COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Cameron Musco

University of Massachusetts Amherst. Fall 2021.

Lecture 12

LOGISTICS

- Problem Set 2 is due Friday, 11:59pm.
- Quiz 6 is due today at 8pm.
- The exam will be held next Tuesday in class. Let me know ASAP if you need accommodations (e.g., extended time).
- We will do some midterm review in class on Thursday. I will also hold additional office hours for midterm prep, **next Monday, 4-6pm**, and potentially Friday afternoon as well.

-Practice problems on schedule.

Last Class: The Johnson-Lindenstrauss Lemma

- Low-distortion embeddings for any set of points via random projection.
- Started on proof of the JL Lemma via the Distributional JL Lemma.

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This Class:

- Finish Up proof of the JL lemma.
- Example applications ~~to classification and~~ clustering.
- Discuss connections to high dimensional geometry.

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

$$\text{For all } i, j: \; (1-\epsilon)\|\vec{x}_i - \vec{x}_j\|_2 \leq \|\tilde{x}_i - \tilde{x}_j\|_2 \leq (1+\epsilon)\|\vec{x}_i - \vec{x}_j\|_2.$$

Further, if $\mathbf{\Pi} \in \mathbb{R}^{m \times d}$ has each entry chosen i.i.d. from $\mathcal{N}(0, 1/m)$ and $m = O\left(\frac{\log n/\delta}{\epsilon^2}\right)$, $\mathbf{\Pi}$ satisfies the guarantee with probability $\geq 1 - \delta$.

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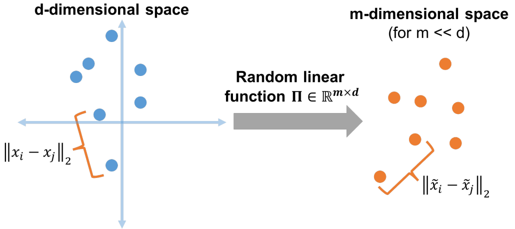
Further, if $\mathbf{\Pi} \in \mathbb{R}^{m\times d}$ has each entry chosen i.i.d. from $\mathcal{N}(0, 1/m)$ and $m = O\left(\frac{\log n/\delta}{\epsilon^2}\right)$, $\mathbf{\Pi}$ satisfies the guarantee with probability $\geq 1-\delta$.



We showed that the Johnson-Lindenstrauss Lemma follows from:

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

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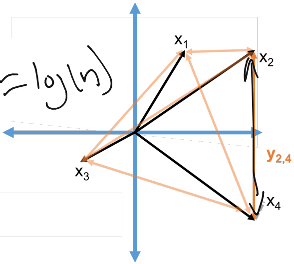
$m << d$

Main Idea: Union bound over $\binom{n}{2}$ difference vectors $\vec{y}_{ij} = \vec{x}_i - \vec{x}_j$.

$\delta = 1/\binom{n}{2}$

$\log(1/\delta) \approx \log(n^2) \approx \log(n)$



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$\vec{y} \in \mathbb{R}^d$: arbitrary vector, $\tilde{\mathbf{y}} \in \mathbb{R}^m$: compressed vector, $\mathbf{\Pi} \in \mathbb{R}^{m \times d}$: random projection. d: original dim. m: compressed dim, ϵ: error, δ: failure prob.

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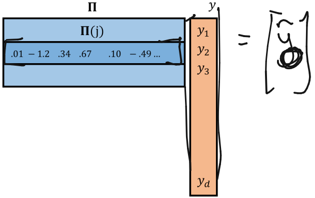

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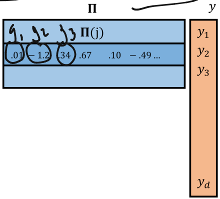
$g_i = \Pi(j,i)$



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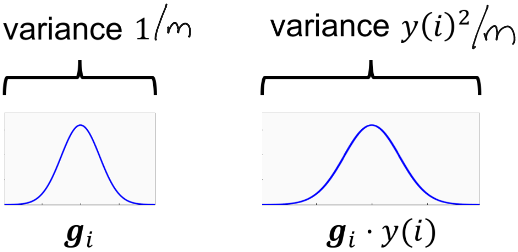

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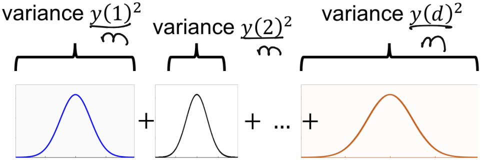

$$\tilde{\mathbf{y}}(j) = \frac{1}{\sqrt{m}}[\boldsymbol{g}_1 \cdot y(1) + \boldsymbol{g}_2 \cdot y(2) + \dots + \boldsymbol{g}_d \cdot y(d)]$$

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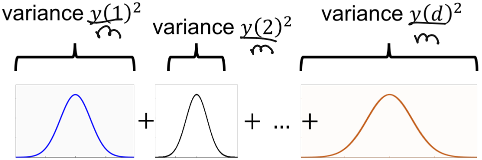

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What is the distribution of $\tilde{\mathbf{y}}(j)$?

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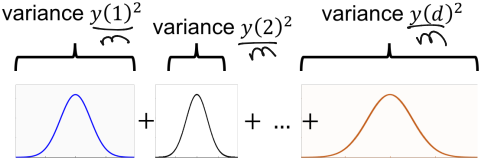

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What is the distribution of $\tilde{\mathbf{y}}(j)$? Also Gaussian!

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Letting $\tilde{\mathbf{y}} = \mathbf{\Pi}\vec{y}$, we have $\tilde{\mathbf{y}}(j) = \langle \mathbf{\Pi}(j), \vec{y} \rangle$ and:

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Stability of Gaussian Random Variables. For independent $a \sim \mathcal{N}(\mu_1, \sigma_1^2)$ and $b \sim \mathcal{N}(\mu_2, \sigma_2^2)$ we have:

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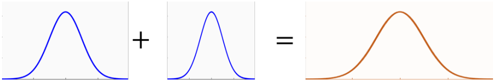

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Thus, $\tilde{\mathbf{y}}(j) \sim \mathcal{N}(0, \frac{\|\vec{y}\|_2^2}{m})$ I.e., $\tilde{\mathbf{y}}$ itself is a random Gaussian vector. Rotational invariance of the Gaussian distribution.

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What is $\mathbb{E}[\|\tilde{\mathbf{y}}\|_2^2]$?

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DISTRIBUTIONAL JL PROOF

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$$\tilde{\mathbf{y}}(j) \sim \mathcal{N}(0, \|\vec{y}\|_2^2/m).$$

$$\mathrm{Var}(\tilde{y}(j)) = \mathbb{E}(\tilde{y}(j) - \mathbb{E}[\tilde{y}(j)])^2 = \mathbb{E}[\tilde{y}(j)^2] = \frac{\|y\|_2^2}{m}$$

What is $\mathbb{E}[\|\tilde{\mathbf{y}}\|_2^2]$?

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$$= \sum_{j=1}^{m} \frac{\|\vec{y}\|_2^2}{m} = \|\vec{y}\|_2^2$$

$\mathbb{E}\,\tilde{y}(j) = 0$

$\mathbb{E}\,\tilde{y}(j)^2 = \frac{\|y\|_2^2}{m}$

So $\tilde{\mathbf{y}}$ has the right norm in expectation.

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So $\tilde{\mathbf{y}}$ has the right norm in expectation.

How is $\|\tilde{\mathbf{y}}\|_2^2$ distributed? Does it concentrate?

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So far: Letting $\boldsymbol{\Pi} \in \mathbb{R}^{d \times m}$ have each entry chosen i.i.d. as $\frac{1}{\sqrt{m}} \cdot \mathcal{N}(0,1)$, for any $\vec{y} \in \mathbb{R}^d$, letting $\tilde{\mathbf{y}} = \boldsymbol{\Pi}\vec{y}$:

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$\|\tilde{\mathbf{y}}\|_2^2 = \sum_{j=1}^m \tilde{\mathbf{y}}(j)^2$ a Chi-Squared random variable with m degrees of freedom (a sum of m squared independent Gaussians)

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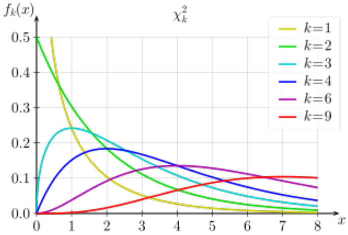

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Lemma: (Chi-Squared Concentration) Letting $\mathbf{Z}$ be a Chi-Squared random variable with m degrees of freedom,

$$\Pr\left[|\mathbf{Z} - \mathbb{E}\mathbf{Z}| \geq \epsilon \mathbb{E}\mathbf{Z}\right] \leq 2e^{-m\epsilon^2/8}.$$

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If we set $m = O\left(\frac{\log(1/\delta)}{\epsilon^2}\right)$, with probability $1 - O(e^{-\log(1/\delta)}) \geq 1 - \delta$:

$$(1-\epsilon)\|\vec{y}\|_2^2 \leq \|\tilde{\mathbf{y}}\|_2^2 \leq (1+\epsilon)\|\vec{y}\|_2^2.$$

$m = 80 \cdot \frac{\log(1/\delta)}{\epsilon^2}$

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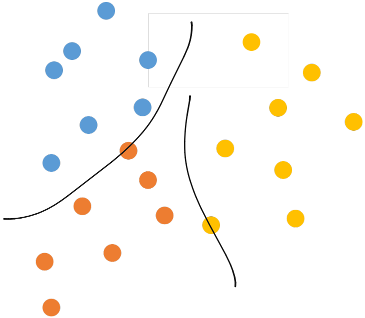
Gives the distributional JL Lemma and thus the classic JL Lemma!

Goal: Separate n points in d dimensional space into k groups.



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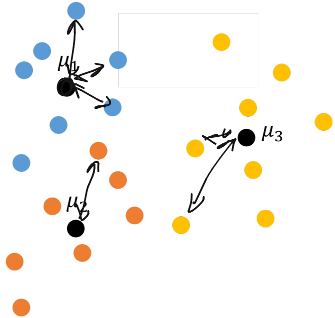

k-means Objective: $Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k) = \min_{\mathcal{C}_1, \ldots \mathcal{C}_k} \sum_{j=1}^{k} \sum_{\vec{x} \in \mathcal{C}_k} \|\vec{x} - \mu_j\|_2^2.$

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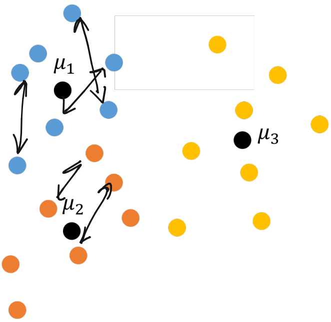

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Write in terms of distances:

$$Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k) = \min_{\mathcal{C}_1, \ldots \mathcal{C}_k} \sum_{j=1}^{k} \sum_{\vec{x}_1, \vec{x}_2 \in \mathcal{C}_k} \|\vec{x}_1 - \vec{x}_2\|_2^2$$

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EXAMPLE APPLICATION: k-MEANS CLUSTERING

k-means Objective: $Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k) = \min_{\mathcal{C}_1, \ldots \mathcal{C}_k} \sum_{j=1}^{k} \sum_{\vec{x}_1, \vec{x}_2 \in \mathcal{C}_k} \|\vec{x}_1 - \vec{x}_2\|_2^2$

If we randomly project to $m = O\left(\frac{\log n}{\epsilon^2}\right)$ dimensions, for all pairs $\vec{x}_1, \vec{x}_2$,

$$(1-\epsilon)\|\vec{x}_1 - \vec{x}_2\|_2^2 \leq \|\tilde{\mathbf{x}}_1 - \tilde{\mathbf{x}}_2\|_2^2 \leq (1+\epsilon)\|\vec{x}_1 - \vec{x}_2\|_2^2$$

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Letting $\overline{Cost}(\mathcal{C}_1, \ldots, \mathcal{C}_k) = \min_{\mathcal{C}_1, \ldots \mathcal{C}_k} \sum_{j=1}^{k} \sum_{\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2 \in \mathcal{C}_k} \|\tilde{\mathbf{x}}_1 - \tilde{\mathbf{x}}_2\|_2^2$

$$(1-\epsilon)Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k) \le \overline{Cost}(\mathcal{C}_1, \ldots, \mathcal{C}_k) \le (1+\epsilon)Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k).$$

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$$(1-\epsilon)Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k) \le \overline{Cost}(\mathcal{C}_1, \ldots, \mathcal{C}_k) \le (1+\epsilon)Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k).$$

Upshot: Can cluster in m dimensional space (much more efficiently) and minimize $\overline{Cost}(\mathcal{C}_1, \ldots, \mathcal{C}_k)$. The optimal set of clusters will have true cost within $1 + c\epsilon$ times the true optimal. Good exercise to prove this.

$1+2\epsilon$

The Johnson-Lindenstrauss Lemma and High Dimensional Geometry

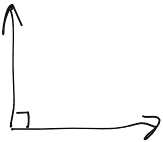
The Johnson-Lindenstrauss Lemma and High Dimensional Geometry

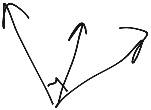
- High-dimensional Euclidean space looks *very different* from low-dimensional space. So how can JL work?
- Is Euclidean distance in high-dimensional meaningless, making JL useless? (The curse of dimensionality)

ORTHOGONAL VECTORS

What is the largest set of mutually orthogonal unit vectors in d-dimensional space?

a) 1   b) $\log d$ c) $\sqrt{d}$ d) d





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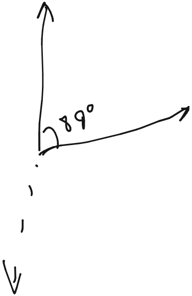
NEARLY ORTHOGONAL VECTORS

What is the largest set of unit vectors in d-dimensional space that have all pairwise dot products $|\langle \vec{x}, \vec{y} \rangle| \leq \epsilon$? (think $\epsilon = .01$)

a) d b) $\Theta(d)$ c) $\Theta(d^2)$ d) $2^{\Theta(d)}$



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a) d b) $\Theta(d)$ c) $\Theta(d^2)$ d) $2^{\Theta(d)}$

In fact, an exponentially large set of random vectors will be nearly pairwise orthogonal with high probability!

$\varepsilon = .01$

$2^{\Theta(d)}$

Claim: $2^{\Theta(\epsilon^2 d)}$ random d-dimensional unit vectors will have all pairwise dot products $|\langle \vec{x}, \vec{y} \rangle| \leq \epsilon$ (be nearly orthogonal) with high probability.

$t =$

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Proof: Let $\vec{x}_1, \ldots, \vec{x}_t$ each have independent random entries set to $\pm 1/\sqrt{d}$.

$\left[\frac{1}{\sqrt{d}}, -\frac{1}{\sqrt{d}}, -\frac{1}{\sqrt{d}} \quad \right]$

ORTHOGONAL VECTORS PROOF

t vectors in d dimensions

Claim: $t = 2^{\Theta(\epsilon^2 d)}$ random d-dimensional unit vectors will have all pairwise dot products $|\langle \vec{x}, \vec{y} \rangle| \leq \epsilon$ (be nearly orthogonal) with high probability.

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$[1/\sqrt{d} \quad -1/\sqrt{d} \quad -1/\sqrt{d} \quad \ldots \quad 1/\sqrt{d}]$

- What is $\|\vec{x}_i\|_2$? $= 1$ $\qquad \|x_i\|_2^2 = \sum_{j=1}^{d} x_i(j)^2 = \sum_{j=1}^{d} 1/d = 1$
- What is $\mathbb{E}[\langle \vec{x}_i, \vec{x}_j \rangle]$? $= 0$

Claim: $2^{\Theta(\epsilon^2 d)}$ random d-dimensional unit vectors will have all pairwise dot products $|\langle \vec{x}, \vec{y} \rangle| \leq \epsilon$ (be nearly orthogonal) with high probability.

Proof: Let $\vec{x}_1, \ldots, \vec{x}_t$ each have independent random entries set to $\pm 1/\sqrt{d}$.

- What is $\|\vec{x}_i\|_2$? Every $\vec{x}_i$ is always a unit vector.
- What is $\mathbb{E}[\langle \vec{x}_i, \vec{x}_j \rangle]$?

Claim: $2^{\Theta(\epsilon^2 d)}$ random d-dimensional unit vectors will have all pairwise dot products $|\langle \vec{x}, \vec{y} \rangle| \leq \epsilon$ (be nearly orthogonal) with high probability.

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$$\|x_i\|_2 = \sqrt{\sum x_i(j)^2} = \sqrt{1} = 1$$

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$$1 = \|x_i\|_2^2 = \sum x_i(j)^2$$

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  $i \neq j$: $\langle x_i, x_i \rangle = \sum x_i(j)^2 = \|x_i\|_2^2 = 1$
- By a Chernoff bound, $\Pr[|\langle \vec{x}_i, \vec{x}_j \rangle| \geq \epsilon] \leq 2e^{-\epsilon^2 d/6}$ (great exercise).

  Bernstein

$$\langle x_i, x_j \rangle = \sum_{k=1}^{d} x_i(k) \cdot x_j(k), \quad x_i(k) \cdot x_j(k) \in \left\{+\frac{1}{d}, -\frac{1}{d}\right\}$$

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- If we chose $t = \frac{1}{2} e^{\epsilon^2 d/12}$, using a union bound over all $\binom{t}{2} \leq \frac{1}{8} e^{\epsilon^2 d/6}$ possible pairs, with probability $\geq 3/4$ all will be nearly orthogonal.

$\leq 2e^{-\epsilon d/6} \cdot \frac{1}{8} \cdot e^{\epsilon^2 d/6} = \frac{1}{4}$

Up Shot: In d-dimensional space, a set of $2^{\Theta(\epsilon^2 d)}$ random unit vectors have all pairwise dot products at most ϵ (think $\epsilon = .01$)

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$$\|\vec{x}_i - \vec{x}_j\|_2^2 = \|\vec{x}_i\|_2^2 + \|\vec{x}_j\|_2^2 - 2\vec{x}_i^T\vec{x}_j$$

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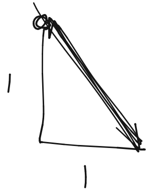

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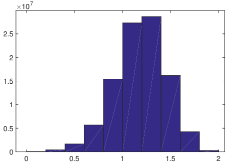
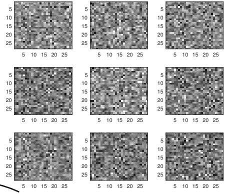
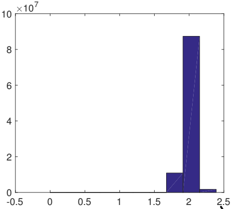
- One version of the 'curse of dimensionality'.
- If all your distances are roughly the same, distance based methods (k-means clustering, nearest neighbors, SVMs, etc.) aren't going to work well.
- Distances are only meaningful if we have lots of structure and our data isn't just independent random vectors.

Distances for MNIST Digits:



Distances for Random Images:





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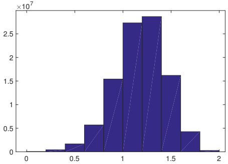

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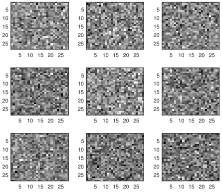

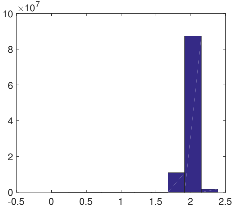

Another Interpretation: Tells us that random data can be a very bad model for actual input data.

Recall: The Johnson Lindenstrauss lemma states that if $\mathbf{\Pi} \in \mathbb{R}^{m \times d}$ is a random matrix (linear map) with $m = O\left(\frac{\log n}{\epsilon^2}\right)$, for $\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$ with high probability, for all i, j:

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

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Implies: If $\vec{x}_1, \ldots, \vec{x}_n$ are nearly orthogonal unit vectors in d-dimensions (with pairwise dot products bounded by $\epsilon/8$), then $\frac{\mathbf{\Pi}\vec{x}_1}{\|\mathbf{\Pi}\vec{x}_1\|_2}, \ldots, \frac{\mathbf{\Pi}\vec{x}_n}{\|\mathbf{\Pi}\vec{x}_n\|_2}$ are nearly orthogonal unit vectors in m-dimensions (with pairwise dot products bounded by ϵ).

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- Algebra is a bit messy but a good exercise to partially work through.

Claim 1: n nearly orthogonal unit vectors can be projected to $m = O\left(\frac{\log n}{\epsilon^2}\right)$ dimensions and still be nearly orthogonal.

Claim 2: In m dimensions, there are at most $2^{O(\epsilon^2 m)}$ nearly orthogonal vectors.

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- $2^{O(\epsilon^2 m)} = 2^{O(\log n)} \geq n$. Tells us that the JL lemma is optimal up to constants.
- m is chosen just large enough so that the odd geometry of d-dimensional space still holds on the n points in question after projection to a much lower dimensional space.