Similarity searching, or how to find your neighbors efficiently

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Background

- **Geometric spaces and techniques are useful in tackling computational problems**
  - Arise in diverse application areas, e.g. data analysis, machine learning, networking, combinatorial optimization

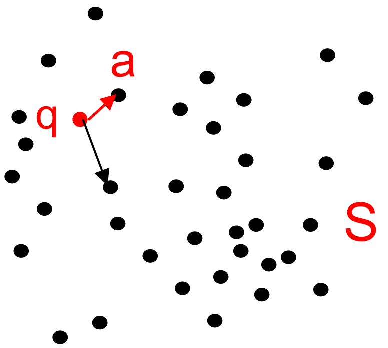
- **Definition: A *metric space* is a set of points M endowed with distance function $d_M(\cdot,\cdot)$**
  - Points can model various data objects e.g. documents, images, biological sequences (or network nodes)
  - Distances can model (dis)similarity between objects (or latency)

  - Common examples: Euclidean, L_p-norms, Hyperbolic, Hamming distance, Edit distance, Earthmover distance

  - Arises also in Linear and Semidefinite Programming (LP,SDP) relaxations

Similarity Searching [Basic Problem]

- **Nearest Neighbor Search (NNS):**
  - **Preprocess:** a dataset S of n points
  - **Query:** given point q, quickly find closest $a \in S$, i.e. $\mathrm{argmin}_{a \in S}\ d_M(a,q)$

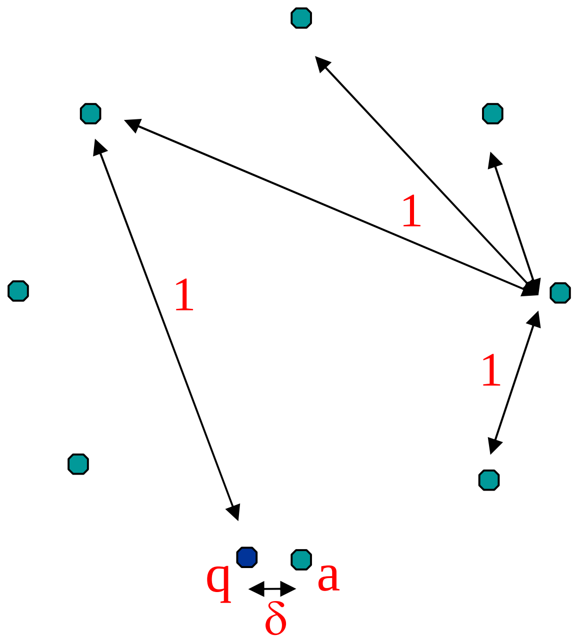


- **Naive solution:**
  - No preprocessing, query time O(n)
- **Ultimate goal (holy grail):**
  - Preprocessing O(n), and query time O(log n)
- **Key problem,**
  - Difficult in hig
  - Algorithms fo
    - Query time
    - Query time

    [Indyk-Motwani

NNS in General Metrics

- **Black-box model:** **Access to pairwise distances (only).**
- **Suppose M is a uniform metric**
  - i.e. $d(x,y) = 1$ for all $x,y \in M$,

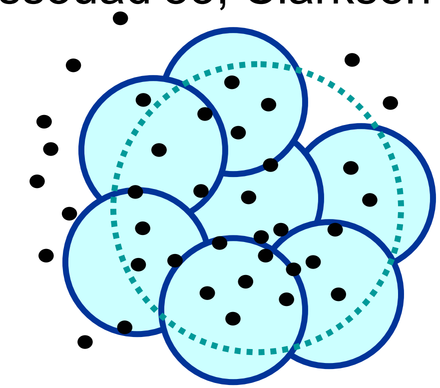


- **For some queries, time $\geq \Omega(n)$, even for approximate NNS.**
- **Depicts difficulty of NNS for high-dimensional data**
  - Such data sets exist in $\mathbb{R}^{\log n}$
- **Is this the only obstacle to efficient NNS?**
  - What about data that "looks" low-dimensional?

A Metric Notion of Dimension

- **Definition: Ball B(x,r) = all points within distance r>0 from $x \in M$.**

- **The dimension of M, denoted dim(M), is the minimum k such that every ball can be covered by 2^k balls of half the radius**
  - Defined by [Gupta-K.-Lee'03], inspired by [Assouad'83, Clarkson'97].
  - Call a metric doubling if dim(M) = O(1)
  - Captures every norm on $\mathbb{R}^k$



Here $2^k \leq 7$.

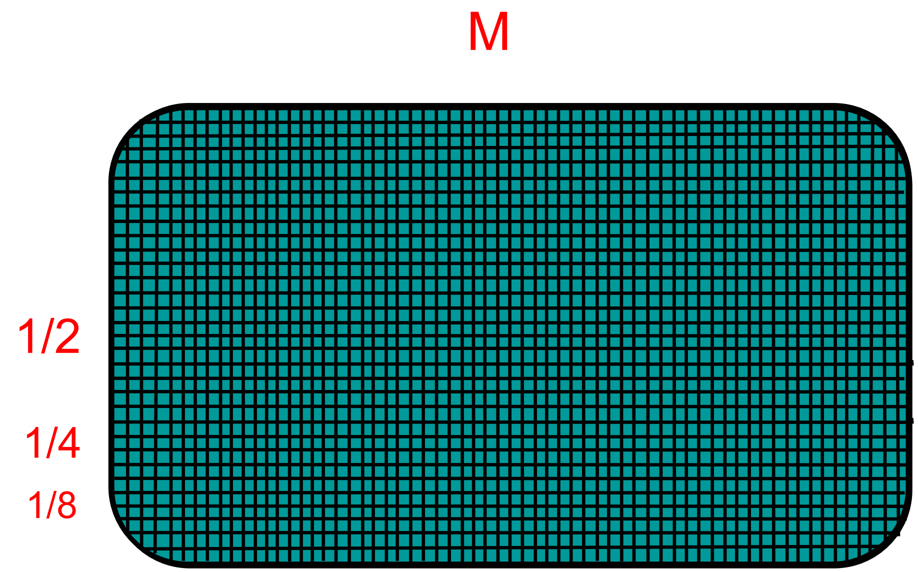
- **Robust to:**
  - taking subsets,
  - union of sets,
  - small distortion in distances, etc.
  - Unlike previous suggestions based on cardinality |B(x,r)| [Plaxton-Richa-Rajaraman'97, Karger-Ruhl'02, Faloutsos-Kamel'94, K.-Lee'03, …]

NNS in Doubling Metrics

- **Theorem [K.-Lee'04a]: There is a *simple* $(1+\varepsilon)$-NNS scheme**
  - Query time: $(1/\varepsilon)^{O(\dim(S))} \cdot \log \Phi$. [$\Phi = d_{max}/d_{min}$ is spread]
  - Preprocessing: $n \cdot 2^{O(\dim(S))}$.
  - Insertion/deletion time: $2^{O(\dim(S))} \cdot \log \Phi \cdot \log\log \Phi$.
- **Outperforms previous schemes [Plaxton-Richa-Rajaraman'98, Clarkson'99, Karger-Ruhl'02]**
  - Simpler, wider applicability, deterministic, no apriori info
  - Nearly matches the Euclidean low-dim. case [Arya et al.'94]
  - Explains empirical successes—it's just easy…
- **Subsequent enhancements**
  - Optimal storage $O(n)$ [Beygelzimer-Kakade-Langford'06]
    - Also implemented and obtained very good empirical results
  - Bounds independent of Φ [K.-Lee'04b, Mendel-HarPeled'05, Gottlieb-Cole'06]
  - Improved for Euclidean metrics [Indyk-Naor'06, Dasgupta-Fruend'08]

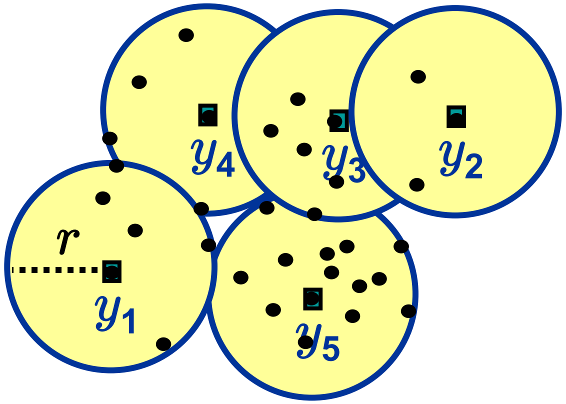
Nets

- Motivation: Approximate the metric at one scale $r>0$.
  - Provide a spatial "sample" of the metric space
  - E.g., grids in $\mathbb{R}^2$.



- General approach:
  - **Choose representatives Y iteratively**

- **Definition: $Y \subseteq S$ is called an r-net if both:**
  1. For all $y_1, y_2 \in Y$, $d(y_1,y_2) \geq r$ [packing]
  2. For all $x \in M \setminus Y$, $d(x,Y) < r$ [covering]



Navigating Nets

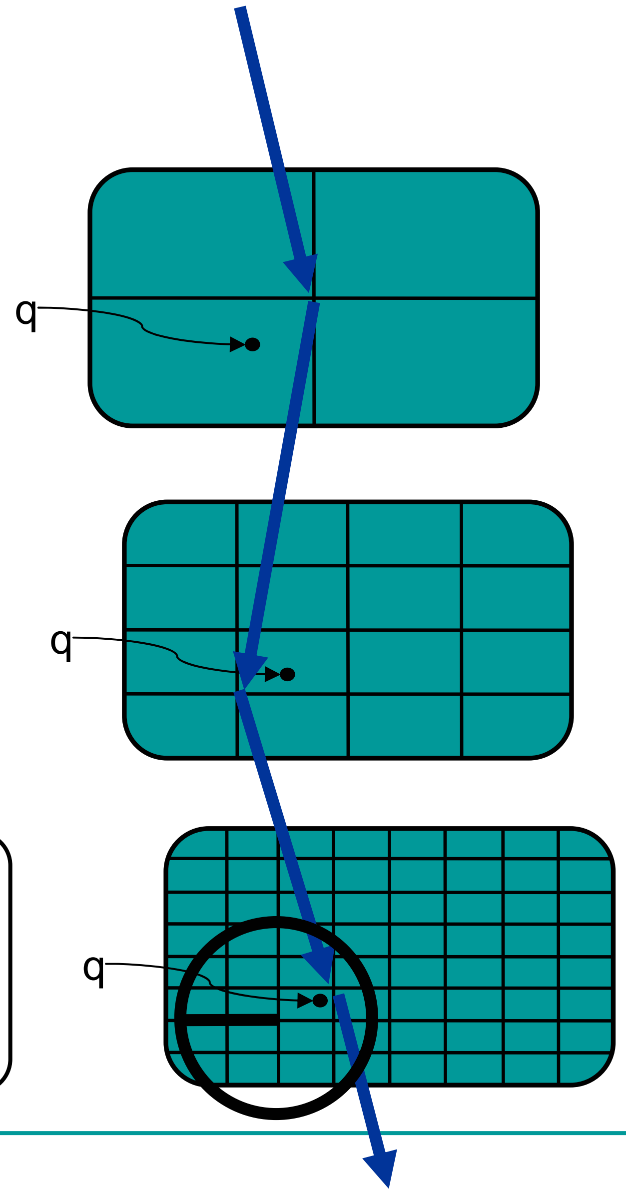
NNS scheme (vanilla version):

- **Preprocessing:**
  - Compute a 2^i-net Y_i for all $i \in \mathbb{Z}$.
  - Add "local links".
- **Query algorithm:**
  - Iteratively go to finer nets
  - Find net-point $\mathbf{y_i} \in \mathbf{Y_i}$ closest to query

From a 2^i-net point to ***nearby*** 2^{i-1}-net points

$d(q,y_i) \le OPT+2^i \Rightarrow d(y_i,y_{i-1}) \le 2OPT+2^i+2^{i-1}$

Thus: # "local" links $\le 2^{O(\dim(S))}$.



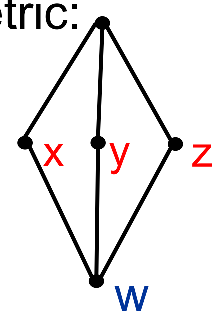
Embeddings [Basic Technique]

- **An *embedding* of M into l_1 is a mapping f: $M \to \mathbb{R}^m$**
  - We say **f** has distortion **K≥1** if

$$d_M(x,y) \le \|f(x)-f(y)\|_1 \le K \cdot d_M(x,y) \qquad \forall x,y \in M$$

- **Example:**

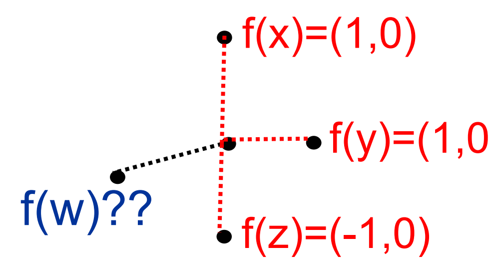
Tree metric:



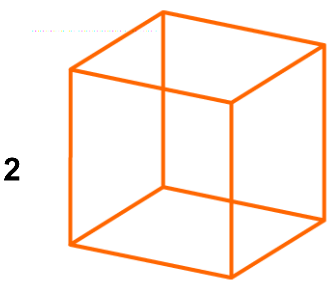
distortion=1

distortion≥4/3

Embedding into $\mathbb{R}^2$:



- **Another example:**
  - discrete cube $\{0,1\}^r$ with $d(x,y)=||x-y||_2$
  - under identity map: $||x-y||_2 \le ||x-y||_1 \le \sqrt{r} \cdot ||x-y||_2$
  - distortion = $\sqrt{r}$? Nah…



- **Very powerful concept, many applications (including NNS)**

A Few Embeddings Theorems

Every n-point ***metric*** embeds

- into l_2 (thus into l_1) with distortion O(log n) [Bourgain'86]
- Tight on expanders

Every n-point ***tree metric*** embeds

- into l_1 isometrically
- into l_2 with distortion $O(\log\log n)^{1/2}$ [Matousek'99]

If M is ***doubling***, $\sqrt{d_M}$ embeds into l_2 (thus into l_1) with distortion O(1) [Assouad'83]

Every doubling **tree metric** embeds into l_2 with distortion O(1) [Gupta-K.-Lee'03]

Some Open Problems [Embeddings]

- **Dimension reduction in l_2:**
  - **Conjecture:** If M is Euclidean (a subset of l_2) and doubling, then it embeds with distortion O(1) into *low-dimensional* l_2 (or l_1)
  - Known: dimension O(log n) where n=# points (not doubling dimension) [Johnson-Lindenstrauss'84]
  - Known: Can embed metric $\sqrt{d_M}$ [Assouad'83]

- **Planar graphs:**
  - **Conjecture:** Every planar metric embeds into l_1 with distortion O(1)

Edit Distance [Specific Metric]

Edit Distance (ED) between two strings $x,y \in \Sigma^d$:

- Minimum number of character insertions / deletions / substitutions to transform one string into the other
- **Extensively used, many applications, variants**

Examples:
ED(and , an)=1
ED(0101010,
1010101) = 2

Computational problems:

1. **Computing ED for two input strings**
   - Currently, best runtime is quadratic $O(d^2/\log^2 d)$ [Masek-Paterson'80]
2. **Quick approximation (near-linear time)**
   - Currently, best approximation is $2^{O(\sqrt{d})}$ [Andoni-Onak'08]
   - Smoothed model: $O(1/\varepsilon)$ approximation in time $d^{1+\varepsilon}$ [Andoni-K.'07]
3. **Estimate ED in restricted computational model**
   - Sublinear time, data-stream model, or limited communication model
4. **NNS under ED** (polynomial preprocessing, sublinear query)
   - Currently, best bounds are obtained via embedding into L_1

Ulam's metric

- **Definitions:**
  - A string $s \in \Sigma^d$ is called a ***permutation*** if it consists of distinct symbols
  - ***Ulam's metric*** = Edit distance on the set of permutations [Ulam'72]
  - For simplicity, suppose **$\Sigma=\{1,\ldots,d\}$** and "ignore" substitutions

x= **123456789**

y= **234657891**

- **Motivations:**
  - A permutation can model ranking, deck of cards, sequence of genes, …
  - A special case of edit distance, useful to develop techniques

Embedding of permutations

Theorem [Charikar-K.'06]: Edit distance on permutations (aka Ulam's metric) embeds into l_1 with distortion O(log d).

Proof. Define $f : \Sigma^d \to R^{|\Sigma|^2}$ **by** $f_{a,b}(P) = \frac{1}{P^{-1}[a] - P^{-1}[b]}$

distortion bound is optimal [Andoni-K.'07]

Intuition:

- sign($f_{a,b}(P)$) indicates whether "a appears before b" in P
- Thus, $|f_{a,b}(P)-f_{a,b}(Q)|$ "measures" if {a,b} is an inversion in P vs. Q

Claim 1: $||f(P)-f(Q)||_1 \le O(\log d)\, ED(P,Q)$

- Assume wlog ED(P,Q)=2, i.e. Q obtained from P by moving one symbol 's'
  - General case then follows by triangle inequality on $P=P_0,P_1,\ldots,P_t=Q$ namely $||f(P)-f(Q)||_1 \le \sum_{j=1}^{t} ||f(P_j)-f(P_{j-1})||_1$
- Total contribution
  - From coordinates where $s \in \{a,b\}$: $\le 2\sum_k (1/k) \le O(\log d)$
  - From other coordinates: $\le \sum_k k(1/k - 1/(k+1)) \le O(\log d)$

Embedding of permutations

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Proof. Define $f : \Sigma^d \to R^{|\Sigma|^2}$ **by** $f_{a,b}(P) = \frac{1}{P^{-1}[a] - P^{-1}[b]}$

Claim 1: $\|f(P)-f(Q)\|_1 \leq O(\log d)\, ED(P,Q)$ ✓

Claim 2: $\|f(P)-f(Q)\|_1 \geq \frac{1}{4} ED(P,Q)$ [alt. proof by Gopalan-Jayram-K.]

- Assume wlog that P=identity
- Edit Q into P=identity using quicksort:
  - Choose a random pivot,
  - Delete all characters inverted wrt to pivot
  - Repeat recursively on left and right portions

pivot

Q= **234657891**

- Now argue **ED(P,Q) ≤ 2 $\mathbb{E}$[#quicksort deletions] ≤ 4** $\|f(P)-f(Q)\|_1$

Surviving subsequence is increasing, thus
ED(P,Q) ≤ 2 #deletions

For every inversion (a,b) in Q:
Pr[a deleted "by" pivot b] ≤
≤ 1 / $|Q^{-1}[a]-Q^{-1}[b]+1|$ ≤ 2 $|f_{a,b}(P) - f_{a,b}(Q)|$

Open Problems [Sublinear Algorithms]

- **Estimate in sublinear time the distance between input permutation P and the identity** [testing distance to monotonicity]
  - If distance = $\delta \cdot d$, use only $\tilde{O}(1/\delta)$ queries to P
  - An $O(\log d)$-approximation follows from the embedding
  - Actually, a factor 2-approximation is known
- **Lower bound for approximation=$1+\varepsilon$?**
  - Question: deciding whether distance is $<d/100$ or $>d/99$ requires $d^{\Omega(1)}$ queries to P?

- **Similar but for block operations [transposition distance]:**
  - Approximation 3 is known (exercise)
  - Is there a lower bound for $1+\varepsilon$ approximation?
  - Remark: distance is not known to be computable in polynomial time

Research Objectives

Two intertwined goals:

1. **Understand the complexity of metric spaces from a mathematical and computational perspective**
   - E.g., identify geometric properties that reveal a simple underlying structure
2. **Develop algorithmic techniques that exploit such characteristics**
   - E.g., design tools that dissect a metric into smaller pieces, or faithfully convert them into simpler metrics

Thank you!

Concrete directions:

- **Find new NNS algorithms for different metrics (in particular for high-dimension)**
- **Classify and characterize metric spaces via embeddings**