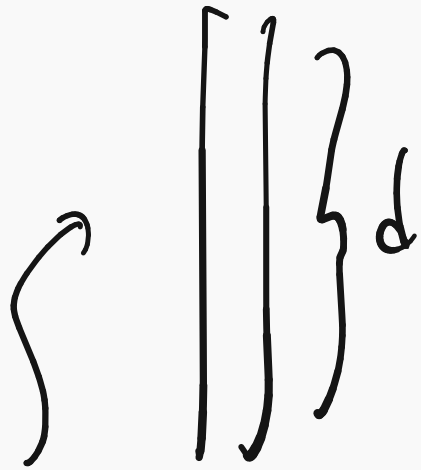
CS-GY 6763: Lecture 6
Near-neighbor search in high dimensions

NYU Tandon School of Engineering, Prof. Christopher Musco

LAST CLASS

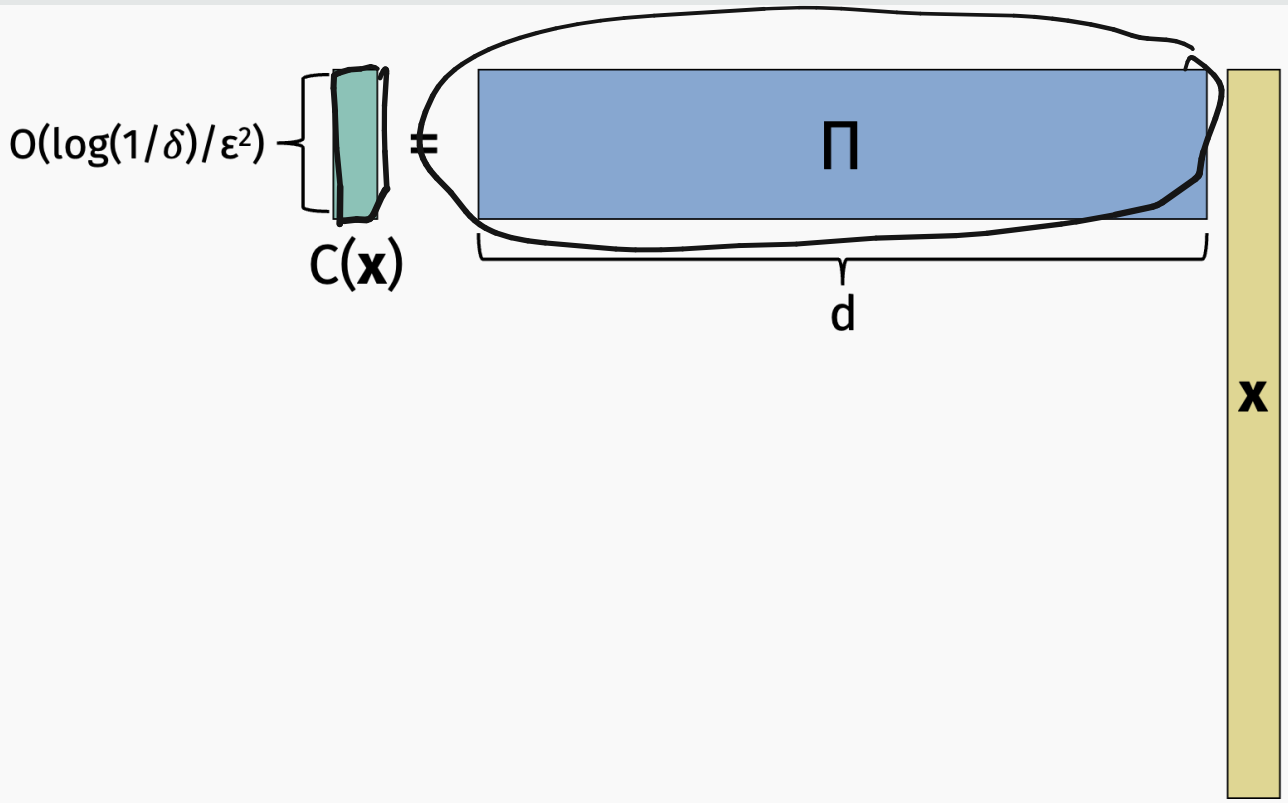


Dimensionality reduction: Given vectors $\mathbf{x}, \mathbf{y}$, compute small space compressions $C(\mathbf{x})$ and $C(\mathbf{y})$ that can be used to estimate the distance or similarity between $\mathbf{x}$ and $\mathbf{y}$.

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* $(1-\delta)$*:*

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

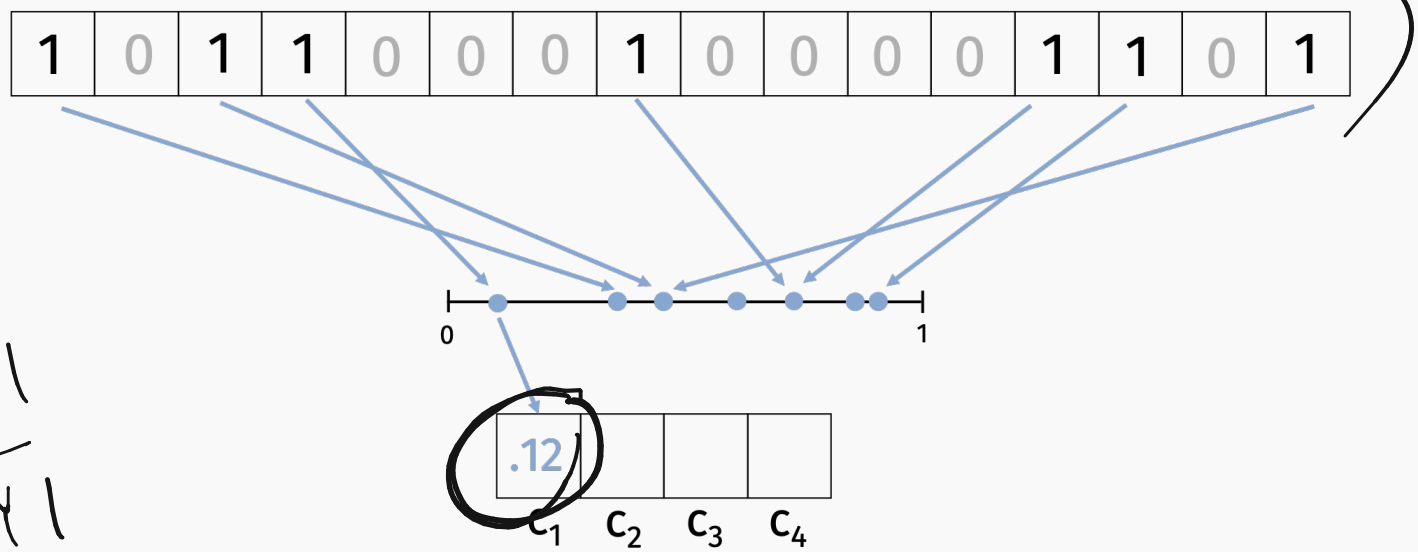


DIMENSIONALITY REDUCTION FOR JACCARD SIMILARITY

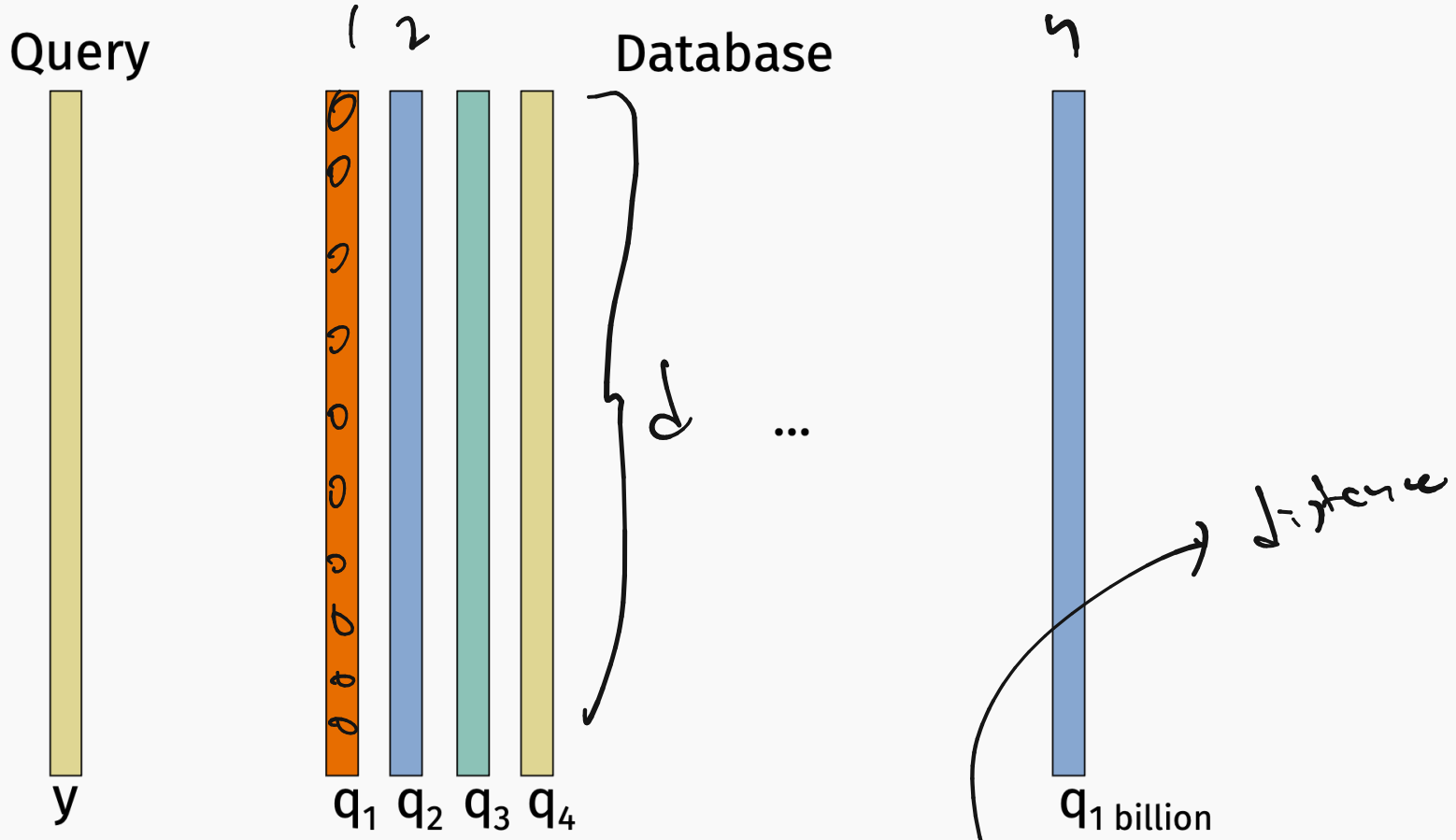
Lemma (MinHash)

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 SEA SEARCH



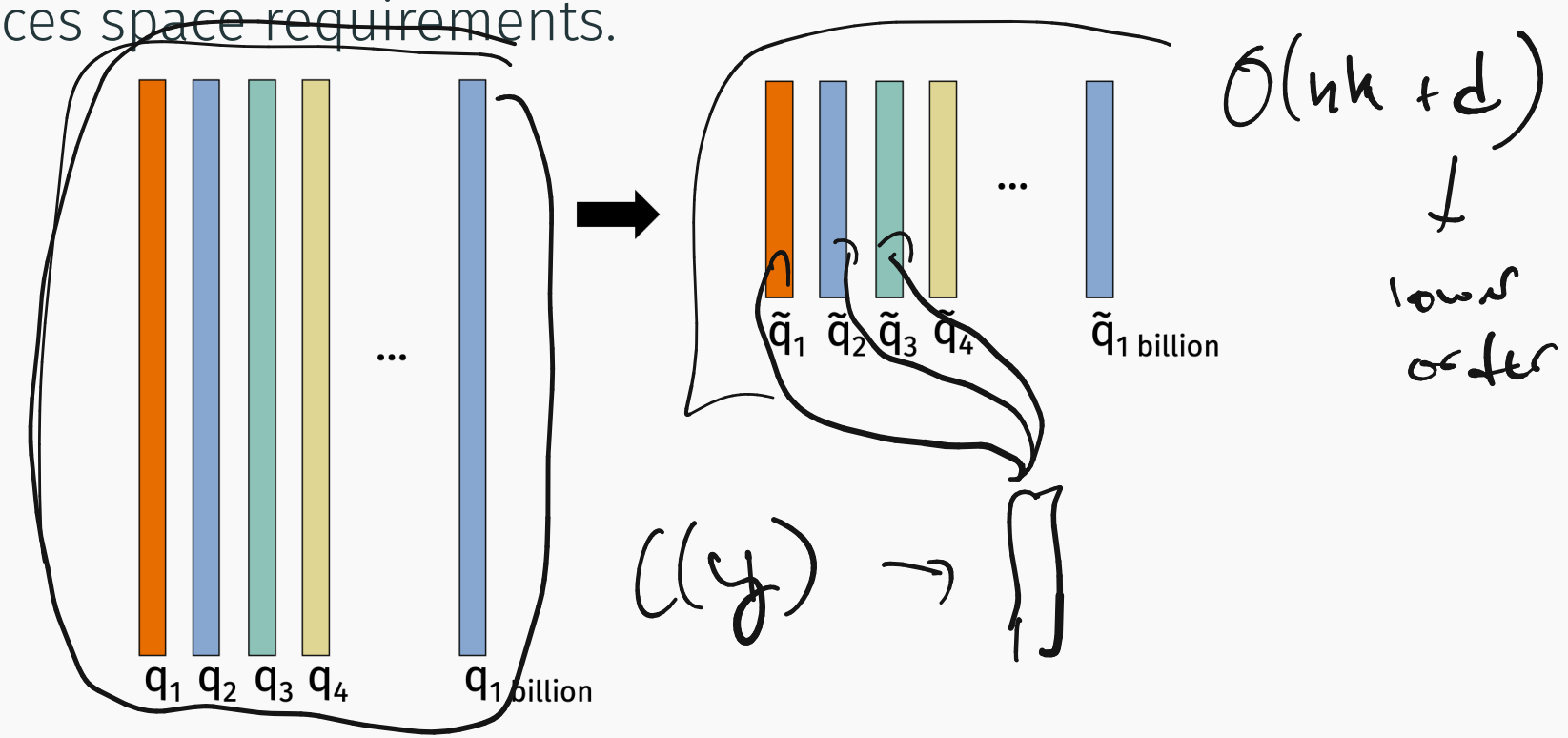
Cost of naive algorithm is $O(nd)$.

$$\arg\min_i d(y, q_i)$$

$$\arg\max_i s(y, q_i)$$

KEY APPLICATION: MODERN VECTOR SEA SEARCH

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



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

Dimensionality reduction methods are typically paired with vector indexing methods.

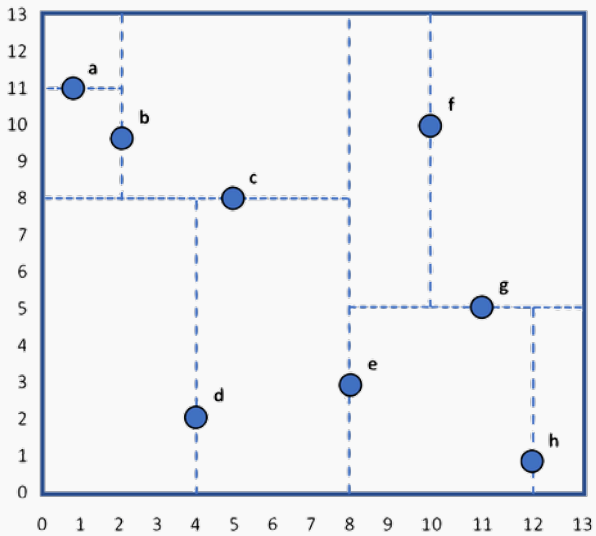
Goal of Dimensionality Reduction: Reduce dependence on d in $O(nd)$ search cost. Reduce space complexity.

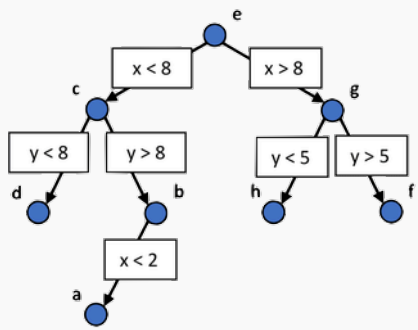
Goal of Vector Indexing: Reduce dependence on n in $O(nd)$ search cost. Often at the cost of added space complexity.

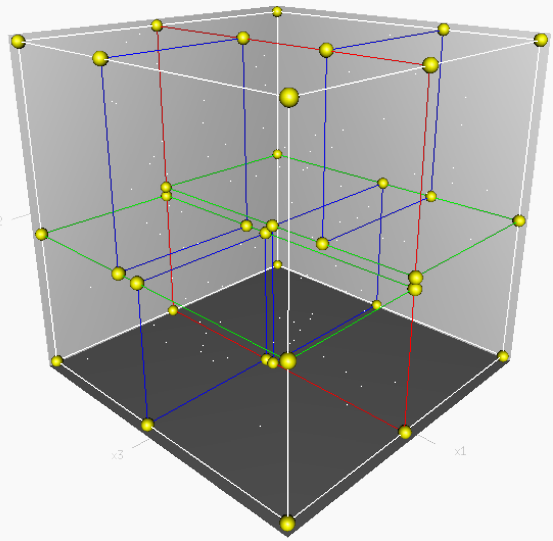
BEYOND A LINEAR SCAN

$O(n)$

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





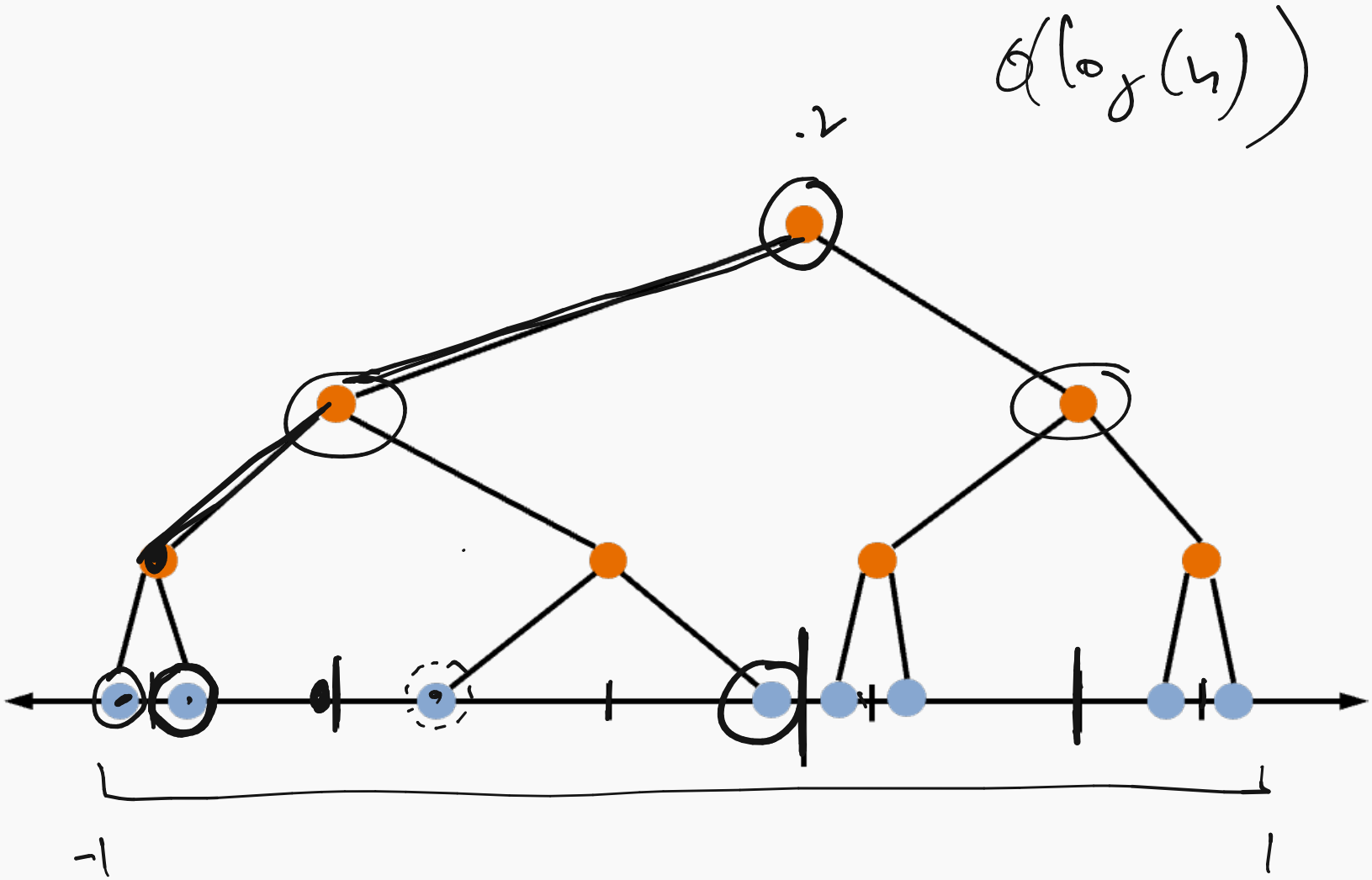


Search time is roughly $O(d \cdot \log n \cdot 2^d)$, which is only sublinear for $d = o(\log n)$.

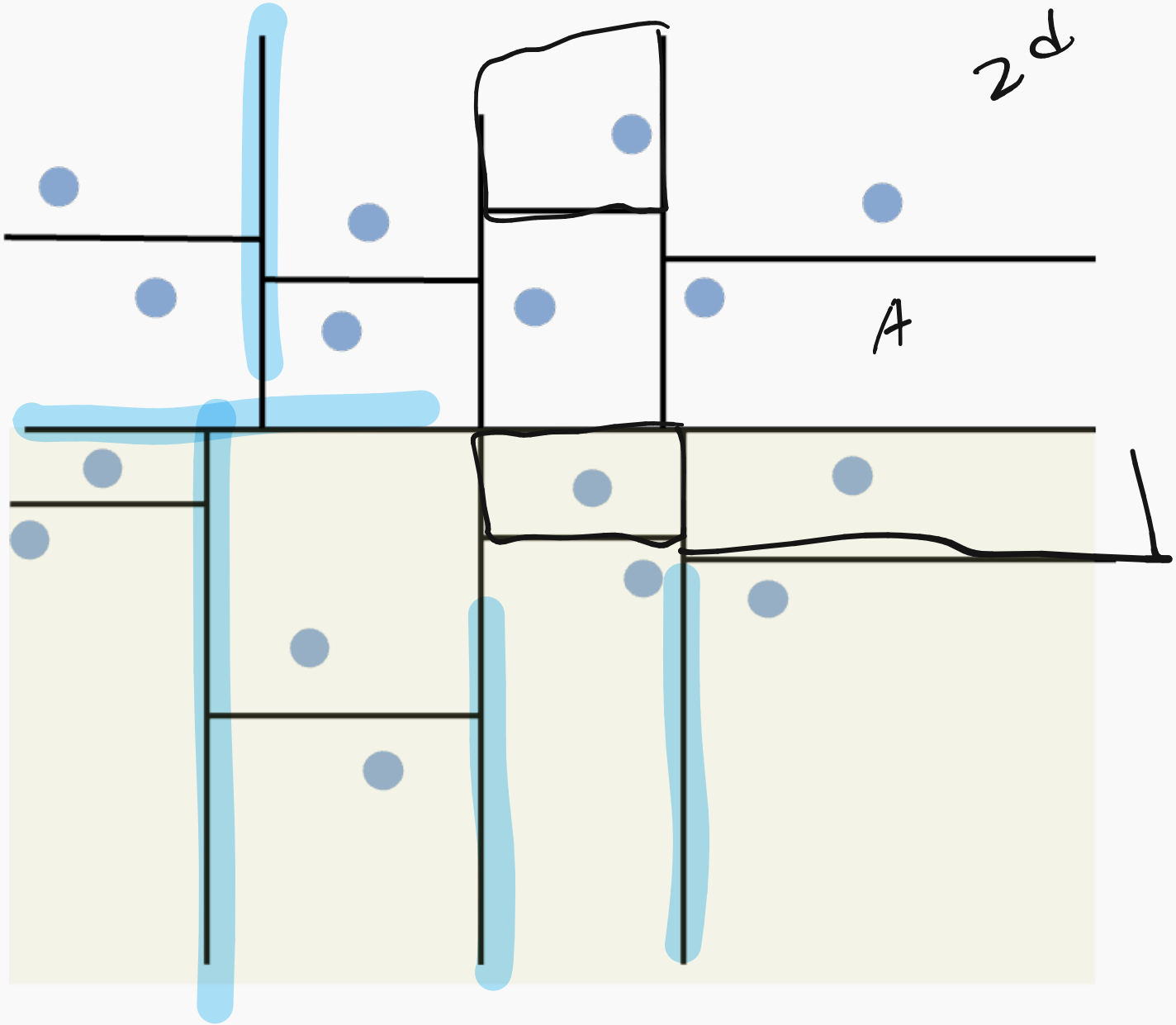
$O(nd)$

$\log(n)$

ISSUE WITH KD-TREES



ISSUE WITH KD-TREES



HIGH DIMENSIONAL NEAR NEIGHBOR SEARCH

Only been attacked much more recently:

- Locality-sensitive hashing [Indyk, Motwani, 1998]
- Spectral hashing [Weiss, Torralba, and Fergus, 2008]
- Vector quantization [Jégou, Douze, Schmid, 2009]
- Graph-based vector search [Malkov, Yashunin, 2016, Subramanya et al., 2019]

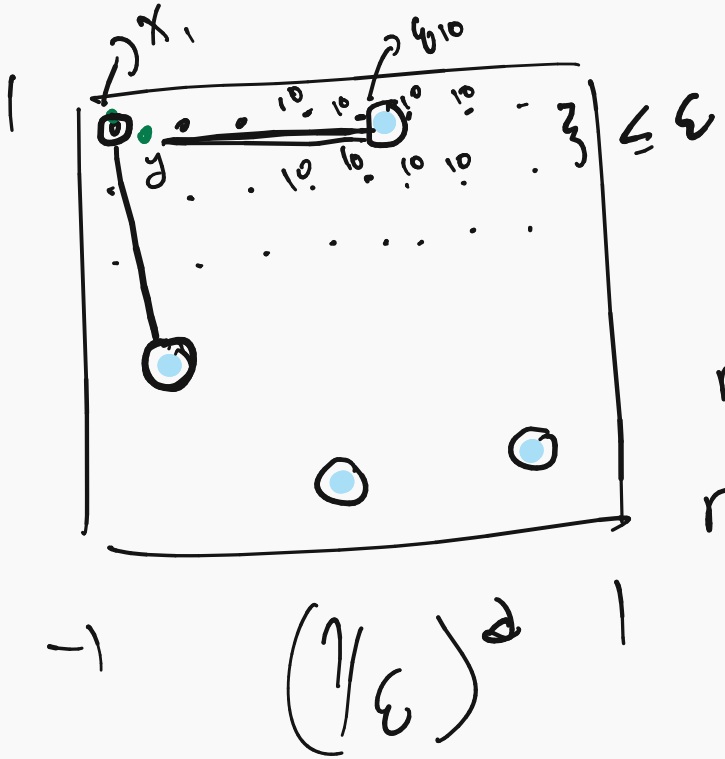
Key ideas behind all of these methods:

1. Trade worse space-complexity + preprocessing time for better time-complexity. I.e., preprocess database in data structure that uses $\Omega(n)$ space.
2. Allow for approximation.

INTUITIVELY WHY DO PREPROCESSING AND SPACE HELP?

Question: Suppose you want to search over points in $[-1,1]^d$ and to achieve accuracy ϵ. I.e., for a given $\mathbf{y} \in [-1,1]^d$, you want to find $\tilde{\mathbf{q}}$ with $\|\mathbf{y} - \tilde{\mathbf{q}}\|_2 \leq \min_i \|\mathbf{y} - \mathbf{q}_i\|_2 + \epsilon$.

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



$O(d)$

query y

round to x_1

return $\min_i \|q_i - x_1\|_2$

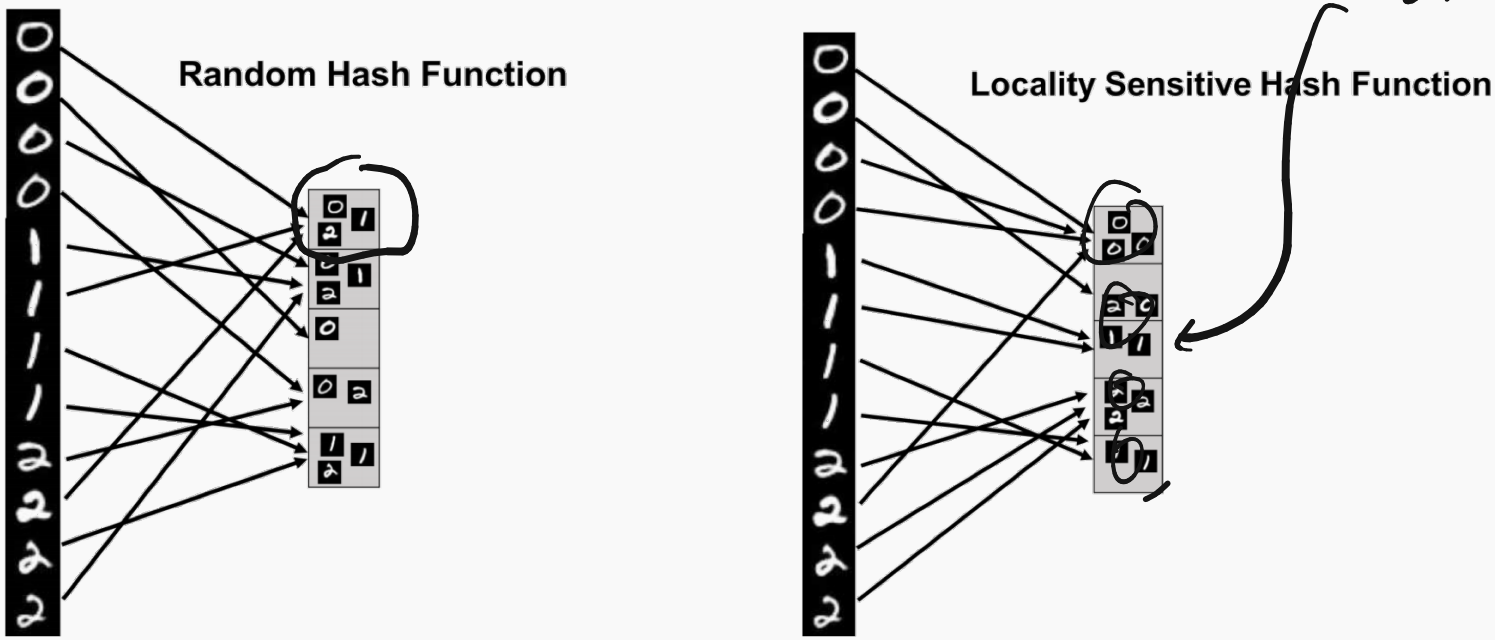
$q_1, \ldots, q_n$

LOCALITY SENSITIVE HASH FUNCTIONS

Let $h : \mathbb{R}^d \to \{1, \ldots, m\}$ be a random hash function.

We call h locality sensitive for similarity function $s(\mathbf{q}, \mathbf{y})$ if $\Pr[h(\mathbf{q}) == h(\mathbf{y})]$ is:

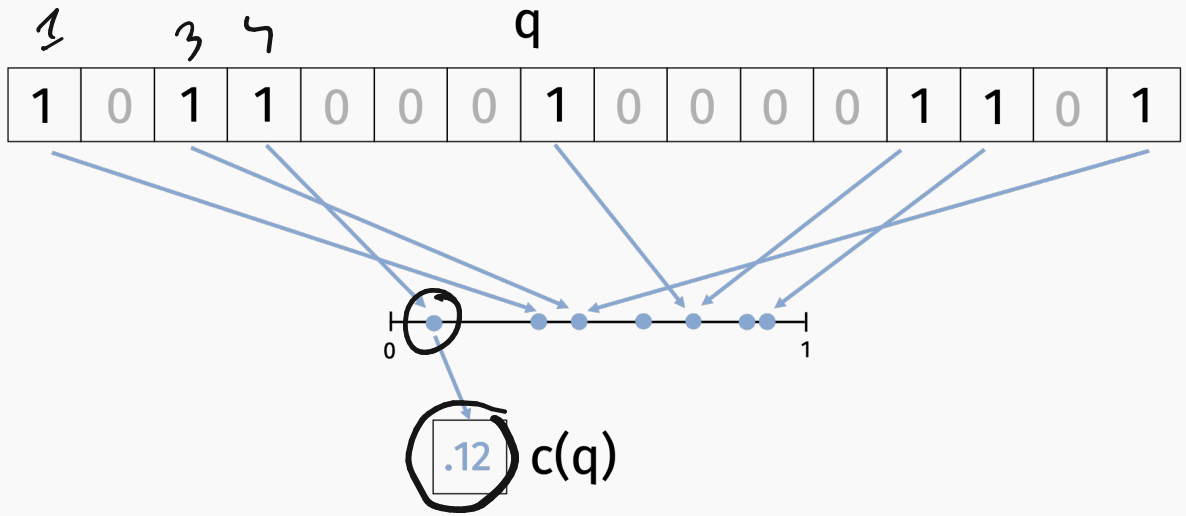
- Higher when $\mathbf{q}$ and $\mathbf{y}$ are more similar, i.e. $s(\mathbf{q}, \mathbf{y})$ is higher.
- Lower when $\mathbf{q}$ and $\mathbf{y}$ are more dissimilar, i.e. $s(\mathbf{q}, \mathbf{y})$ is lower.



LOCALITY SENSITIVE HASH FUNCTIONS

LSH for $s(\mathbf{q}, \mathbf{y})$ equal to Jaccard similarity:

- Let $c : \{0,1\}^d \to [0,1]$ be a single instantiation of MinHash.
- Let $g : [0,1] \to \{1, \ldots, m\}$ be a uniform random hash function.
- Let $h(\mathbf{q}) = g(c(\mathbf{q}))$.



LOCALITY SENSITIVE HASH FUNCTIONS

$\Pr[c(q) == c(y)] = J(q, y)$

LSH for Jaccard similarity:

- Let $c : \{0,1\}^d \to [0,1]$ be a single instantiation of MinHash.
- Let $g : [0,1] \to \{1, \ldots, m\}$ be a uniform random hash function.
- Let $h(\mathbf{x}) = g(c(\mathbf{x}))$.

$g(c(q)) = g(c(y))$ if $c(q) = c(y)$

$h(q)$ $h(y)$

If $J(\mathbf{q}, \mathbf{y}) = v$,

$$\Pr[h(\mathbf{q}) == h(\mathbf{y})] = J(q,y) + (1 - J(q,y)) \cdot \frac{1}{m}$$

negligible

Assume $m = \mathcal{O}(n)$

n: # of items in database

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

Pre-processing:

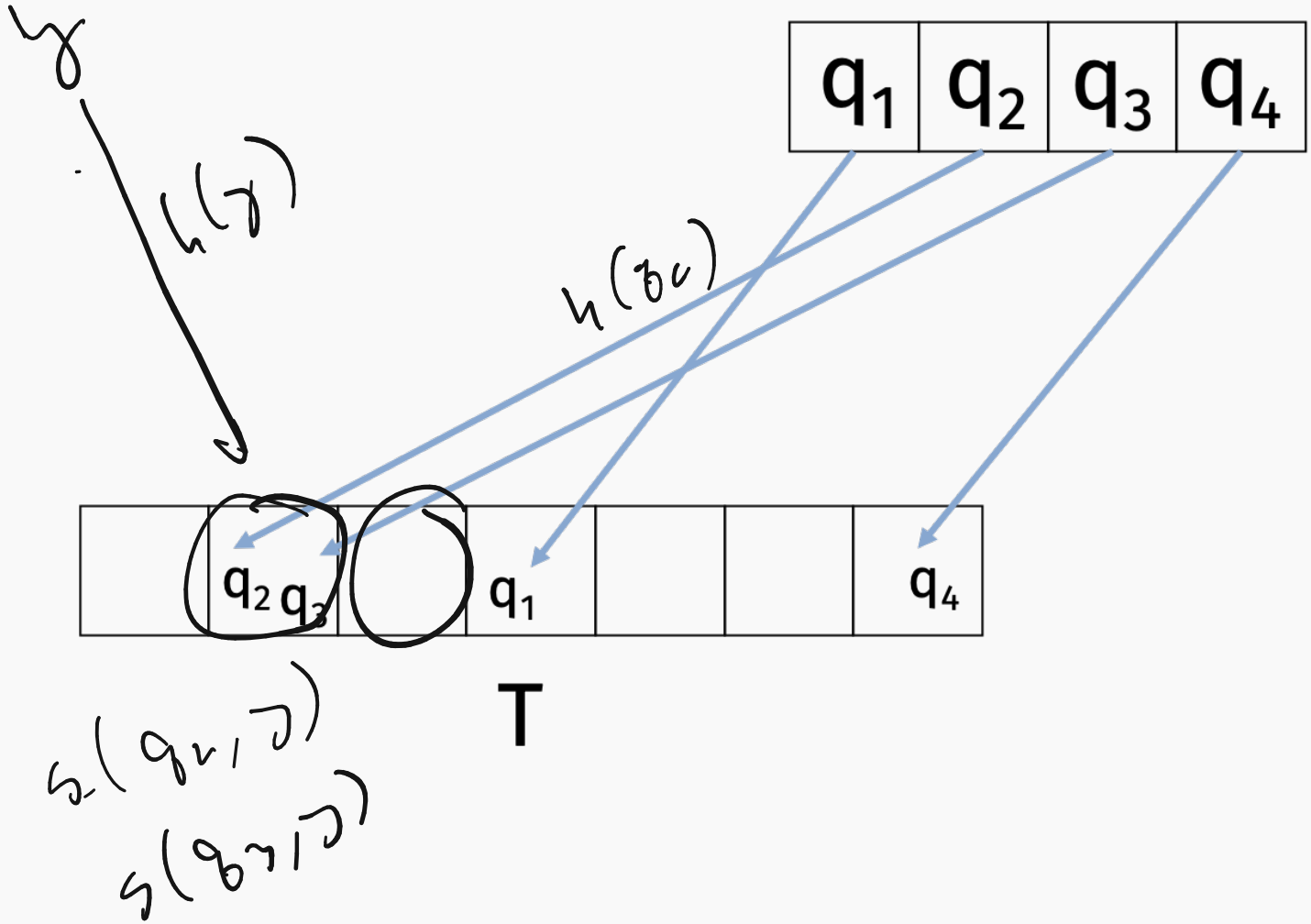
- Select random LSH function $h : \{0,1\}^d \to 1, \ldots, m$.
- Create table T with $m = O(n)$ slots.[1]
- For $i = 1, \ldots, n$, insert $\mathbf{q}_i$ into $T(h(\mathbf{q}_i))$.

Query:

- Want to find near neighbors of input $\mathbf{y} \in \{0,1\}^d$.
- Linear scan through all vectors $\mathbf{q} \in T(h(\mathbf{y}))$ and return any that are close to $\mathbf{y}$. Time required is $O(d \cdot |T(h(\mathbf{y})|)$.

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

NEAR NEIGHBOR SEARCH



Two main considerations:

- **False Negative Rate**: What's the probability we do not find a vector that is close to $\mathbf{y}$?
- **False Positive Rate**: What's the probability that a vector in $T(h(\mathbf{y}))$ is not close to $\mathbf{y}$?

A higher false negative rate means we miss near neighbors.

A higher false positive rate means increased runtime – we need to compute $S(\mathbf{q}, \mathbf{y})$ for every $\mathbf{q} \in T(h(\mathbf{y}))$ to check if it's actually close to $\mathbf{y}$.

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. We will discuss LSH for inner product/Euclidean distance as well. Suppose the nearest database point $\mathbf{q}$ has $J(\mathbf{y}, \mathbf{q}) = .4$.

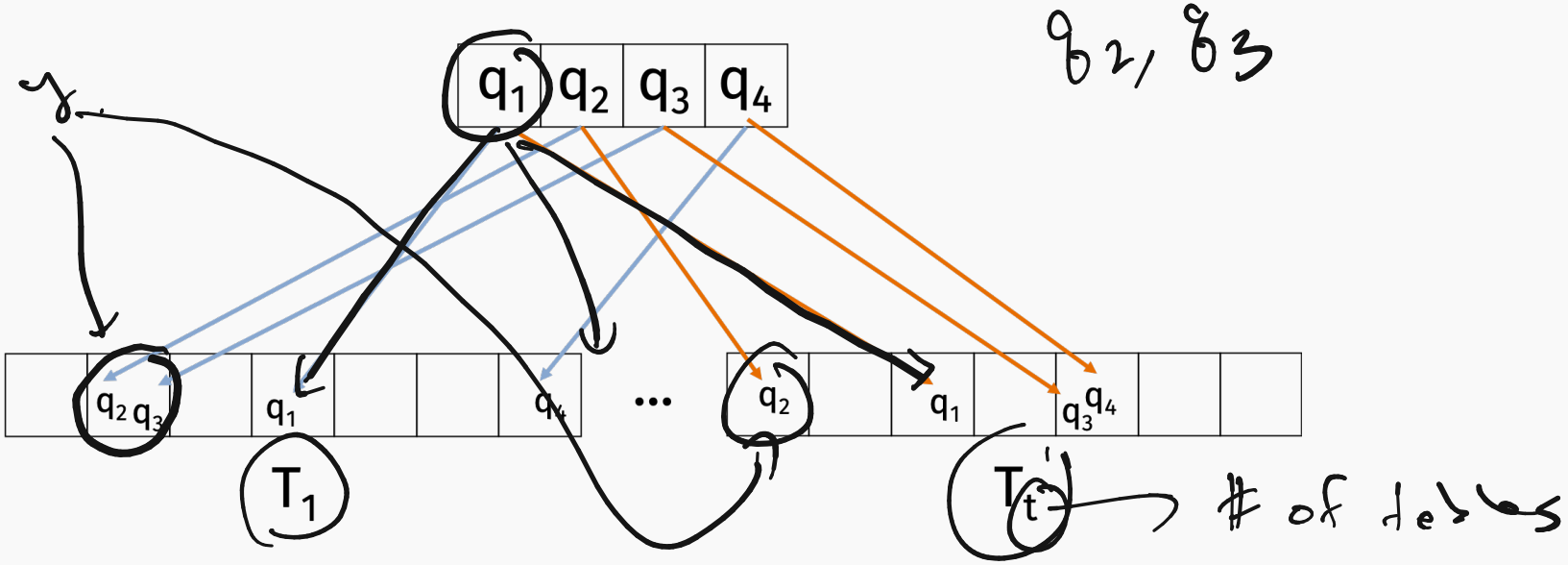
What's the probability we do not find q?

$$\Pr[q \in T(h(y))]$$

$$= \Pr(h(q) = h(y)) = J(y, q) = .4$$

False negative prob. $= 1 - .4 = .6$.

REDUCING FALSE NEGATIVE RATE



Pre-processing:

- Select t independent LSH's $h_1, \ldots, h_t : \{0,1\}^d \to 1, \ldots, m$.
- 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 $T_j(h_j(\mathbf{q}_i))$.

REDUCING FALSE NEGATIVE RATE

Query:

- Want to find near neighbors of input $\mathbf{y} \in \{0,1\}^d$.
- Linear scan through all vectors in $T_1(h_1(\mathbf{y})) \cup T_2(h_2(\mathbf{y})) \cup \ldots, T_t(h_t(\mathbf{y}))$.

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

What's the probability we find q?

$1 - (1 - .4)^t = 1 - .6^t$

(10, 99%)

$t = 10$

WHAT HAPPENS TO FALSE POSITIVES?

Suppose there is some other database point $\mathbf{z}$ with $J(\mathbf{y}, \mathbf{z}) = .2$.

What is the probability we will need to compute $J(\mathbf{z}, \mathbf{y})$ in our hashing scheme with one table? I.e. the probability that $\mathbf{y}$ hashes into at least one bucket containing $\mathbf{z}$.

In the new scheme with $t = 10$ tables?

$1 - (1 - .2)^t = 1 - .8^t = 89\%$

$t = 10$

if $t = 10$.

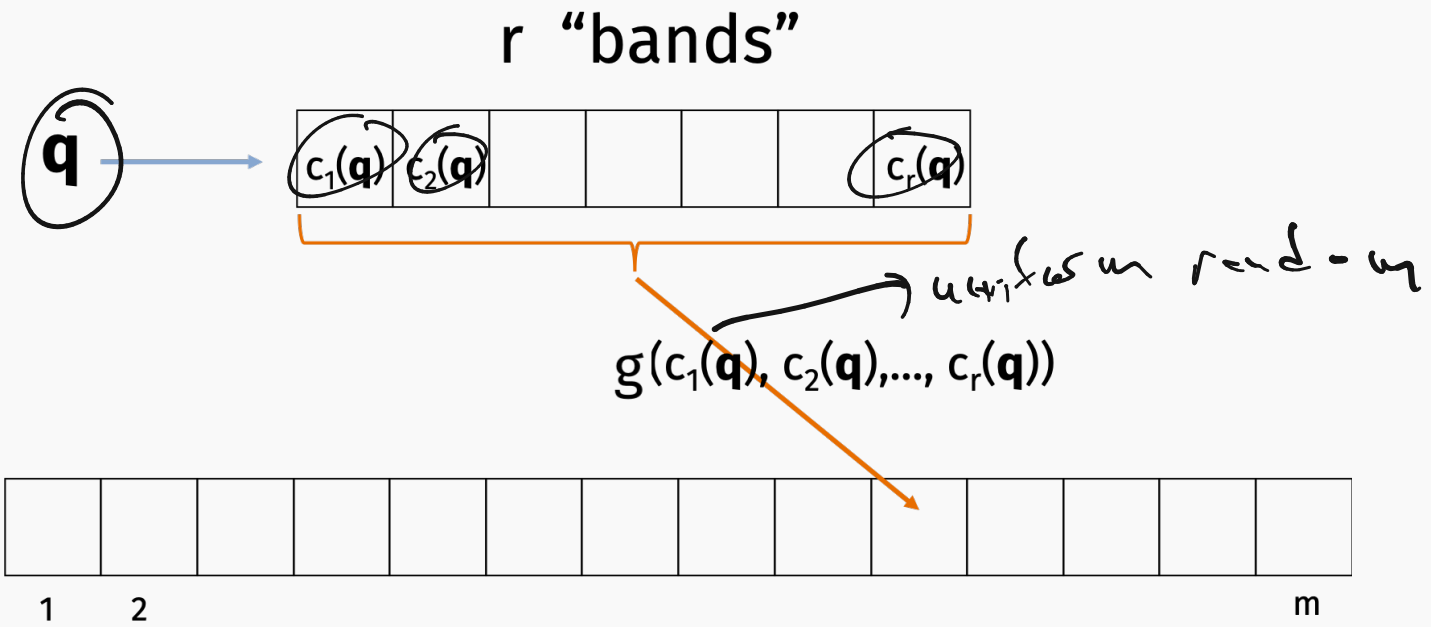
(89%)

REDUCING FALSE POSITIVES

Change our locality sensitive hash function.

Tunable LSH for Jaccard similarity:

- Choose parameter $r \in \mathbb{Z}^+$.
- Let $c_1, \ldots, c_r : \{0,1\}^d \to [0,1]$ be independnt random MinHash's.
- Let $g : [0,1]^r \to \{1, \ldots, m\}$ be a uniform random hash function.
- Let $h(x) = g(c_1(x), \ldots, c_r(x))$.



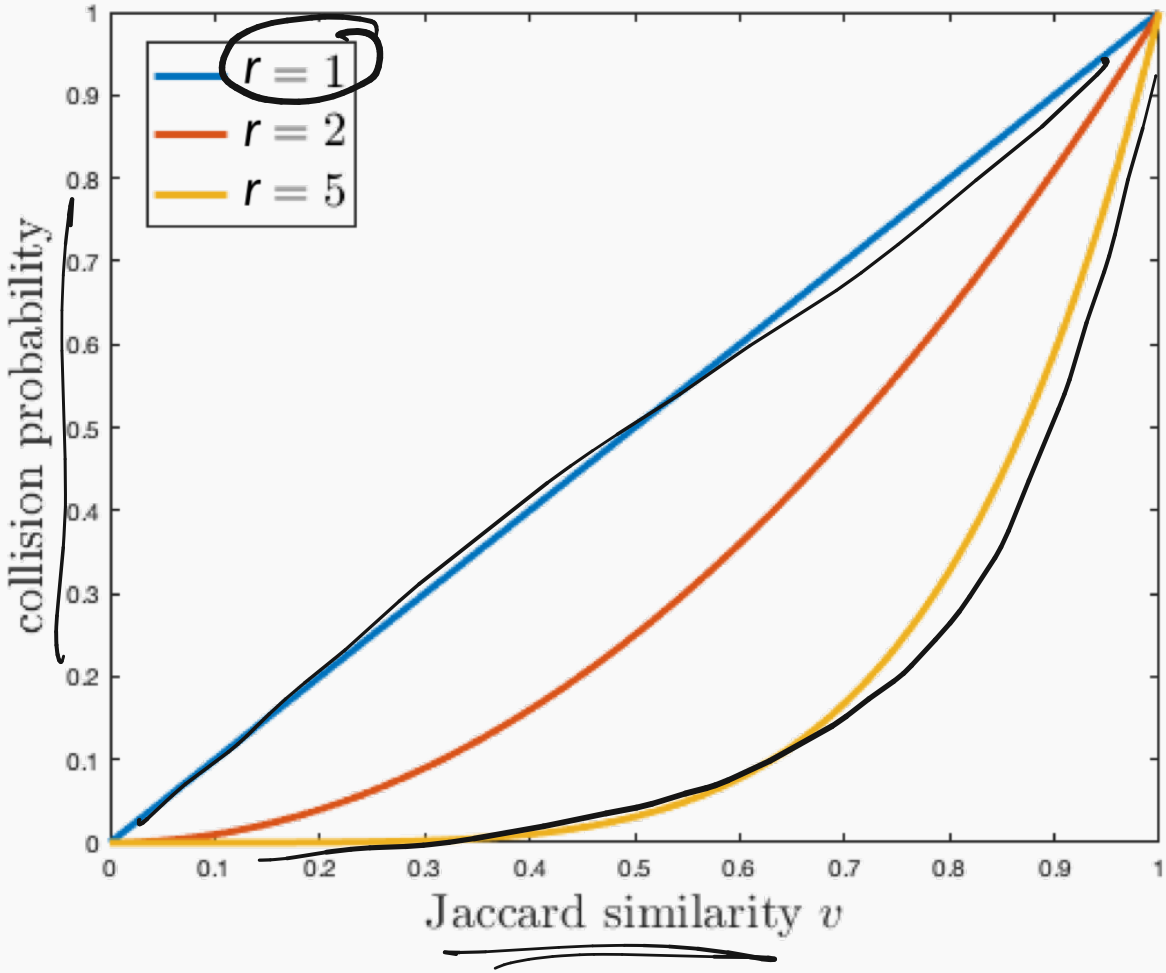
REDUCING FALSE POSITIVES

Tunable LSH for Jaccard similarity:

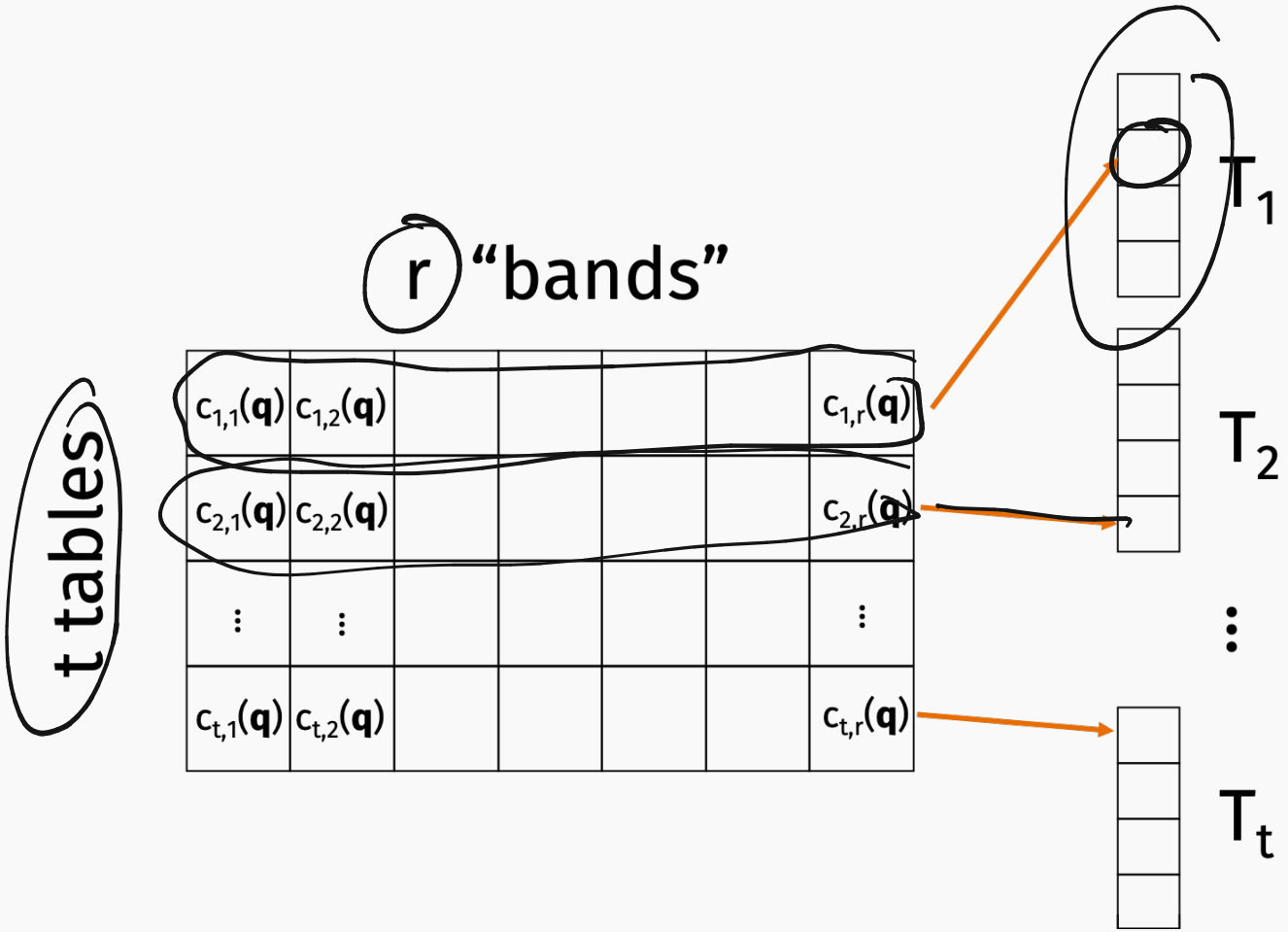
- Choose parameter $r \in \mathbb{Z}^+$.
- Let $c_1, \ldots, c_r : \{0,1\}^d \to [0,1]$ be random MinHash.
- Let $g : [0,1]^r \to \{1, \ldots, m\}$ be a uniform random hash function.
- Let $h(\mathbf{x}) = g(c_1(\mathbf{x}), \ldots, c_r(\mathbf{x}))$.

If $J(\mathbf{q}, \mathbf{y}) = v$, then $\Pr[h(\mathbf{q}) == h(\mathbf{y})] =$ $v^r + (1 - v^r) \cdot \frac{1}{m}$

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

Full LSH cheme has two parameters to tune:



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

False Negatives ↓

False Positives ↑

Effect of **increasing number of bands** *r* on:

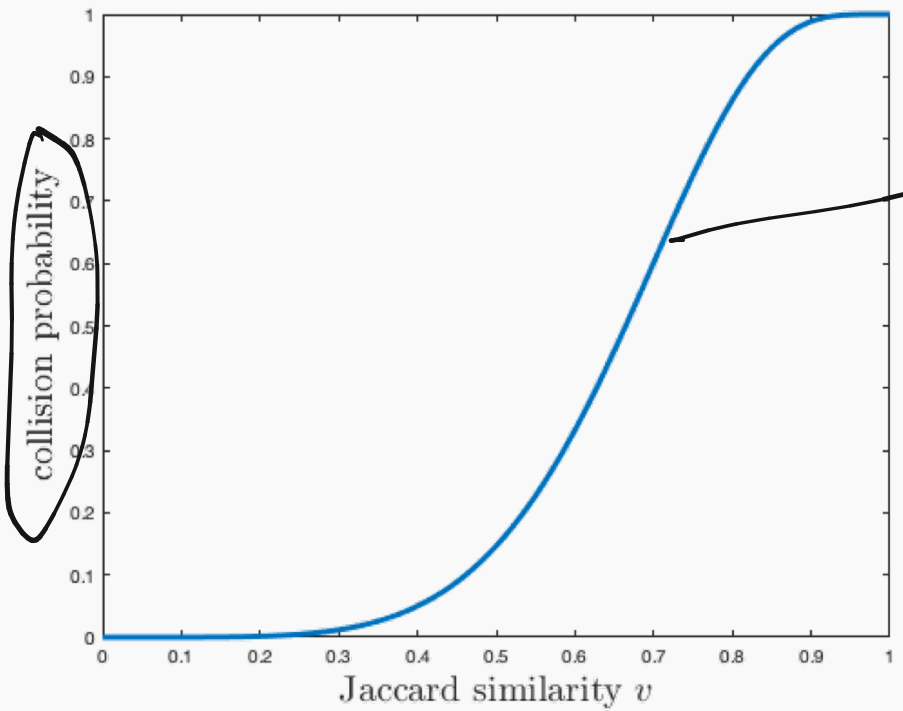
False Negatives ↑

False Positives ↓

s-curve tuning

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

$\Pr[q \in T_i(h(y)) \text{ for some } i \in 1, \ldots, t]$



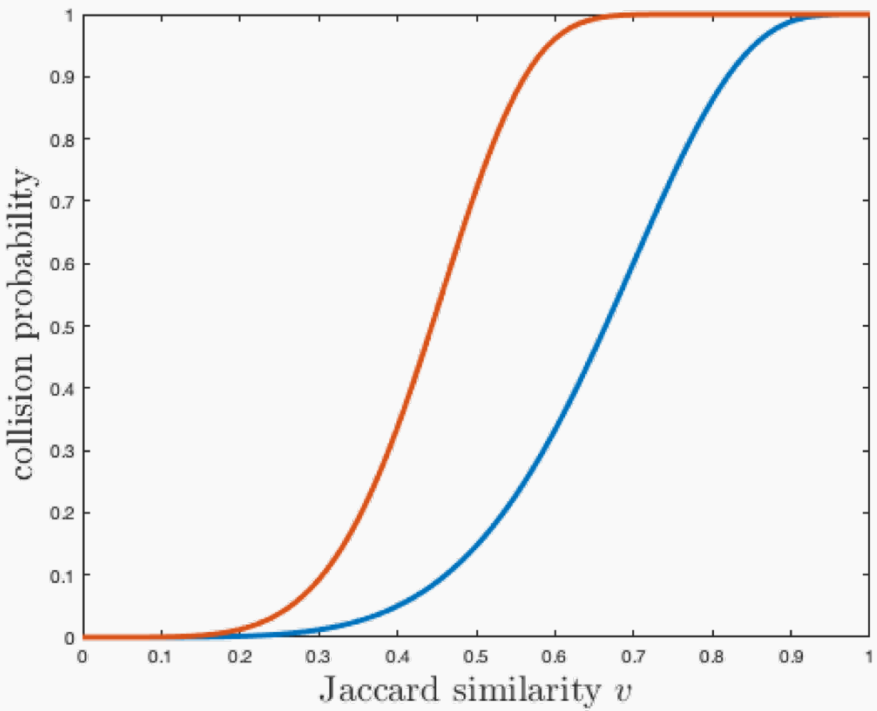
$1 - (1 - v^r)^t$

$r = 5, t = 5$

S-CURVE TUNING

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

$$\approx 1 - (1 - v^r)^t$$

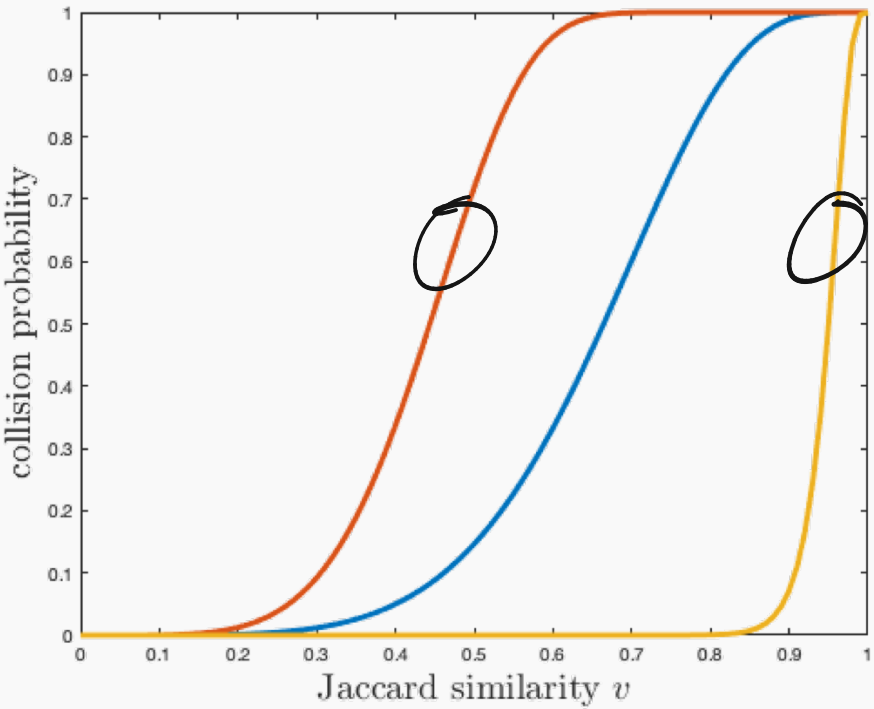


$$r = 5, t = 40$$

S-CURVE TUNING

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

$$\approx 1 - (1 - v^r)^t$$

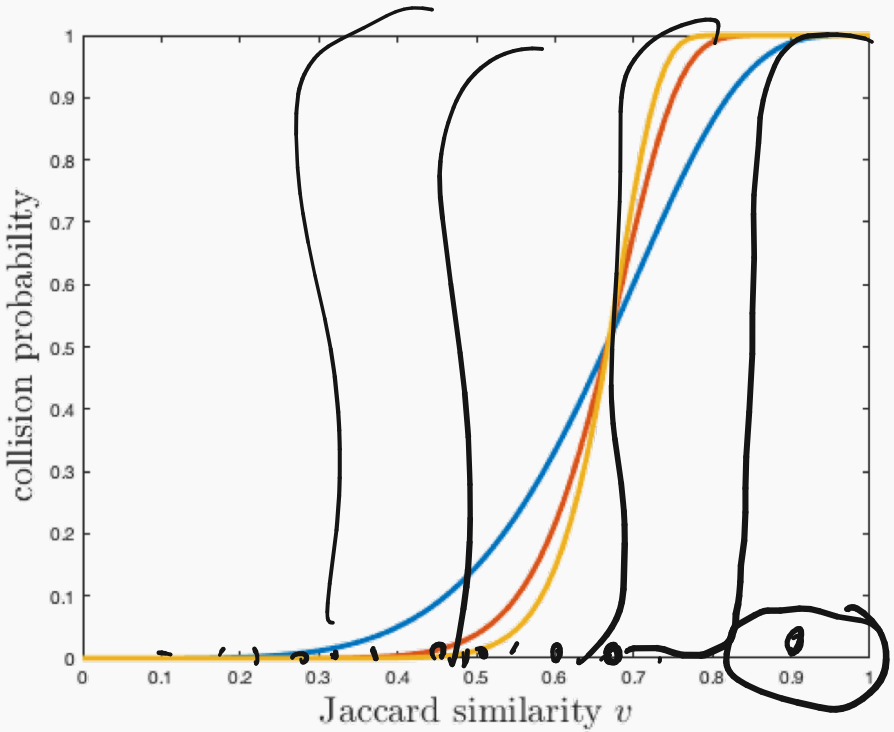


$$r = 40, t = 5$$

S-CURVE TUNING

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

$$1 - (1 - v^r)^t$$



Increasing both r and t gives a steeper curve.

Better for search, but worse space complexity.

FIXED THRESHOLD

Use Case 1: Fixed threshold.

- Shazam wants to find match to audio clip $\mathbf{y}$ in a database of 10 million clips.
- There are 10 true matches with $J(\mathbf{y}, \mathbf{q}) > .9$.
- There are 10,000 near matches with $J(\mathbf{y}, \mathbf{q}) \in [.7, .9]$.
- All other items have $J(\mathbf{y}, \mathbf{q}) < .7$.

With $r = 25$ and $t = 40$,

- Hit probability for $J(\mathbf{y}, \mathbf{q}) > .9$ is $\gtrsim 1 - (1 - .9^{25})^{40} = .95$
- Hit probability for $J(\mathbf{y}, \mathbf{q}) \in [.7, .9]$ is $\lesssim 1 - (1 - .9^{25})^{40} = .95$
- 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 $\approx 40 \cdot O(n)$. $+ O(nd)$

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:

- *Time: $O\left(n^{1/C}\right)$.*
- *Space: $O\left(n^{1+1/C} + nd\right)$.*

$\|\mathbf{q} - \mathbf{y}\|_0 =$ "hamming distance" = number of elements that differ between $\mathbf{q}$ and $\mathbf{y}$.

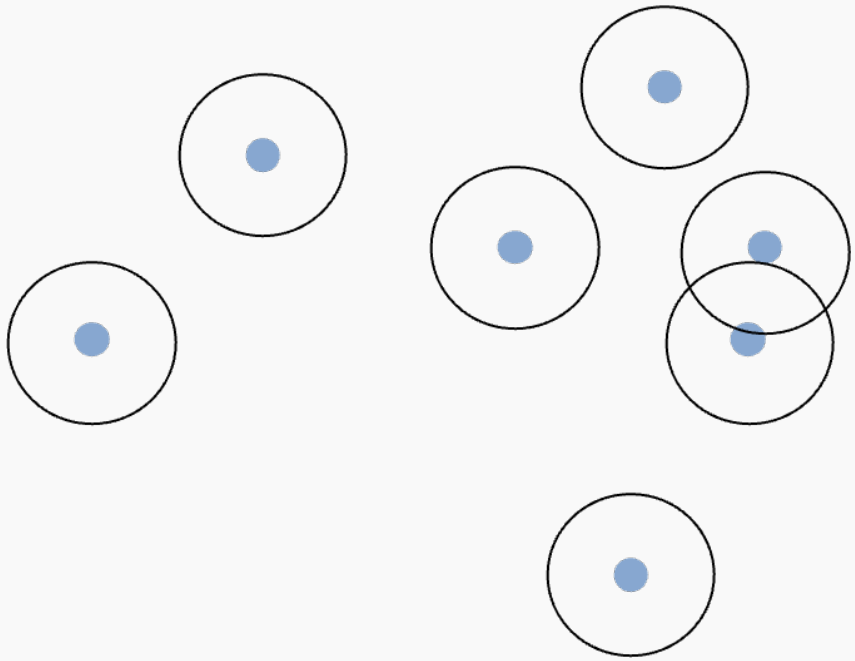
If there is no point at distance R, algorithm does not need to return anything.

LSH based nearest-neighbor in theory

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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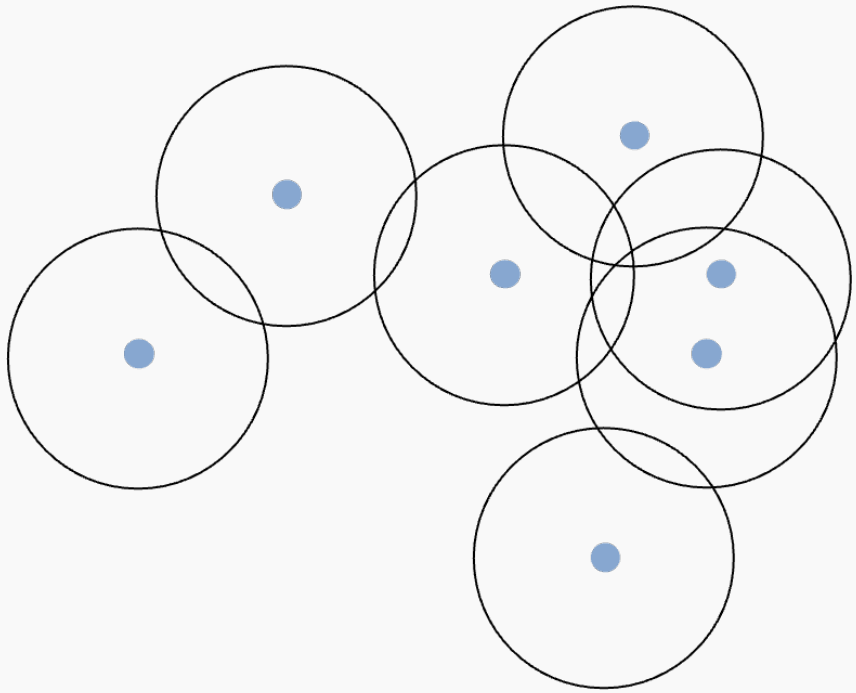

LSH based nearest-neighbor in theory

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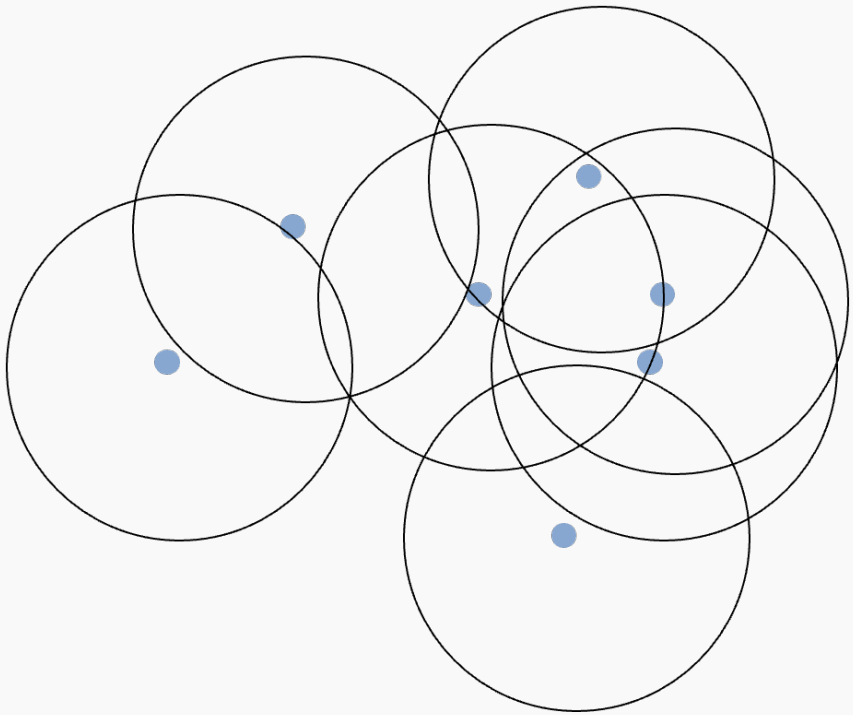


Total number of levels = $O(\log(d_{\max}/d_{\min}))$, where $d_{\max} = \max_{i,j} \|\mathbf{q}_i - \mathbf{q}_j\|$ and $d_{\min} = \min_{i,j} \|\mathbf{q}_i - \mathbf{q}_j\|$. $d_{\max}/d_{\min}$ is called the dynamic range.

Theorem (Indyk, Motwani, 1998)

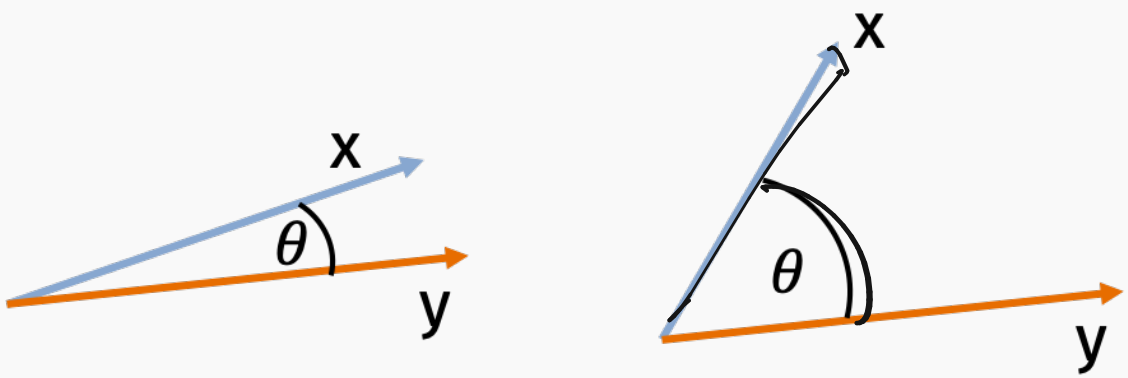
Let q^* be the closest database vector to $\mathbf{y}$. Return a vector $\tilde{\mathbf{q}}$ with $\|\tilde{\mathbf{q}} - \mathbf{y}\|_0 \leq C \cdot \|\mathbf{q}^* - \mathbf{y}\|_0$ in:

- *Time: $\tilde{O}\left(n^{1/C}\right)$.*
- *Space: $\tilde{O}\left(n^{1+1/C} + nd\right)$.*

Similar results can be proven for other metrics, including Euclidean distance. But you need a good LSH function.

Good locality sensitive hash functions exists for other similarity measures.

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



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

COSINE SIMILARITY

Cosine similarity is natural "inverse" for Euclidean distance when $\|\mathbf{x}\|_2^2 = \|\mathbf{y}\|_2^2 = 1$ (often the case for ML-based embeddings).

$$\cos(\theta(x,y)) = \langle x, y \rangle = 1 - \frac{\|x-y\|_2^2}{2}$$

$$\|x-y\|_2^2 = \|x\|_2^2 + \|y\|_2^2 - 2\langle x, y \rangle = 2 - 2\langle x, y \rangle$$

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

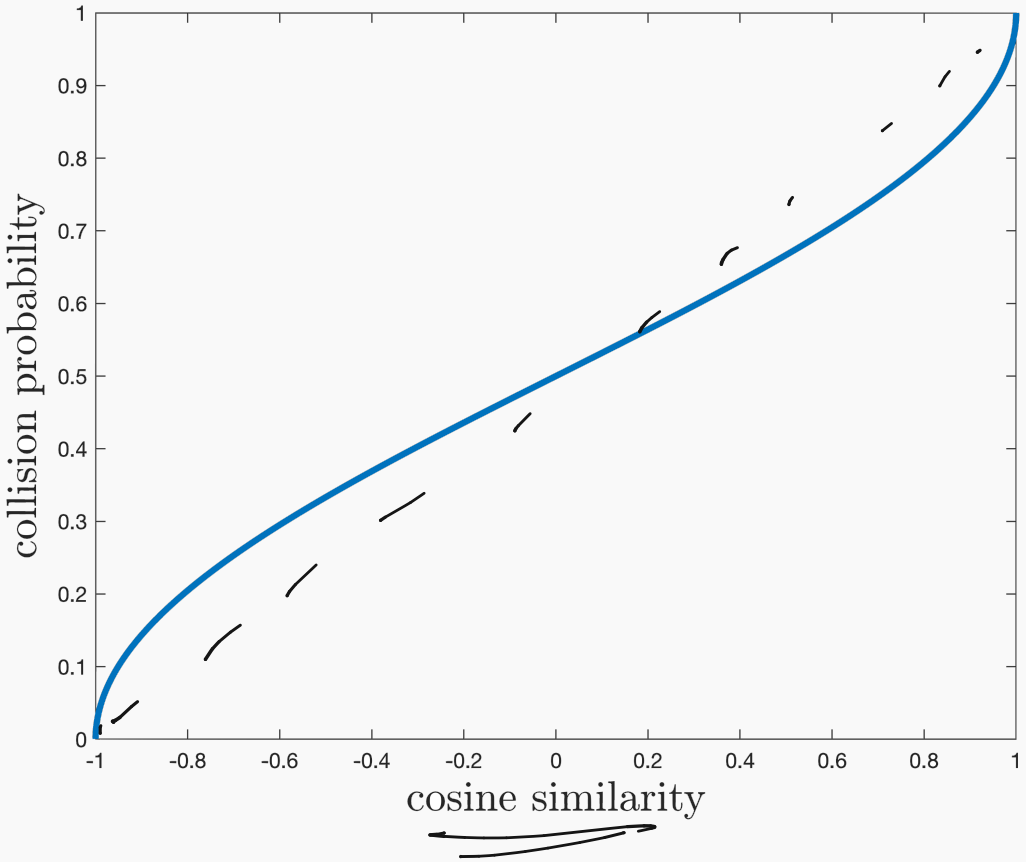
Locality sensitive hash for **cosine similarity**:

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

If $\cos(\theta(\mathbf{x}, \mathbf{y})) = v$, what is $\Pr[h(\mathbf{x}) == h(\mathbf{y})]$?

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

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



SIMHASH

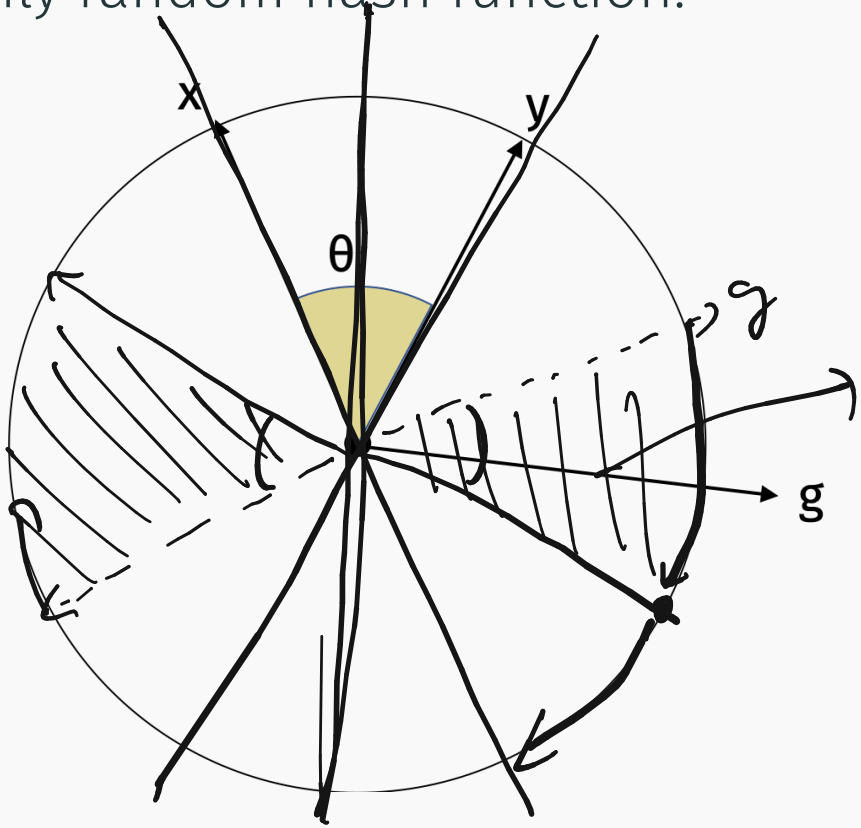
SimHash can be banded, just like our MinHash based LSH function for Jaccard similarity:

- 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 $h(\mathbf{x}) = f([\mathsf{sign}(\langle \mathbf{g}_1, \mathbf{x} \rangle), \ldots, \mathsf{sign}(\langle \mathbf{g}_r, \mathbf{x} \rangle)])$.

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

SIMHASH ANALYSIS IN 2D

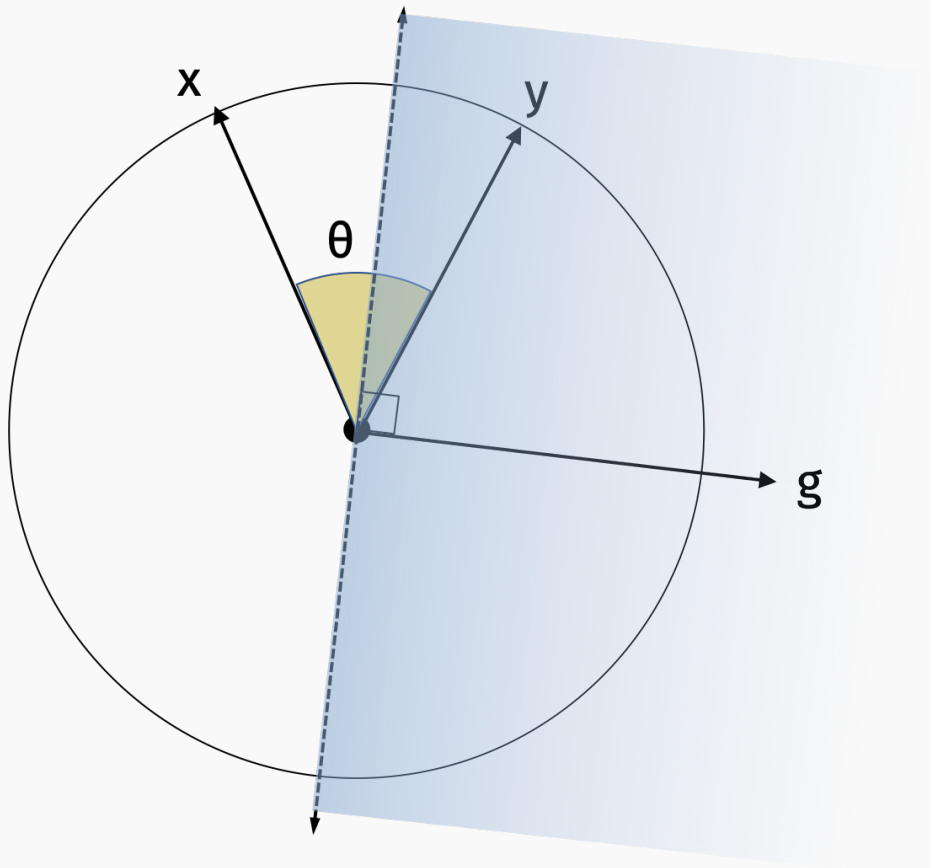
To prove: $\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx 1 - \frac{\theta}{\pi}$, where $h(\mathbf{x}) = f(\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle))$ and f is uniformly random hash function.



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

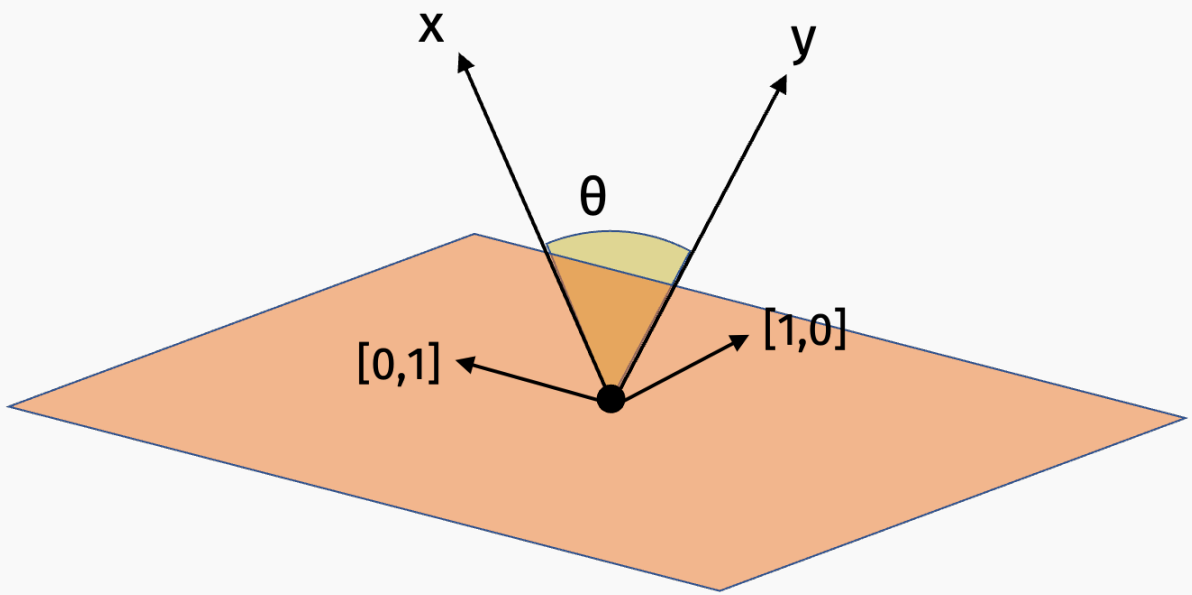
where $z = \Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)]$

SIMHASH ANALYSIS 2D

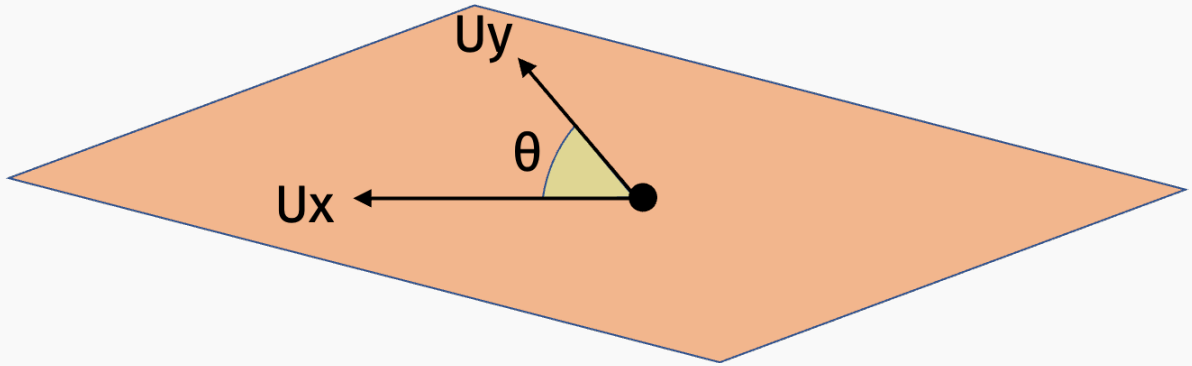


$\Pr[\mathsf{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \mathsf{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)] =$ probability $\mathbf{x}$ and $\mathbf{y}$ are on the same side of hyperplane orthogonal to $\mathbf{g}$.

SIMHASH ANALYSIS HIGHER DIMENSIONS



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



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

Note: A rotation matrix $\mathbf{U}$ has the property that $\mathbf{U}^T\mathbf{U} = \mathbf{I}$. I.e., $\mathbf{U}^T$ is a rotation matrix itself, which reverses the rotation of $\mathbf{U}$.

Claim:

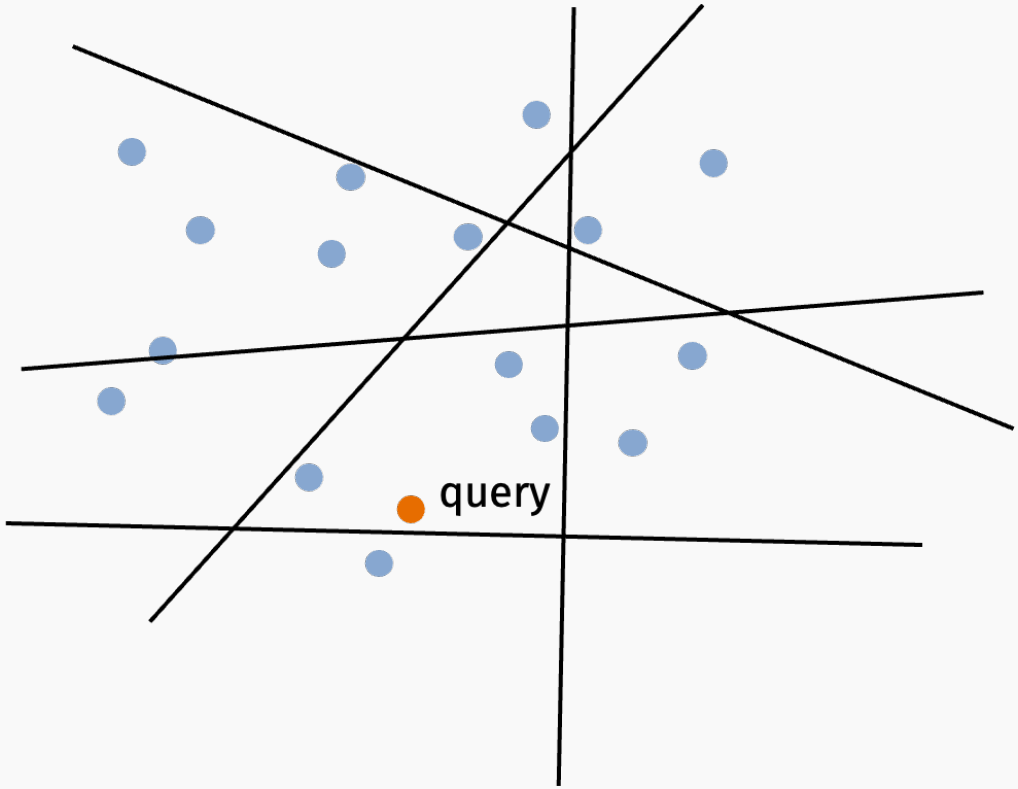
$$\begin{aligned}\Pr[\mathsf{sign}(\langle \mathbf{g}, \mathbf{x}\rangle) == \mathsf{sign}(\langle \mathbf{g}, \mathbf{y}\rangle) &= \Pr[\mathsf{sign}(\langle \mathbf{g}, \mathbf{U}\mathbf{x}\rangle) == \mathsf{sign}(\langle \mathbf{g}, \mathbf{U}\mathbf{y}\rangle)] \\ &= \Pr[\mathsf{sign}(\langle \mathbf{g}[1,2],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

The first step is the trickiest here. Why does it hold?

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.

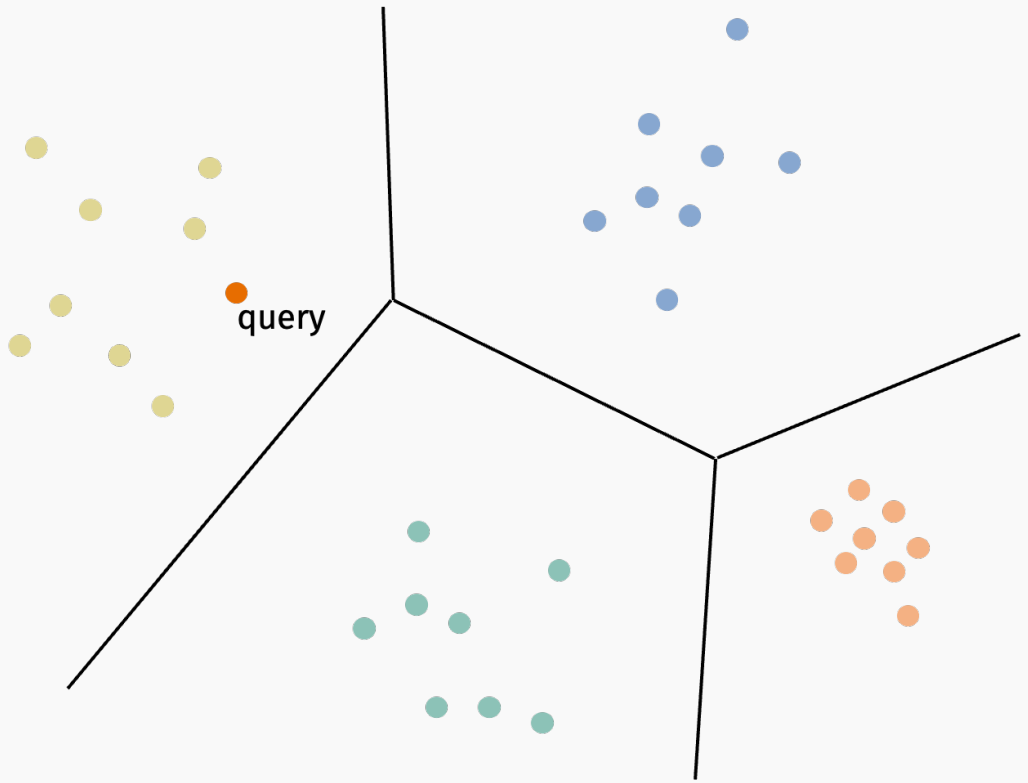
Starting point: Think of LSH as a randomized space-partitioning method.



NEAREST-NEIGHBOR SEARCH IN PRACTICE

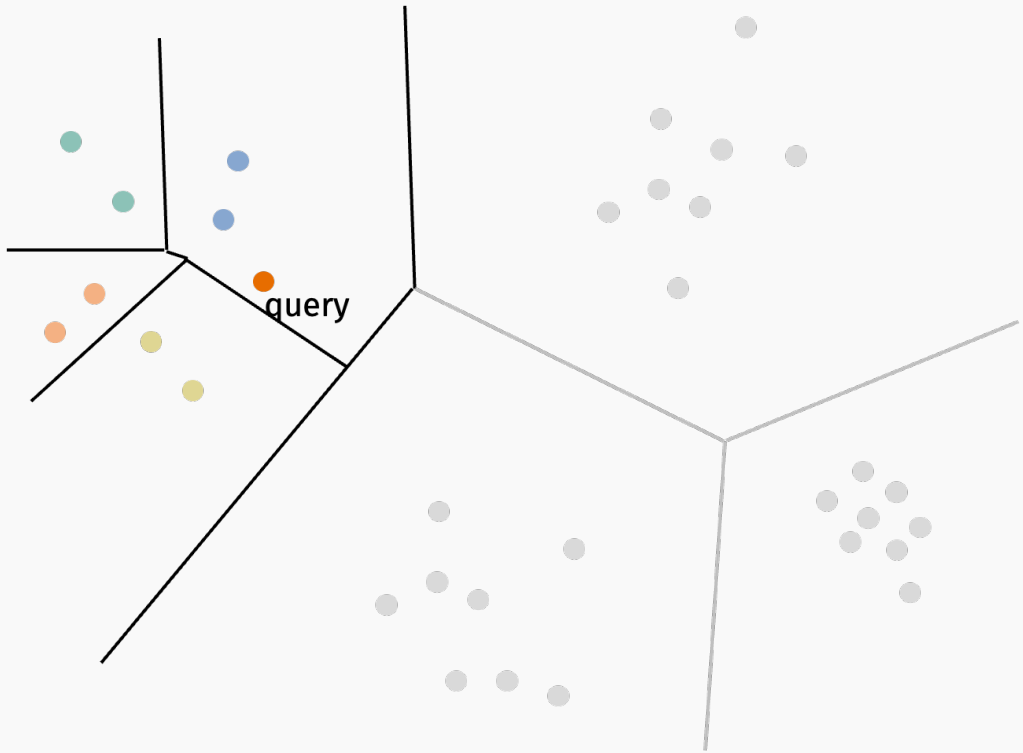
In practice, we can often get partitions with better margin but partitioning in a data-dependent way.

Common approach: Split data using k-means clustering.



NEAREST-NEIGHBOR SEARCH IN PRACTICE

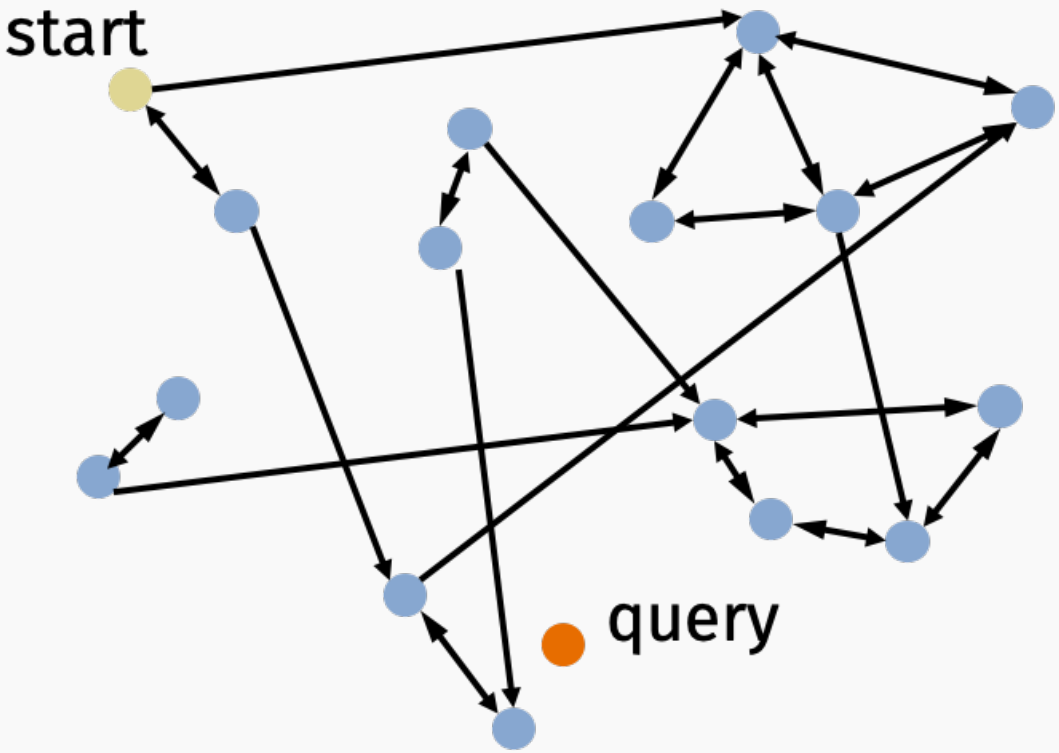
Common approach: Split data using k-means clustering.



Main approach behind “k-means tree” and “inverted file index” based near-neighbor search methods like Meta’s FAISS library and Google’s SCANN.

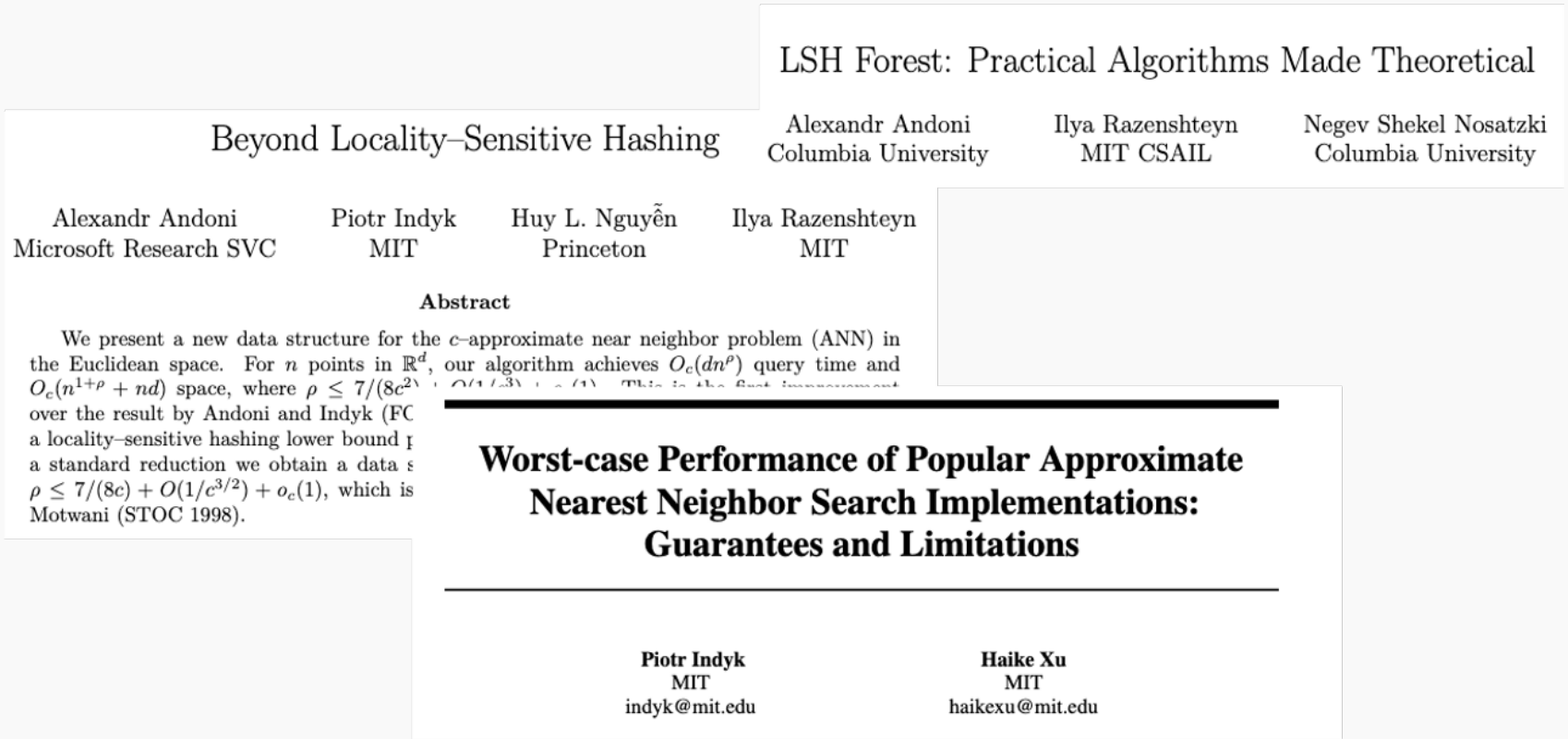
NEAREST-NEIGHBOR SEARCH IN PRACTICE

New kid on the block: Graph-based nearest neighbor search.



Idea behind methods like NSG, HNSW, DiskANN, etc. Inspired by Milgram's famous "small-world" experiments from the 1960's.

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



LSH Forest: Practical Algorithms Made Theoretical

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Beyond Locality–Sensitive Hashing

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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 $\rho \leq 7/(8c^2) + O(1/c^3) + o_c(1)$. This is the first improvement over the result by Andoni and Indyk (FC
a locality–sensitive hashing lower bound p
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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