## President's Day Lecture: Advanced Nearest Neighbor Search

[Advanced Algorithms, Spring'17]

## Announcements

- Evaluation on CourseWorks
- If you think homework is too easy (or too hard):
" mark "appropriateness of workload"


## Time-Space Trade-offs (Euclidean)

| space | query | Space | Time | Comment | Reference |
| :---: | :---: | :---: | :---: | :---: | :---: |
| low | high | $\approx n$ | $n^{\sigma}$ | $\sigma=2.09 / c$ | [Ind'01, Par'06] |
|  |  |  |  | $\sigma=O\left(1 / c^{2}\right)$ | [A100] |
| medium | medium | ${ }^{n^{1+\rho}}$ | $n^{\rho}$ | $\rho=1 / c$ | [IM 98 , DIIM $\left.{ }^{\prime} 04\right]$ |
|  |  |  |  | $\rho=1 / c^{2}$ | [A106] |
|  |  |  |  | $\rho \geq 1 / c^{2}$ | [MNP'06, OWZ'11] |
|  |  | $n^{1+o\left(1 / c^{2}\right.}$ | $\omega(1) \mathrm{m}$ | bry lookups | [PTW ${ }^{\text {'08, PTW' }}$ '10] |
| high | low | mem lookup |  |  |  |
|  |  | $n^{4 / \epsilon^{2}}$ | Ofog | $c=1+\epsilon$ | [KOR'98, IM'98, Pan'06] |
|  |  | $n^{0\left(1 / \epsilon^{2}\right)}$ | $\omega(1) \mathrm{m}$ | ry lookups | [AIP'06] |

## Near-linear Space for $\{0,1\}^{d}$

[Indyk'OI, Panigrahy'06]

## Sample a few buckets in the same hash table!

- Setting:
, Close: $r=\frac{d}{2 c} \Rightarrow P_{1}=1-\frac{1}{2 c}$
( Far: $c r=\frac{d}{2} \Rightarrow P_{2}=\frac{1}{2}$
- Algorithm:
, Use one hash table with $k=\frac{\log n}{\log 1 / P_{2}}=\alpha \cdot \ln n$
, On query $q$ :
, compute $w=g(q) \in\{0,1\}^{k}$
- Repeat $R=n^{\sigma}$ times:
$\square w^{\prime}$ : flip each $w_{j}$ with probability $1-P_{1}$
$\square$ look up bucket $w^{\prime}$ and compute distance to all points there
- If found an approximate near neighbor, stop


## Near-linear Space

- Theorem: for $\sigma=\Theta\left(\frac{\log c}{c}\right)$, we have:
- $\operatorname{Pr[find~an~approx~near~neighbor]~} \geq 0.1$
- Expected runtime: $O\left(n^{\sigma}\right)$
- Proof:
- Let $p^{*}$ be the near neighbor: $\left\|q-p^{*}\right\| \leq r$
, $w=g(q), t=\left\|w-g\left(p^{*}\right)\right\|_{1}$
- Claim I: $\operatorname{Pr}\left[t \leq \frac{k}{c}\right] \geq \frac{1}{2}$
, Claim 2: $\underset{g, w^{\prime}}{\operatorname{Pr}}\left[w^{\prime}=g(p) \left\lvert\,\|q-p\|_{1} \geq \frac{d}{2}\right.\right] \leq \frac{1}{n}$
- Claim 3: $\operatorname{Pr}\left[w^{\prime}=g\left(p^{*}\right) \mid \operatorname{Claim} 1\right] \geq 2 n^{-\sigma}$
- If $w^{\prime}=g\left(p^{*}\right)$ at least for one $w^{\prime}$, we are guaranteed to output either $p^{*}$ or an approx. near neighbor


## Beyond LSH

## Space $\quad$ Time Exponent $\quad c=2$ Reference

| Hamming <br> space | $n^{1+\rho}$ | $n^{\rho}$ | $\rho=1 / c$ | $\rho=\mathbf{1} / \mathbf{2}$ | $\left[\mathrm{IM}^{\prime} 98\right]$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  | $\rho \geq 1 / c$ |  | $\left[\mathrm{MNP}^{\prime} 06\right.$, OWZ'।I] |
|  | $n^{1+\rho}$ | $n^{\rho}$ | $\rho \approx \frac{1}{2 c-1}$ | $\rho=\mathbf{1} / \mathbf{3}$ | $[$ [AINR'।4, AR'।5] |


| Euclidean space | $n^{1+\rho}$ | $n^{\rho}$ | $\rho \approx 1 / c^{2}$ | $\rho=\mathbf{1} / 4$ | [Al'06] |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | $\rho \geq 1 / c^{2}$ |  | [MNP'06, OWZ'II] |
|  | $n^{1+\rho}$ | $n^{\rho}$ | $\rho \approx \frac{1}{2 c^{2}-1}$ | $\rho=1 / 7$ | [AINR'I4,AR'I5] |

## New approach?

## Data-dependent hashing

- A random hash function, chosen after seeing the given dataset
- Efficiently computable


## Construction of hash function

[A.-Indyk-Nguyen-Razenshteyn'।4, A.-Razenshteyn'I5]
, Two components:

- Nice geometric structure
- Reduction to such structure


## Nice geometric structure

- Points on a unit sphere, where
- $c r \approx \sqrt{2}$, i.e., far pair is (near) orthogonal
b this would be distance if the dataset were random on sphere
, Close pair: $r=\sqrt{2} / c$
, Query:
, at angle 45' from near-neighbor



## Alg 1: Hyperplanes

[Charikar'02]

- Sample unit $r$ uniformly, hash $p$ into $\operatorname{sgn}\langle r, p\rangle$
- $\begin{aligned} \operatorname{Pr}[h(p)= & h(q)] ? \\ & =1-\alpha / \pi\end{aligned}$
- where $\alpha$ is the angle between $p$ and $q$
- $P_{1}=3 / 4$
- $P_{2}=1 / 2$
- $\rho \approx 0.42$



## Alg 2: Voronoi

[A.-Indyk-Nguyen-Razenshteyn'14] based on [Karger-Motwani-Sudan'94]

- Sample $T$ i.i.d. standard $d$ dimensional Gaussians

$$
g_{1}, g_{2}, \ldots, g_{T}
$$

- Hash $p$ into

$$
h(p)=\operatorname{argmax}_{1 \leq i \leq T}\left\langle p, g_{i}\right\rangle
$$

- $T=2$ is simply Hyperplane LSH



## Hyperplane vs Voronoi

- Hyperplane with $k=6$ hyperplanes
- Means we partition space into $2^{6}=64$ pieces
- Voronoi with $T=2^{k}=64$ vectors
- $\rho=0.18$
b grids vs spheres



## Reduction to nice structure (very HL)

- Idea: iteratively decrease the radius of minimum enclosing ball OR make more isotopic
- Algorithm:
- find dense clusters
with smaller radius large fraction of points
- recurse on dense clusters
> apply VoronoiLSH on the rest
- recurse on each "cap"
- eg, dense clusters might reappear

Why ok?

- no dense clusters
- like "random dataset" with radius $=100 \mathrm{cr}$
- even better!

$$
\text { radius }=99 \mathrm{cr}
$$

## Hash function

- Described by a tree (like a hash table)



## Dense clusters

- Current dataset: radius $R$
- A dense cluster:
- Contains $n^{1-\delta}$ points
- Smaller radius: $\left(1-\Omega\left(\epsilon^{2}\right)\right) R$
- After we remove all clusters:
- For any point on the surface, there are $\epsilon$ trade-off points within distance $(\sqrt{2}-\epsilon) R$
, The other points are essentially orthogonal !
- When applying Cap Carving with parameters $\frac{\&}{2}$ - Empirical number of far pts collifling with query: $n P_{2}+n n^{1-\delta}$ - As long as $n P_{2} \gg n^{1-\delta}$, the "impurity" doesn't matter!


## Tree recap

- During query:
- Recurse in all clusters
- Just in one bucket in VoronoiLSH
- Will look in >I leaf!
- How much branching?
- Claim: at most $\left(n^{\delta}+1\right)^{O\left(1 / \epsilon^{2}\right)}$
- Each time we branch
- at most $n^{\delta}$ clusters (+1)
- a cluster reduces radius by $\Omega\left(\epsilon^{2}\right)$
> cluster-depth at most $100 / \Omega\left(\epsilon^{2}\right)$
- Progress in 2 ways:
- Clusters reduce radius

- CapCarving nodes reduce the \# of far points (empirical $P_{2}$ )
- A tree succeeds with probability $\geq n^{-\frac{1}{2 c^{2}-1}-o(1)}$


## NNS: conclusion

- I.Via sketches
- 2. Locality Sensitive Hashing
- Random space partitions
- Better space bound
, Even near-linear!

3. Data-dependent hashing even better

- Used in practice a lot these days

