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

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DIMENSIONALITY REDUCTION

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.**

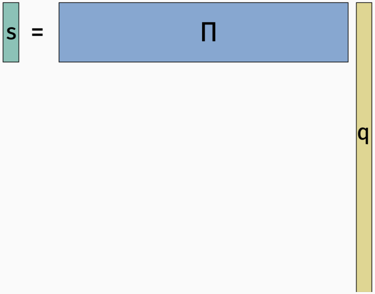
We will be very careful not to compress things <u>too</u> far. An extremely simple method known as Johnson-Lindenstrauss Random Projection pushes right up to the edge of how much compression is possible.

EUCLIDEAN DIMENSIONALITY REDUCTION

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,

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



EUCLIDEAN DIMENSIONALITY REDUCTION

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 $(1-\epsilon)^2 = 1 - O(\epsilon)$.

TONS OF APPLICATIONS

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.

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

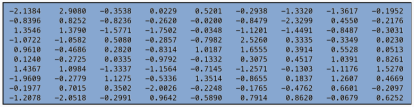
The map $\mathbf{\Pi}$ is **oblivious to the data set**. This stands in contrast to other vector compression methods you might know like PCA.

[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.

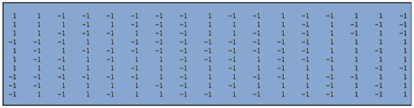
Let $\mathbf{\Pi} \in \mathbb{R}^{k\times d}$ be chosen so that each entry equals $\frac{1}{\sqrt{k}}\mathcal{N}(0,1)$.

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



```
-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;
```



```
 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   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
```

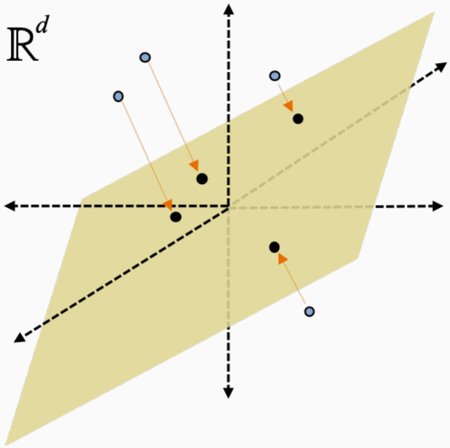
```
>> Pi = 2*randi(2,m,d)-3;
>> s = (1/sqrt(m))*Pi*q;
```

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.

RANDOM PROECTION

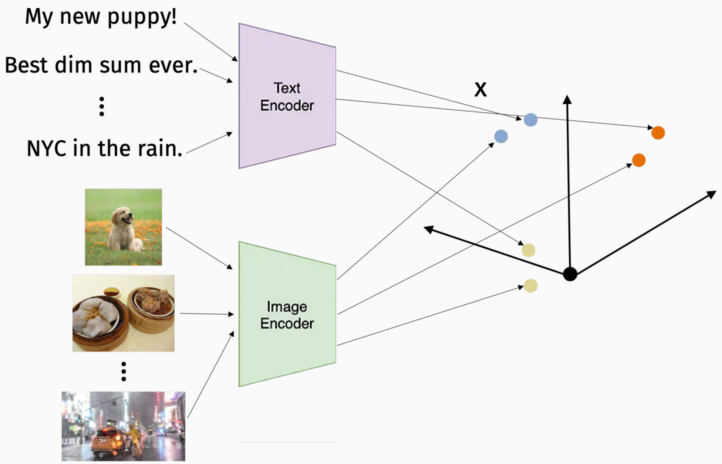
Can anyone see why $\mathbf{\Pi}$ is similar to a projection matrix? I.e., a matrix satisfying $\mathbf{Q}\mathbf{Q}^T = \mathbf{I}_{k\times k}$.

RANDOM PROJECTION



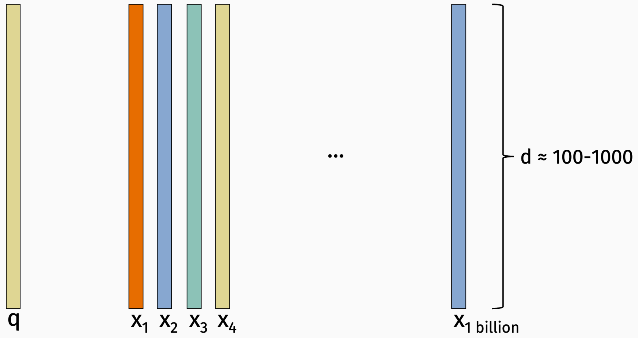
Intuition: Multiplying by a random matrix mimics the process of projecting onto a random k dimensional subspace in d dimensions.

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.

APPLICATION: THE NEW PARADIGM FOR SEARCH



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!**

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.

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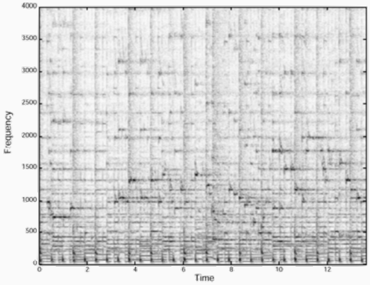
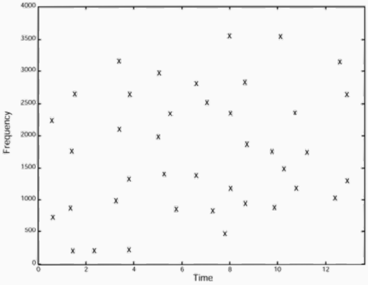
Shazam can match a song clip against a library of 8 million songs (32 TB of data) in a fraction of a second. Whole system based on vector embeddings + search.



Spectrogram extracted from audio clip.



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

VECTOR SEARCH

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

Weaviate qdrant

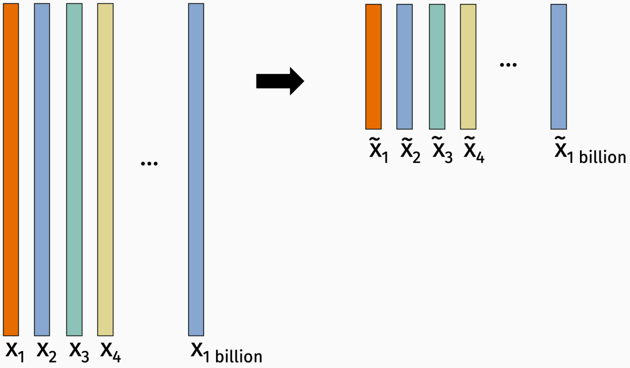
Pinecone zilliz

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 $\mathbf{x}_i$.



x_1 x_2 x_3 x_4 ... $x_{1\text{ billion}}$
$\tilde{x}_1$ $\tilde{x}_2$ $\tilde{x}_3$ $\tilde{x}_4$ ... $\tilde{x}_{1\text{ billion}}$

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* *<u>for all i, j</u>,*

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

EUCLIDEAN DIMENSIONALITY REDUCTION

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* <u>*any vector* $\mathbf{x}$</u>, *with probability* $(1-\delta)$:

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

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

JL FROM DISTRIBUTIONAL JL

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 $1 - \delta$,

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

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 <u>for all</u> i, j, as long as we compress to:

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

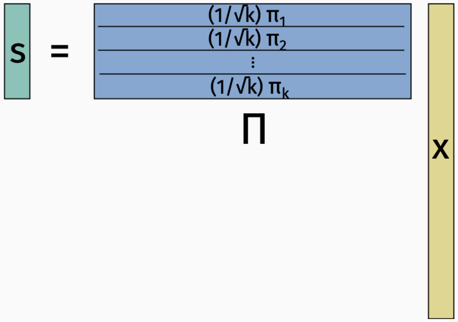
PROOF OF DISTRIBUTIONAL JL

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.

PROOF OF DISTRIBUTIONAL JL

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

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

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

PROOF OF DISTRIBUTIONAL JL

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

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.

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

STABLE RANDOM VARIABLES

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.

PROOF OF DISTRIBUTIONAL JL

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.

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

"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.

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

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

CONNECTION TO EARLIER PART OF LECTURE

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?

CONNECTION TO DIMENSIONALITY REDUCTION

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

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

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

CONNECTION TO DIMENSIONALITY REDUCTION

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

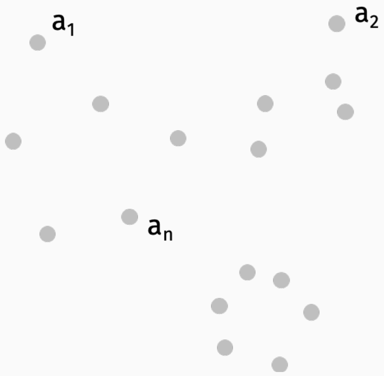
$$\|\mathbf{x}_i - \mathbf{x}_j\|_2^2 = 2 \qquad \text{for all } i, j.$$

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.

SECOND APPLICATION

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:

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



SAMPLE APPLICATION

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

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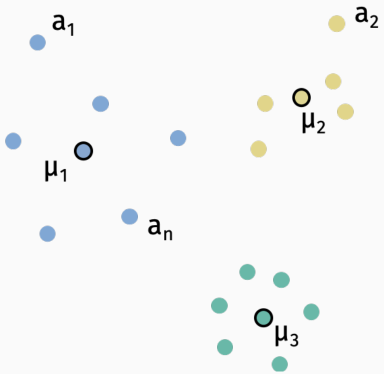

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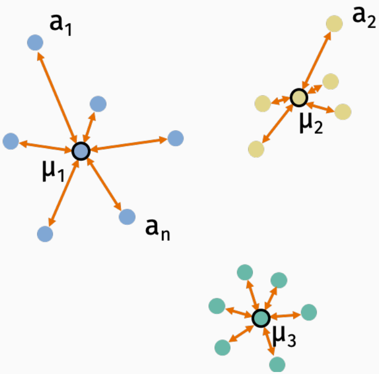
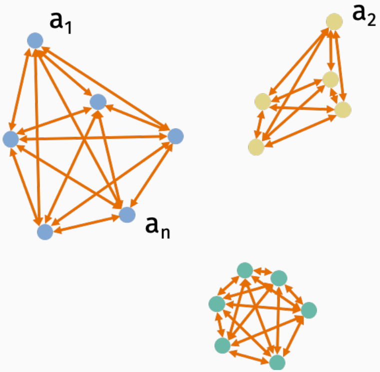


k-means clustering

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

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

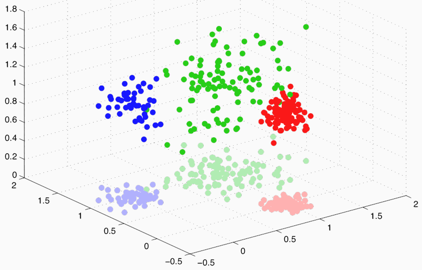


Exercise: Prove this to your self.

k-means clustering

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 $C_1,\ldots,C_k$:

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

K-MEANS CLUSTERING

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

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.

JACCARD SIMILARITY

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.

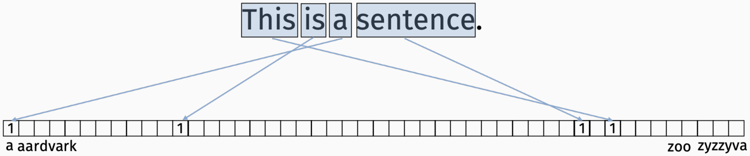
Definition (Jaccard Similarity)

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

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

JACCARD SIMILARITY FOR DOCUMENT COMPARISON

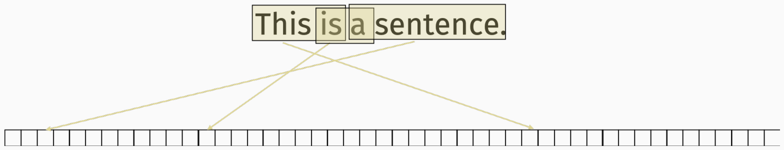
"Bag-of-words" model:



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

JACCARD SIMILARITY FOR DOCUMENT COMPARISON

“Bag-of-words” model:

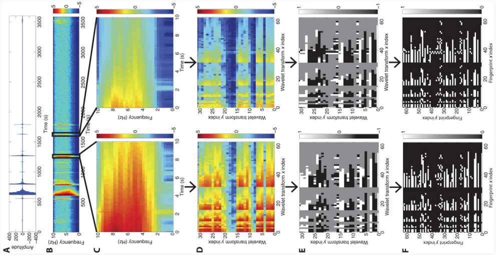


How many bigrams do a pair of documents have in common?

APPLICATIONS: DOCUMENT SIMILARITY

- 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.

JACCARD SIMILARITY FOR SEISMIC DATA

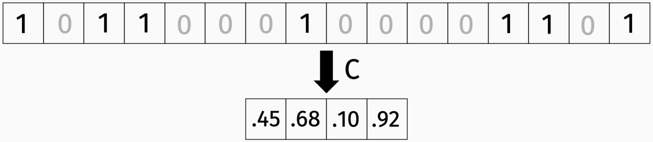


Feature extract pipeline for earthquake data.

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

SIMILARITY ESTIMATION

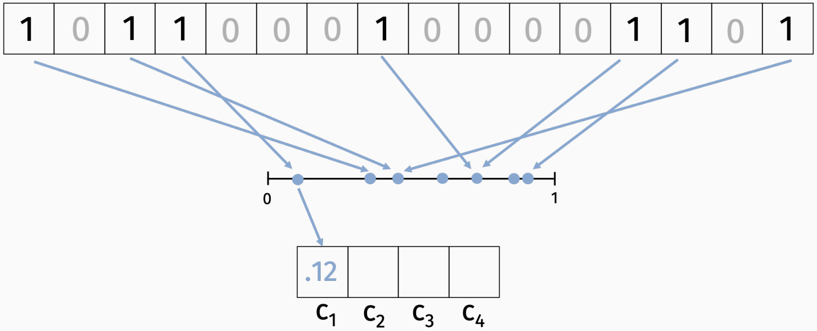
Goal: Design a compact sketch $C : \{0,1\} \to \mathbb{R}^k$:



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):

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



MINHASH

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- For $i \in 1, \ldots, k$,
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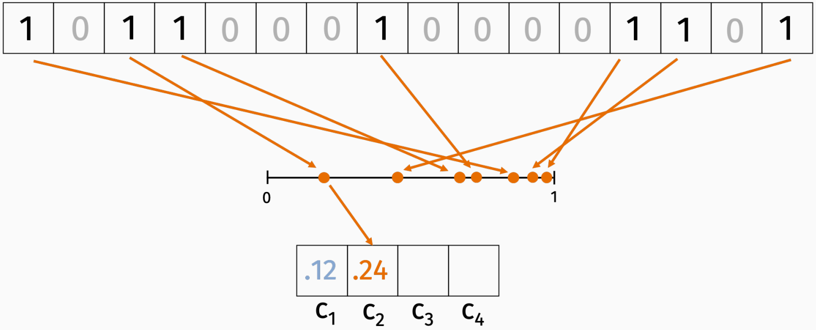
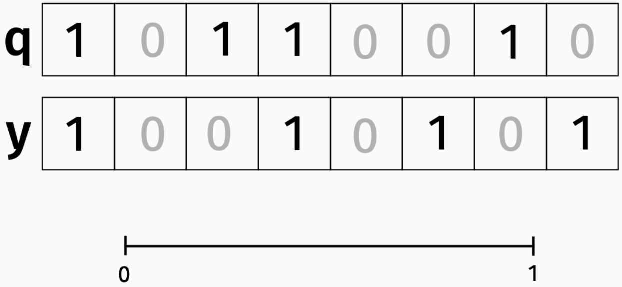
- $C(\mathbf{q}) = [c_1, \ldots, c_k]$.



MINHASH ANALYSIS

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

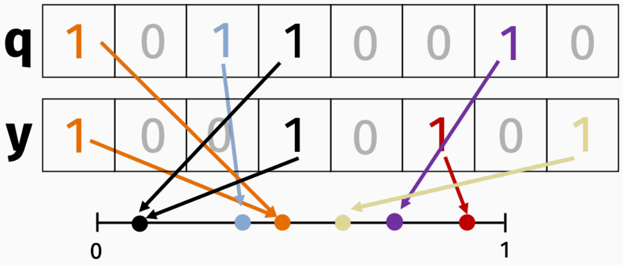


Proof:

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

MINHASH ANALYSIS

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:

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

MINHASH ANALYSIS

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:

$$\mathbb{E}\tilde{J} =$$

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

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

The more repetitions, the lower the variance.

MINHASH ANALYSIS

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

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

$$\mathrm{Var}[\tilde{J}] =$$

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

MINHASH ANALYSIS

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

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

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.

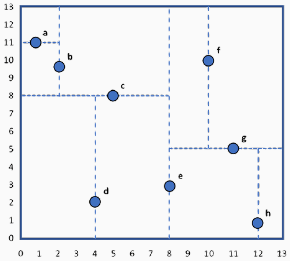
Can we also reduce the dependence on n?

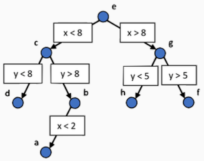
BEYOND A LINEAR SCAN

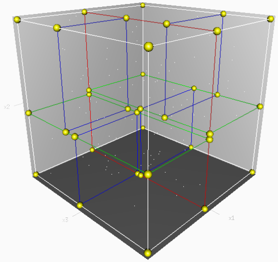
Goal: <u>Sublinear</u> $o(n)$ time to find near neighbors.

BEYOND A LINEAR SCAN

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







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

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:

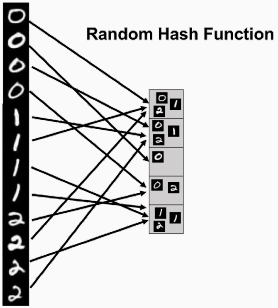
1. Trade worse space-complexity + preprocessing time for better time-complexity. I.e., preprocess database in data structure that uses $\Omega(n)$ space.
2. Allow for approximation.

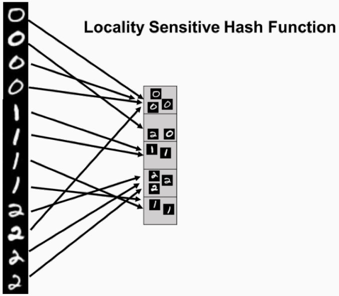
LOCALITY SENSITIVE HASH FUNCTIONS

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.

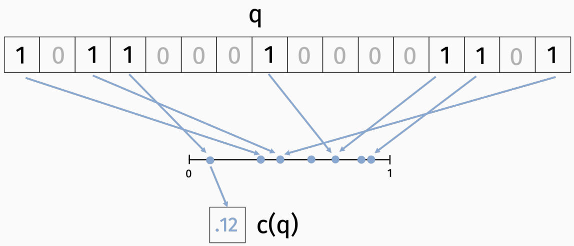




LOCALITY SENSITIVE HASH FUNCTIONS

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

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

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

NEAR NEIGHBOR SEARCH

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

Pre-processing:

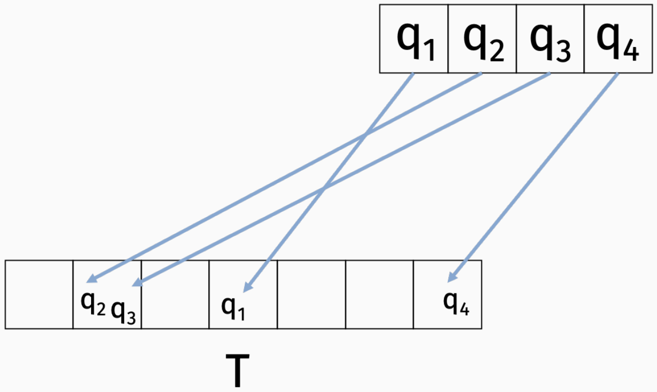
- Select random LSH function $h : \{0,1\}^d \to 1, \ldots, m$.
- Create table T with $m = O(n)$ slots.[1]
- For $i = 1, \ldots, n$, insert $\mathbf{q}_i$ into $T(h(\mathbf{q}_i))$.

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



NEAR NEIGHBOR SEARCH

Two main considerations:

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

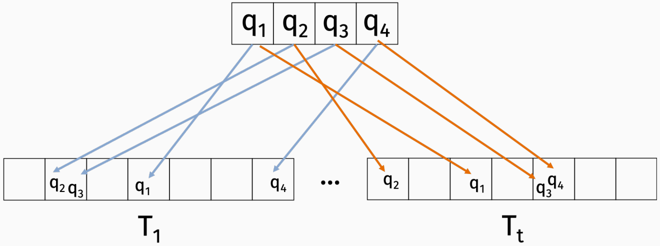
Note: The meaning of "close" and "not close" is application dependent. E.g. we might specify that we want to find anything with Jaccard similarity $> .4$, but not with Jaccard similarity $< .2$.

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?

REDUCING FALSE NEGATIVE RATE



Pre-processing:

- Select t independent LSH's $h_1, \ldots, h_t : \{0,1\}^d \rightarrow 1, \ldots, m$.
- 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?

(10, 99%)

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?

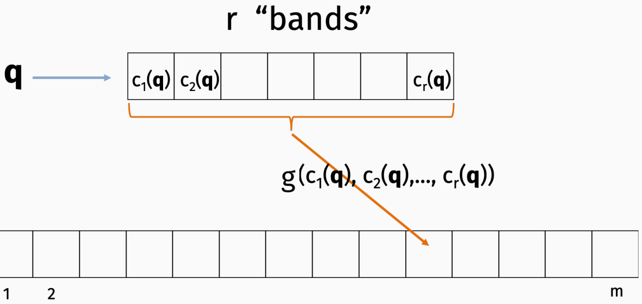
(89%)

REDUCING FALSE POSITIVES

Change our locality sensitive hash function.

Tunable LSH for Jaccard similarity:

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



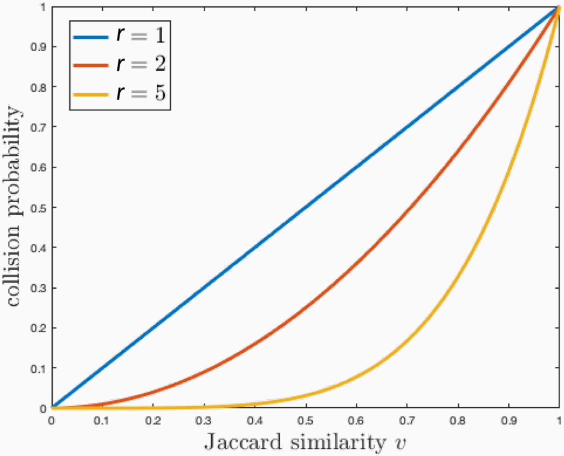
REDUCING FALSE POSITIVES

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

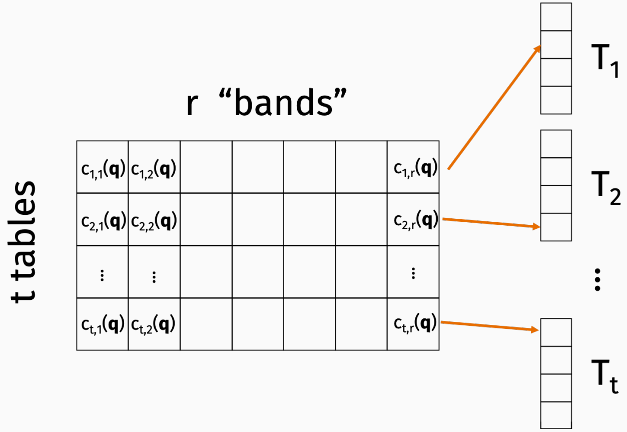
TUNABLE LSH



$r = 1$
$r = 2$
$r = 5$
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 cheme has two parameters to tune:



TUNABLE LSH

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

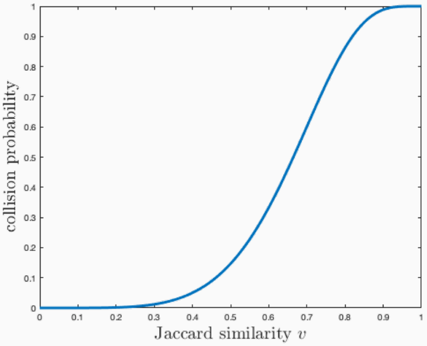
False Negatives False Positives

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

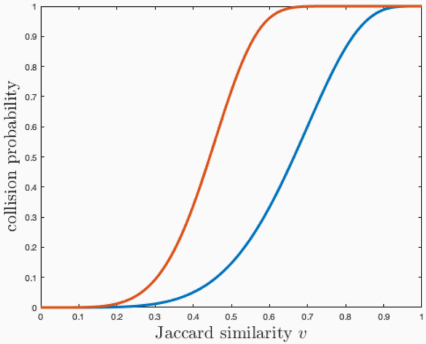


$r = 5, t = 5$

s-curve tuning

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

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

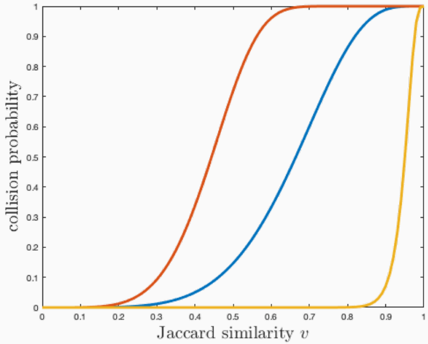


$$r = 5, t = 40$$

s-CURVE TUNING

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

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

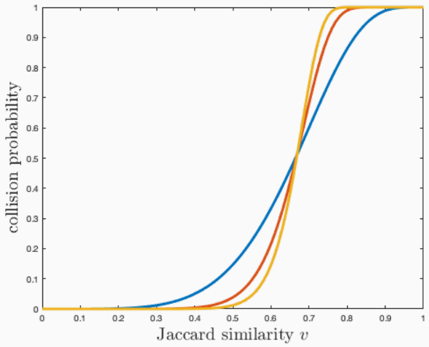


$$r = 40, t = 5$$

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 <u>true matches</u> with $J(\mathbf{y}, \mathbf{q}) > .9$.
- There are 10,000 <u>near matches</u> 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 $\approx 40 \cdot O(n)$.

Directly trade space for fast search.

WORSE CASE GUARANTEES

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 $\mathbf{y}$.

APPROXIMATE NEAREST NEIGHBOR SEARCH

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:

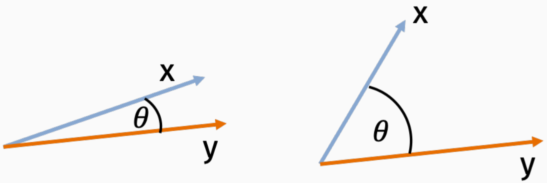
- *Time: $\tilde{O}\left(n^{1/C}\right)$.*
- *Space: $\tilde{O}\left(n^{1+1/C}\right)$.*

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

OTHER LSH FUNCTIONS

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.

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

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

SIMHASH

Locality sensitive hash for **cosine similarity**:

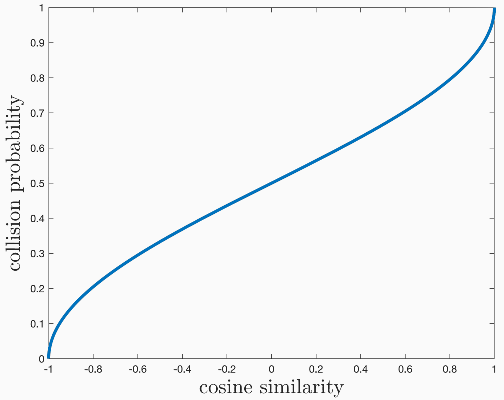
- Let $\mathbf{g} \in \mathbb{R}^d$ be randomly chosen with each entry $\mathcal{N}(0,1)$.
- Let $f : \{-1,1\} \to \{1,\ldots,m\}$ be a uniformly random hash function.
- $h : \mathbb{R}^d \to \{1,\ldots,m\}$ is definied $h(\mathbf{x}) = f(\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle))$.

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

SIMHASH ANALYSIS IN 2D

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

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



SIMHASH

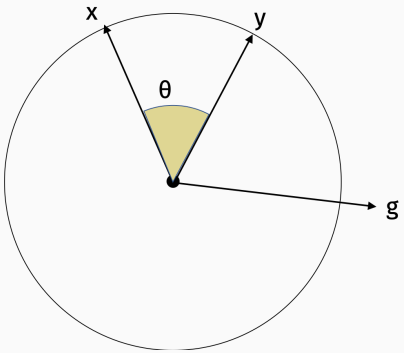
SimHash can be banded, just like our MinHash based LSH function for Jaccard similarity:

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

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

SIMHASH ANALYSIS IN 2D

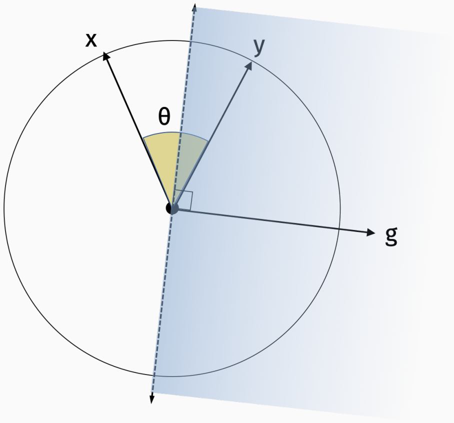
To prove: $\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx 1 - \frac{\theta}{\pi}$, where $h(\mathbf{x}) = f(\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle))$ and f is uniformly random hash function.



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

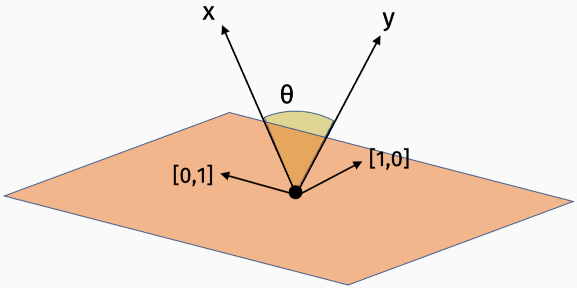
where $z = \Pr[\text{sign}(\langle \mathbf{g}, \mathbf{x} \rangle) == \text{sign}(\langle \mathbf{g}, \mathbf{y} \rangle)]$

SIMHASH ANALYSIS 2D



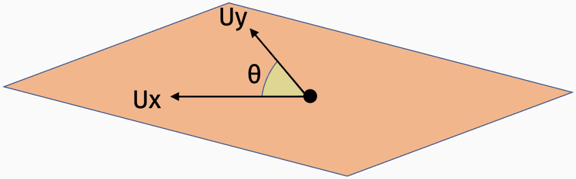
$\Pr[h(\mathbf{x}) == h(\mathbf{y})] \approx$ probability $\mathbf{x}$ and $\mathbf{y}$ are on the same side of hyperplane orthogonal to $\mathbf{g}$.

SIMHASH ANALYSIS HIGHER DIMENSIONS



There is always some rotation matrix $\mathbf{U}$ 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 $\mathbf{y}$.

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: 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 $\mathbf{U}$.

SIMHASH ANALYSIS HIGHER DIMENSIONS

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?