CS-GY 6763: Lecture 6
Near-neighbor search in high dimensions

NYU, Prof. Ainesh Bakshi

Last Class

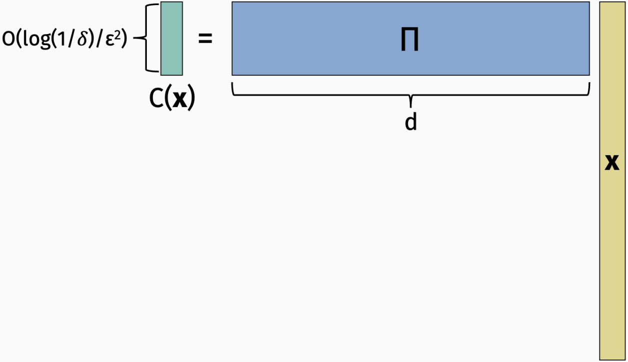
Dimensionality reduction: Given vectors $\mathbf{x}, \mathbf{y}$, compute small space compressions $C(\mathbf{x})$ and $C(\mathbf{y})$ that can be used to estimate the distance or similarity between $\mathbf{x}$ and $\mathbf{y}$.

Euclidean Dimensionality Reduction

Lemma (Distributional JL Lemma)

Let $\mathbf{\Pi}$ *be a random matrix that compresses to* $k = O\left(\frac{\log(1/\delta)}{\epsilon^2}\right)$ *rows. Then with probability* $(1-\delta)$*:*

$$(1-\epsilon)\|\mathbf{x}-\mathbf{y}\|_2^2 \leq \|\mathbf{\Pi x}-\mathbf{\Pi y}\|_2^2 \leq (1+\epsilon)\|\mathbf{x}-\mathbf{y}\|_2^2$$

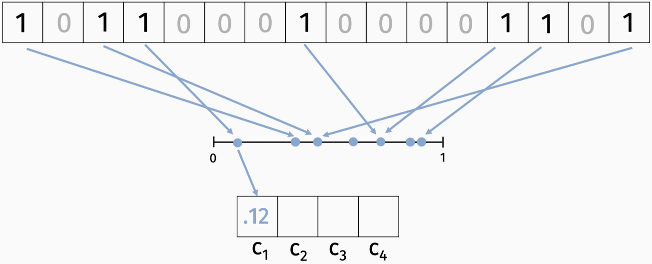


Dimensionality Reduction for Jaccard Similarity

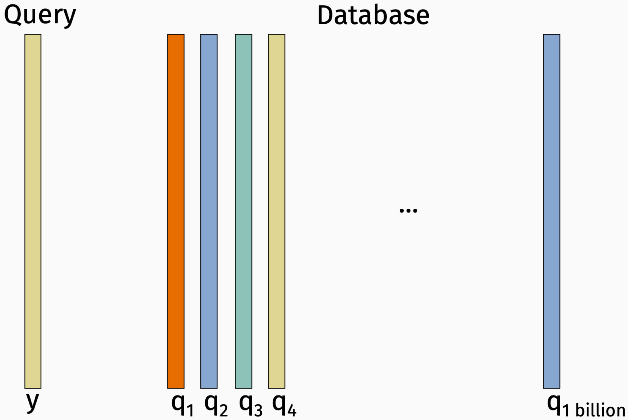
Lemma (MinHash)

Let C be a length $k = O\left(\frac{\log(1/\delta)}{\epsilon^2}\right)$ MinHash sketch. Then with probability $(1-\delta)$, we can return an estimate $\tilde{J}$ based on $C(\mathbf{x})$ and $C(\mathbf{y})$ with:

$$J(\mathbf{x},\mathbf{y}) - \epsilon \leq \tilde{J} \leq J(\mathbf{x},\mathbf{y}) + \epsilon.$$



Key Application: Modern Vector Search



Goal: Find $\arg\max_i \mathrm{dist}(\mathbf{q}_i, \mathbf{q})$

Cost of naive algorithm is

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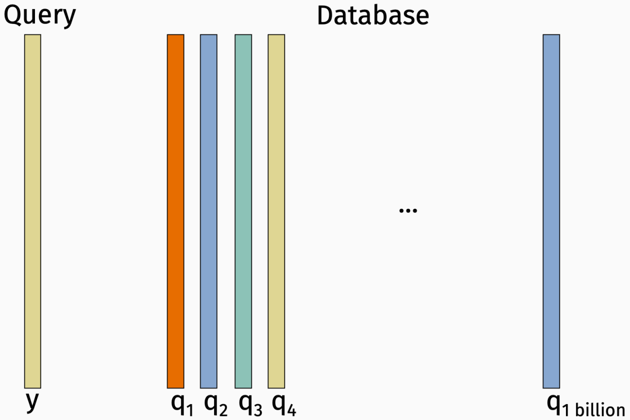

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Cost of naive algorithm is $O(nd)$.

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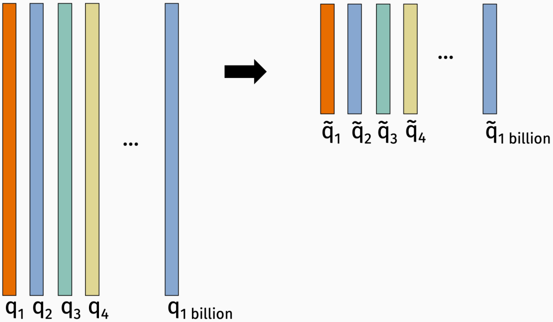
Dimensionality reduction reduces search cost to $O(nk)$ and reduces space requirements.



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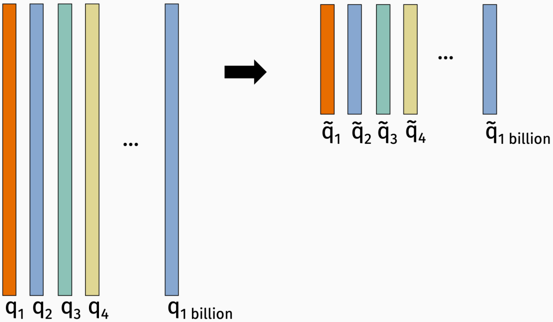


All modern vector search systems use "fancier" versions of methods studied in this class:

- Quantized JL/SimHash
- b-bit MinHash
- Product Quantization
- PCA-based methods

Vector Indexing / Near Neighbor Search

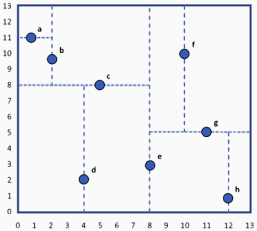
Dimensionality reduction methods are typically paired with vector indexing methods.

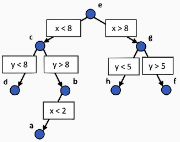
Goal of Dimensionality Reduction: Reduce **dependence on** d in $O(nd)$ search cost. Reduce space complexity.

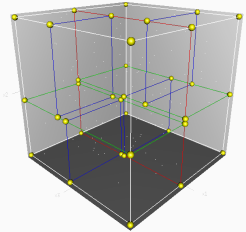
Goal of Vector Indexing: Reduce **dependence on** n in $O(nd)$ search cost. Often at the cost of added space complexity.

Beyond a Linear Scan

This problem can already be solved in low-dimensions using space partitioning approaches (namely, kd-trees).







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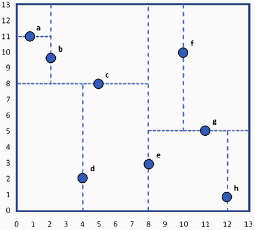
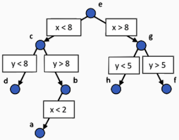
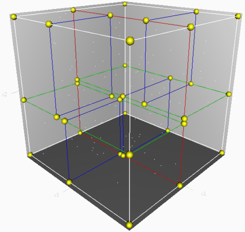


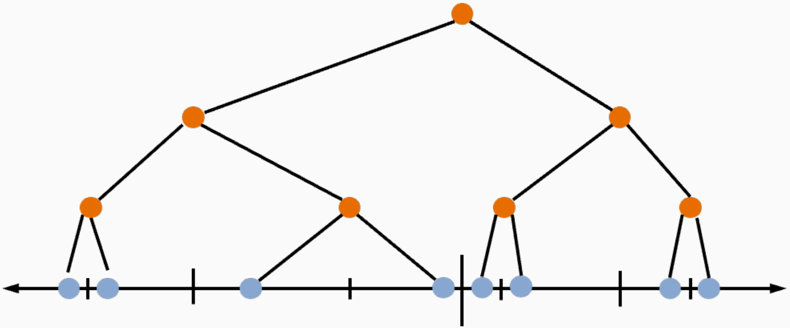




Search time is roughly $O(d \cdot \log n \cdot 2^d))$, which is only sublinear for $d = o(\log n)$.

Issue with KD-Trees

How do we build the tree?



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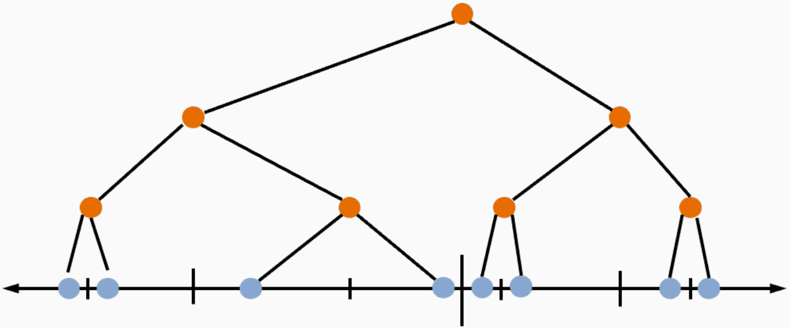

Given a query q, how do we find the nearest neighbor?

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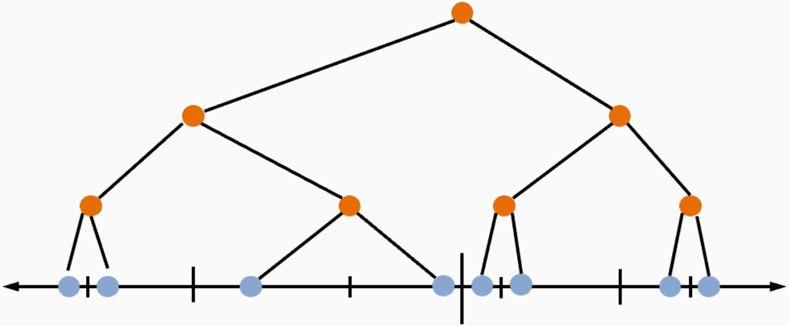

Are we guaranteed to get the nearest neighbor in the worst case?

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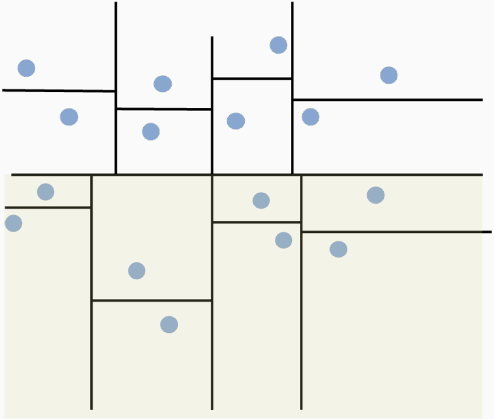

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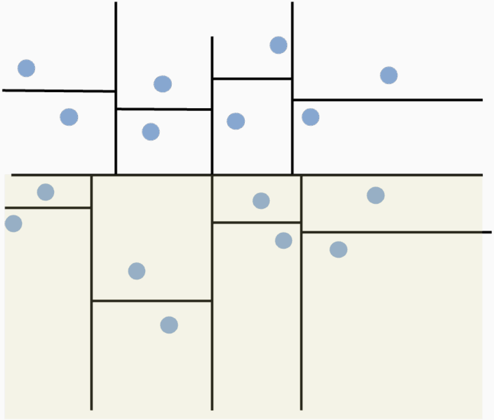

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2^d in d dimensions, so query time is exponential in d.

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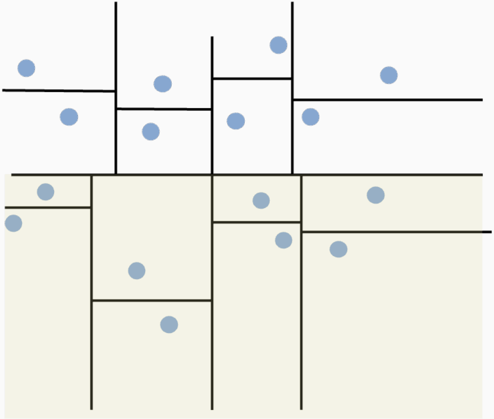

Theorem (informal): Exact nearest neighbor search in d dimensions requires exponential (in d) space and time.

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Key ideas behind all of these methods:

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1. Trade worse space-complexity + preprocessing time for better query time.
2. Preprocess and create data structure that uses $\Omega(n)$ space.
3. Allow for approximation.

Intuitively Why Do Preprocessing and Space Help?

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Question: Dataset is n points in the cube $[-1,1]^d$. Given ϵ and a query $\mathbf{q} \in [-1,1]^d$, you want to find $\tilde{\mathbf{y}}$ with

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Can you construct a data structure that supports $O(d)$ time search but uses exponential space?

Locality Sensitive Hashing

Key Idea: Map close by points in R^d to the same bucket. Map far away points to different buckets.

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Why does such a function even exist? It's the complete opposite of uniformly random hash functions.

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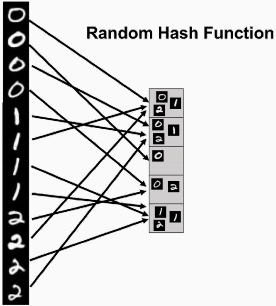

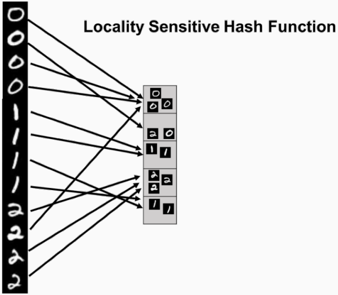

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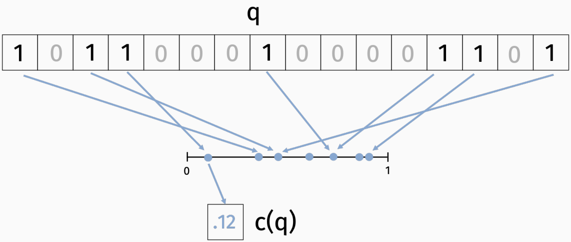

Why should this be locality sensitive?

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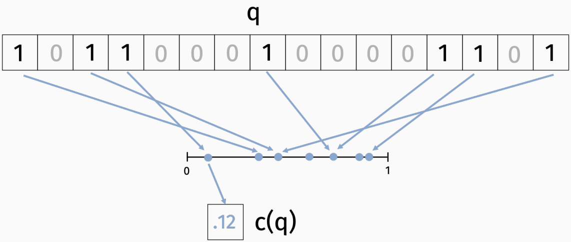

$$Pr[c(\mathbf{q}) == c(\mathbf{y})] = J(\mathbf{q}, \mathbf{y}) \text{ and } c(\mathbf{q}) = c(\mathbf{y}) \text{ implies } g(c(\mathbf{q})) = g(c(\mathbf{y})).$$

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$$= J(\mathbf{q}, \mathbf{y}) + \underbrace{(1 - J(\mathbf{q}, \mathbf{y}))\frac{1}{m}}_{\text{negligible}}$$

Near Neighbor Search

Basic approach for LSH-based near neighbor search in a database.

Pre-processing:

- Select random LSH function $h : \{0, 1\}^d \rightarrow 1, \ldots, m$.

[1]Enough to make the $O(1/m)$ term negligible.

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Time required is $O(d \cdot |T(h(\mathbf{y})|)$.

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Note: The meaning of "close" and "not close" is application dependent. E.g. we might specify that we want to find anything with Jaccard similarity $> .4$, but not with Jaccard similarity $< .2$.

Reducing False Negative Rate

Let's use Jaccard similarity as a running example.

Suppose the nearest database point $\mathbf{q}$ has $J(\mathbf{y}, \mathbf{q}) = .4$.

What's the probability we do not find q?

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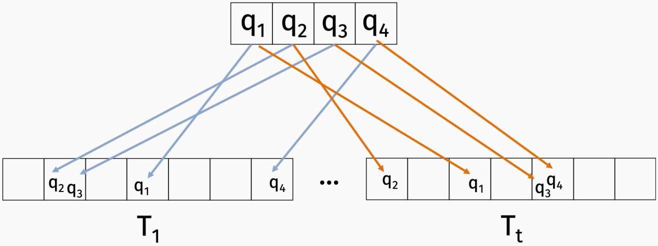
This is quite bad, how do we dampen the false negative rate?

Reducing False Negative Rate



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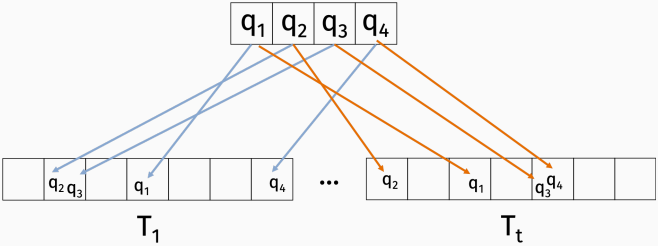

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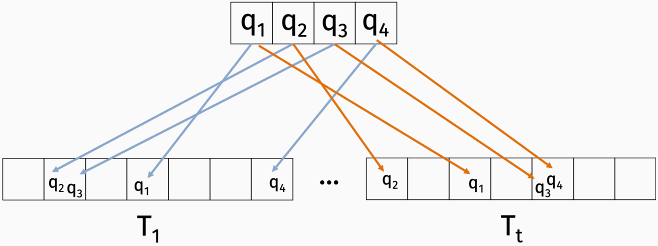

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- Create tables $T_1, \ldots, T_t$, each with m slots.
- For $i = 1, \ldots, n$, $j = 1, \ldots, t$,
  - Insert $\mathbf{q}_i$ into $T_j(h_j(\mathbf{q}_i))$.

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- Linear scan through all vectors in $T_1(h_1(\mathbf{y})) \cup T_2(h_2(\mathbf{y})) \cup \ldots, T_t(h_t(\mathbf{y}))$.

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This is really bad! All the other points could have similarity .2

We have to search over $\Omega(n)$ points anyway.

Reducing False Positives

Secret Sauce: **Change our locality sensitive hash function.**

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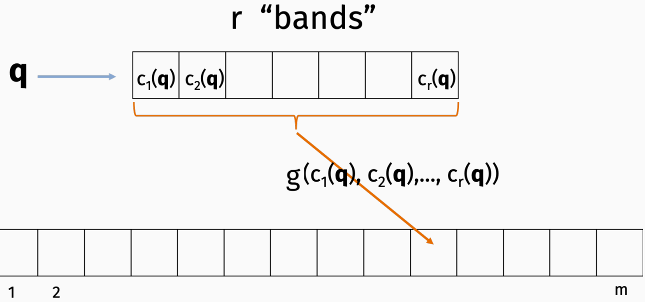

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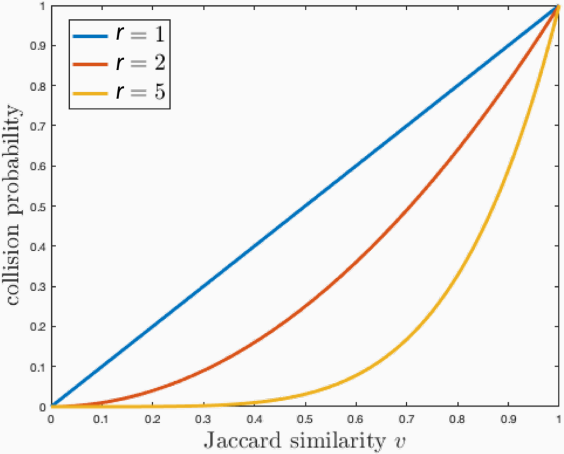
$$= v \cdot v \cdots v + \text{correction} = v^r + (1 - v^r)\frac{1}{m}$$

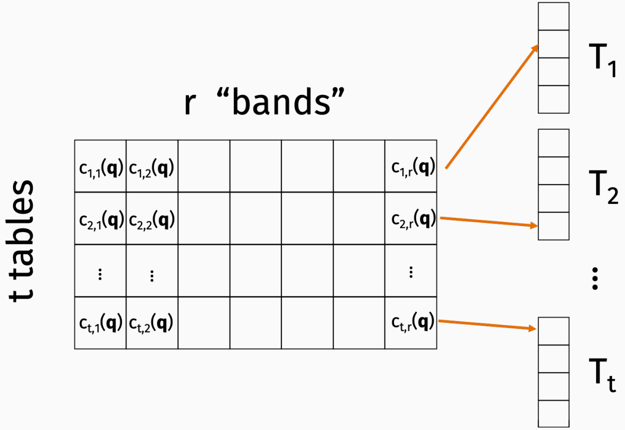
Tunable LSH



$r = 1$
$r = 2$
$r = 5$
collision probability
Jaccard similarity v
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Tunable LSH

Full LSH scheme has two parameters to tune:



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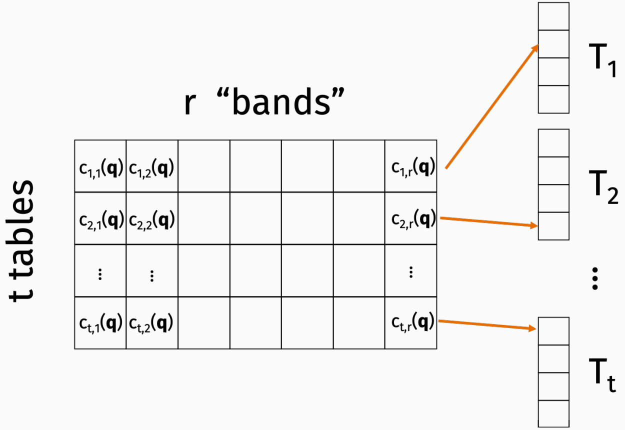

Still unclear why this is useful

Tunable LSH

Effect of **increasing number of tables** t on:

False Negatives

False Positives

Tunable LSH

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False Negatives	False Positives
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s-curve tuning

Probability we check $\mathbf{q}$ when querying $\mathbf{y}$ if $J(\mathbf{q},\mathbf{y}) = v$:

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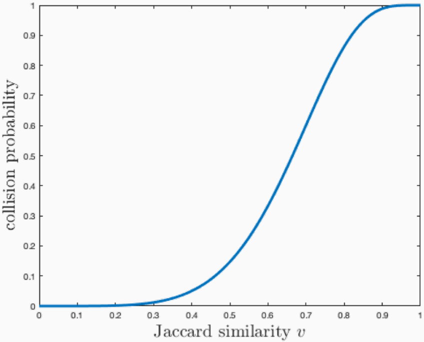

$r = 5, t = 5$

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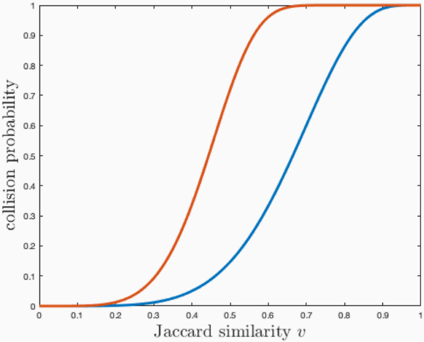

$r = 5, t = 40$

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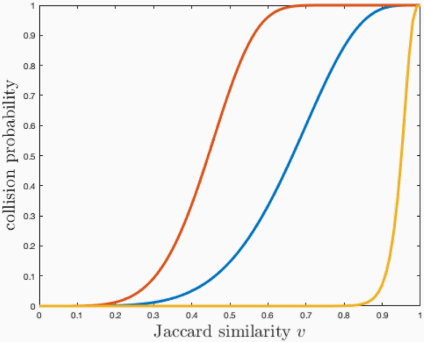

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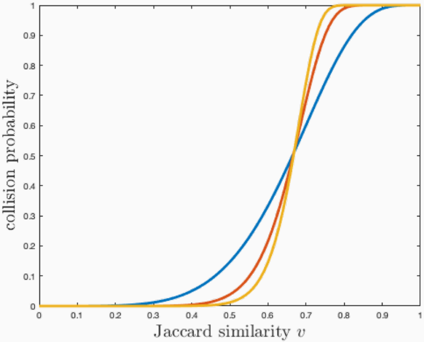

Increasing both r and t gives a steeper curve, approaching a step function.

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- Hit probability for $J(\mathbf{y}, \mathbf{q}) < .7$ is $\lesssim 1 - (1 - .7^{25})^{40} = .005$

Upper bound on total number of items checked:

$$10 + .95 \cdot 10,000 + .005 \cdot 9,989,990 \approx 60,000 \ll 10,000,000.$$

Fixed Threshold

Space complexity: 40 hash tables $\approx 40 \cdot O(n)$.

Directly trade space for fast search.

LSH Based Nearest-Neighbor in Theory

Possible to prove concrete worst-case results for distance functions that satisfy triangle inequality.

Theorem (Indyk, Motwani, 1998. Point Location in Ball)

Fix a distance R. If there exists some q with $\|\mathbf{q}-\mathbf{y}\|_0 \leq R$, return a vector $\tilde{\mathbf{q}}$ with $\|\tilde{\mathbf{q}}-\mathbf{y}\|_0 \leq C \cdot R$ in:

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If there is no point at distance R, algorithm does not need to return anything.

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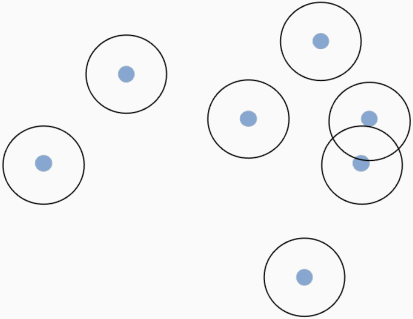
To obtain a nearest-neighbor search algorithm build multiple data structures for exponentially growing distances:

$$R \qquad 2R \qquad 4R \qquad 8R \qquad \ldots$$

Search from most accurate level to least accurate.



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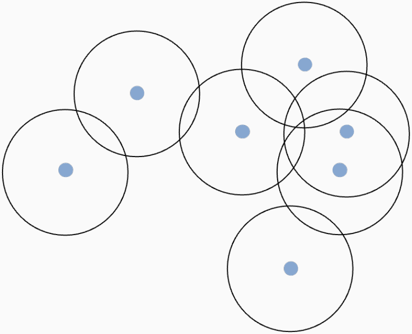

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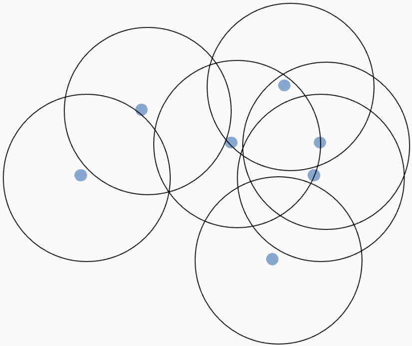

Approximate Nearest Neighbor Search

Total number of levels $= O(\log(d_{\max}/d_{\min}))$, where $d_{\max} = \max_{i,j} \|\mathbf{q}_i - \mathbf{q}_j\|$ and $d_{\min} = \min_{i,j} \|\mathbf{q}_i - \mathbf{q}_j\|$. $d_{\max}/d_{\min}$ is called the **dynamic range**.

Theorem (Indyk, Motwani, 1998)

Let q be the closest database vector to $\mathbf{y}$. Return a vector $\tilde{\mathbf{q}}$ with $\|\tilde{\mathbf{q}} - \mathbf{y}\|_0 \leq C \cdot \|\mathbf{q} - \mathbf{y}\|_0$ in:

- *Time:* $\tilde{O}\left(n^{1/C}\right)$.
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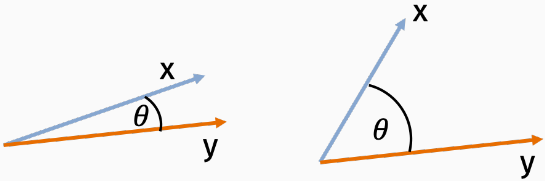
Similar results can be proven for other metrics, including Euclidean distance. But you need a good LSH function.

Other LSH Functions

Good locality sensitive hash functions exists for other similarity measures.

Cosine similarity $\cos(\theta(\mathbf{x}, \mathbf{y})) = \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\|_2 \|\mathbf{y}\|_2}$**:**



$$-1 \leq \cos(\theta(\mathbf{x}, \mathbf{y})) \leq 1.$$

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LSH functions also exist for Euclidean distance, but are a bit more complex to describe/analyze. See [Andoni, Indyk, 2006] if you are interested.

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Locality sensitive hash for **cosine similarity**:

- Let $\mathbf{g} \in \mathbb{R}^d$ be randomly chosen with each entry $\mathcal{N}(0,1)$.

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$$\textbf{Claim: } \Pr[h(\mathbf{x}) == h(\mathbf{y})] = 1 - \frac{\theta}{\pi} + \frac{\theta}{\pi m}$$

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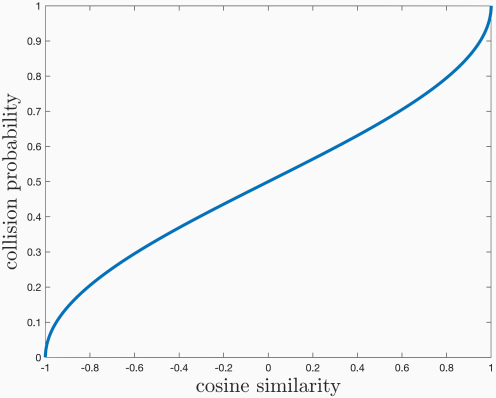
$$\approx 1 - \frac{\cos^{-1}(v)}{\pi}$$

SimHash Analysis in 2D

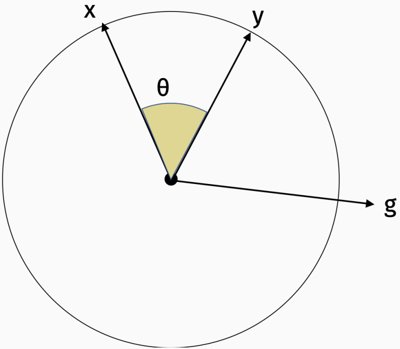
Theorem (to be proven): If $\cos(\theta(\mathbf{x}, \mathbf{y})) = v$, then

$$\Pr[h(\mathbf{x}) == h(\mathbf{y})] = 1 - \frac{\theta}{\pi} + \frac{\theta/\pi}{m} \approx 1 - \frac{\cos^{-1}(v)}{\pi}$$



SimHash Analysis in 2D

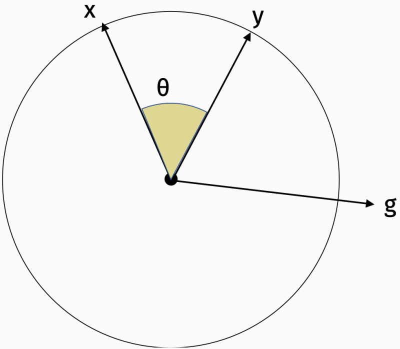
To prove: $\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx 1 - \frac{\theta}{\pi}$, where $h(\mathbf{x}) = f(\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle))$ and f is uniformly random hash function.



$$\Pr[h(\mathbf{x}) == h(\mathbf{y})] = z + \frac{1-z}{m} \approx z \,,$$

SimHash Analysis in 2D

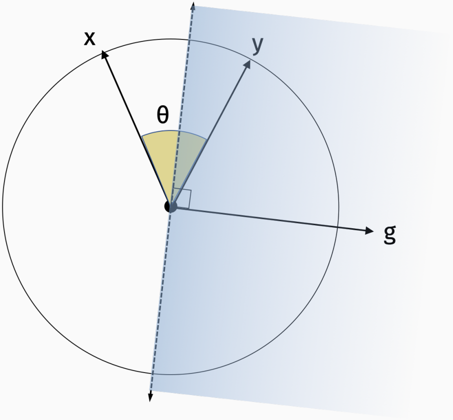
To prove: $\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx 1 - \frac{\theta}{\pi}$, where $h(\mathbf{x}) = f(\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle))$ and f is uniformly random hash function.



$$\Pr[h(\mathbf{x}) == h(\mathbf{y})] = z + \frac{1-z}{m} \approx z\,,$$

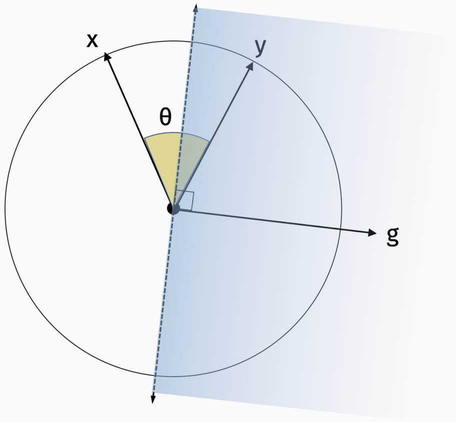
$$\text{where } z = \Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)]$$

SimHash Analysis 2D



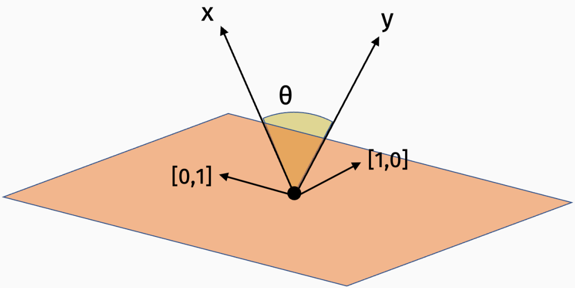
- $\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) \neq \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)$ when $\mathbf{g}$ lands between $\mathbf{x}$ and $\mathbf{y}$.
- By rotational invariance of Gaussian
  $\Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) \neq \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)] = \frac{2\theta}{2\pi} = \frac{\theta}{\pi}$

SimHash Analysis 2D



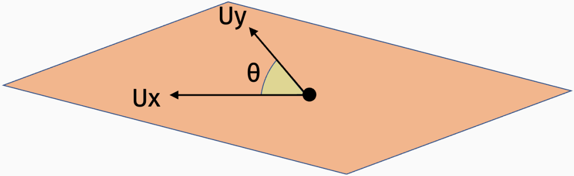
$$\Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)] = 1 - \frac{\theta}{\pi}$$

SimHash Analysis Higher Dimensions



There is always some rotation matrix $\mathbf{U}$ such that $\mathbf{Ux}, \mathbf{Uy}$ are spanned by the first two-standard basis vectors and have the same cosine similarity as $\mathbf{x}$ and $\mathbf{y}$.

SimHash Analysis Higher Dimensions



There is always some rotation matrix $\mathbf{U}$ such that $\mathbf{x}, \mathbf{y}$ are spanned by the first two-standard basis vectors.

Note: We have now reduced to the 2D case (we can also revert this rotation at the end)

SimHash Analysis Higher Dimensions

Analysis: Let U be the rotation matrix that maps **x** and **y** to the XY plane

$$\Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)]$$

SimHash Analysis Higher Dimensions

Analysis: Let U be the rotation matrix that maps $\mathbf{x}$ and $\mathbf{y}$ to the XY plane

$$\begin{aligned}&\Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x}\rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y}\rangle)]\\ &= \Pr[\text{sign}(\langle \mathbf{U}^T\mathbf{g}, \mathbf{x}\rangle) == \text{sign}(\langle \mathbf{U}^T\mathbf{g}, \mathbf{y}\rangle)]\end{aligned}$$

SimHash Analysis Higher Dimensions

Analysis: Let U be the rotation matrix that maps **x** and **y** to the XY plane

$$\begin{aligned}
&\Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{U}^T \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{U}^T \mathbf{g}, \mathbf{y} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{g}, \mathbf{Ux} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{Uy} \rangle)]
\end{aligned}$$

SimHash Analysis Higher Dimensions

Analysis: Let U be the rotation matrix that maps $\mathbf{x}$ and $\mathbf{y}$ to the XY plane

$$\begin{aligned}
&\Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{U}^T \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{U}^T \mathbf{g}, \mathbf{y} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{g}, \mathbf{U}\mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{U}\mathbf{y} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{g}[1,2], (\mathbf{U}\mathbf{x})[1,2] \rangle) == \text{sign}(\langle \mathbf{g}[1,2], (\mathbf{U}\mathbf{y}[1,2] \rangle)]
\end{aligned}$$

SimHash Analysis Higher Dimensions

Analysis: Let U be the rotation matrix that maps $\mathbf{x}$ and $\mathbf{y}$ to the XY plane

$$
\begin{aligned}
&\Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{U}^T \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{U}^T \mathbf{g}, \mathbf{y} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{g}, \mathbf{Ux} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{Uy} \rangle)] \\
&= \Pr[\text{sign}(\langle \mathbf{g}[1,2], (\mathbf{Ux})[1,2] \rangle) == \text{sign}(\langle \mathbf{g}[1,2], (\mathbf{Uy}[1,2] \rangle)] \\
&= 1 - \frac{\theta}{\pi}.
\end{aligned}
$$

Banded SimHash

SimHash can be banded, just like our MinHash based LSH function for Jaccard similarity:

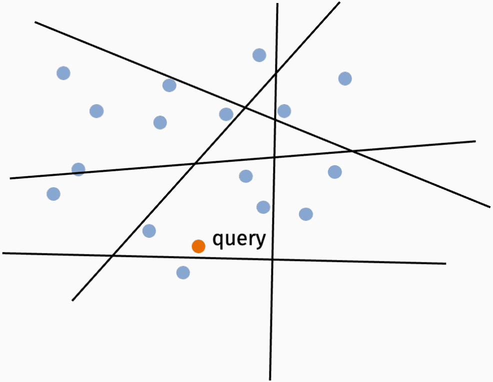
- Let $\mathbf{g}_1, \ldots, \mathbf{g}_r \in \mathbb{R}^d$ be randomly chosen with each entry $\mathcal{N}(0, 1)$.
- Let $f : \{-1, 1\}^r \to \{1, \ldots, m\}$ be a uniformly random hash function.
- $h : \mathbb{R}^d \to \{1, \ldots, m\}$ is defined $h(\mathbf{x}) = f\left([\text{sign}(\langle \mathbf{g}_1, \mathbf{x} \rangle), \ldots, \text{sign}(\langle \mathbf{g}_r, \mathbf{x} \rangle)]\right)$.

$$\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx \left(1 - \frac{\theta}{\pi}\right)^r$$

Nearest-Neighbor Search in Practice

LSH is widely used in practice, but is starting to get replaced by other methods. Most of these are data dependent in some way.

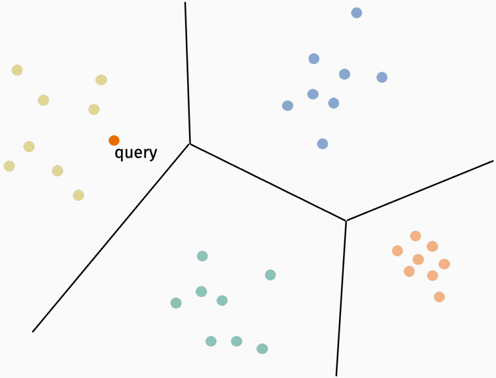
Starting point: Think of LSH as a randomized space-partitioning method.



Nearest-Neighbor Search in Practice

In practice, we can often get partitions with better margin by partitioning in a data-dependent way.

Common approach: Split data using k-means clustering.



Open Theory Challenge

Can we better explain the success of data-dependent nearest-neighbor search methods?

LSH Forest: Practical Algorithms Made Theoretical

Alexandr Andoni, Columbia University
Ilya Razenshteyn, MIT CSAIL
Negev Shekel Nosatzki, Columbia University

Beyond Locality–Sensitive Hashing

Alexandr Andoni, Microsoft Research SVC
Piotr Indyk, MIT
Huy L. Nguyễn, Princeton
Ilya Razenshteyn, MIT

Abstract

We present a new data structure for the c–approximate near neighbor problem (ANN) in the Euclidean space. For n points in $\mathbb{R}^d$, our algorithm achieves $O_c(dn^\rho)$ query time and $O_c(n^{1+\rho} + nd)$ space, where $\rho \leq 7/(8c^2$ …
over the result by Andoni and Indyk (FC …
a locality–sensitive hashing lower bound …
a standard reduction we obtain a data s…
$\rho \leq 7/(8c) + O(1/c^{3/2}) + o_c(1)$, which is …
Motwani (STOC 1998).

Worst-case Performance of Popular Approximate Nearest Neighbor Search Implementations: Guarantees and Limitations

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