Nearest Neighbor Classifiers and the Curse of Dimensionality

Machine Learning Course - CS-433

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Supervised machine learning

We observe some data $S_{\text{train}} = \{x_i, y_i\}_{i=1}^{n} \in \mathcal{X} \times \mathcal{Y}$

<u>Goal</u>: given a new x, we want to predict its label y

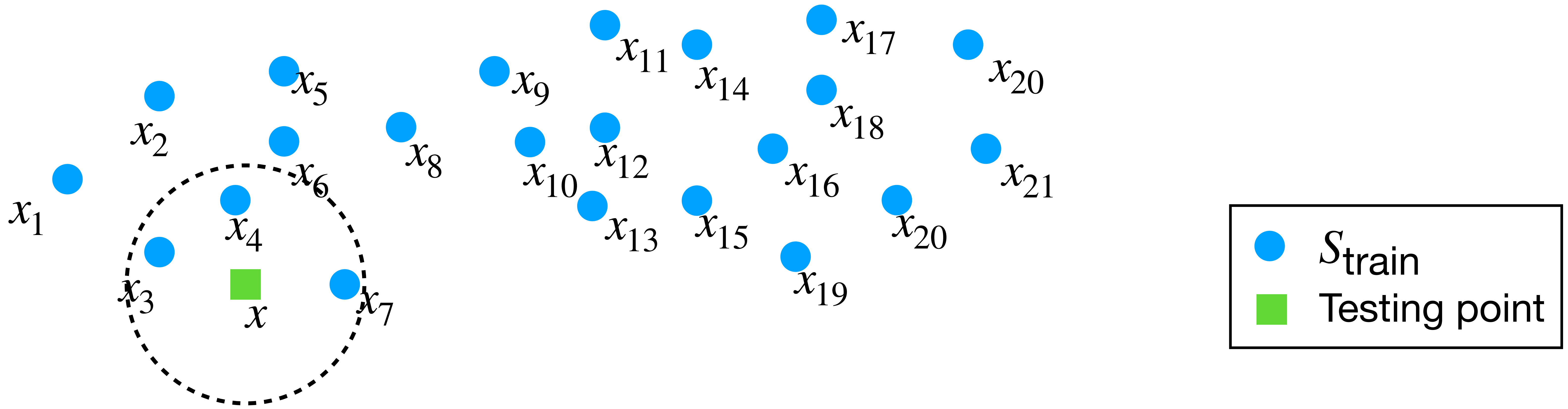
<u>How:</u>

$S_{\text{train}} = \{x_i, y_i\}_{i=1}^{n}$ $\mathcal{A}$ $f_S = \mathcal{A}(S)$

Nearest neighbor function

$$\mathrm{nbh}_{S_{train},k} : \mathcal{X} \to \mathcal{X}^k$$

$$x \mapsto \{k \text{ elements of } S_{\text{train}} \text{ the closest to } x\}$$

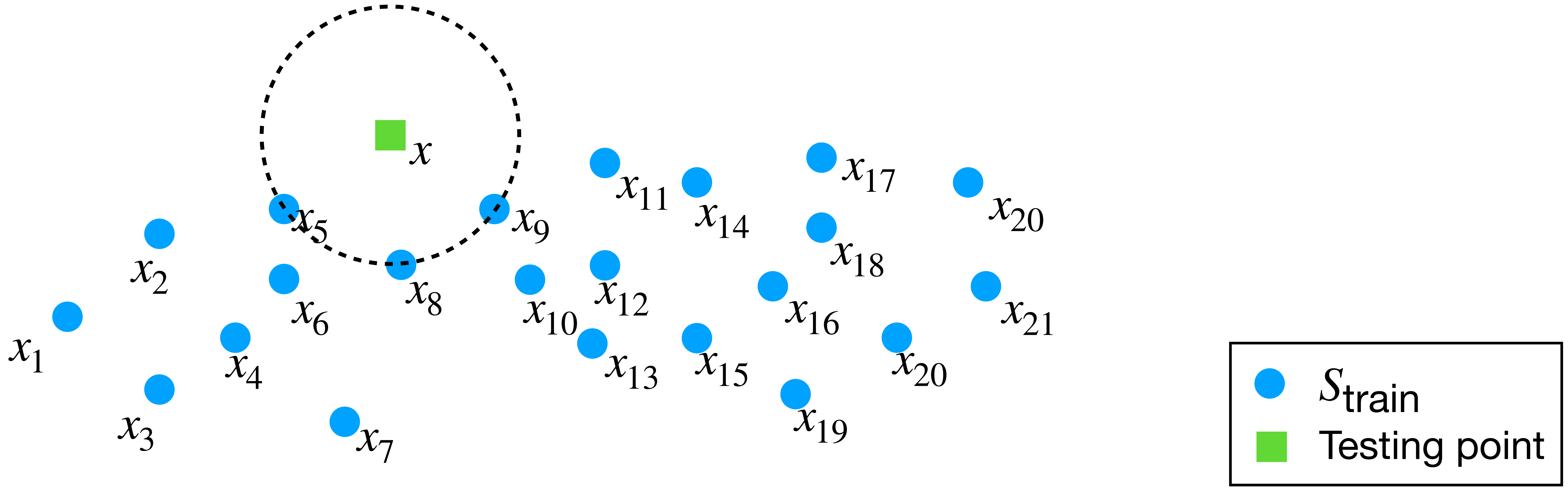


$$\mathrm{nbh}_{S_{train},3}(x) = \{x_3, x_4, x_7\}$$

Nearest neighbor function

$$\text{nbh}_{S_{train},k} : \mathcal{X} \to \mathcal{X}^k$$

$$x \mapsto \{k \text{ elements of } S_{\text{train}} \text{ the closest to } x\}$$



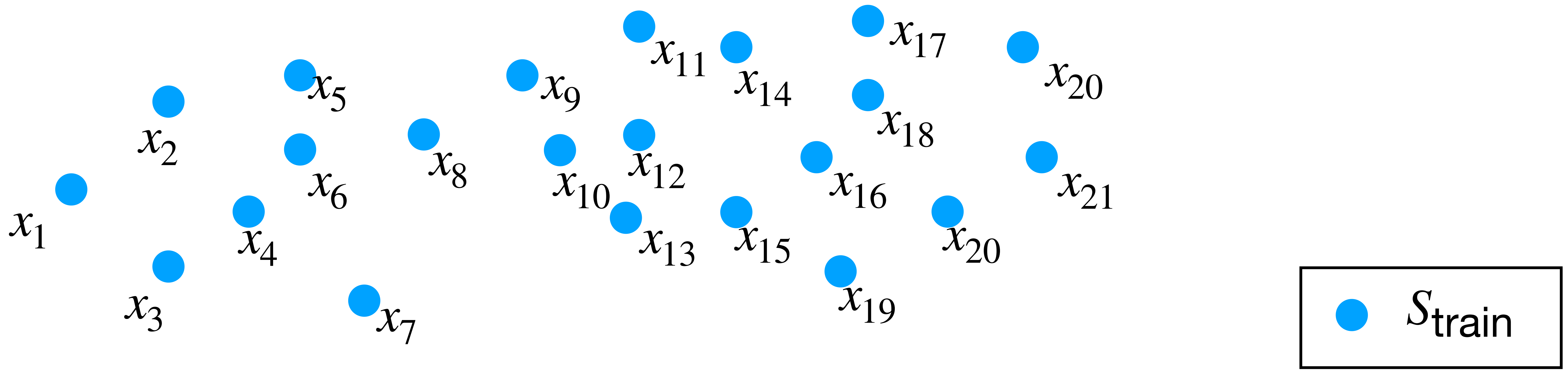
$$\text{nbh}_{S_{train},2}(x) = \{x_5, x_8\}$$

Not uniquely defined!
It will depend on the implementation
Often ties are broken randomly

Nearest neighbor function

$$\text{nbh}_{S_{train},k} : \mathscr{X} \to \mathscr{X}^k$$

$$x \mapsto \{k \text{ elements of } S_{\text{train}} \text{ the closest to } x\}$$

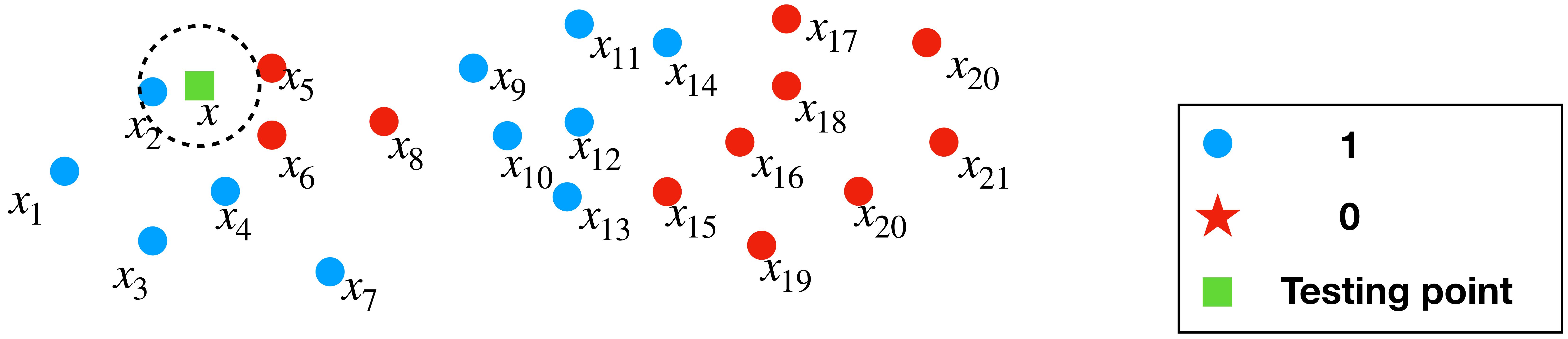


Rmq:

- Different metrics can be used
- Computational complexity when n is large (but efficient data structure may exist)

k-NN can be used for classification ($y \in \{0,1\}$)

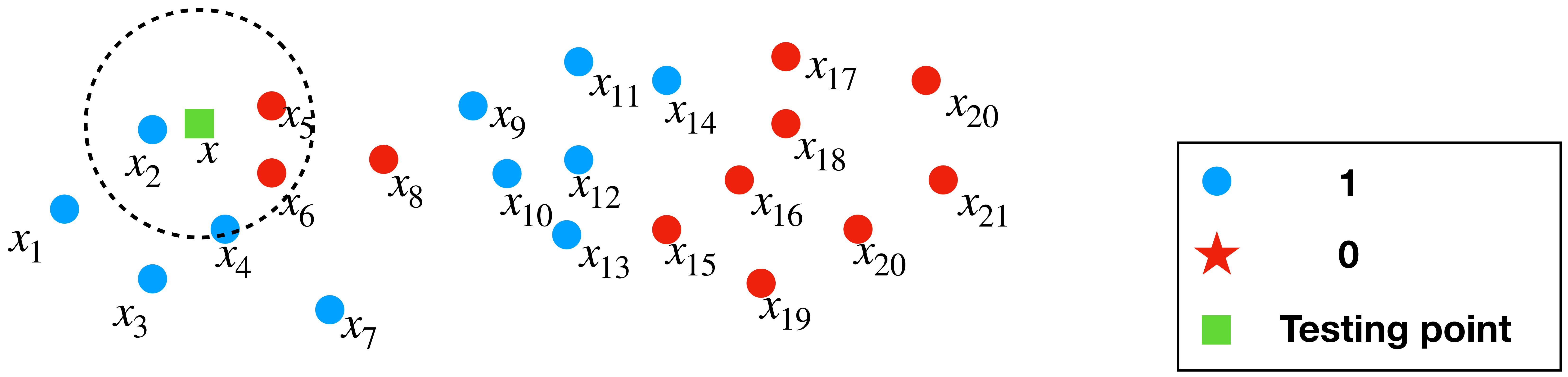
$$f_{S_{train},k}(x) = \text{majority}\{y_i : x_i \in \text{nbh}_{S_{train},k}(x)\}$$



$$f_{S_{train},1}(x) = 1$$

k-NN can be used for classification ($y \in \{0,1\}$)

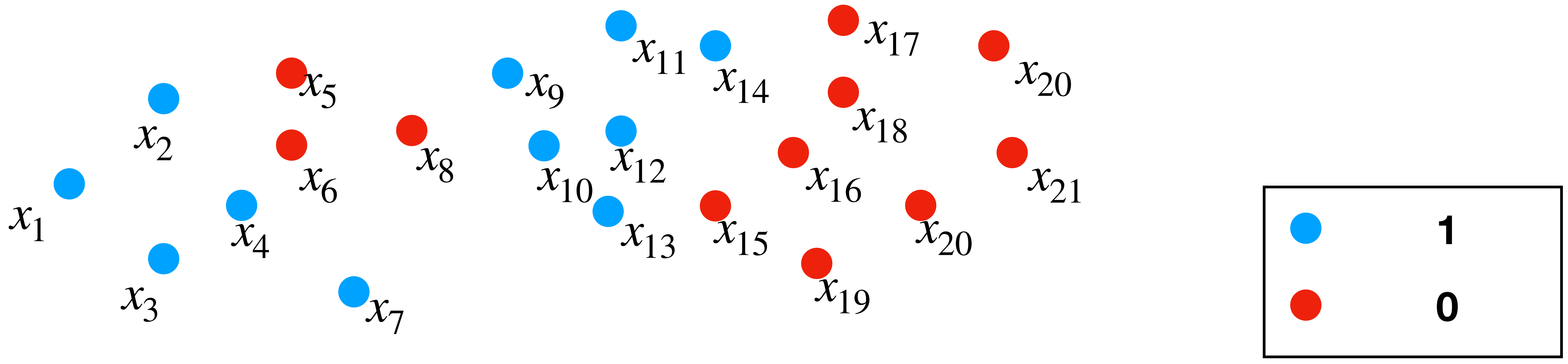
$$f_{S_{train},k}(x) = \text{majority}\left\{y_i : x_i \in \text{nbh}_{S_{train},k}(x)\right\}$$



$f_{S_{train},4}(x) = ?$ **Tie!**

k-NN can be used for classification ($y \in \{0,1\}$)

$$f_{S_{train},k}(x) = \text{majority}\left\{y_i : x_i \in \text{nbh}_{S_{train},k}(x)\right\}$$

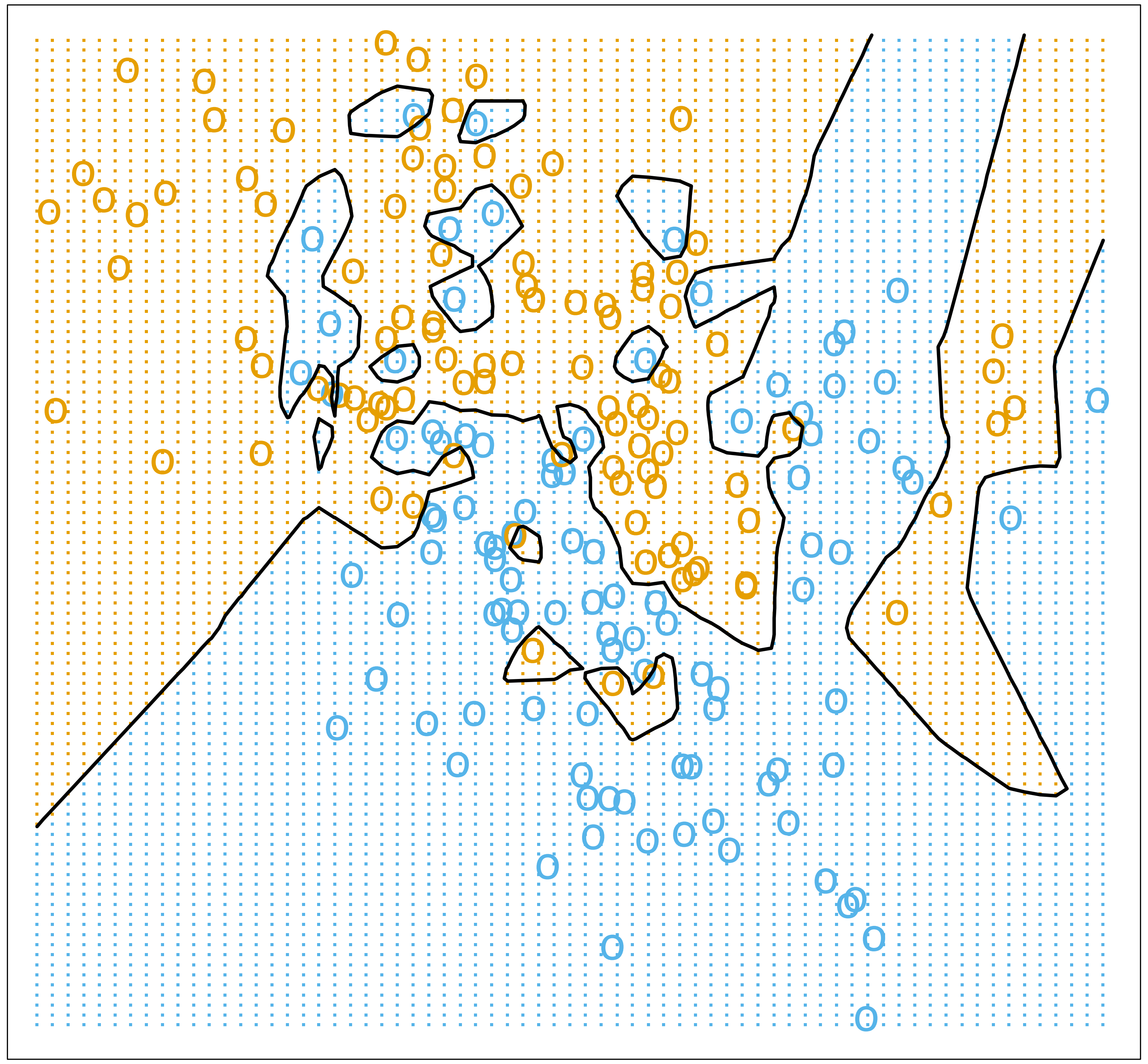


Rmq:

- k is often chosen odd to avoid ties
- Generalization: smoothing kernels; weighted linear combination of elements

Why does it make sense?

- Meaningful when there is spatial correlation
- Implicitly learns very complex decision boundaries in low dimension



Bias Variance for k-NN

Small k:

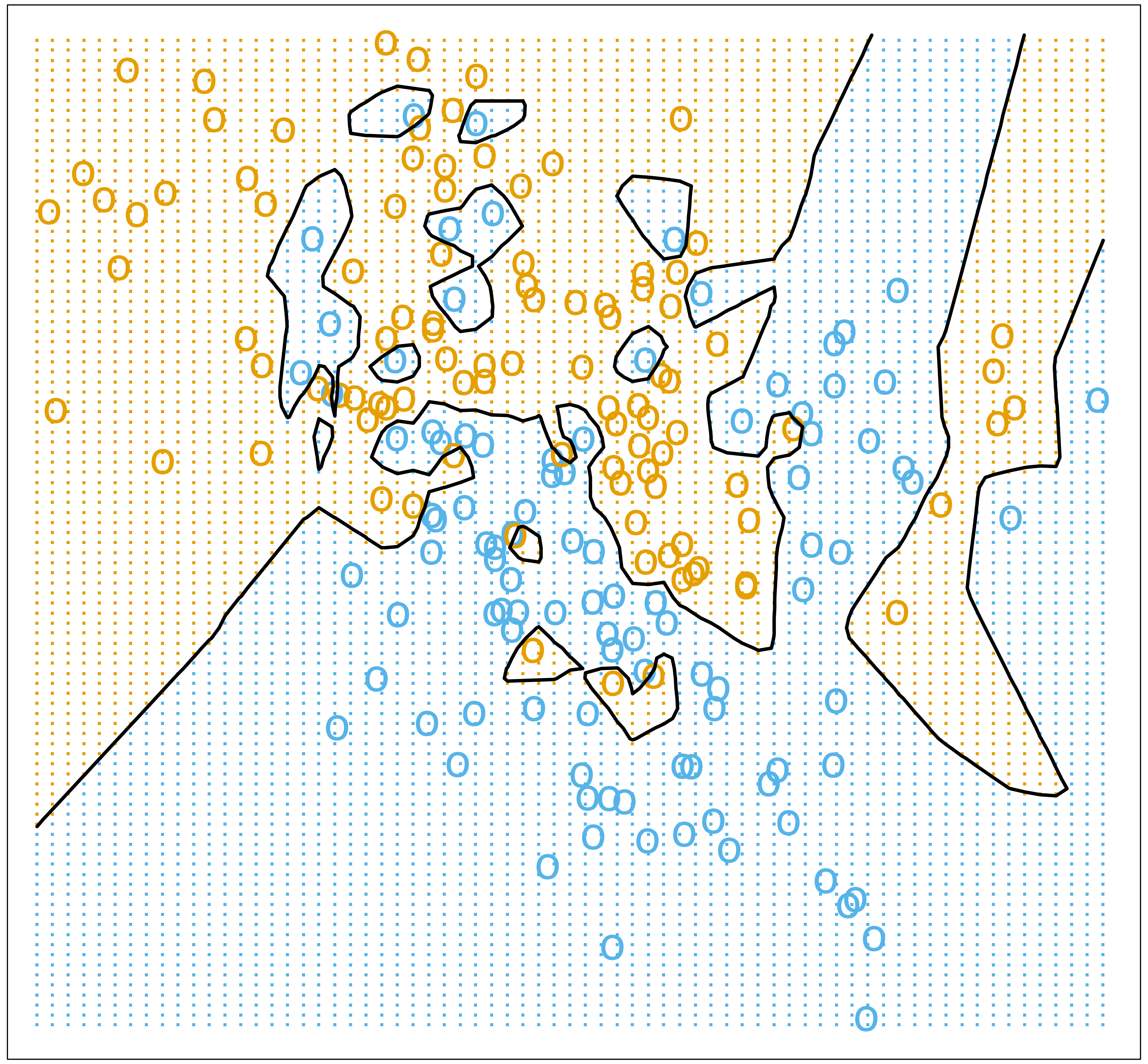
Small bias - complex decision boundary

Large variance - overfitting

Large k: ($k = n$ constant prediction)

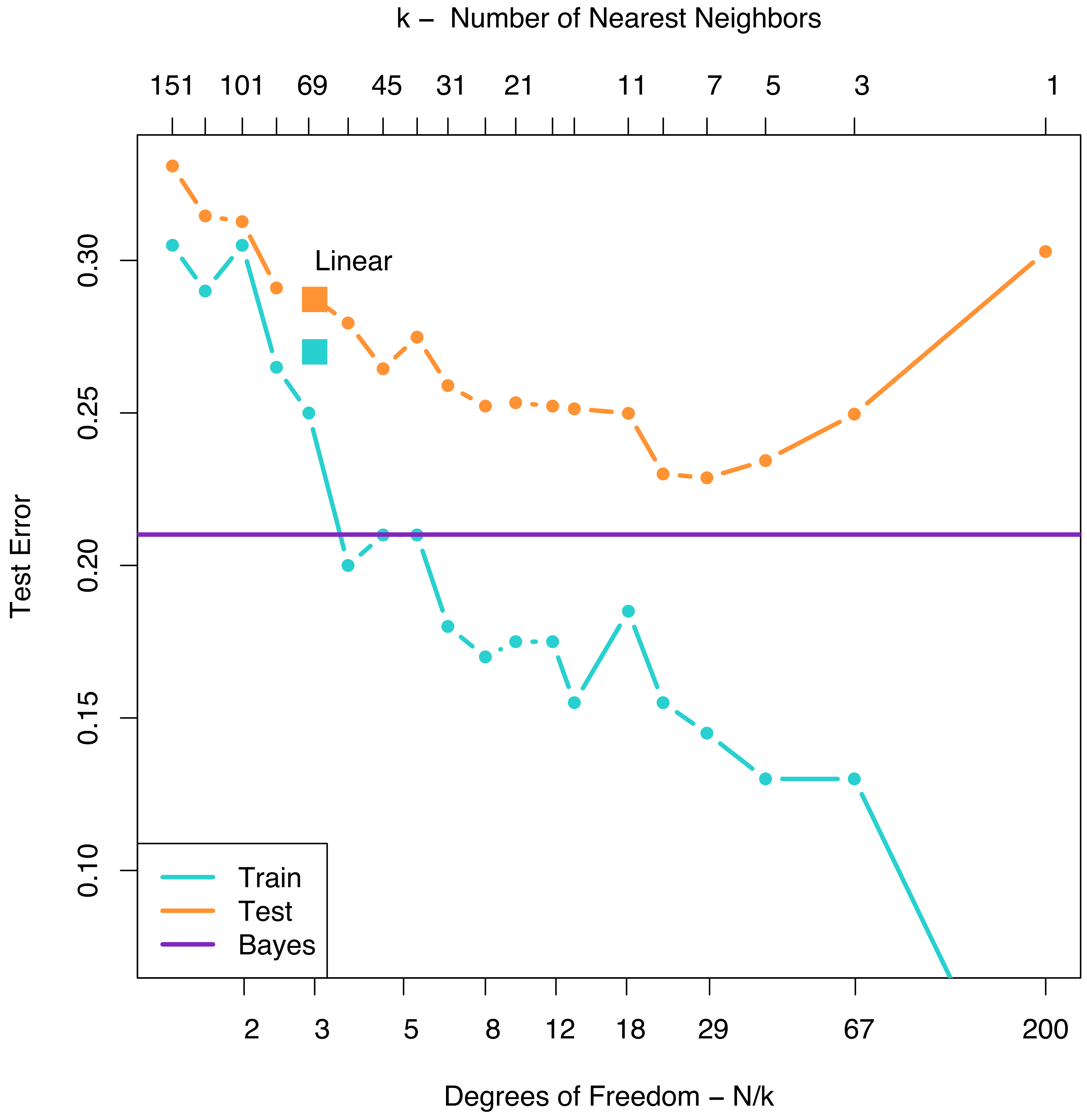
Large bias

Small variance



1-nearest neighbor classification

U-shape curve for k-NN bias-variance tradeoff



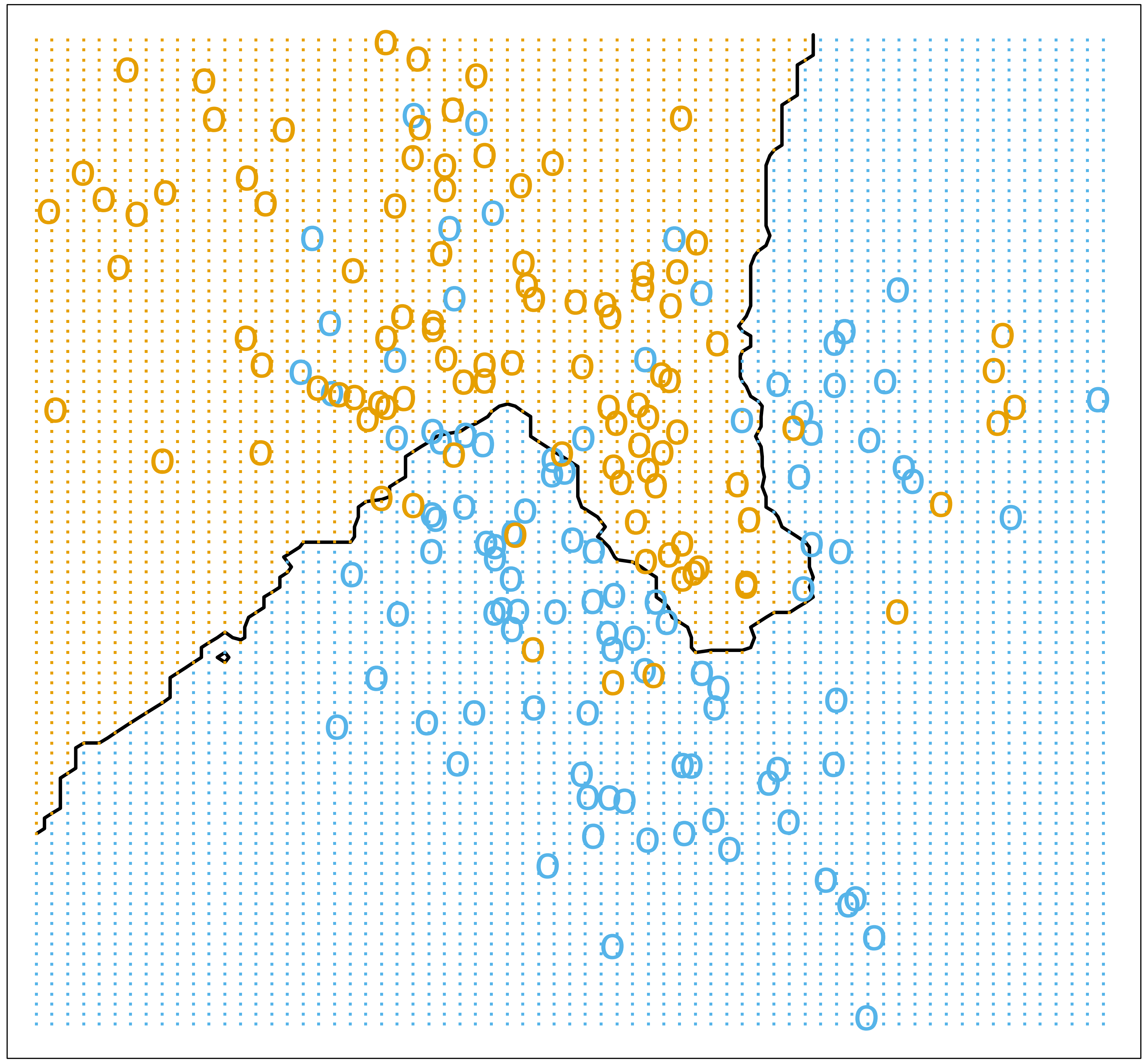
Complexity increases when k decreases

Find a k which balances the bias and the variance

<u>Good k:</u>

Small bias - complex enough decision boundary

Small variance - no overfitting



15-nearest neighbor classification

Curse of dimensionality

Claim 1: As the dimensionality grows, fixed-size training sets cover a dwindling fraction of the input space.

Assume the data $x \sim \mathcal{U}([0,1]^d)$

Consider a blue box around the center x_0 of size r

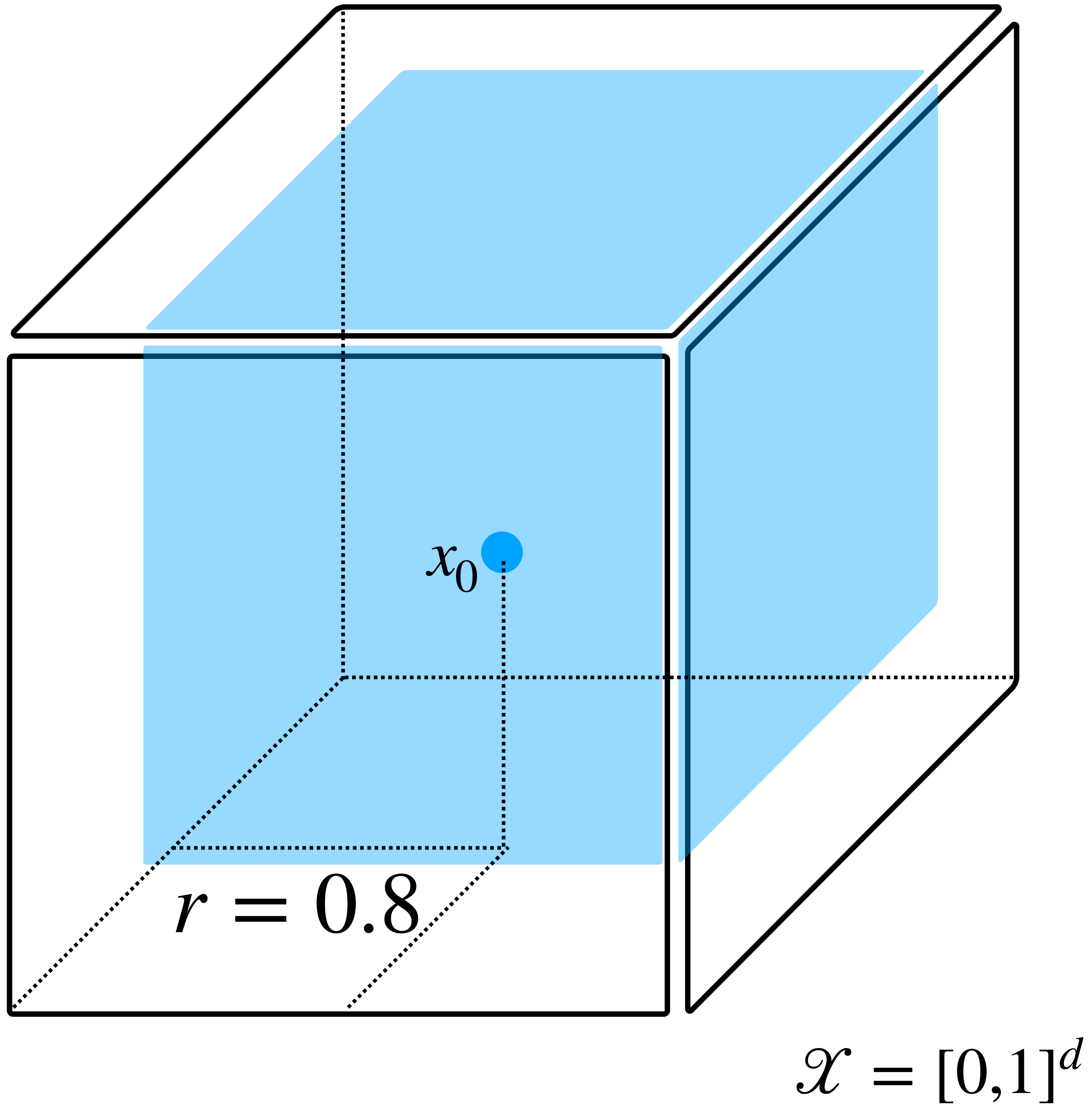
$\mathbb{P}(x \in$ $) = r^d := \alpha$

If $d = 10$, to have:

$\alpha = 0.01$ we need $r = 0.63$

$\alpha = 0.1$ we need $r = 0.8$

We need to explore almost the whole box



Curse of dimensionality

Claim 2: In high-dimension, data-points are far from each other.

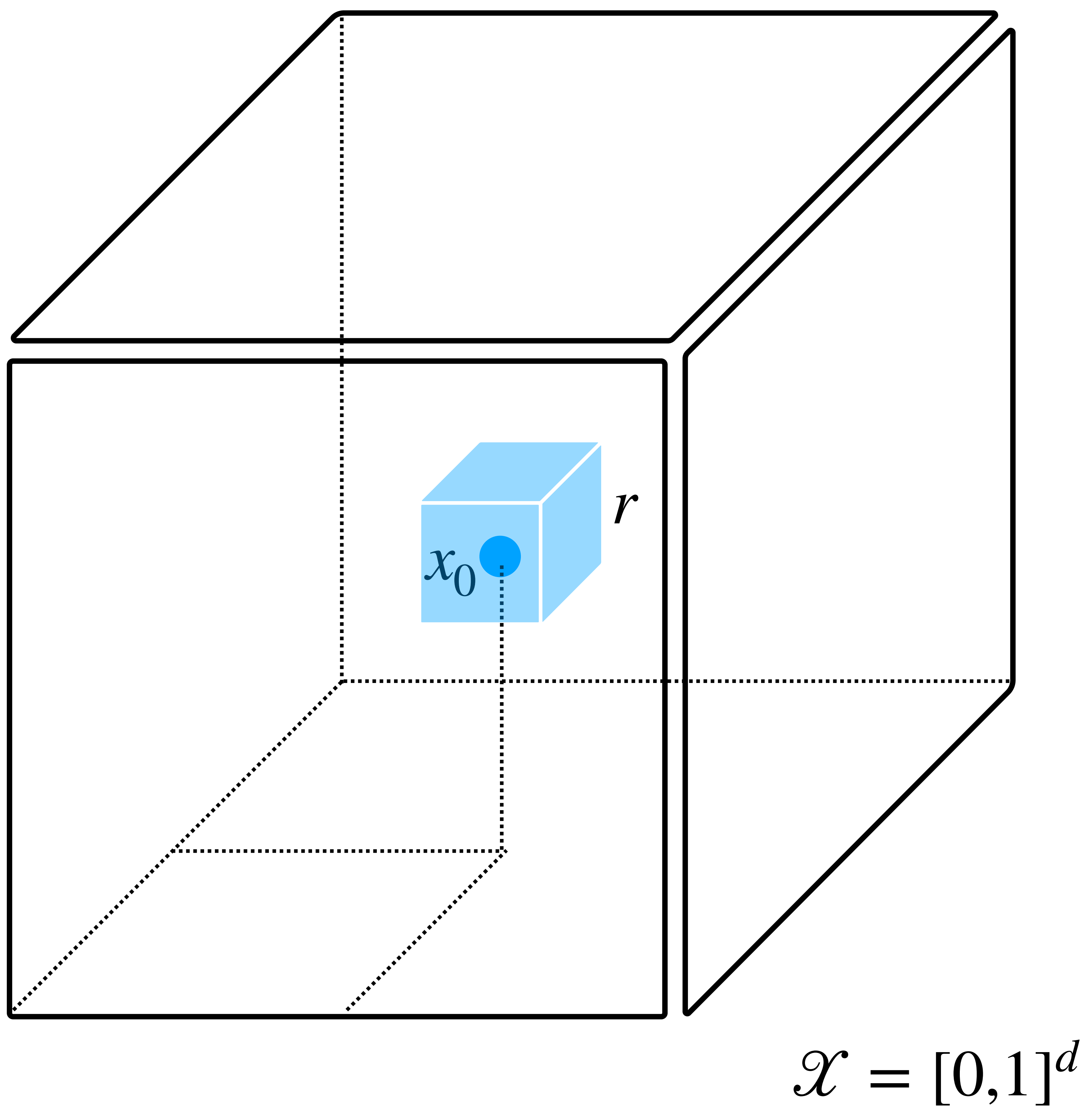
Consider n i.i.d. points uniform in the $[0,1]^d$

$$\mathbb{P}(\exists x_i \in \quad) \geq 1/2 \implies r \geq \left(1 - \frac{1}{2^{1/n}}\right)^{1/d}$$

Proof: $\mathbb{P}(x \notin \quad) = 1 - r^d$

$$\mathbb{P}(x_i \notin \quad , \forall i \leq n) = (1 - r^d)^n$$

$$\mathbb{P}(\exists x_i \in \quad) = 1 - (1 - r^d)^n$$



Curse of dimensionality

<u>Claim 2</u>: In high-dimension, data-points are far from each other.

Consider n i.i.d. points uniform in the $[0,1]^d$

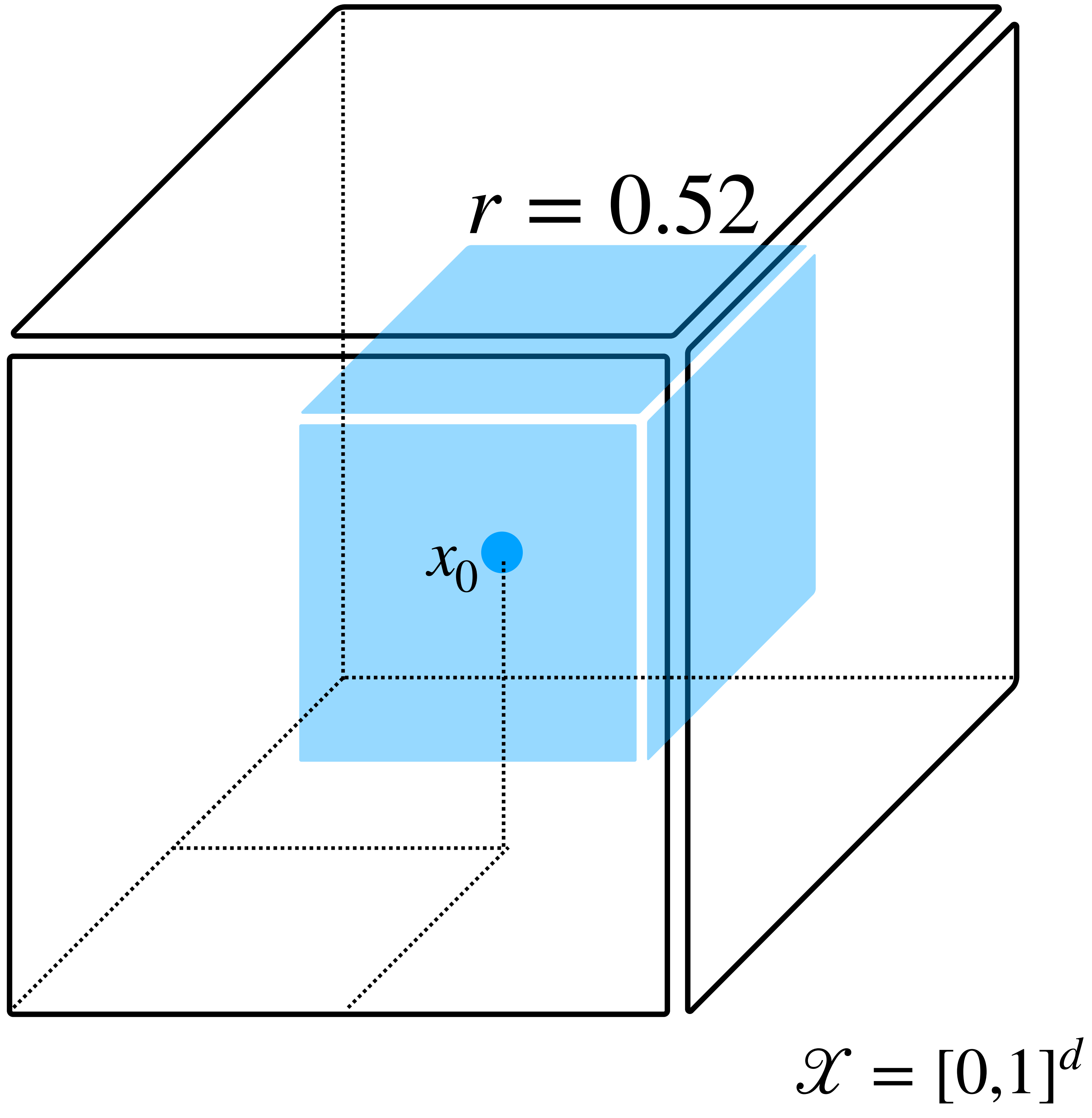
$\mathbb{P}(\exists x_i \in$ $) \geq 1/2 \implies r \geq \left(1 - \frac{1}{2^{1/n}}\right)^{1/d}$

Proof: $\mathbb{P}(x \notin$ $) = 1 - r^d$

$\mathbb{P}(x_i \notin$ $, \forall i \leq n) = (1 - r^d)^n$

$\mathbb{P}(\exists x_i \in$ $) = 1 - (1 - r^d)^n$

For $d = 10,\ n = 500$, we have $r \geq 0.52$



Generalization bound for 1-NN

Setup: $(X, Y) \sim \mathscr{D}$ over $\mathscr{X} \times \mathscr{Y} = [0,1]^d \times \{0,1\}$

Goal: Bound the classification error:

$$L(g) = \mathbb{P}_{(X,Y)\sim\mathscr{D}}(Y \neq g(X))$$

Baseline:

- Bayes classifier - minimizes L over all classifiers

$$g_*(x) = 1_{\eta(x)\geq 1/2} \text{ where } \eta(x) = \mathbb{P}(Y = 1 \,|\, X = x)$$

- Bayes risk - smallest probability of misclassification

$$L(g_*) = \mathbb{P}(g_*(X) \neq Y) = \mathbb{E}_{X\sim\mathscr{D}_X}[\min\{\eta(X), 1 - \eta(X)\}]$$

Generalization bound for 1-NN

Setup: $(X, Y) \sim \mathscr{D}$ ov

Goal: Bound the classi

Proof 1:

$$\eta(x) \geq 1/2 \iff \mathbb{P}(Y=1\,|\,X=x) \geq 1/2$$
$$\iff \mathbb{P}(Y=1\,|\,X=x) \geq \mathbb{P}(Y=0\,|\,X=x)$$
$$\iff 1 \in \arg\max_{y\in\{0,1\}} P(Y=y\,|\,X=x)$$

Baseline:

- Bayes classifier - minimizes L over all classifiers

$$g_*(x) = 1_{\eta(x)\geq 1/2} \text{ where } \eta(x) = \mathbb{P}(Y=1\,|\,X=x)$$

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$$L(g_*) = \mathbb{P}(g_*(X) \neq Y) = \mathbb{E}_{X\sim\mathscr{D}_X}[\min\{\eta(X), 1-\eta(X)\}]$$

Generalization bound for 1-NN

Proof 2:

$$
\begin{aligned}
L(g_*) &= \mathbb{E}_{(X,Y)\sim\mathscr{D}}[1_{g_*(X)\neq Y}] \\
&= \mathbb{E}_{X\sim\mathscr{D}_X}[\mathbb{E}_{Y\sim\mathscr{D}_{Y|X}}[1_{g_*(X)\neq Y}\,|\,X]] \\
&= \mathbb{E}_{X\sim\mathscr{D}_X}[\mathbb{E}_{Y\sim\mathscr{D}_{Y|X}}[1_{g_*(X)\neq Y}\,|\,X]1_{\eta(X)\geq 1/2} + E_{Y\sim\mathscr{D}_{Y|X}}[1_{g_*(X)\neq Y}\,|\,X]1_{\eta(X)>1/2}] \\
&= \mathbb{E}_{X\sim\mathscr{D}_X}[\mathbb{E}_{Y\sim\mathscr{D}_{Y|X}}[1_{1\neq Y}\,|\,X]1_{\eta(X)\geq 1/2} + E_{Y\sim\mathscr{D}_{Y|X}}[1_{0\neq Y}\,|\,X]1_{\eta(X)>1/2}] \\
&= \mathbb{E}_{X\sim\mathscr{D}_X}[\mathbb{P}(Y=0\,|\,X)1_{\eta(X)\geq 1/2} + \mathbb{P}(Y=1\,|\,X)1_{\eta(X)>1/2}] \\
&= \mathbb{E}_{X\sim\mathscr{D}_X}[\min\{\eta(X), 1-\eta(X)\}]
\end{aligned}
$$

- Bayes risk - smallest probability of misclassification

$$L(g_*) = \mathbb{P}(g_*(X)\neq Y) = \mathbb{E}_{X\sim\mathscr{D}_X}[\min\{\eta(X), 1-\eta(X)\}]$$

Generalization bound for 1-NN

Assumption: $\exists c \geq 0, \forall x, x' \in \mathcal{X}$:

$$|\eta(x) - \eta(x')| \leq c\|x - x'\|_2$$

➡ Nearby points are likely to have the same label

Claim:

$$\mathbb{E}_{S_{train}}[L(g_{S_{train}})] \leq 2L(g_*) + c\mathbb{E}_{S_{train}, X\sim\mathcal{D}_X}[\|X - \text{nbh}_{S_{train},1}(X)\|]$$

$$\leq 2L(g_*) + 4c\sqrt{d}N^{-\frac{1}{d+1}}$$

geometric term:
average distance between
a random point and x

Interpretation:

Fixed d and $N \to \infty$: $\mathbb{E}_{S_{train}}[L(g_{S_{train}})] \leq 2L(g_*)$

Fixed N and $d \to \infty$: error increases exponentially fast

Interpolation method can generalize well: against common belief

Proof

We want to bound

$$\mathbb{E}_{S_{train}}[L(g_{S_{train}})] = \mathbb{E}_{S_{train}}[\mathbb{P}_{(X,Y)\sim\mathscr{D}}[g_{S_{train}}(X) \neq Y]]$$

We first sample n unlabeled examples $S_{train,X} = (X_1, \cdots X_n) \sim \mathscr{D}_X$, an unlabeled example $X \sim \mathscr{D}$ and define $X' = \text{nbh}_{S_{train},1}(X)$

Finally we sample $Y \sim \eta(X)$ and $Y' \sim \eta(X')$

We have:

$$\begin{aligned}
\mathbb{E}_{S_{train}}[L(g_{S_{train}})] &= \mathbb{E}_{S_{X,train},X\sim\mathscr{D}_X,Y\sim\eta(X),Y'\sim\eta(X')}[1_{Y\neq g_{S_{train}(X)}}] \\
&= \mathbb{E}_{S_{X,train},X\sim\mathscr{D}_X,Y\sim\eta(X),Y'\sim\eta(X')}[1_{Y\neq Y'}] \\
&= \mathbb{E}_{S_{train,X}X\sim\mathscr{D}_X}[\mathbb{P}_{Y\sim\eta(X),Y'\sim\eta(X')}(Y \neq Y')]
\end{aligned}$$

Proof

Consider two points $x, x' \in [0,1]^d$.

Sample their labels $Y \sim \eta(x)$ and $Y' \sim \eta(x')$

Claim:

$$\mathbb{P}(Y' \neq Y) \leq 2\min\{\eta(x), 1 - \eta(x)\} + c\|x - x'\|$$

- Simple case: $x = x'$

$$\begin{aligned}
\mathbb{P}(Y' \neq Y) &= \mathbb{E}[1_{Y' \neq Y} 1_{Y'=1} + 1_{Y' \neq Y} 1_{Y'=0}] \\
&= \mathbb{P}(Y' = 1)\mathbb{P}(Y = 0) + \mathbb{P}(Y' = 1)\mathbb{P}(Y = 0) \\
&= 2\eta(x)(1 - \eta(x)) \\
&\leq 2\min\{\eta(x), 1 - \eta(x)\}
\end{aligned}$$

Case 1:

Y=0 $(1 - \eta(x))$

Y'=1 $\eta(x)$

Case 2:

Y=1 $\eta(x)$

Y'=0 $(1 - \eta(x))$

Proof

- General case:

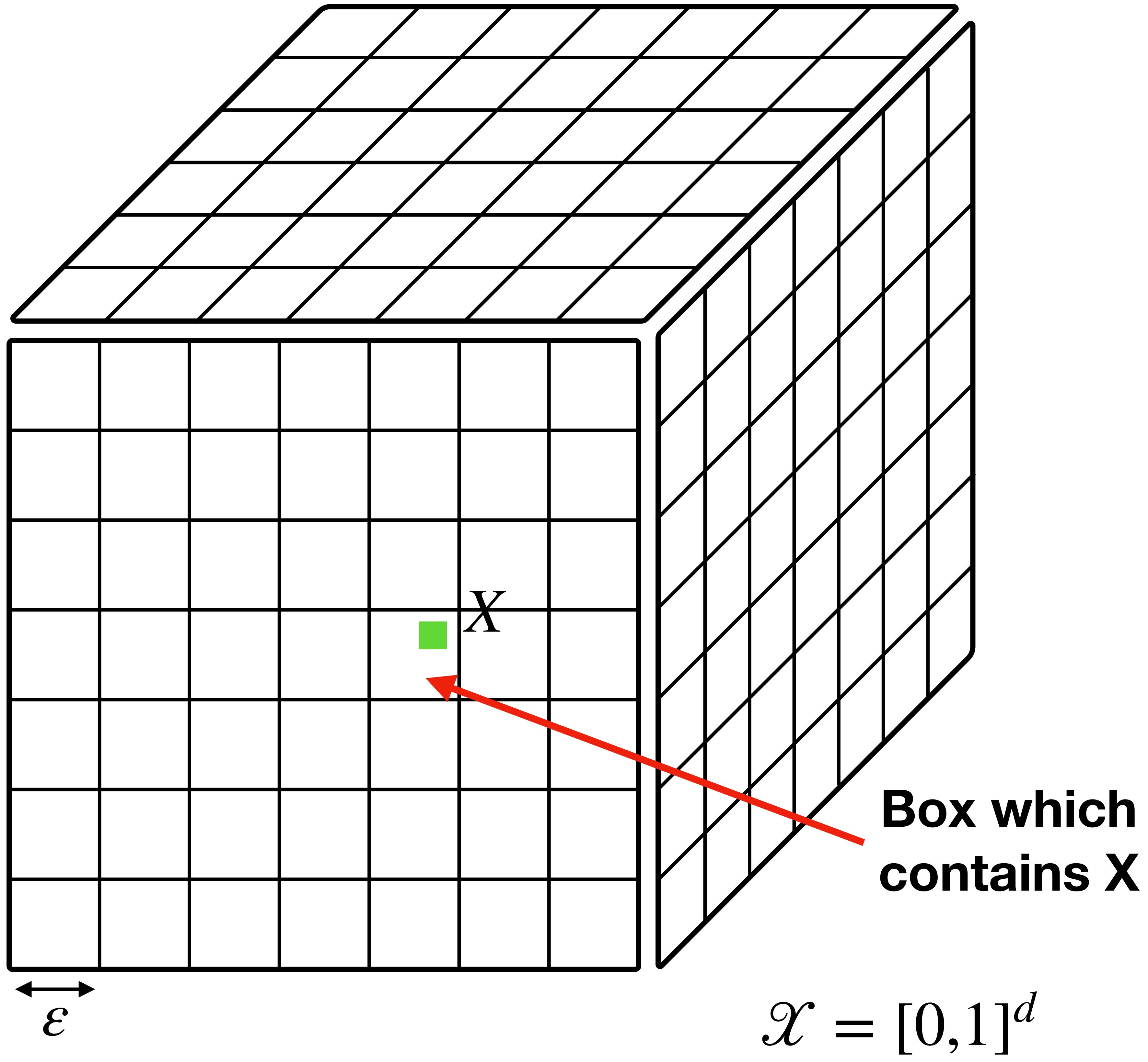
$$
\begin{aligned}
\mathbb{P}(Y \neq Y') &= \eta(x)(1-\eta(x')) + \eta(x')(1-\eta(x)) \\
&= \eta(x)(1-\eta(x)) + \eta(x)(\eta(x) - \eta(x')) \\
&\qquad + \eta(x)(1-\eta(x)) + (\eta(x') - \eta(x))(1-\eta(x)) \\
&= 2\eta(x)(1-\eta(x)) + (2\eta(x)-1)(\eta(x) - \eta(x')) \\
&\leq 2\eta(x)(1-\eta(x)) + |(2\eta(x)-1)||\eta(x) - \eta(x')| \\
&\leq 2\eta(x)(1-\eta(x)) + |\eta(x) - \eta(x')| \\
&\leq 2\eta(x)(1-\eta(x)) + c\|x - x'\| \\
&\leq 2\min\{\eta(x), 1-\eta(x)\} + c\|x - x'\|
\end{aligned}
$$

Proof

$$
\begin{aligned}
\mathbb{E}_{S_{train}}[L(g_{S_{train}})] &= \mathbb{E}_{S_{X,train},X\sim\mathcal{D}_X,Y\sim\eta(X),Y'\sim\eta(X')}[1_{Y\neq g_{S_{train}(X)}}] \\
&= \mathbb{E}_{S_{X,train},X\sim\mathcal{D}_X,Y\sim\eta(X),Y'\sim\eta(X')}[1_{Y\neq Y'}] \\
&= \mathbb{E}_{S_{train,X}X\sim\mathcal{D}_X}[\mathbb{P}_{Y\sim\eta(X),Y'\sim\eta(X')}(Y\neq Y')] \\
&\leq 2\mathbb{E}_{S_{train,X}X\sim\mathcal{D}_X}[2\min\{\eta(X),1-\eta(X)\}+c\|X-X'\|] \\
&\leq 2L(g_*)+c\mathbb{E}_{S_{train}X\sim\mathcal{D}_X}[\|X-\mathsf{nbh}_{S_{train},1}(X)\|]
\end{aligned}
$$

Bound on the geometric term

Consider a fresh sample $X \sim \mathscr{D}$ and denote by
$p_k = \mathbb{P}(X \in \text{Box}_k)$
Consider the box which contains X. Two options:



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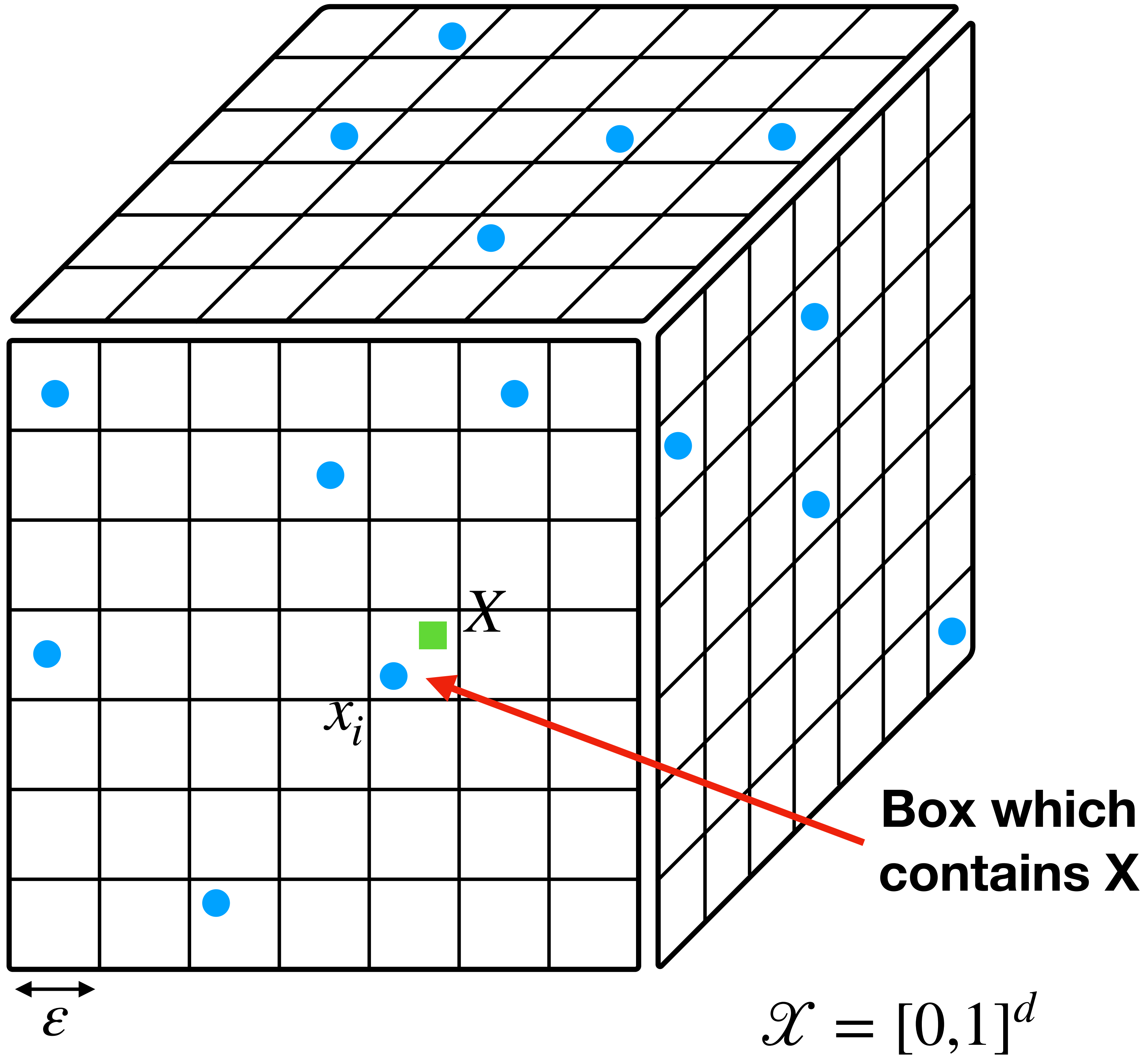
$p_k = \mathbb{P}(X \in \text{Box}_k)$
Consider the box which contains X. Two options:

- The box contains an element of S_{train}. X has a neighbor in S_{train} at distance at most $\sqrt{d}\varepsilon$

It happens with probability $1 - (1 - p_k)^n$



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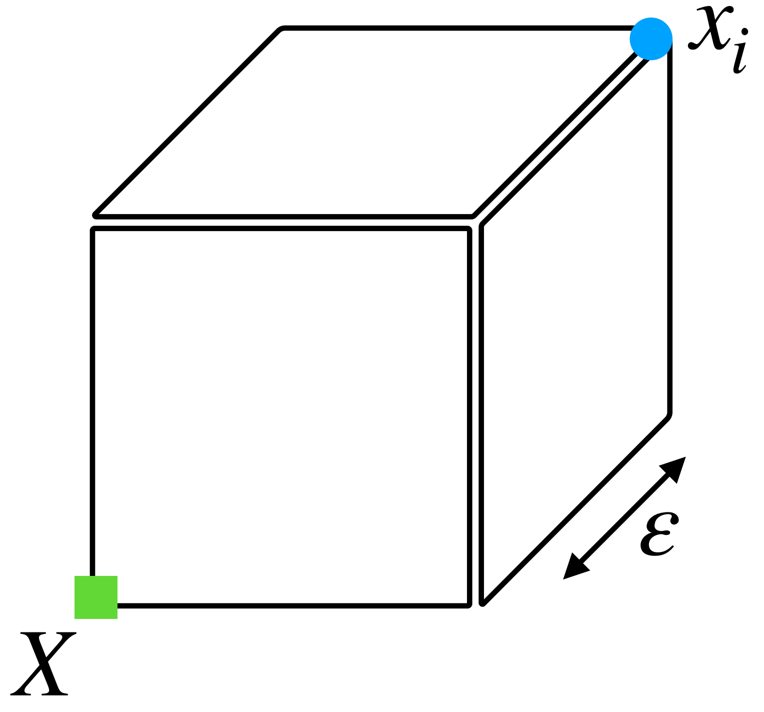
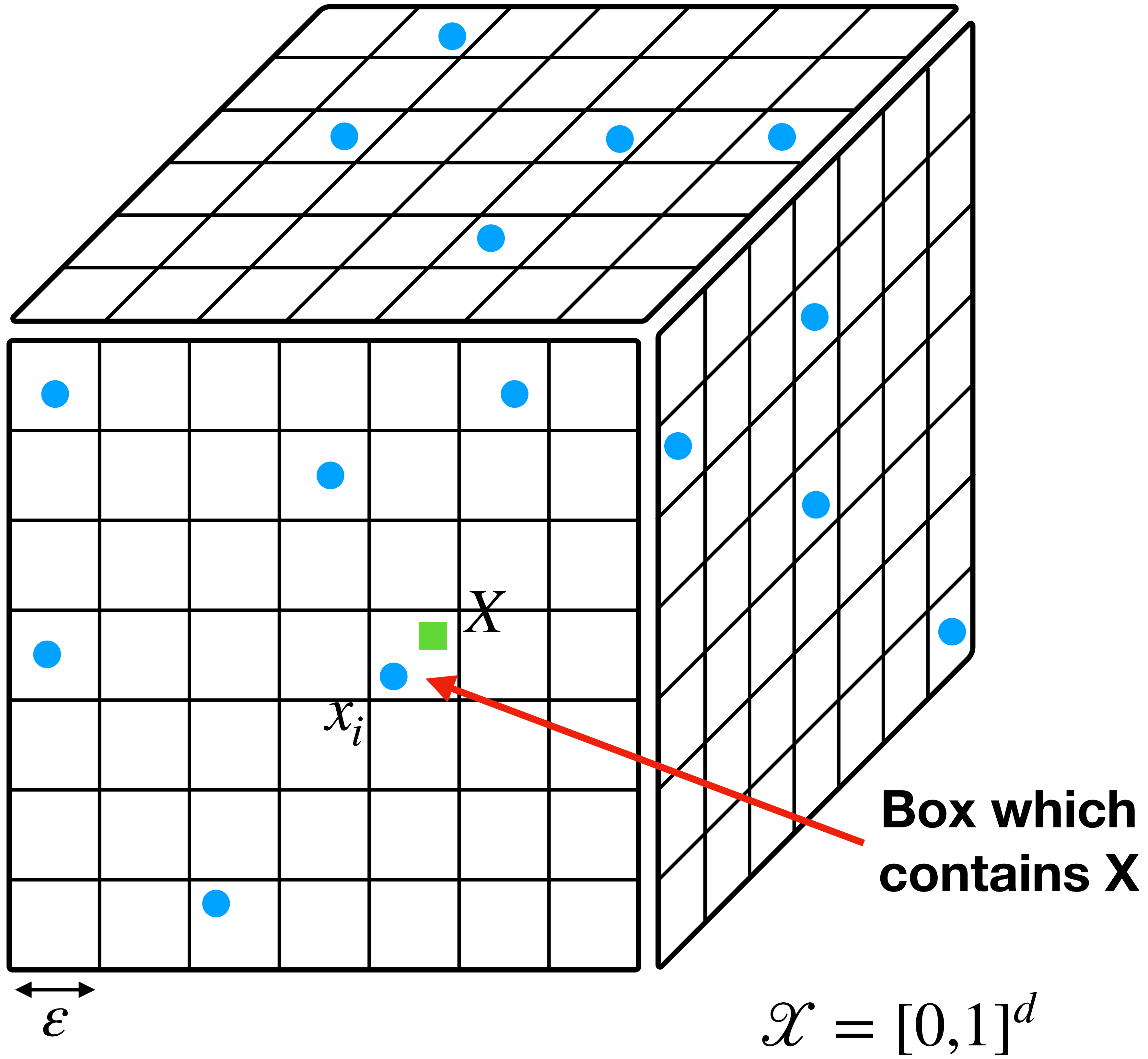
- The box contains an element of S_{train}. X has a neighbor in S_{train} at distance at most $\sqrt{d}\varepsilon$

It happens with probability $1 - (1 - p_k)^n$

Proof: Consider the worst case:

$$\|X - x_i\| = \sqrt{\sum_{i=1}^{d} \varepsilon^2} = \sqrt{d}\varepsilon$$





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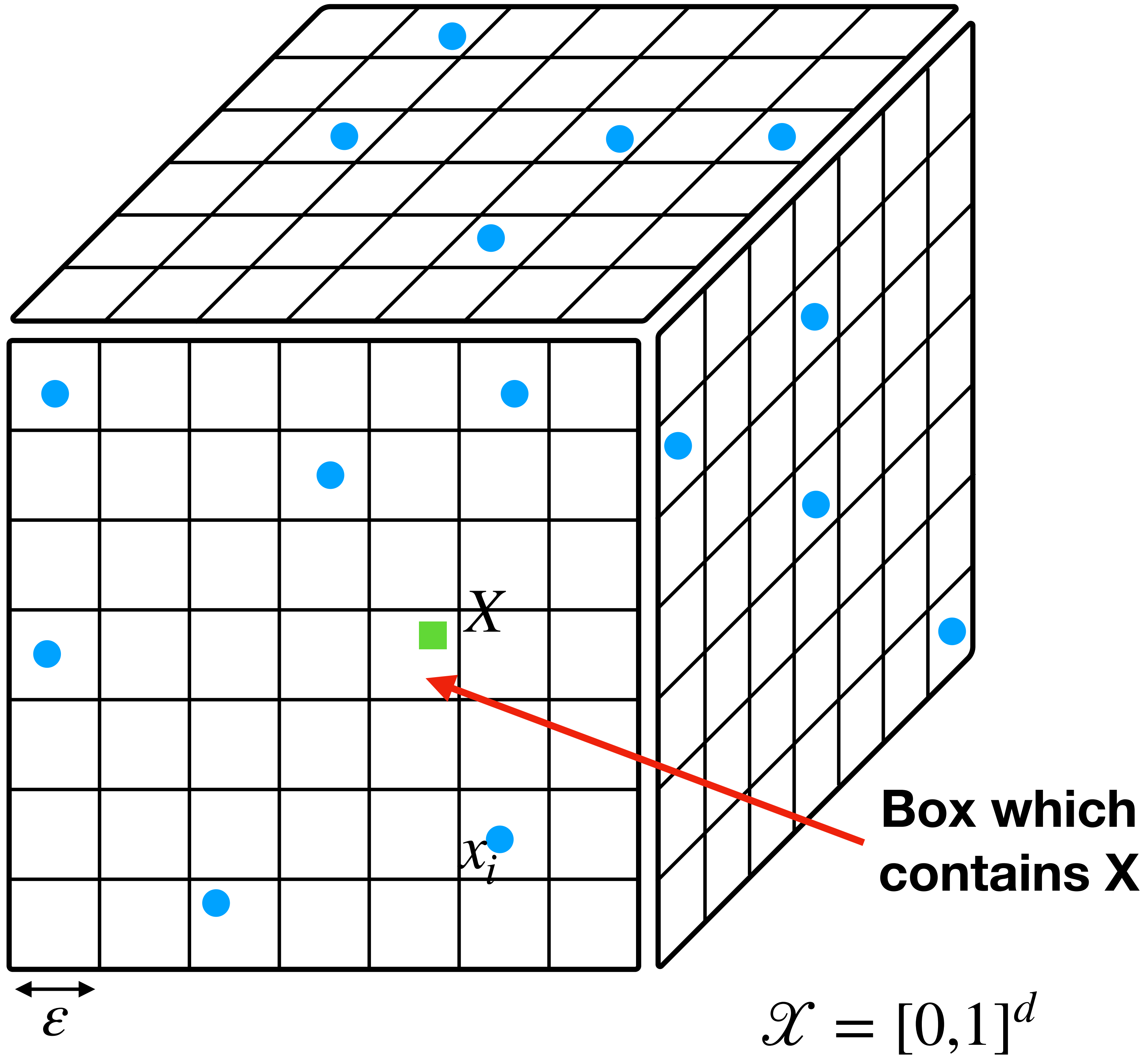
Consider a fresh sample $X \sim \mathscr{D}$ and denote by
$p_k = \mathbb{P}(X \in \text{Box}_k)$
Consider the box which contains X. Two options:

- The box contains an element of S_{train}. X has a neighbor in S_{train} at distance at most $\sqrt{d}\varepsilon$

It happens with probability $1 - (1 - p_k)^n$

- There is no element of S_{train}. The nearest neighbor of X can be at worst at a distance $\sqrt{d}$

It happens with probability $(1 - p_k)^n$



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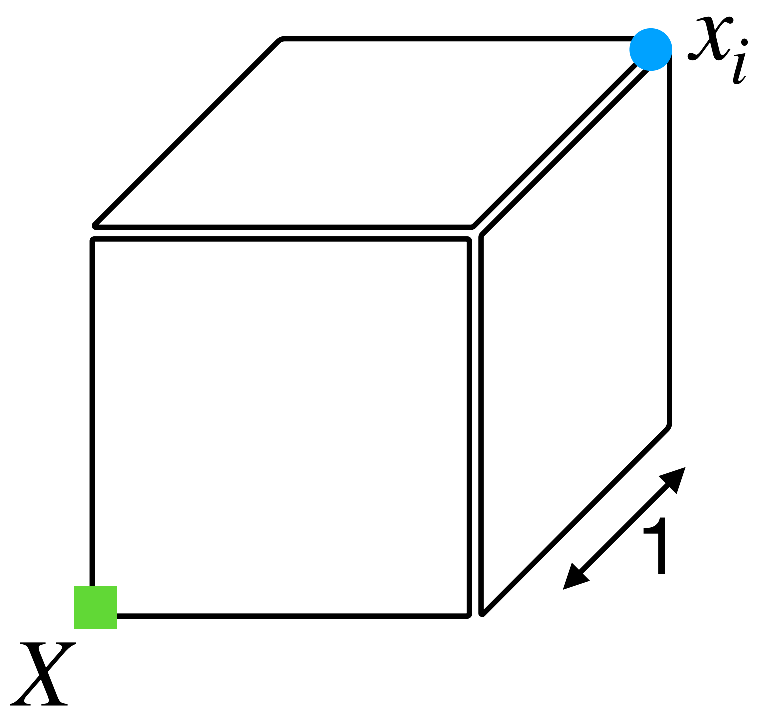
C

Proof: Consider the worst case:

$$\|X - x_i\| = \sqrt{\textstyle\sum_{i=1}^{d} 1} = \sqrt{d}$$

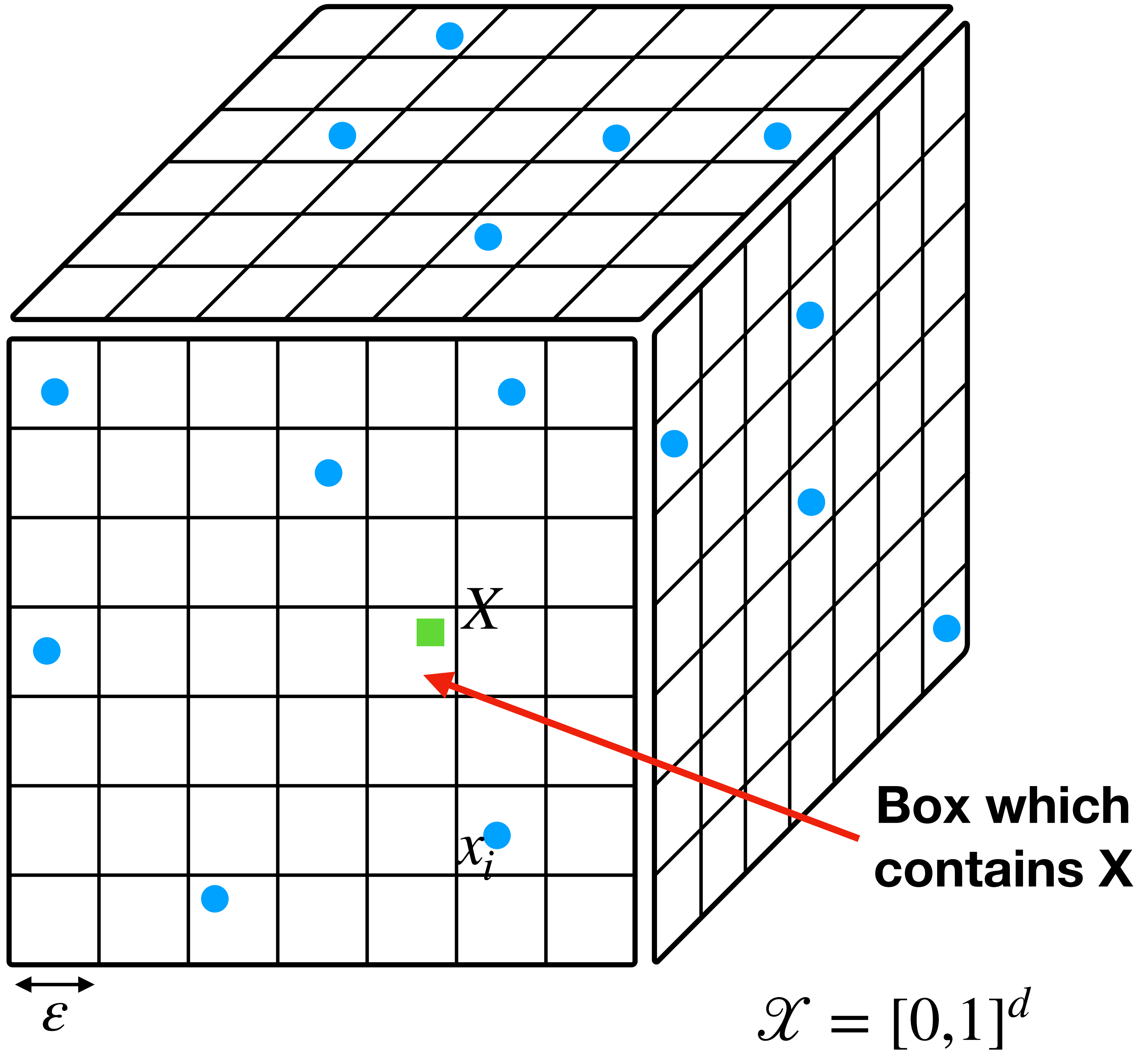


of

train

X can be at worst at a distance $\sqrt{d}$

It happens with probability $(1 - p_k)^n$



Bound on the geometric term

$$\mathbb{E}[X - \text{nbh}(X)] = \sum_k p_k[(1-p_k)^n\sqrt{d} + (1-(1-p_k)^n)\sqrt{d}\varepsilon]$$

Claim: we get the bound by maximizing over p_k and ε

Intuition:

- If p_k is large: it is likely that I pick that box but it is also likely that I find a training point in that box
- If p_k is small, then we are fine since by definition this does not happen very often.