Introduction to Supervised Learning

Problem setup, feature types, assumptions about data

Machine Learning and Data Mining, 2022

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LAMBDA • HSE

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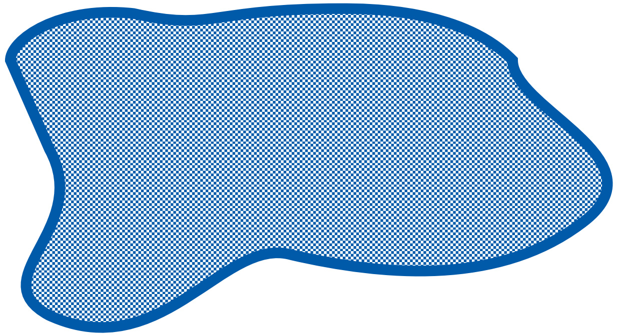
Supervised Learning

Problem setup

$\mathcal{X}$ – a set of objects



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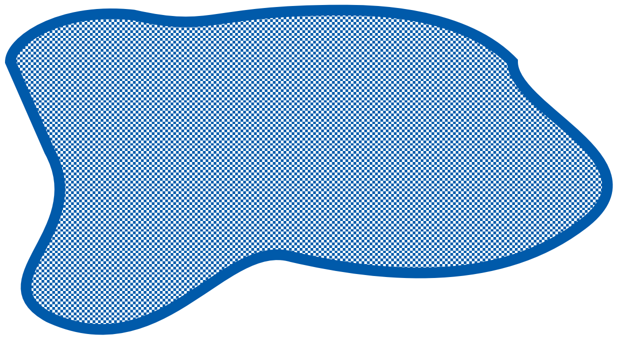
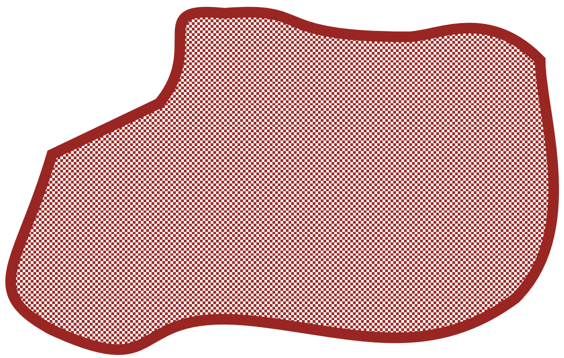


$\mathcal{Y}$ – a set of targets



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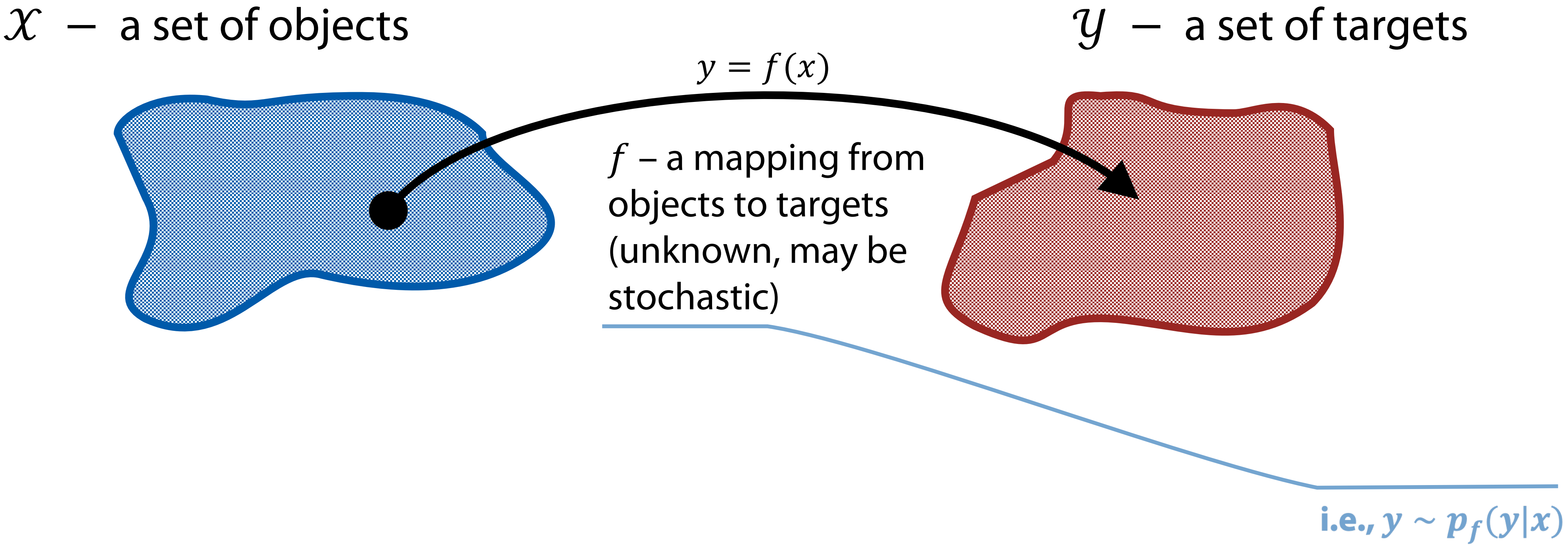

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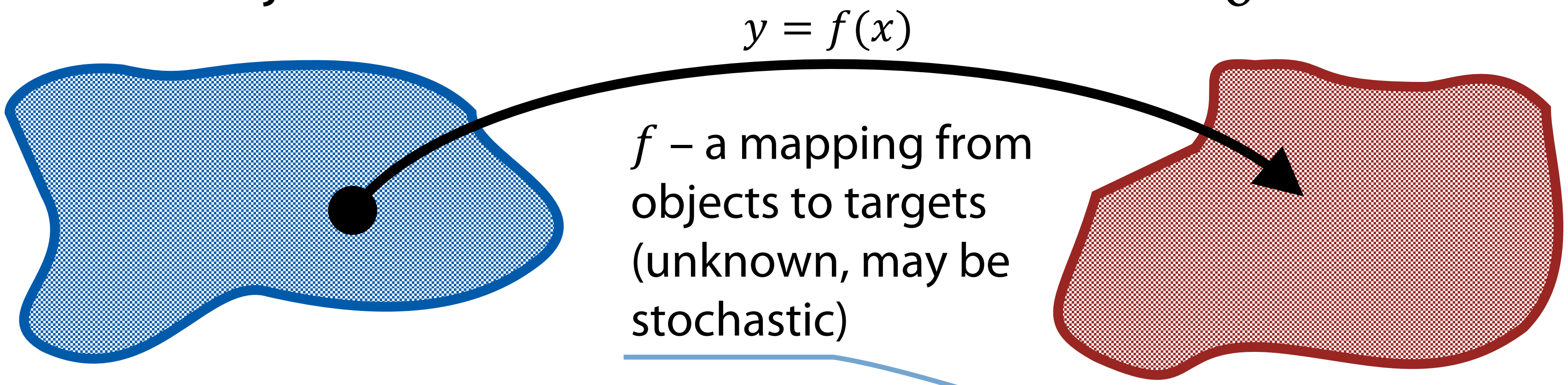

i.e., $y \sim p_f(y|x)$

A dataset: $D = \{(x_i,\ y_i) : i = 1,\ 2, \ldots ,\ N\}$

$$x_i \in \mathcal{X}, \qquad y_i = f(x_i) \in \mathcal{Y}$$

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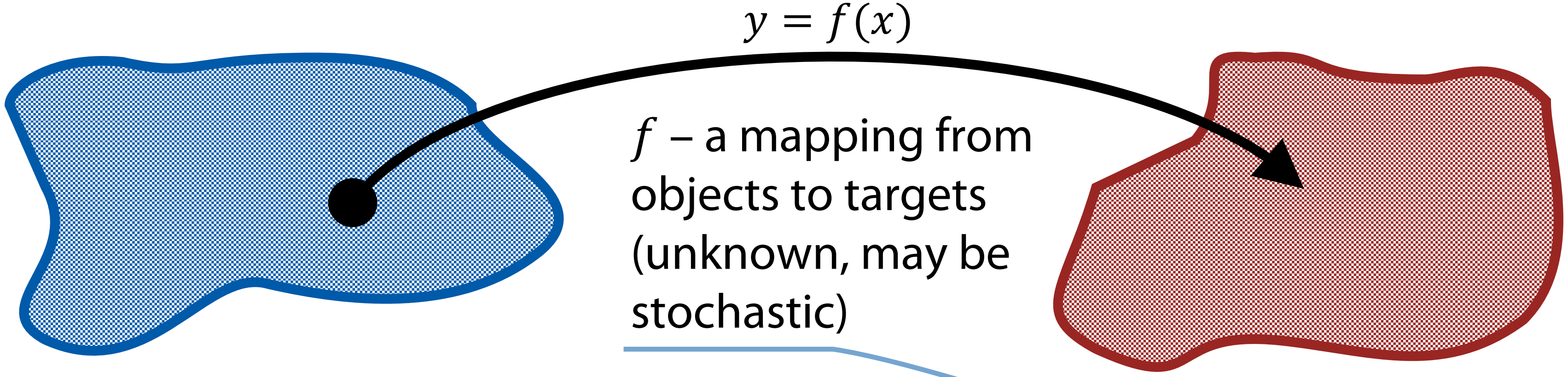

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Goal: **approximate *f* given *D***
i.e. learn to **recover targets from objects**

Examples

- Iris flower species classification

Objects

Individual flowers, described by the length and width of their sepals and petals

Targets

Species to which this particular flower belongs

Mapping

Different shapes of sepals and petals correspond to different species

(non-deterministic)

images source: wikipedia.org

Examples

- Spam filtering

Objects

E-mails (sequences of characters)

Targets

“spam” / ”not spam”

Mapping

Message content defines whether it’s spam or not

(non-deterministic, varies from person to person)

Icon made by Freepik from www.flaticon.com

Examples

- CAPTCHA recognition

Objects

CAPTCHA images (vectors of pixel brightness levels)

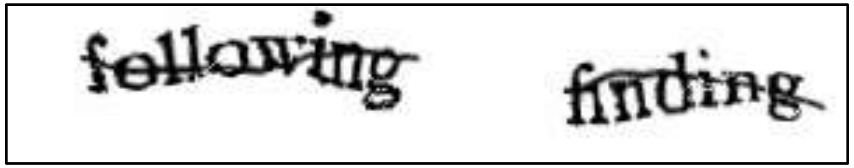
Targets

Sequences of characters

Mapping

Inverse of CAPTCHA generating algorithm

(almost deterministic, depending on the level of distortion)



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Features

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- Objects x_i are described by features x_i^j, i.e.:
  - It's a vector $x_i = (x_i^1, x_i^2, \dots, x_i^d)$

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- many algorithms require that the dimensionality d of the data is same for all objects
  - In such case the objects may be organised in a design matrix:

$$X = \begin{array}{cc} & \xrightarrow{\textit{features}} \\ & \begin{bmatrix} x_1^1 & x_1^2 & \cdots & x_1^d \\ x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \cdots & x_N^d \end{bmatrix} \Big\downarrow \textit{objects} \end{array}$$

Example: Iris dataset

sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)
5.1	3.5	1.4	0.2
4.9	3.0	1.4	0.2
4.7	3.2	1.3	0.2
4.6	3.1	1.5	0.2
5.0	3.6	1.4	0.2
...	...	...	...
6.7	3.0	5.2	2.3
6.3	2.5	5.0	1.9
6.5	3.0	5.2	2.0
6.2	3.4	5.4	2.3
5.9	3.0	5.1	1.8

In this example, all featuers are real numbers

Feature types

- Individual features x_i^j may be of various nature
- Common cases:
  - **Numeric features**, e.g.:
    - Sepal length
    - Height of a building
    - Temperature
    - Price
    - Age
    - Etc.

Feature types

- Individual features x_i^j may be of various nature
- Common cases:
  - **Categorical**

nominal (no order implied), e.g.:

Color
City of birth
Name

ordinal (values can be compared, though pairwise differences are not defined), e.g.:

Level of education
Age category (child, teen, adult, etc.)

Feature types

- Individual features x_i^j may be of various nature
- Common cases:
  - **Binary**, e.g.:
    - True / False
  - Can be treated as numeric (0/1 or –1/+1)

One-hot encoding

- How does one convert categorical feature to numeric?

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- How does one convert categorical feature to numeric?
  - Assigning each category a number (e.g. ”red” = 1, “green” = 2, etc.) may have negative effect on the learning algorithm
- One-hot encoding – simple trick to convert categorical feature to numeric:

color
“red”
“red”
“blue”
“green”
“blue”

→

is_blue	is_red	is_green
0	1	0
0	1	0
1	0	0
0	0	1
1	0	0

A trick for ordinal features

- One-hot encoding may be used, though it loses the information about the relations between the categories

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- One-hot encoding may be used, though it loses the information about the relations between the categories
- Similar trick:

Academic degree	**is_bachelor**	**is_master**	**is_PhD**
"none"	0	0	0
"bachelor"	1	0	0
"master"	1	1	0
"PhD"	1	1	1
"master"	1	1	0

More advanced encoding techniques

- See https://contrib.scikit-learn.org/category_encoders/index.html

Learning Algorithms

Machine Learning Algorithm

Algorithm $\mathcal{A}$:

given a dataset $D = \{(x_i,\ y_i) : i = 1,\ 2, \dots ,\ N\}$

$$x_i \in \mathcal{X},\ y_i = f(x_i) \in \mathcal{Y}$$

returns an approximation $\hat{f} = \mathcal{A}(D)$ to the true dependence f.

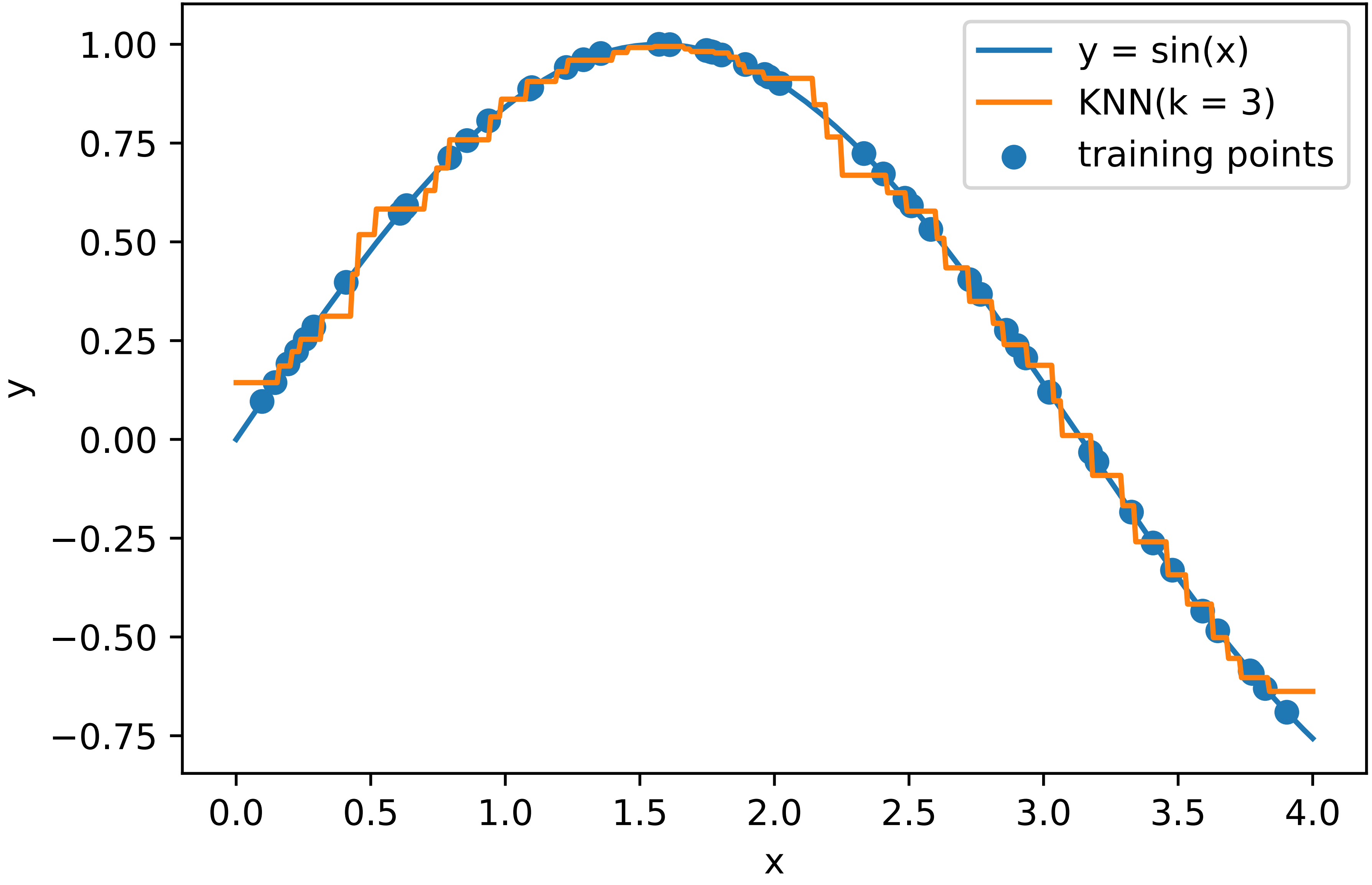
Example: k nearest neighbors (kNN)

- Idea: close objects should have similar targets
- Why don't we look up k closest (by some metric of the feature space) objects in the dataset and average their targets:

$$\hat{f}(x) = \frac{1}{k} \sum_{i:\, x_i \in D_x^k} y_i$$

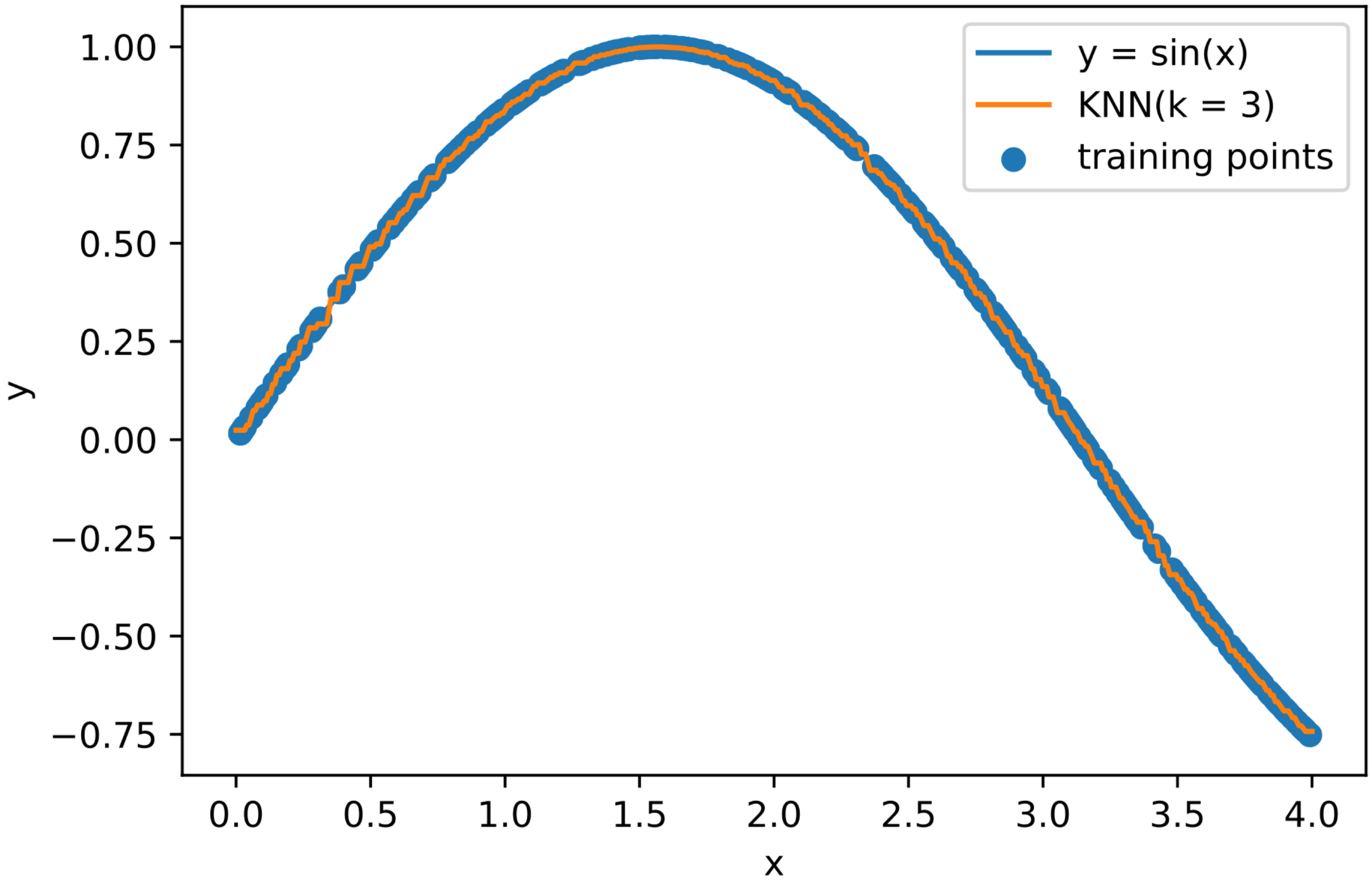
D_x^k – set of k objects from D closest to x

Example: k nearest neighbors



training points: 50

Example: k nearest neighbors



training points: 250

More data = **better approximation**

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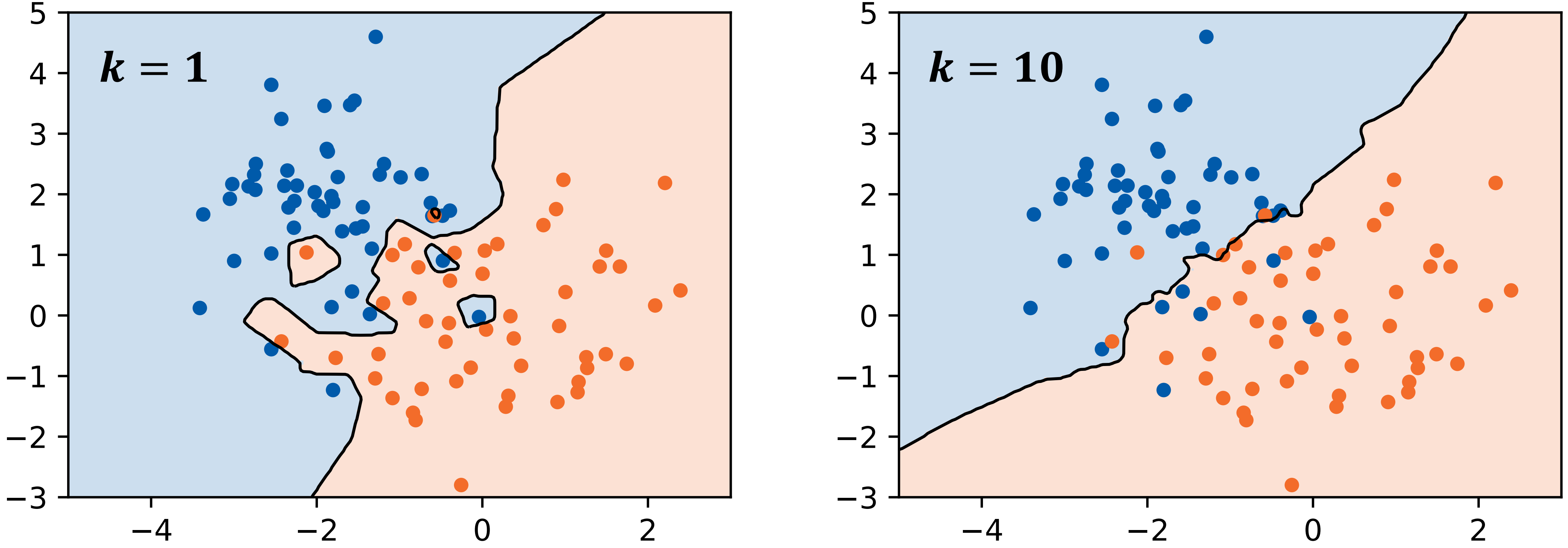

$$\hat{f}(x) = \underset{C}{\operatorname{argmax}} \sum_{i:\, x_i \in D_x^k} \mathbb{I}[y_i = C]$$

Classification example

D_x^k – set of k objects from D closest to x

Loss function

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- Many algorithms work by solving an **optimization task**
- We can measure the quality of a prediction for a single object x_i with a **loss function** $\mathcal{L} = \mathcal{L}\left(y_i, \hat{f}(x_i)\right)$

E.g. squared error:
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Loss function

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- We can measure the quality of a prediction for a single object x_i with a **loss function** $\mathcal{L} = \mathcal{L}\left(y_i, \hat{f}(x_i)\right)$
- Then, learning (or training) can be formulated as a **loss minimization** problem:

$$\hat{f} = \underset{\tilde{f}}{\operatorname{argmin}} \underset{(x,y)\in D}{\mathbb{E}} \mathcal{L}\left(y, \tilde{f}(x)\right)$$

E.g. squared error:
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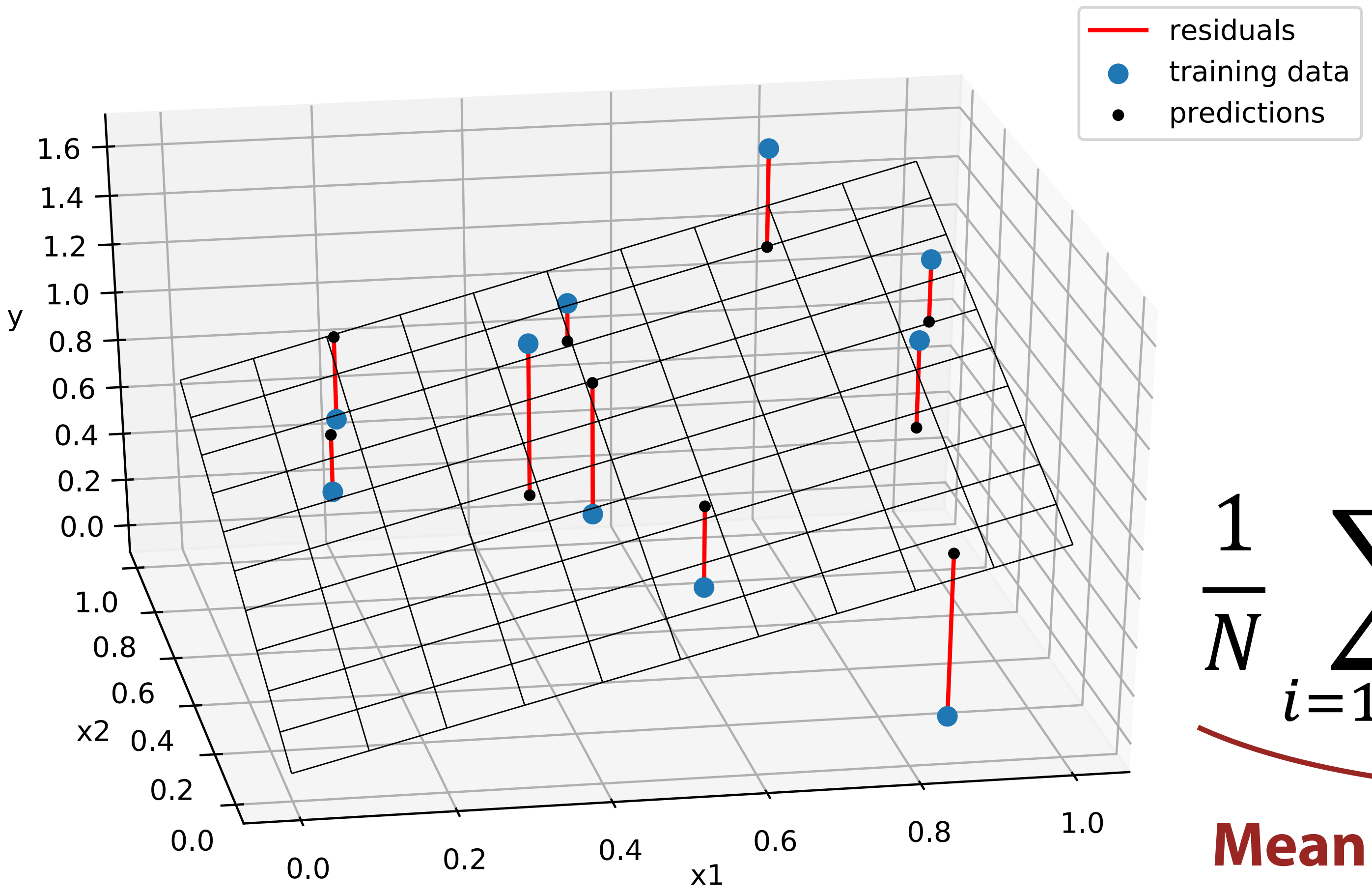
Example: linear regression



$$\hat{f}_{w,b}(x) = w^{\mathrm{T}}x + b$$

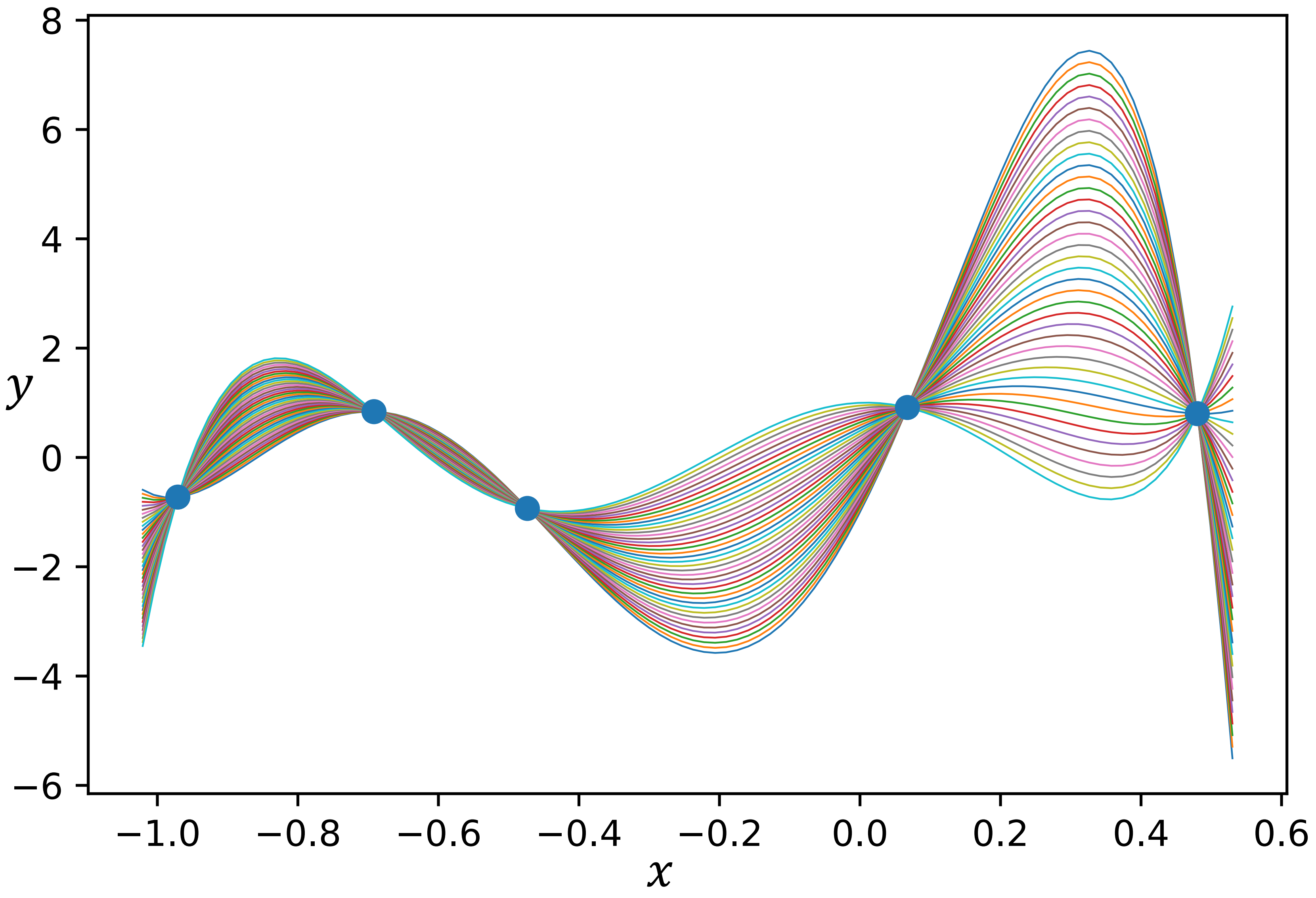
$$w \in \mathbb{R}^d$$
$$b \in \mathbb{R}$$
$$x \in \mathcal{X} \subset \mathbb{R}^d$$

$$\underbrace{\frac{1}{N}\sum_{i=1\dots N}\left(y_i - \hat{f}_{w,b}(x_i)\right)^2}_{\text{Mean Squared Error (MSE loss)}} \xrightarrow[w,b]{} \min$$

Mean Squared Error
(MSE loss)

Assumptions about data

No assumptions = Infinitely many solutions



Any of these curves minimizes the loss

We want **expected loss over population** to be minimized

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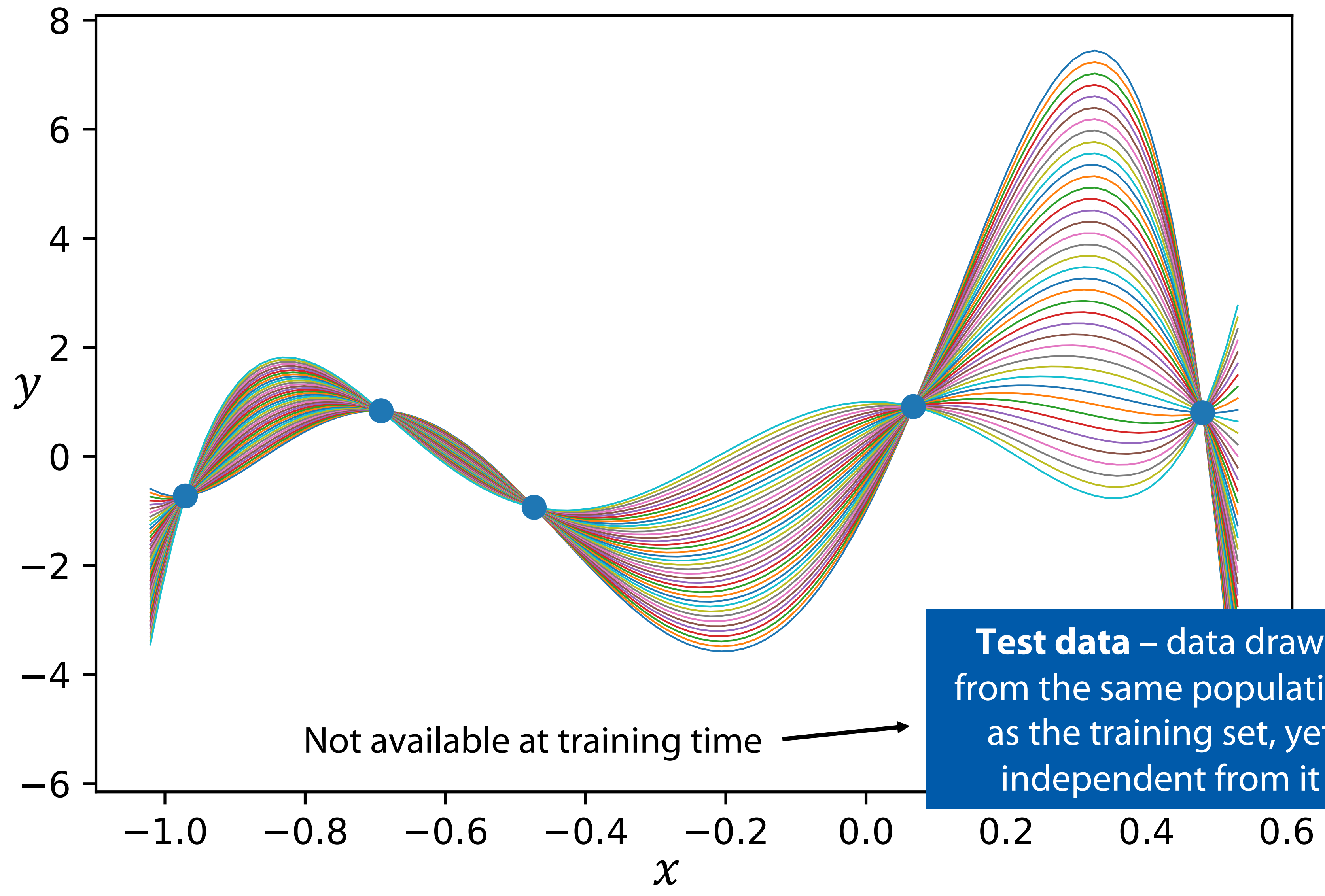

Test data – data drawn from the same population as the training set, yet independent from it

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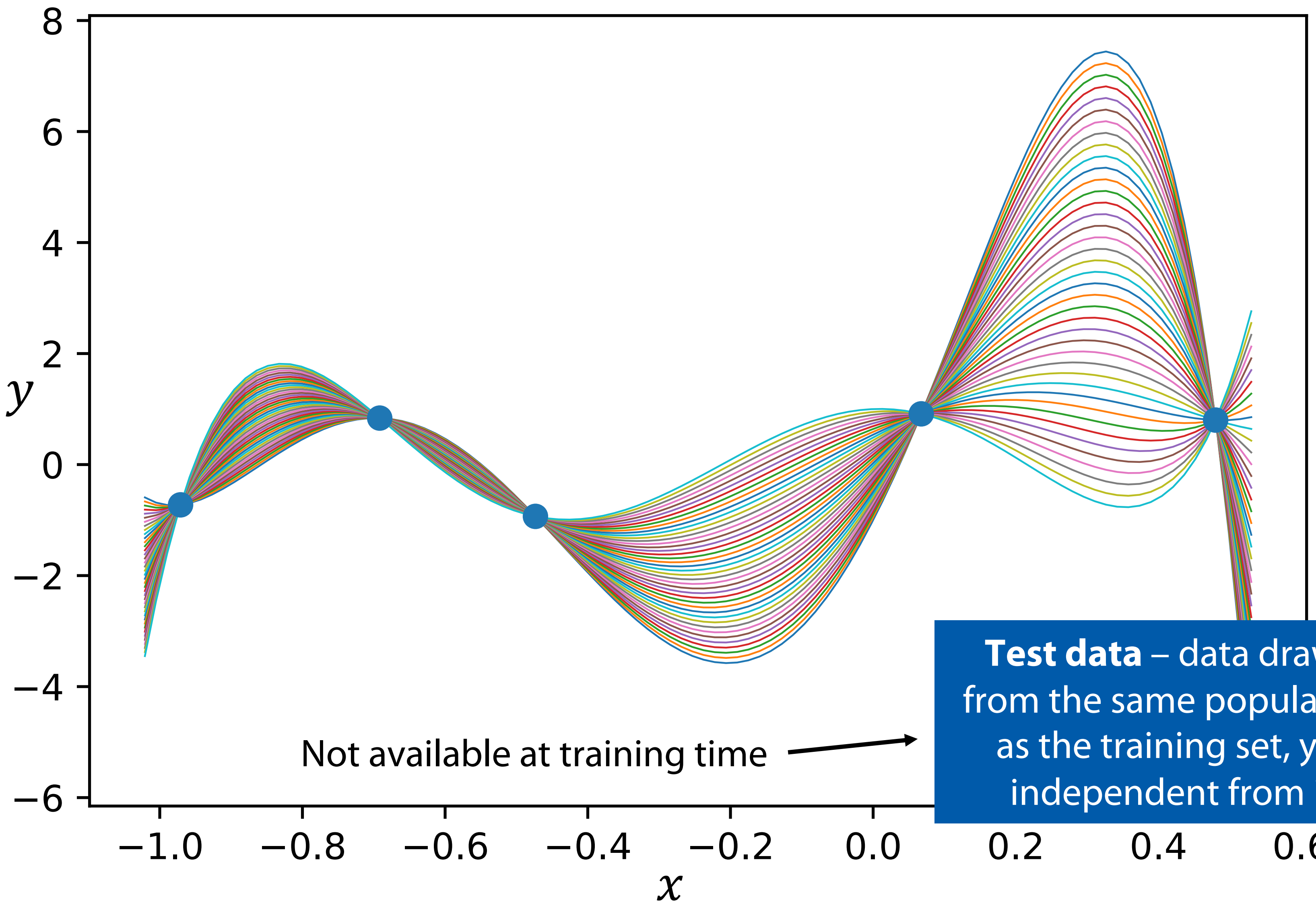

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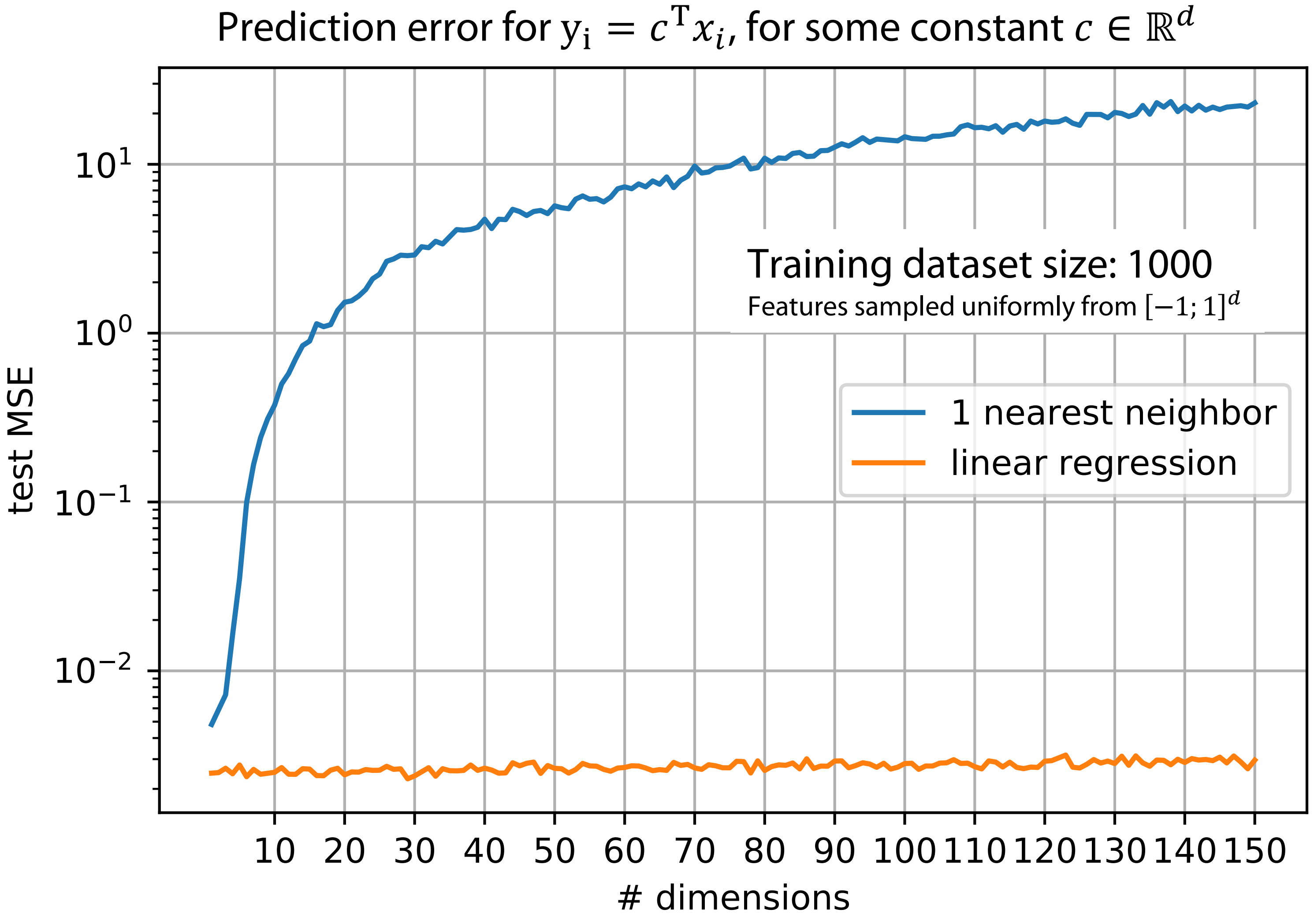
Need to **assume some structure** of the data, common to **training** and **testing** data

Example: kNN(k = 1) VS Linear Regression



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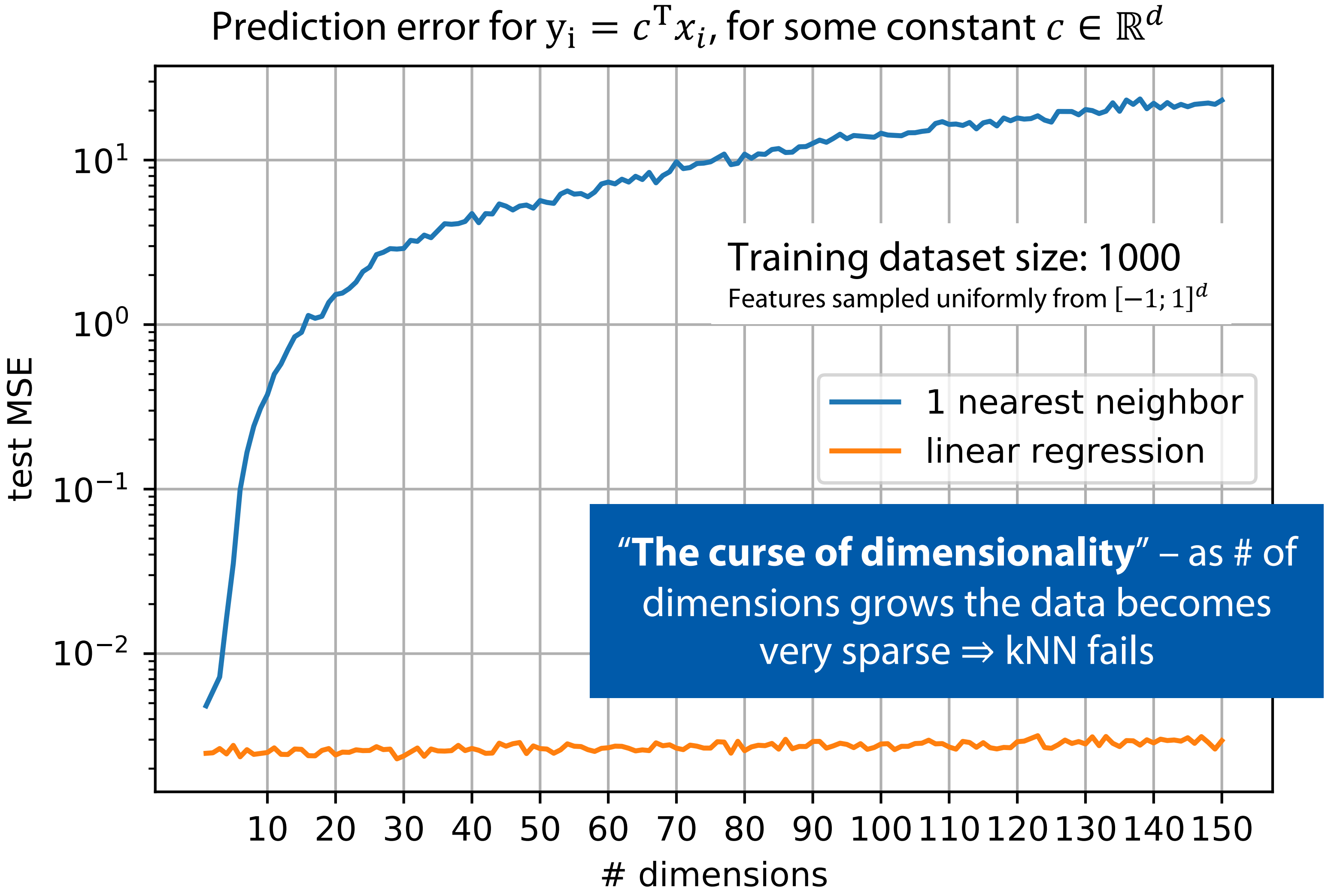

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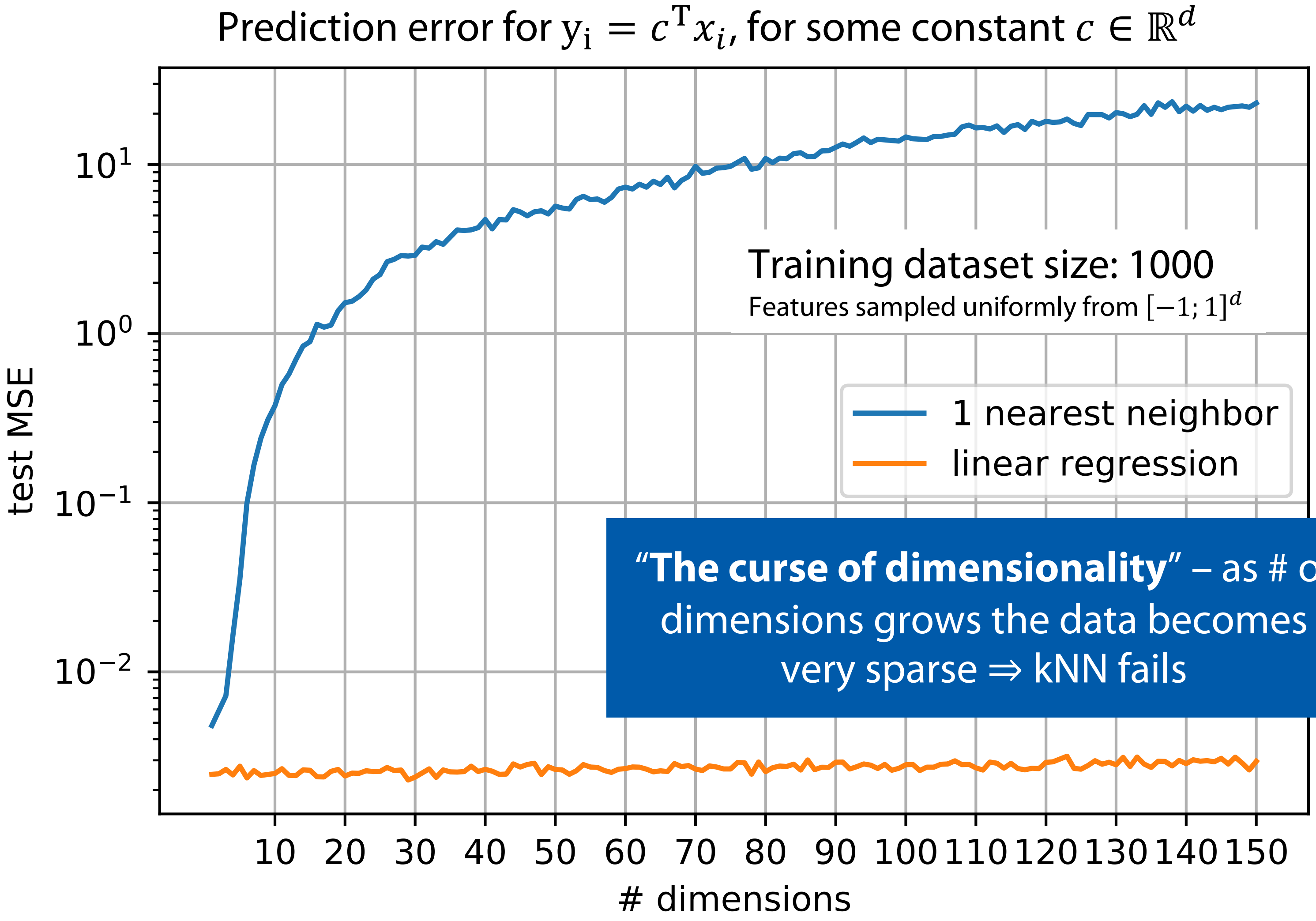

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Assumption for kNN:
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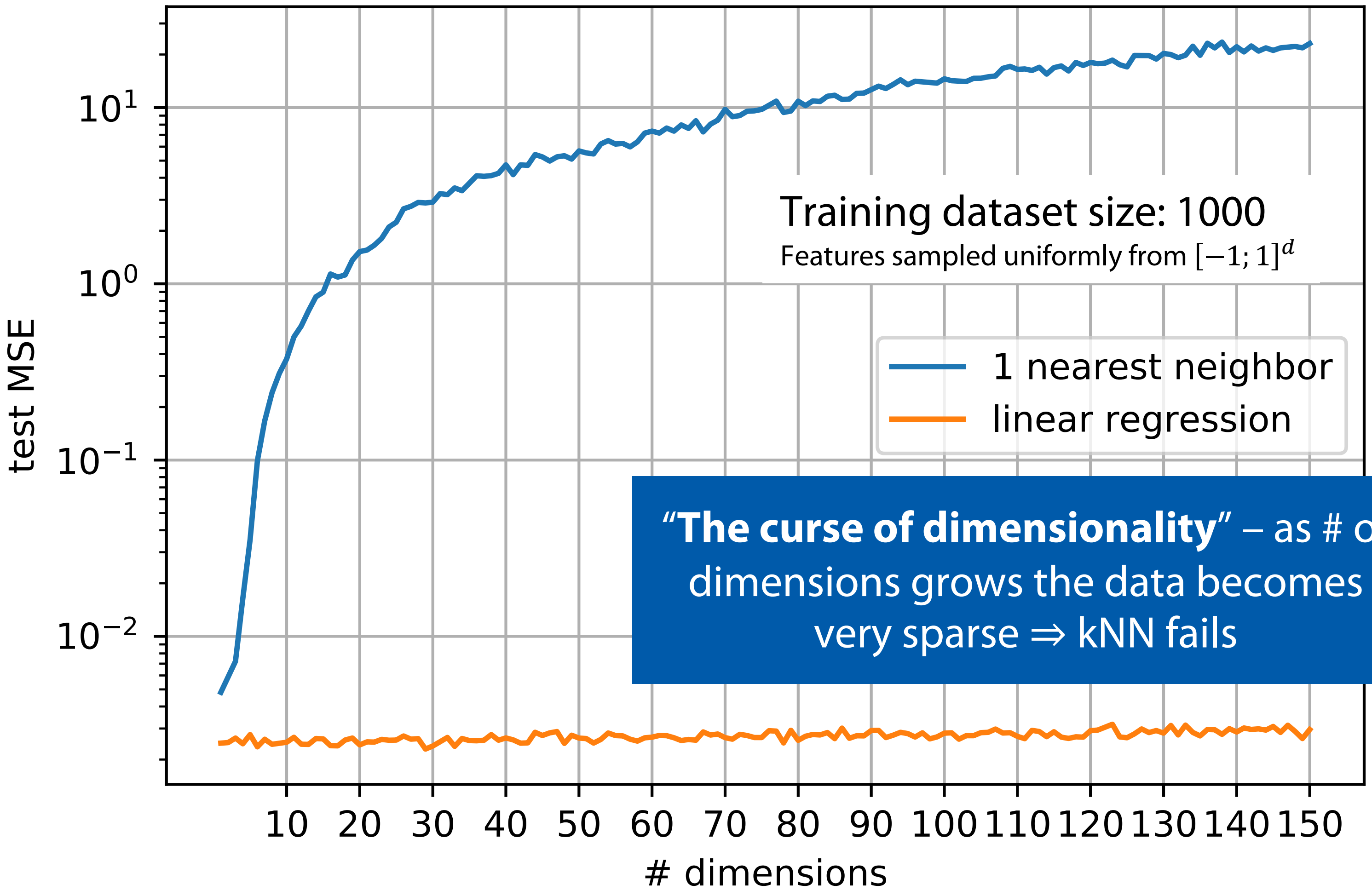
Prediction error for $y_i = c^T x_i$, for some constant $c \in \mathbb{R}^d$



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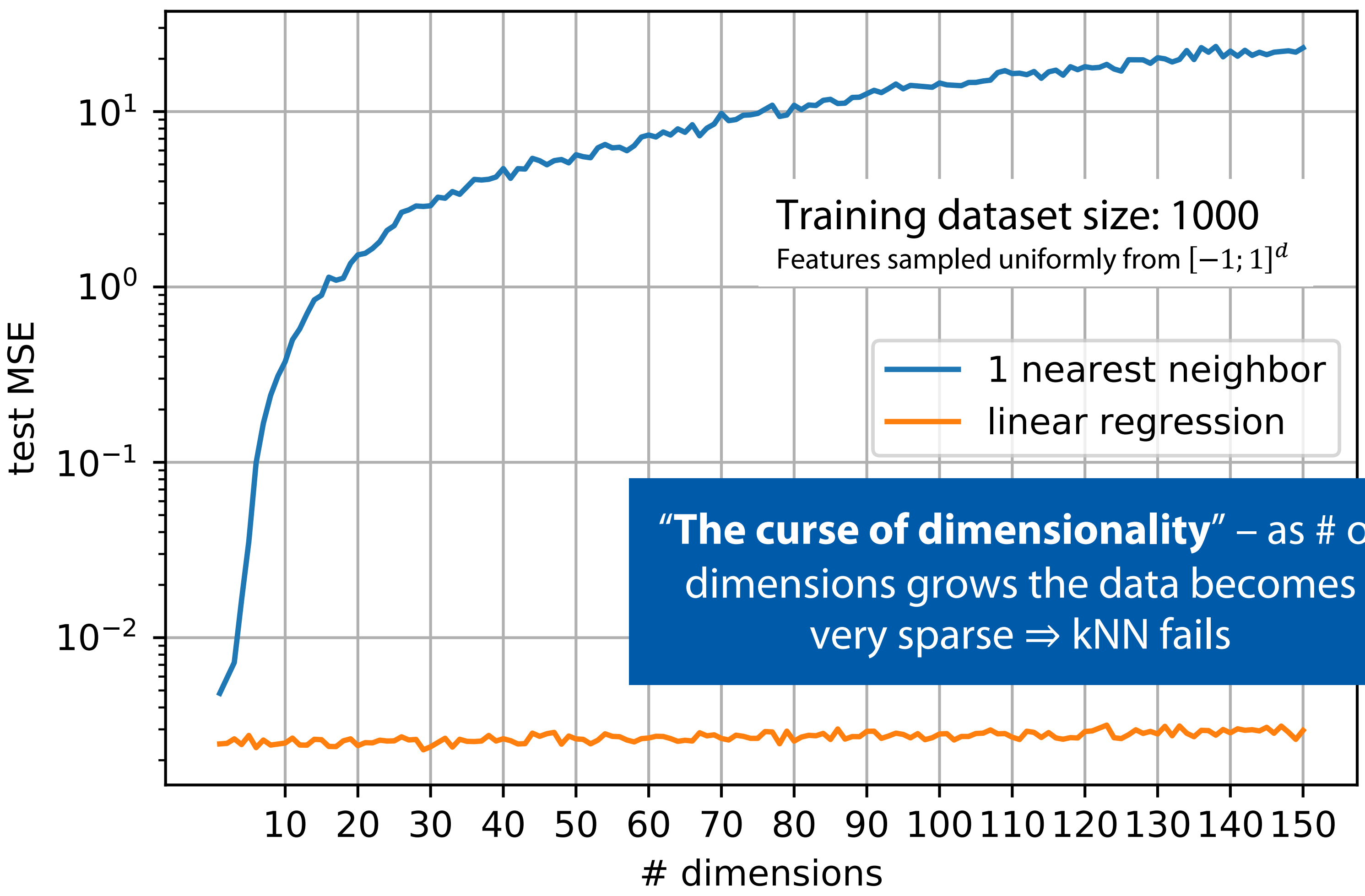

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For this example, both assumptions are correct, but one is **stronger** than the other

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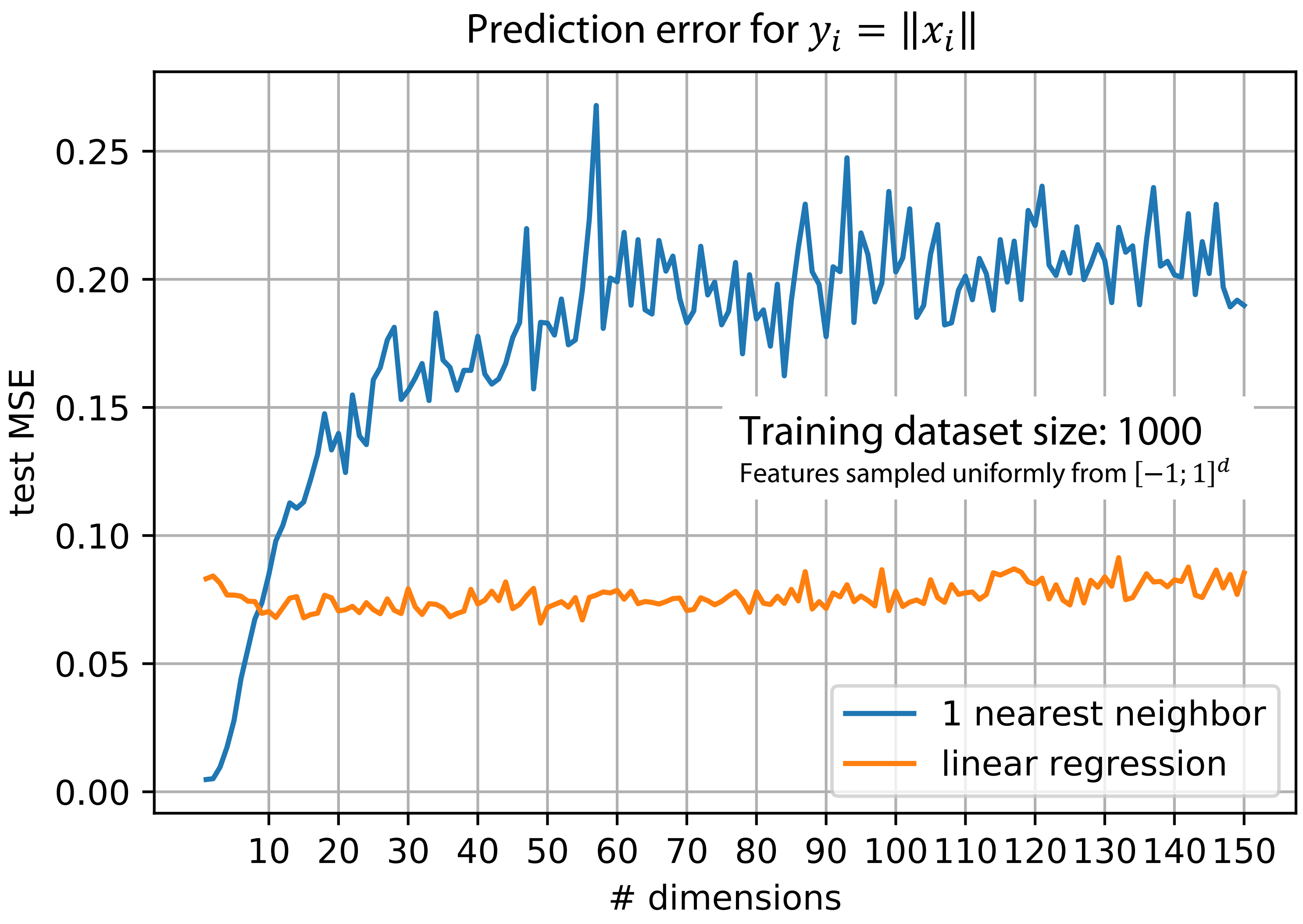

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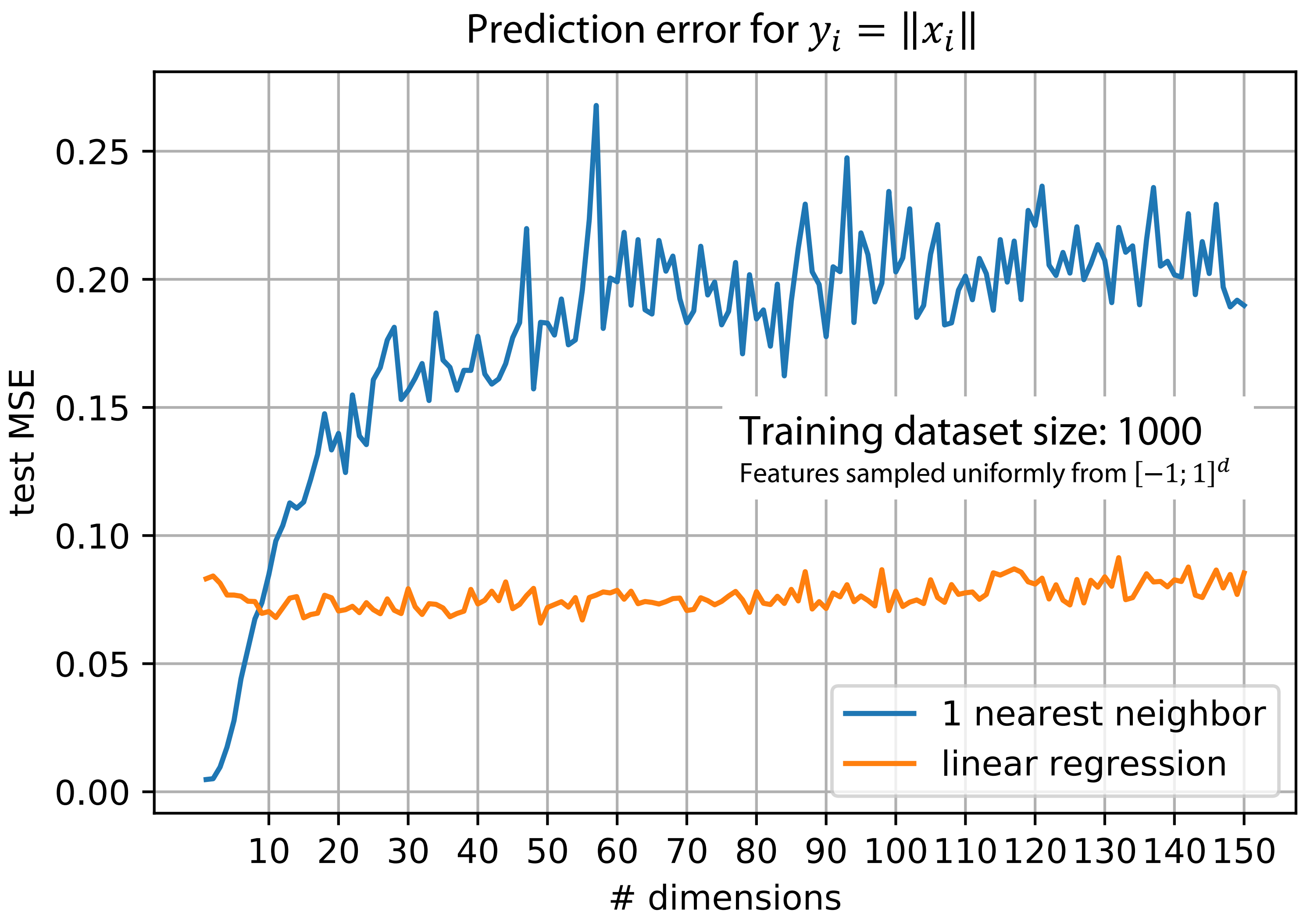

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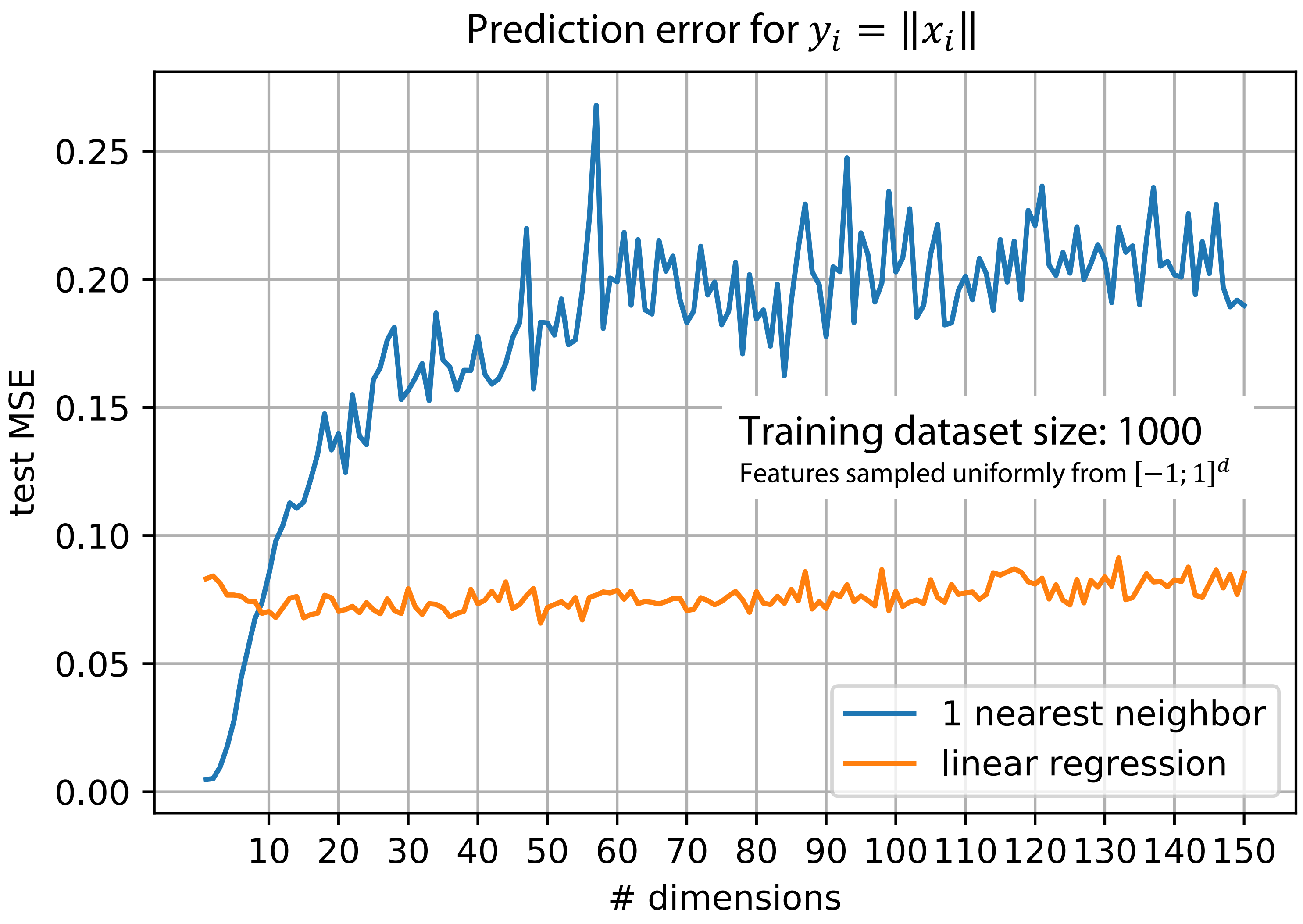

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Imposing assumptions about the data **restricts the space of possible solutions**

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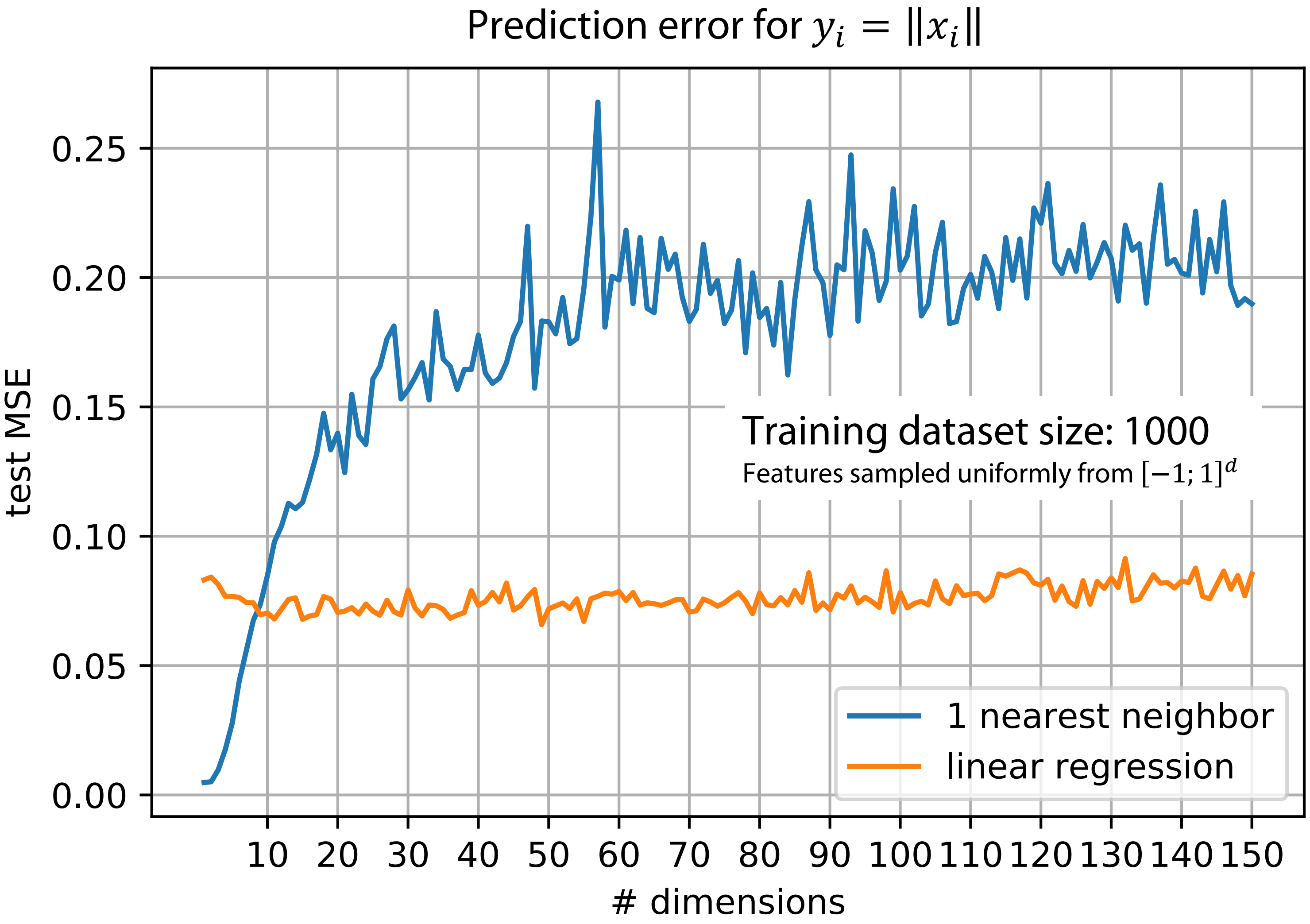

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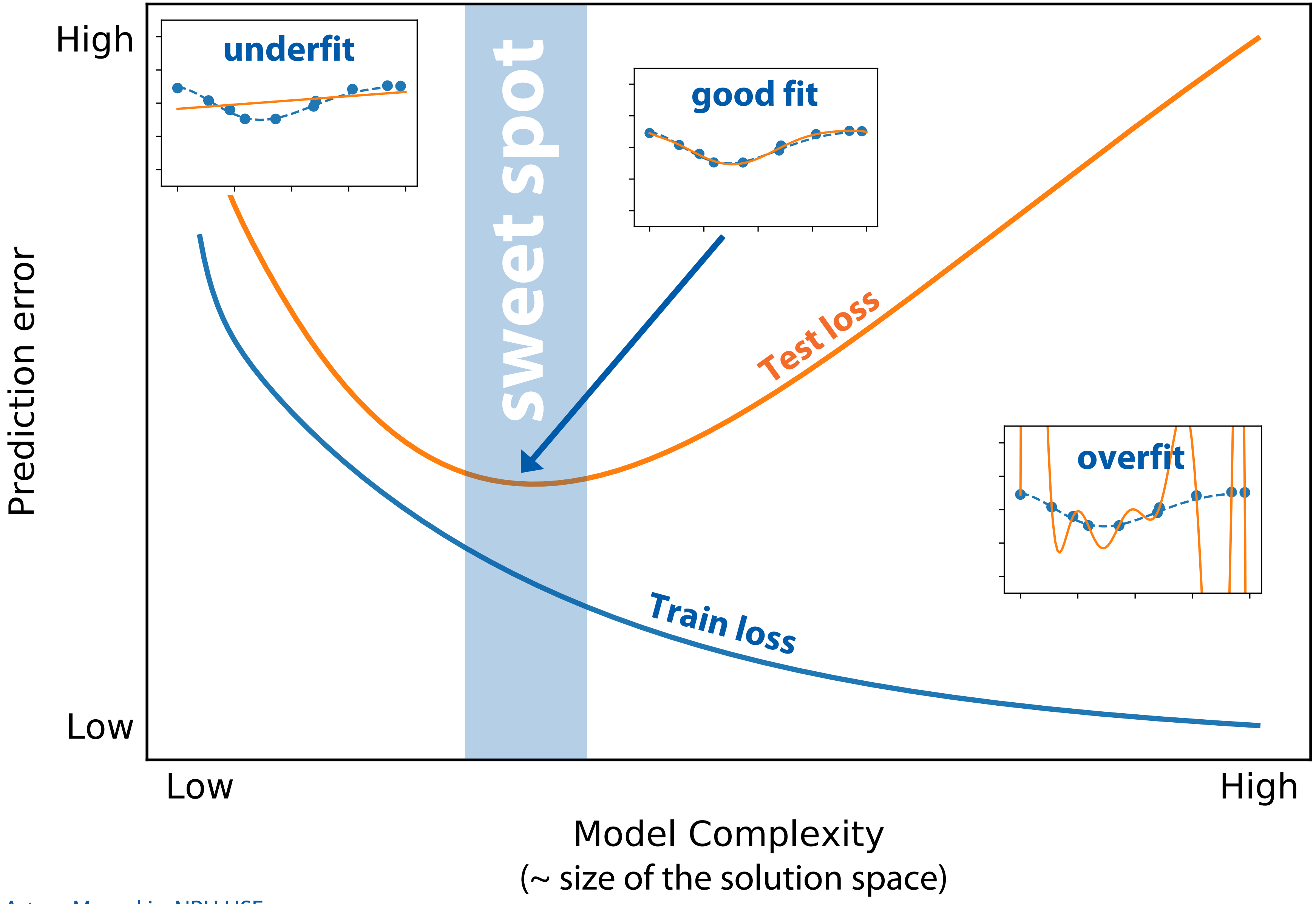
Imposing assumptions about the data **restricts the space of possible solutions**

This restriction allows to **overcome the curse of dimensionality**

(Though, wrong assumptions lead to wrong solutions)

How to check whether a model is good?



Check the loss on the **test data** – i.e. data that the learning algorithm "hasn't seen"

The goal is to find the **right level of limitations** – not too strict, not too loose

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- Food for thought: how can Linear Regression model be used to fit a n-th degree polynomial?

Thank you!

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