CS-GY 6763: Lecture 5
Dimensionality reduction, near neighbor search in high dimensions

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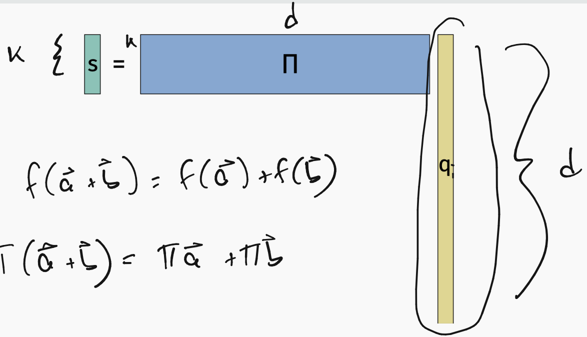
Despite all our warning from last class that low-dimensional space looks nothing like high-dimensional space, next we are going to learn about how to **compress high dimensional vectors to low dimensions.**

We will be very careful not to compress things too far. An extremely simple method known as Johnson-Lindenstrauss Random Projection pushes right up to the edge of how much compression is possible.

Lemma (Johnson-Lindenstrauss, 1984)

For any set of n data points $\mathbf{q}_1, \ldots, \mathbf{q}_n \in \mathbb{R}^d$ there exists a linear map $\mathbf{\Pi} : \mathbb{R}^d \to \mathbb{R}^k$ where $k = O\left(\frac{\log n}{\epsilon^2}\right)$ such that for all i, j,

$$(1-\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2 \leq \|\mathbf{\Pi}\mathbf{q}_i - \mathbf{\Pi}\mathbf{q}_j\|_2 \leq (1+\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2.$$



$f(\vec{a})$ $\quad f(\vec{a}+\vec{b}) = f(\vec{a}) + f(\vec{b})$

$\Pi(\vec{a}+\vec{b}) = \Pi\vec{a} + \Pi\vec{b}$

This is equivalent to:

Lemma (Johnson-Lindenstrauss, 1984)

For any set of n data points $\mathbf{q}_1, \ldots, \mathbf{q}_n \in \mathbb{R}^d$ *there exists a linear map* $\mathbf{\Pi} : \mathbb{R}^d \to \mathbb{R}^k$ *where* $k = O\left(\frac{\log n}{\epsilon^2}\right)$ *such that for all* i, j,

$$(1-\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2^2 \leq \|\mathbf{\Pi}\mathbf{q}_i - \mathbf{\Pi}\mathbf{q}_j\|_2^2 \leq (1+\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2^2.$$

because for small ϵ, $(1+\epsilon)^2 = 1 + O(\epsilon)$ and $(1-\epsilon)^2 = 1 - O(\epsilon)$.

$(1-\epsilon)^2$ $(1+\epsilon)^2$

$(1-\epsilon)^2 \geq 1-2\epsilon$

$(1+\epsilon)^2 \leq 1+3\epsilon$

Make pretty much any computation involving vectors faster and more space efficient.

- Faster vector search (used in image search, AI-based web search, Retrieval Augmented Generation (RAG), etc.).
- Faster machine learning (today we will see an application to speeding up clustering).
- Faster numerical linear algebra.

Only useful if we can explicity construct a JL map $\mathbf{\Pi}$ and apply efficiently to vectors.

Remarkably, Π can be chosen (completely at random!)

One possible construction: Random Gaussian.

$$\Pi_{i,j} = \frac{1}{\sqrt{k}} \mathcal{N}(0,1)$$

→ # of rows (dimension we reduce to)

The map $\mathbf{\Pi}$ is **oblivious to the data set**. This stands in contrast to other vector compression methods you might know like PCA.

[Indyk, Motwani 1998] [Arriage, Vempala 1999] [Achlioptas 2001] [Dasgupta, Gupta 2003].

Many other possible choices suffice – you can use random $\{+1, -1\}$ variables, sparse random matrices, pseudorandom $\mathbf{\Pi}$. Each with different advantages.

72 x 1000

Let $\mathbf{\Pi} \in \mathbb{R}^{k \times d}$ be chosen so that each entry equals $\frac{1}{\sqrt{k}}\mathcal{N}(0,1)$.

... or each entry equals $\frac{1}{\sqrt{k}} \pm 1$ with equal probability.

d

n

-2.1384	2.9080	-0.3538	0.0229	0.5201	-0.2938	-1.3320	-1.3617	-0.1952
-0.8396	0.8252	-0.8236	-0.2620	-0.0200	-0.8479	-2.3299	0.4550	-0.2176
1.3546	1.3790	-1.5771	-1.7502	-0.0348	-1.1201	-1.4491	-0.8487	-0.3031
-1.0722	-1.0582	0.5080	-0.2857	-0.7982	2.5260	0.3335	-0.3349	0.0230
0.9610	-0.4686	0.2820	-0.8314	1.0187	1.6555	0.3914	0.5528	0.0513
0.1240	-0.2725	0.0335	-0.9792	-0.1332	0.3075	0.4517	1.0391	0.8261
1.4367	1.0984	-1.3337	-1.1564	-0.7145	-1.2571	-0.1303	-1.1176	1.5270
-1.9609	-0.2779	1.1275	-0.5336	1.3514	-0.8655	0.1837	1.2607	0.4669
-0.1977	0.7015	0.3502	-2.0026	-0.2248	-0.1765	-0.4762	0.6601	-0.2097
-1.2078	-2.0518	-0.2991	0.9642	-0.5890	0.7914	0.8620	-0.0679	0.6252

```
>> Pi = randn(m,d);
>> s = (1/sqrt(m))*Pi*q;
```

Q

1	1	-1	-1	-1	-1	-1	-1	1	-1	-1	1	-1	-1	1	1	-1
1	1	1	-1	1	-1	-1	-1	1	1	1	1	-1	1	-1	-1	-1
1	1	-1	-1	-1	1	-1	-1	1	1	-1	1	-1	1	-1	1	-1
-1	-1	-1	1	1	-1	-1	-1	[illegible]	-1	-1	-1	-1	1	1	1	1
1	-1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1	1	-1	1
1	-1	-1	1	-1	1	1	-1	-1	-1	1	-1	-1	-1	1	1	1
1	1	-1	1	1	-1	1	-1	1	-1	1	-1	1	1	1	-1	-1
-1	-1	-1	-1	-1	-1	1	-1	1	1	-1	-1	1	-1	-1	1	1
-1	-1	1	1	1	1	-1	-1	1	-1	1	1	1	-1	1	-1	1
-1	1	-1	1	-1	1	1	-1	-1	1	-1	1	-1	-1	1	-1	1

```
>> Pi = 2*randi(2,m,d)-3;
>> s = (1/sqrt(m))*Pi*q;
```

$\sqrt{d/k}$

q

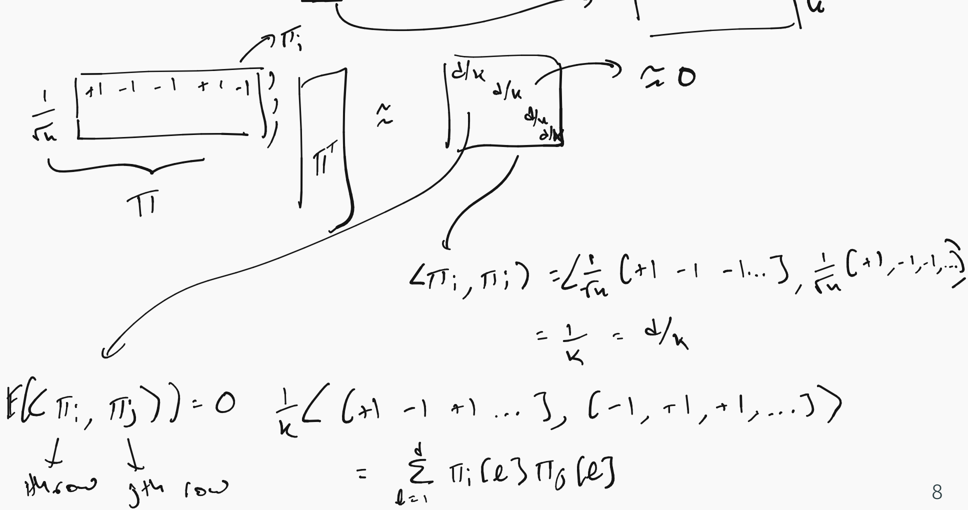
A random orthogonal matrix $\mathbf{Q}$ also works. I.e. with $\mathbf{Q}\mathbf{Q}^T = \mathbf{I}_{k \times k}$. For this reason, the JL operation is often called a "random projection", even though it technically is not a projection when $\mathbf{\Pi}$'s entries are i.i.d.

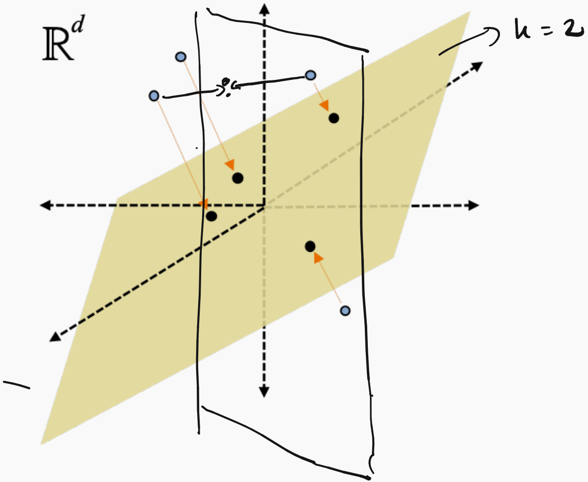
Vershynin Book

requirement on entries:

1) mean 0 2) variance 1 3) "sub-gaussian r.v."

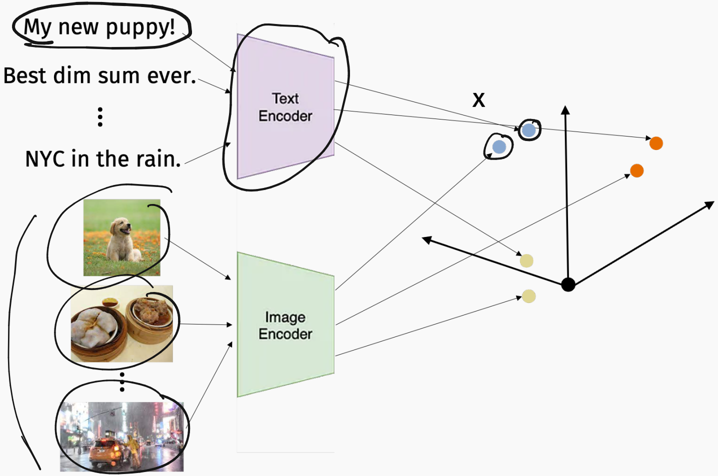
Can anyone see why $\mathbf{\Pi}$ is similar to a projection matrix? I.e., a matrix satisfying $\mathbf{Q}\mathbf{Q}^T = \mathbf{I}_{k\times k}$.



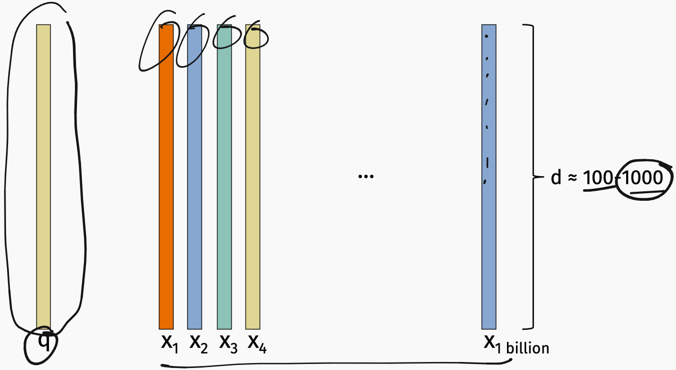


Intuition: Multiplying by a random matrix mimics the process of projecting onto a random k dimensional subspace in d dimensions.

APPLICATION: THE NEW PARADIGM FOR SEARCH



Use neural network (BERT, CLIP, etc.) to convert documents, images, etc. to high dimensional vectors. Results matching search should have similar vector embeddings.



Finding results for a query reduces to finding the nearest vector in a vector database, with similarity typically measured by Euclidean distance. **This is a massive algorithmic challenge!**

$\min_i \|q - x_i\|_2 \qquad \max_i \langle q, x_i \rangle$

ANOTHER EXAMPLE OF VECTOR SEARCH

Shazam can match a song clip against a library of 8 million songs (32 TB of data) in a fraction of a second. Whole system based on vector embeddings + search.

$x_1, \dots, x_n \in \mathbb{R}^d$

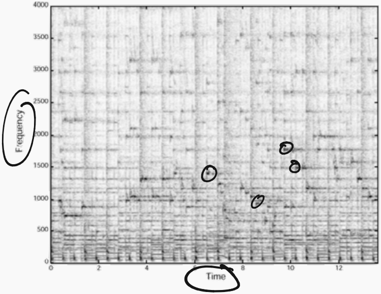
$s_1, \dots, s_n \in \mathbb{R}^k$

$$\min_{s_1,\dots,s_n} \sum_{ij} \left(\langle x_i, x_j\rangle - \langle s_i, s_j\rangle\right)^2$$

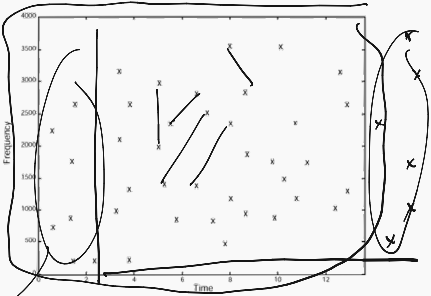
$$\min_{s_1,\dots,s_n} \max_{ij} \left(\langle x_i, x_j\rangle - \langle s_i, s_j\rangle\right)^2$$

$$\min \max_{ij} \left| \|x_i - x_j\|_2^2 - \|s_i - s_j\|_2^2 \right|$$

Shazam can match a song clip against a library of 8 million songs (32 TB of data) in a fraction of a second. Whole system based on vector embeddings + search.



Spectrogram extracted from audio clip.



Processed spectrogram: used to construct audio "fingerprint" $\mathbf{x} \in \mathbb{R}^d$.

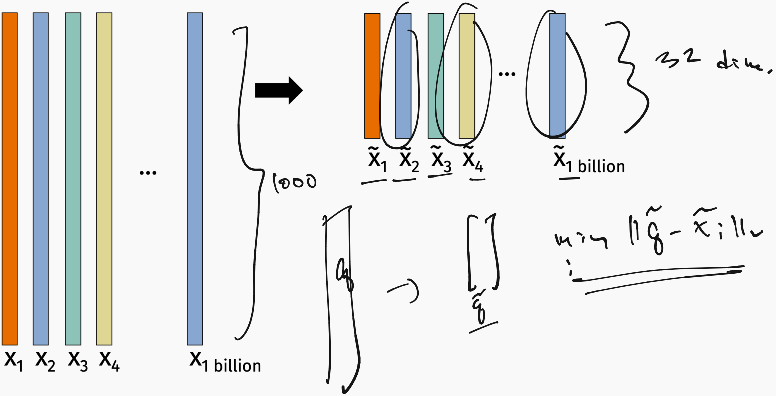
Tons of new startups in the space (offering managed vector databases) and all major tech companies are frantic[redacted] working on speeding up vector search.

Two main ingredients:

1. Vector indexing methods (second half of lecture).
2. Vector compression methods (like Johnson-Lindenstrauss).

APPLICATION: THE NEW PARADIGM FOR SEARCH

Main computational cost is repeatedly computing $\|\mathbf{q} - \mathbf{x}_i\|_2$ for candidate result $\mathbf{x}_i$.



Vector compression leads to faster distance computations. Not only is computational complexity reduced, but we can fit more database vectors in memory.

EUCLIDEAN DIMENSIONALITY REDUCTION

Lemma (Johnson-Lindenstrauss, 1984)

Let $\mathbf{\Pi} \in \mathbb{R}^{k \times d}$ be chosen so that each entry equals $\frac{1}{\sqrt{k}}\mathcal{N}(0,1)$, where $\mathcal{N}(0,1)$ denotes a standard Gaussian random variable.

If we choose $k = O\left(\frac{\log(n)}{\epsilon^2}\right)$, then with probability 99/100, for for all i, j,

$$(1-\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2^2 \leq \|\mathbf{\Pi}\mathbf{q}_i - \mathbf{\Pi}\mathbf{q}_j\|_2^2 \leq (1+\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2^2.$$

$1-\delta \rightarrow O\left(\frac{\log(n/\delta)}{\epsilon^2}\right)$

Intermediate result:

Lemma (Distributional JL Lemma)

Let $\mathbf{\Pi} \in \mathbb{R}^{k \times d}$ *be chosen so that each entry equals* $\frac{1}{\sqrt{k}}\mathcal{N}(0,1)$, *where* $\mathcal{N}(0,1)$ *denotes a standard Gaussian random variable.*

If we choose $k = O\left(\frac{\log(1/\delta)}{\epsilon^2}\right)$, *then for any vector* $\mathbf{x}$, *with probability* $(1-\delta)$*:*

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

$x = q_i - q_j$

$(1-\epsilon)\|q_i - q_j\|_2^2 \leq \|\Pi(q_i - q_j)\|_2^2 \leq (1+\epsilon)\|q_i - q_j\|_2^2$

$\|\Pi q_i - \Pi q_j\|_2^2$

Given this lemma, how do we prove the traditional Johnson-Lindenstrauss lemma?

Union bound

We have a set of vectors $\mathbf{q}_1, \ldots, \mathbf{q}_n$. Fix $i, j \in 1, \ldots, n$.

Let $\mathbf{x} = \mathbf{q}_i - \mathbf{q}_j$. By linearity, $\mathbf{\Pi x} = \mathbf{\Pi}(\mathbf{q}_i - \mathbf{q}_j) = \mathbf{\Pi q}_i - \mathbf{\Pi q}_j$.

By the Distributional JL Lemma, with probability $1 - \delta$,

$$(1-\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2 \le \|\mathbf{\Pi q}_i - \mathbf{\Pi q}_j\|_2 \le (1+\epsilon)\|\mathbf{q}_i - \mathbf{q}_j\|_2.$$

Finally, set $\delta = \frac{1}{100n^2}$. Since there are $< n^2$ total i, j pairs, by a union bound we have that with probability 99/100, the above will hold for all i, j, as long as we compress to: $\le \delta \cdot n^2 = 1/100$

$\log(1/\delta)$

$$k = O\left(\frac{\log(1/(1/100n^2))}{\epsilon^2}\right) = O\left(\frac{\log n}{\epsilon^2}\right) \text{ dimensions.} \quad \square$$

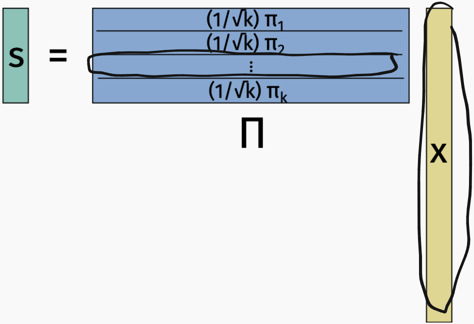
$\log(100n^2) = O(\log(n))$

Want to argue that, with probability $(1 - \delta)$,

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

Claim: $\mathbb{E}\|\mathbf{\Pi x}\|_2^2 = \|\mathbf{x}\|_2^2$.

Some notation:



So each $\boldsymbol{\pi}_i$ contains $\mathcal{N}(0, 1)$ entries.

Intermediate Claim: Let $\boldsymbol{\pi}$ be a length d vector with $\mathcal{N}(0,1)$ entries.

$$\mathbb{E}\left[\|\boldsymbol{\Pi}\mathbf{x}\|_2^2\right] = \mathbb{E}\left[(\langle \boldsymbol{\pi}, \mathbf{x}\rangle)^2\right].$$

$$\sum_{i=1}^{k} [\Pi x]_i^2 = \sum_{i=1}^{k} \langle 1/\sqrt{k}\, \pi_i, x\rangle^2 = \sum_{i=1}^{k} \frac{1}{k} \langle \pi_i, x\rangle^2$$

$$\mathbb{E}\left[\|\Pi x\|_2^2\right] = \sum_{i=1}^{k} \frac{1}{k} \mathbb{E}\left[\langle \pi_i, x\rangle^2\right] = \sum_{i=1}^{k} \frac{1}{k} \mathbb{E}\left[\langle \pi, x\rangle^2\right]$$

$$= \mathbb{E}\left[(\langle \pi, x\rangle)^2\right].$$

Goal: Prove $\mathbb{E}\|\boldsymbol{\Pi}\mathbf{x}\|_2^2 = \|\mathbf{x}\|_2^2$.

$Z_1, \ldots, Z_d$

$$\langle \boldsymbol{\pi}, \mathbf{x} \rangle = Z_1 \cdot x[1] + Z_2 \cdot x[2] + \ldots + Z_d \cdot x[d]$$

where each $Z_1, \ldots, Z_d$ is a standard normal $\mathcal{N}(0, 1)$.

We have that $Z_i \cdot x[i]$ is a normal $\mathcal{N}(0, x[i]^2)$ random variable.

$\mathbb{E}[\langle \pi, x \rangle^2] = \|x\|_2^2$

non random scalar

$\text{Var}[\langle \pi, x \rangle] = \text{var}\left(\sum_{i=1}^{d} N(0, x[i]^2)\right) = \sum_{i=1}^{d} x[i]^2 = \|x\|_2^2.$

independence of $Z_1, \ldots Z_d$.

$= \mathbb{E}[\langle \pi, x \rangle^2] - \mathbb{E}[\langle \pi, x \rangle]^2$

Goal: Prove $\mathbb{E}\|\boldsymbol{\Pi}\mathbf{x}\|_2^2 = \|\mathbf{x}\|_2^2$. Established: $\mathbb{E}\|\boldsymbol{\Pi}\mathbf{x}\|_2^2 = \mathbb{E}\left[(\langle \boldsymbol{\pi}, \mathbf{x} \rangle)^2\right]$

What type of random variable is $\langle \boldsymbol{\pi}, \mathbf{x} \rangle$?

Fact (Stability of Gaussian random variables)

$$\mathcal{N}(\mu_1, \sigma_1^2) + \mathcal{N}(\mu_2, \sigma_2^2) = \mathcal{N}(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2)$$

$$\begin{aligned}\langle \boldsymbol{\pi}, \mathbf{x} \rangle &= \mathcal{N}(0, x[1]^2) + \mathcal{N}(0, x[2]^2) + \ldots + \mathcal{N}(0, x[d]^2) \\ &= \mathcal{N}(0, \|\mathbf{x}\|_2^2).\end{aligned}$$

So $\mathbb{E}\|\boldsymbol{\Pi}\mathbf{x}\|_2^2 = \mathbb{E}\left[(\langle \boldsymbol{\pi}, \mathbf{x} \rangle)^2\right] = \mathbb{E}\left[\mathcal{N}(0, \|\mathbf{x}\|_2^2)^2\right] = \|\mathbf{x}\|_2^2$, as desired.

$k = O\left(\frac{\log 1/\delta}{\epsilon^2}\right)$

Want to argue that, with probability $(1-\delta)$,

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

1. $\mathbb{E}\|\mathbf{\Pi x}\|_2^2 = \|\mathbf{x}\|_2^2$.
2. Need to use a concentration bound.

$\pi_1, \ldots, \pi_k$ are i.i.d Gaussian random vectors.

$$\|\mathbf{\Pi x}\|_2^2 = \frac{1}{k}\sum_{i=1}^{k}(\langle \boldsymbol{\pi}_i, \mathbf{x}\rangle)^2 = \frac{1}{k}\sum_{i=1}^{k}\mathcal{N}(0, \|\mathbf{x}\|_2^2)^2$$

"Chi-squared random variable with k degrees of freedom."

CONCENTRATION OF CHI-SQUARED RANDOM VARIABLES

Lemma

Let H be a Chi-squared random variable with k degrees of freedom.

$$\Pr[|\mathbb{E}H - H| \geq \epsilon \mathbb{E}H] \leq 2e^{-k\epsilon^2/8}$$

$$\Pr\left[\left| \|x\|_2^2 - \|\Pi x\|_2^2 \right| \geq \epsilon \|x\|_2^2 \right] \leq 2e^{-k\epsilon^2/8}$$

want $= \delta$

$$2e^{-k\epsilon^2/8} = \delta$$

$$-k\epsilon^2/8 = \log(\delta/2) \qquad k\epsilon^2/8 = \log(2/\delta)$$

$$k = \frac{\log(2/\delta)\cdot 8}{\epsilon^2} = O\left(\frac{\log 1/\delta}{\epsilon^2}\right)$$

Goal: Prove $\|\mathbf{\Pi x}\|_2^2$ concentrates within $1 \pm \epsilon$ of its expectation, which equals $\|\mathbf{x}\|_2^2$.

If high dimensional geometry is so different from low-dimensional geometry, why is dimensionality reduction possible?

Doesn't Johnson-Lindenstrauss tell us that high-dimensional geometry can be approximated in low dimensions?

nearly orthogonal 2^d

Hard case: $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ are all mutually orthogonal unit vectors:

$\langle x_i, x_j \rangle \leq \epsilon$

$$\|\mathbf{x}_i - \mathbf{x}_j\|_2^2 = 2 - 2\epsilon \qquad \text{for all } i, j.$$

When we reduce to k dimensions with JL, we still expect these vectors to be nearly orthogonal. Why?

$$\langle \Pi x_i, \Pi x_j \rangle = \frac{1}{2}\left(\|\Pi x_i\|_2^2 + \|\Pi x_j\|_2^2 - \|\Pi x_i - \Pi x_j\|_2^2 \right) \leq O(\epsilon).$$

($\|\Pi x_i\|_2^2 \approx 1$, $\|\Pi x_j\|_2^2 \approx 1$, $\|\Pi x_i - \Pi x_j\|_2^2 \approx \|x_i - x_j\|_2^2 = 2 - 2\epsilon$)

$$\|\Pi x_i - \Pi x_j\|_2^2 = \|\Pi x_i\|_2^2 + \|\Pi x_j\|_2^2 - 2\langle \Pi x_i, \Pi x_j \rangle$$

Hard case: $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ are all mutually orthogonal unit vectors:

$$\|\mathbf{x}_i - \mathbf{x}_j\|_2^2 = 2 \qquad\qquad \text{for all } i, j.$$

From our result last class, in $O(\log n/\epsilon^2)$ dimensions, there exists $2^{O(\epsilon^2 \cdot \log n/\epsilon^2)} \geq n$ unit vectors that are close to mutually orthogonal. $O(\log n/\epsilon^2)$ = just enough dimensions.

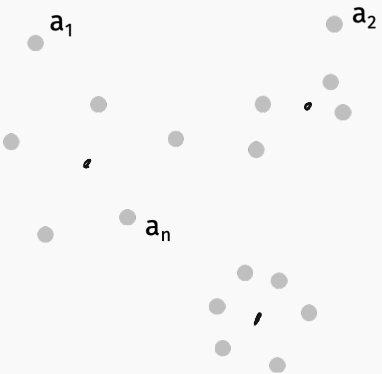
$2^{O(k \cdot \varepsilon^2)}$ = # of ε-nearly orthogonal unit vectors in k dimensional space.

$k = O(\log(n)/\varepsilon^2)$

$2^{O(\log(n))} \geq n$.

k-means clustering: Give data points $a_1, \ldots, a_n \in \mathbb{R}^d$, find centers $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k \in \mathbb{R}^d$ to minimize:

$$Cost(\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_k) = \sum_{i=1}^{n} \min_{j=1,\ldots,k} \|\boldsymbol{\mu}_j - a_i\|_2^2$$



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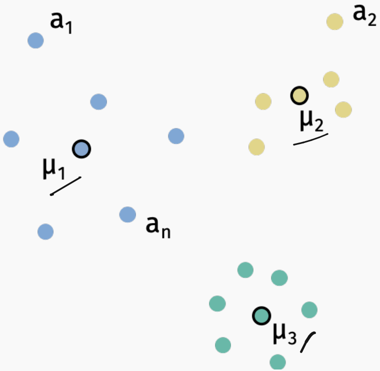

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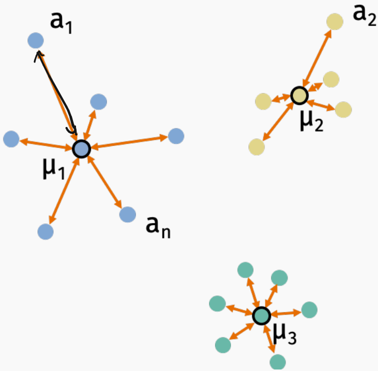
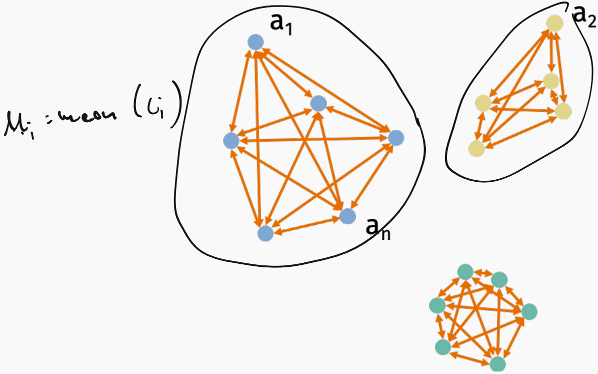


Equivalent form: Find clusters $C_1, \ldots, C_k \subseteq \{1, \ldots, n\}$ to minimize:

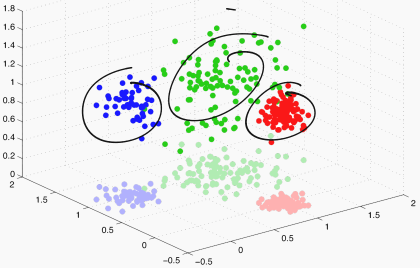
$$Cost(C_1, \ldots, C_k) = \sum_{j=1}^{k} \left(\frac{1}{2|C_j|}\right) \sum_{u,v \in C_j} \|\mathbf{a}_u - \mathbf{a}_v\|_2^2.$$



Exercise: Prove this to your self.

NP-hard to solve exactly, but there are many good approximation algorithms. All depend at least linearly on the dimension d.

Approximation scheme: Find clusters $\tilde{C}_1, \ldots, \tilde{C}_k$ for the $k = O\left(\frac{\log n}{\epsilon^2}\right)$ dimension data set $\mathbf{\Pi a}_1, \ldots, \mathbf{\Pi a}_n$.



Argue these clusters are near optimal for $\mathbf{a}_1, \ldots, \mathbf{a}_n$.

K-MEANS CLUSTERING

$$Cost(C_1, \ldots, C_k) = \sum_{j=1}^{k} \frac{1}{2|C_j|} \sum_{u,v \in C_j} \|\mathbf{a}_u - \mathbf{a}_v\|_2^2$$

$$\widetilde{Cost}(C_1, \ldots, C_k) = \sum_{j=1}^{k} \frac{1}{2|C_j|} \sum_{u,v \in C_j} \|\Pi\mathbf{a}_u - \Pi\mathbf{a}_v\|_2^2$$

Claim: For any clusters $C_1, \ldots, C_k$:

$$(1-\epsilon)Cost(C_1, \ldots, C_k) \leq \widetilde{Cost}(C_1, \ldots, C_k) \leq (1+\epsilon)Cost(C_1, \ldots, C_k)$$

$\frac{1}{1-\epsilon}$

$\sum_{j=1}^{k} \frac{1}{2|C_j|} \sum_{u,v \in C_j} \|\Pi a_u - \Pi a_v\|_2^2 \leq (1+\epsilon) \sum \sum \|a_u - a_v\|_2^2$

$\leq (1+\epsilon) \|a_u - a_v\|_2^2$

Suppose we use an approximation algorithm to find clusters $B_1, \ldots, B_k$ such that:

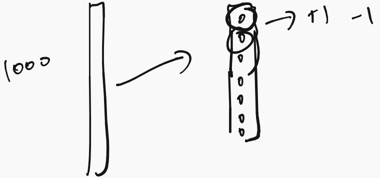
$$\widetilde{Cost}(B_1, \ldots, B_k) \leq (1+\alpha)\widetilde{Cost}^*$$

Then:

$$\begin{aligned} Cost(B_1, \ldots, B_k) &\leq \frac{1}{1-\epsilon}\widetilde{Cost}(B_1, \ldots, B_k) \\ &\leq (1+O(\epsilon))(1+\alpha)\widetilde{Cost}^* \\ &\leq (1+O(\epsilon))(1+\alpha)(1+\epsilon)Cost^* \\ &= (1+O(\alpha+\epsilon))\, Cost^* \end{aligned}$$

$Cost^* = \min_{C_1,\ldots,C_k} Cost(C_1, \ldots, C_k)$ and
$\widetilde{Cost}^* = \min_{C_1,\ldots,C_k} \widetilde{Cost}(C_1, \ldots, C_k)$

DIMENSIONALITY REDUCTION



Product Quantization

The Johnson-Lindenstrauss Lemma let us sketch vectors and preserve their ℓ_2 **Euclidean distance.**

We also have dimensionality reduction techniques that preserve alternative measures of similarity.

q = [0 0 1 0 0 0 1]

y = [1 1 1 0 0 0 0]

1/4

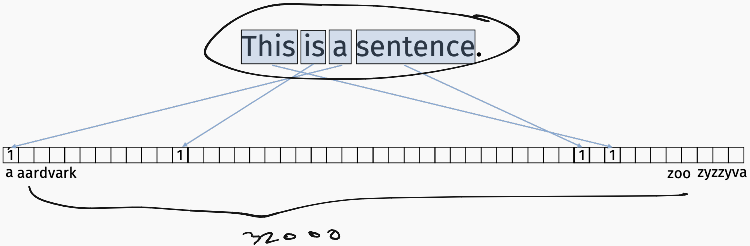
Often vector embeddings used in semantic search are binary.
For such vectors, Jaccard similarity is often used instead of Euclidean distance or inner product to compute similarity.

Definition (Jaccard Similarity)

$$J(\mathbf{q}, \mathbf{y}) = \frac{|\mathbf{q} \cap \mathbf{y}|}{|\mathbf{q} \cup \mathbf{y}|} = \frac{\text{\# of non-zero entries in common}}{\text{total \# of non-zero entries}}$$

Natural similarity measure for binary vectors. $0 \leq J(\mathbf{q}, \mathbf{y}) \leq 1$.

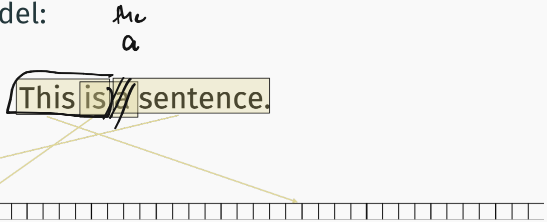
"Bag-of-words" model:



How many words do a pair of documents have in common?

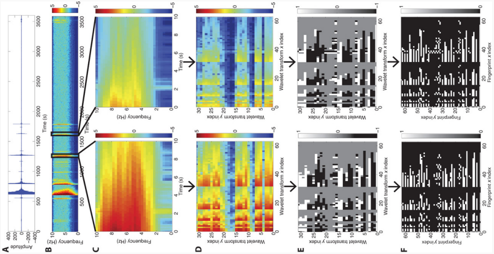
SPLADE

"Bag-of-words" model:



How many bigrams do a pair of documents have in common?

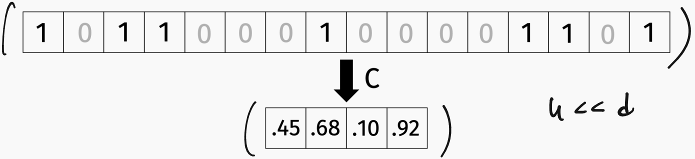
- Finding duplicate or new duplicate documents or webpages.
- Change detection for high-speed web caches.
- Finding near-duplicate emails or customer reviews which could indicate spam.



Feature extract pipeline for earthquake data.

(see paper by Rong et al. posted on course website)

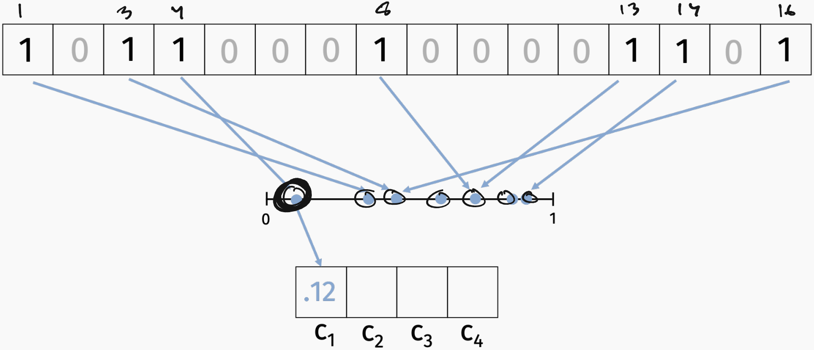
Goal: Design a compact sketch $C : \{0, 1\}^d \rightarrow \mathbb{R}^k$:



Want to use $C(\mathbf{q}), C(\mathbf{y})$ to approximately compute the Jaccard similarity $J(\mathbf{q}, \mathbf{y}) = \frac{|\mathbf{q} \cap \mathbf{y}|}{|\mathbf{q} \cup \mathbf{y}|}$.

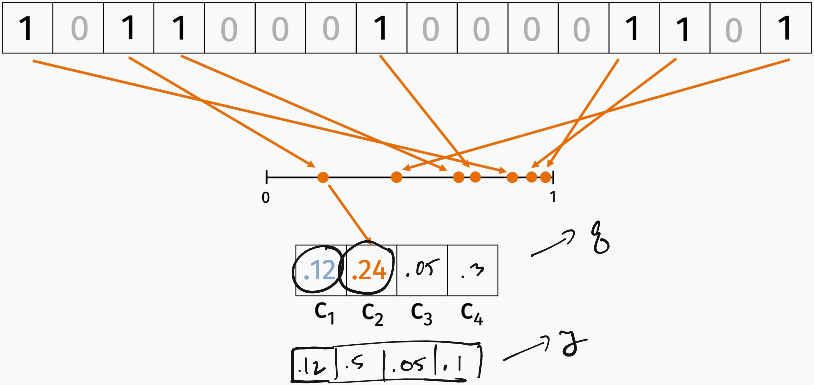
MinHash (Broder, '97): → sketch dimension

- Choose k random hash functions $h_1, \ldots, h_k : \{1, \ldots, d\} \to [0, 1]$.
- For $i \in 1, \ldots, k$,
  - Let $c_i = \min_{j, \mathbf{q}_j = 1} h_i(j)$.
- $C(\mathbf{q}) = [c_1, \ldots, c_k]$.



MINHASH

- Choose k random hash functions $h_1, \ldots, h_k : \{1, \ldots, n\} \to [0, 1]$.
- For $i \in 1, \ldots, k$,
  - Let $c_i = \min_{j, \mathbf{q}_j = 1} h_i(j)$.
- $C(\mathbf{q}) = [c_1, \ldots, c_k]$.



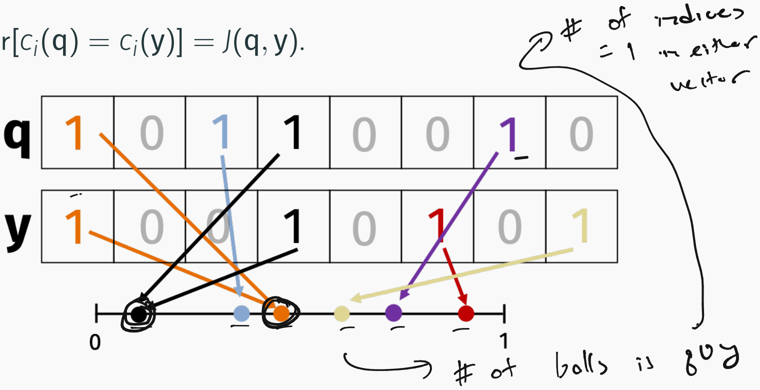
Claim: For all i, $\Pr[c_i(\mathbf{q}) = c_i(\mathbf{y})] = J(\mathbf{q}, \mathbf{y}) = \frac{|\mathbf{q} \cap \mathbf{y}|}{|\mathbf{q} \cup \mathbf{y}|}$.

q	1	0	1	1	0	0	1	0
y	1	0	0	1	0	1	0	1

Proof:

1. For $c_i(\mathbf{q}) = c_i(\mathbf{y})$, we need that $\arg\min_{i,\, q_i \neq 0} h(i) = \arg\min_{i,\, y_i \neq 0} h(i)$.

Claim: $\Pr[c_i(\mathbf{q}) = c_i(\mathbf{y})] = J(\mathbf{q}, \mathbf{y})$.



2. Every non-zero index in $\mathbf{q} \cup \mathbf{y}$ is equally likely to produce the lowest hash value. $c_i(\mathbf{q}) = c_i(\mathbf{y})$ only if this index is 1 in both $\mathbf{q}$ and $\mathbf{y}$. There are $\mathbf{q} \cap \mathbf{y}$ such indices. So:

$$\Pr[c_i(\mathbf{q}) = c_i(\mathbf{y})] = \frac{|\mathbf{q} \cap \mathbf{y}|}{|\mathbf{q} \cup \mathbf{y}|} = J(\mathbf{q}, \mathbf{y})$$

approx similarity.

Let $J = J(\mathbf{q}, \mathbf{y})$ denote the Jaccard similarity between **q** and **y**.

Return: $\tilde{J} = \frac{1}{k}\sum_{i=1}^{k} \mathbb{1}[c_i(\mathbf{q}) = c_i(\mathbf{y})]$.

Unbiased estimate for Jaccard similarity:

$$\mathbb{E}\tilde{J} = \frac{1}{k}\sum_{i=1}^{k} \mathbb{E}\left[\mathbb{1}(c_i(q) = c_i(y))\right] = \frac{1}{k}\cdot k \cdot J(q,y)$$

$$= J(q,y).$$

C(q)	.12	.24	.76	.35

C(y)	.12	.98	.76	.11

$\tilde{J} = 1/2$

The more repetitions, the lower the variance.

Let $J = J(\mathbf{q}, \mathbf{y})$ denote the true Jaccard similarity. $\to J$ $\quad J - J^2$

Estimator: $\tilde{J} = \frac{1}{k}\sum_{i=1}^{k} \mathbb{1}[c_i(\mathbf{q}) = c_i(\mathbf{y})]$.

$$\mathrm{Var}[\tilde{J}] = \frac{1}{k^2}\sum_{i=1}^{k} \mathrm{Var}\left(\mathbb{1}[c_i(q) = c_i(y)]\right) = \frac{1}{k^2}\sum_{i=1}^{k} J - J^2$$

$$\leq 1/k.$$

Plug into Chebyshev inequality. How large does k need to be so that with probability $> 1-\delta$, $|J - \tilde{J}| \leq \epsilon$?

$$k = O\left(\frac{\log(1/\delta)}{\epsilon}\right)$$

$$\Pr[|J - \tilde{J}| \geq \alpha\sigma] \leq 1/\alpha^2 = \delta \qquad \alpha = 1/\sqrt{\delta}$$

$$\Pr\left[|J - \tilde{J}| \geq \overbrace{\frac{1}{\sqrt{\delta}}\sigma}^{\epsilon}\right] \leq \delta \qquad \sigma = 1/\sqrt{k}$$

$$\frac{1}{\sqrt{\delta}\sqrt{k}} = \epsilon \qquad \sqrt{k} = \frac{1}{\sqrt{\delta}\,\epsilon}$$

$$\boxed{k = \frac{1}{\epsilon^2\delta}}$$

Chebyshev inequality: As long as $k = O\left(\frac{1}{\epsilon^2 \delta}\right)$, then with prob. $1 - \delta$,

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

And $\tilde{J}$ only takes $O(k)$ time to compute! Independent of original vector dimension, d.

Can be improved to $\log(1/\delta)$ dependence?

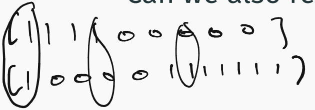
VECTOR SEARCH / NEAR NEIGHBOR SEARCH

Goal: Find all vectors in database $\mathbf{q}_1, \ldots, \mathbf{q}_n \in \mathbb{R}^d$ that are close to some input query vector $\mathbf{y} \in \mathbb{R}^d$. I.e. find all of $\mathbf{y}$'s "nearest neighbors" in the database.

How does similarity sketching help in these applications?

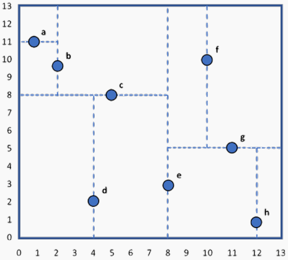
- Improves runtime of "linear scan" from $O(nd)$ to $O(nk)$.
- Improves space complexity from $O(nd)$ to $O(nk)$. This can be super important – e.g. if it means the linear scan only accesses vectors in fast memory.

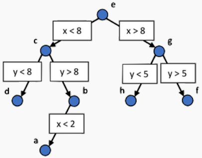
Can we also reduce the dependence on n?

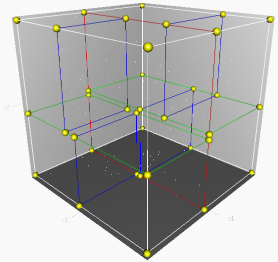


Goal: Sublinear $o(n)$ time to find near neighbors.

This problem can already be solved in low-dimensions using space partitioning approaches (e.g. kd-tree).

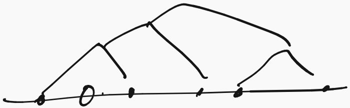






Runtime is roughly ~~$O(d \cdot \min(n, 2^d))$~~ $\cdot \log(n)$, which is only sublinear for $d = o(\log n)$.

$O(\log(n) \cdot 2^d)$



$O(\log(n))$ time

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]

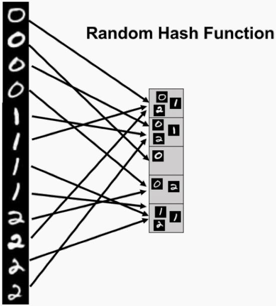
Key ideas behind all of these methods:

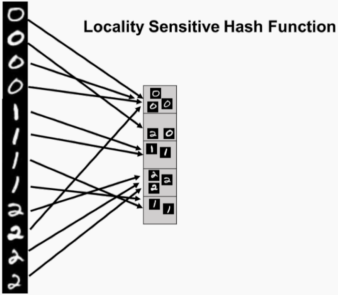
1. Trade worse space-complexity + preprocessing time for better time-complexity. I.e., preprocess database in data structure that uses $\Omega(n)$ space.
2. Allow for approximation.

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:

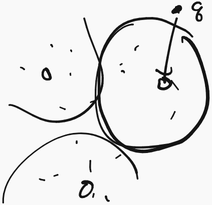
- Higher when $\mathbf{q}$ and $\mathbf{y}$ are more similar, i.e. $s(\mathbf{q}, \mathbf{y})$ is higher.
- Lower when $\mathbf{q}$ and $\mathbf{y}$ are more dissimilar, i.e. $s(\mathbf{q}, \mathbf{y})$ is lower.

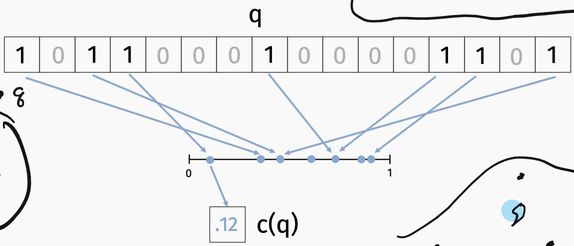


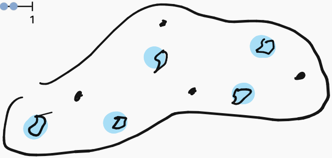


LSH for $s(\mathbf{q}, \mathbf{y})$ equal to Jaccard similarity:

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







LSH for Jaccard similarity:

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

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

$$\Pr\left[h(\mathbf{q}) == h(\mathbf{y})\right] =$$

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

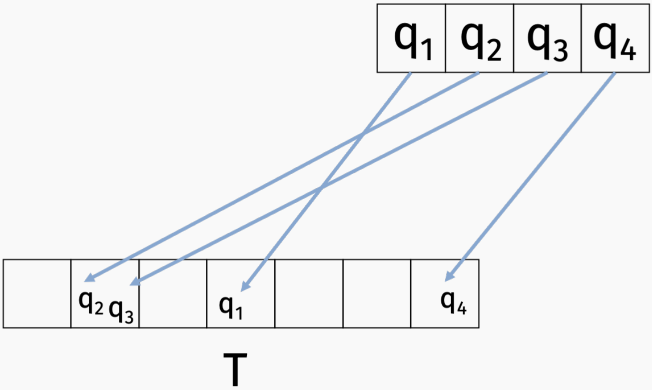
Pre-processing:

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


q1
q2
q3
q4
q2 q3
q1
q4
T

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 $\mathbf{y}$?

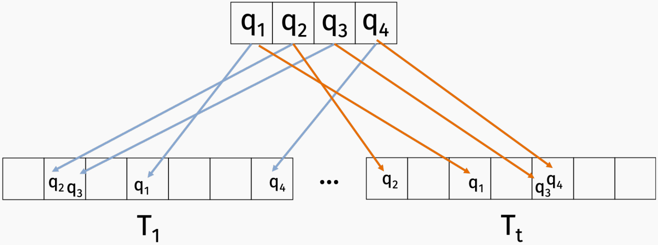
A higher false negative rate means we miss near neighbors.

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 $< .2$.

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?



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 $T_j(h_j(\mathbf{q}_i))$.

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?

(10, 99%)

WHAT HAPPENS TO FALSE POSITIVES?

Suppose there is some other database point **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 **y** hashes into at least one bucket containing **z**.

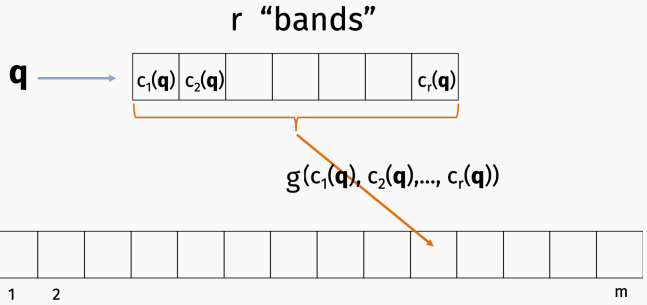
In the new scheme with $t = 10$ tables?

(89%)

Change our locality sensitive hash function.

Tunable LSH for Jaccard similarity:

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

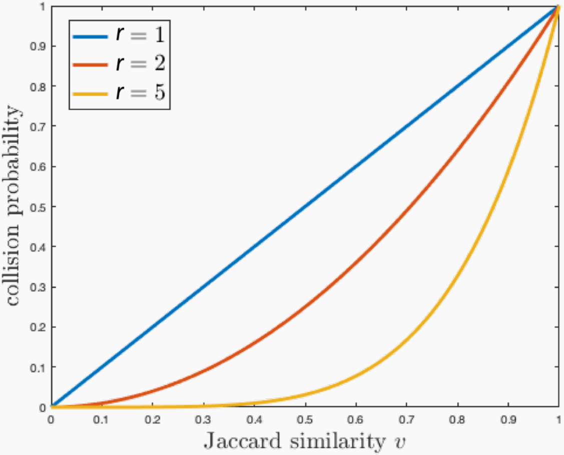


Tunable LSH for Jaccard similarity:

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

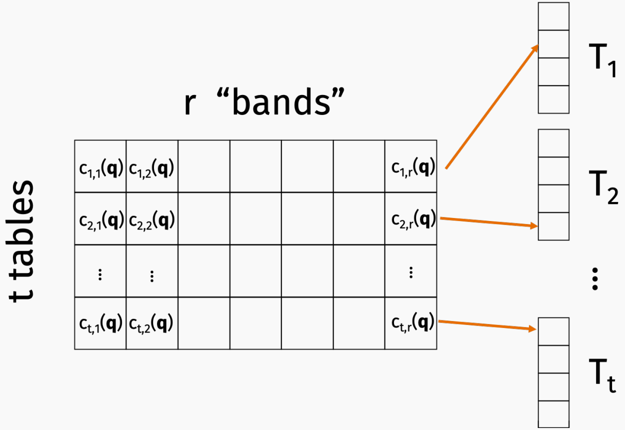
If $J(\mathbf{q}, \mathbf{y}) = v$, then $\Pr[h(\mathbf{q}) == h(\mathbf{y})] =$

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:



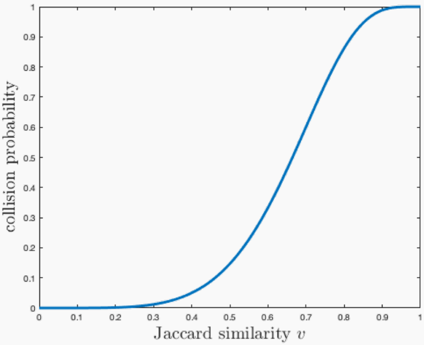
Effect of **increasing number of tables** t on:

False Negatives | False Positives

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

False Negatives | False Positives

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

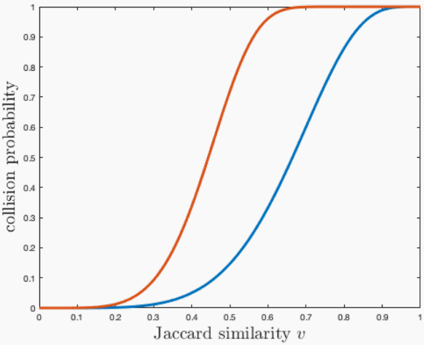


$r = 5, t = 5$

s-curve tuning

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

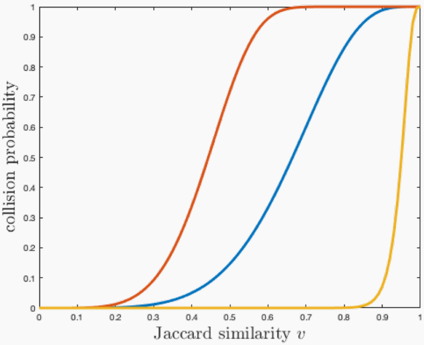
$$\approx 1 - (1 - v^r)^t$$



$r = 5, t = 40$

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

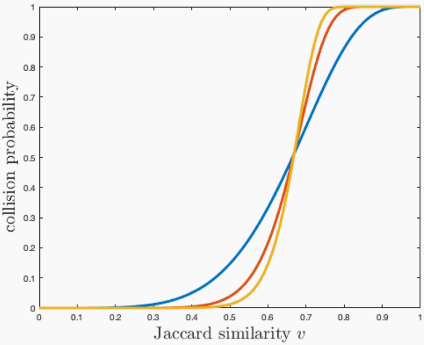
$$\approx 1 - (1 - v^r)^t$$



$$r = 40, t = 5$$

Probability we check **q** when querying **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.

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:

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

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

Directly trade space for fast search.

Near Neighbor Search Problem

Concrete worst case result:

Theorem (Indyk, Motwani, 1998)

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

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

Theorem (Indyk, Motwani, 1998)

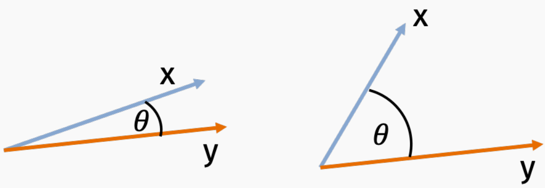
Let q be the closest database vector to $\mathbf{y}$*. Return a vector* $\tilde{\mathbf{q}}$ *with* $\|\tilde{\mathbf{q}} - \mathbf{y}\|_0 \leq C \cdot \|\mathbf{q} - \mathbf{y}\|_0$ *in:*

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

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



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

Cosine similarity is natural "inverse" for Euclidean distance.

Euclidean distance $\|\mathbf{x}-\mathbf{y}\|_2^2$:

- Suppose for simplicity that $\|\mathbf{x}\|_2^2 = \|\mathbf{y}\|_2^2 = 1$.

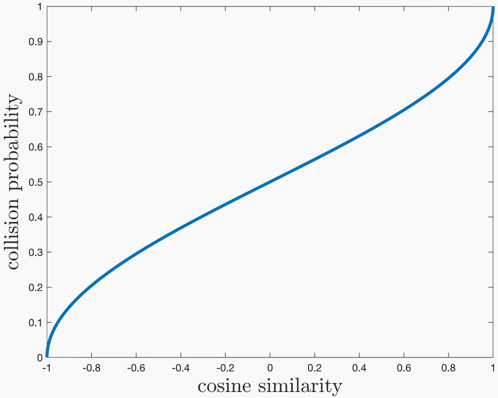
Locality sensitive hash for **cosine similarity**:

- Let $\mathbf{g} \in \mathbb{R}^d$ be randomly chosen with each entry $\mathcal{N}(0, 1)$.
- Let $f : \{-1, 1\} \rightarrow \{1, \ldots, m\}$ be a uniformly random hash function.
- $h : \mathbb{R}^d \rightarrow \{1, \ldots, m\}$ 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

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

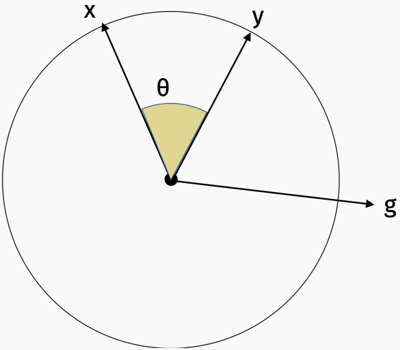


SimHash can be banded, just like our MinHash based LSH function for Jaccard similarity:

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

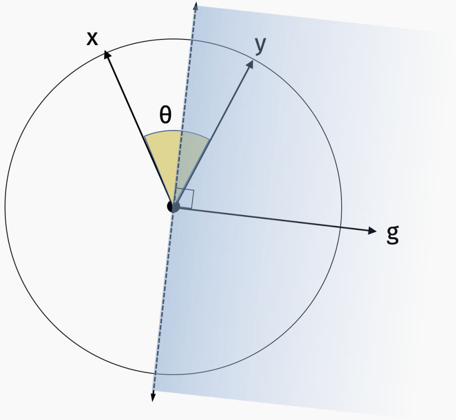
$$\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx \left(1 - \frac{\theta}{\Pi}\right)^r$$

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.

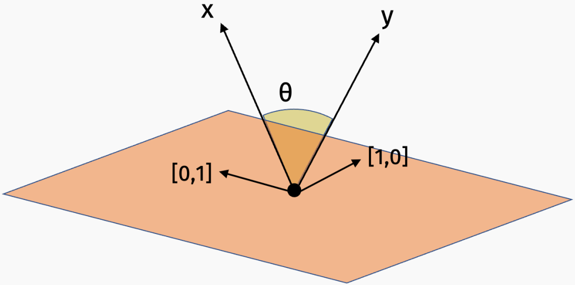


$$\Pr[h(\mathbf{x}) == h(\mathbf{y})] = z + \frac{1-z}{m} \approx z.$$

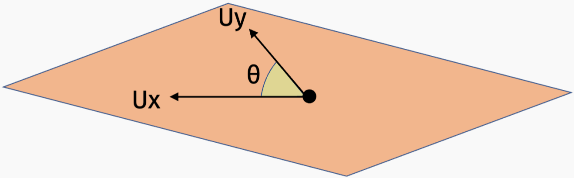
where $z = \Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)]$



$\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx$ probability **x** and **y** are on the same side of hyperplane orthogonal to **g**.



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



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:

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

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