

COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2020.

Lecture 12

- Midterm will be next Thursday-Friday. See webpage for study guide/practice questions.
- No quiz this upcoming week.
- I will hold extra office hours next Wednesday at 2pm.
- Pratheba has expanded her office hours to: Monday 2-3pm, Wednesday 1-2pm, and Friday 1-2pm, starting this upcoming week.

Last Class: Finished Up Johnson-Lindenstrauss Lemma

- Completed the proof of the Distributional JL lemma.
- Discussed an application to k -means clustering.
- Started discussion of high-dimensional geometry.

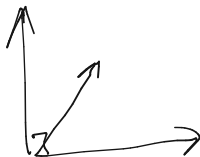
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This Class: High-Dimensional Geometry

- Bizarre phenomena in high-dimensional space.
- Connections to JL lemma and random projection.

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

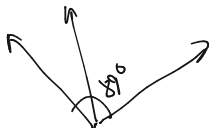


What is the largest set of mutually orthogonal unit vectors in d -dimensional space? Answer: d .

$$\langle x, y \rangle = 0$$

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 $\epsilon = .01$)

Answer: $2^{\Theta(\epsilon^2 d)}$.



ORTHOGONAL VECTORS

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

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 $\epsilon = .01$)
Answer: $2^{\Theta(\epsilon^2 d)}$.

An exponentially large set of **random vectors** will be nearly pairwise orthogonal with high probability!

$$\left[\begin{array}{ccc} +1/\sqrt{d} & -1/\sqrt{d} & -1/\sqrt{d} \end{array} \right]$$

union +
Cheb. off bound

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

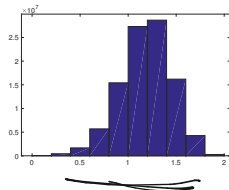
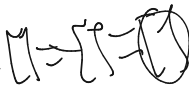
Implies: $\|\vec{x}_i - \vec{x}_j\|_2^2$ = $\|\vec{x}_i\|_2^2$ + $\|\vec{x}_j\|_2^2$ - $2\vec{x}_i^T \vec{x}_j$ \in $[1.98, 2.02]$.

Even with an exponential number of random vector samples, we don't see any nearby vectors.

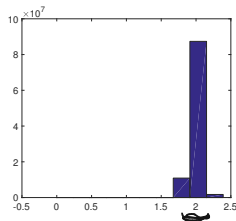
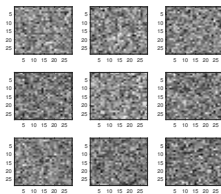
- One version of the 'curse of dimensionality'.
- If all your distances are roughly the same, distance based methods (k -means clustering, nearest neighbors, SVMs, etc.) aren't going to work well.
- Distances are only meaningful if we have lots of structure and our data isn't just independent random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

CURSE OF DIMENSIONALITY

Distances for MNIST Digits:



Distances for Random Images:



CONNECTION TO DIMENSIONALITY REDUCTION

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 $\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$ with high probability, for all i, j :

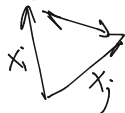
$$(1 - \epsilon) \|\vec{x}_i - \vec{x}_j\|_2^2 \leq \|\mathbf{\Pi}\vec{x}_i - \mathbf{\Pi}\vec{x}_j\|_2^2 \leq (1 + \epsilon) \|\vec{x}_i - \vec{x}_j\|_2^2.$$

Handwritten diagram illustrating the Johnson-Lindenstrauss lemma. It shows a mapping from a d -dimensional space to an m -dimensional space. A box labeled Π is shown mapping a vector x_i from \mathbb{R}^d to a vector \hat{x}_i in \mathbb{R}^m .

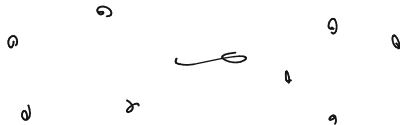
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Implies: If $\vec{x}_1, \dots, \vec{x}_n$ are nearly orthogonal unit vectors in d -dimensions (with pairwise dot products bounded by $\epsilon/8$), then $\frac{\mathbf{P}\vec{x}_1}{\|\mathbf{P}\vec{x}_1\|_2}, \dots, \frac{\mathbf{P}\vec{x}_n}{\|\mathbf{P}\vec{x}_n\|_2}$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



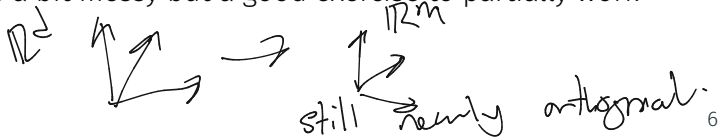
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- Algebra is a bit messy but a good exercise to partially work through.



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

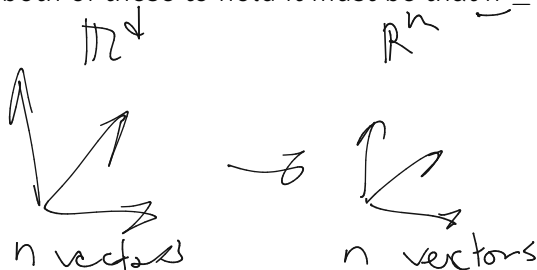
Claim 2: In m dimensions, there can be roughly $2^{O(\epsilon^2 m)}$ nearly orthogonal unit vectors.

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$$\log n \leq m \epsilon^2 \quad \curvearrowright$$

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- Tells us that the JL lemma is optimal up to constants.
- m is chosen just large enough so that the geometry of d -dimensional space still holds on the n points in question after projection to a much lower dimensional space.

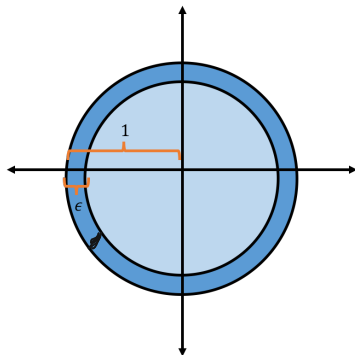
BIZARRE SHAPE OF HIGH-DIMENSIONAL BALLS

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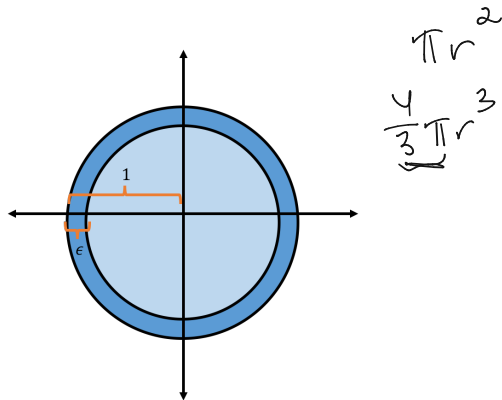
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Volume of a radius R ball is $\frac{\pi^{\frac{d}{2}}}{(d/2)!} \cdot R^d$.

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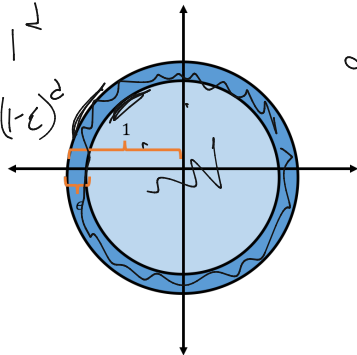
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What percentage of the volume of \mathcal{B}_d falls within ϵ distance of its surface? Answer: all but a $(1 - \epsilon)^d \leq \underline{e^{-\epsilon d}}$ fraction. Exponentially small in the dimension d !

$$\text{Vol}(\mathcal{B}_d) = \frac{\pi^{d/2}}{(d/2)!} \cdot 1^d$$

$$\text{Vol}(\mathcal{B}_d(1-\epsilon)) = \frac{\pi^{d/2}}{(d/2)!} \cdot (1-\epsilon)^d$$

$$\underline{(1-\epsilon)^d}$$



$$\epsilon = .1$$

$$d = 100$$

$$e^{-\epsilon d} = e^{-.1 \cdot 100} = e^{-10}$$

$$\approx .0000001$$

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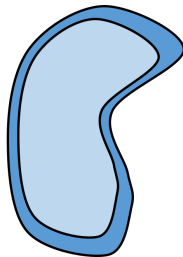
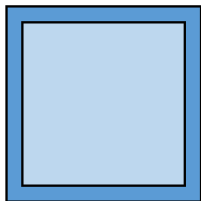
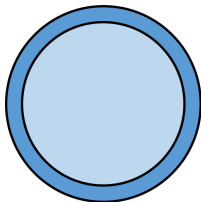
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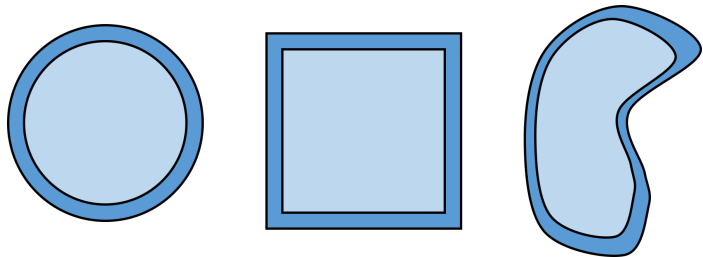
- **Isoperimetric inequality:** the ball has the minimum surface area/volume ratio of any shape.



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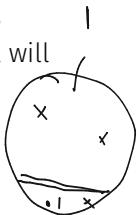
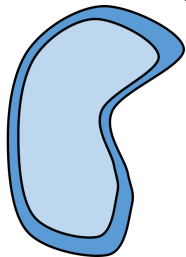
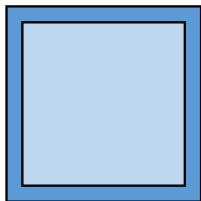
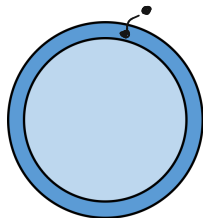


- If we randomly sample points from **any high-dimensional shape**, nearly all will fall near its surface.

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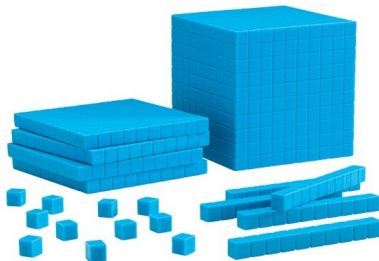


- If we randomly sample points from **any high-dimensional shape**, nearly all will fall near its surface.
- *curly* 'All points are outliers.'

BIZARRE SHAPE OF HIGH-DIMENSIONAL BALLS

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

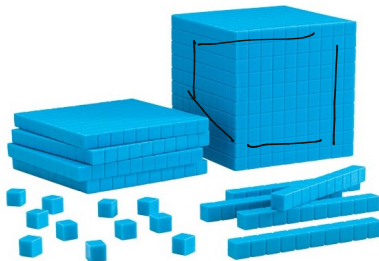
- a) 80% b) 50% c) 25% d) 10%



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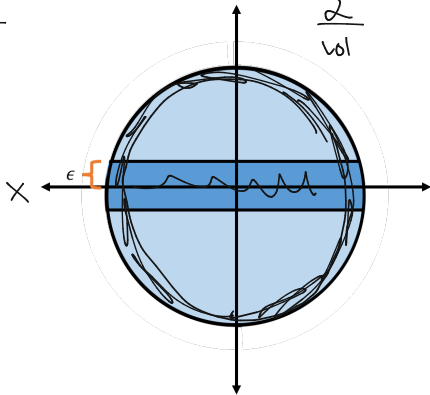
$$\frac{10^3 - 8^3}{10^3} = \frac{1000 - \underline{512}}{1000} = .488.$$

BIZARRE SHAPE OF HIGH-DIMENSIONAL BALLS

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

$$\frac{\epsilon}{d}$$

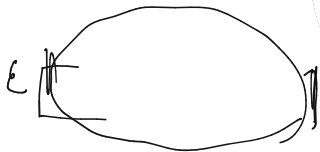
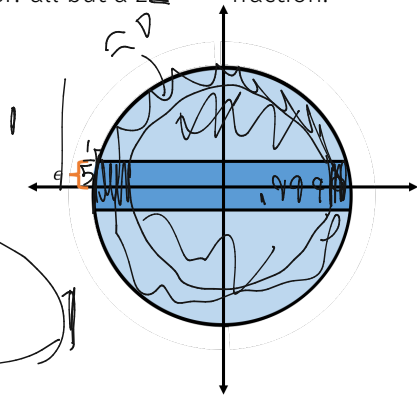
$$\frac{2^\epsilon}{\text{Vol}}$$



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

BIZARRE SHAPE OF HIGH-DIMENSIONAL BALLS

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.



$$\epsilon = 0.2 \quad d = 500$$
$$2^{-0.2^2 \cdot 500} = 2^{-20} \approx 0$$

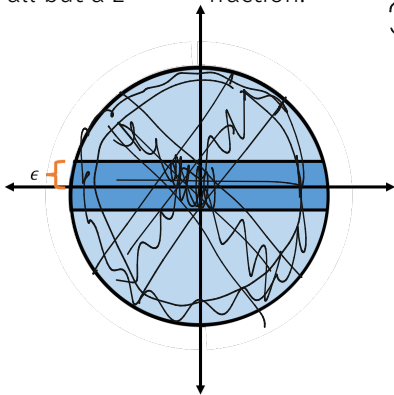
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What percentage of the volume of \mathcal{B}_d falls within ϵ distance of its equator? Answer: all but a $2^{\Theta(-\epsilon^2 d)}$ fraction.

$$\mathcal{B}_r = \{x : \|x\|_2 \leq r\}$$



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**! $S = \{x \in \mathcal{B}_d : |\langle x, t \rangle| \leq \epsilon\}$

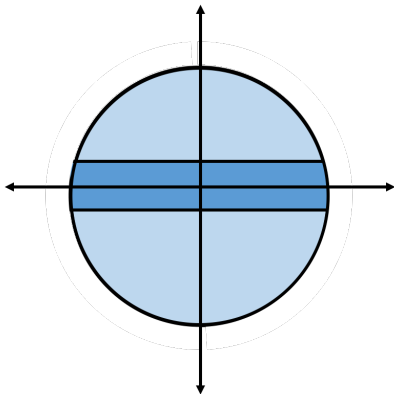
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Claim 2: All but a $2^{\Theta(-\epsilon d)}$ fraction falls within ϵ of its surface.

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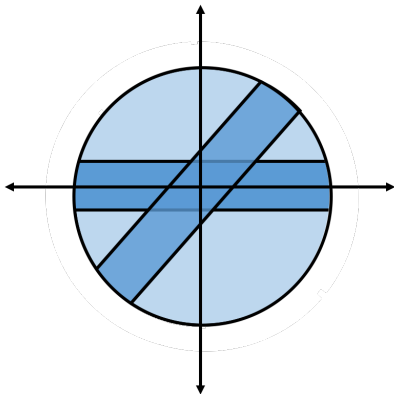
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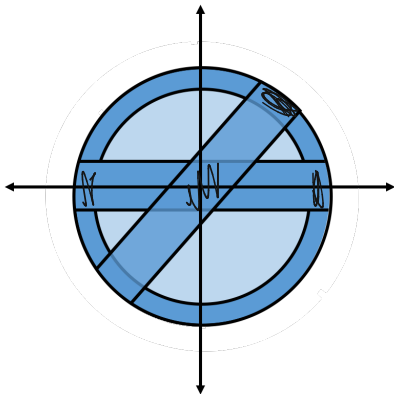
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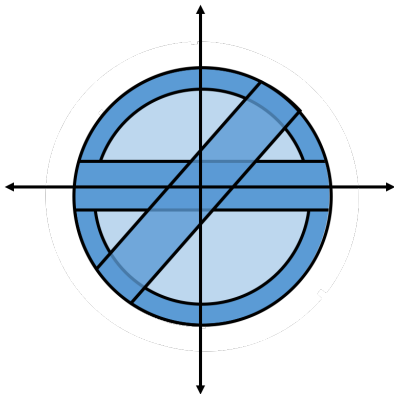
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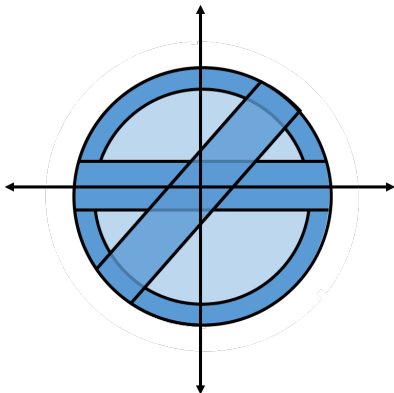


How is this possible?

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

CONCENTRATION OF VOLUME AT EQUATOR

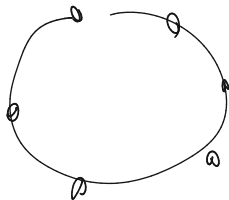
Claim: All but a $2^{\Theta(-\epsilon^2 d)}$ fraction of the volume of a ball falls within ϵ of its equator. I.e., in $S = \{x \in \mathcal{B}_d : |x(1)| \leq \epsilon\}$.

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Proof Sketch:

- Let x have independent Gaussian $\mathcal{N}(0, 1)$ entries and let $\bar{x} = \frac{x}{\|x\|_2}$. \bar{x} is selected uniformly at random from the surface of the ball.

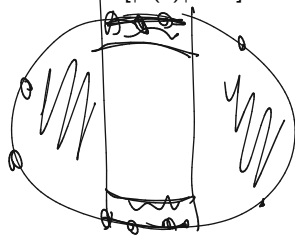


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- $\bar{x}(1) = \frac{x(1)}{\|x\|_2}$. What is $\mathbb{E}[\|x\|_2^2]$?

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- $\bar{x}(1) = \frac{x(1)}{\|x\|_2}$. $\mathbb{E}[\|x\|_2^2] = \sum_{i=1}^d \mathbb{E}[x(i)^2] = \underline{d}$.

Claim: All but a $2^{\Theta(-\epsilon^2 d)}$ fraction of the volume of a ball falls within ϵ of its equator. I.e., in $S = \{x \in \mathcal{B}_d : |x(1)| \leq \epsilon\}$.

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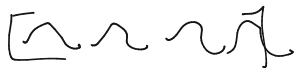
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 $\|x\|_2 \geq \sqrt{d/2}$

$$\begin{aligned} \Pr[|\bar{x}(1)| > \epsilon] &= \Pr[|x(1)| > \epsilon \cdot \|x\|_2] \\ &\leq \Pr[|x(1)| > \epsilon \cdot \sqrt{d/2}] \end{aligned}$$

CONCENTRATION OF VOLUME AT EQUATOR

Claim: All but a $2^{-\Theta(\epsilon^2 d)}$ fraction of the volume of a ball falls within ϵ of its equator. I.e., in $S = \{x \in \mathcal{B}_d : |x(1)| \leq \epsilon\}$.

Proof Sketch:



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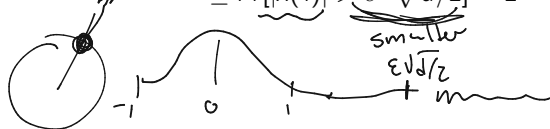
- Suffices to show that $\Pr[|\bar{x}(1)| > \epsilon] \leq 2^{-\Theta(\epsilon^2 d)}$. Why?

$$\bar{x}(1) = \frac{x(1)}{\|x\|_2} \cdot \mathbb{E}[\|x\|_2^2] = \sum_{i=1}^d \mathbb{E}[x(i)^2] = d. \quad \Pr[\|x\|_2^2 \leq d/2] \leq 2^{-\Theta(d)}$$

- Conditioning on $\|x\|_2^2 \geq d/2$, since $x(1)$ is normally distributed, $\|x\|_2^2 \geq d/2$

$$\Pr[|\bar{x}(1)| > \epsilon] = \Pr[|x(1)| > \epsilon \cdot \|x\|_2]$$

$$\leq \Pr[|x(1)| > \epsilon \cdot \sqrt{d/2}] = 2^{-\Theta(\epsilon^2 d/2)} = 2^{-\Theta(\epsilon^2 d)}$$



$$e^{-x^2/2} \quad \sqrt{d/2}$$

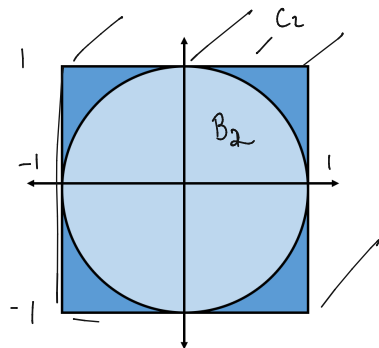
$$e^{-\epsilon^2 d/2} \approx 2^{-\Theta(\epsilon^2 d)}$$

Let \mathcal{C}_d be the d -dimensional cube: $\mathcal{C}_d = \{x \in \mathbb{R}^d : |x(i)| \leq 1 \forall i\}$.

HIGH-DIMENSIONAL CUBES

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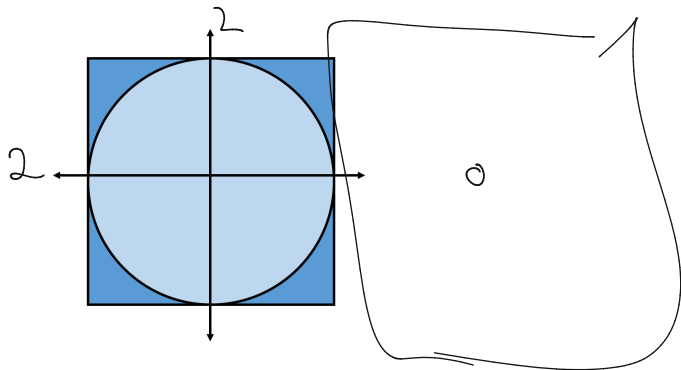
In low-dimensions, the cube is not that different from the ball.



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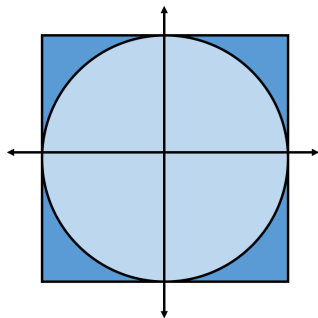


But volume of \mathcal{C}_d is 2^d while volume of \mathcal{B}^d is $\frac{\pi^{d/2}}{(d/2)!} = \frac{1}{d^{\Theta(d)}}$. A huge gap!

HIGH-DIMENSIONAL CUBES

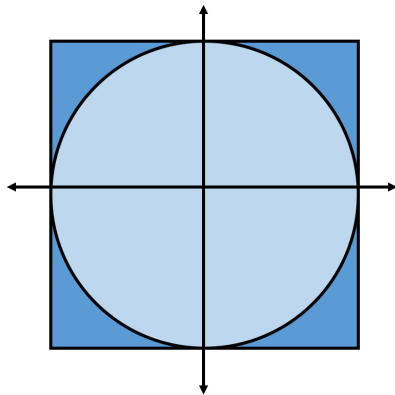
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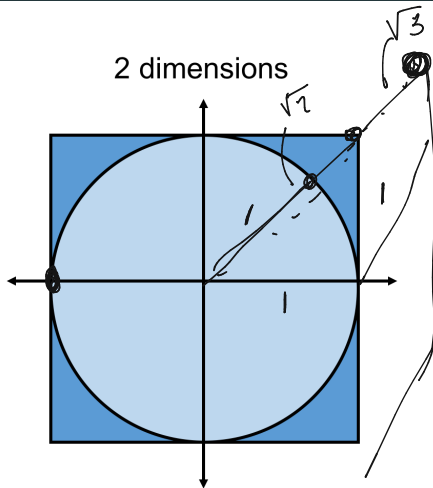


But volume of \mathcal{C}_d is 2^d while volume of \mathcal{B}^d is $\frac{\pi^{\frac{d}{2}}}{(d/2)!} = \frac{1}{d^{\Theta(d)}}$. A huge gap! So something is very different about these shapes...

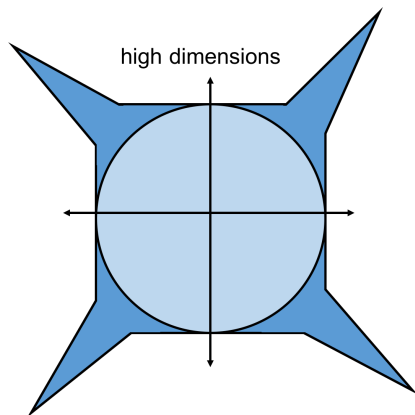
2 dimensions



HIGH-DIMENSIONAL CUBES



Corners of cube are \sqrt{d} times further away from the origin than the surface of the ball.



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Data generated from the ball \mathcal{B}_d will behave very differently than data generated from the cube \mathcal{C}_d .

HIGH-DIMENSIONAL CUBES

Data generated from the ball \mathcal{B}_d will behave very differently than data generated from the cube \mathcal{C}_d .

• $x \sim \mathcal{B}_d$ has $\|x\|_2^2 \leq 1$.

• $x \sim \mathcal{C}_d$ has $\mathbb{E}[\|x\|_2^2] = ?$,

$[x^{(1)} \quad x^{(2)} \quad \dots \quad x^{(d)}]$
↓
uniform random
on $[-1, 1]$

$$\mathbb{E}[\|x\|_2^2] = \sum_{i=1}^d \mathbb{E}[x^{(i)2}] = \sum_{i=1}^d \text{Var}(x_i) = \frac{d}{3}$$

$O(\dots)$

HIGH-DIMENSIONAL CUBES

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- $x \sim \mathcal{B}_d$ has $\|x\|_2^2 \leq 1$.

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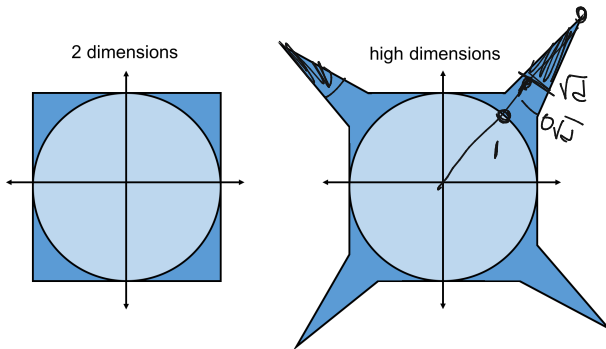
- $x \sim \mathcal{B}_d$ has $\|x\|_2^2 \leq 1$.
- $x \sim \mathcal{C}_d$ has $\mathbb{E}[\|x\|_2^2] = d/3$, and $\Pr[\|x\|_2^2 \leq d/6] \leq 2^{-\Theta(d)}$.

HIGH-DIMENSIONAL CUBES

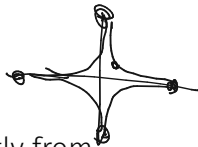
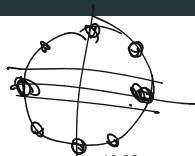
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- $x \sim \mathcal{B}_d$ has $\|x\|_2^2 \leq 1$.
- $x \sim \mathcal{C}_d$ has $\mathbb{E}[\|x\|_2^2] = d/3$, and $\Pr[\|x\|_2^2 \leq d/6] \leq 2^{-\Theta(d)}$.
- Almost all the volume of the unit cube falls far away from the origin – i.e., far outside the unit ball.

$$1 - 2^{-d}$$



TAKAWAYS



- High-dimensional space behaves very differently from low-dimensional space.
- Random projection (i.e., the JL Lemma) reduces to a much lower-dimensional space that is still large enough to capture this behavior on a subset of n points.
- Need to be careful when using low-dimensional intuition for high-dimensional vectors.

Need to be careful when modeling data as ^{uniform} random vectors in high-dimensions.

$\epsilon > \frac{1}{\sqrt{d}}$

$$\begin{bmatrix} \pm \frac{1}{\sqrt{d}} & \pm \frac{1}{\sqrt{d}} & \pm \frac{1}{\sqrt{d}} \\ \pm 1 & 0 & 0 & 0 \\ 0 & \pm 1 & 0 & 0 \end{bmatrix}$$

$\|x\| = \begin{cases} \epsilon \sqrt{d} \\ \frac{1}{\sqrt{d}} \\ 1 \end{cases}$