Nearest-Neighbor Classifiers and the Curse of Dimensionality

Machine Learning Course - CS-433
15 Oct 2025
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EPFL

Supervised machine learning

We observe some data $S_{\text{train}} = \{x_n, y_n\}_{n=1}^{N} \in \mathcal{X} \times \mathcal{Y}$

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

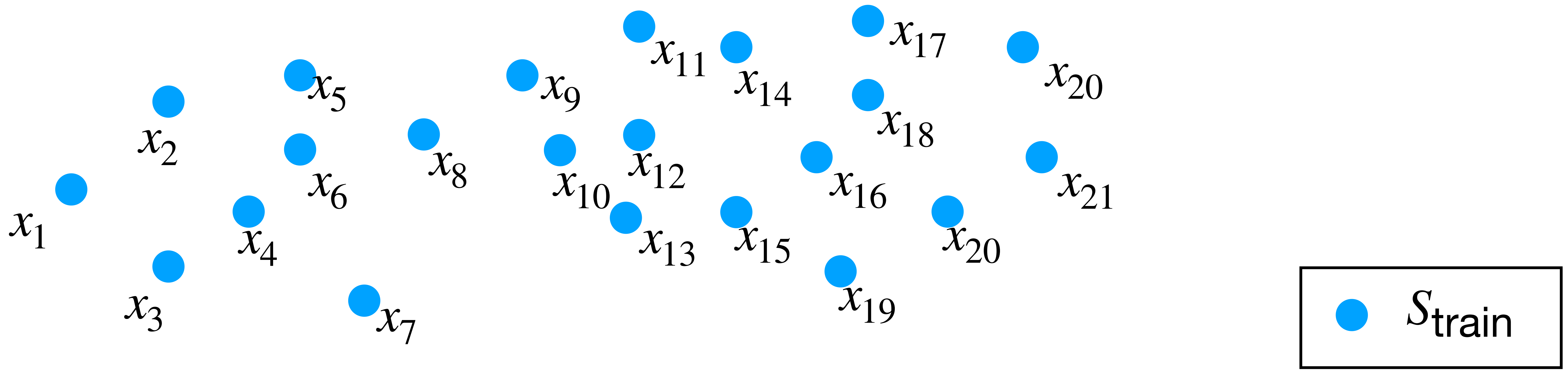
<u>How:</u>

$S_{\text{train}} = \{x_n, y_n\}_{n=1}^{N}$ $\qquad$ $\mathcal{A}$ $\qquad$ $f_S = \mathcal{A}(S)$

Nearest neighbor function

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

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



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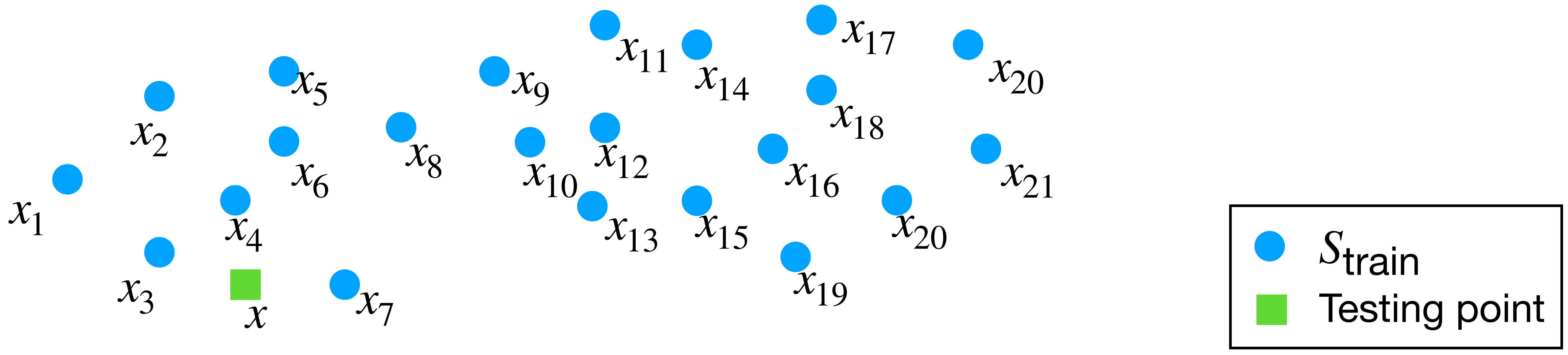

$$\text{nbh}_{S_{train},3}(x) = ?$$

Nearest neighbor function

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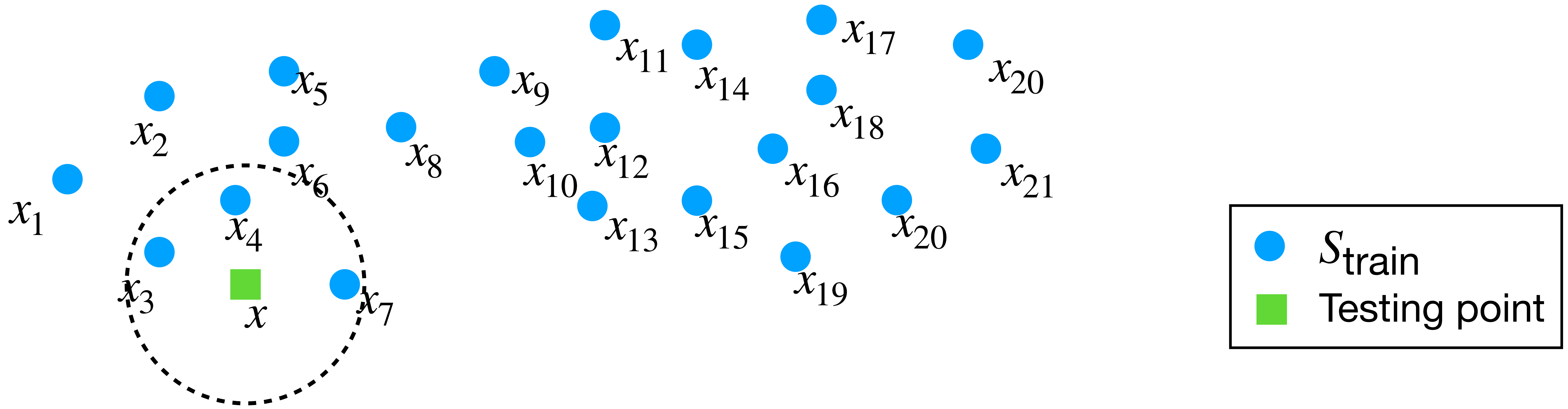

$$\text{nbh}_{S_{train},3}(x) = \{x_3, x_4, x_7\}$$

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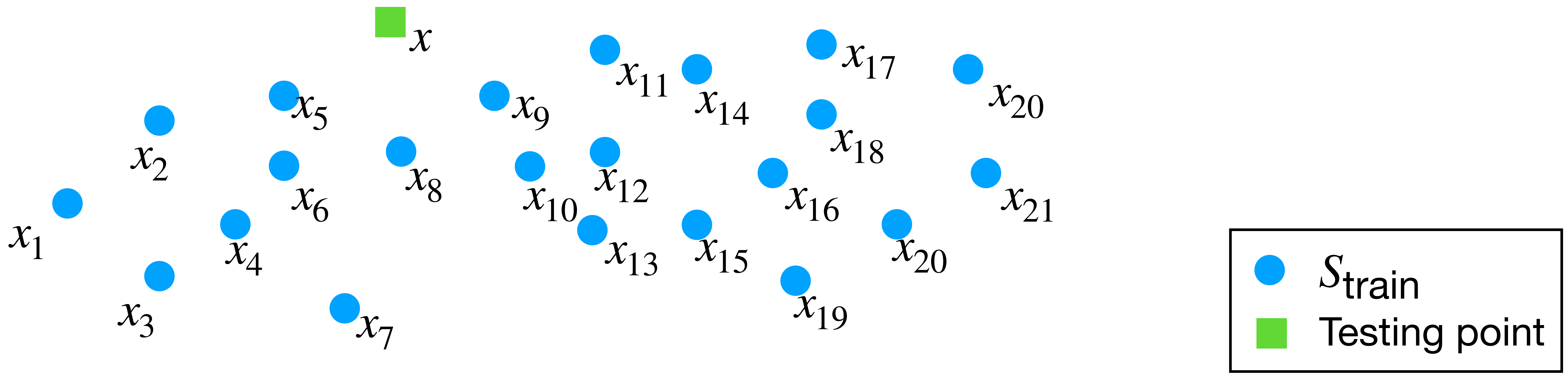

$$\text{nbh}_{S_{train},2}(x) = ?$$

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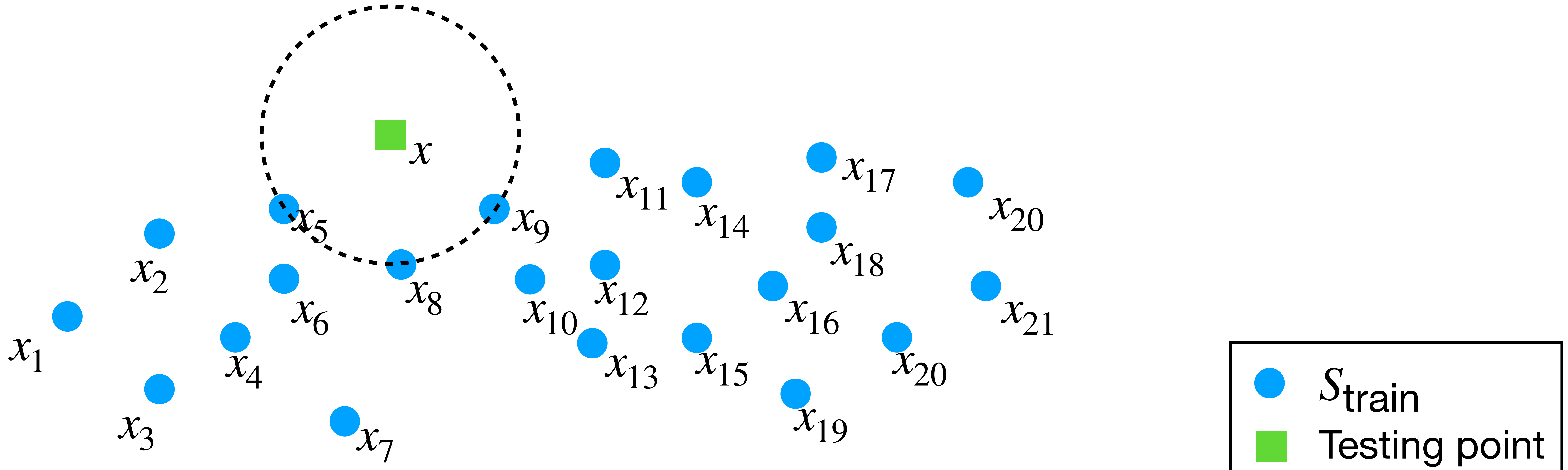

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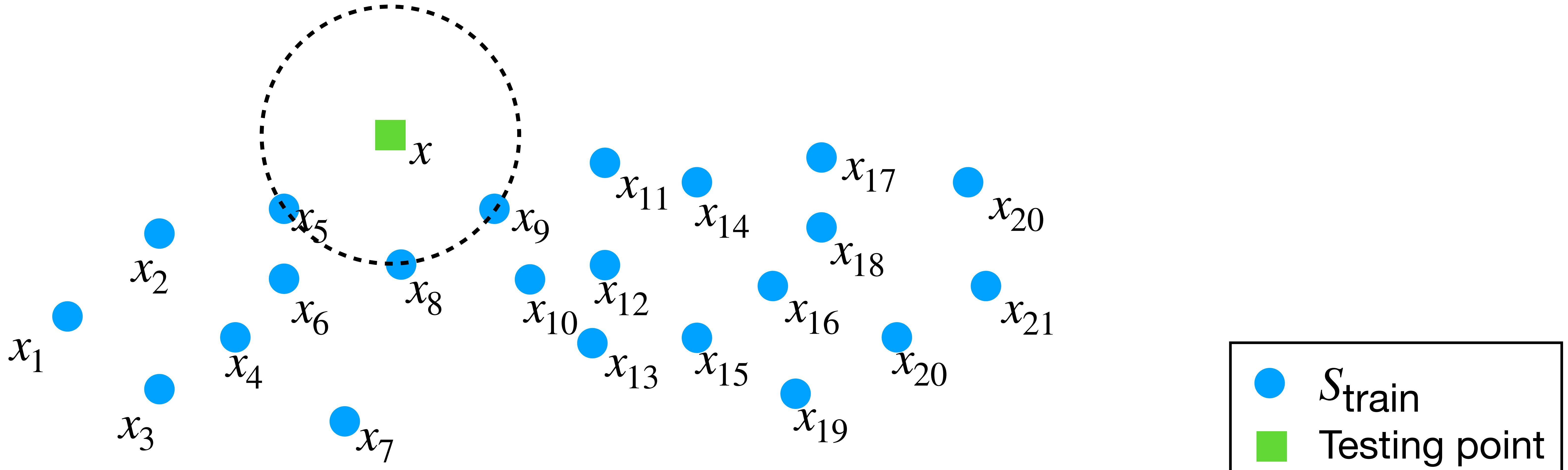

$$\text{nbh}_{S_{train},2}(x) = \{x_5, x_8\}$$

Not uniquely defined!
The result depends on the implementation
Ties are often broken randomly

Nearest neighbor function

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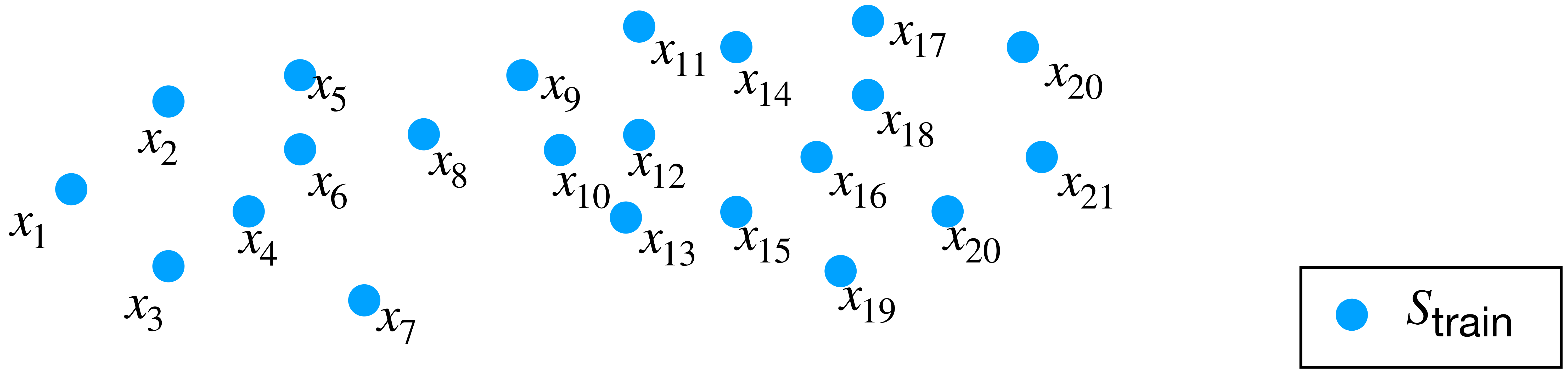
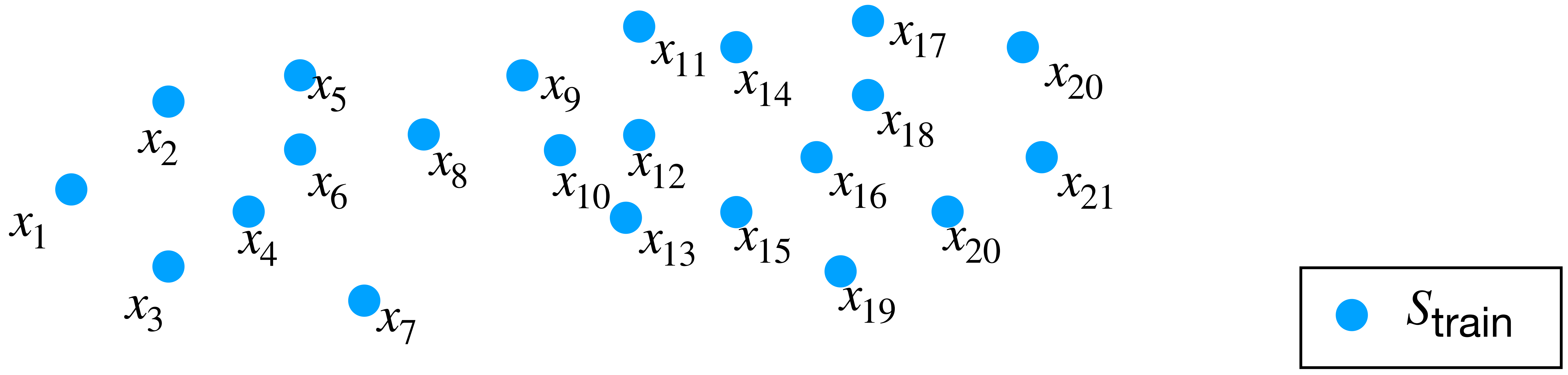


<u>Remarks:</u>

- Different metrics can be employed
- High computational complexity for large N (but efficient data structure may exist)

k-NN can be used for regression ($y \in \mathbb{R}$)

$$f_{S_{train},k}(x) = \frac{1}{k} \sum_{n: x_n \in nbh_{S_{train},k}(x)} y_n$$



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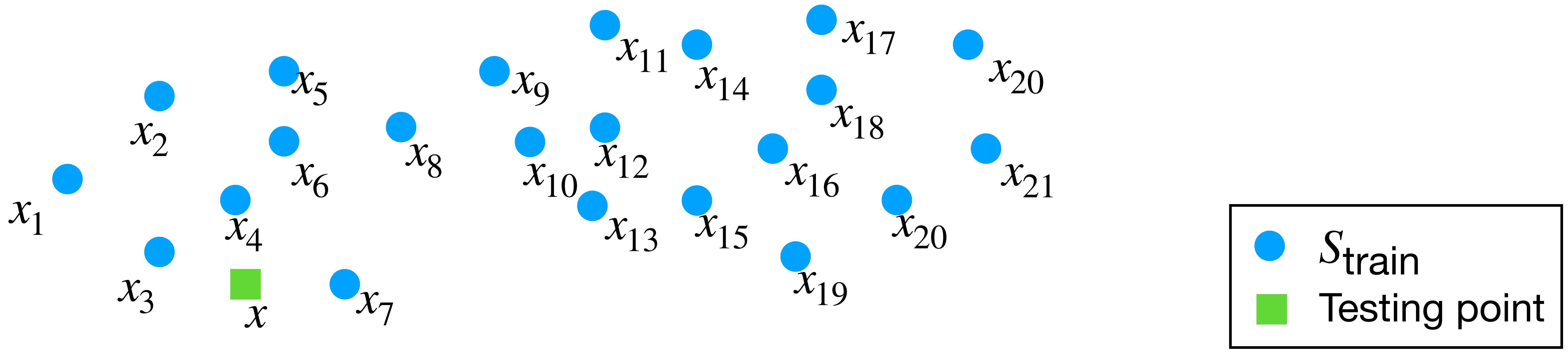

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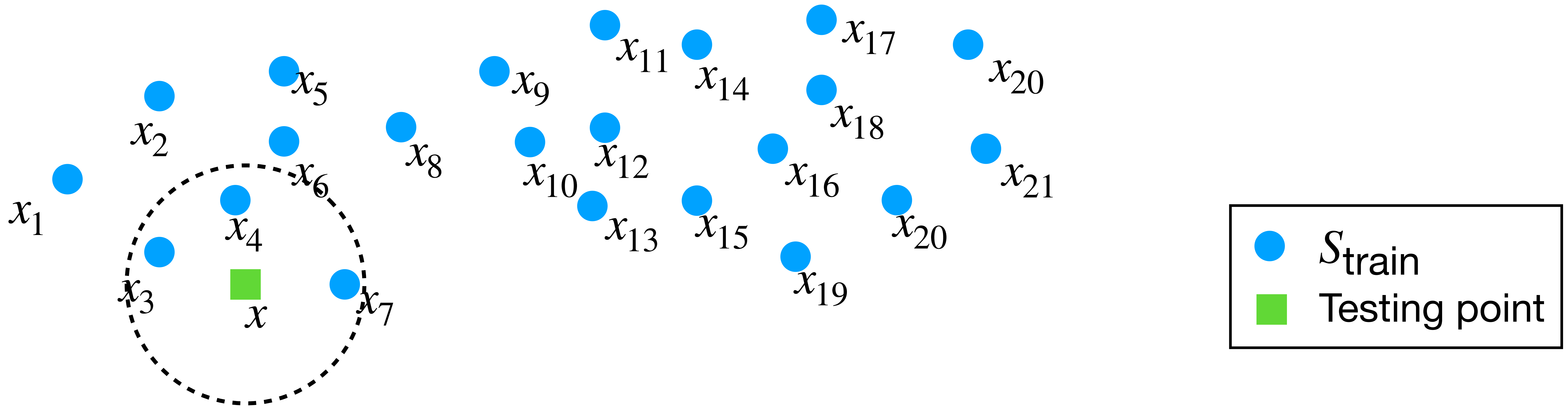

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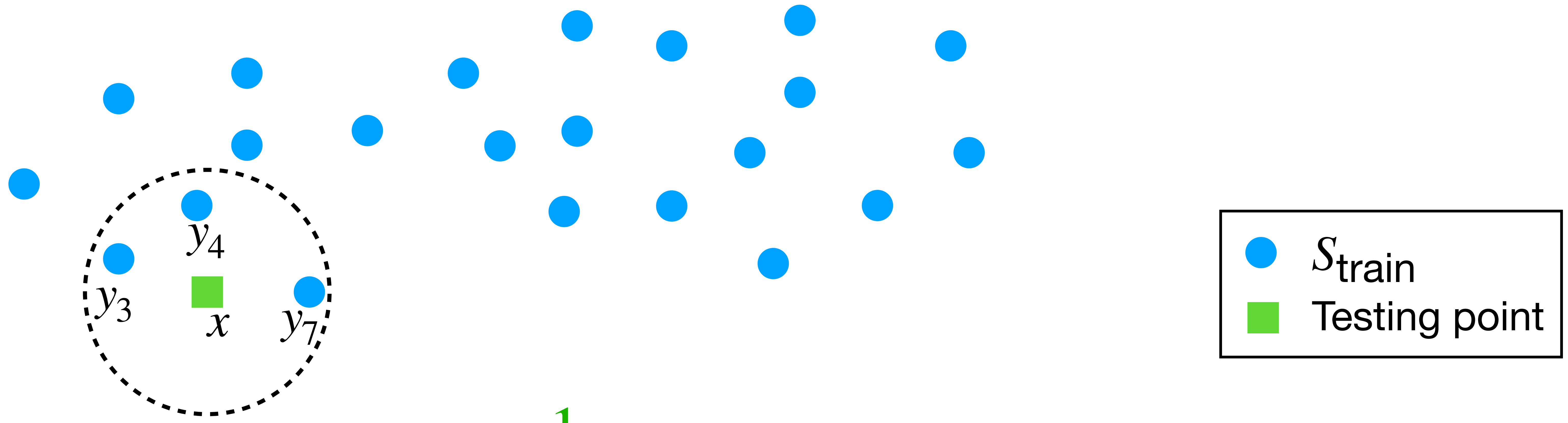
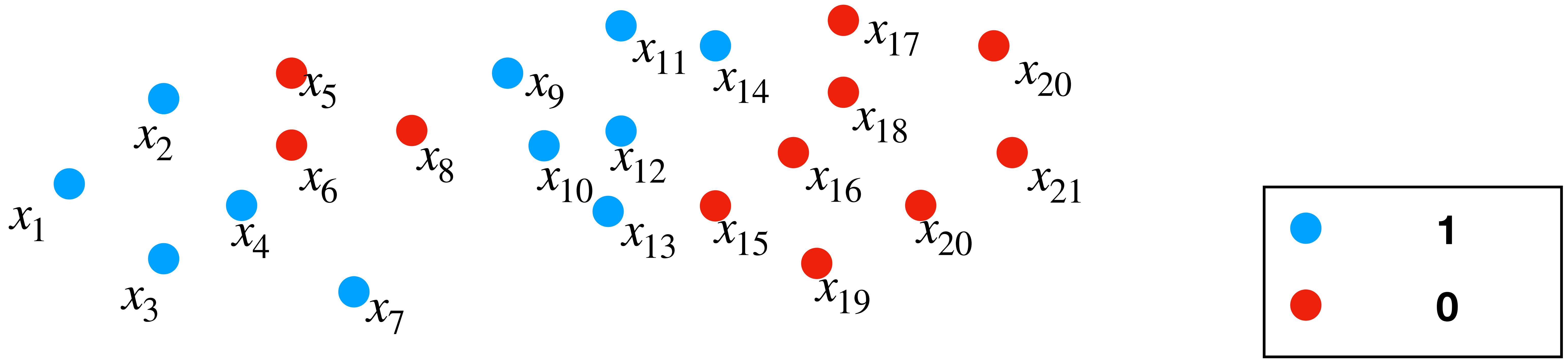


$$f_{S_{train},3}(x) = \frac{1}{3}\left(y_3 + y_4 + y_7\right)$$

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

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



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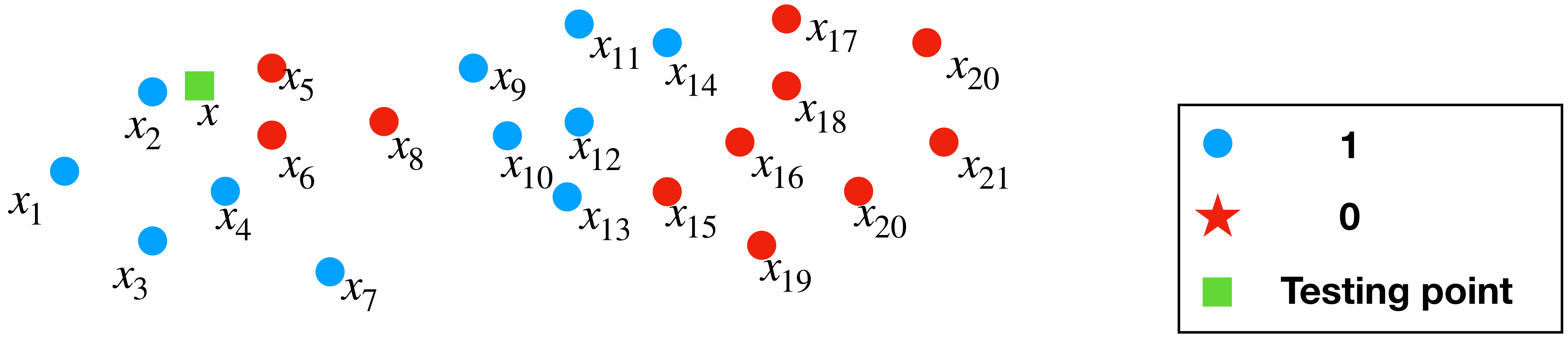

$$f_{S_{train},1}(x) = ?$$

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

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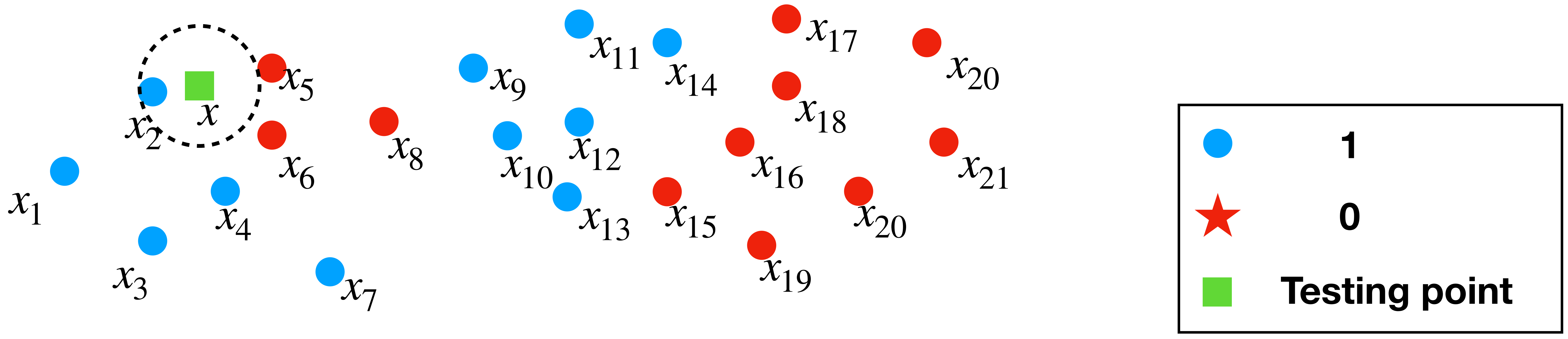

$$f_{S_{train},1}(x) = 1$$

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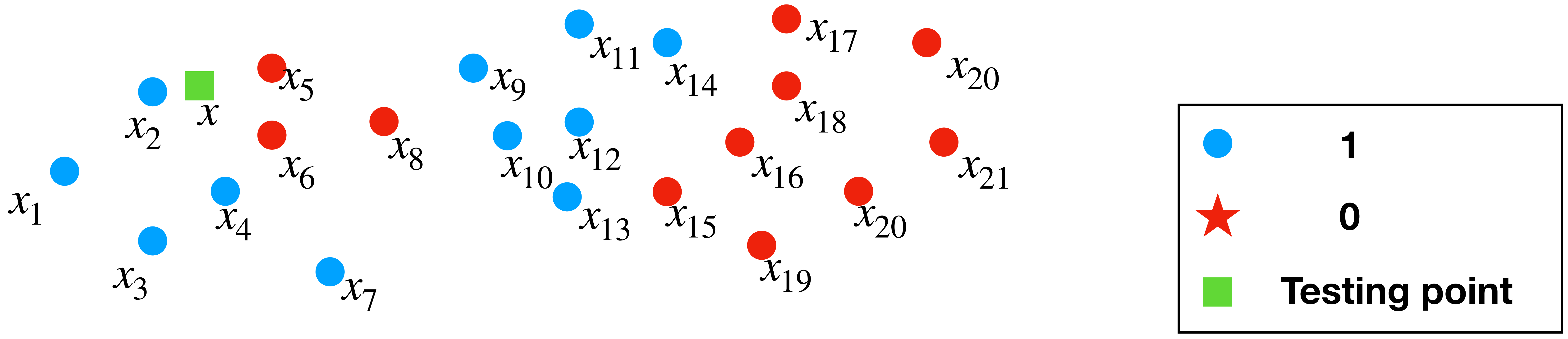

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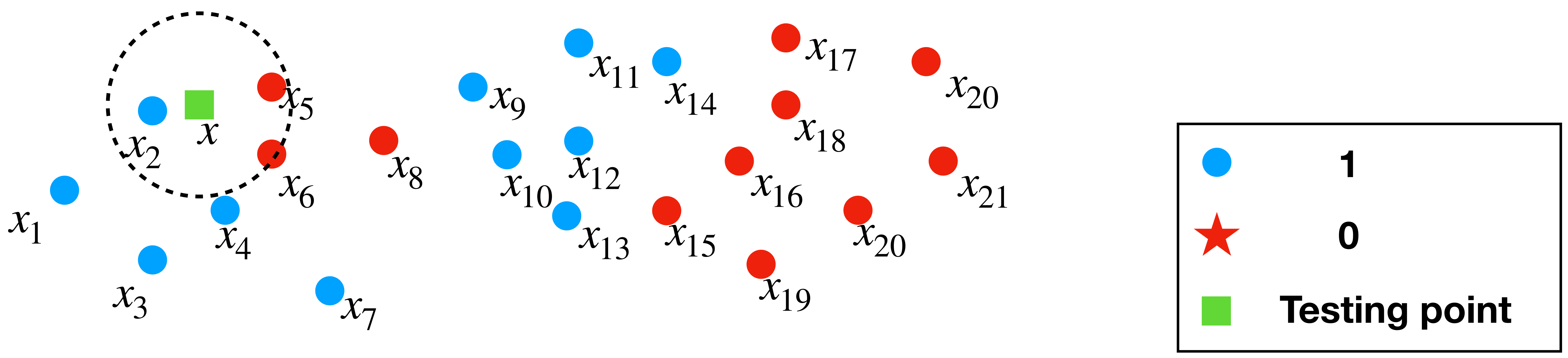

$$f_{S_{train},3}(x) = 0$$

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

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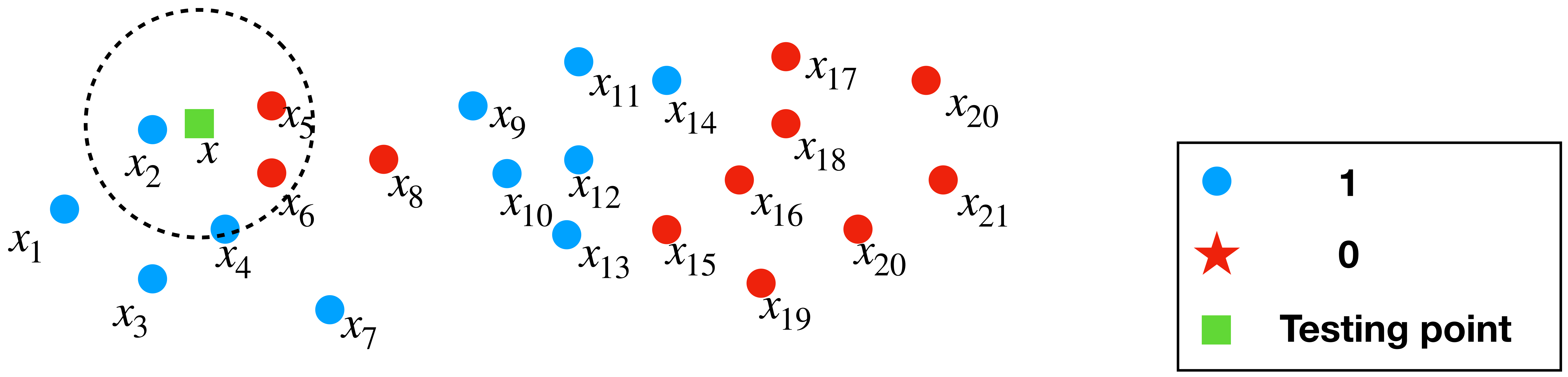
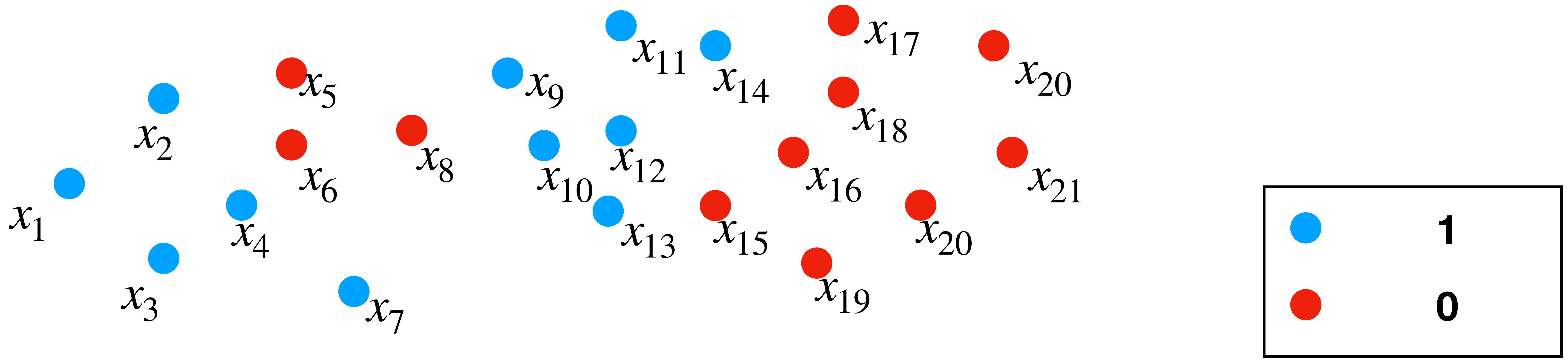


$f_{S_{train},4}(x) = ?$ **Tie!**

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

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

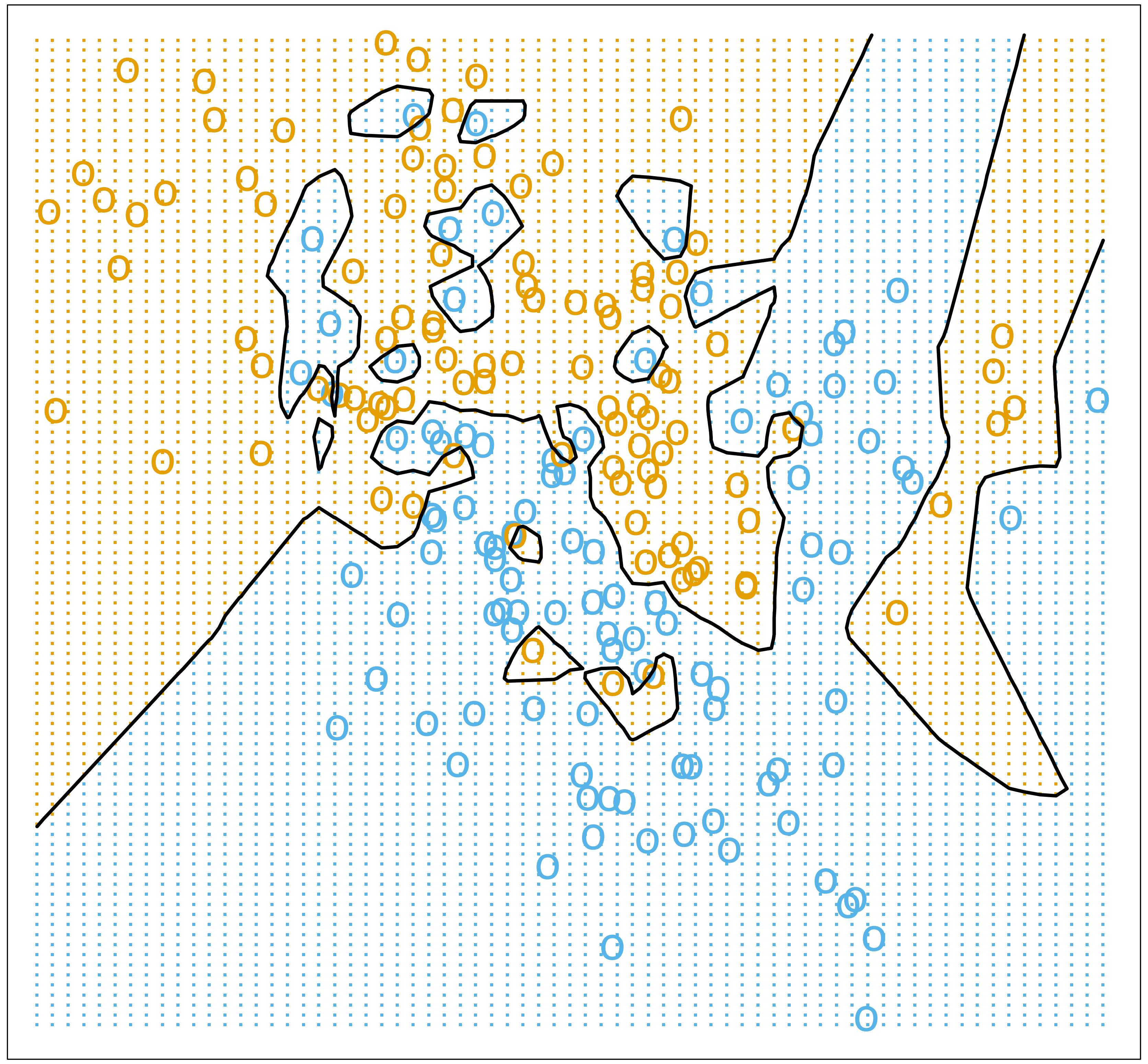


<u>Remarks:</u>

- Choose an odd value for k to prevent ties
- Generalization: smoothing kernels; weighted linear combination of elements

Why does it make sense?

- Relevant in the presence of spatial correlation
- Implicitly models intricate decision boundaries in low-dimensional spaces



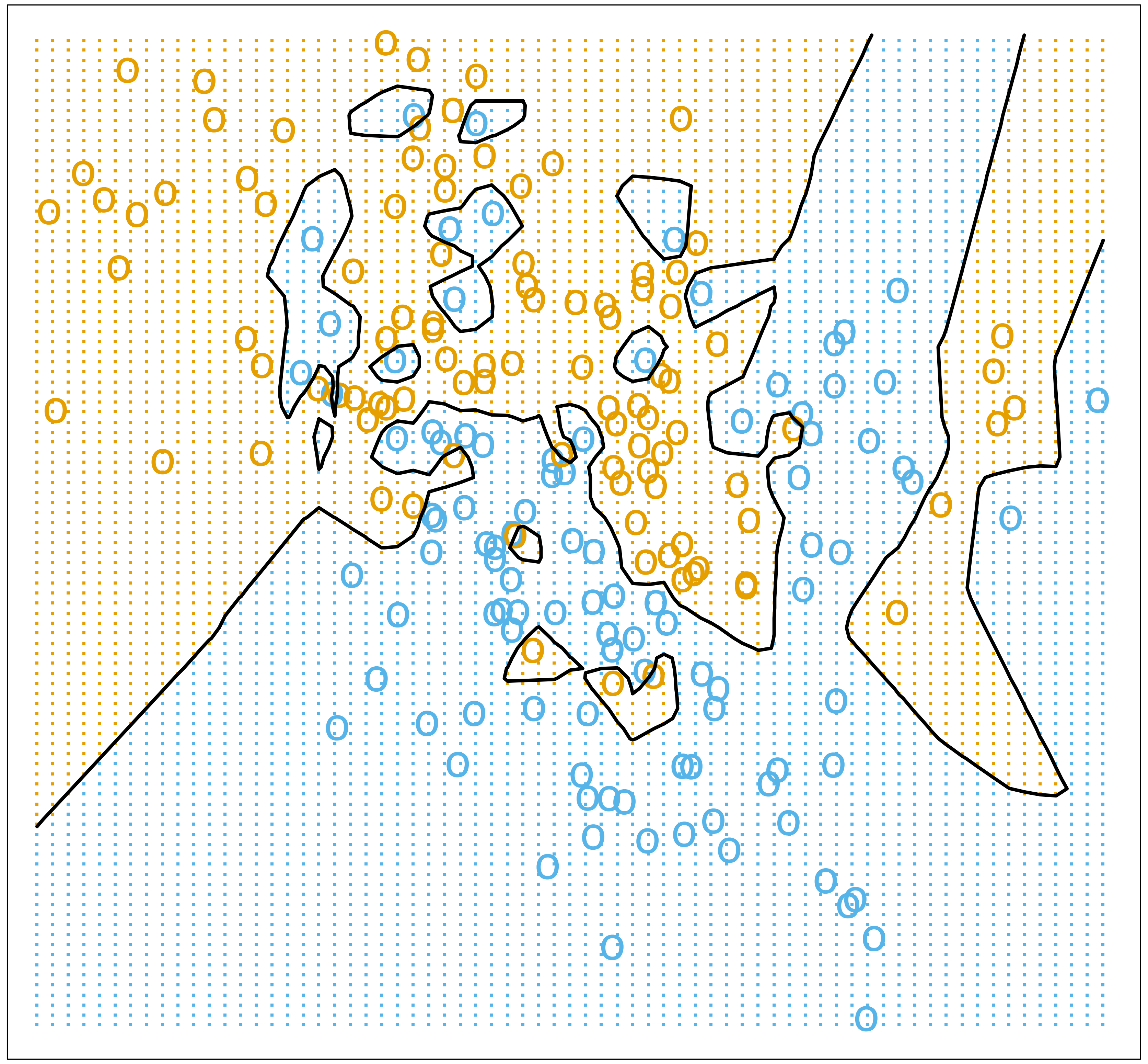
Bias-variance tradeoff in k-NN

For small k:

- Low bias - complex decision boundary
- High variance - overfitting

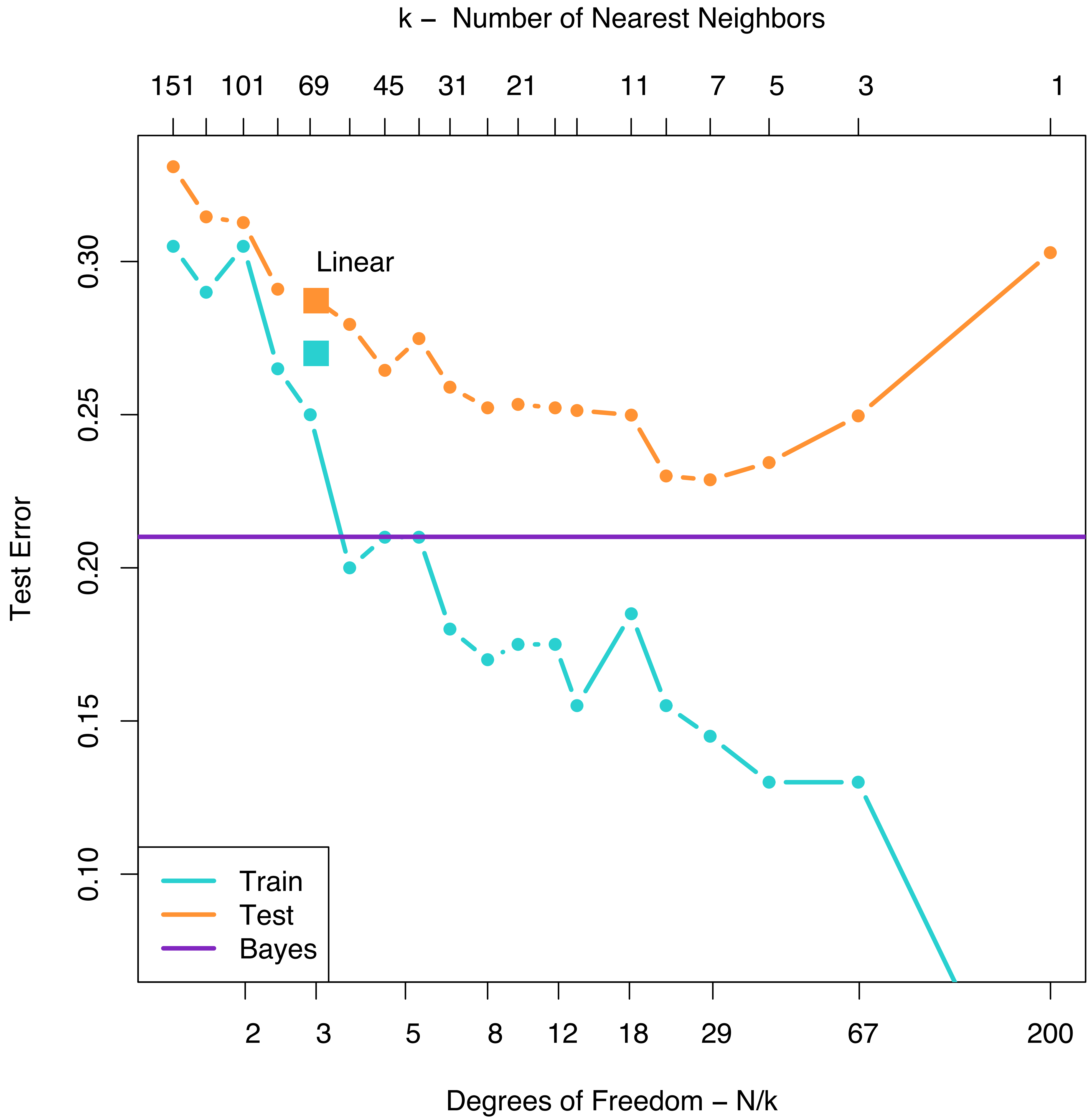
For large k:
(When $k = N$, prediction is constant)

- High bias
- Low variance



1-nearest neighbor classification

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

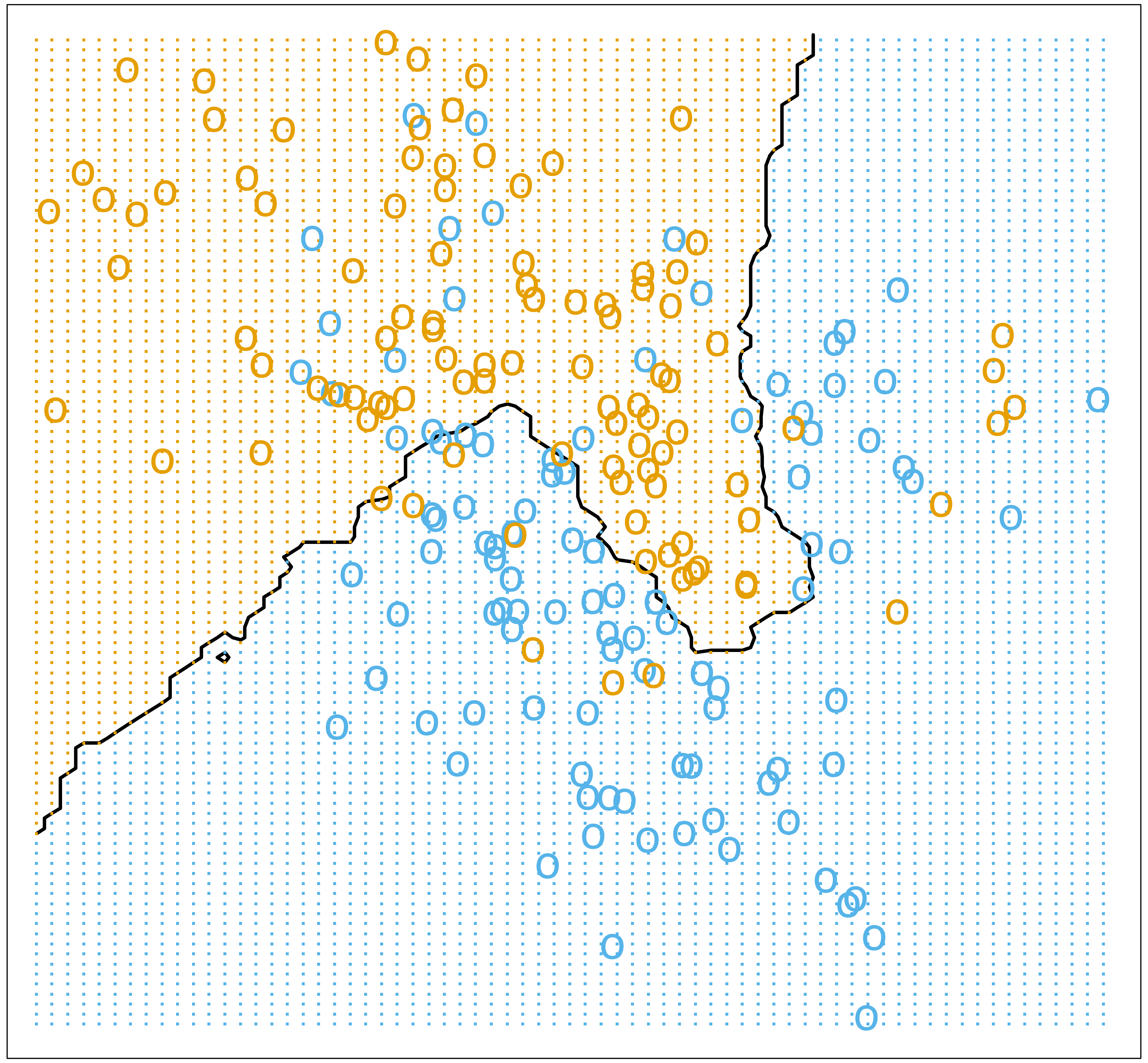


Complexity increases as k decreases

Find a k that balances bias and variance

Characteristics of an optimal k:

- Low bias: Ensures a sufficiently complex decision boundary
- Low variance: Prevents overfitting



15-nearest neighbor classification

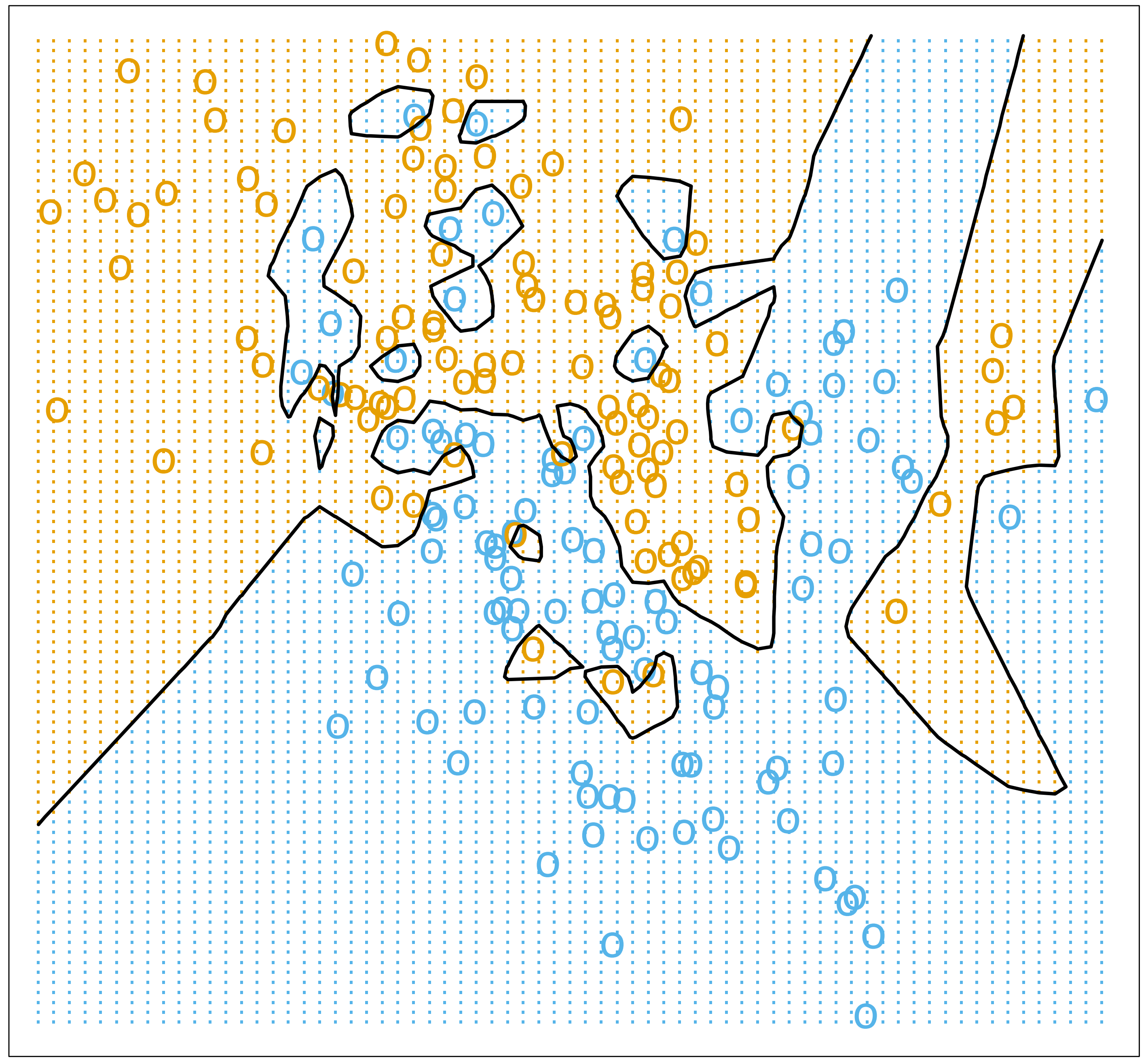
Summary: k-Nearest Neighbor

Pros:

- **No optimization** or training
- **Easy** to implement
- Works well in **low dimensions,** allowing for very complex decision boundaries

Cons:

- **Slow** at query time
- Not suitable for high-dimensional data
- Choosing the right local distance is crucial



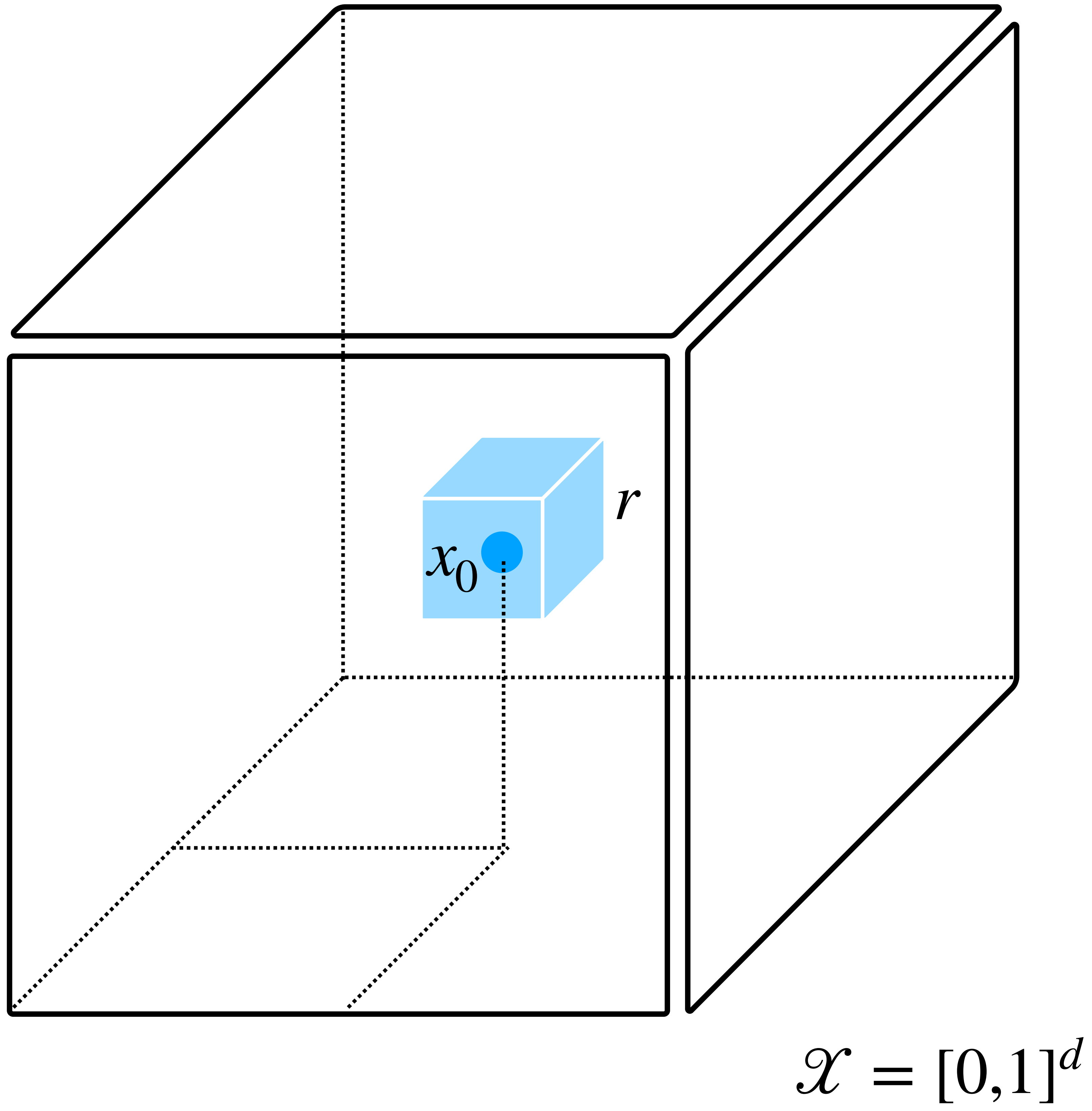
Curse of dimensionality

<u>Claim 1</u>: As the dimensionality grows, fixed-size training sets cover a diminishing 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

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



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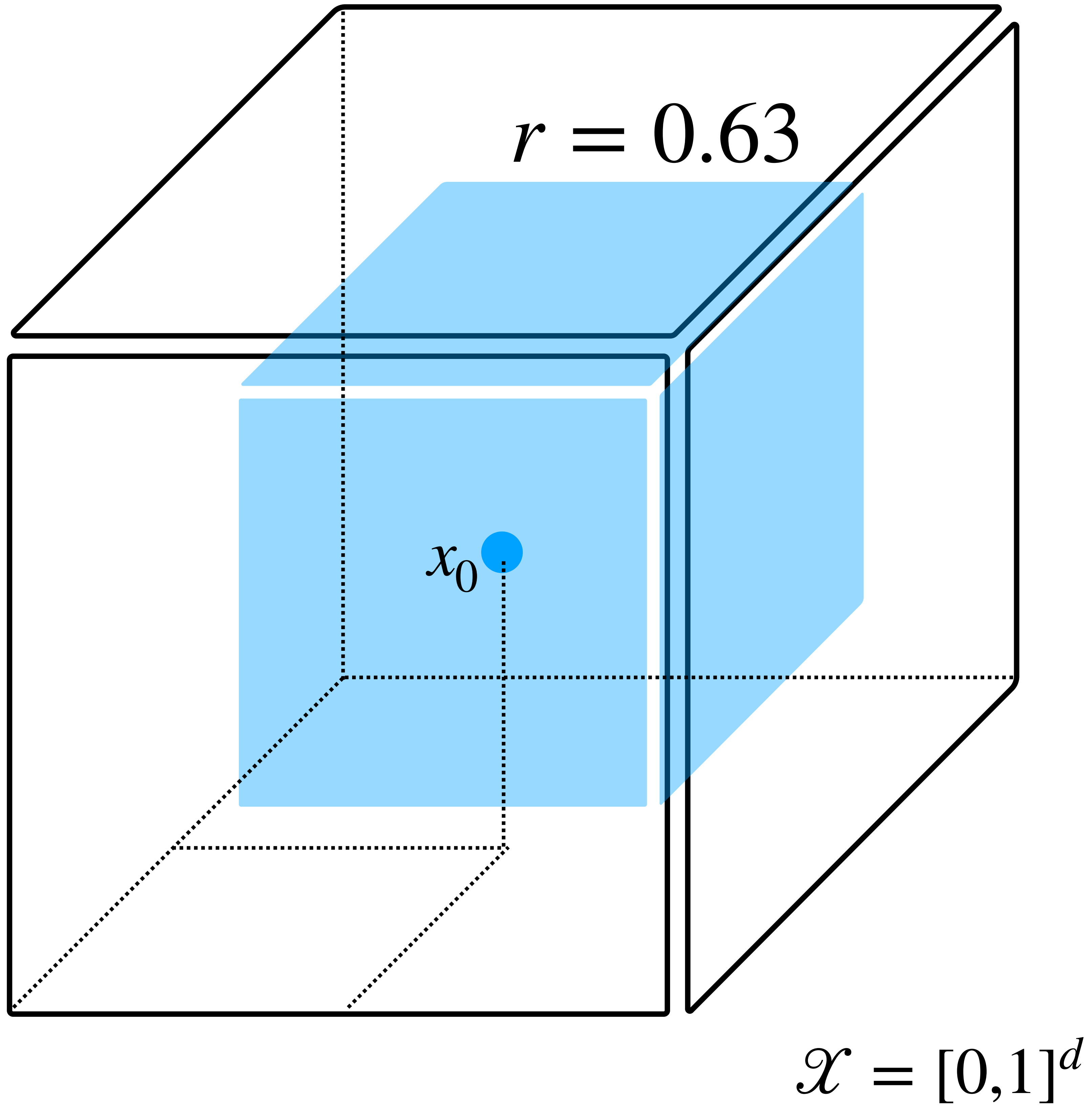
If $\alpha = 0.01$, to have:

$d = 10$, we need $r = 0.63$



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If $\alpha = 0.01$, to have:

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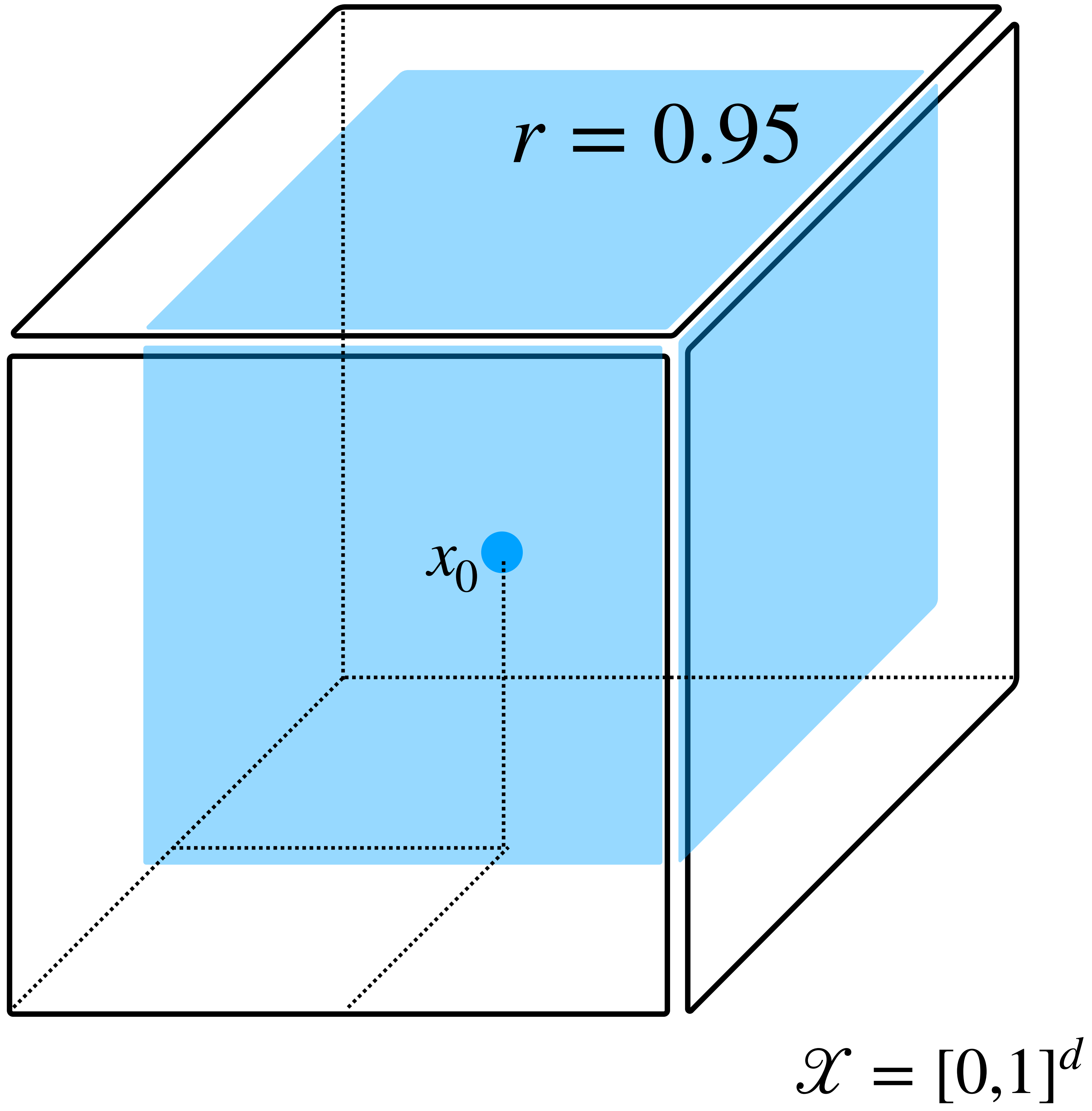
$d = 100$, we need $r = 0.95$

We need to explore almost the whole box



Curse of dimensionality

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

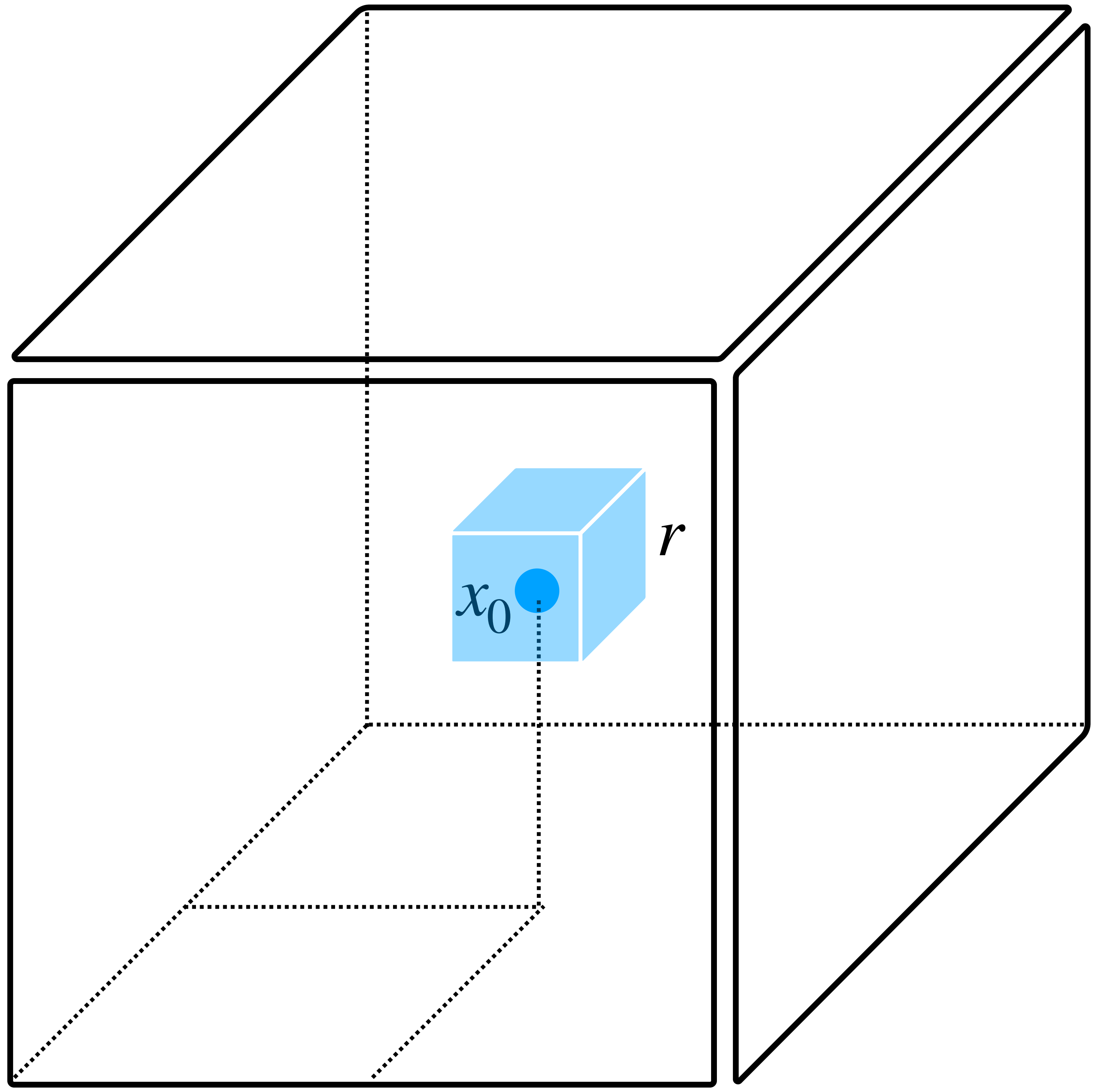
Consider N i.i.d. points uniform in the $[0,1]^d$

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

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

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

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



$\mathscr{X} = [0,1]^d$

Curse of dimensionality

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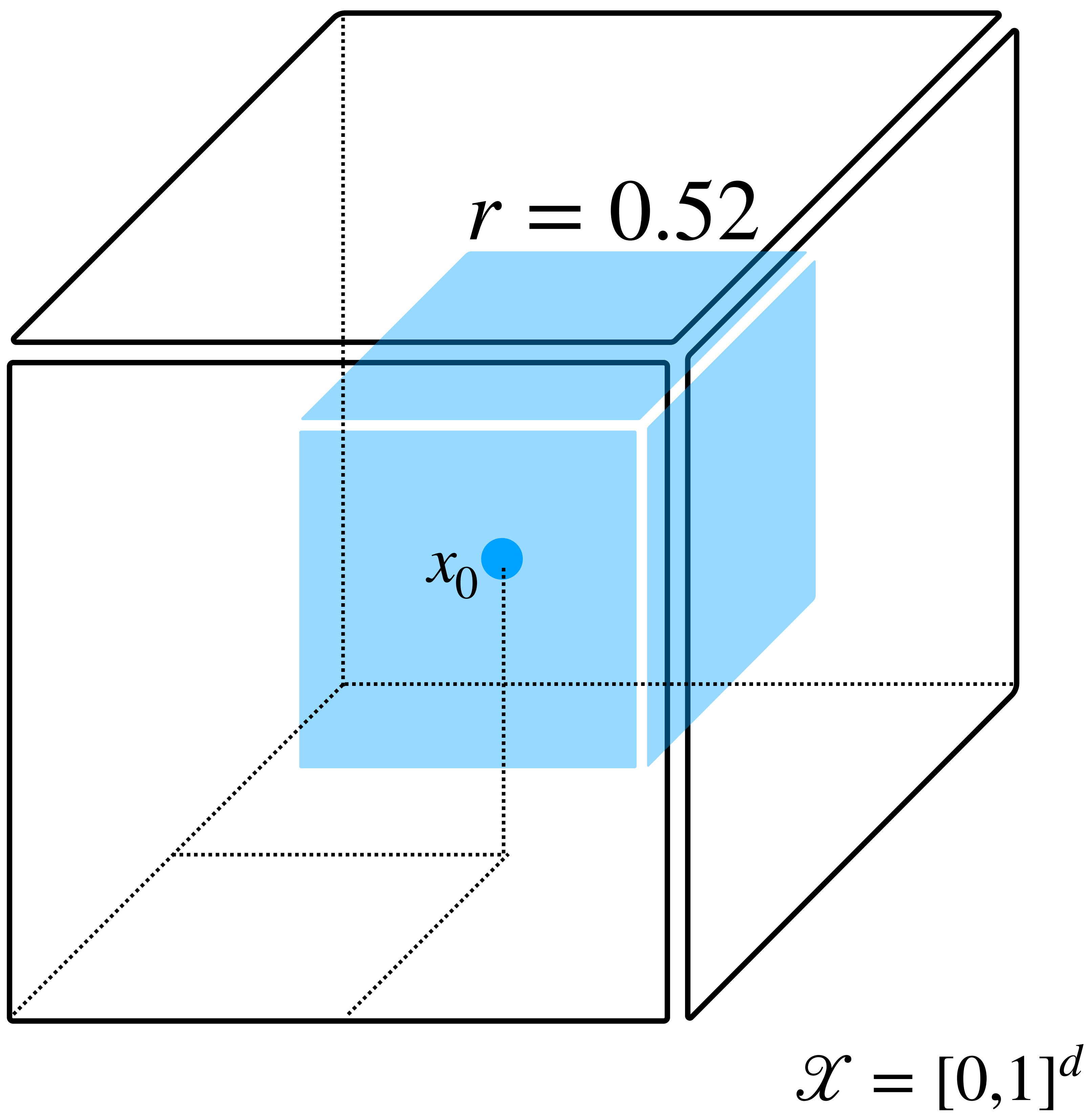
$$\mathbb{P}(x_i \notin \quad, \forall i \leq N) = (1 - r^d)^N$$

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

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:

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

Baseline:

- Bayes classifier: minimizes L over all classifiers

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

- Bayes risk: represents the minimum probability of misclassification

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

Generalization bound for 1-NN

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

Goal: Bound the classif

Proof 1:

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

Thus $1_{\eta(x) \geq 1/2} = \arg\max_{y \in \{0,1\}} \mathbb{P}(Y=y \mid X=x) = f_*(x)$

Baseline:

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Generalization bound for 1-NN

<u>Proof 2:</u>

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

- Bayes risk: represents the minimum probability of misclassification

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

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 share the same label

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Claim:

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

geometric term: average distance between a random point and its closest neighbor

Generalization bound for 1-NN

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

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➡ Nearby points are likely to share the same label

<u>Claim:</u>

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

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

<u>Interpretation</u>:

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

To achieve a constant error, we need $N \propto d^{(d+1)/2}$ - curse of dimensionality

Despite common belief: Interpolation method can generalize well

Proof

We want to bound

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

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

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

We have:

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

Proof

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

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

<u>Claim:</u>

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

- Simple case: $x = x'$

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

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

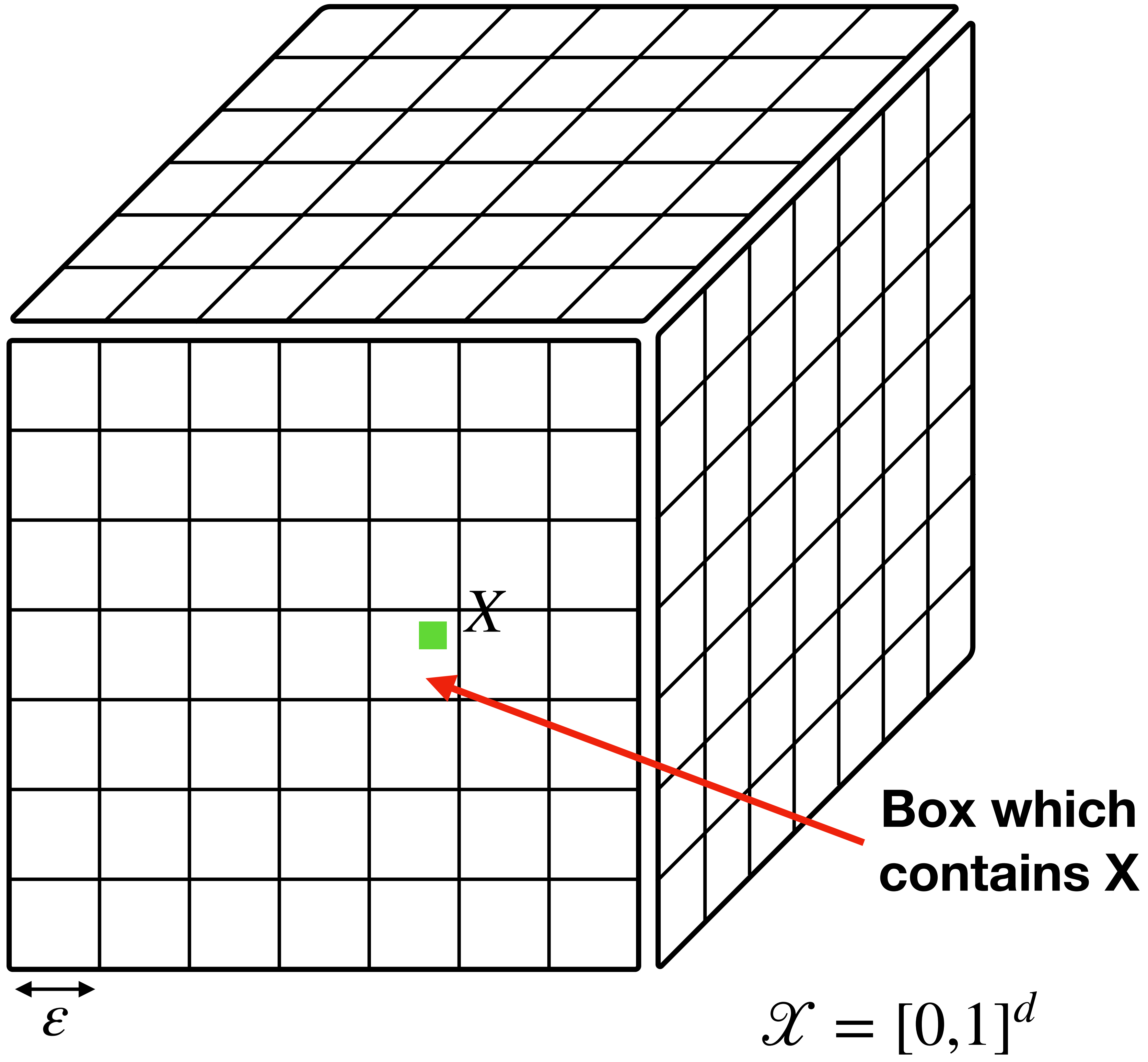
$$
\begin{aligned}
\mathbb{E}_{S_{train}}[L(f_{S_{train}})] &= \mathbb{E}_{S_{train,X},X\sim\mathscr{D}_X,Y\sim\eta(X),Y'\sim\eta(X')}[1_{Y\neq f_{S_{train}}(X)}] \\
&= \mathbb{E}_{S_{train,X},X\sim\mathscr{D}_X,Y\sim\eta(X),Y'\sim\eta(X')}[1_{Y\neq Y'}] \\
&= \mathbb{E}_{S_{train,X},X\sim\mathscr{D}_X}[\mathbb{P}_{Y\sim\eta(X),Y'\sim\eta(X')}(Y\neq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

Bound on the geometric term

Consider a fresh sample $X \sim \mathscr{D}_X$ and denote by

$p_k = \mathbb{P}(X \in \text{Box}_k)$

Consider the box which contains X. Two options:



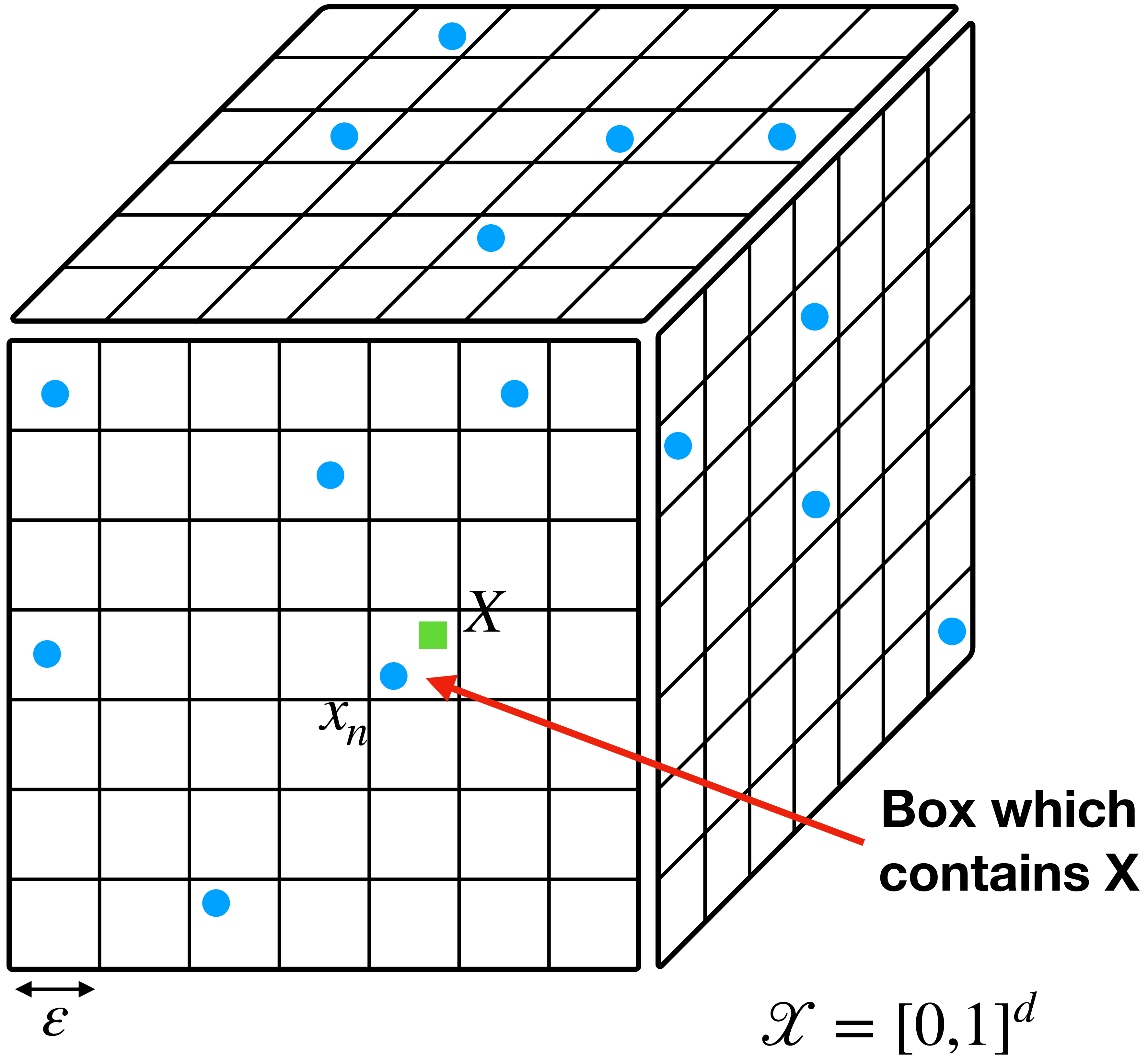
ε- **cover of the Hypercube**

Bound on the geometric term

Consider a fresh sample $X \sim \mathscr{D}_X$ 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 $1 - (1 - p_k)^N$



ε- cover of the Hypercube

Bound on the geometric term

Consider a fresh sample $X \sim \mathscr{D}_X$ and denote by $p_k = \mathbb{P}(X \in \text{Box}_k)$

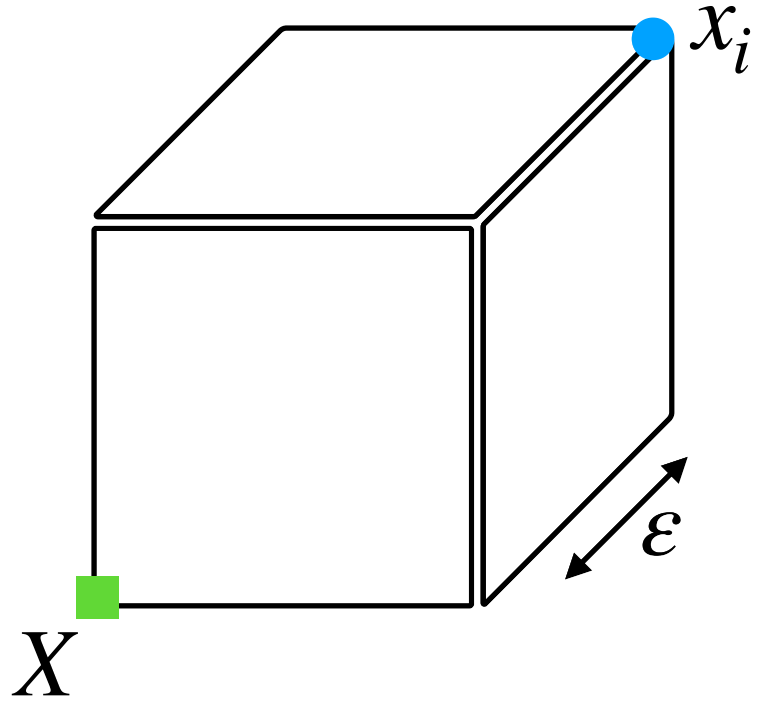
Consider the box which contains X. Two options:

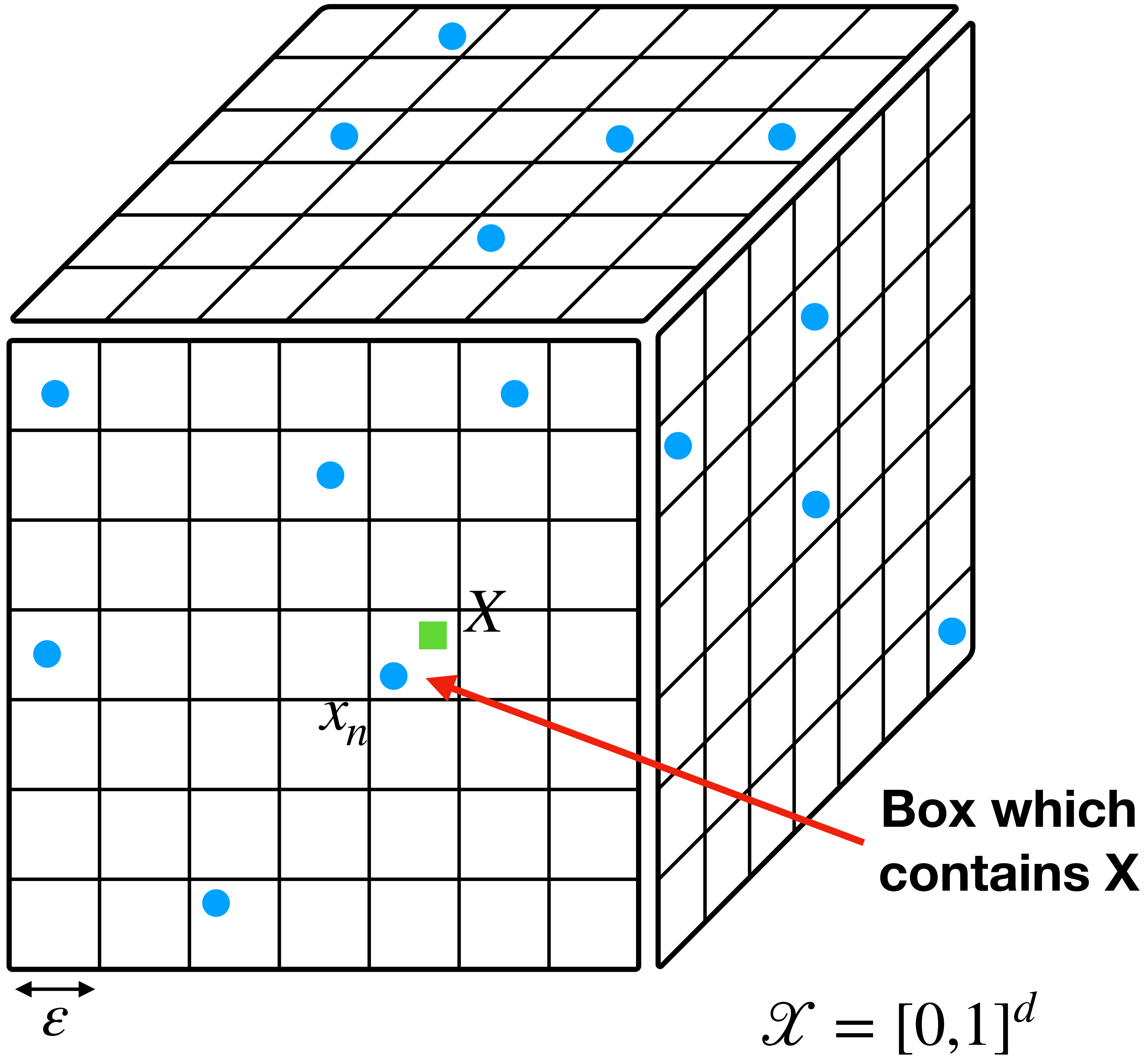
- The box contains an element of S_{train}. X has a neighbor in S_{train} at distance at most $\sqrt{d}\varepsilon$

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

Proof: Consider the worst case:

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





ε- cover of the Hypercube

Bound on the geometric term

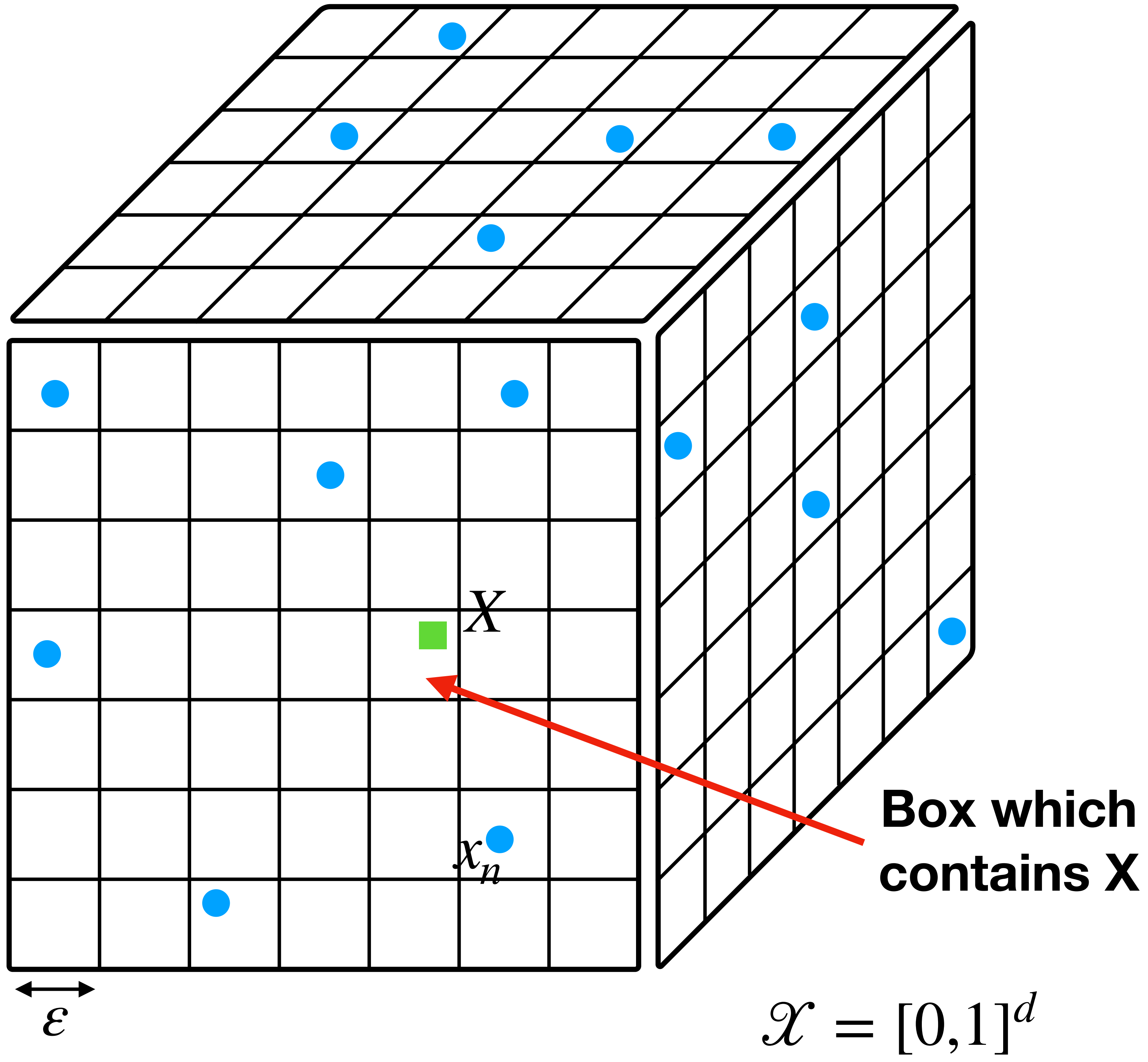
Consider a fresh sample $X \sim \mathcal{D}_X$ and denote by
$p_k = \mathbb{P}(X \in \text{Box}_k)$
Consider the box which contains X. Two options:

- 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 $(1 - p_k)^N$



ε- cover of the Hypercube

Bound on the geometric term

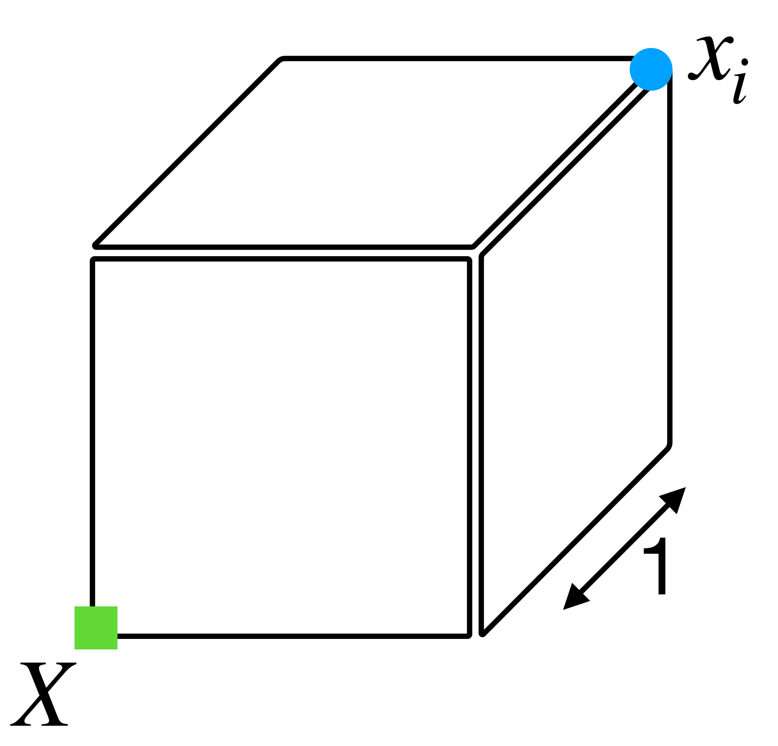
Consider a fresh sample $X \sim \mathscr{D}_X$ and denote by

$p_k = \mathbb{P}(X \in \text{Box}_k)$

C

Proof: Consider the worst case:

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

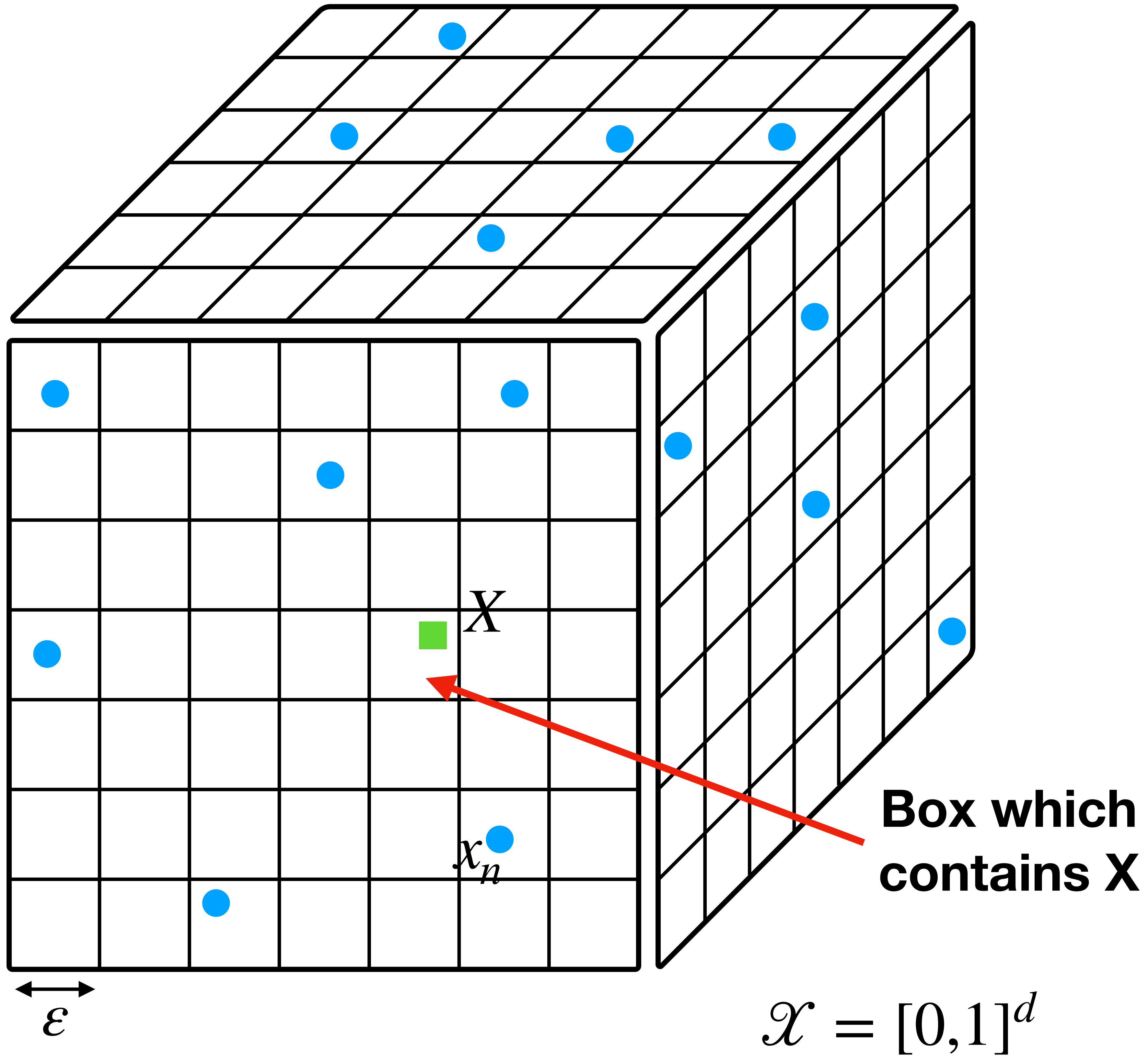


of

train

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

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



ε- cover of the Hypercube

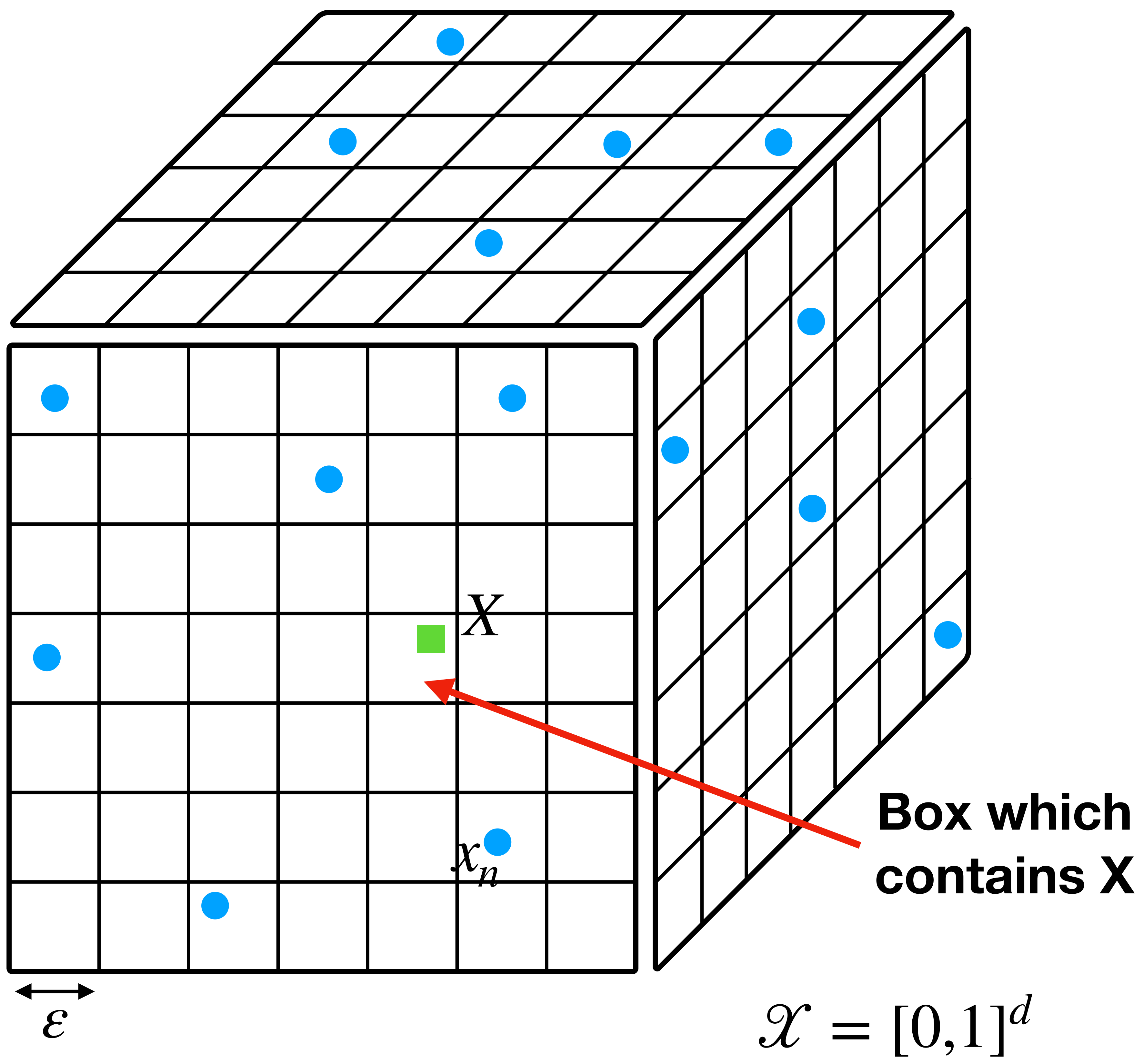
Bound on the geometric term

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

<u>Claim:</u> The bound is derived by optimizing over p_k and ε

<u>Intuition:</u>

- If p_k is large: it is likely that we pick that box but it is also likely that we find a training point in that box
- If p_k is small, we are generally safe, as by its definition, this scenario occurs infrequently



ε- **cover of the Hypercube**

Nearest Neighbors is a local averaging method

Local averaging methods aim to approximate the Bayes predictor directly - without the need for optimization

This is achieved by approximating the conditional distribution $p(y|x)$ by some $\hat{p}(y|x)$

These "plug-in" estimators are:

- $f(x) \in \arg\max_{y \in \mathcal{Y}} \hat{\mathbb{P}}(Y = y|x)$ for classification with the 0-1 loss
- $f(x) = \hat{\mathbb{E}}[Y|x] = \int_{\mathcal{Y}} y\hat{p}(y|x)dy$ for regression with the square loss

In the case of nearest neighbors:

$$\hat{p}(y|x) = \sum_{n=1}^{N} \hat{w}_n(x) 1_{y=y_n}$$

where $\hat{w}(x) = 1/k$ for the k nearest neighbors (0 otherwise)

Recap

- k-NN: a local averaging method for regression and classification
  - use a notion of distance to define *neighborhoods* (= k nearest neighbors)
  - the prediction is a function of these neighborhoods

    e.g., majority selection for classification, weighted sum for regression
- Bias-variance: small/large k leads to low/high bias and high/low variance
- Curse of dimensionality: as $d \nearrow \infty$, it is harder to define local neighborhoods
- For $N \to \infty$, 1-NN is competitive with Bayes classifier
- N needs to scale exponentially in d to achieve the same error