K-nearest Neighbor

Announcements:

1. HW1 will be out today / early tomorrow and Due Sep 12

2. P1 will be out later this week

3. First paper reading quiz will be out later this week (for 5780)

Recap on ML basics

T/F: A hypothesis that achieves zero training error is always good

T/F: zero-one loss is a good loss function for regression

T/F: We can use validation dataset to check if our model overfits

Objective

Understand KNN — our first ML algorithm that can do both regression and classification

Outline for Today

1. The K-NN Algorithm

2. Why/When does K-NN work

3. Curse of dimensionality (i.e., when it can fail)

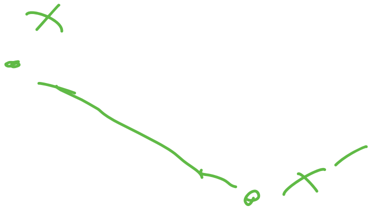
The K-NN Algorithm

Input: classification training dataset $\{x_i, y_i\}_{i=1}^n$, and parameter $K \in \mathbb{N}^+$,

and a distance metric $d(x, x')$ (e.g., $\|x - x'\|_2$ euclidean distance)

$x - x' = \sqrt{(x-x')^T (x-x')}$

K-NN Algorithm:



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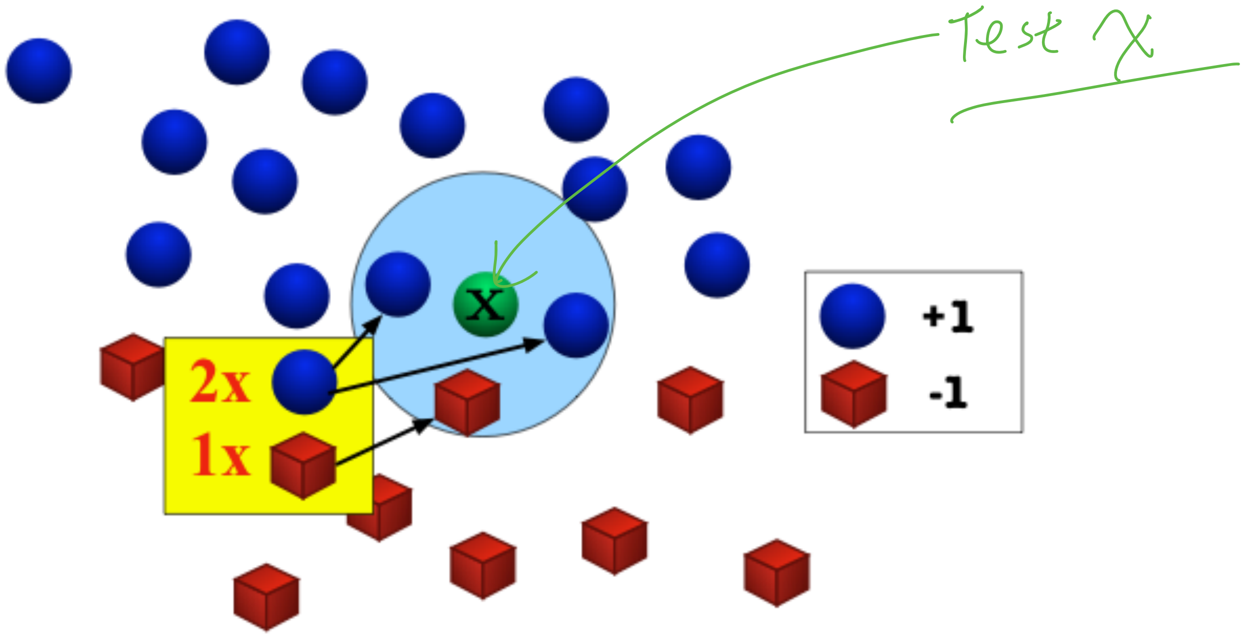
(If for regression, return the average value of the K neighbors)

The K-NN Algorithm

Example: 3-NN for binary classification using Euclidean distance



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Examples that are close to each other under distance d share similar labels

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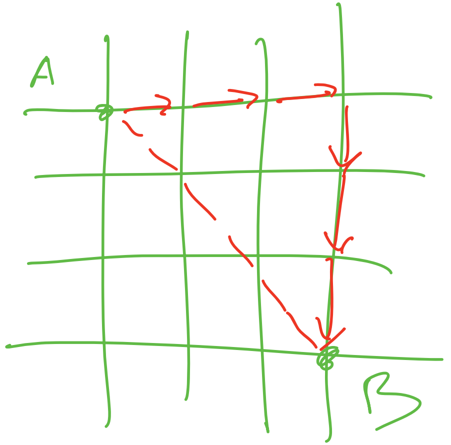
Another example: Manhattan distance (ℓ_1)

$$d(x, x') = \sum_{j=1}^{d} |x[j] - x'[j]|$$



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$K = n$

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(What about the training error when K = 1?)

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Bayes Optimal Predictor

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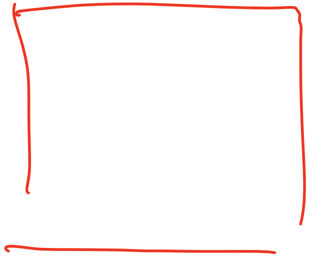
$$\epsilon_{opt} = 1 - P(y_b \mid x) = 0.2$$

Guarantee of KNN when $K = 1$ and $n \to \infty$

Assume $x \in [-1,1]^2$, $P(x)$ has support everywhere $P(x) > 0, \forall x \in [-1,1]^2$



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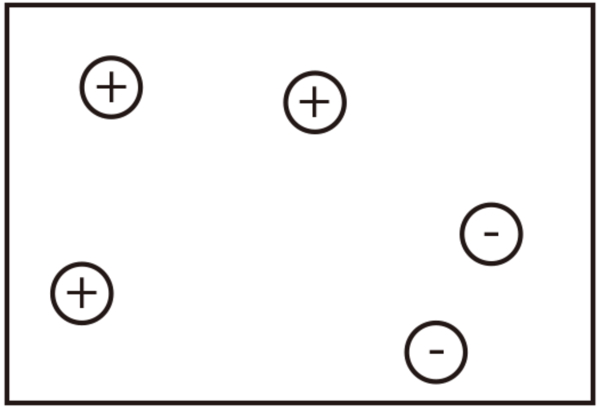

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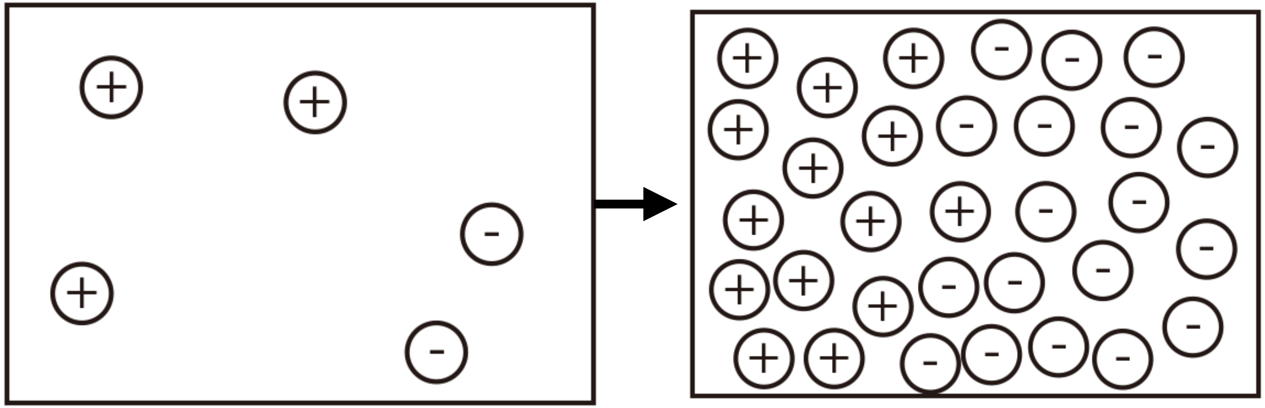

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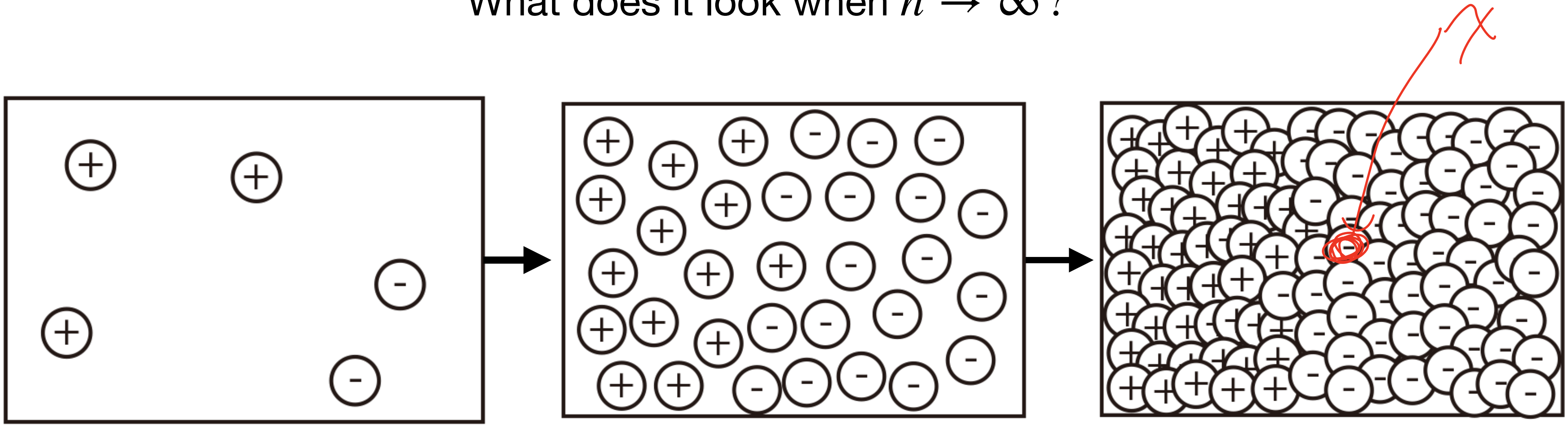

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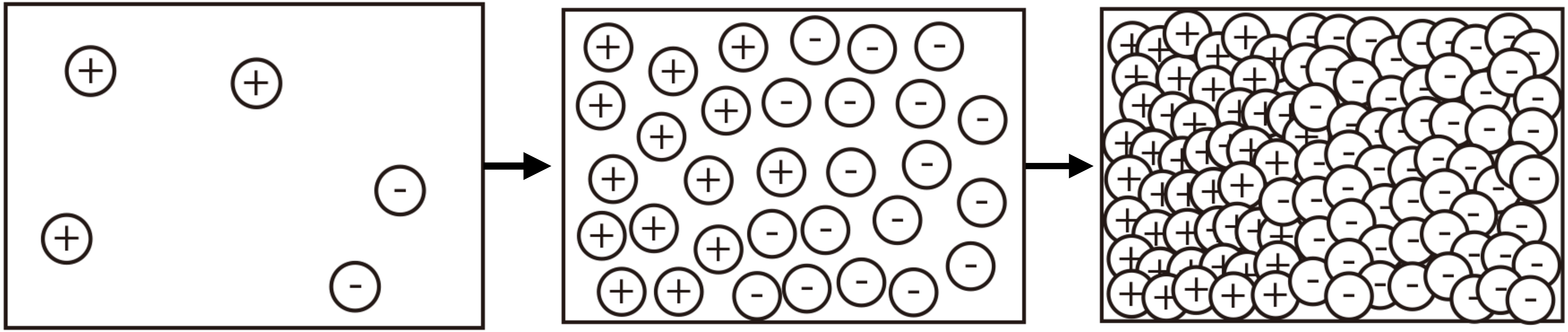

Given test x, as $n \to \infty$, its nearest neighbor x_{NN} is super close, i.e., $d(x, x_{NN}) \to 0$!

Guarantee of KNN when $K = 1$ and $n \to \infty$

Theorem: as $n \to \infty$, 1-NN prediction error is **no more than twice** of the error of the Bayes optimal classifier

Proof:

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$= 1 - P(y_b \mid x)$

$y_b = 1$

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Case 2 when $y_{NN} = -1$ (it happens w/ prob $P(-1 \mid x_{NN}) = P(-1 \mid x)$):

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Final prediction error at x:

$$P(1 \mid x)(1 - P(y_b \mid x)) + P(-1 \mid x)P(y_b \mid x) = P(1 \mid x)(1 - P(y_b \mid x)) + (1 - P(y_b \mid x))P(y_b \mid x)$$

$$\leq (1 - P(y_b \mid x)) + (1 - P(y_b \mid x)) = 2\epsilon_{opt}$$

What happens if K is large?

(e.g., $K = 1e6, n \to \infty$)

$$\frac{K}{n} \to 0$$

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A: Given any x, the K-NN should return the y_b — the solution of the Bayes optimal

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2. Why/When does K-NN work ✓

3. Curse of dimensionality (i.e., why it can fail in high-dimension data)

<u>Finite sample</u> error rate of 1-NN in <u>high-dimension</u> setting

(Informal result and no proof)

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Fix $n \in \mathbb{N}^+$, assume $x \in [0,1]^d$, assume $P(y|x)$ is Lipschitz continuous with respect to x, i.e., $|P(y|x) - P(y|x')| \leq d(x, x')$

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$$\mathbb{E}_{x,y \sim P}\left[\mathbf{1}(y \neq \text{1NN}(x))\right] \leq 2\mathbb{E}_{x,y \sim P}\left[\mathbf{1}(y \neq h_{opt}(x))\right] + O\left(\left(\frac{1}{n}\right)^{1/d}\right)$$

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$\to 1, d \to \infty$

The bound is meaningless when $d \to \infty$, while n is some finite number!

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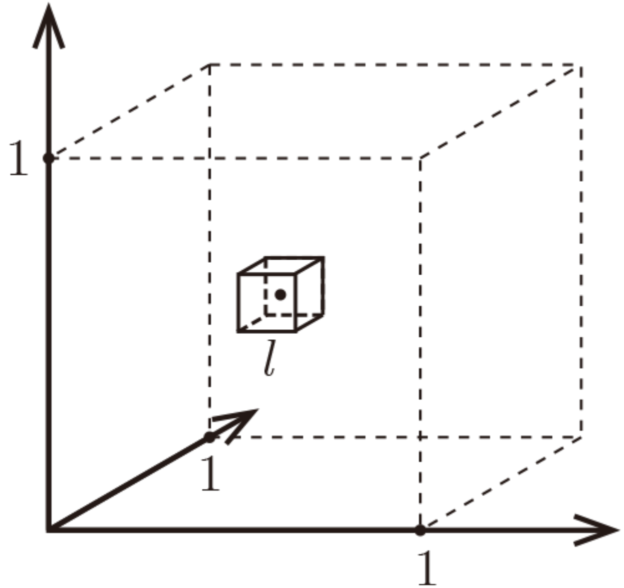
Curse of dimensionality!

Curse of Dimensionality Explanation

Key problem: in high dimensional space, points that are draw from a distribution tends to be far away from each other!



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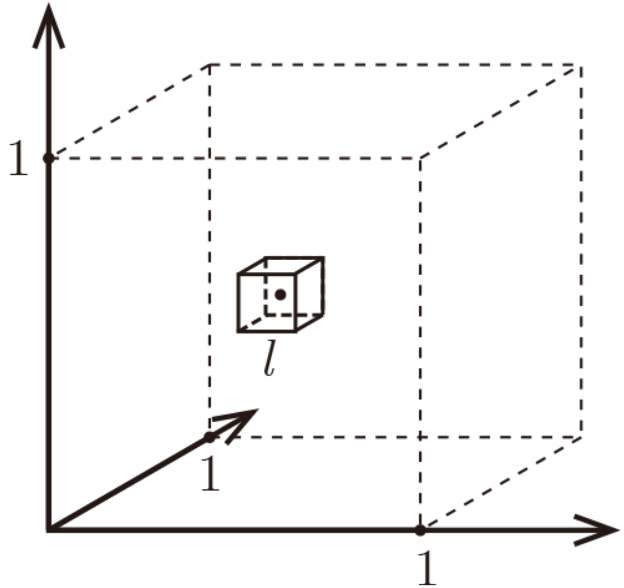
Example: let us consider uniform distribution over a cube $[0,1]^d$



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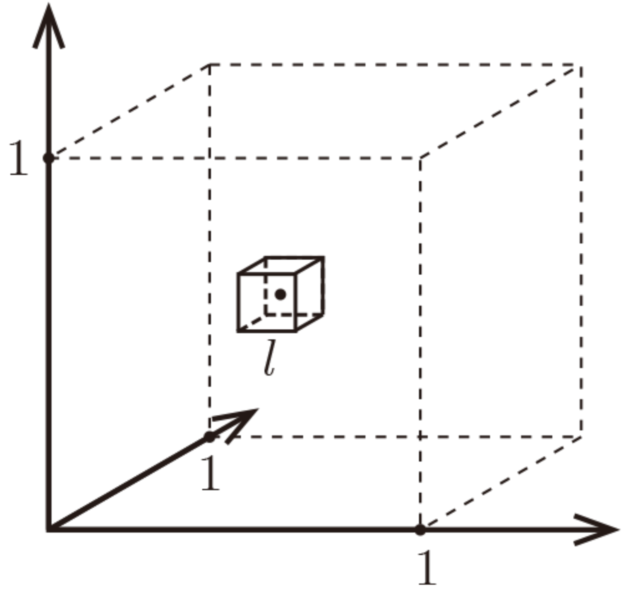

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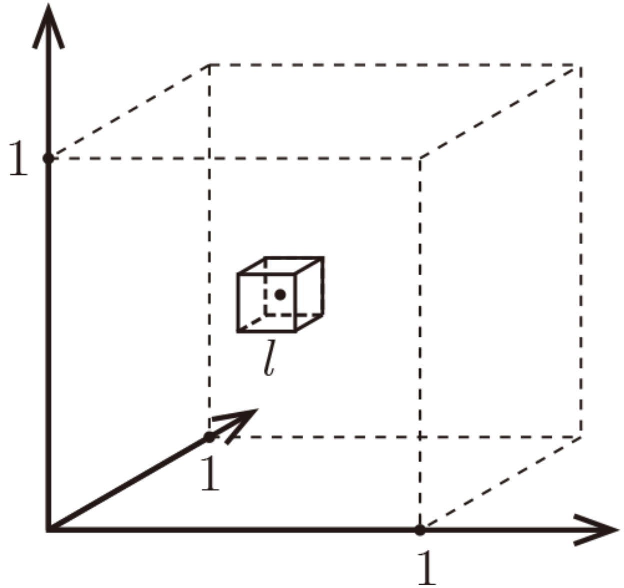

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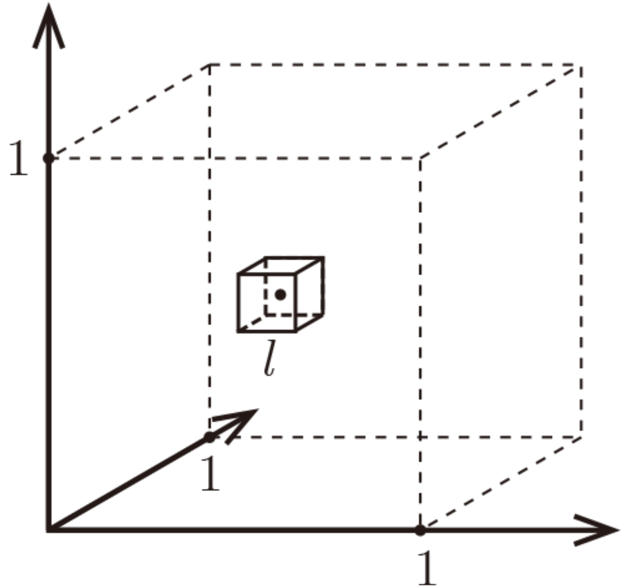

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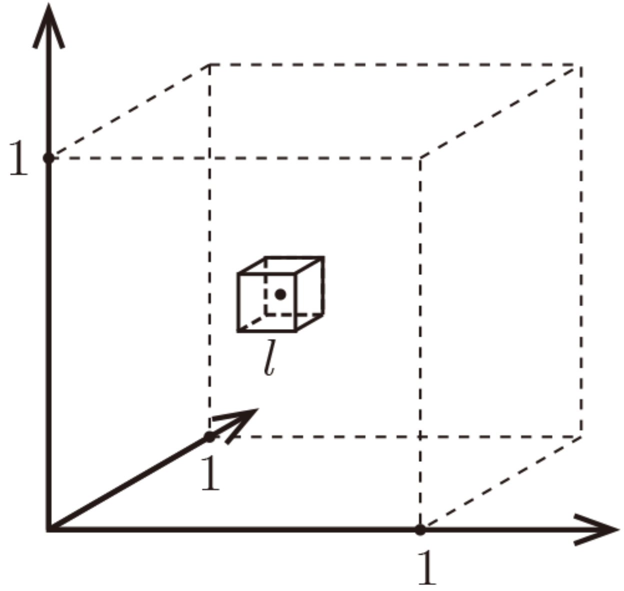

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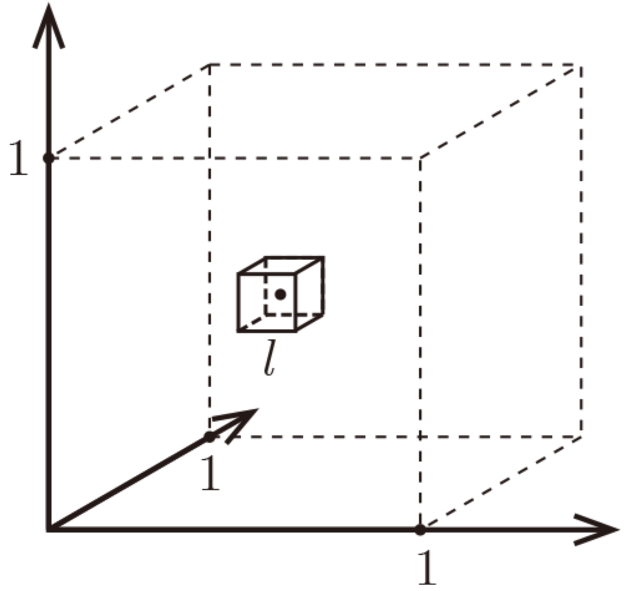

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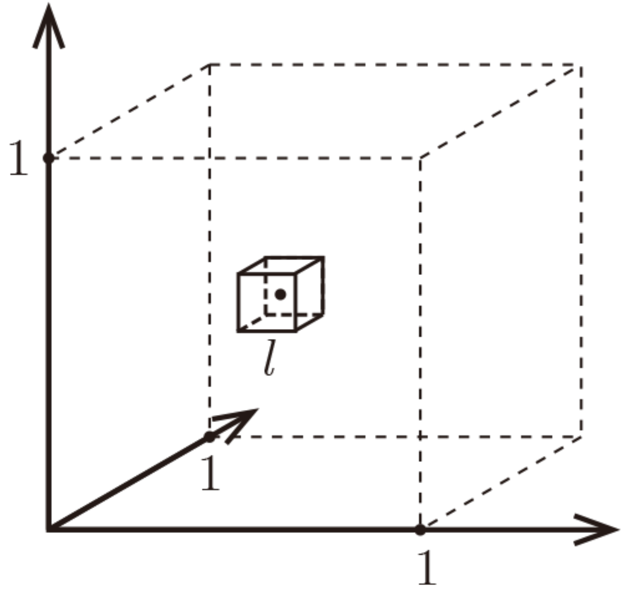

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Thus, we have $l^d \approx \frac{K}{n}$

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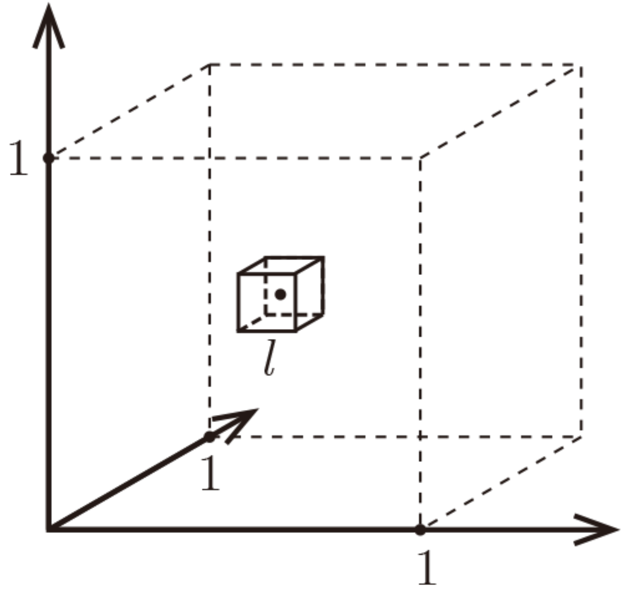

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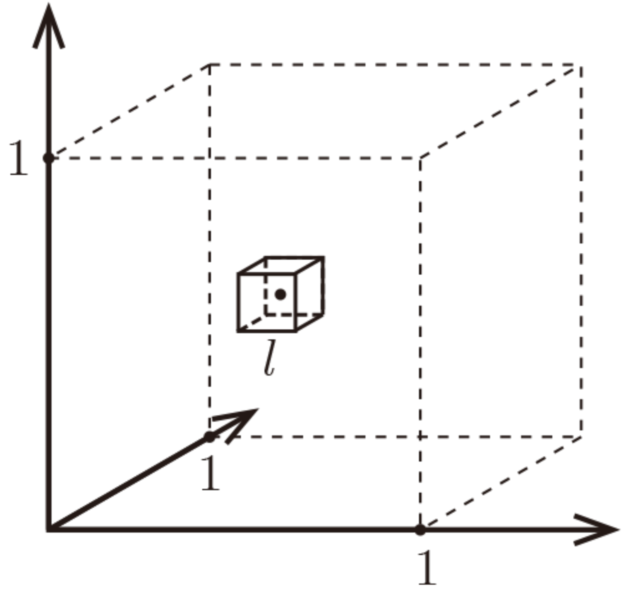

Q: how large we should set l, s.t., we will have K examples (out of n) fall inside the small cube?

$l = \left(\frac{K}{n}\right)^{1/d}$

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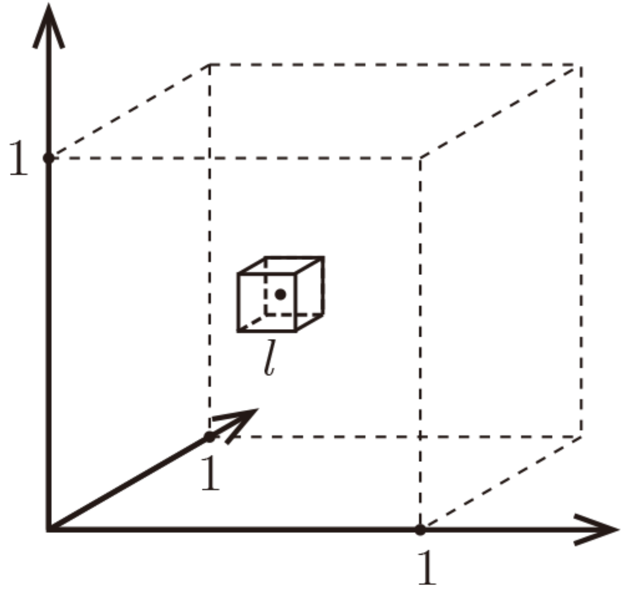

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$$l \approx (K/n)^{1/d}$$

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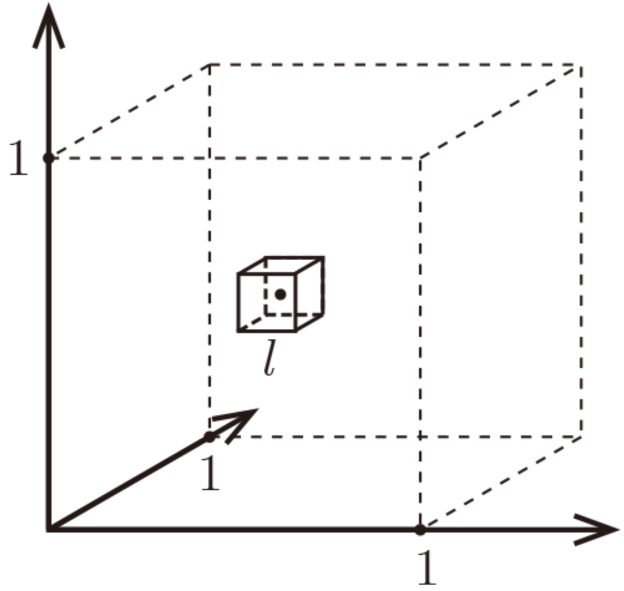

Q: how large we should set l, s.t., we will have K examples (out of n) fall inside the small cube?

$$l \approx (K/n)^{1/d} \rightarrow 1, \text{ as } d \rightarrow \infty$$

Curse of Dimensionality Explanation

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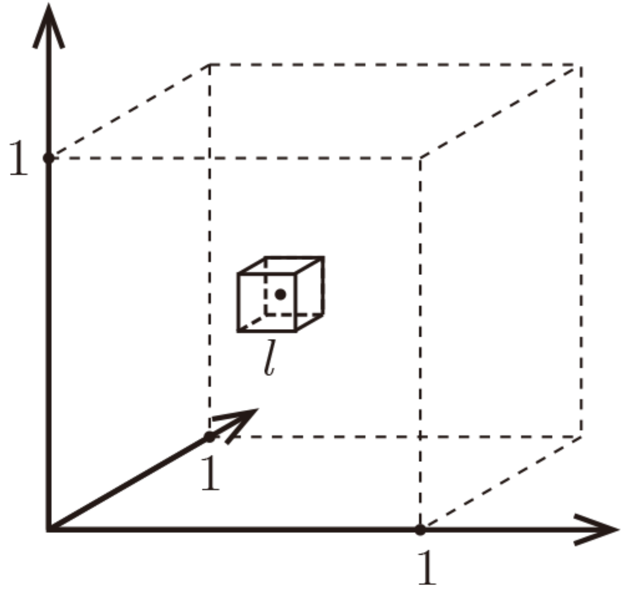

Q: how large we should set l, s.t., we will have K examples (out of n) fall inside the small cube?

$$l \approx (K/n)^{1/d} \to 1, \text{ as } d \to \infty$$

Bad news: when $d \to \infty$, the K nearest neighbors will be all over the place! (Cannot trust them, as they are not nearby points anymore!)

The distance between two sampled points increases as d grows

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In $[0,1]^d$, we uniformly sample two points x, x', calculate

$$d(x, x') = \|x - x'\|_2$$

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Let's plot the distribution of such distance:

d ← Random number

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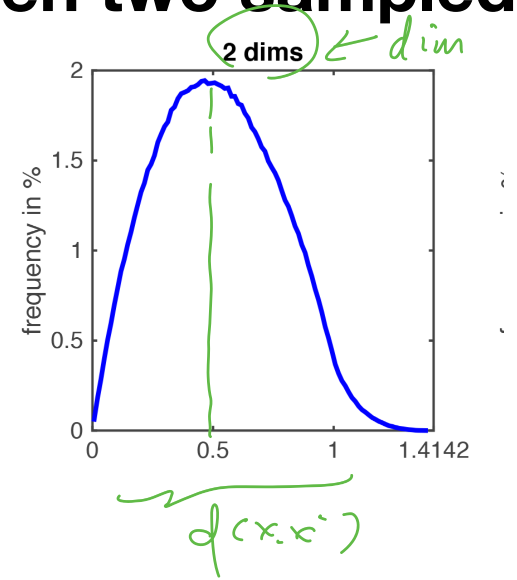

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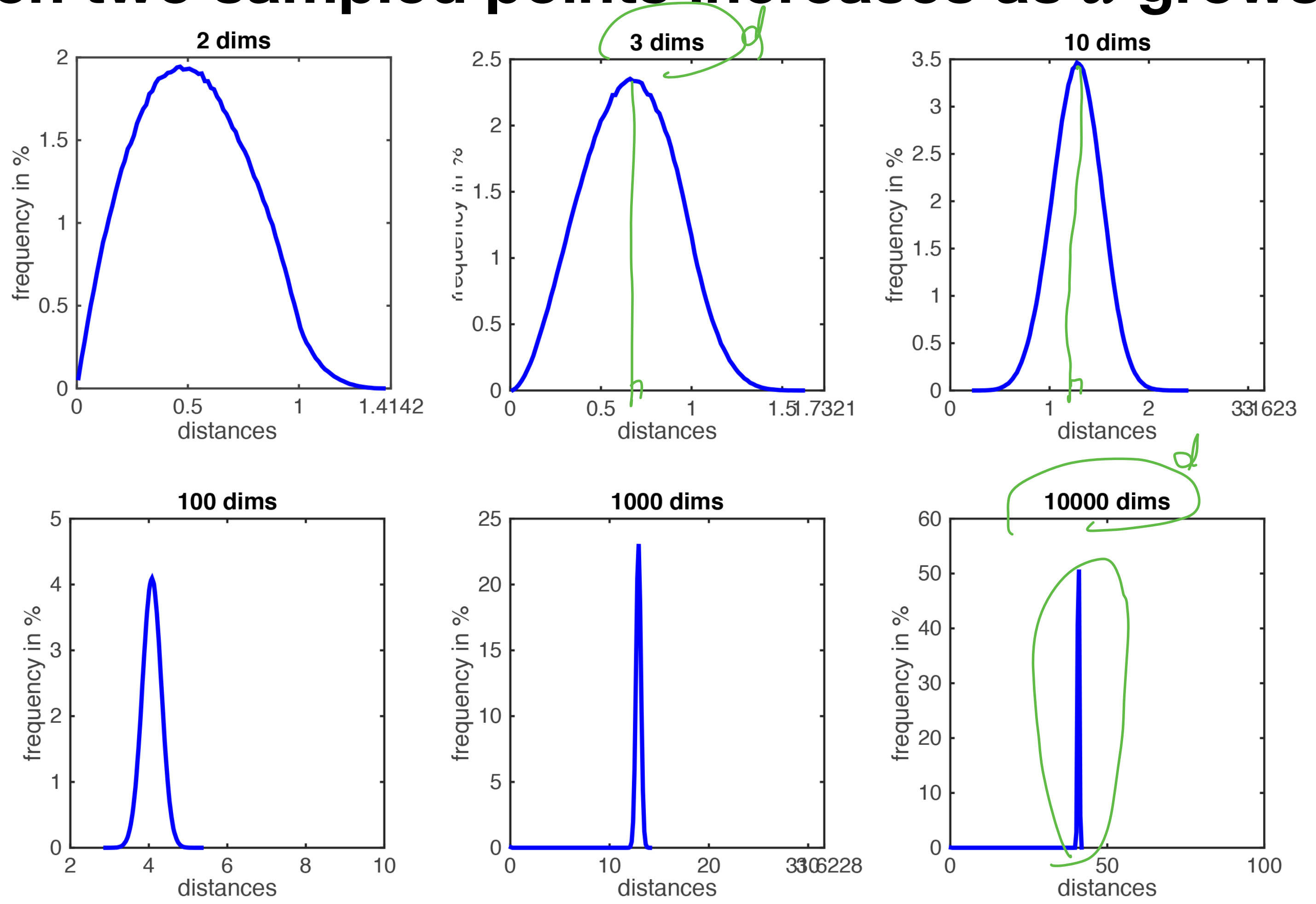

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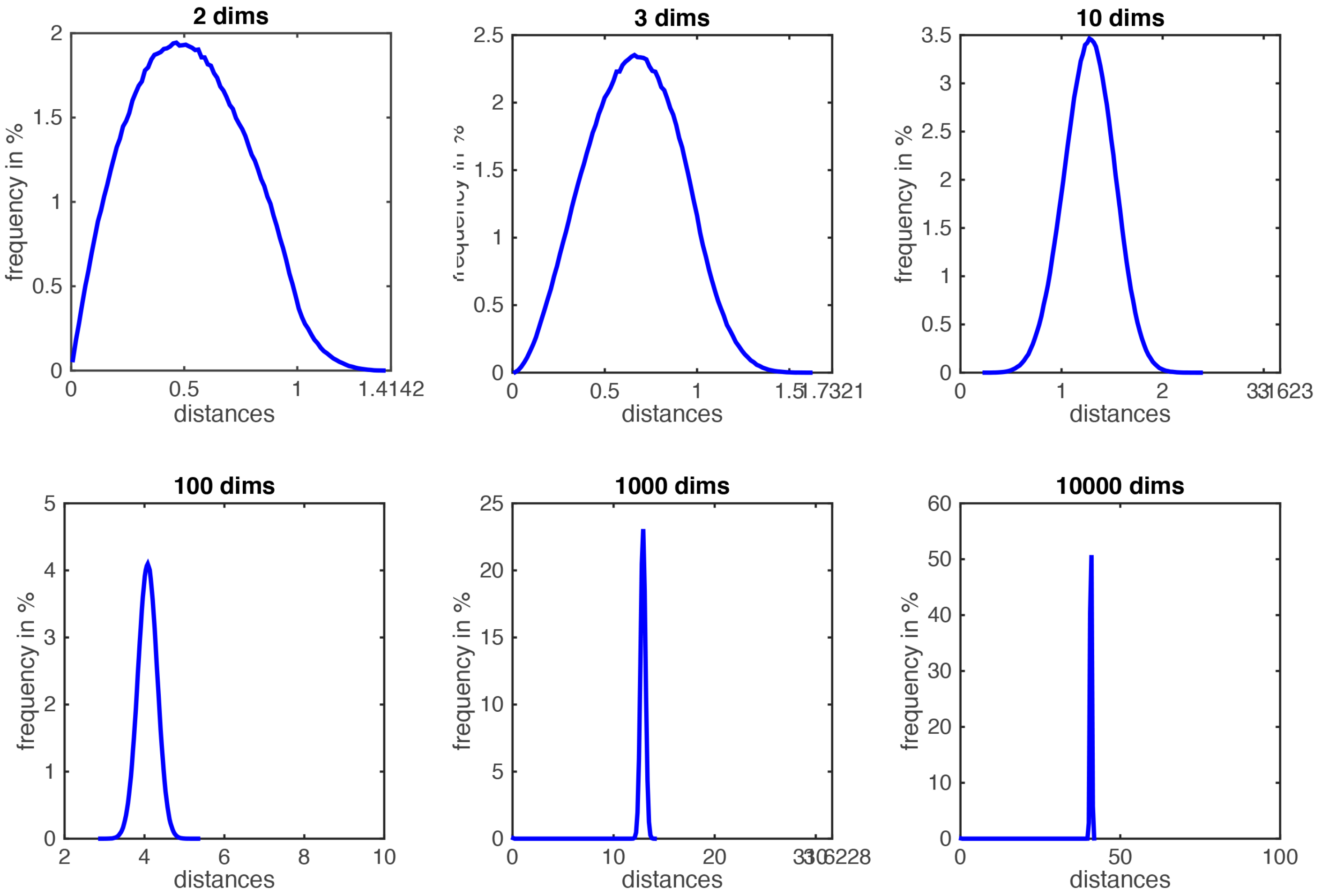

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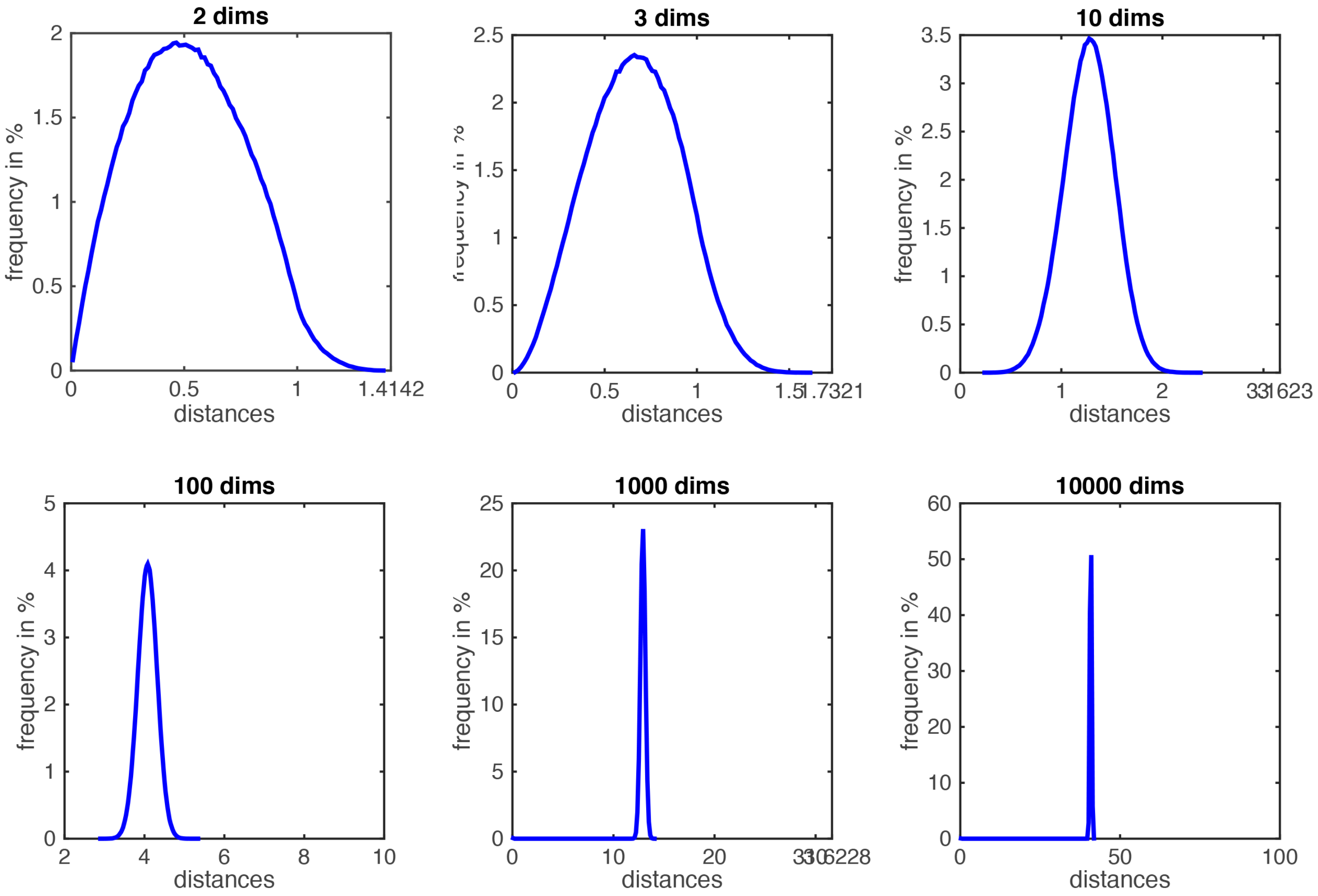
Q: can you compute $\mathbb{E}_{x,x'}\|x - x'\|_2^2$?



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Well, can we just increase n to avoid this?

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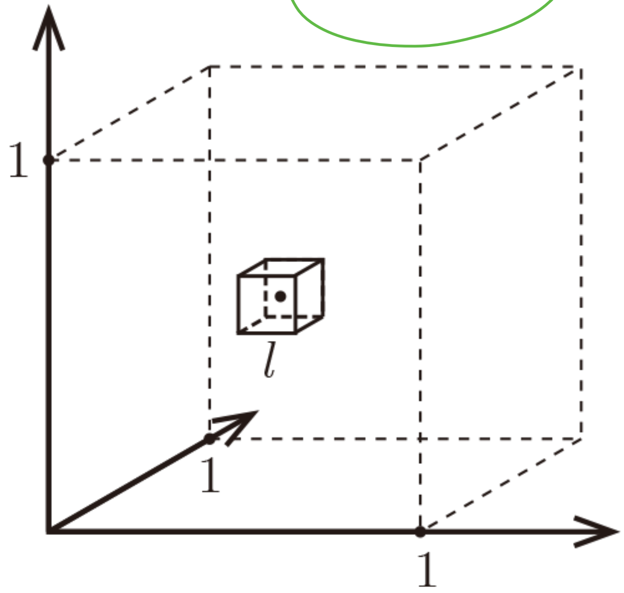

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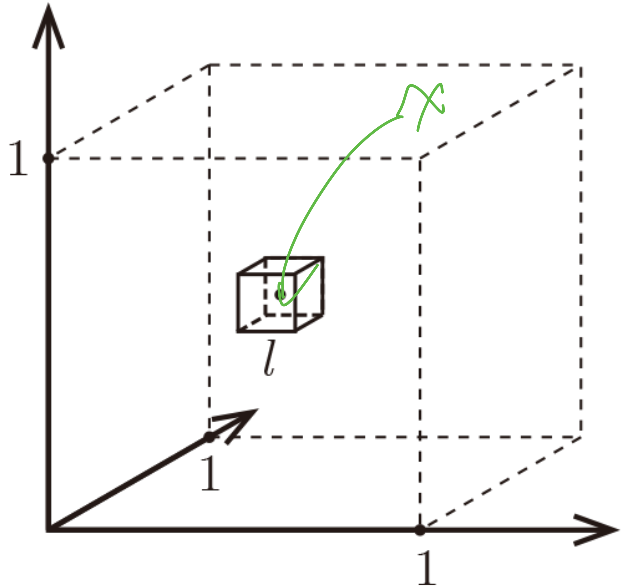

Q: to make sure that we have one sample inside a small cube, how large n needs to be?

$n = \dfrac{K}{l^d}$ $K = 1$

$= 1/l^d$

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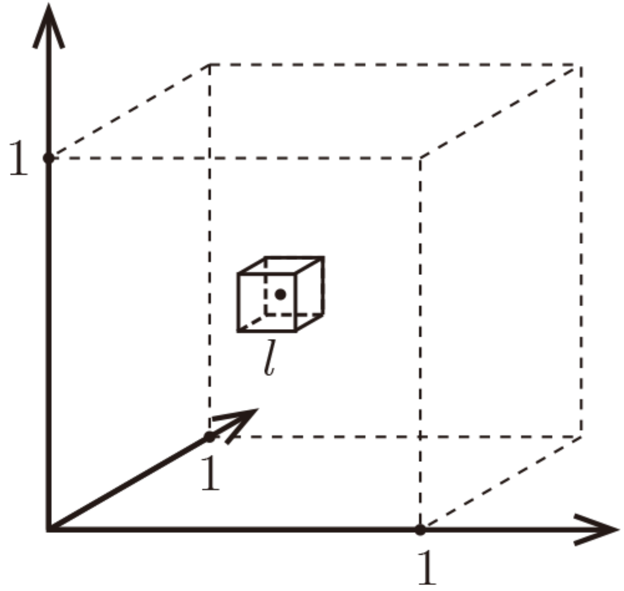

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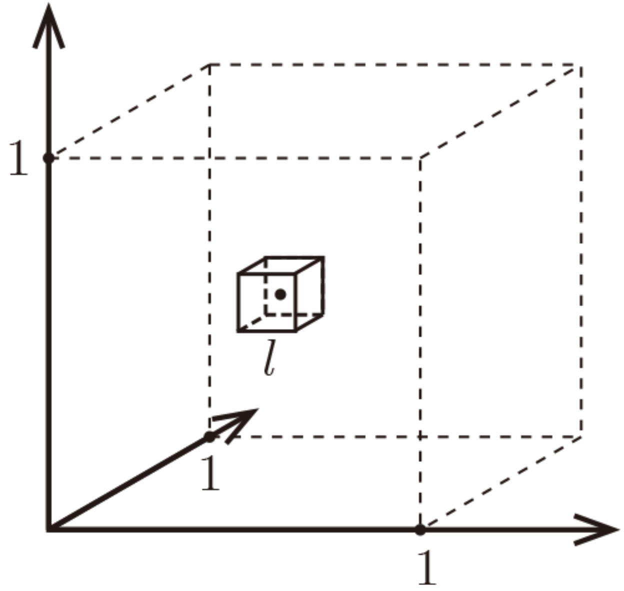

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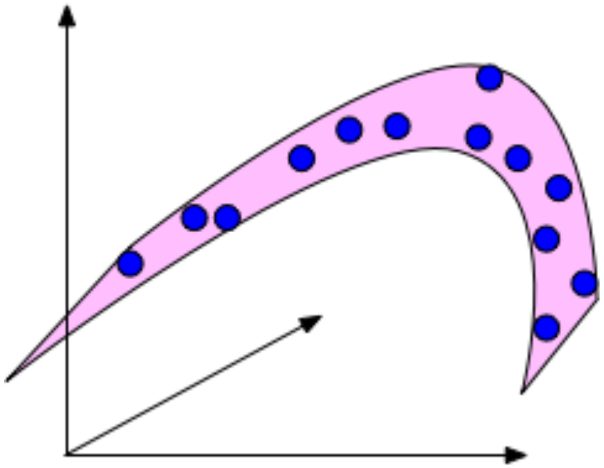
Bad news: when $d \geq 100$, # of samples needs to be larger than total # of atoms in the universe!

Luckily, real world data often has low-dimensional structure!



Data lives in 2-d manifold

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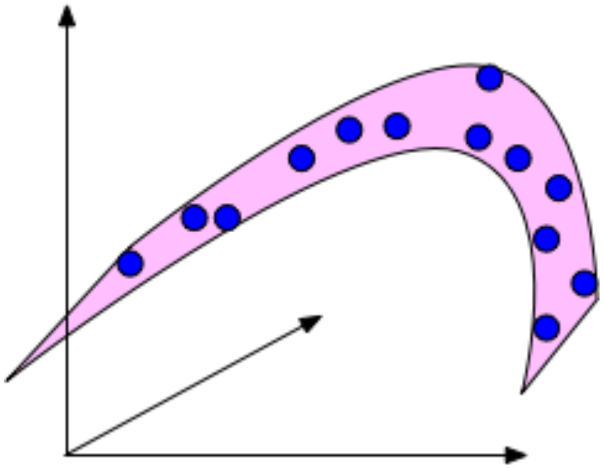

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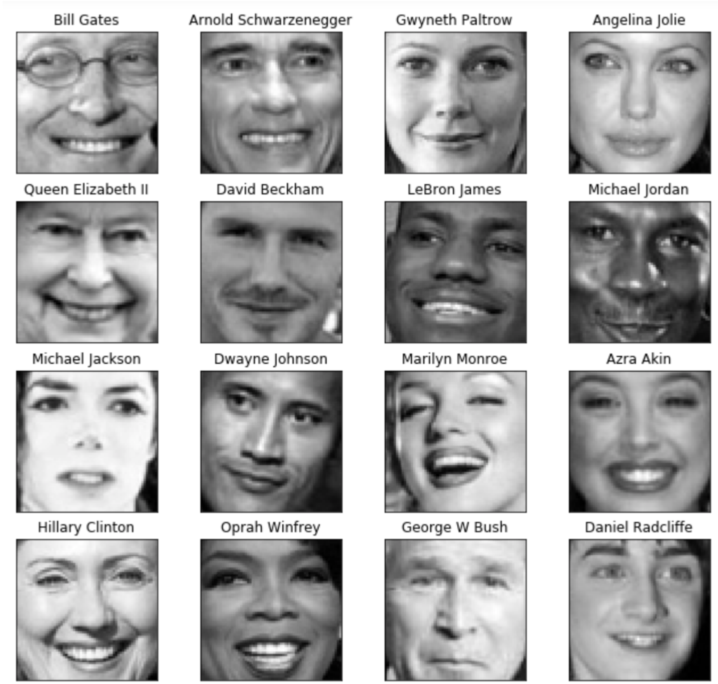

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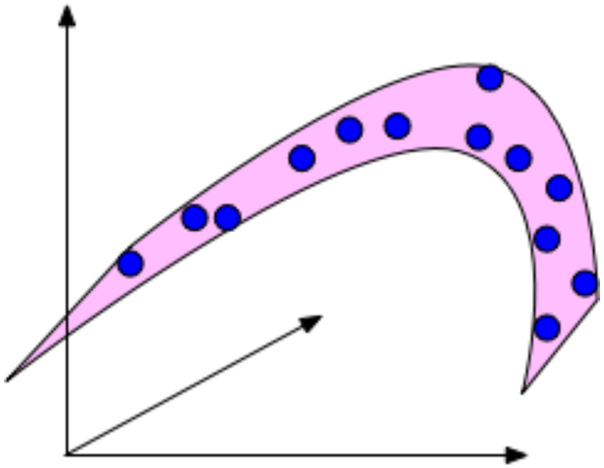

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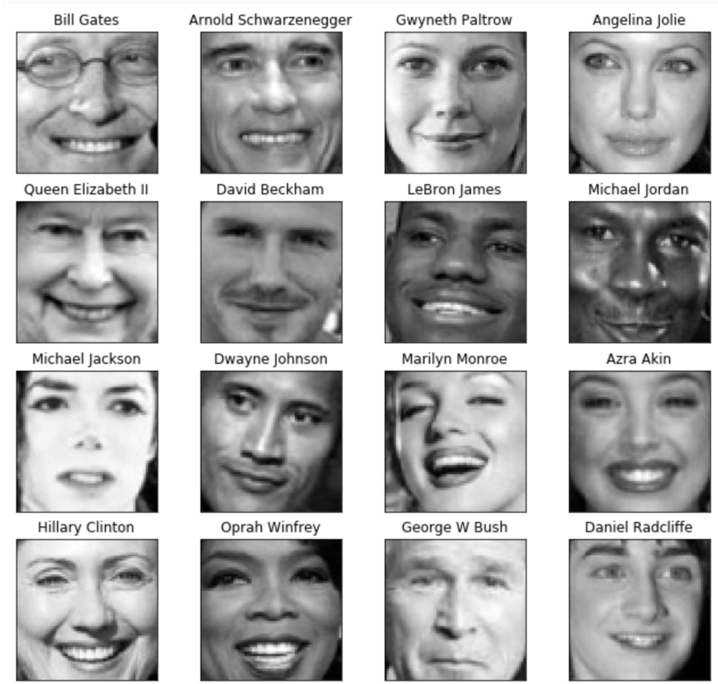

Original image: $\mathbb{R}^{64^2}$

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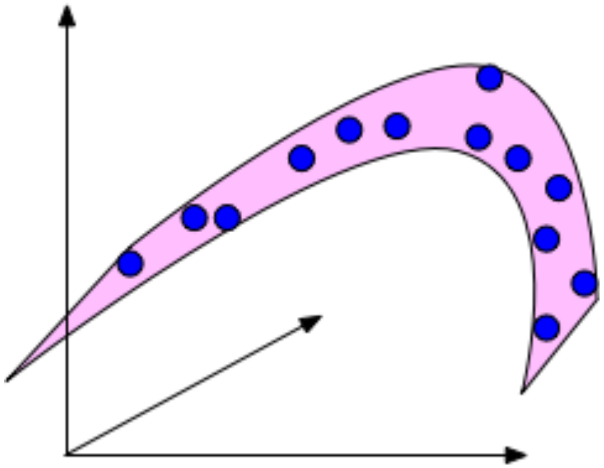

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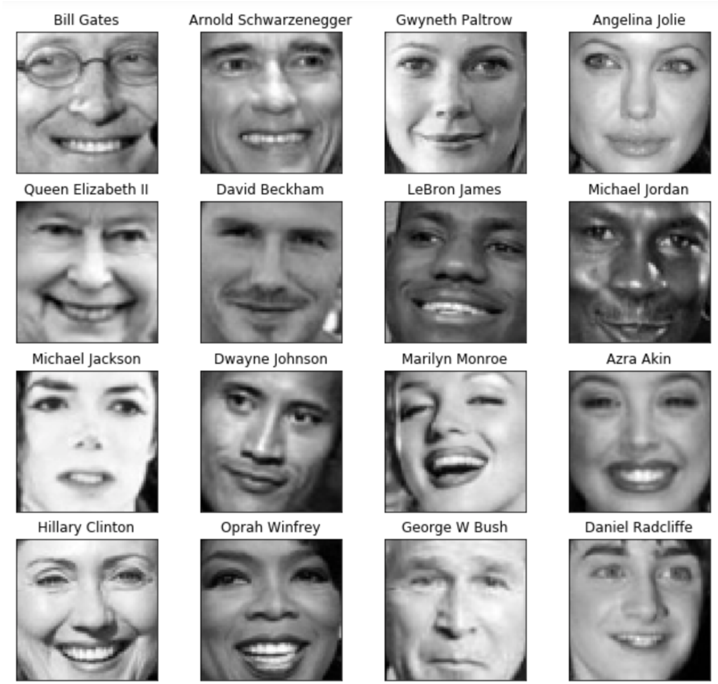

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Next week: we will see that these faces approximately live in 100-d space!

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2. Works well when data is low-dimensional (e.g., can compare against the Bayes optimal)

3. Suffer when data is high-dimensional, due to the fact that in high-dimension space, data tends to spread far away from each other