Introduction to Supervised Learning

Intro to Machine Learning, Supervised Learning

Programming and Statistical Analysis, 2025

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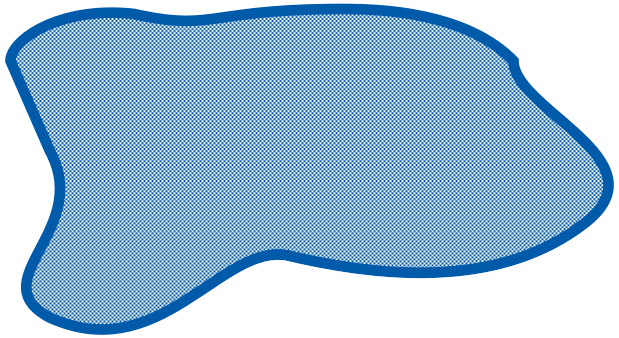
Supervised Learning

Problem setup

$\mathcal{X}$ – a set of objects



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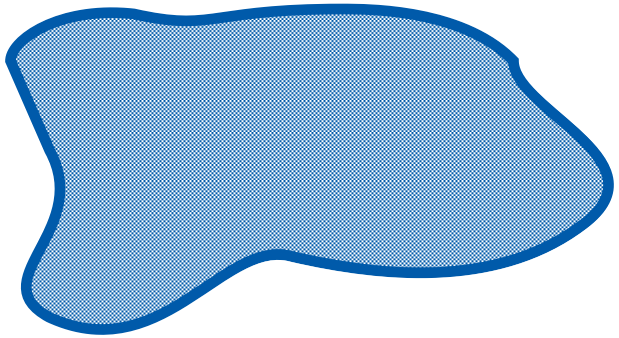
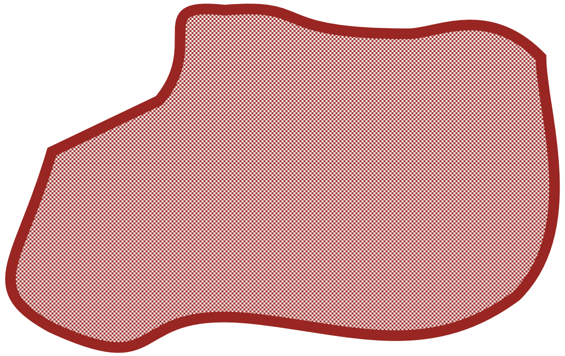


$\mathcal{Y}$ − a set of targets



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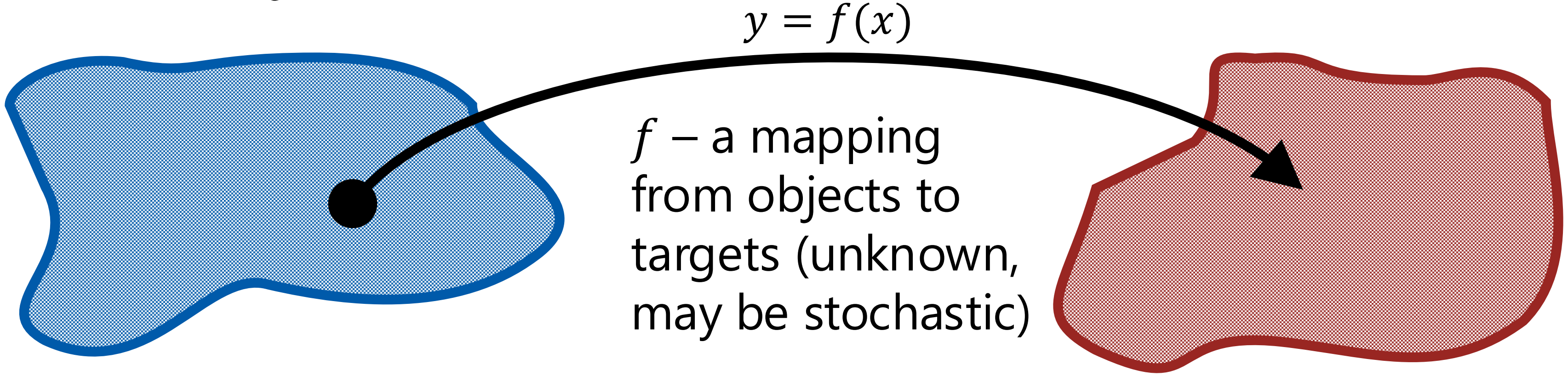

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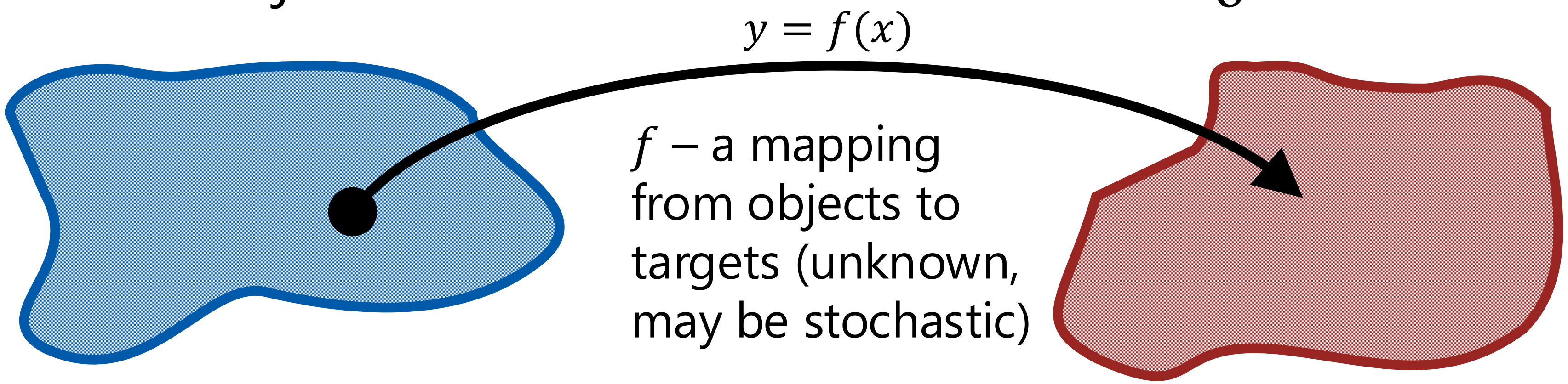

A dataset: $D = \{(x_i,\ y_i) : i = 1,\ 2, \dots,\ N\}$

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

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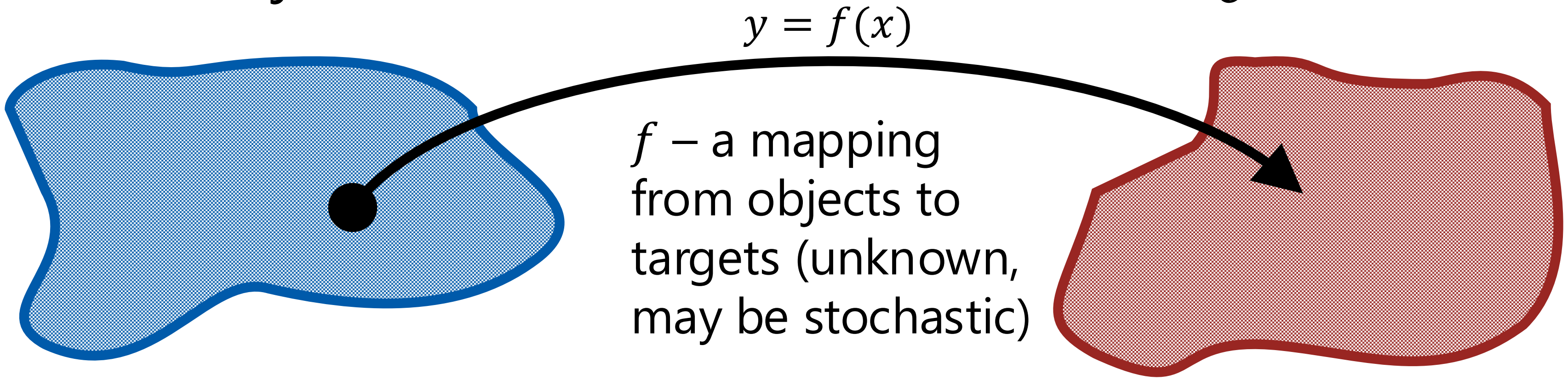

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Goal: **approximate f given D**
i.e. learn to **recover targets from objects**

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)

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)

image source: wikipedia.org

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:

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

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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  - Assigning each category a number (e.g. ″red″ = 1, “green″ = 2, etc.) may have negative effect on the learning algorithm

One-hot encoding

- 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

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A trick for ordinal features

- 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.

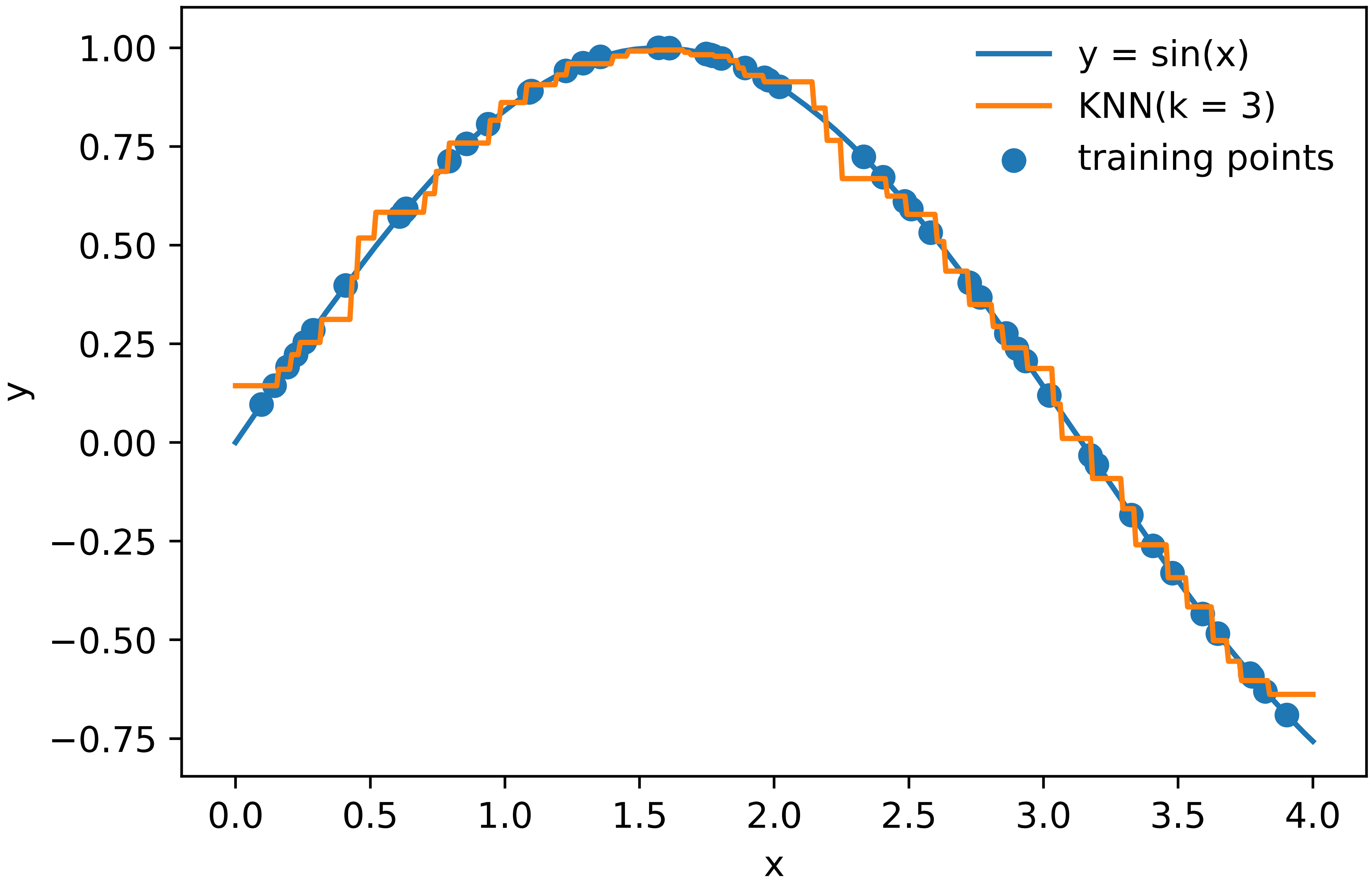
Example: k nearest neighbors (kNN)

- 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:

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

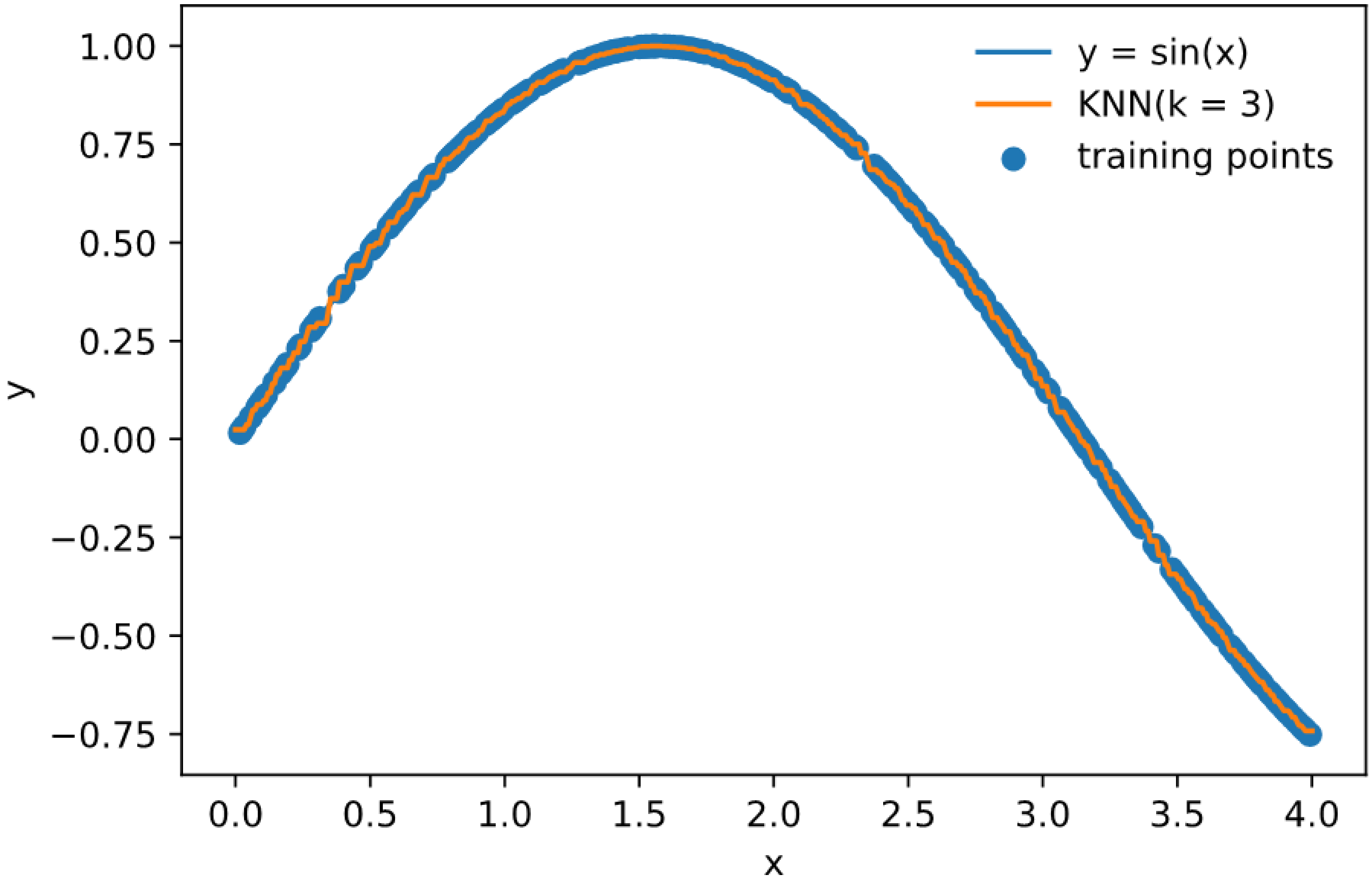
D_x^k – set of k objects from D closest to x

Example: k nearest neighbors



training points: 50

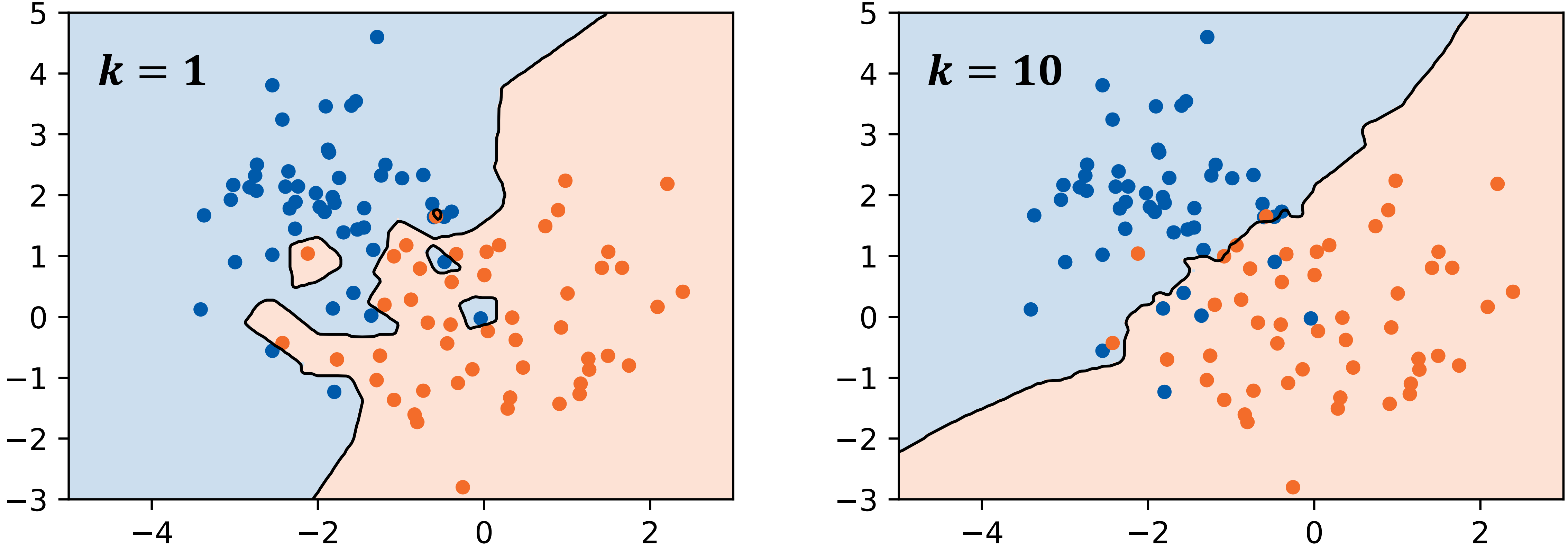
Example: k nearest neighbors



training points: 250

More data = **better approximation**

Example: k nearest neighbors



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

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:
$\boldsymbol{\mathcal{L} = \left(y_i - \hat{f}(x_i)\right)^2}$

Loss function

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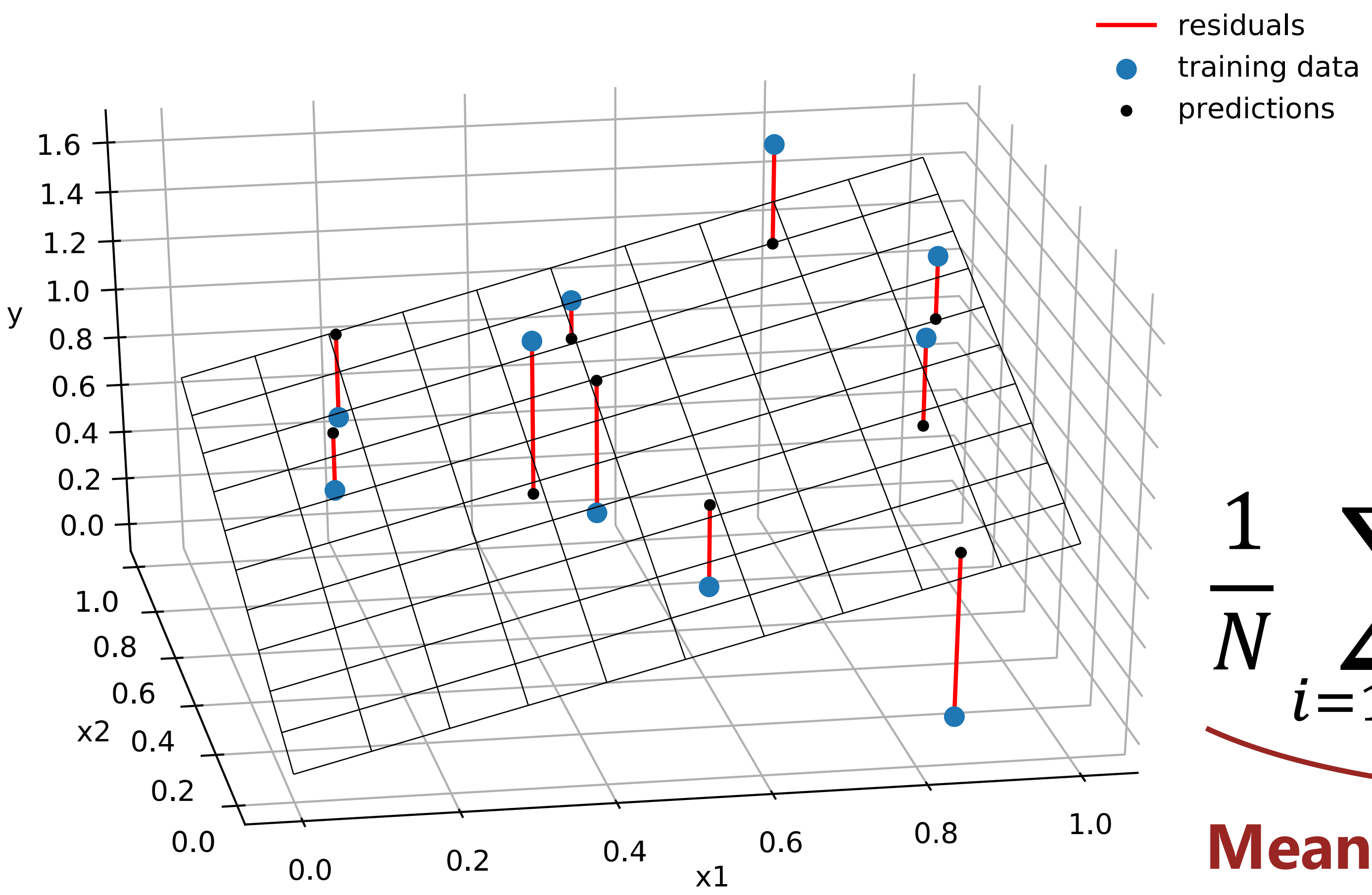
- We can measure the quality of a prediction for a single object x_i with a **loss function** $\mathcal{L} = \mathcal{L}\left(y_i, \hat{f}(x_i)\right)$
- Then, learning (or training) can be formulated as a **loss minimization** problem:

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

E.g. squared error:
$$\boldsymbol{\mathcal{L} = \left(y_i - \hat{f}(x_i)\right)^2}$$

Example: linear regression



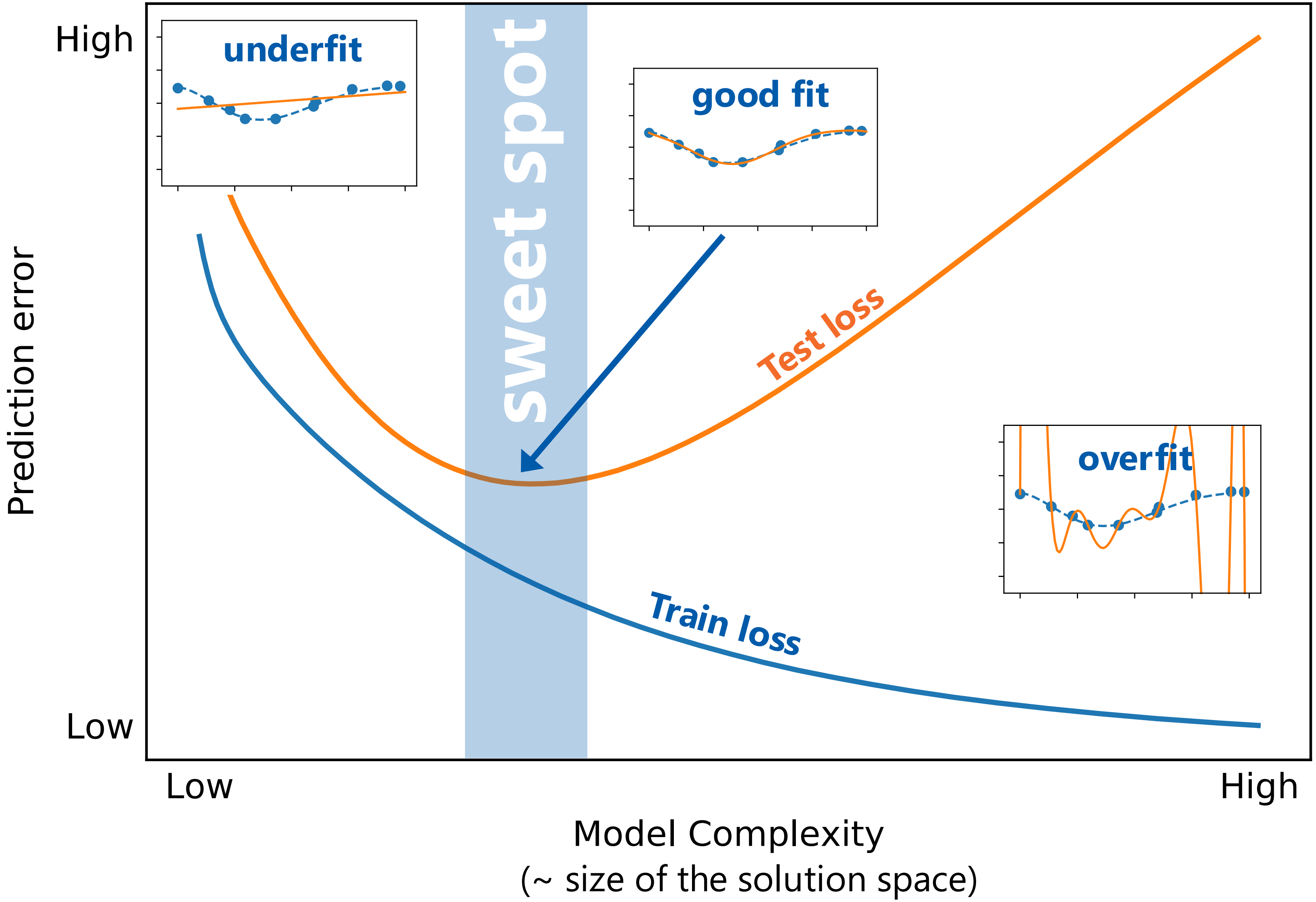
$$\hat{f}_{w,b}(x) = w^{\mathrm{T}}x + b$$

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

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

Mean Squared Error (MSE loss)

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

Summary

- Supervised Machine Learning algorithms build approximations $\hat{f} = \mathcal{A}(D)$ to the true dependence f
- Features may be of various nature, one-hot encoding is useful to convert categorical features to numeric
- Machine Learning algorithms can be defined as expected loss minimization tasks
- Choosing the right model = applying the right assumptions about the data
- Use test data to detect underfitting and overfitting

Thank you!

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