K-nearest Neighbor

Announcement:

1. HW1 will be out today / early tomorrow and Due Sep 13

Recap

$D = \{x_i, y_i\}_{i=1}^{n}$

$x = \begin{bmatrix} 0.1 \\ 0.2 \\ \vdots \\ -0.1 \end{bmatrix} \in \mathbb{R}^d$

$y \in \{-1, +1\}$

$x_i, y_i \sim P$

$\ell(h, x, y) = \mathbb{1}[y \neq h(x)]$

$= \begin{cases} +1, & \text{if } y \neq h(x) \\ 0 & \text{else} \end{cases}$

$h(x) = y$

$\mathcal{H} = \{h\}$

$\hat{h} = \arg\min_{h \in \mathcal{H}} \sum_{i=1}^{n} \ell(h; x_i, y_i)$

Ex: $h(x) = \text{sign}(w^T x)$

$\mathcal{H} = \{\text{sign}(w^T x) : \|w\|_2 \leq 1\}$,

Generalization Err: $\mathbb{E}_{x, y \sim P}[\ell(\hat{h}, x, y)]$

Outline for Today

1. The K-NN Algorithm

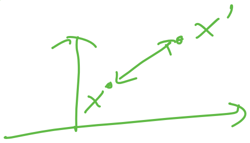
2. Why/When does K-NN work

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)

$\sqrt{(x-x')^\top (x-x')}$



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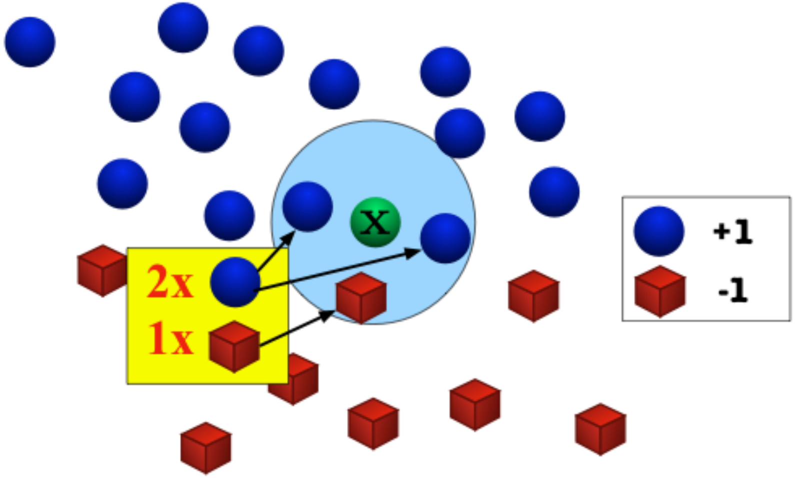
(If for regression, return the average value of the K neighbors)

The K-NN Algorithm

Example: 3-NN for binary classification using Euclidean distance



The choice of metric

$\|x - x'\|_2 = 0 \Leftrightarrow x = x'$

1. We believe our metric d captures similarities between examples:

Examples that are close to each other share similar labels

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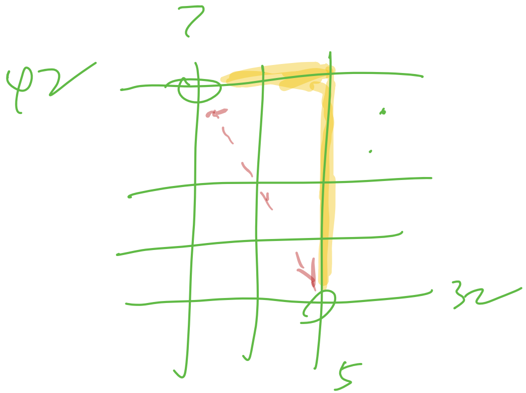
$$\ell_2(x, x') = \sqrt{\sum_{j=1}^{d} (x[j] - x'[j])^2}$$

Another example: Manhattan distance (ℓ_1)

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



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

= 0

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Assume our data is collected in an i.i.d fashion, i.e., $(x, y) \sim P$ (say $y \in \{-1, 1\}$)

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$$\begin{cases} P(1 \mid x) = 0.8 \\ P(-1 \mid x) = 0.2 \end{cases}$$

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Q: What's the probability of h_{opt} making a mistake on x?

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

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

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

$P(x, y)$

$P(x) = p(x, +1) + p(x, -1)$

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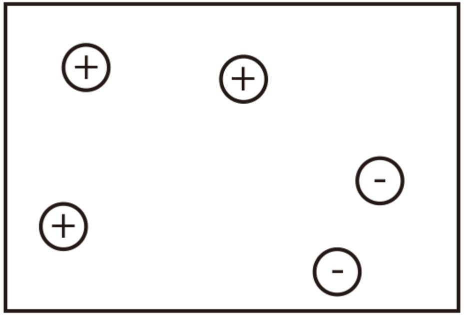

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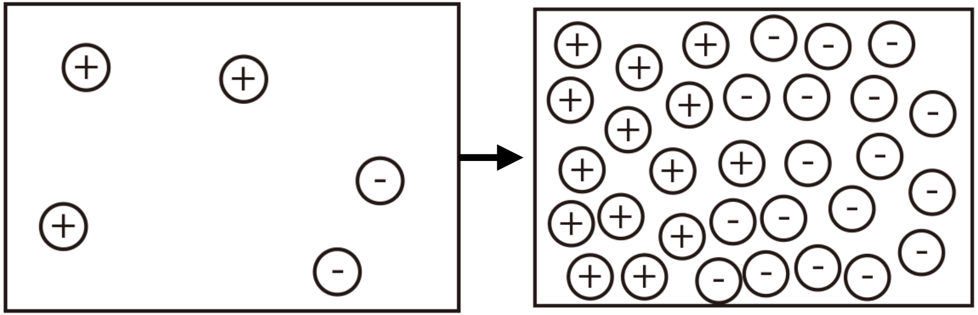

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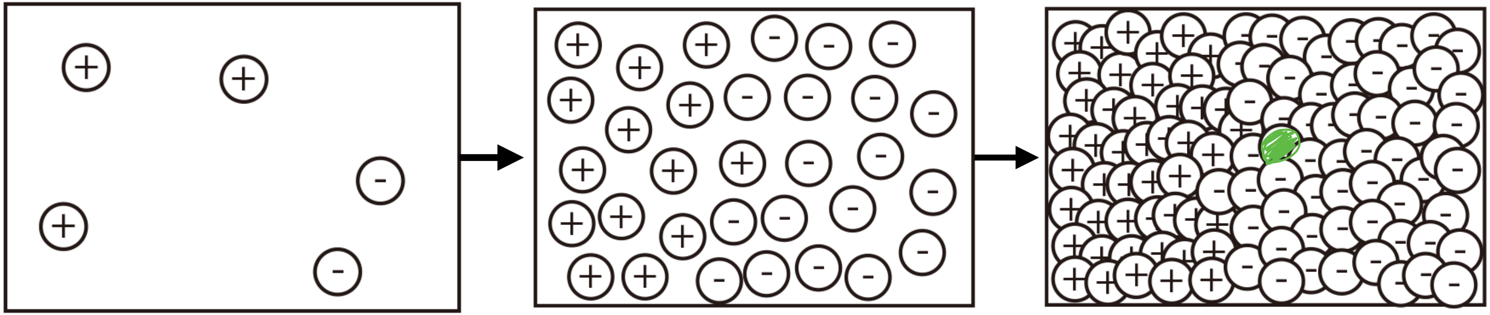

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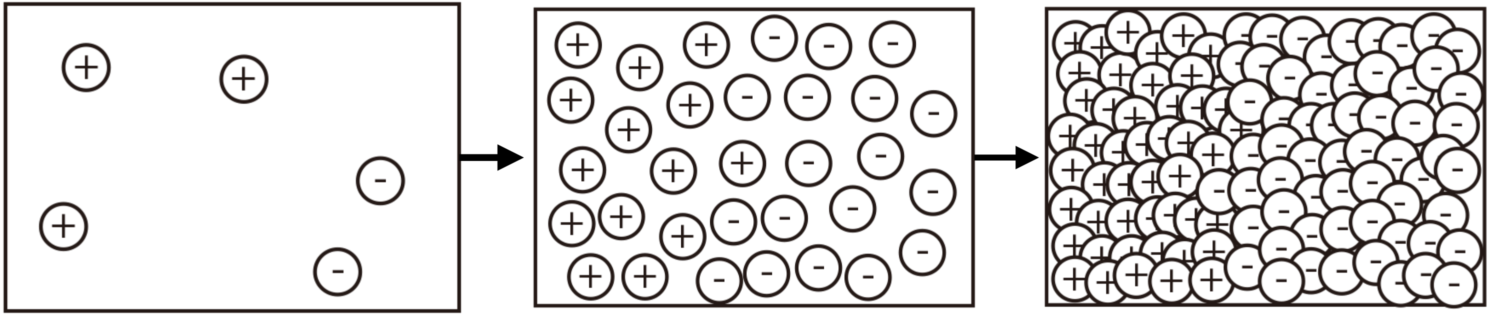

Given test x, as $n \to \infty$, its nearest neighbor x_{NN} is super close, i.e., $d(x, x_{NN}) \to 0$!

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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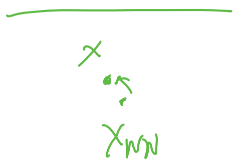

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$(y_b = 1)$

↑

Bayes opt

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Our prediction error at x:

$$P(1|x)\left(1 - P(y_b|x)\right) + P(-1|x)P(y_b|x)$$

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$1 - P(y_b|x)$ ($\because y_b = 1$)

≤ 1, ≤ 1

$\leq (1 - P(y_b|x)) + (1 - P(y_b|x))$

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

ϵ_{opt}

What happens if K is large?

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

$x_{nn} \mapsto x$

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

\# of +1 : 1e6 × 80%

\# of −1 : 1e6 × 20%

$$\begin{cases} P(y=+1 \mid x) = 80\% \\ P(y=-1 \mid x) = 20\% \end{cases}$$

What happens if K is large?

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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)

Finite sample error rate of 1-NN in high-dimension setting

(Informal result and no proof)

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

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

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

Bayes opt

n → ∞ d is fixed

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→ 1, when $d \to \infty$

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

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Curse of dimensionality!

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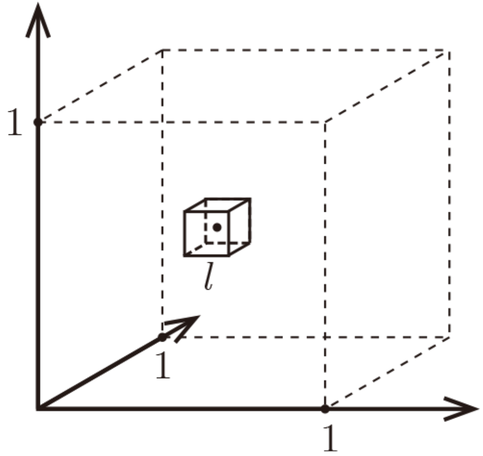
Curse of Dimensionality Explanation

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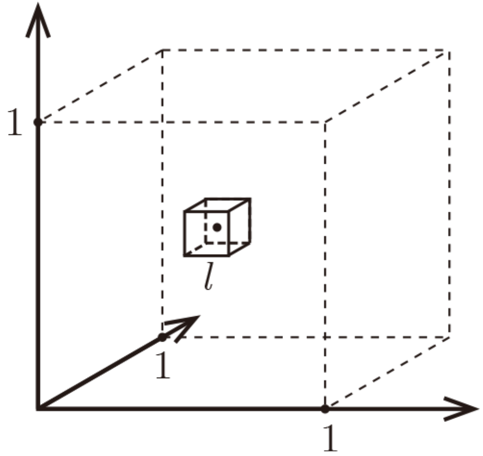
Example: let us consider uniform distribution over a cube $[0,1]^d$



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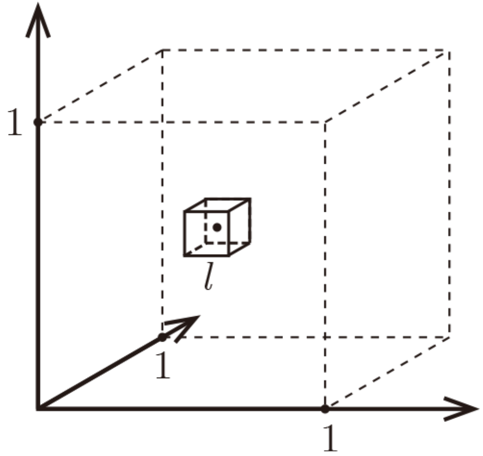
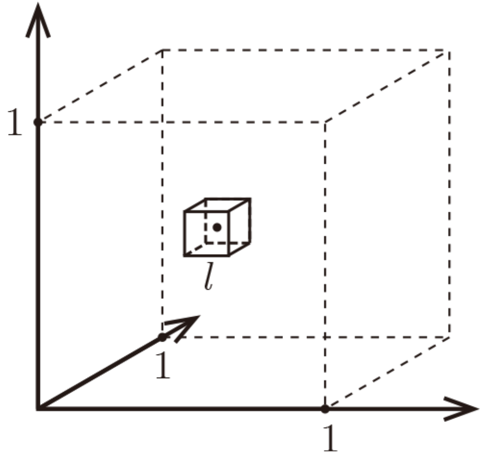


Q: sample x uniformly, what is the probability that x is inside the small cube?

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!

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



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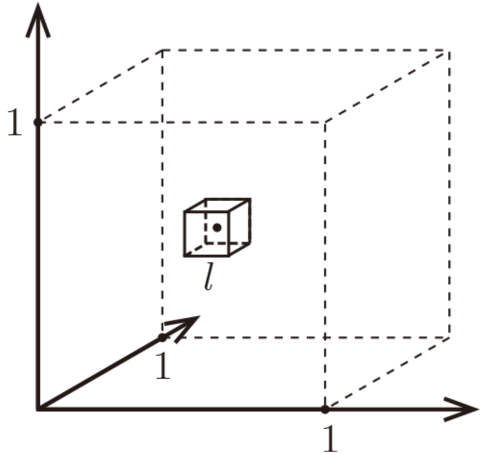

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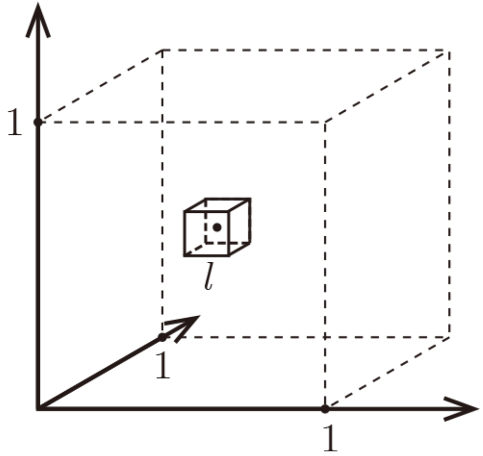

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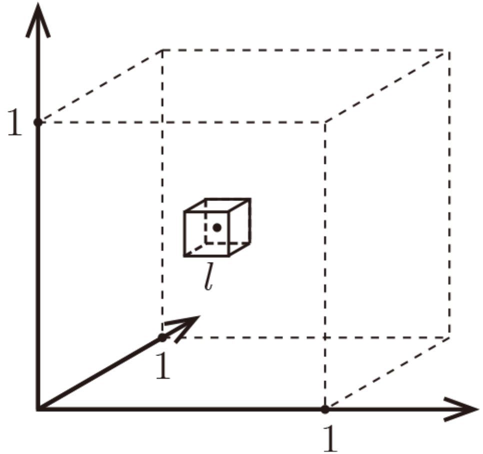

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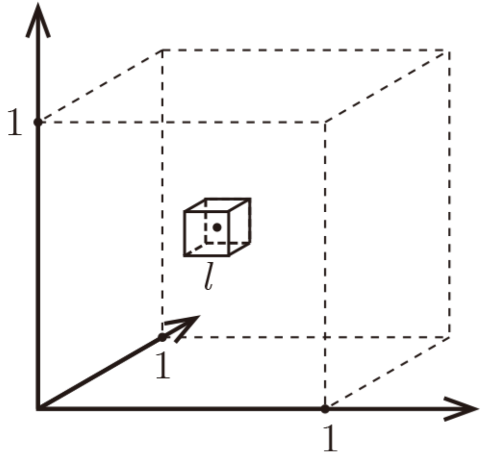

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Thus, we have $$l^d \approx \frac{K}{n}$$

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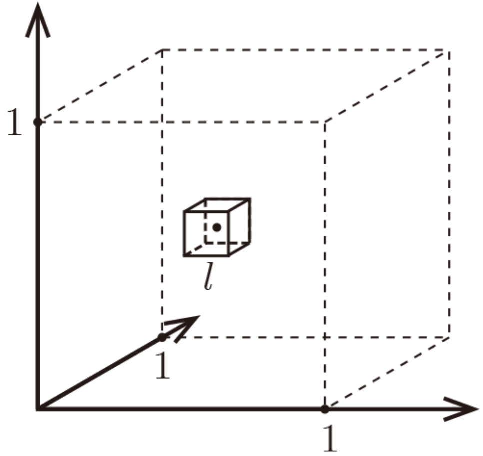

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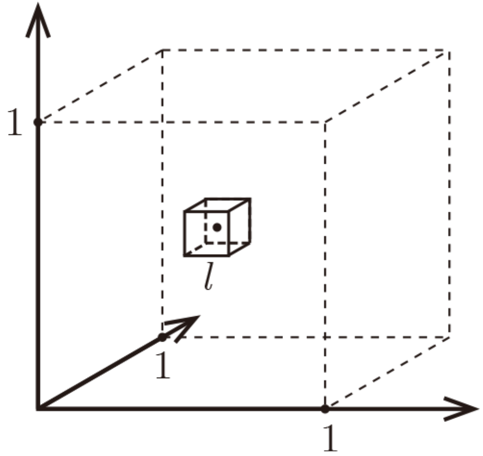

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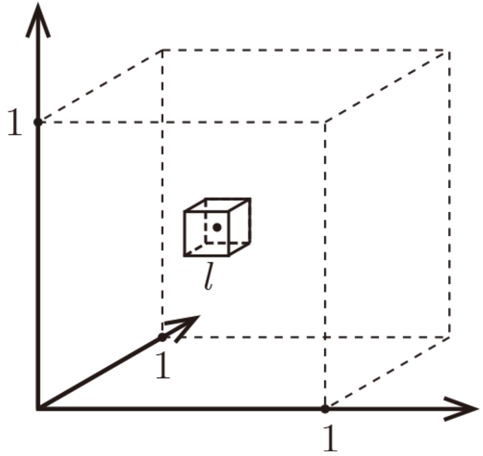

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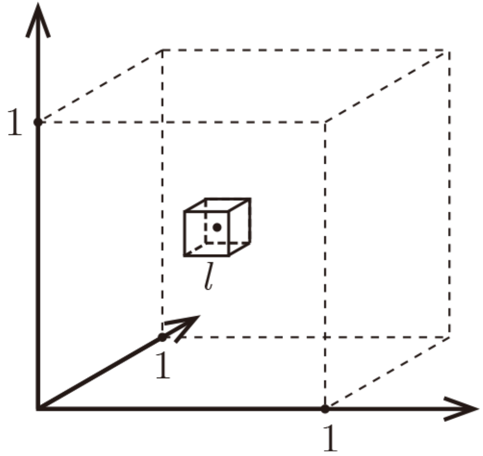

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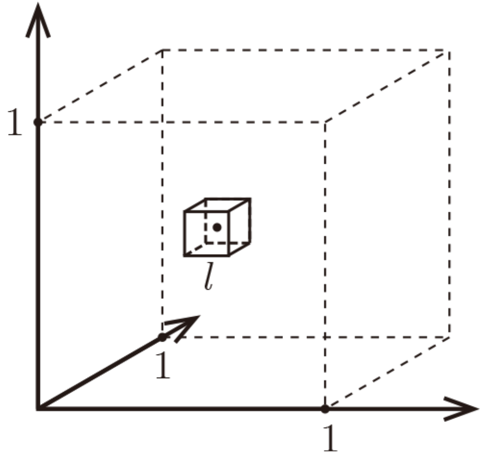

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$$l \approx (K/n)^{1/d} \rightarrow 1, \text{ as } d \rightarrow \infty$$

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

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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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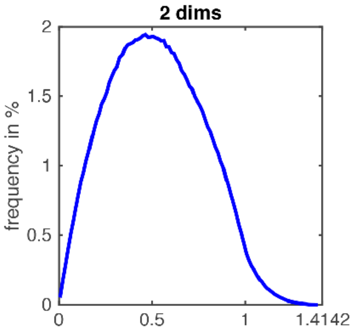

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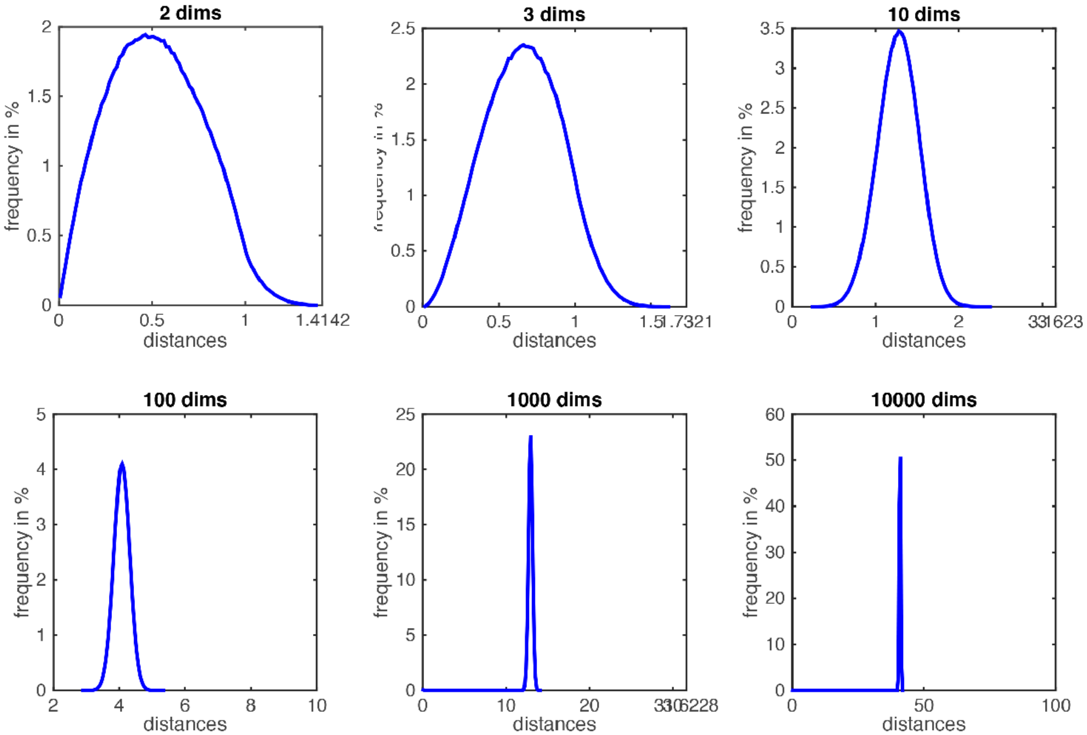

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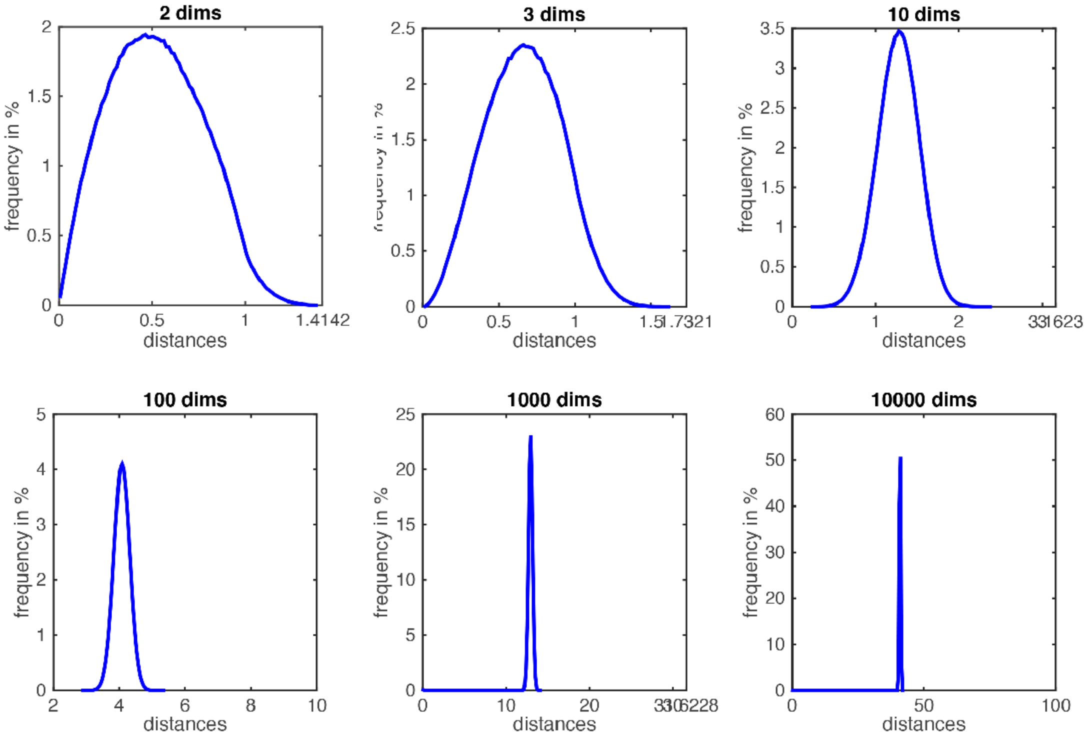
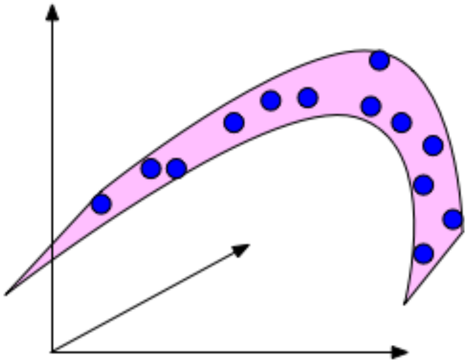


Distance increases as $d \to \infty$

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



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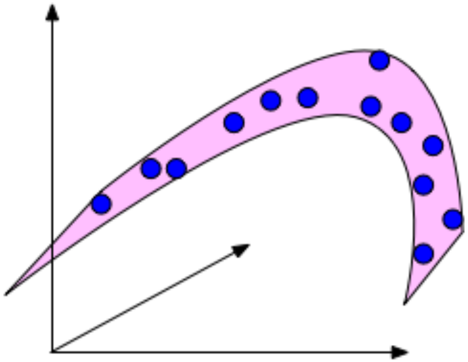

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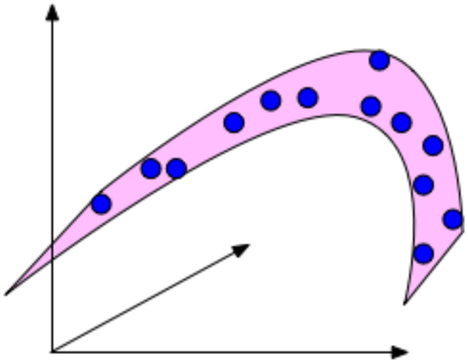

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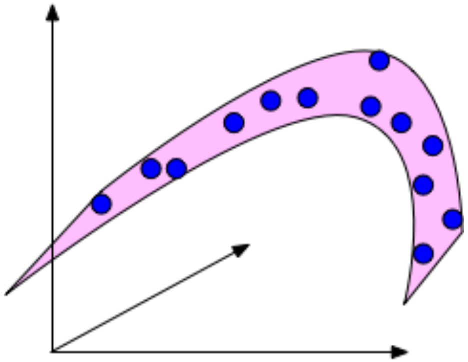

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Next week: we will see that these faces approximately live in 100-d space!

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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