Machine Learning: High-dimensional statistics

Hao Tang

March 22, 2024

High-dimensional objects in machine learning

- A 28×28 image
- A one-hot vector that represents a word in a 20000-word vocabulary set

Intuitions

- We tend to extrapolate our intuitions from two- or three-dimensional space to high-dimensional spaces.

- Many intuitions in two- and three-dimensional spaces fail to hold in high dimensions.

Volume concentration

- The volume of a ball with radius r is

$$V(r) = \frac{\pi^{d/2}}{\Gamma(d/2+1)} r^d. \tag{1}$$

Volume concentration

- The volume of a ball with radius r is

$$V(r) = \frac{\pi^{d/2}}{\Gamma(d/2+1)} r^d. \tag{1}$$

- If we shrink the radius by a small amount ϵ, the volume shrinks by

$$\frac{V((1-\epsilon)r)}{V(r)} = \frac{(1-\epsilon)^d V(r)}{V(r)} = (1-\epsilon)^d \leq e^{-\epsilon d}. \tag{2}$$

- The last inequality uses $1 - x \leq e^{-x}$.

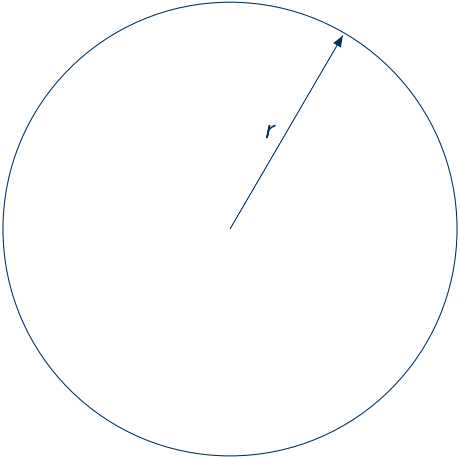
Volume concentration

- As d becomes large, $V((1-\epsilon)r)$ is only a small fraction of $V(r)$.
- The volume of a ball in high dimensions concentrates on the thin crust of the ball.

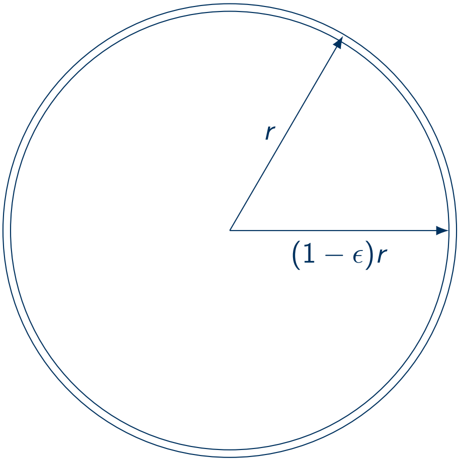
Volume concentration

- As d becomes large, $V((1-\epsilon)r)$ is only a small fraction of $V(r)$.
- The volume of a ball in high dimensions concentrates on the thin crust of the ball.
- If you uniformly sample a point, you will likely end up at the crust of the ball.

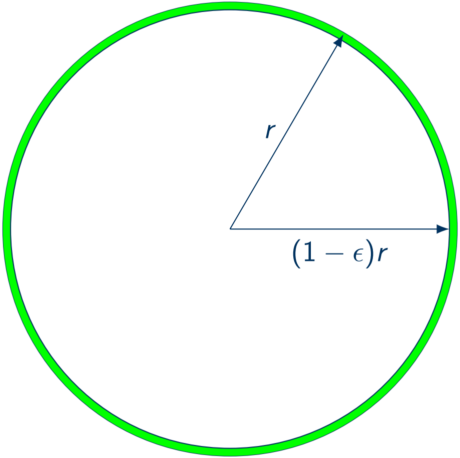
Volume concentration



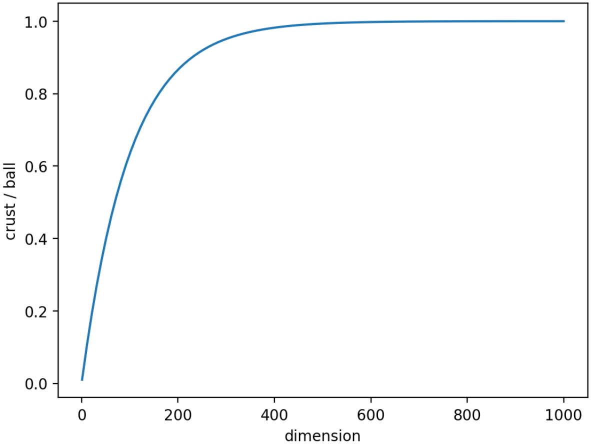
Volume concentration



Volume concentration



Volume concentration



Volume of a unit ball

- The volume of a unit ball ($r = 1$) is

$$V(1) = \frac{\pi^{d/2}}{\Gamma(d/2 + 1)}. \tag{3}$$

- $\Gamma(x + 1) \sim \sqrt{2\pi x} \left(\frac{x}{e}\right)^x$

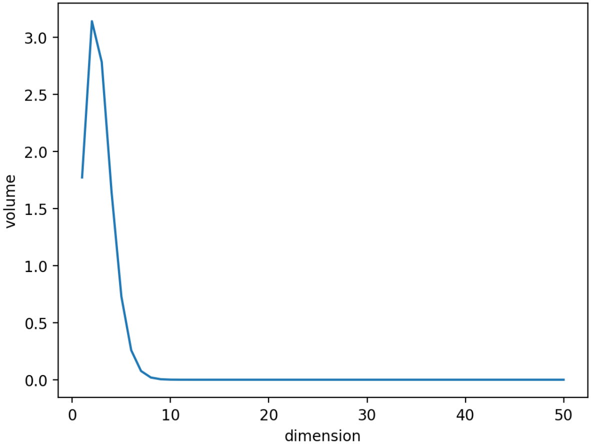
Volume of a unit ball

- The volume of a unit ball ($r = 1$) is

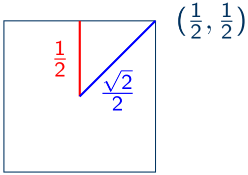
$$V(1) = \frac{\pi^{d/2}}{\Gamma(d/2+1)}. \tag{3}$$

- $\Gamma(x+1) \sim \sqrt{2\pi x}\left(\frac{x}{e}\right)^x$
- $V(1) \to 0$ when $d \to \infty$.

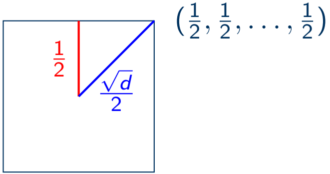
Volume of a unit ball



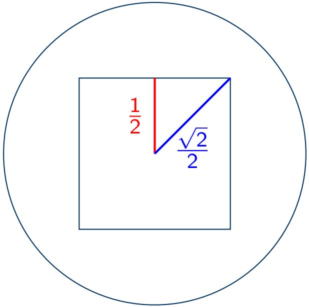
Corners of the unit cube



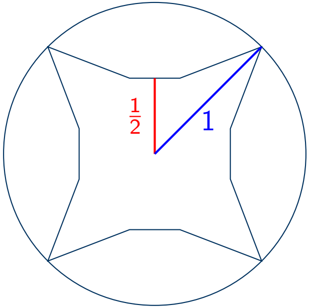
Corners of the unit cube



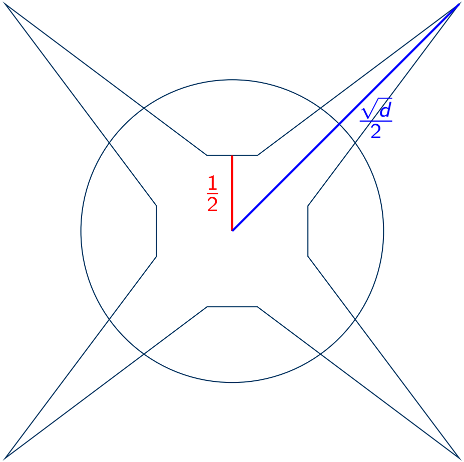
Corners of the unit cube ($d = 2$)



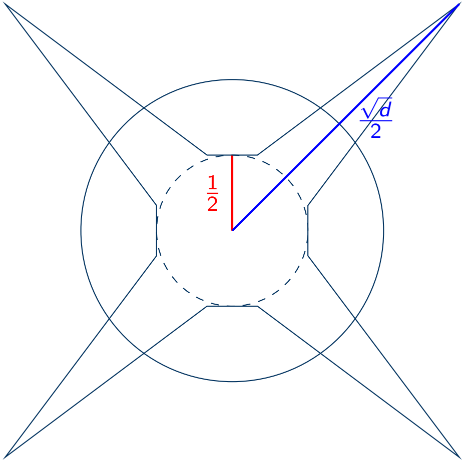
Corners of the unit cube ($d = 4$)



Corners of the unit cube



Corners of the unit cube



Corners of the unit cube

- The distance between the origin and the corner is $\frac{\sqrt{d}}{2}$.
- For example, one corner is $(1/2, 1/2, \ldots, 1/2)$.
- The distance between the origin and one of the faces is $\frac{1}{2}$.
- The distances to the faces stay the same, while the distances to the corners becomes large, when d is large.

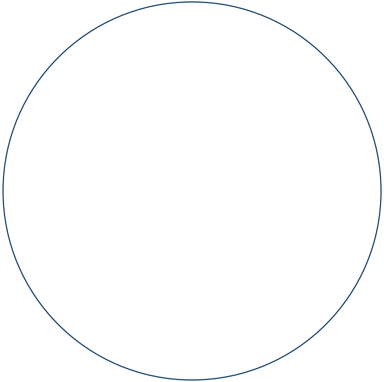
Volume near the equator

- Pick a north direction.
- Pick $\epsilon > 0$, the width of a slab. The volume above is about $\frac{2}{\epsilon\sqrt{d}}e^{-d\epsilon^2/2}$.

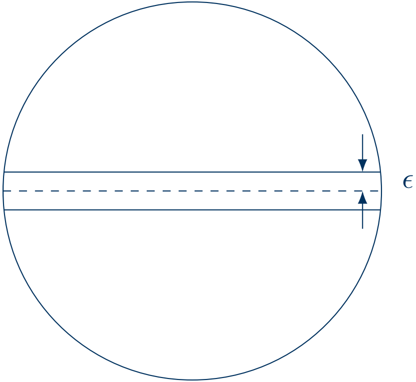
Volume near the equator

- Pick a north direction.
- Pick $\epsilon > 0$, the width of a slab. The volume above is about $\frac{2}{\epsilon\sqrt{d}} e^{-d\epsilon^2/2}$.
- The volume is concentrated at the equator.

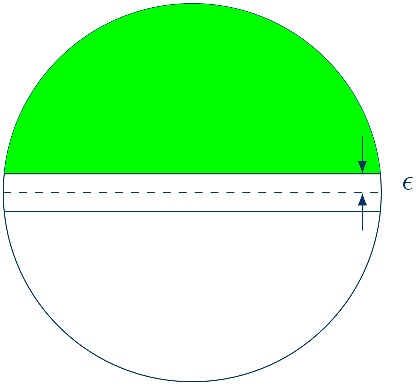
Volume near the equator



Volume near the equator



Volume near the equator



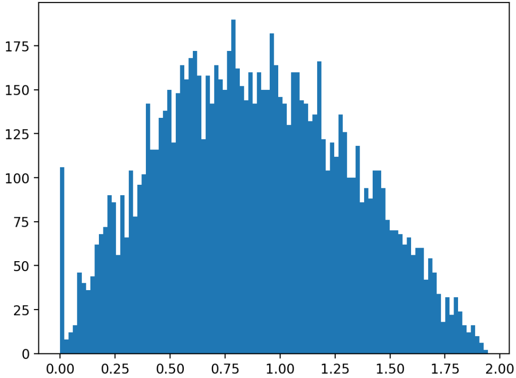
Two random vectors inside a unit ball

- Pick a random vector u inside the unit ball.
- Set u to be the north.
- Since most of the volume is concentrated at the equator, another random vector v will likely lies on the equator.
- The dot product $u^\top v$ will likely be close to 0.

Distances of two random vectors

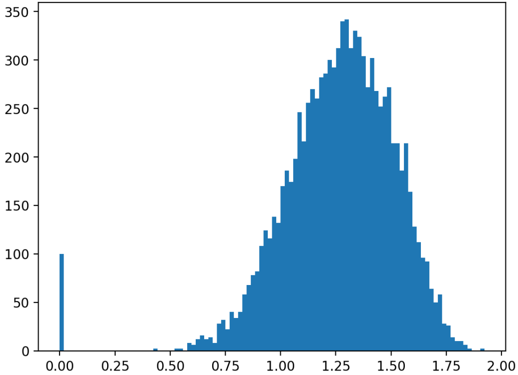
- Any two random vectors u and v in a unit ball are likely to be orthogonal, meaning $u^\top v$ is likely to be small.
- The volume is concentrated at the crust, so $\|u\|_2$ and $\|v\|_2$ are likely to be close to 1.
- The distance of any two random vectors u and v is likely to be about $\sqrt{2}$.

Distances of two random vectors



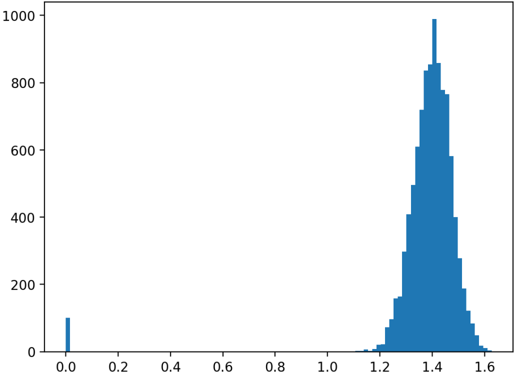
$d = 2$

Distances of two random vectors



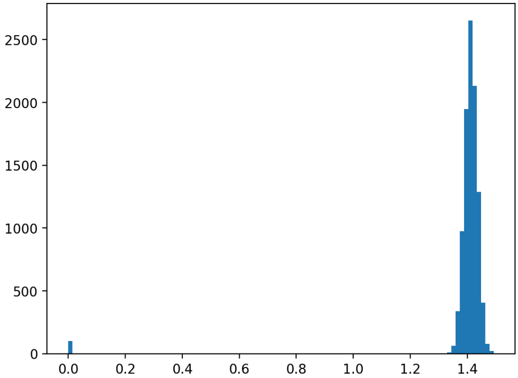
$d = 10$

Distances of two random vectors



$d = 100$

Distances of two random vectors



$d = 1000$

Distances of two random vectors

- Distances of two random vectors in a unit ball concentrate at $\sqrt{2}$.
- Most points have similar distances!

Norm of random Gaussian vectors

- For any $x \sim \mathcal{N}(0, I)$,

$$\mathbb{P}\left(\frac{\|x\|_2^2}{d} - 1 > \epsilon\right) \leq \exp\left(\frac{-d\epsilon^2}{8}\right). \tag{4}$$

Norm of random Gaussian vectors

- For any $x \sim \mathcal{N}(0, I)$,

$$\mathbb{P}\left(\frac{\|x\|_2^2}{d} - 1 > \epsilon\right) \leq \exp\left(\frac{-d\epsilon^2}{8}\right). \tag{4}$$

- In words, for any $x \sim \mathcal{N}(0, I)$, $\|x\|_2$ is about $\sqrt{d}$.

Norm of random Gaussian vectors

- For any $x \sim \mathcal{N}(0, I)$,

$$\mathbb{P}\left(\frac{\|x\|_2^2}{d} - 1 > \epsilon\right) \leq \exp\left(\frac{-d\epsilon^2}{8}\right). \tag{4}$$

- In words, for any $x \sim \mathcal{N}(0, I)$, $\|x\|_2$ is about $\sqrt{d}$.

- "High-dimension Gaussian is like a soap buble."