COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2020.

Lecture 11

LOGISTICS

- Problem Set 2 was due yesterday. Solutions posted.
- Quiz 5 is due **today at 8pm.**
- The exam will be held next Thursday-Friday. Let me know ASAP if you need accommodations (e.g., extended time).
- My office hours this week and next will focus on exam review and going through practice questions.

SUMMARY

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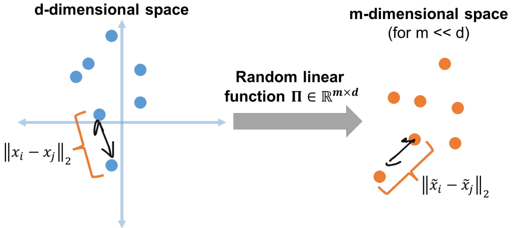
Further, if $\mathbf{\Pi} \in \mathbb{R}^{m \times d}$ has each entry chosen i.i.d. from $\mathcal{N}(0, 1/m)$ and $m = O\left(\frac{\log n/\delta}{\epsilon^2}\right)$, $\mathbf{\Pi}$ satisfies the guarantee with probability $\geq 1 - \delta$.



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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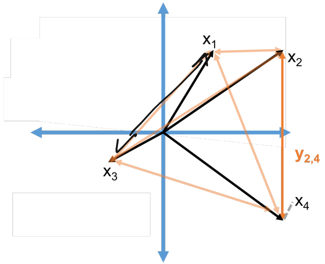
$\frac{\log(1/\delta)}{\epsilon^2} \to \frac{\log(n/\delta)}{\epsilon^2}$

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

$\|\tilde{x}_i - \tilde{x}_j\| \approx \|x_i - x_j\|$



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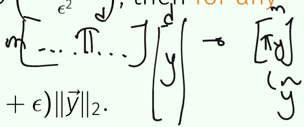

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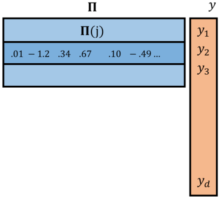

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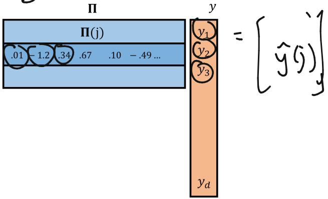

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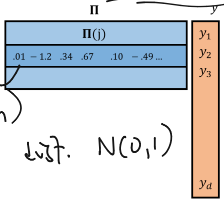

each entry: N(0,1/m)

$\frac{1}{\sqrt{m}}$ · each entry is dist. N(0,1)

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$\|\tilde{y}\| \approx \|y\|$

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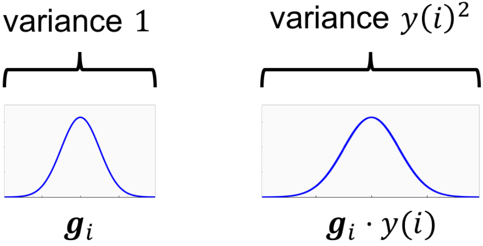

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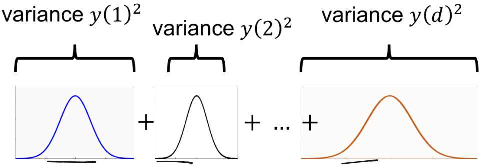

$$\tilde{\mathbf{y}}(j) = \frac{1}{\sqrt{m}}[\boldsymbol{g}_1 \cdot y(1) + \boldsymbol{g}_2 \cdot y(2) + \dots + \boldsymbol{g}_n \cdot y(d)]$$

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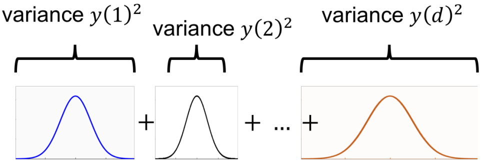

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What is the distribution of $\tilde{\mathbf{y}}(j)$? / still normal.

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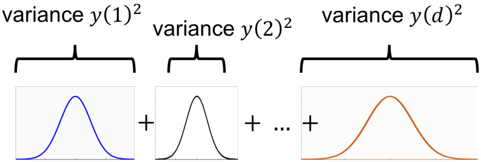

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What is the distribution of $\tilde{\mathbf{y}}(j)$? Also Gaussian!

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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:

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

linearity of variance

linear expectation

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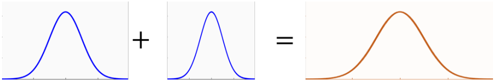

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Thus, $\tilde{\mathbf{y}}(j) \sim \frac{1}{\sqrt{m}} \mathcal{N}(0, \underbrace{\vec{y}(1)^2 + \vec{y}(2)^2 + \ldots + \vec{y}(d)^2}_{\|y\|_2^2})$ $\quad \tilde{y}(j) \sim \frac{1}{\sqrt{m}} N(0, \|y\|_2^2)$

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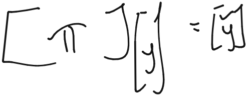
DISTRIBUTIONAL JL PROOF

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



$$\tilde{\mathbf{y}}(j) = \frac{1}{\sqrt{m}} \sum_{i=1}^{d} \mathbf{g}_i \cdot \vec{y}(i) \text{ where } \mathbf{g}_i \cdot \vec{y}(i) \sim \mathcal{N}(0, \vec{y}(i)^2).$$

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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Πy has i.i.d Gaussian entries

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Stability is another explanation for the central limit theorem.

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goal: $\|\tilde{y}\| = \|\Pi y\| \approx \|y\|$

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

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Goal: show that $\|\tilde{y}\|_2^2 \approx \|y\|_2^2$ with high prob.

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

$\mathrm{Var}(\tilde{y}(j))$

$\vec{y} \in \mathbb{R}^d$: arbitrary vector, $\tilde{\mathbf{y}} \in \mathbb{R}^m$: compressed vector, $\mathbf{\Pi} \in \mathbb{R}^{m \times d}$: random projection mapping $\vec{y} \to \tilde{\mathbf{y}}$. $\mathbf{\Pi}(j)$: j^{th} row of $\mathbf{\Pi}$, d: original dimension. m: compressed dimension, $\mathbf{g}_i$: normally distributed random variable

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

$$\mathrm{Var}[\tilde{y}(j)] = \mathbb{E}(\tilde{y}(j)^2) - \mathbb{E}[\tilde{y}(j)]^2 \quad (\mathbb{E}[\tilde{y}(j)] \to 0)$$

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

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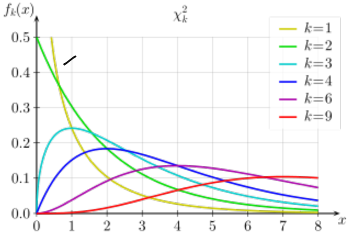

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Lemma: (Chi-Squared Concentration) Letting $\mathbf{Z}$ be a Chi-Squared random variable with m degrees of freedom, $\varepsilon > 0$,

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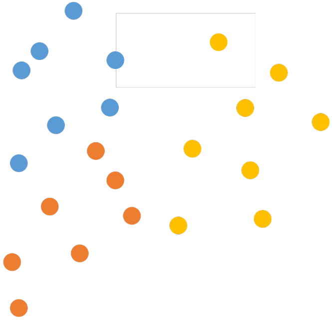
Gives the distributional JL Lemma and thus the classic JL Lemma!

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



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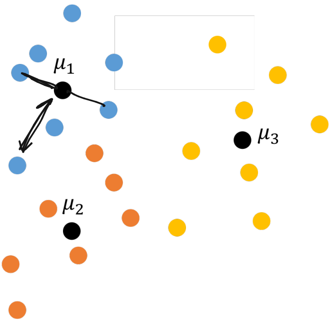

k-means Objective: $Cost(\mathcal{C}_1, \ldots, \mathcal{C}_k) = \min_{\mathcal{C}_1, \ldots \mathcal{C}_k} \sum_{j=1}^{k} \sum_{\vec{x} \in \mathcal{C}_k} \|\vec{x} - \mu_j\|_2^2.$

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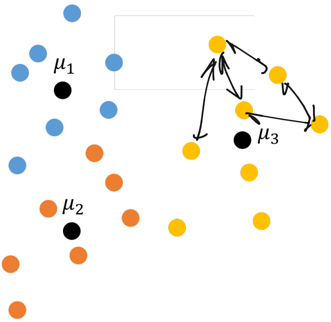

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Write in terms of distances:

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

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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 $\vec{x}_1, \vec{x}_2$,

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

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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.

$\epsilon < \frac{1}{2}$, $c = 2, 3$

$C(\ldots)$ = object function, "cost"

The Johnson-Lindenstrauss Lemma and High Dimensional Geometry

$C_1^* \ldots C_k^*$ be the true best clusters.

$\tilde{C}_1, \ldots \tilde{C}_k$ be the best low. dim. clustering

(1) $\bar{C}(\hat{C}_1 \ldots \bar{C}_k) \leq \bar{C}(C_1^*, \ldots C_k^*)$

$$C(\tilde{C}_1, \ldots \tilde{C}_k) \leq \frac{1}{1-\varepsilon} \bar{C}(\tilde{C}_1, \ldots \tilde{C}_k) \overset{(1)}{\leq} \frac{1}{(1-\varepsilon)} \bar{C}(C_1^*, \ldots C_k^*)$$

$$\leq \frac{1+\varepsilon}{1-\varepsilon} C(C_1^*, \ldots C_k^*)$$

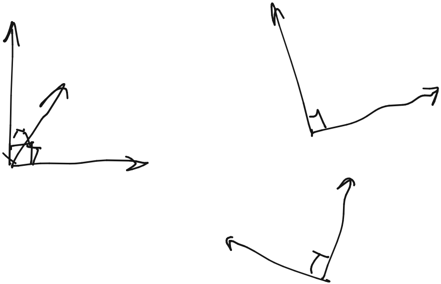
$$1 + c\varepsilon = \frac{1+\varepsilon}{1-\varepsilon}$$

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)

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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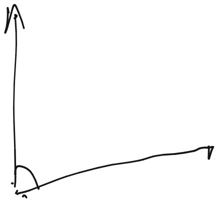
NEARLY ORTHOGONAL VECTORS

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

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).

ORTHOGONAL VECTORS PROOF

$t = 2^{\Theta(d)}$ $\quad [+\frac{1}{\sqrt{d}} \ +\frac{1}{\sqrt{d}} \ -\frac{1}{\sqrt{d}} \quad]$

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).

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

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

- What is $\|\vec{x}_i\|_2$? = 1
- What is $\mathbb{E}[\langle \vec{x}_i, \vec{x}_j \rangle]$?

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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 $\mathbb{E}[\langle \vec{x}_i, \vec{x}_j \rangle]$?

$\|x\|_2 = \sqrt{\sum_{i=1}^{d} x(i)^2} = \sqrt{\sum_{i=1}^{d} \frac{1}{d}} = \sqrt{1} = 1$

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$$\mathbb{E}\left[\sum_{k=1}^{d} x_i(k) \cdot x_j(k)\right] = \sum_{k=1}^{d} \mathbb{E}\, x_i(k)\, x_j(k), \quad \mathbb{E}\, x_i(k)\, x_j(k) = \mathbb{E}\, x_i(k) \cdot \mathbb{E}\, x_j(k) = 0 \cdot 0 = 0$$

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  $t = 2^{\Theta(d)}$

- 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.

  w.p. $> 3/4$ $\forall i, j,$ $|\langle x_i, x_j \rangle| < \epsilon$

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 $\epsilon = .01$)

$$\frac{1}{8} e^{\epsilon^2 d/12}$$

$$\epsilon = .1 \rightarrow \epsilon^2 = .01 = \frac{1}{100}$$

$$d > 1200 \cdot 3 \qquad \epsilon^2 \cdot d/12 = 3$$

$$\frac{1}{8} \cdot e^3 > 1$$

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 $\epsilon = .01$)

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

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

$x_i^T x_j = \langle x_i, x_j \rangle$

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 $\epsilon = .01$)

$$\|\vec{x}_i - \vec{x}_j\|_2^2 = \|\vec{x}_i\|_2^2 + \|\vec{x}_j\|_2^2 - 2\vec{x}_i^T\vec{x}_j \geq 1.98.$$

1 1 ≤ .01 in magnitude

≤ 2.02

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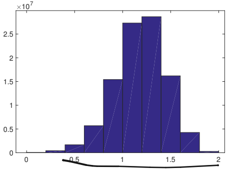
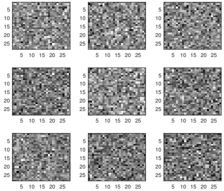
Curse of dimensionality for sampling/learning functions in high-dimensional space – samples are very 'sparse' unless we have a huge amount of data.

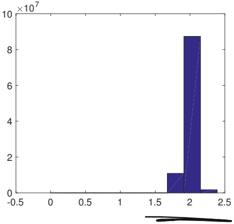
- Only hope is if we lots of structure (which we typically do...)

Distances for MNIST Digits:



Distances for Random Images:





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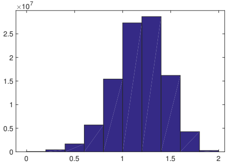

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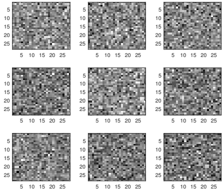

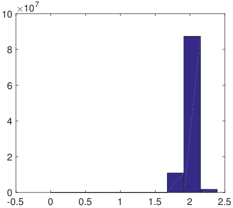

Another Interpretation: Tells us that random data can be a very bad model for actual input data.

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.

BIZARRE SHAPE OF HIGH-DIMENSIONAL BALLS

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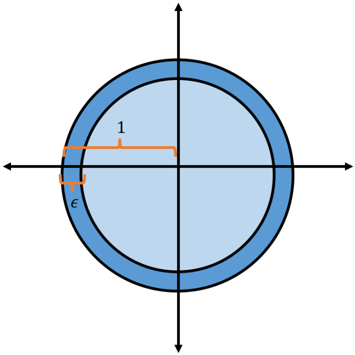
What percentage of the volume of $\mathcal{B}_d$ falls within ϵ distance of its surface?



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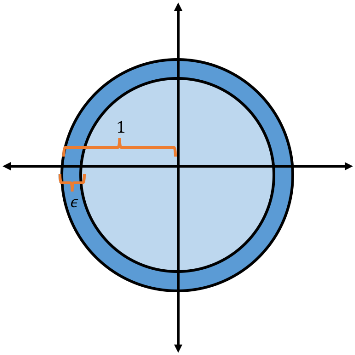

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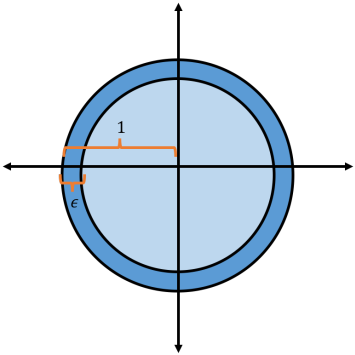
What percentage of the volume of $\mathcal{B}_d$ falls within ϵ distance of its surface? Answer: all but a $(1-\epsilon)^d \leq e^{-\epsilon d}$ fraction. Exponentially small in the dimension d!



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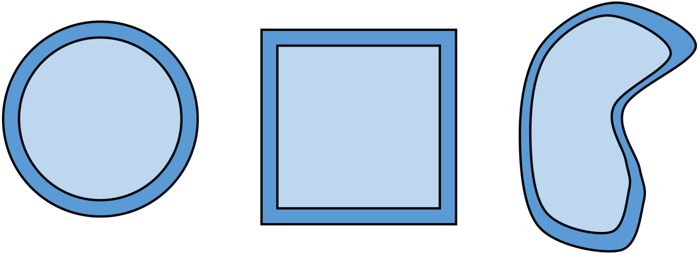
- **Isoperimetric inequality**: the ball has the minimum surface area/volume ratio of any shape.



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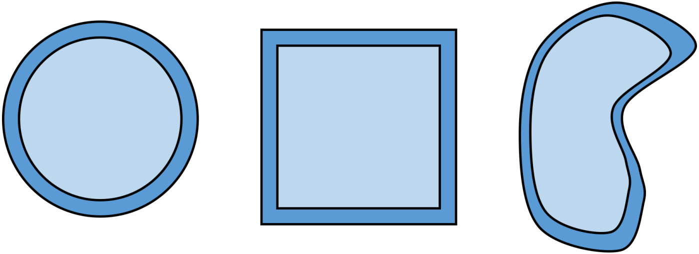

- If we randomly sample points from any high-dimensional shape, nearly all will fall near its surface.

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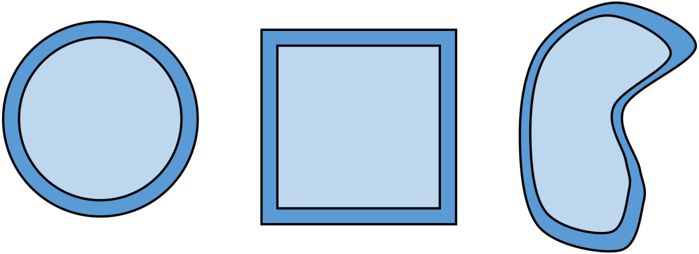
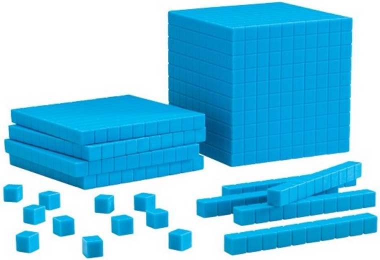


- If we randomly sample points from any high-dimensional shape, nearly all will fall near its surface.
- 'All points are outliers.'

What fraction of the cubes are visible on the surface of the cube?



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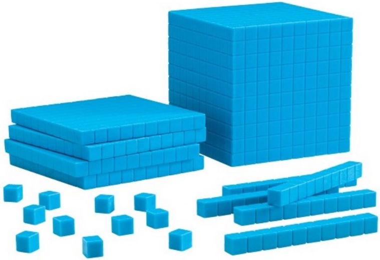
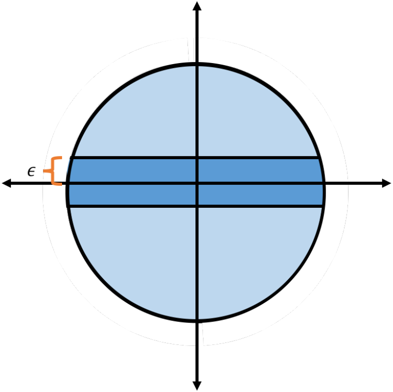


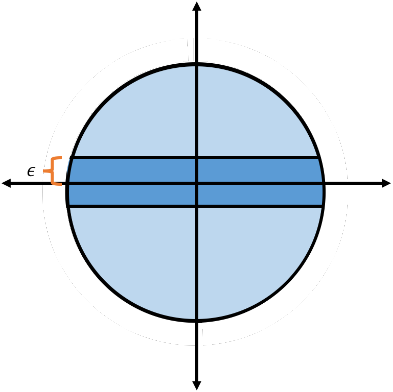
$$\frac{10^3 - 8^3}{10^3} = \frac{1000 - 512}{1000} = .488.$$

What percentage of the volume of $\mathcal{B}_d$ falls within ϵ distance of its equator?



Formally: volume of set $S = \{x \in \mathcal{B}_d : |x(1)| \leq \epsilon\}$.

What percentage of the volume of $\mathcal{B}_d$ falls within ϵ distance of its equator? Answer: all but a $2^{\Theta(-\epsilon^2 d)}$ fraction.



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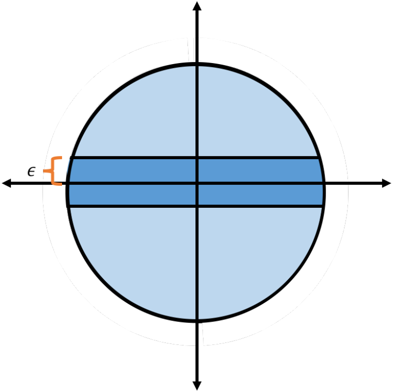

Formally: volume of set $S = \{x \in \mathcal{B}_d : |x(1)| \leq \epsilon\}$.

By symmetry, all but a $2^{\Theta(-\epsilon^2 d)}$ fraction of the volume falls within ϵ of any equator! $S = \{x \in \mathcal{B}_d : |\langle x, t\rangle| \leq \epsilon\}$

BIZARRE SHAPE OF HIGH-DIMENSIONAL BALLS

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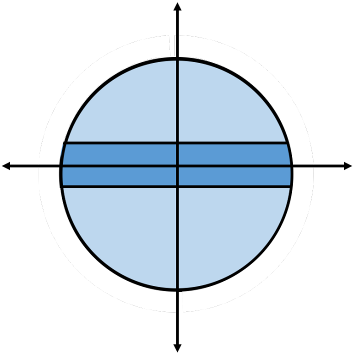

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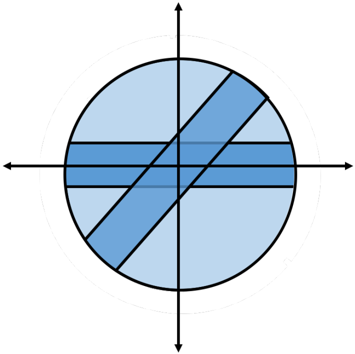

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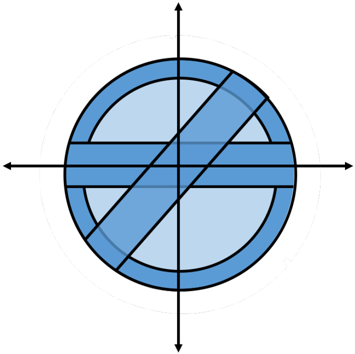

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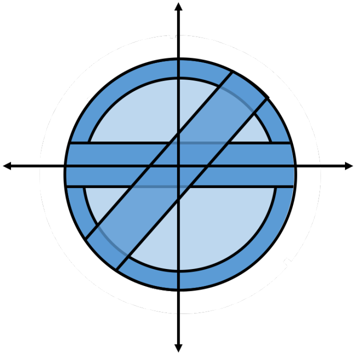
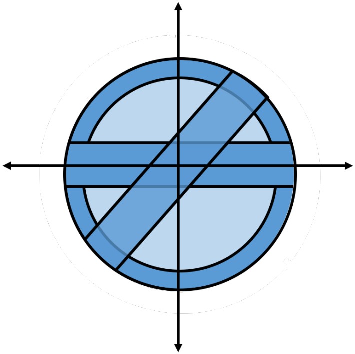


How is this possible?

Claim 1: All but a $2^{\Theta(-\epsilon^2 d)}$ fraction of the volume of a ball falls within ϵ of any equator.

Claim 2: All but a $2^{\Theta(-\epsilon d)}$ fraction falls within ϵ of its surface.



How is this possible? High-dimensional space looks nothing like this picture!

Summary: