High Dimensional Space

longhuan@sjtu.edu.cn
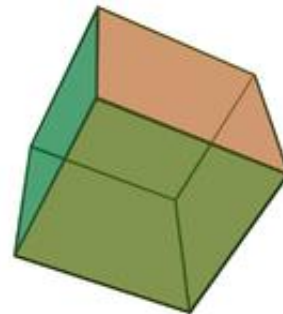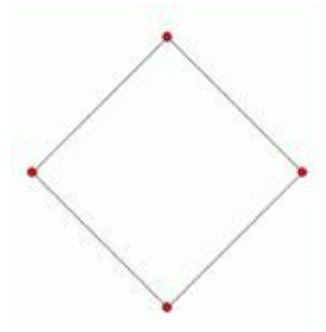
Word Vector Model

Web Page Model

web page 4 → $(1,0,1,0,0,1)$

web page 5 → $(1,1,1,0,0,1)$
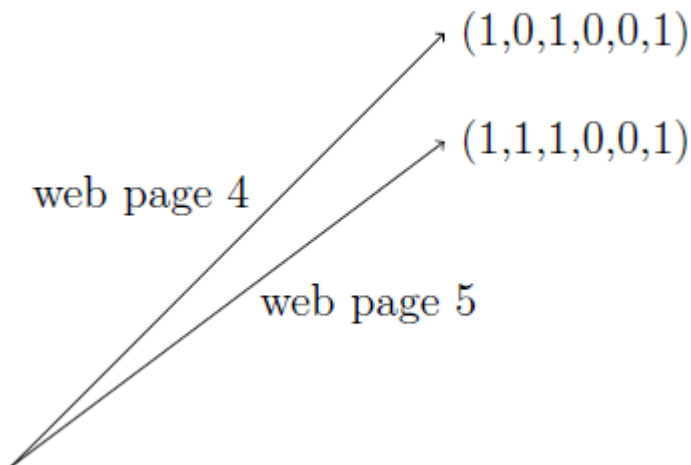
- Nearest neighbor query
- Information retrieval
- Web page rank
- Online recommendation
- ……

The law of Large numbers

Properties of High-Dimensional space, unit ball

Generating points uniformly at random from a ball

Gaussians in High Dimension

Random Projection and Johnson-Lindenstrauss Lemma

Seperating Gaussians

Normal distribution (Gauss Distribution)

$X \sim N(\mu, \sigma^2)$, with density function:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}, \qquad -\infty < x < +\infty$$

Variance

$$Var(X) = E((X - E[X])^2)$$

$$= E(X^2 + E[X]^2 - 2XE[X])$$

$$= E(X^2 - E[X]^2)$$

$$= E[X^2] - E[X]^2$$

Chebyshev's Inequality

$$\forall a > 0, \Pr(|X - E(X)| \geq a) \leq \frac{Var[X]}{a^2}$$

Law of Large Numbers

- In probability theory, the **law of large numbers** (**LLN**) is a theorem that describes the result of performing the same experiment a large number of times.

- According to the law, the average of the results obtained from a large number of trials should be close to the expected value, and will tend to become closer as more trials are performed.

Law of large numbers

Let $x_1, x_2, \ldots, x_n$ be n independent samples of a random variable x, then

$$\Pr\left(\left|\frac{x_1 + x_2 + \cdots x_n}{n} - E(x)\right| \geq \epsilon\right) \leq \frac{Var(x)}{n\epsilon^2}$$

Proof. (Chebychev's Inequality)

$$\Pr\left(\left|\frac{x_1 + x_2 + \cdots x_n}{n} - E(x)\right| \geq \epsilon\right) \leq \frac{Var\left(\frac{x_1 + x_2 + \cdots x_n}{n}\right)}{\epsilon^2}$$

$$= \frac{Var(x_1 + x_2 + \cdots x_n)}{n^2 \epsilon^2}$$

$$= \frac{Var(x)}{n\epsilon^2}$$

Application

- x be a $d-$dimensional random point whose coordinates are each selected from $N\left(0, \frac{1}{2\pi}\right)$,

- i.e. $x = [x_1, x_2, \ldots, x_d]$ with $x_i \sim N\left(0, \frac{1}{2\pi}\right)$

- By LLN: $|x|^2 = \sum_{i=1}^{d} x_i^2 = \frac{d}{2\pi} = \Theta(d)$ with high probability.

- The probability that point x lie in the unit ball is *vanishingly small*.

Application

- $x, y : [z_1, z_2, \ldots, z_d]$ with $z_i \sim N(0, 1)$
- $|x|^2 \approx d, |y|^2 \approx d,$
- $|x - y|^2 \approx ?$

Application

- $x, y : [z_1, z_2, \ldots, z_d]$ with $z_i \sim N(0, 1)$

- $|x|^2 \approx d, |y|^2 \approx d,$

- $|x - y|^2 = \sum_{i=1}^{d} (x_i - y_i)^2$

$$E(x_i - y_i)^2 = E(x_i^2) + E(y_i^2) - 2E(x_i y_i)$$

$$= 1 + 1 - 2E(x_i)E(y_i) = 2.$$

Application

- $x, y : [z_1, z_2, \ldots, z_d]$ with $z_i \sim N(0, 1)$
- $|x|^2 \approx d, |y|^2 \approx d,$
- $|x - y|^2 = \sum_{i=1}^{d}(x_i - y_i)^2 = 2d$

$$E(x_i - y_i)^2 = E(x_i^2) + E(y_i^2) - 2E(x_i y_i)$$
$$= 1 + 1 - 2E(x_i)E(y_i) = 2.$$

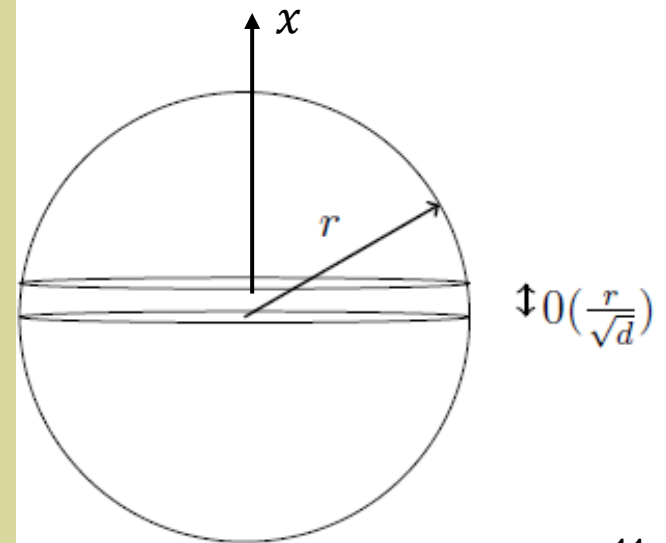- $|x - y|^2 \approx |x|^2 + |y|^2$
- <mark>Pythagorean theorem</mark> $\Rightarrow$ random $d-$dimensional x, y are approximately orthogonal.

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Application

- $x, y : [z_1, z_2, \ldots, z_d]$ with $z_i \sim N(0, 1)$
- Pythagorean theorem $\Rightarrow$ random $d-$dimensional x, y are approximately orthogonal.
- If we scale these random points to be unit length and call x the North Pole, *much of the surface area of the unit ball must lie near the equator.*

$\updownarrow O\left(\frac{r}{\sqrt{d}}\right)$

Table of tail bounds

	Condition	Tail bound
Markov	$x \geq 0$	$\mathrm{Prob}(x \geq a) \leq \frac{E(x)}{a}$
Chebychev	Any x	$\mathrm{Prob}(|x - E(x)| \geq a) \leq \frac{\mathrm{Var}(x)}{a^2}$
Chernoff	$x = x_1 + x_2 + \cdots + x_n$ $x_i \in [0, 1]$ i.i.d. Bernoulli;	$\mathrm{Prob}(|x - E(x)| \geq \varepsilon E(x))$ $\leq 3e^{-c\varepsilon^2 E(x)}$
Higher Moments	r positive even integer	$\mathrm{Prob}(|x| \geq a) \leq E(x^r)/a^r$
Gaussian Annulus	$x = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$ $x_i \sim N(0, 1); \beta \leq \sqrt{n}$ indep.	$\mathrm{Prob}(|x - \sqrt{n}| \geq \beta) \leq 3e^{-c\beta^2}$
Power Law for x_i; order $k \geq 4$	$x = x_1 + x_2 + \ldots + x_n$ x_i i.i.d ; $\varepsilon \leq 1/k^2$	$\mathrm{Prob}(|x - E(x)| \geq \varepsilon E(x))$ $\leq (4/\varepsilon^2 kn)^{(k-3)/2}$

The law of Large numbers
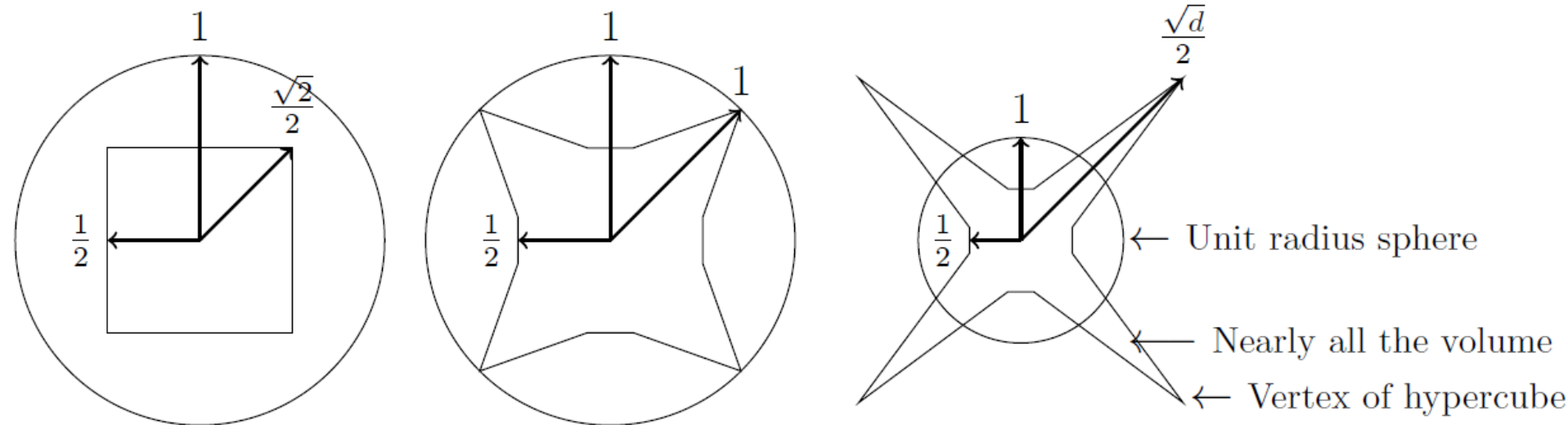
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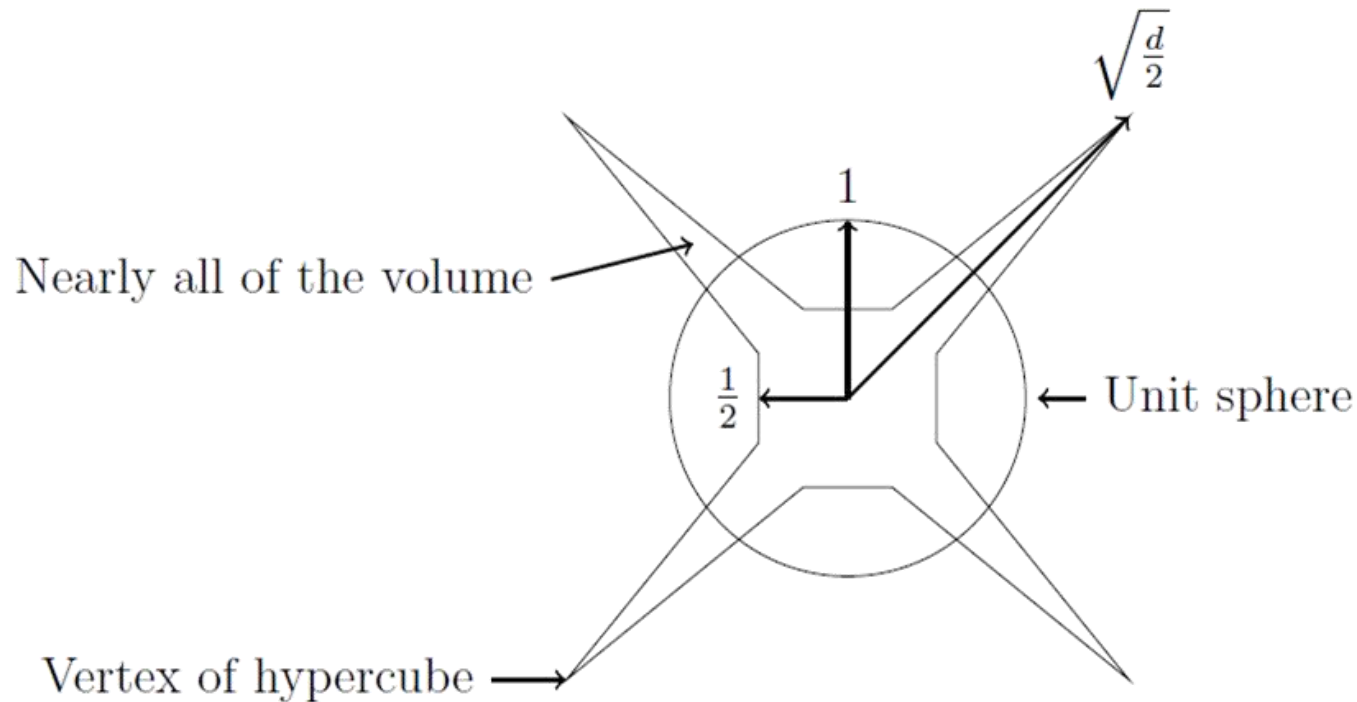
Random Projection and Johnson-Lindenstrauss Lemma

Seperating Gaussians

Relationship between the <mark>sphere and cube</mark>

The difference between the volume of a cube with unit-length sides and the volume of a unit-radius sphere at the dimensions: $2, 4$ and d.

Conceptual drawing of a sphere and a cube

For large d, almost all the volume of the cube is located outside the sphere.

Geometry of High Dimensions

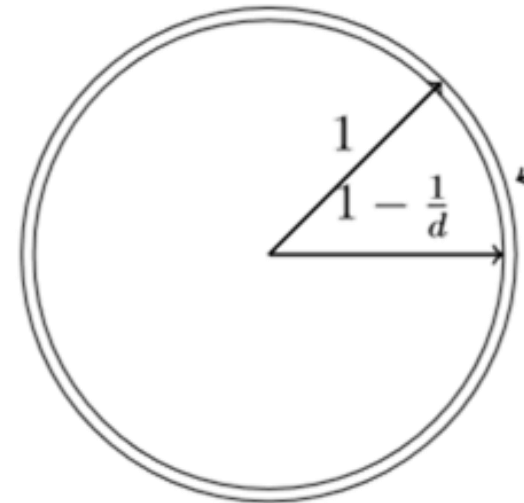- Most of the volume of the high-dimensional objects is near the surface:

$$\frac{Volume\big((1 - \epsilon)A\big)}{Volume(A)} = (1 - \epsilon)^d \leq e^{-\epsilon d}$$

Fix ϵ and letting $d \to \infty$, the above quantity rapidly approaches zero.

- **Application:**

S be the unit ball in $d -$dimensions (i.e., the set of points within distance 1 of the origin). Then $1 - e^{-\epsilon d}$ fraction of the volume is in $S \backslash (1 - \epsilon)S$.

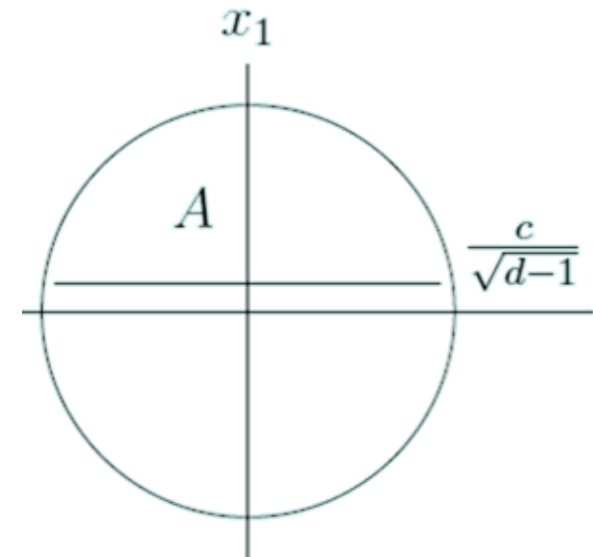Especially, consider $\epsilon = \frac{1}{d}$.

Unit ball in $d-$dimensions

- Surface: $A(d) = \dfrac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)}$, Volume: $\mathrm{V}(d) = \dfrac{2}{d}\dfrac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)}$.

- $V(2) = \pi, V(3) = \dfrac{4}{3}\pi$, $\quad \lim_{n\to\infty} V(d) = 0.$ 随着维度增加，单位球的体积会无限趋近于0

- Most of the volume of a unit ball in high dimensions is concentrated near its equator no matter which direction is defined to be the North Pole.

Theorem: For $c \geq 1$ and $d \geq 3$, at least a $1 - \dfrac{2}{c}e^{-c^2/2}$ fraction of the volume of the $d-$dimensional unit ball has $|x_1| \leq \dfrac{c}{\sqrt{d-1}}$.

x_1

A

$\dfrac{c}{\sqrt{d-1}}$

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The law of Large numbers

Properties of High-Dimensional space, unit ball
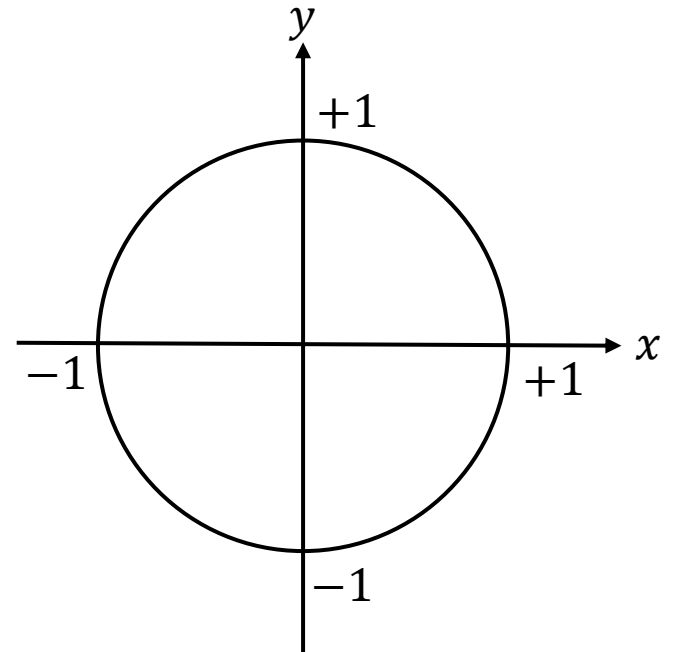
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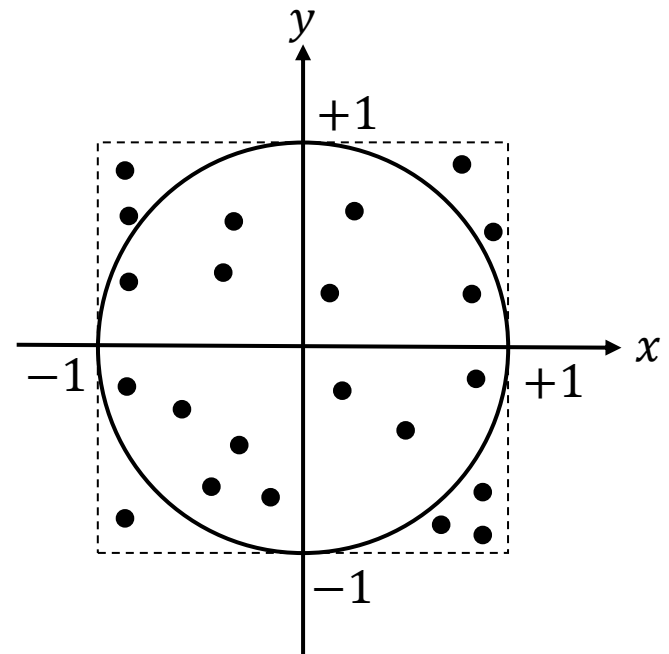
Seperating Gaussians

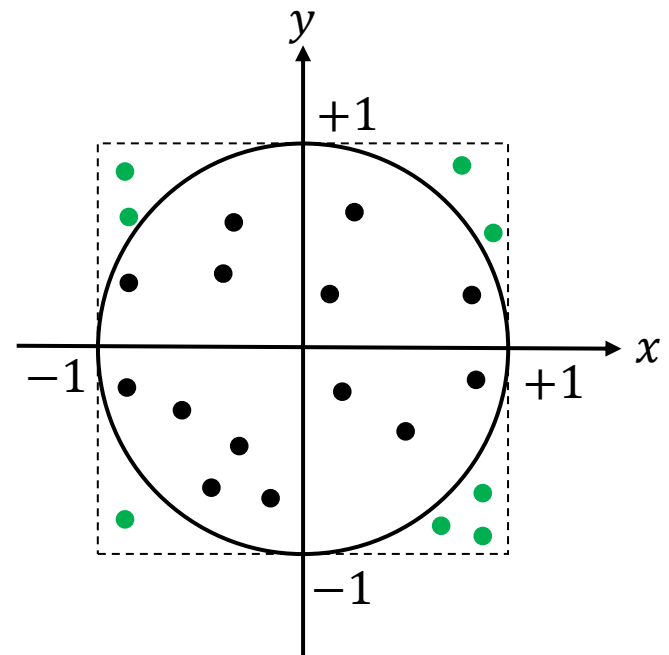# Generating points uniformly at random on the surface of the unit ball

- $d = 2$

Generating points uniformly at random on the surface of the unit ball

- $d = 2$
  - Generate x_i, y_i u.a.r from the interval $[-1,1]$;

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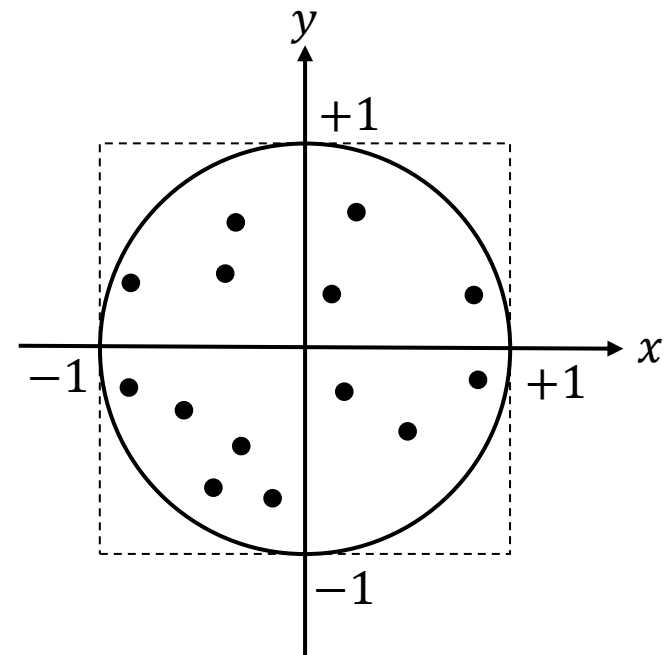 - Discard the points outside the unit circle;

Generating points uniformly at random on the surface of the unit ball

- $d = 2$
  - Generate x_i, y_i u.a.r from the interval $[-1,1]$;
  - Discard the points outside the unit circle;
  - Project the remaining points onto the circle.

- How about d is large?
  - The above strategy would fail. (why?)
  ① Surface: Spherical normal distribution + Normalizing.
  ② Surface+interior: Scale the point on the surface.
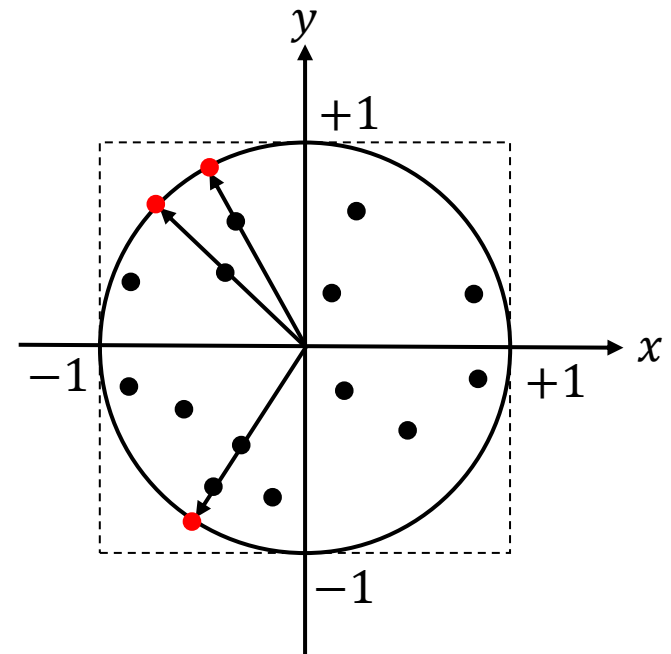
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- 1-dimensional Gaussian

Gaussian or "normal" distribution

$f_g(x)$

.0214   .0214

.00135   .1359   .3413   .3413   .1359   .00135

-3σ -2σ $-\sigma$ 0 σ 2σ 3σ

x

- <mark>d −dimensional spherical Gaussian with 0 means and variance σ^2 in each coordinate has density function</mark>:

$$p(x) = \frac{1}{(2\pi)^{d/2}\sigma^d} \, exp\left(-\frac{|x|^2}{2\sigma^2}\right)$$

- Integrate the PDF over a unit ball centered at the origin will cover almost 0 mass, for the volume of such a ball is negligible.

- The radius of the ball need to be nearly $\sqrt{d}$ before there is a significant volume and hence significant probability mass.

Gaussian Annulus Theorem

- For a $d-$dimensional spherical Gaussian with unit variance in each direction ,for any $\beta \leq \sqrt{d}$, all but at most $3e^{-c\beta^2}$ of the probability mass lies within the annulus

$$\sqrt{d} - \beta \leq |x| \leq \sqrt{d} + \beta$$

where c is a fixed positive constant.

The law of Large numbers

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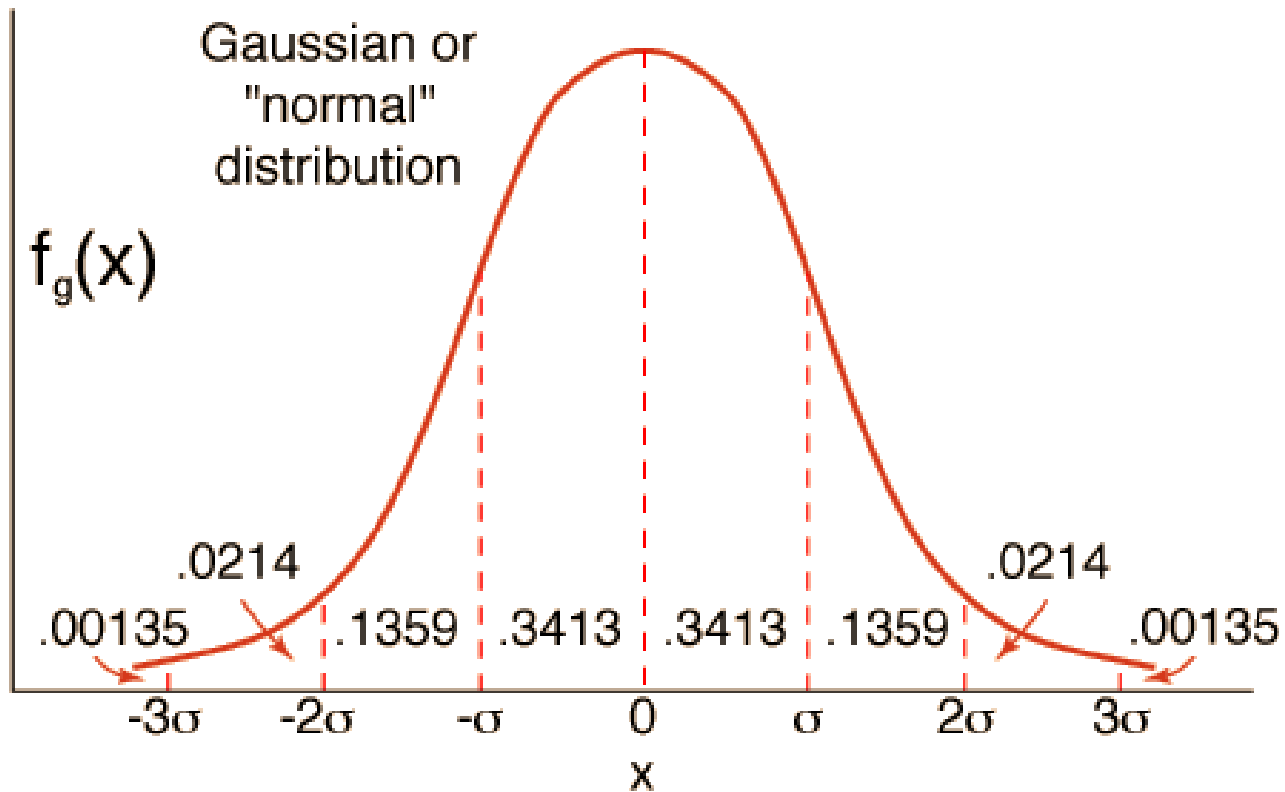
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Separating Gaussians

Database query: Nearest neighbor search

n points from R^d:
$$\begin{bmatrix} v_{11} & v_{21} & \vdots & v_{n1} \\ v_{12} & v_{22} & \vdots & v_{n2} \\ \vdots & \vdots & \vdots & \vdots \\ v_{1d} & v_{2d} & \vdots & v_{nd} \end{bmatrix}$$

- Nearest neighbor search: find the nearest or approximately nearest database point to the query point.

- When d is large, it could cost more than expected.

- Dimension reduction : *Project* the database points to a k dimensional space with $k \ll d$. It will work so long as the relative distances between points are approximately preserved.

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Projection function

- Pick k vectors $\boldsymbol{u_1}, \boldsymbol{u_2}, \dots, \boldsymbol{u_k}$, independently from the Gaussian distribution $\frac{1}{(2\pi)^{d/2}\sigma^d} exp\left(-\frac{|x|^2}{2\sigma^2}\right)$, for any vector $\boldsymbol{\color{red}v}$, the projection $f: R^d \to R^k$ is:

$$f(\boldsymbol{\color{red}v}) = (\boldsymbol{u_1} \cdot \boldsymbol{\color{red}v}, \boldsymbol{u_2} \cdot \boldsymbol{\color{red}v}, \dots, \boldsymbol{u_k} \cdot \boldsymbol{\color{red}v})$$

Projection function

Pick k vectors $\boldsymbol{u_1, u_2, \ldots, u_k}$, independently from the Gaussian distribution $\frac{1}{(2\pi)^{d/2}\sigma^d} exp\left(-\frac{|x|^2}{2\sigma^2}\right)$, for any vector $\boldsymbol{v}$, the projection $f: R^d \to R^k$ is:

$$f(\boldsymbol{v}) = (\boldsymbol{u_1 \cdot v, u_2 \cdot v, \ldots, u_k \cdot v})$$

- $f(v_1 - v_2) = f(v_1) - f(v_2)$

- $|f(v)| \approx \sqrt{k}|v|$ w.h.p.

- To estimate $|v_1 - v_2|$, it suffices to compute $|f(v_1) - f(v_2)|$

Random Projection Theorem

- Let v be a fixed vector in R^d and let f be defined as above. Then there exists constant $c > 0$ such that for $\epsilon \in (0,1)$

$$\Pr\left(\left|\|f(v) - \sqrt{k}|v|\right| \geq \epsilon\sqrt{k}|v|\right|\right) \leq 3e^{-ck\epsilon^2}$$

Johnson-Lindenstrass Lemma

- For any $0 < \epsilon < 1$ and any integer n, let $k \geq \frac{3}{c\epsilon^2} \ln n$ for c as in the Gaussian Annulus theorem, for any set of n points in R^d, the random projection f defined above has the property that for all pairs of points v_i and v_j, with probability at least $1 - \frac{1.5}{n}$

$$(1 - \epsilon)\sqrt{k}\left|v_i - v_j\right| \leq \left|f(v_i) - f(v_j)\right| \leq (1 + \epsilon)\sqrt{k}\left|v_i - v_j\right|.$$

Comments

- JL lemma works for all pairs of points,
- k depends on $\ln n$,
- To the database, JL Lemma says the algorithm will yield the right answer with high probability whatever the query is.
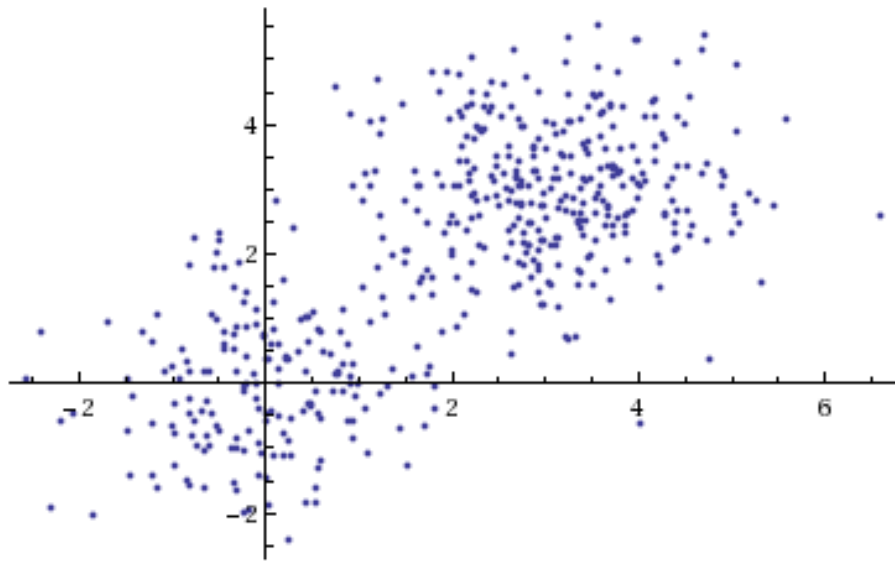
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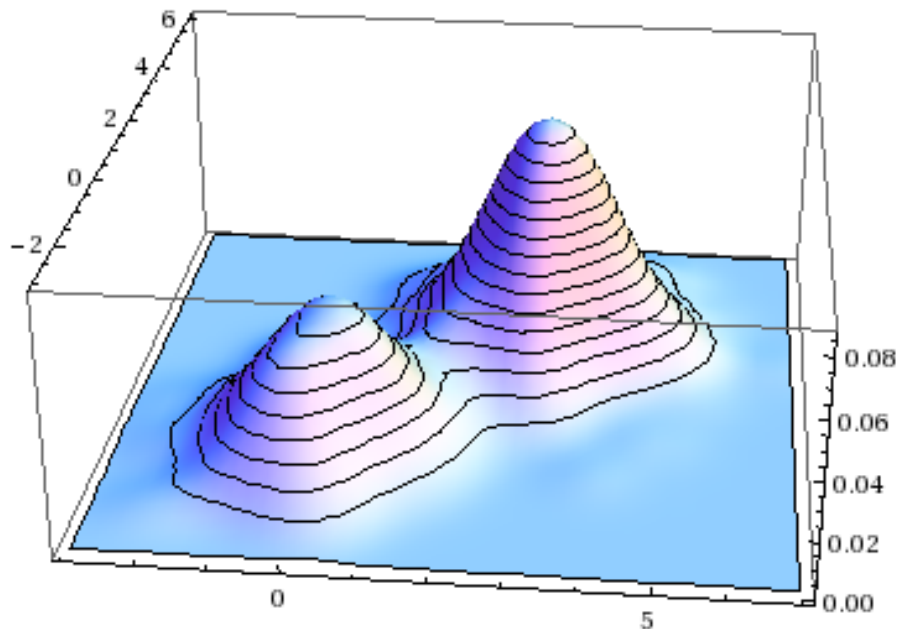Generating points uniformly at random from a ball

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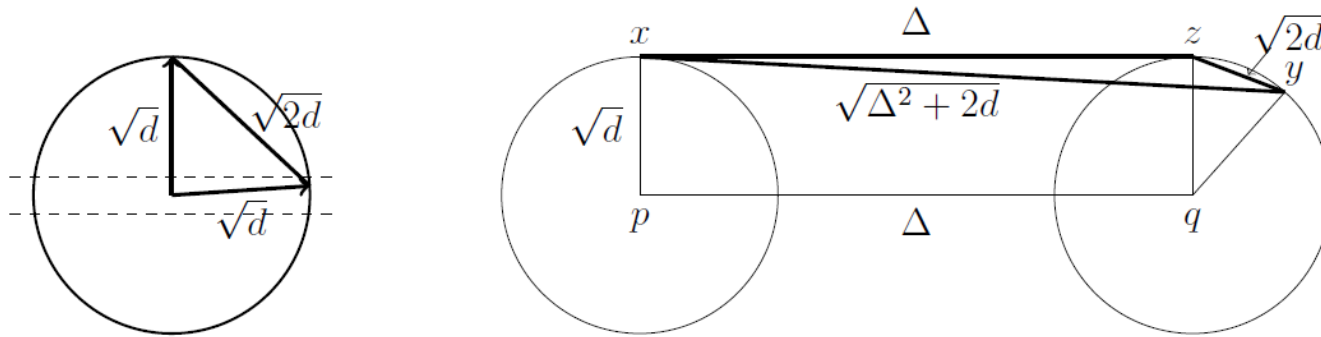
Separating Gaussians

- Mixtures of Gaussians

- Parameter estimation problem

- When $\Delta \in \Omega(d^{1/4})$

- Algorithm for separating points from two Gaussians: Calculate all pairwise distance between points. The cluster of smallest pairwise distances must come from a single Gaussian. Remove these points. The remaining points come from the second Gaussian.