From NNS to MIPS

CS 5968/6968: Data Str & Alg for Scalable Computing Spring 2023

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Learning Outcomes

Nearest neighbor

What is the nearest neighbor?

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Definition (Nearest Neighbor)

Given a universe Ω and a distance function $D : \Omega^2 \to \mathbb{R}$, the nearest neighbor of a query point $q \in \Omega$ in a finite set of points $P \subseteq \Omega$ is,

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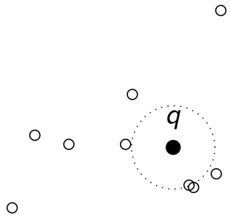
For example, $\Omega = \mathbb{R}^2$



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- Reasonable preprocessing time: $\mathrm{poly}(n, d)$
- Fast query time: $\mathrm{poly}(\log n, d)$

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- When the objective is to maximizing a similarity function, we call it similarity search.

Common distance functions

- For $\mathbb{R}^d$:
  - L_p distance: $L_p(p,q) := \left(\sum_{i=1}^{d} |p_i - q_i|^p\right)^{1/p}$ for $p \geq 1$. When $p = 2$ we get the Euclidean distance. Other common choices are $p = 1$ (Manhattan distance) and $p = \infty$ (Chebyshev distance).
  - Cosine similarity: $S_C(p,q) = \frac{p^T q}{\|p\|_2 \|q\|_2}$.
  - Dot product (similarity): $S_D(p,q) = p^T q$.
- For strings:
  - Edit distance, Hamming distance.
- For the power set of a finite set:
  - Jacard similarity, Jacard distance,
- For nodes in a graph:
  - Length of the shortest path.
- For point sets:
  - Kernel distance, Gromov-Hausdorff distance.

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  - Vector data (low/high dimensional).
  - Efficient NNS system is crucial.

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I'd see NNS as a searching problem, as the name suggests.

Applications

The rest lecture mostly focuses on the most common data space, d-dimensional vectors, i.e. $\Omega = \mathbb{R}^d$.

$d = 1$

- Sort the data points. Binary search.
  - Space: $O(n)$; query time: $O(\log n)$.
- Balanced binary search tree.
  - Space: $O(n)$; query time: $O(\log n)$.
- vEB-tree, x-fast trie...
  - Space: $O(n)$; query time: $O(\log \log u)$.

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$d = 2$

- Voronoi diagram
  - Space: $O(n)$; query time: $O(\log n)$. [Lipton-Tarjan'80]
- kd-Tree
  - Space: $O(n)$; query time: $O(\log n)$. [Lipton-Tarjan'80]

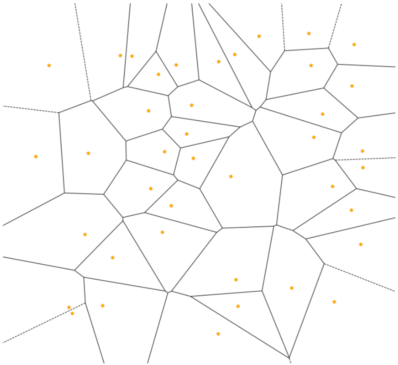


Image by Hristo Hristov

Space: $O(n)$; query time: $O(\log n)$ on average.

Curse of dimensionality

- All known data structures that beat $O(dn)$ linear scan query time require $O(2^d)$ space.
- Observation (Number of partitions). Splits the data space in each dimension into two halves, end with 2^d partitions.
- Think $n = 10^6$, $d = 100$.

Point Location in Equal Balls (PLEB)

Definition (ε-NN)

Given a point set P and a query point q, we say $\hat{p} \in P$ is an ε-NN of q in P if

$$D(\hat{p}, q) \leq (1+\varepsilon) \min_{p \in P} D(p, q)$$

Definition (ε-Point Location in Equal Balls (ε-PLEB))

Given a point set P and $r \in \mathbb{R}^+$, for any query point q,

- if $\min_{p \in P} D(p, q) \leq r$, return a point p' s.t. $D(p', q) \leq (1+\varepsilon)r$.
- if $(1+\varepsilon)r \leq \min_{p \in P} D(p, q)$, return $\emptyset$.
- if $r \leq \min_{p \in P} D(p, q) \leq (1+\varepsilon)r$, return p' or $\emptyset$.

Indyk-Motwani'98

Algorithm 1 Preprocess

Input: point set $P \subset \{0,1\}^d$, size ℓ
i.i.d. drawn $H \leftarrow \mathcal{H}^{\ell \times k}$
ℓ hash tables $T \leftarrow \{\} * \ell$
for $p \in P$ **do**
  for $j = 1$ to ℓ **do**
    $T_j[(H_{j,1}(p), \ldots, H_{j,k}(p))] \leftarrow p$
return T, H

$k = O(\log n), \ell = O(n^{1/\varepsilon})$
space: $O(nd + n^{1+1/\varepsilon})$
Where $\mathcal{H}$ is a family of LSH.

Algorithm 2 Query

Input: ℓ hash tables T, $\ell \times k$ hash functions H, query point $q \in \{0,1\}^d$
$A \leftarrow \emptyset$
for $j = 1$ to ℓ **do**
  $p \leftarrow T_j[(H_{j,1}(q), \ldots, H_{j,k}(q))]$
  if $D(q,p) \leq r_2$ **then**
    return p

time: $O(n^{1/\varepsilon} d)$

Indyk-Motwani'98 - Result

Definition (Locality-Sensitive Hashing)

A family $\mathcal{H} = \{h : \Omega \to S\}$ is called (r_1, r_2, p_1, p_2)-sesitive for metric D if for any $q, p \in \Omega$

- if $D(p, q) \le r_1$ then $\Pr_{h \sim \mathcal{H}}[h(q) = h(p)] \ge p_1$,
- if $D(p, q) \ge r_2$ then $\Pr_{h \sim \mathcal{H}}[h(q) = h(p)] \le p_2$,

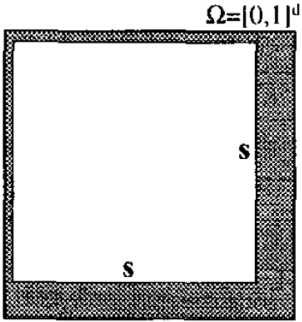
where $p_1 > p_2$ and $r_1 < r_2$.

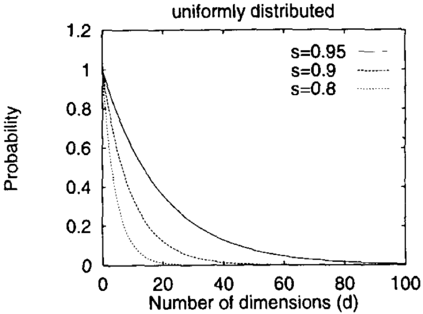
For d dimensional hamming space $\Omega = \{0, 1\}^d$ and hamming distance $D(p, q) = \sum_{i=1}^{d} \mathbb{1}(p_i \ne q_i)$, $\mathcal{H} = \{h_i : h_I(p) := p_i, i = 1, \dots, d\}$ is $(r, r(1+\varepsilon), 1 - \frac{r}{d}, 1 - \frac{r(1+\varepsilon)}{d})$-sensitive.

Theorem

For any $\varepsilon > 1$, there exists an algorithm for ε-PLEB in $\{0, 1\}^d$ using $O(dn + n^{1+1/\varepsilon})$ space and $O(dn^{1/\varepsilon})$ query time.

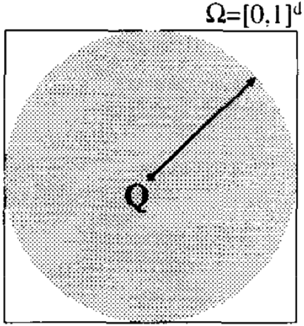
hyper-cube range query





Random sample a point from a hypercube $[0,1]^d$. Then the probability of the point lies within the lenght s hypercube.

hyper-sphere range query

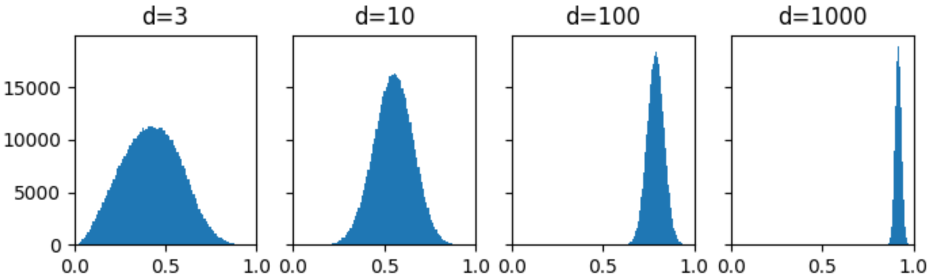


d	$P[R \in sp^d(Q, 0.5)]$
2	0.785
4	0.308
10	0.002
20	$2.461 \cdot 10^{-8}$
40	$3.278 \cdot 10^{-21}$
100	$1.868 \cdot 10^{-70}$

Random sample a point from a hypercube $[0, 1]^d$. Then the probability of the point lies within the largest ball that fits entirely within the hypercube.

Euclidean distance in high dimensional space

In the high dimensional space, the distance between two points is not a good indicator of their similarity.



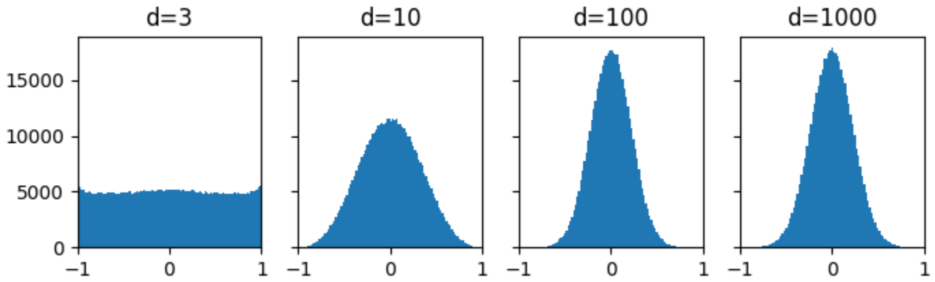
Randomly sample 1000 points from a uniform distribution in $[-1, 1]^d$. Then plot the histogram of the pairwise distances normalized by the max distance.

When $d = 1000$, $2/24$ error will include more than 50% of the points; $3/24$ error will include almost all the points.

Embedded data

- In the AI era, everything is a vector. And the dimension is quite large.
  - Google's Universal Sentence Encoder embeds sentences into a space of dimension 512.
  - GPT-3 embeds documents into space of dimension from 1024 to 12288.
- These embeds are not fixed, but learned by minimizing some loss function.
- The loss function can be defined in terms of the distances, or the similarities.

Cosine similarity in high dimensional space



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High dimensional MIPS

There are two main tasks required to develop an efficient MIPS system.

- To reduce the number of candidates. e.g. space/data partitioning.
    - Tree search methods [Muja-Lowe'14; Dasgupta-Freund'08]
    - Locality sensitive hashing [Shrivastava-Li'14; Neyshabur-Srebro'15; Indyk-Motwani,'98; Andoni-Indyk-Laarhoven-Razenshteyn-Schmidt'15]
    - Graph search [Malkov-Yashunin'16; Harwood-Drummond'16]
- To speed up evaluation.
    - Quantization.
    - Random projection (dimension reduction) [Ailon-Liberty'13]

Conclusion

- A NNS system preprocesses the dataset for fast query.
- The objective can be minimizing a distance function or maximizing a similarity function.
- There are many methods exist for low dimensional data.
- In high dimensional space, the euclidean distance is not a good measurement of similarity, people usually use cosine similarity, e.g. MIPS.
- In addition to space(data) partitioning, speeding up evaluation is also important in high dimensional space.