

COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2021.

Lecture 11

LOGISTICS

- Problem Set 2 is due next Friday 10/15.
- Midterm is in class on Tuesday, 10/19.
- I have posted a study guide and practice questions on the course schedule.
- This week's quiz due Tues. 8pm.

Last Class:

- Introduced the k -frequent elements problem – identify all elements of a stream of n elements that occur $\geq n/k$ times.
- Saw how to solve approximately in $O(k \log n / \epsilon)$ space using the Count-min sketch algorithm.
- Simple analysis based on Markov's inequality and repeated random hashing.

This Class:

- Randomized methods for dimensionality reduction.
- The Johnson-Lindenstrauss Lemma.

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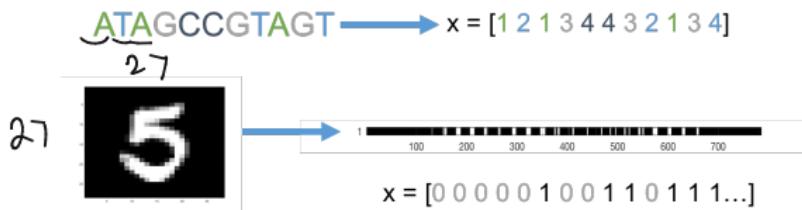
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- The human genome contains 3 billion+ base pairs. Genetic datasets often contain information on **100s of thousands+** mutations and genetic markers.

DATA AS VECTORS AND MATRICES

In data analysis and machine learning, data points with many attributes are often stored, processed, and interpreted as **high dimensional vectors**, with real valued entries.

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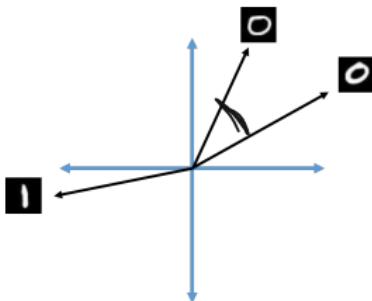
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ATAGCCGTAGT → $x = [1 \ 2 \ 1 \ 3 \ 4 \ 4 \ 3 \ 2 \ 1 \ 3 \ 4]$



Similarities/distances between vectors (e.g., $\langle x, y \rangle$, $\|x - y\|_2$) have meaning for underlying data points.

DATASETS AS VECTORS AND MATRICES

Data points are interpreted as **high dimensional vectors**, with real valued entries. Data set is interpreted as a matrix.

Data Points: $\vec{x}_1, \vec{x}_2, \dots, \vec{x}_n \in \mathbb{R}^d$.

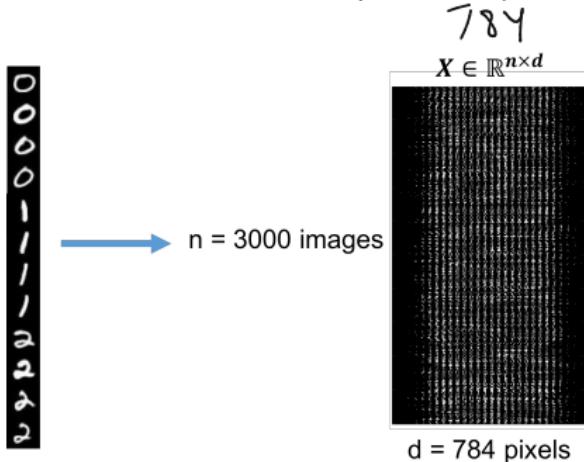
Data Set: $X \in \mathbb{R}^{n \times d}$ with i^{th} row equal to \vec{x}_i .

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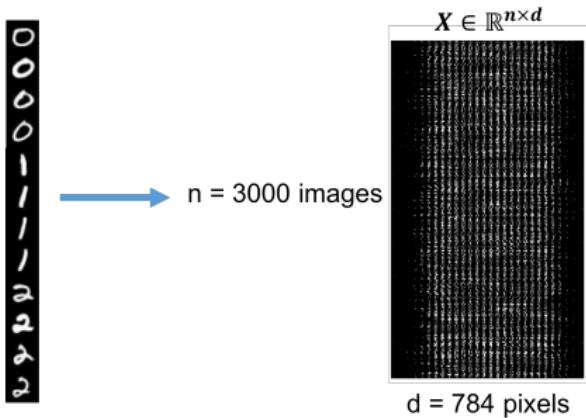


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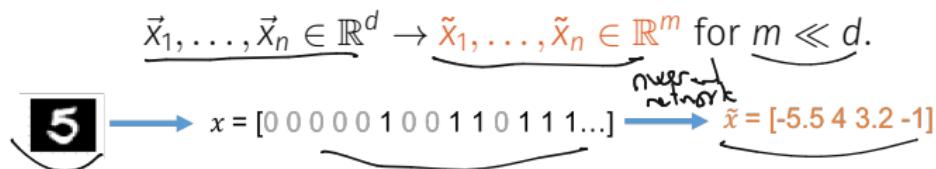
Many data points $n \implies$ tall. Many dimensions $d \implies$ wide.

DIMENSIONALITY REDUCTION

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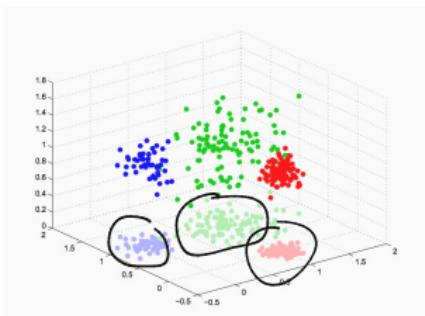
$$\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d \rightarrow \tilde{\vec{x}}_1, \dots, \tilde{\vec{x}}_n \in \mathbb{R}^m \text{ for } m \ll d.$$

5 → $x = [0\ 0\ 0\ 0\ 0\ 1\ 0\ 0\ 1\ 1\ 0\ 1\ 1\ 1\dots] \rightarrow \tilde{x} = [-5.5\ 4\ 3.2\ -1]$

'Lossy compression' that still preserves important information about the relationships between $\vec{x}_1, \dots, \vec{x}_n$.

$$d=3$$

$$m=2$$



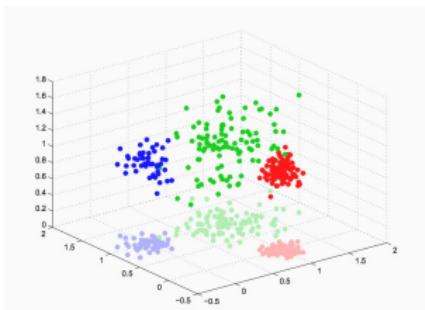
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Generally will not consider directly how well $\tilde{\vec{x}}_i$ approximates \vec{x}_i .

DIMENSIONALITY REDUCTION

Dimensionality reduction is one of the most important techniques in data science. **What methods have you heard of?**

SVD - principal component analysis

linear discriminant analysis

LSI

TSNE

multi dimensional
scaling.

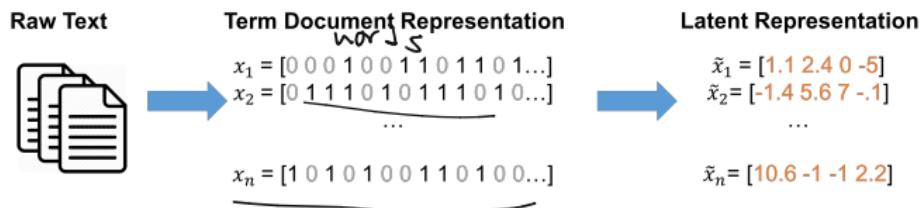
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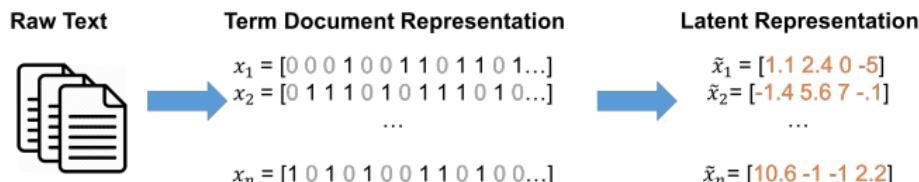


- Linear discriminant analysis
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- Linear discriminant analysis
- Autoencoders

Compressing data makes it more efficient to work with. May also remove extraneous information/noise.

EMBEDDINGS FOR EUCLIDEAN SPACE

Euclidean Low Distortion Embedding: Given $\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$ and error parameter $\epsilon \geq 0$, find $\tilde{x}_1, \dots, \tilde{x}_n \in \mathbb{R}^m$ (where $m \ll d$) such that for all $i, j \in [n]$:

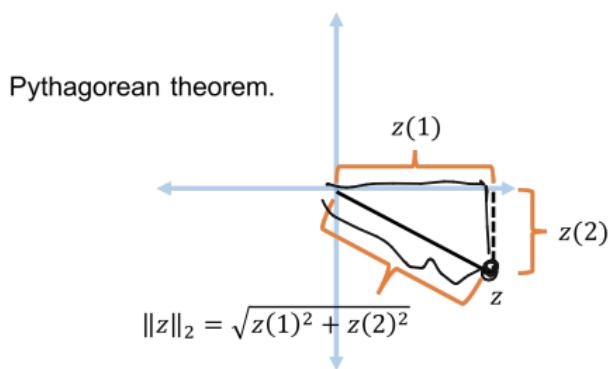
$$(1 - \epsilon) \underbrace{\|\vec{x}_i - \vec{x}_j\|_2}_{\leq} \leq \underbrace{\|\tilde{x}_i - \tilde{x}_j\|_2} \leq (1 + \epsilon) \|\vec{x}_i - \vec{x}_j\|_2.$$

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$$(1 - \epsilon) \underbrace{\|\vec{x}_i - \vec{x}_j\|_2}_{\text{Euclidean distance}} \leq \|\tilde{x}_i - \tilde{x}_j\|_2 \leq (1 + \epsilon) \|\vec{x}_i - \vec{x}_j\|_2.$$

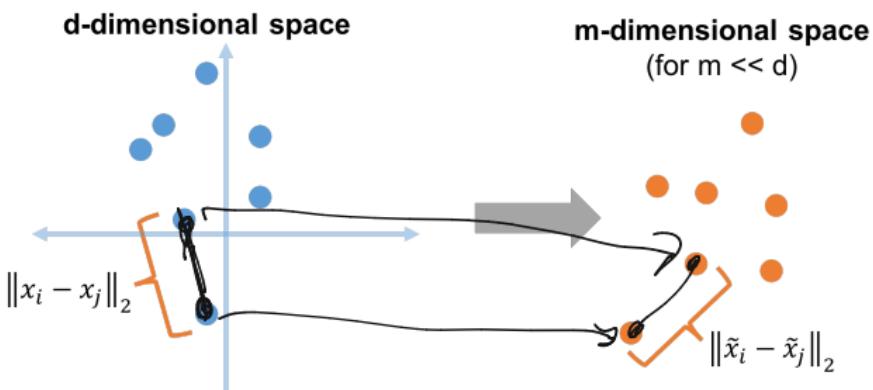
Recall that for $\vec{z} \in \mathbb{R}^n$, $\|\vec{z}\|_2 = \sqrt{\sum_{i=1}^n z(i)^2}$.



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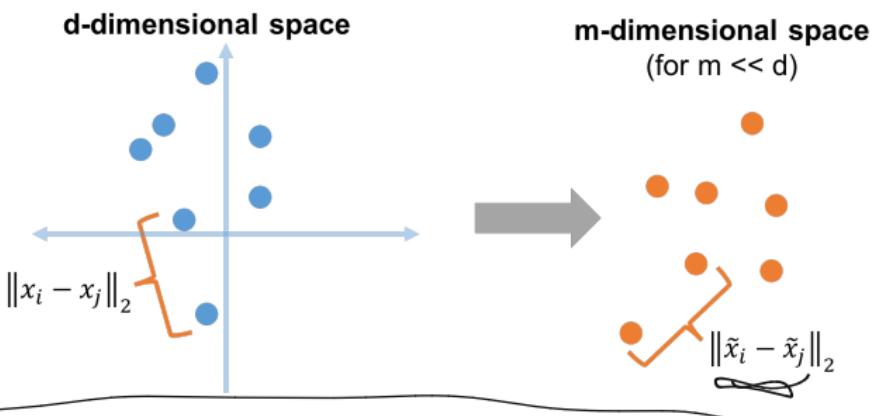
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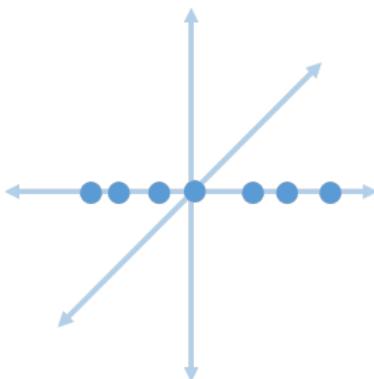


Can use $\tilde{x}_1, \dots, \tilde{x}_n$ in place of $\vec{x}_1, \dots, \vec{x}_n$ in clustering, SVM, linear classification, near neighbor search, etc.

EMBEDDING WITH ASSUMPTIONS

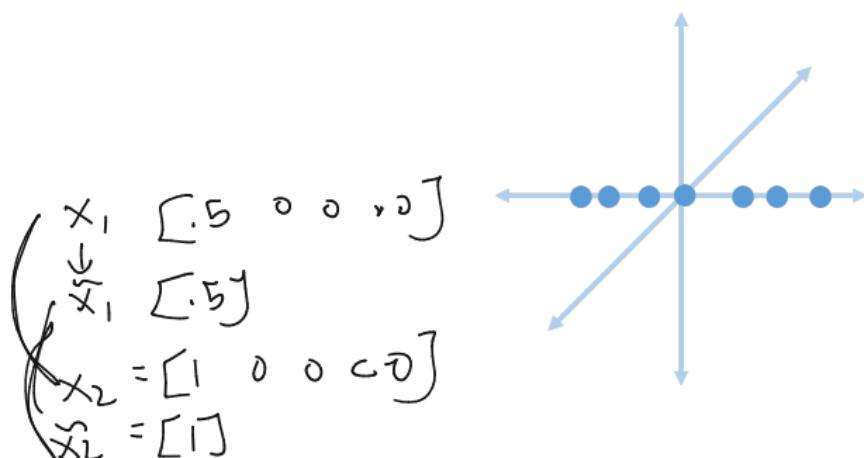
A very easy case: Assume that $\vec{x}_1, \dots, \vec{x}_n$ all lie on the 1st axis in \mathbb{R}^d .

$$\begin{bmatrix} .5 & 0 & 0 & 0 \end{bmatrix}$$
$$\begin{bmatrix} .6 & 0 & 0 & 0 \end{bmatrix}$$
$$\begin{bmatrix} -.5 & 0 & 0 & 0 \end{bmatrix}$$



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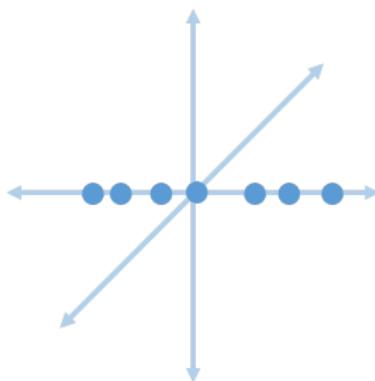


Set $m = 1$ and $\tilde{x}_i = \underbrace{[\vec{x}_i(1)]}$ (i.e., \tilde{x}_i contains just a single number).

$$\cdot \underbrace{\|\tilde{x}_i - \tilde{x}_j\|_2}_{= \sqrt{[\vec{x}_i(1) - \vec{x}_j(1)]^2}} = \underbrace{|\vec{x}_i(1) - \vec{x}_j(1)|}_{= \|\vec{x}_i - \vec{x}_j\|_2} = \|\vec{x}_i - \vec{x}_j\|_2.$$

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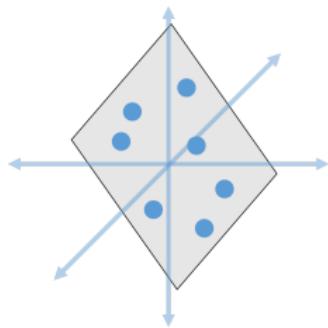


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- An embedding with **no distortion** from any d into $m = 1$.

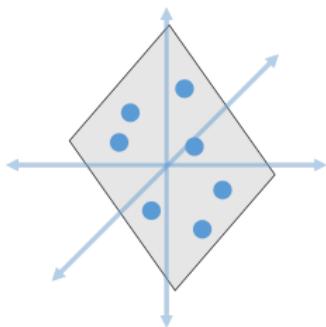
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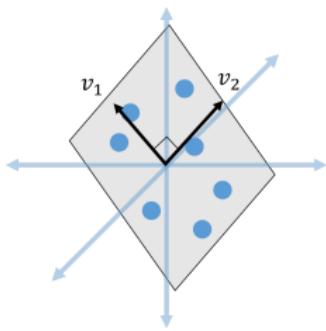
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- Let $\vec{v}_1, \vec{v}_2, \dots, \vec{v}_k$ be an orthonormal basis for \mathcal{V} and let $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns.

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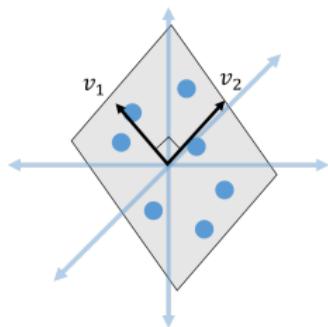


$$V = \begin{bmatrix} | & | & | \\ v_1 & v_2 & v_3 \\ | & | & | \end{bmatrix}$$

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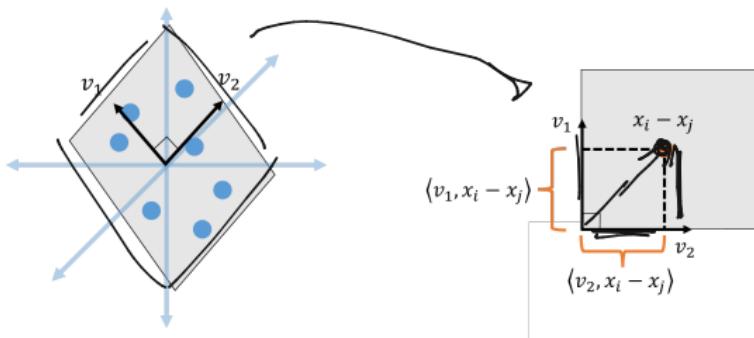


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- For all i, j we have $\vec{x}_i - \vec{x}_j \in \mathcal{V}$ and (a good exercise!):

$$\underbrace{\|\vec{x}_i - \vec{x}_j\|_2}_{\cdot} = \sqrt{\sum_{\ell=1}^k \underbrace{\langle v_\ell, \vec{x}_i - \vec{x}_j \rangle^2}_{\cdot}}.$$

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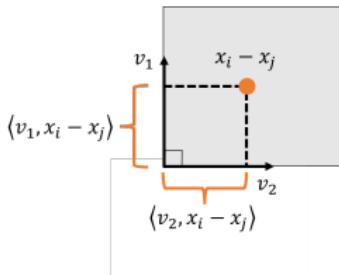
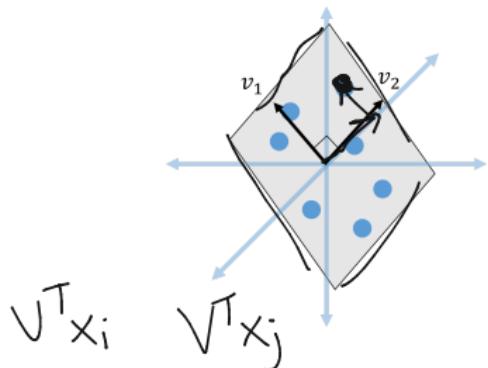


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$$\sqrt{v_1^T} x_i \quad \sqrt{v_1^T} x_j$$

$$\|\vec{x}_i - \vec{x}_j\|_2 = \sqrt{\sum_{\ell=1}^k \langle v_\ell, \vec{x}_i - \vec{x}_j \rangle^2} = \|\mathbf{V}^T(\vec{x}_j - \vec{x}_i)\|_2.$$

10

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$k \times d \rightarrow k$

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~~\tilde{x}_i~~ ~~\tilde{x}_j~~

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$$\|\tilde{x}_i - \tilde{x}_j\|_2 = \|\mathbf{V}^T \vec{x}_i - \underbrace{\mathbf{V}^T \vec{x}_j}_{\mathbf{V}^T(\vec{x}_i - \vec{x}_j)}\|_2 = \|\mathbf{V}^T(\vec{x}_i - \vec{x}_j)\|_2 = \|\vec{x}_i - \vec{x}_j\|_2.$$

- An embedding with **no distortion** from any d into $m = k$.
- $\underline{\mathbf{V}^T} : \mathbb{R}^d \rightarrow \mathbb{R}^k$ is a linear map giving our embedding.

EMBEDDING WITH NO ASSUMPTIONS

What about when we don't make any assumptions on $\vec{x}_1, \dots, \vec{x}_n$. I.e., they can be scattered arbitrarily around d -dimensional space?

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What about when we don't make any assumptions on $\vec{x}_1, \dots, \vec{x}_n$. I.e., they can be scattered arbitrarily around d -dimensional space?

- Can we find a no-distortion embedding into $m < d$ dimensions? **No. Require $m = d$.**
- Can we find an ϵ -distortion embedding into $m \ll d$ dimensions for $\epsilon > 0$? **Yes! Always, with m depending on ϵ .**

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THE JOHNSON-LINDENSTRAUSS LEMMA

$$m \left[\begin{array}{c} \xrightarrow{d} \\ \boldsymbol{\Pi} \end{array} \right] \left[\begin{array}{c} x_i \\ \xrightarrow{?} \end{array} \right]$$

Johnson-Lindenstrauss Lemma: For any set of points $\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$ and $\epsilon > 0$ there exists a linear map $\boldsymbol{\Pi} : \mathbb{R}^d \rightarrow \mathbb{R}^m$ such that $m = O\left(\frac{\log n}{\epsilon^2}\right)$ and letting $\tilde{x}_i = \underbrace{\boldsymbol{\Pi} \vec{x}_i}_{\text{underbrace}}$:

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~~1 query.~~
For $d \geq 1$ trillion, $\epsilon = .05$, and $n = 100,000$, $m \approx 6600$.

THE JOHNSON-LINDENSTRAUSS LEMMA

$n = \# \text{ data points}$ $d = \dim \text{ of data.}$

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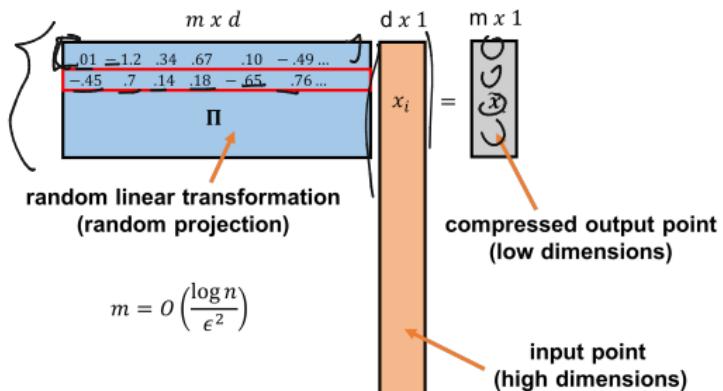
For $d = 1$ trillion, $\epsilon = .05$, and $n = 100,000$, $m \approx 6600$.

Very surprising! Powerful result with a simple construction: applying a random linear transformation to a set of points preserves distances between all those points with high probability.

RANDOM PROJECTION

For any $\vec{x}_1, \dots, \vec{x}_n$ and $\Pi \in \mathbb{R}^{m \times d}$ with each entry chosen i.i.d. from $\mathcal{N}(0, 1/m)$, with high probability, letting $\tilde{\vec{x}}_i = \underline{\Pi \vec{x}_i}$:

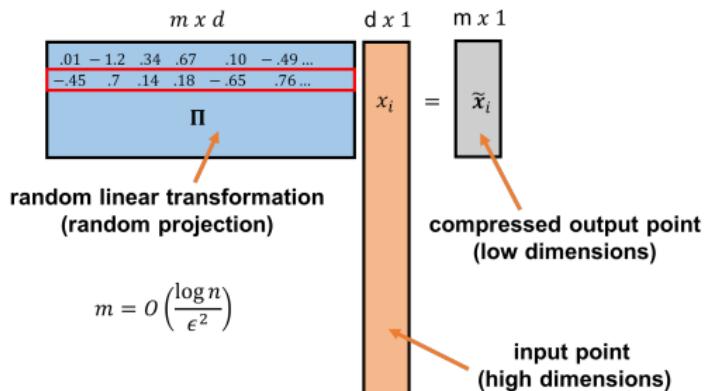
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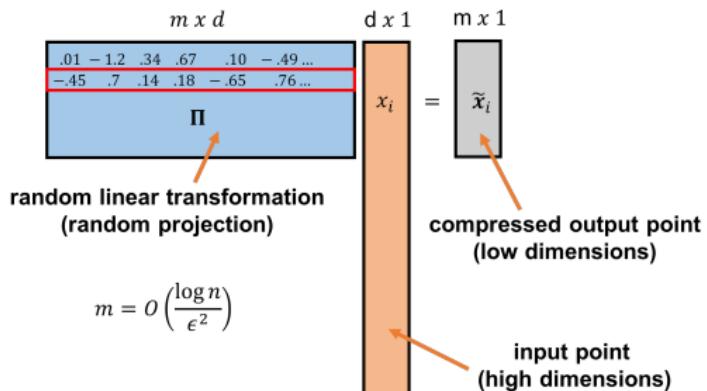


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Π is **data oblivious**. Stark contrast to methods like PCA.

ALGORITHMIC CONSIDERATIONS

- Many alternative constructions: ± 1 entries, sparse (most entries 0), Fourier structured, etc. \implies more efficient computation of $\tilde{\mathbf{x}}_i = \underline{\mathbf{\Pi} \vec{\mathbf{x}}_i}$.

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- Compression can also be easily performed in parallel on different servers.
 - When new data points are added, can be easily compressed, without updating existing points.

CONNECTION TO SIMHASH

Compression operation is $\tilde{\vec{x}}_i = \underbrace{\boldsymbol{\Pi} \vec{x}_i}_{\text{so for any } j}$,

$$\tilde{\vec{x}}_i(j) = \underbrace{\langle \boldsymbol{\Pi}(j), \vec{x}_i \rangle}_{\sum_{k=1}^d \underbrace{\boldsymbol{\Pi}(j, k)}_{\text{compression}} \cdot \underbrace{\vec{x}_i(k)}_{\text{original point}}} = \sum_{k=1}^d \boldsymbol{\Pi}(j, k) \cdot \vec{x}_i(k).$$



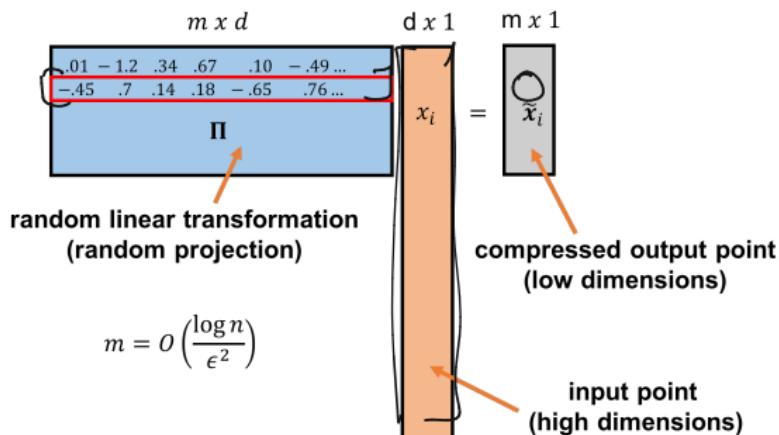
$\vec{x}_1, \dots, \vec{x}_n$: original points (d dims.), $\tilde{\vec{x}}_1, \dots, \tilde{\vec{x}}_n$: compressed points ($m < d$ dims.), $\boldsymbol{\Pi} \in \mathbb{R}^{m \times d}$: random projection (embedding function)

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$$\tilde{x}_i(j) = \langle \Pi(j), \vec{x}_i \rangle = \sum_{k=1}^d \Pi(j, k) \cdot x_i(k).$$

$\Pi(j)$ is a vector with independent random Gaussian entries.



$$m = O\left(\frac{\log n}{\epsilon^2}\right)$$

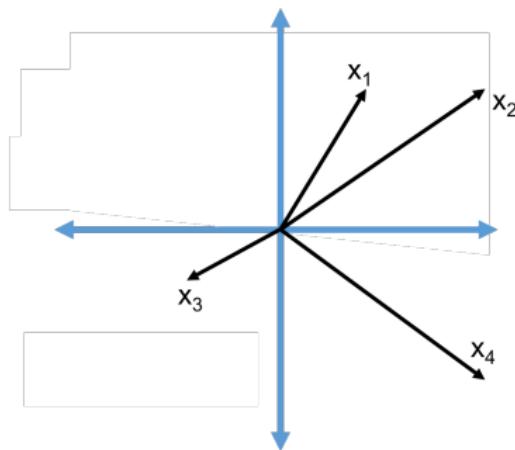
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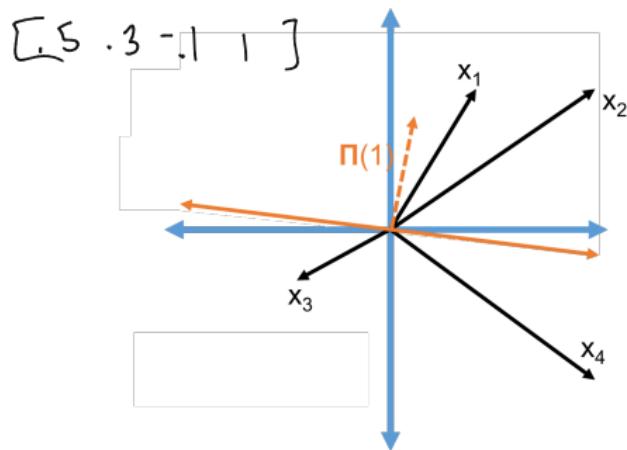
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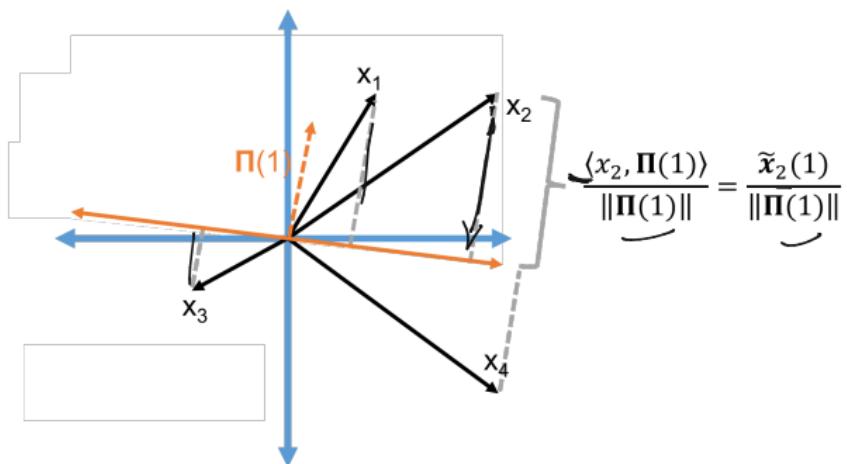
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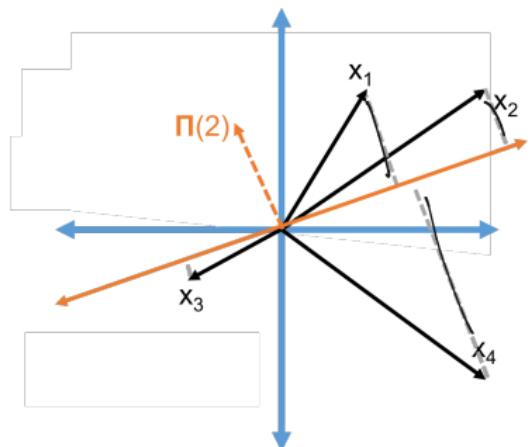
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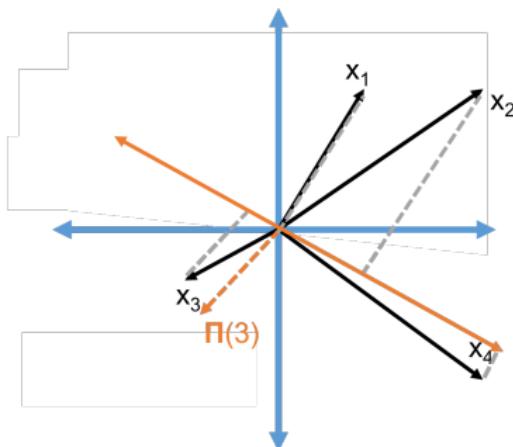
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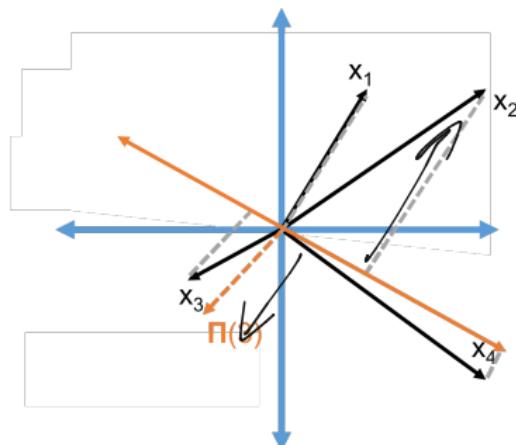
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$$\begin{array}{c} \xrightarrow{\tilde{\mathbf{x}}_i = [1.1 \ -2.4 \ 0.1 \ -5]} \\ \downarrow \\ \text{SimHash Signature } [1 \ -1 \ 1 \ -1] \end{array}$$

Points with high cosine similarity have similar random projections.

Computing a length m SimHash signature $SH_1(\vec{\mathbf{x}}_i), \dots, SH_m(\vec{\mathbf{x}}_i)$ is identical to computing $\tilde{\mathbf{x}}_i = \boldsymbol{\Pi} \vec{\mathbf{x}}_i$ and then taking $\text{sign}(\tilde{\mathbf{x}}_i)$.

The Johnson-Lindenstrauss Lemma is a direct consequence of a closely related lemma:

Distributional JL Lemma: Let $\Pi \in \mathbb{R}^{m \times d}$ have each entry chosen i.i.d. as $\mathcal{N}(0, 1/m)$. If we set $\underline{m} = O\left(\frac{\log(1/\delta)}{\epsilon^2}\right)$, then **for any** $\vec{y} \in \mathbb{R}^d$, with probability $\geq 1 - \delta$

$$\underbrace{(1 - \epsilon)\|\vec{y}\|_2}_{\text{lower bound}} \leq \underbrace{\|\Pi\vec{y}\|_2}_{\text{projection}} \leq \underbrace{(1 + \epsilon)\|\vec{y}\|_2}_{\text{upper bound}}$$

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- Can be proven from first principles.

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Questions?

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Distributional JL Lemma \implies JL Lemma: Distributional JL show that a random projection Π preserves the **norm** of any y . The main JL Lemma says that Π preserves **distances** between vectors.

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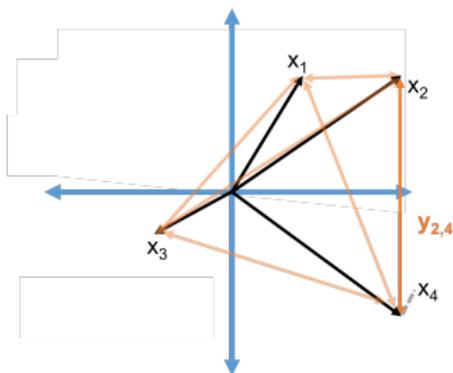


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$$\underbrace{(1 - \epsilon)\|\vec{x}_i - \vec{x}_j\|_2}_{(1 - \epsilon)\|\tilde{x}_i - \tilde{x}_j\|_2} \leq \|\tilde{x}_i - \tilde{x}_j\|_2 \leq (1 + \epsilon)\|\vec{x}_i - \vec{x}_j\|_2$$

$\vec{x}_1, \dots, \vec{x}_n$: original points, $\tilde{x}_1, \dots, \tilde{x}_n$: compressed points, $\Pi \in \mathbb{R}^{m \times d}$: random projection matrix. d : original dimension. m : compressed dimension, ϵ : embedding error, δ : embedding failure prob.

DISTRIBUTIONAL JL \implies JL

Claim: If we choose $\mathbf{\Pi}$ with i.i.d. $\mathcal{N}(0, 1/m)$ entries and $m = O\left(\frac{\log(1/\delta')}{\epsilon^2}\right)$, letting $\tilde{\mathbf{x}}_i = \underbrace{\mathbf{\Pi} \vec{\mathbf{x}}_i}_{\geq 1 - \delta'}$, for each pair $\vec{\mathbf{x}}_i, \vec{\mathbf{x}}_j$ with probability $\geq 1 - \delta'$ we have:

$$(1 - \epsilon) \|\vec{\mathbf{x}}_i - \vec{\mathbf{x}}_j\|_2 \leq \|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|_2 \leq (1 + \epsilon) \|\vec{\mathbf{x}}_i - \vec{\mathbf{x}}_j\|_2.$$

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With what probability are all pairwise distances preserved?

↳ apply union bound

$\vec{\mathbf{x}}_1, \dots, \vec{\mathbf{x}}_n$: original points, $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n$: compressed points, $\Pi \in \mathbb{R}^{m \times d}$: random projection matrix. d : original dimension. m : compressed dimension, ϵ : embedding error, δ : embedding failure prob.

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With what probability are all pairwise distances preserved?

Union bound: With probability $\geq 1 - \binom{n}{2} \cdot \delta'$ all pairwise distances are preserved. $|-\mathcal{J}^1 \cdot \binom{n}{2}$

$\vec{\mathbf{x}}_1, \dots, \vec{\mathbf{x}}_n$: original points, $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n$: compressed points, $\Pi \in \mathbb{R}^{m \times d}$: random projection matrix. d : original dimension. m : compressed dimension, ϵ : embedding error, δ : embedding failure prob.

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With what probability are all pairwise distances preserved?

Union bound: With probability $\geq 1 - \binom{n}{2} \cdot \delta'$ all pairwise distances are preserved.

Apply the claim with $\delta' = \delta / \binom{n}{2}$.

$\vec{\mathbf{x}}_1, \dots, \vec{\mathbf{x}}_n$: original points, $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n$: compressed points, $\Pi \in \mathbb{R}^{m \times d}$: random projection matrix. d : original dimension. m : compressed dimension, ϵ : embedding error, δ : embedding failure prob.

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With what probability are all pairwise distances preserved?

Union bound: With probability $\geq 1 - \underbrace{\binom{n}{2} \cdot \delta'}_{\text{all pairwise distances}}$ all pairwise distances are preserved.

Apply the claim with $\underline{\delta'} = \underline{\delta / \binom{n}{2}}$. \implies for $\underline{m} = O\left(\frac{\log(1/\delta')}{\epsilon^2}\right)$, all pairwise distances are preserved with probability $\geq \underline{1 - \delta}$.

$\vec{\mathbf{x}}_1, \dots, \vec{\mathbf{x}}_n$: original points, $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n$: compressed points, $\Pi \in \mathbb{R}^{m \times d}$: random projection matrix. d : original dimension. m : compressed dimension, ϵ : embedding error, δ : embedding failure prob.

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$$m = O\left(\frac{\log(1/\delta')}{\epsilon^2}\right) = O\left(\frac{\log(\binom{n}{2}/\delta)}{\epsilon^2}\right)$$

$\vec{\mathbf{x}}_1, \dots, \vec{\mathbf{x}}_n$: original points, $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_n$: compressed points, $\mathbf{\Pi} \in \mathbb{R}^{m \times d}$: random projection matrix. d : original dimension. m : compressed dimension, ϵ : embedding error, δ : embedding failure prob.

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Union bound: With probability $\geq 1 - \binom{n}{2} \cdot \delta'$ all pairwise distances are preserved.

Apply the claim with $\delta' = \delta / \binom{n}{2}$. \implies for $m = O\left(\frac{\log(1/\delta')}{\epsilon^2}\right)$, all pairwise distances are preserved with probability $\geq 1 - \delta$.

$$\overbrace{m} = O\left(\frac{\log(1/\delta')}{\epsilon^2}\right) = O\left(\frac{\log(\binom{n}{2}/\delta)}{\epsilon^2}\right) = O\left(\frac{\log(n^2/\delta)}{\epsilon^2}\right) = O\left(\frac{\log(n/\delta)}{\epsilon^2}\right)$$

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Yields the JL lemma.