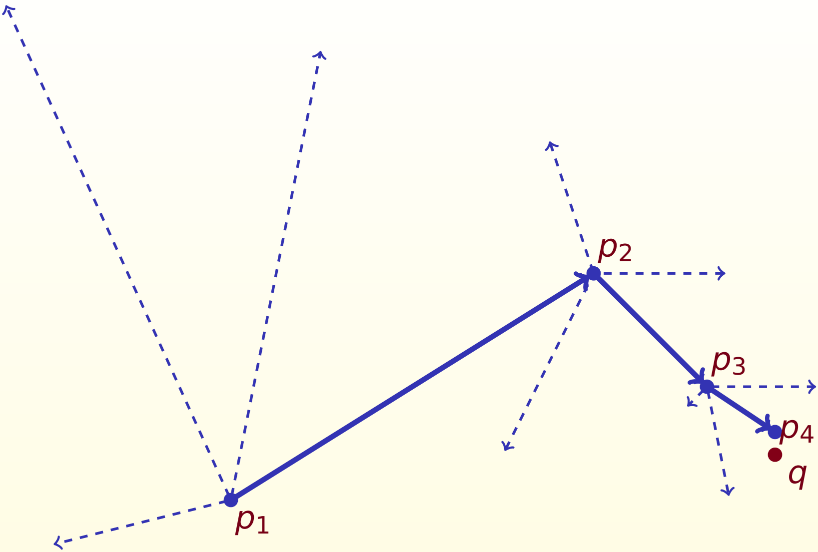
p_1
p_2
q



p_2
p_3
q
p_1



p_2
p_3
p_1
q


p_1
p_2
p_3
p_4
q

Definition of Visibility

A center c_i in the $\frac{n}{2^i}$-net is visible from some object p iff

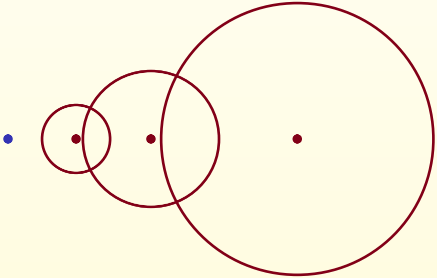
$$rank_p(c_i) \leq 3D^2 \frac{n}{2^i}$$

Definition of Visibility

A center c_i in the $\frac{n}{2^i}$-net is visible from some object p iff

$$rank_p(c_i) \leq 3D^2 \frac{n}{2^i}$$

Interpretation: the farther you are the larger radius you need to be visible

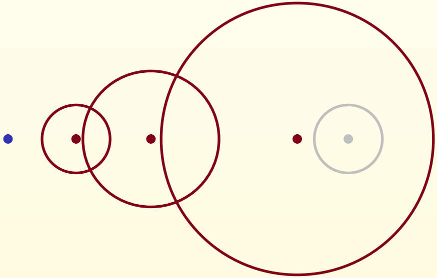


Definition of Visibility

A center c_i in the $\frac{n}{2^i}$-net is visible from some object p iff

$$rank_p(c_i) \leq 3D^2 \frac{n}{2^i}$$

Interpretation: the farther you are the larger radius you need to be visible



Analysis

Three claims:

- Out-degrees are $\mathcal{O}(D^4 \log n)$
- After i steps we reach a point that is at least as close to q as the best center in $\frac{n}{2^i}$-net
- Visibility graph can be constructed in $poly(D) n \log^2 n$ time

Bound on Degrees

Connecting p with centers of r-net:

- By construction, centers have ranks at most $3D^2r$ to p
- There are disjoint $\frac{r}{2D}$ balls around these centers
- Members of these disjoint balls have $\mathcal{O}(D^3)r$ rank to p
- Thus, there are at most $\mathcal{O}(D^4)$ such centers

Fast Convergence

After i steps we reach a point that is at least as close to q as the best point in $\frac{n}{2^i}$-net

Inductive proof. From i to $i+1$:

- For the best center in i-th level $rank_q(c_i^*) \le Dr_i$.

  Similarly, c_{i+1}^* satisfies $rank_q(c_{i+1}^*) \le \frac{Dr_i}{2}$

Fast Convergence

After i steps we reach a point that is at least as close to q as the best point in $\frac{n}{2^i}$-net

Inductive proof. From i to $i+1$:

- For the best center in i-th level $rank_q(c_i^*) \leq Dr_i$.

  Similarly, c_{i+1}^* satisfies $rank_q(c_{i+1}^*) \leq \frac{Dr_i}{2}$

- From inductive conjecture: after i steps in a greedy walk the current point $p^{(i)}$ also has $rank_q(p^{(i)}) \leq Dr_i$

Fast Convergence

After i steps we reach a point that is at least as close to q as the best point in $\frac{n}{2^i}$-net

Inductive proof. From i to $i+1$:

- For the best center in i-th level $rank_q(c_i^*) \leq Dr_i$.

  Similarly, c_{i+1}^* satisfies $rank_q(c_{i+1}^*) \leq \frac{Dr_i}{2}$
- From inductive conjecture: after i steps in a greedy walk the current point $p^{(i)}$ also has $rank_q(p^{(i)}) \leq Dr_i$
- By disorder inequality $p^{(i)}$ is connected to c_{i+1}^*

  Therefore $p^{(i+1)}$ is at least as good as c_{i+1}^* is

Directions for Further Research

- Other problems in combinatorial framework:
  - Low-distortion embeddings
  - Closest pairs
  - Community discovery
  - Linear arrangement
  - Distance labelling
  - Dimensionality reduction
- What if disorder inequality has exceptions, but holds in average?
- Insertions, deletions, changing metric
- Metric regularizations
- Experiments & implementation

Call for Feedback

- What do you like the most in these results?
- What is the most important question for further studies?
- Relevant literature?

Call for Feedback

- What do you like the most in these results?
- What is the most important question for further studies?
- Relevant literature?
- Are you interested in further discussions?

  I am around this evening and the whole Friday.

Call for Feedback

- What do you like the most in these results?
- What is the most important question for further studies?
- Relevant literature?
- Are you interested in further discussions?

  I am around this evening and the whole Friday.

Another talk: YL, “Open Problems TO GO”

Friday Nov 30, 4pm, 56-154, MIT Theory Reading Group

Sponsored Links

http://yury.name

http://simsearch.yury.name

Tutorial, bibliography, people, links, open problems

Yury Lifshits and Shengyu Zhang
Similarity Search via Combinatorial Nets
http://yury.name/papers/lifshits2008similarity.pdf

Navin Goyal, Yury Lifshits, Hinrich Schütze
Disorder Inequality: A Combinatorial Approach to Nearest Neighbor Search
http://yury.name/papers/goyal2008disorder.pdf

Benjamin Hoffmann, Yury Lifshits, Dirk Novotka
Maximal Intersection Queries in Randomized Graph Models
http://yury.name/papers/hoffmann2007maximal.pdf

Summary

- Combinatorial framework:
  comparison oracle + disorder inequality
- Near-linear construction of combinatorial nets
- Nearest neighbor search in almost logarithmic time
- Deterministic detection of near-duplicates in subquadratic time
- Visibility graph: small degrees and deterministic convergence in $\log n$ steps

Summary

- Combinatorial framework:
  comparison oracle + disorder inequality
- Near-linear construction of combinatorial nets
- Nearest neighbor search in almost logarithmic time
- Deterministic detection of near-duplicates in subquadratic time
- Visibility graph: small degrees and deterministic convergence in $\log n$ steps

Thanks for your attention!

Questions?