

Introduction to Supervised Learning

Problem setup, feature types, assumptions about data

Machine Learning and Data Mining, 2024

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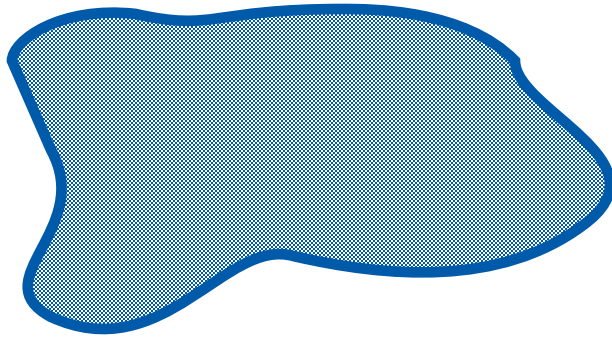
September 04, 2024

Supervised Learning



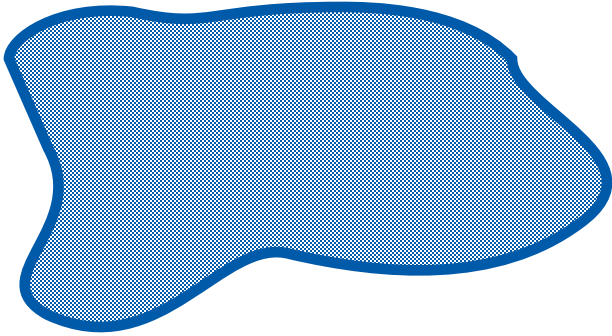
Problem setup

\mathcal{X} – a set of objects

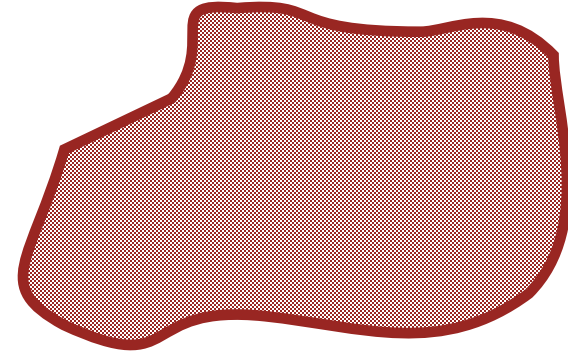


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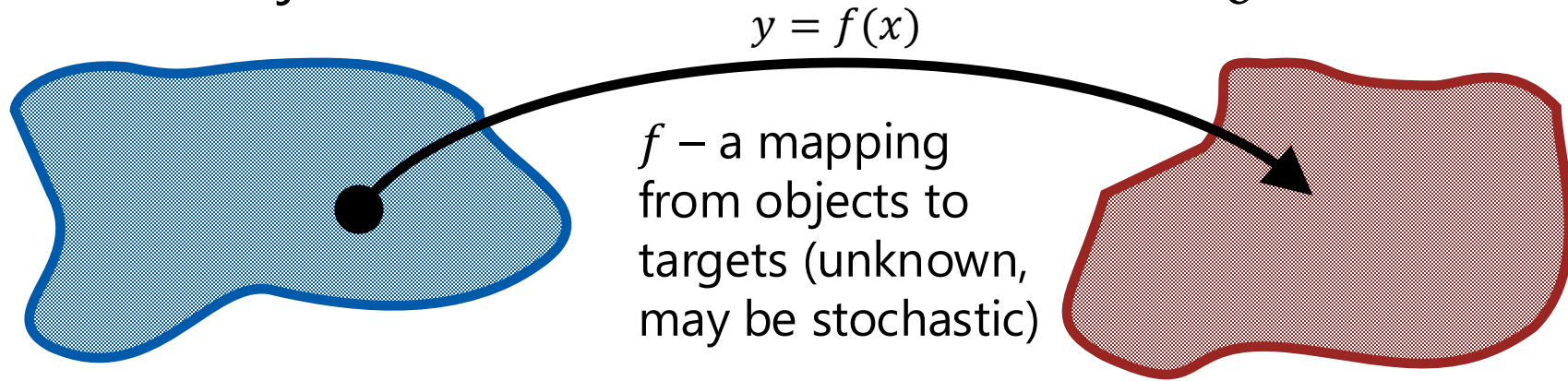
\mathcal{Y} – a set of targets



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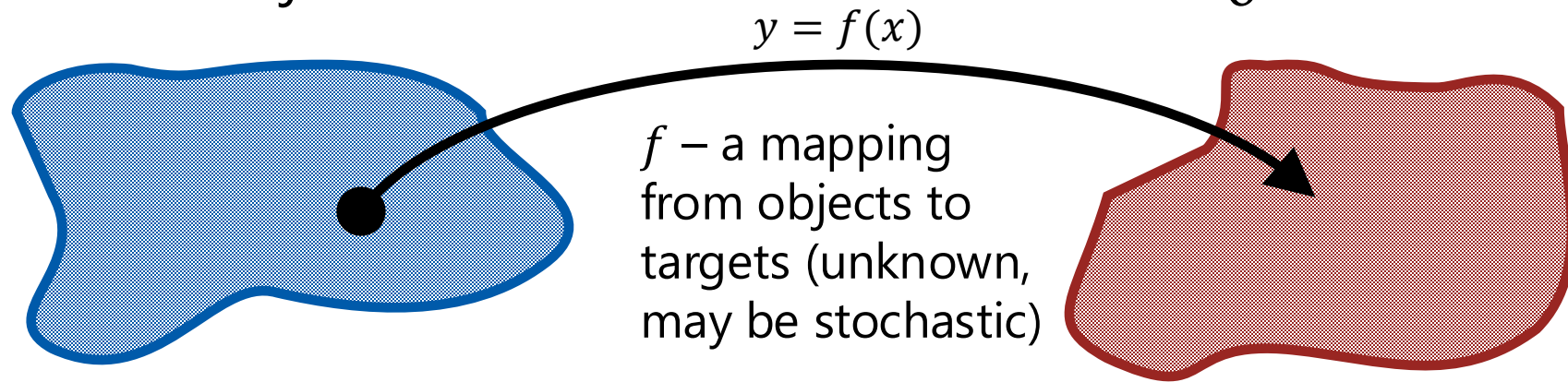
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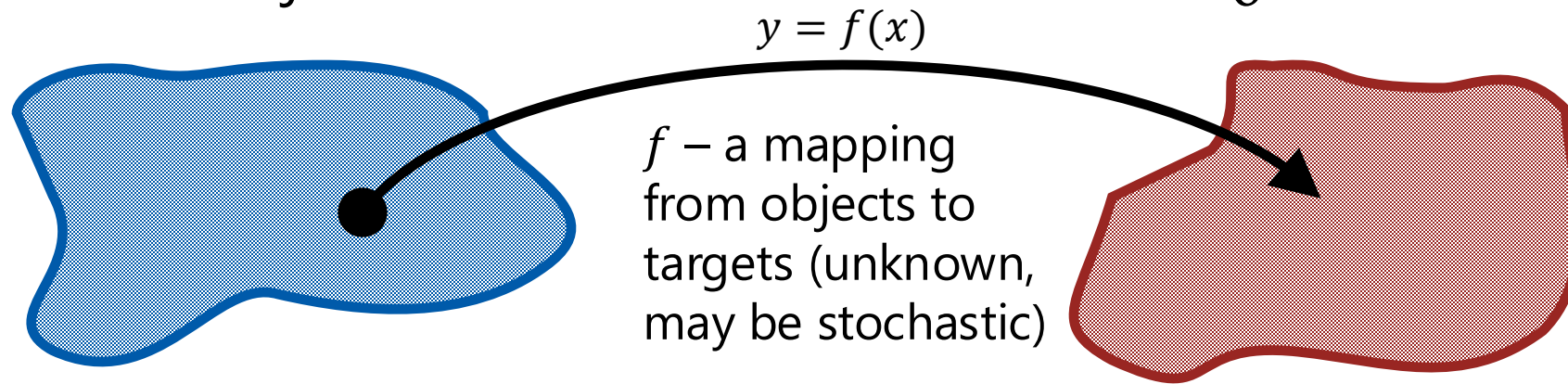
A dataset: $D = \{(x_i, y_i) : i = 1, 2, \dots, N\}$

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

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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)

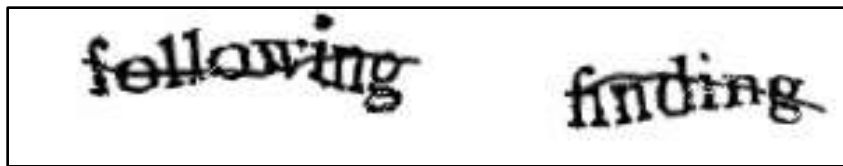


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Features



Features

- ▶ 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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 - It's a vector $x_i = (x_i^1, x_i^2, \dots, x_i^d)$
- ▶ 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**:

$$X = \begin{array}{c} \xrightarrow{\text{features}} \\ \left[\begin{array}{cccc} x_1^1 & x_1^2 & \cdots & x_1^d \\ x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \cdots & x_N^d \end{array} \right] \downarrow \text{objects} \end{array}$$

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 features 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 – simple trick to convert categorical feature to numeric:

color	is_blue	is_red	is_green
"red"	0	1	0
"red"	0	1	0
"blue"	1	0	0
"green"	0	0	1
"blue"	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 .

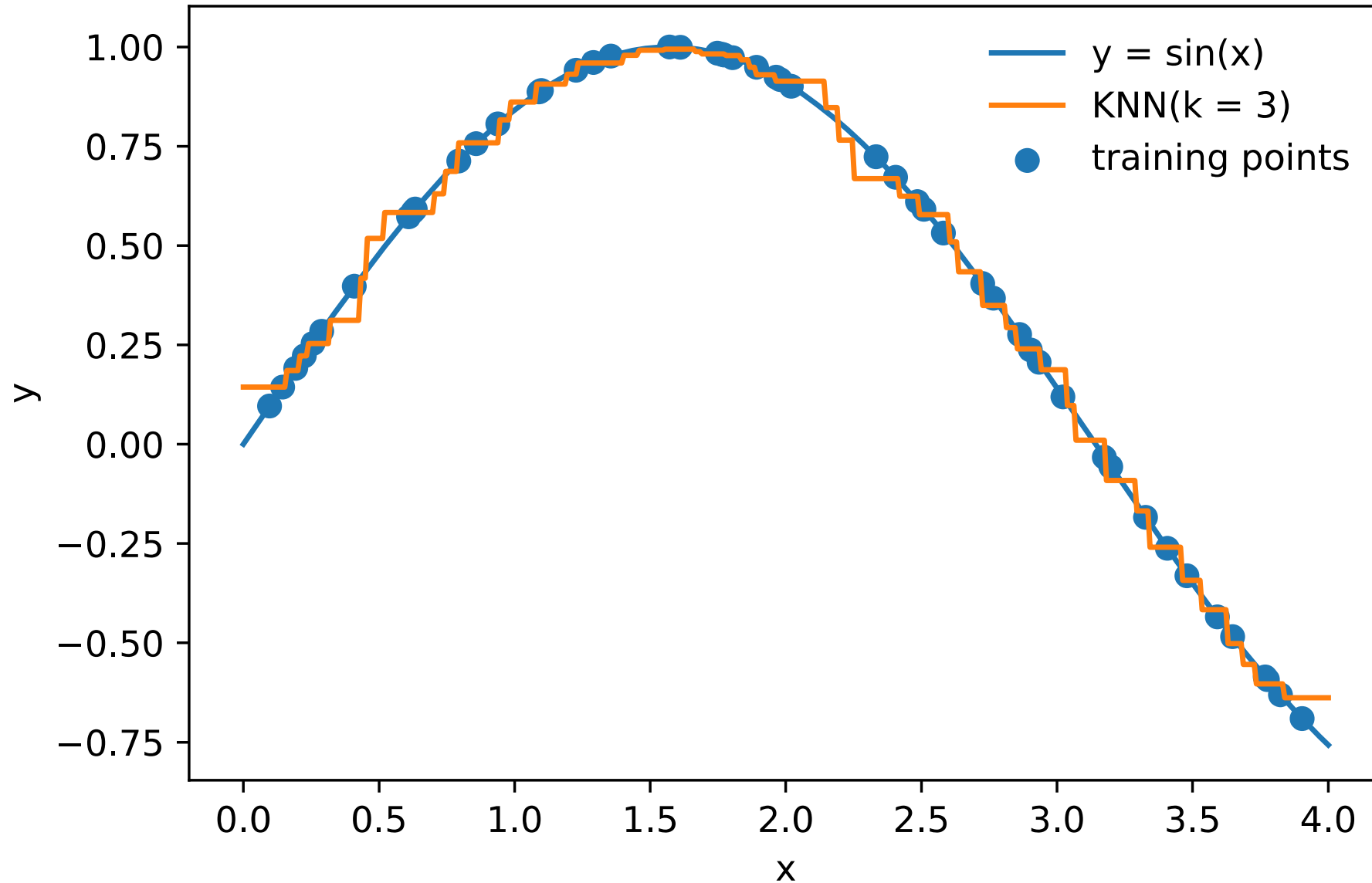
Example: k nearest neighbors (kNN)

- ▶ 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:

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

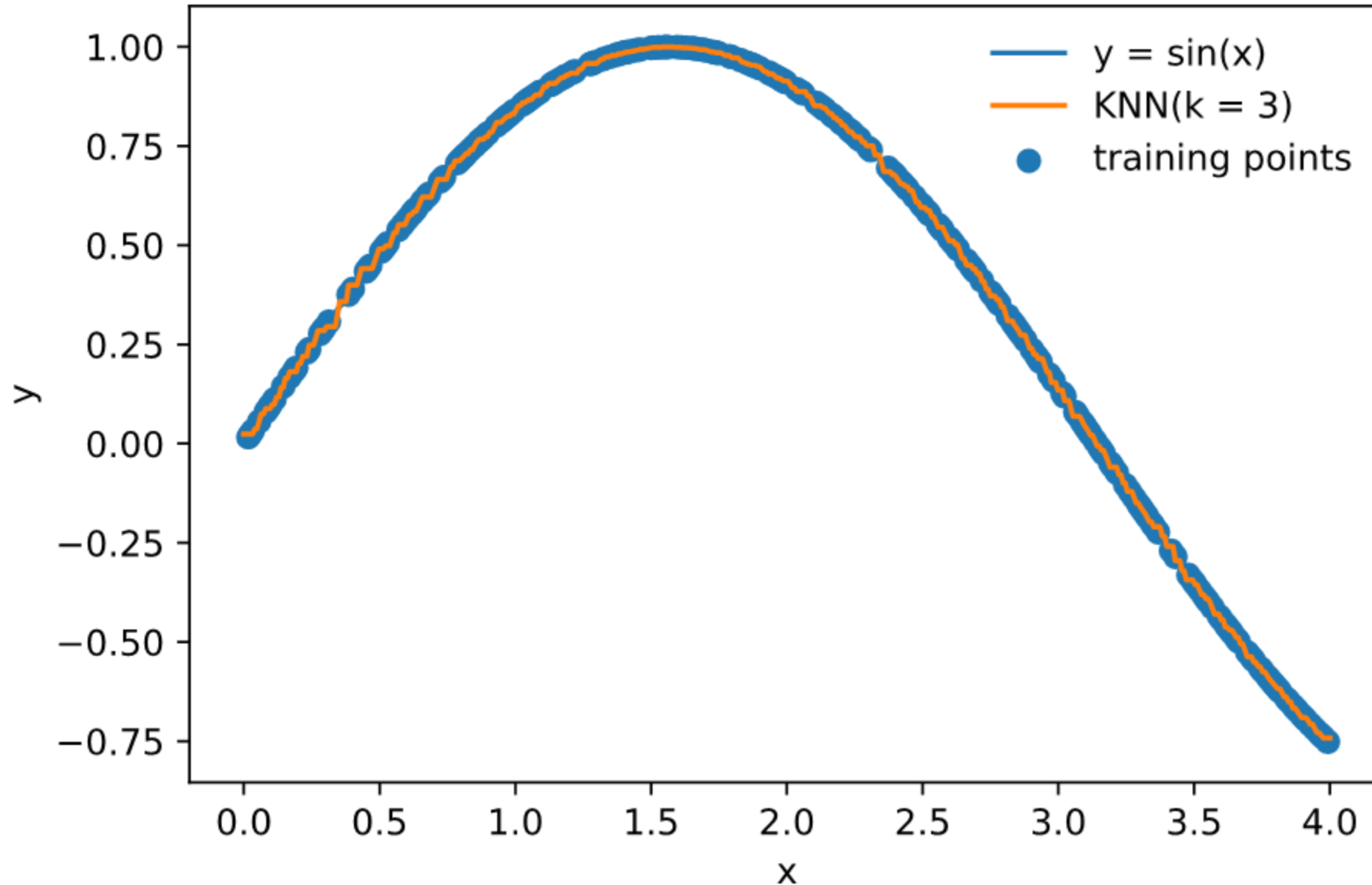
D_x^k – set of k objects from D closest to x

Example: k nearest neighbors



training points: 50

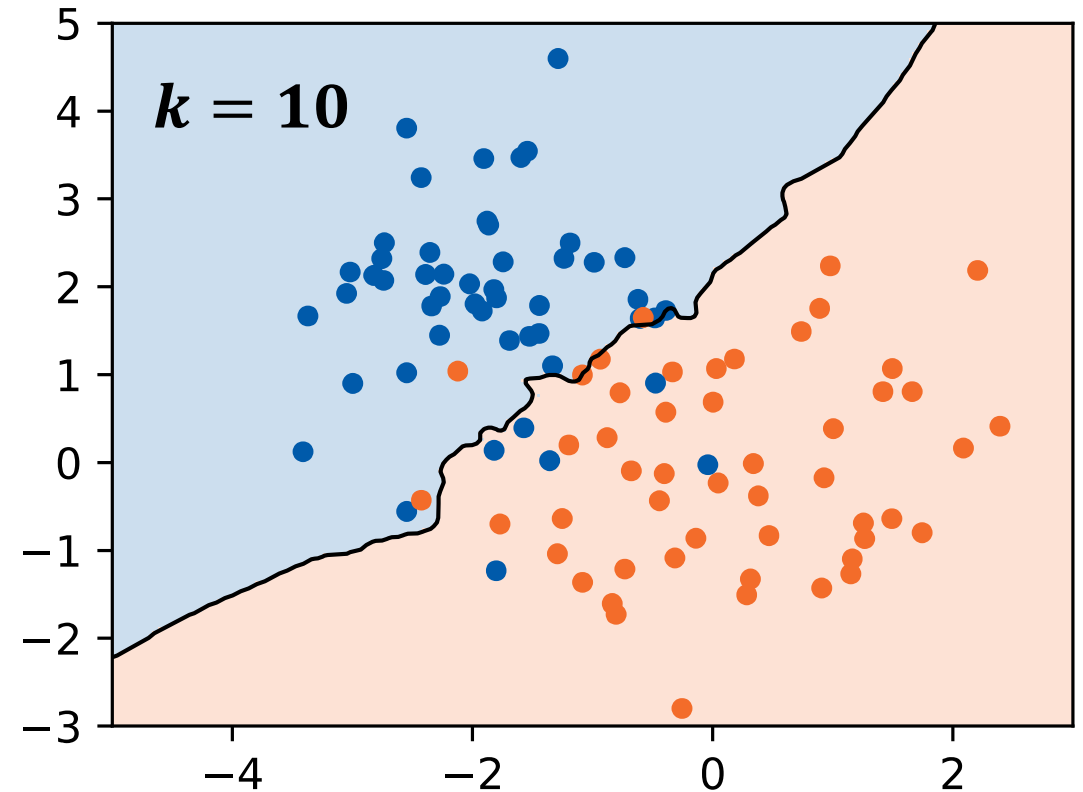
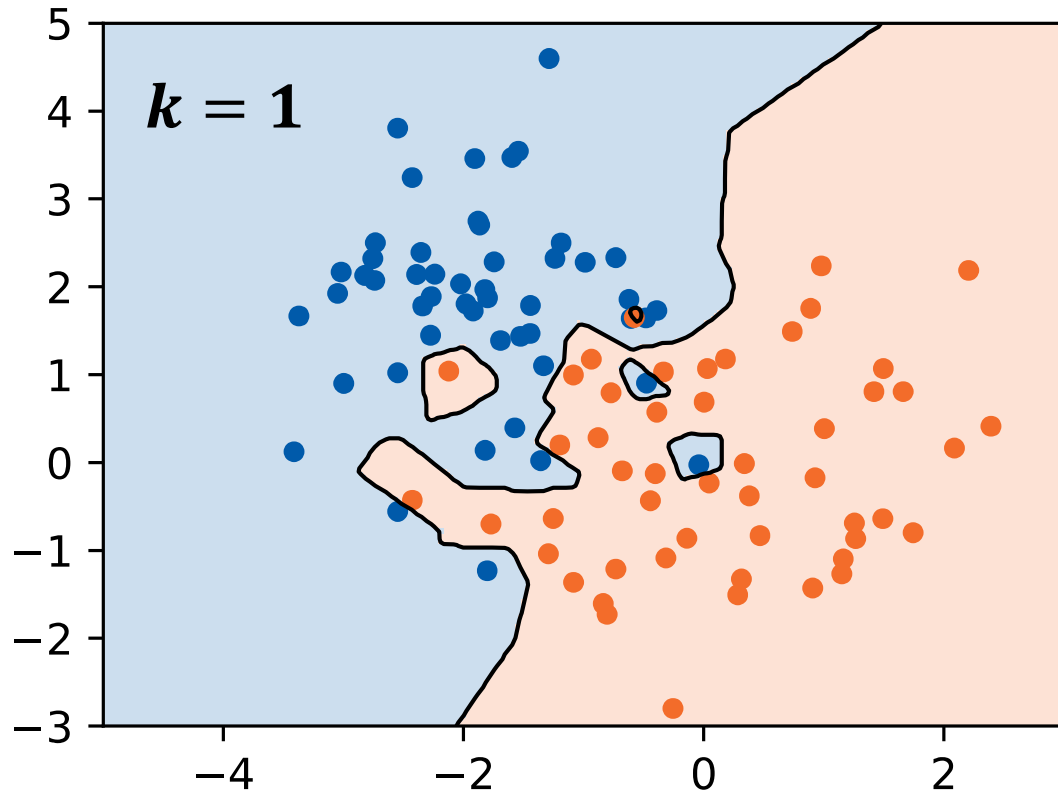
Example: k nearest neighbors



training points: 250

**More data =
better
approximation**

Example: k nearest neighbors



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

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** $\mathcal{L} = \mathcal{L}(y_i, \hat{f}(x_i))$

E.g. squared
error:

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

Loss function

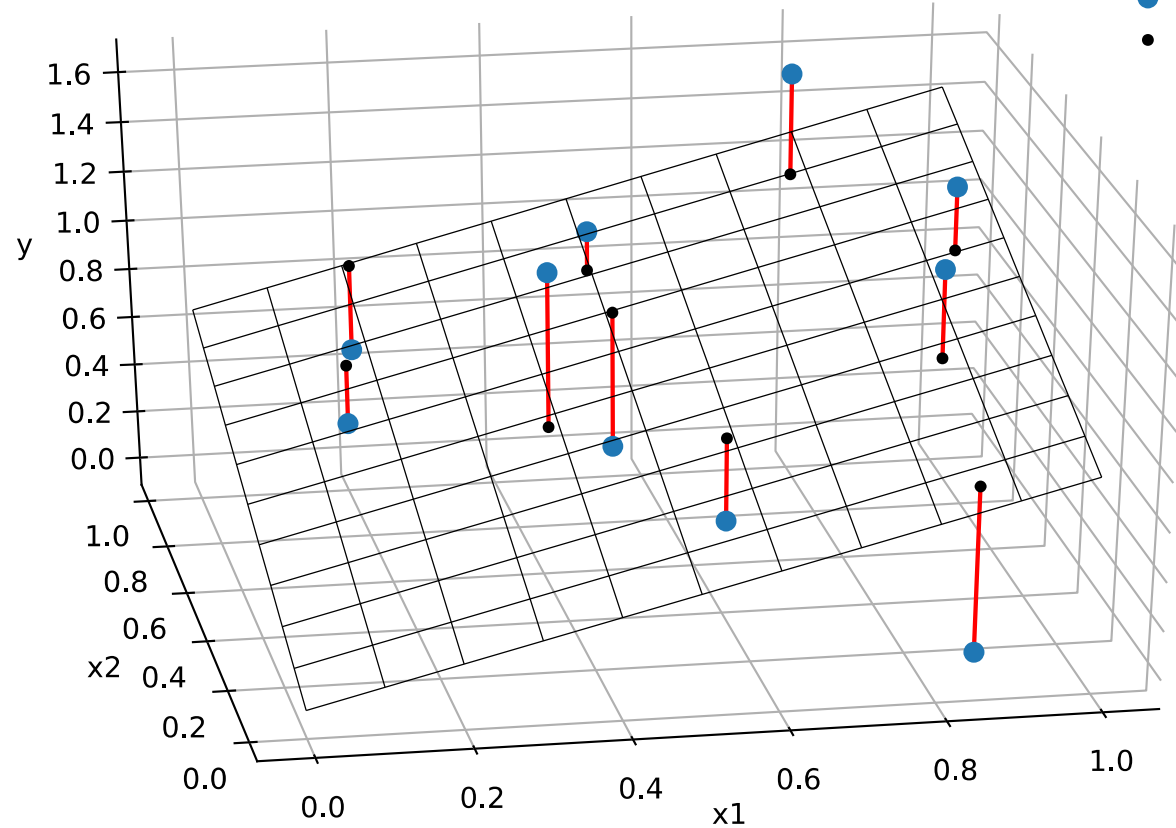
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- ▶ We can measure the quality of a prediction for a single object x_i with a **loss function** $\mathcal{L} = \mathcal{L}(y_i, \hat{f}(x_i))$
- ▶ Then, learning (or training) can be formulated as a **loss minimization** problem:

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

E.g. squared
error:

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Example: linear regression



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

$$w \in \mathbb{R}^d$$

$$b \in \mathbb{R}$$

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

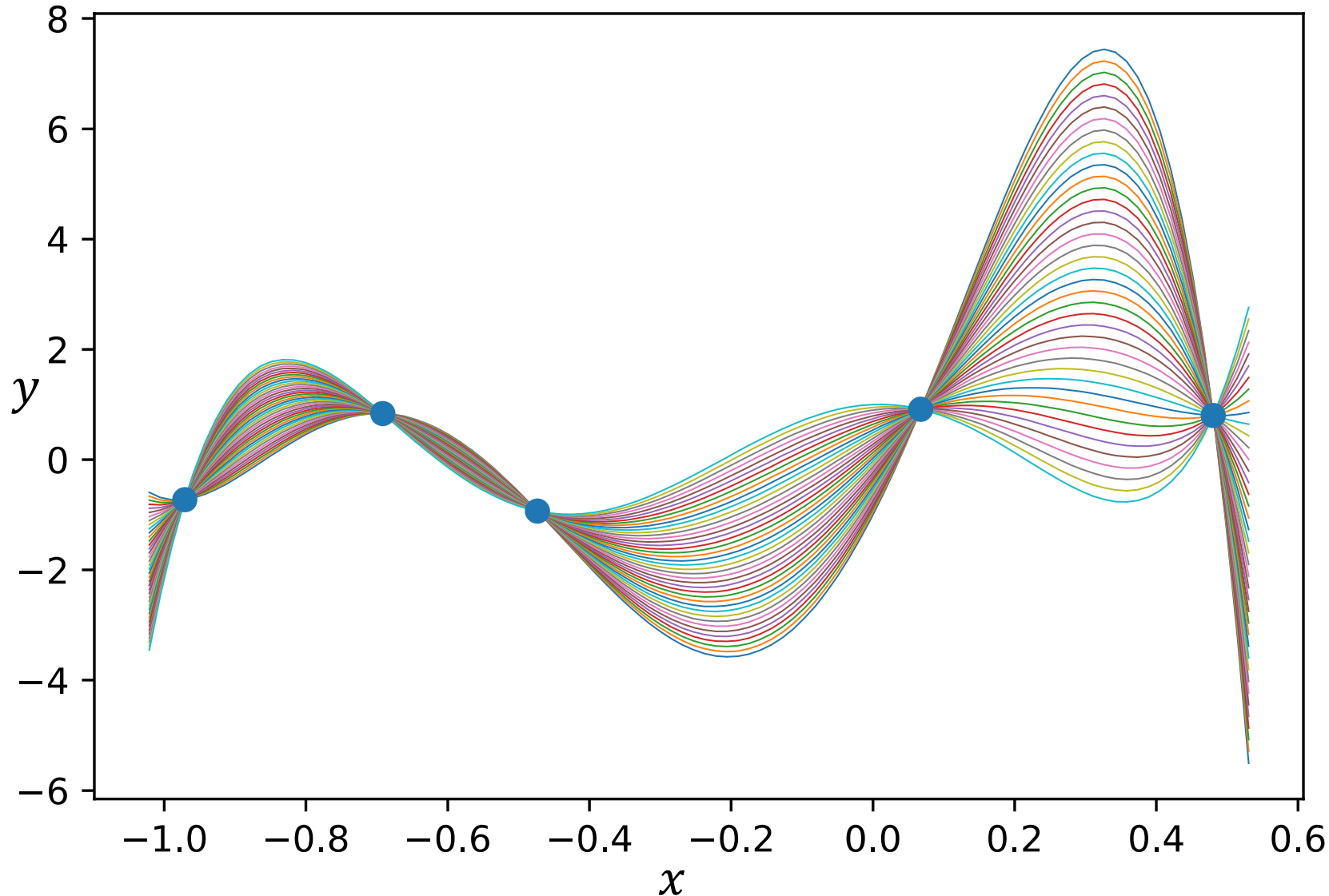
$$\frac{1}{N} \sum_{i=1 \dots N} \left(y_i - \hat{f}_{w,b}(x_i) \right)^2 \xrightarrow{w,b} \min$$

**Mean Squared Error
(MSE loss)**

Assumptions about data



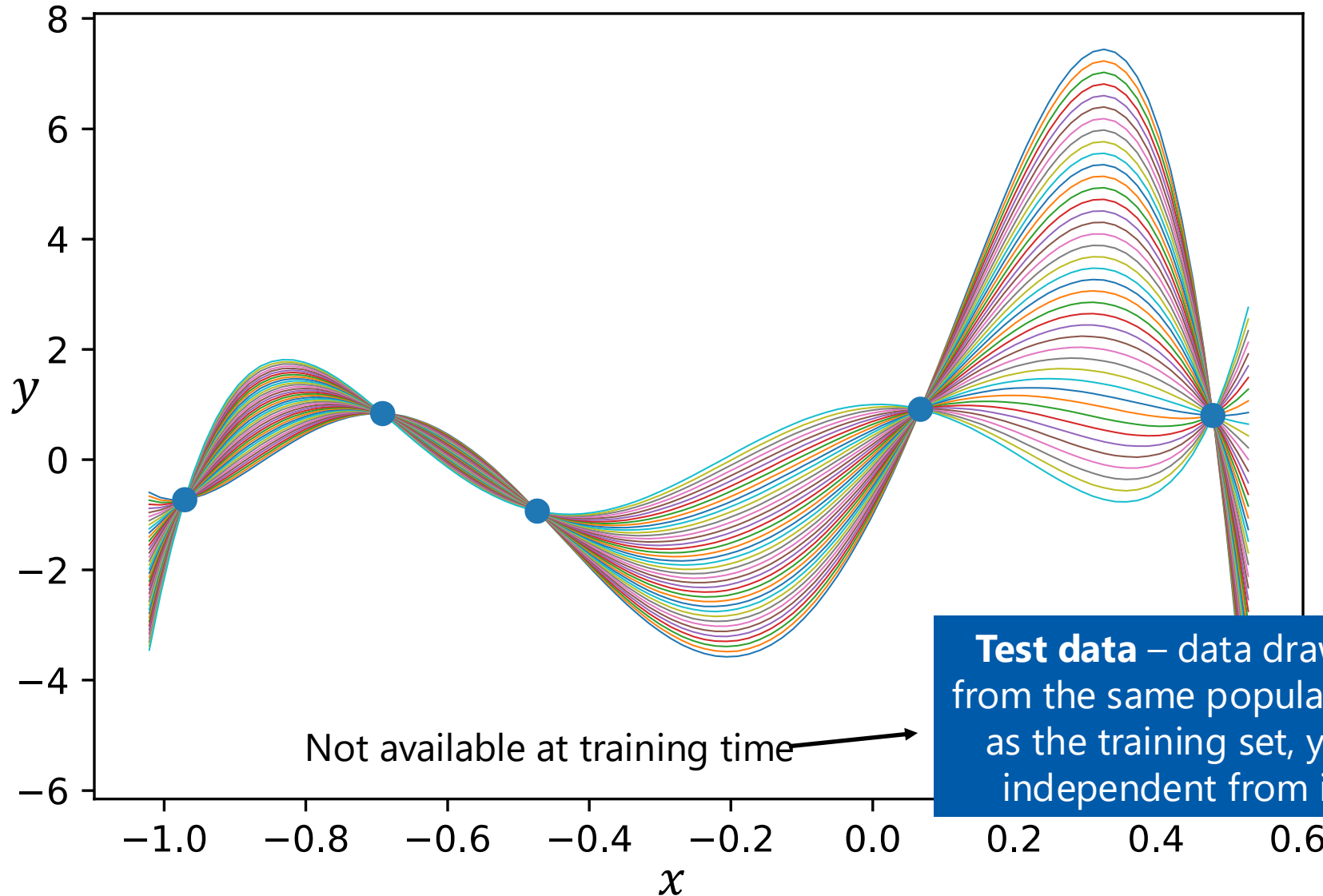
No assumptions = Infinitely many solutions



Any of these curves
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We want **expected loss
over population** to be
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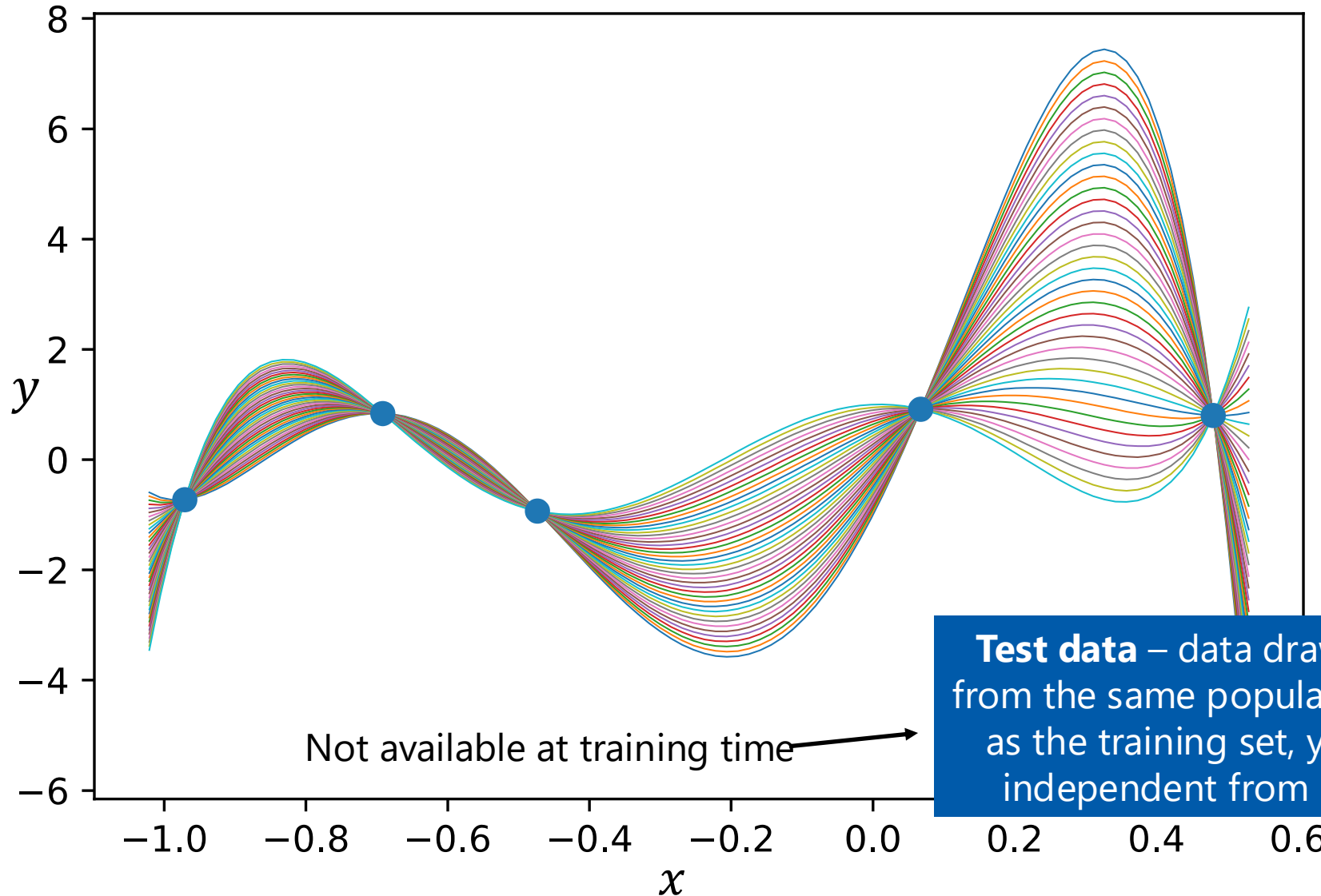


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Test data – data drawn
from the same population
as the training set, yet
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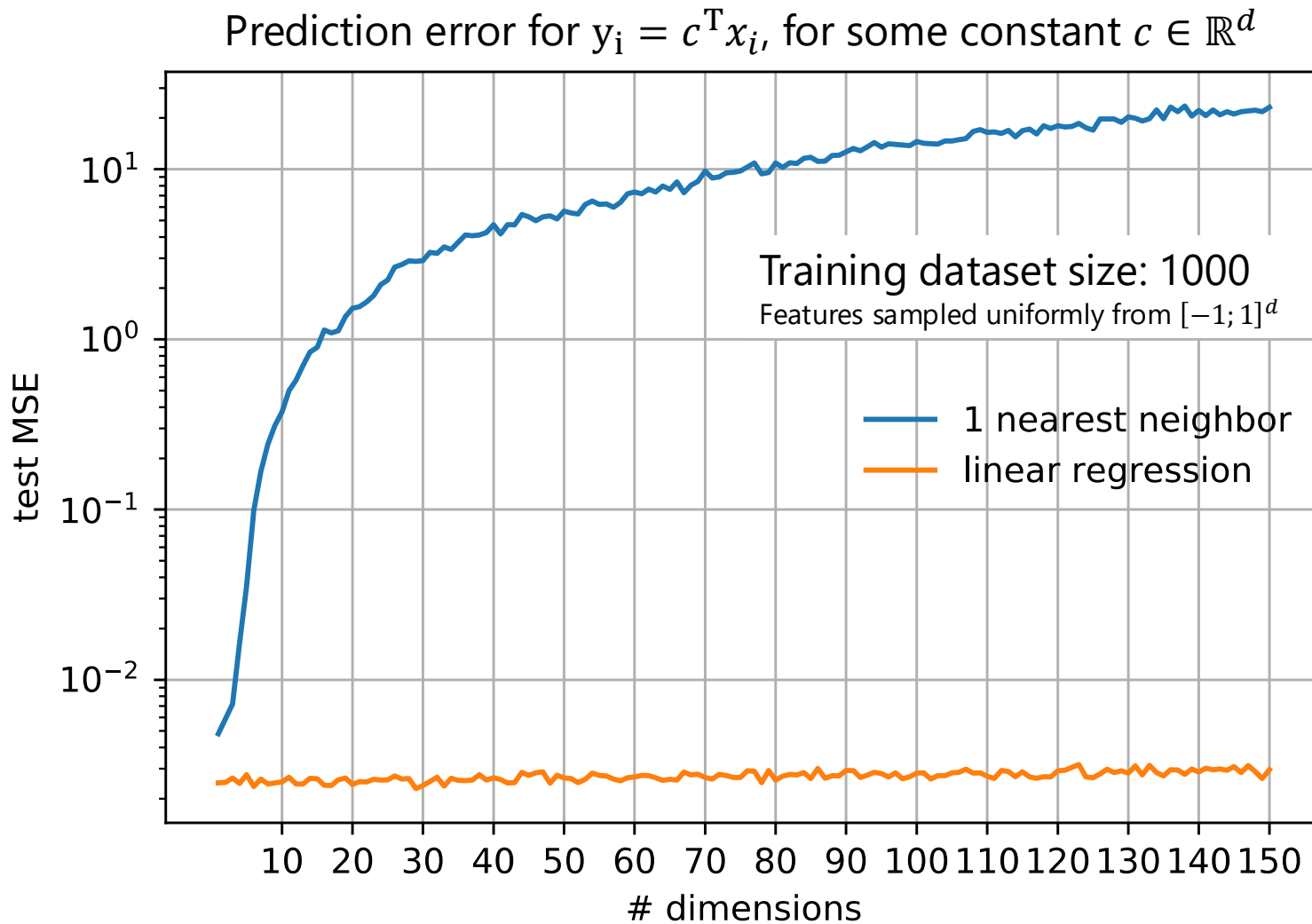
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Need to **assume some
structure** of the data,
common to **training** and
testing data

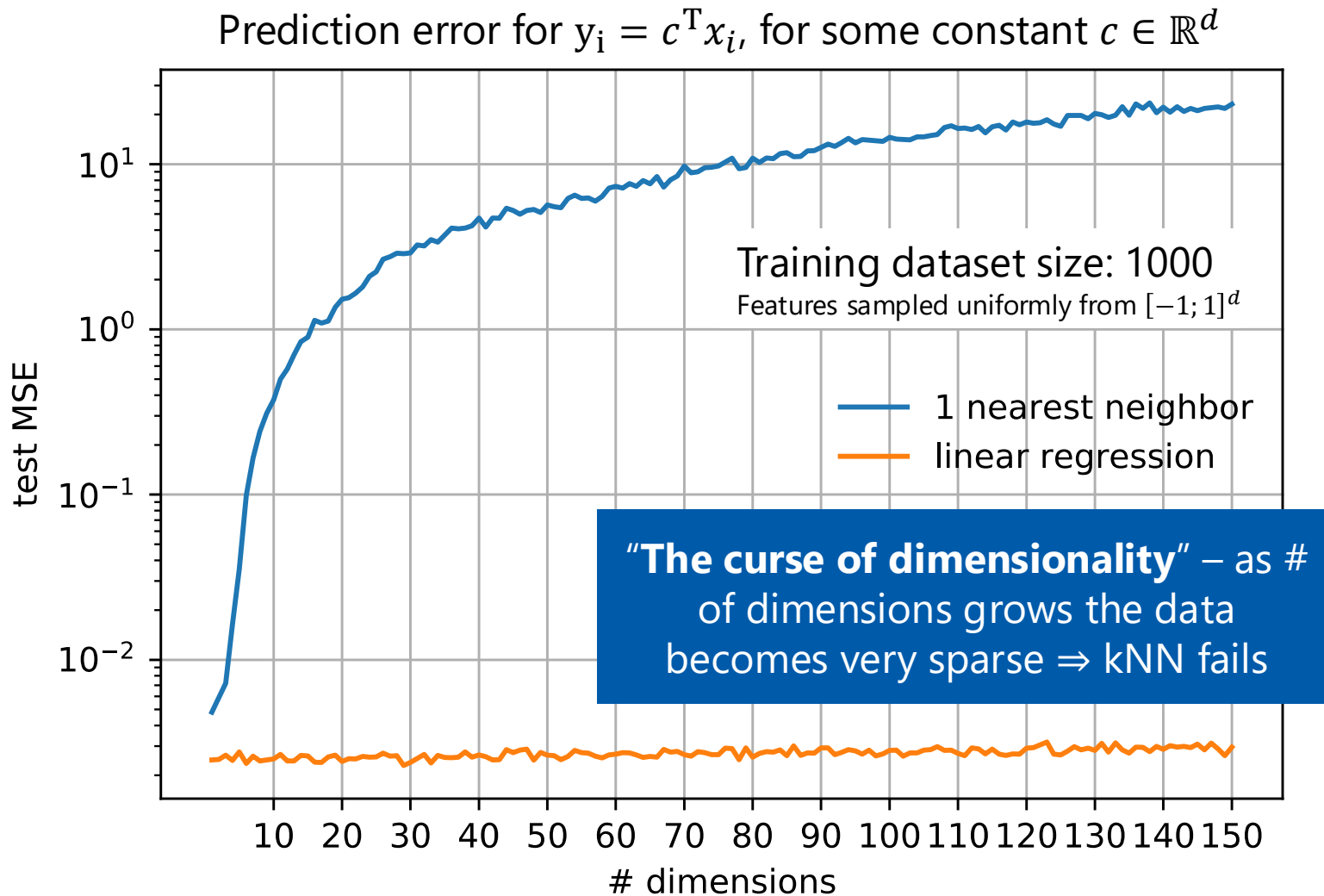
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Not available at training time

Example: kNN(k = 1) VS Linear Regression

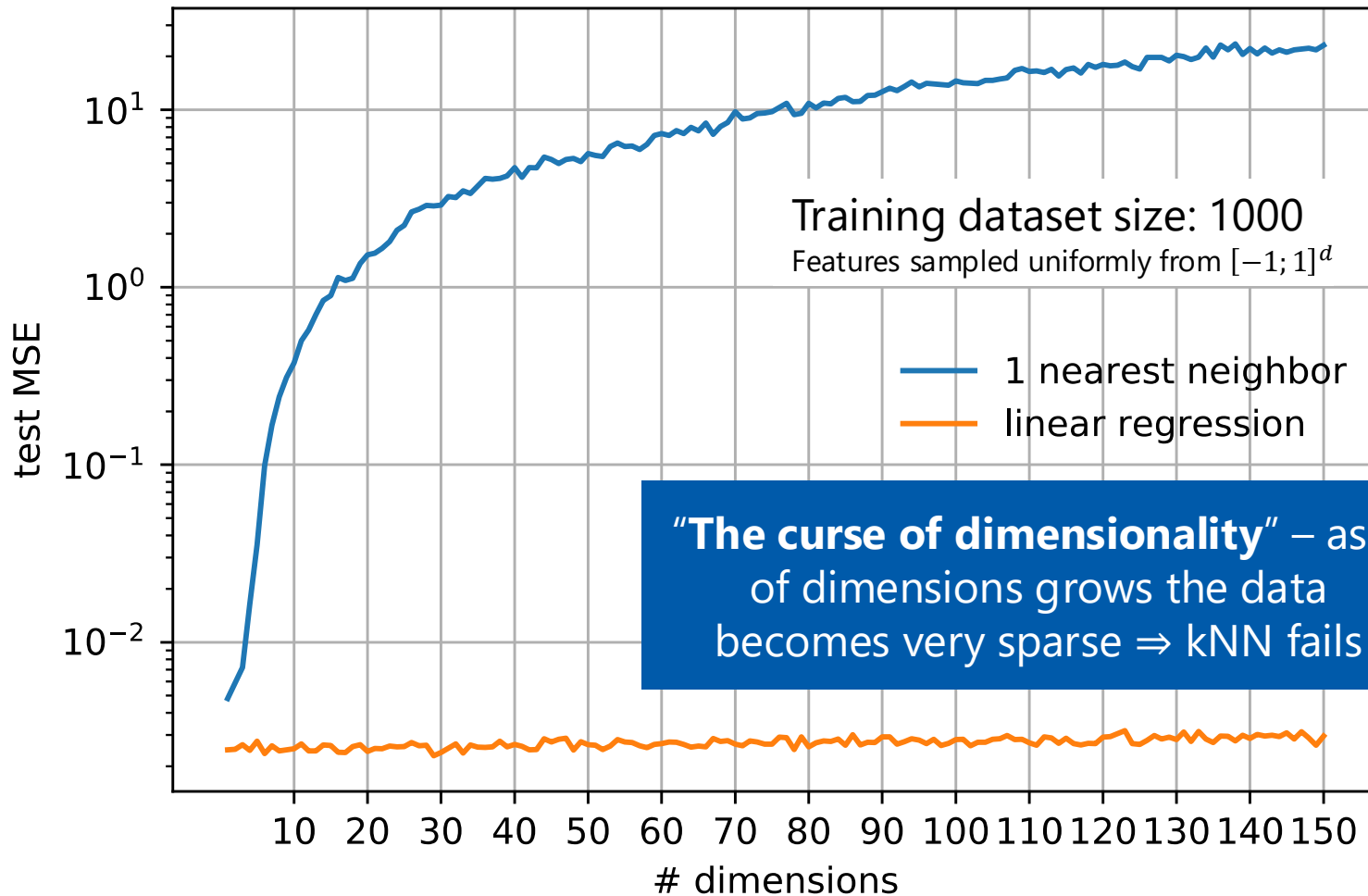


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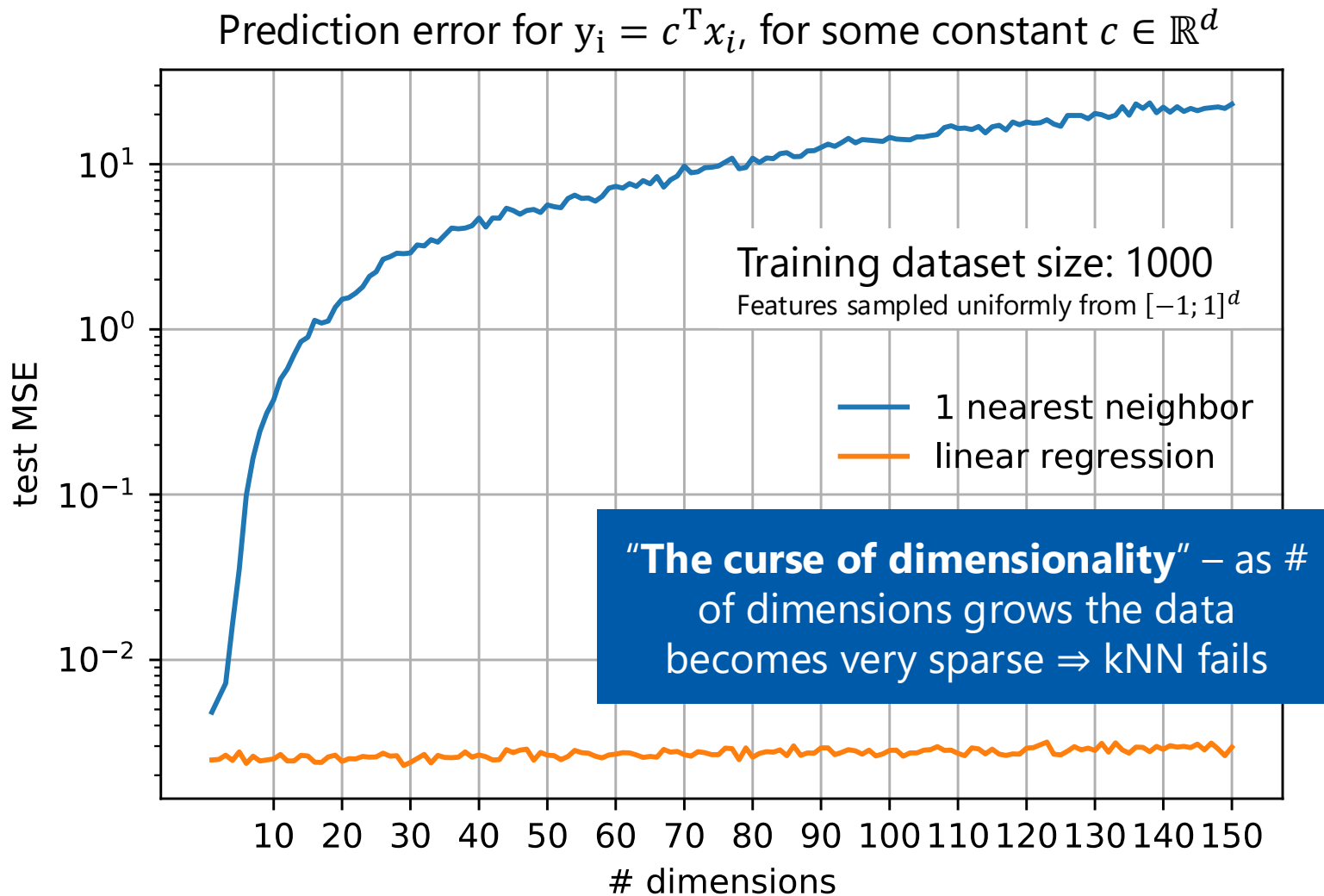
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Prediction error for $y_i = c^T x_i$, for some constant $c \in \mathbb{R}^d$



Assumption for kNN:
"similar objects have similar targets"

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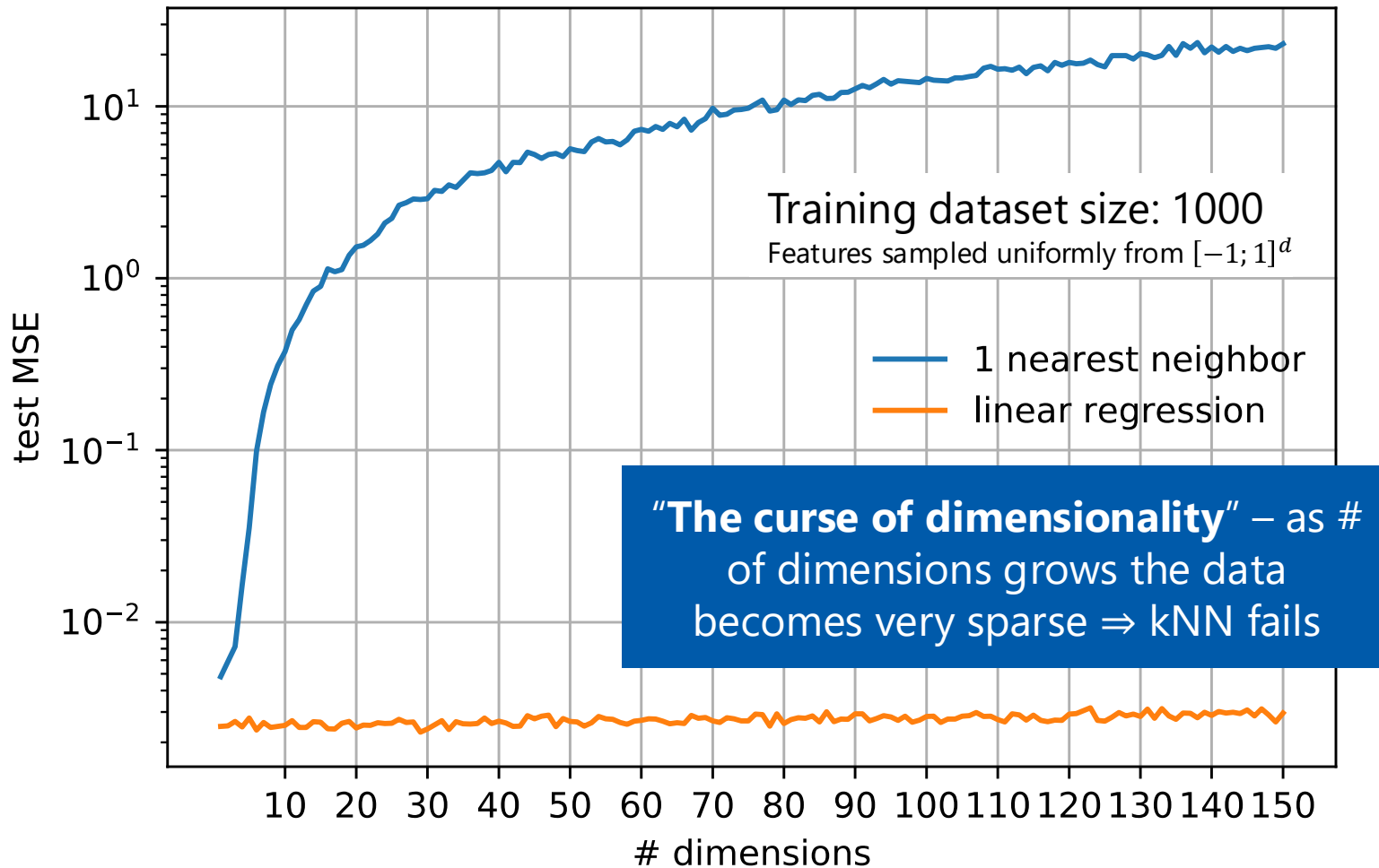


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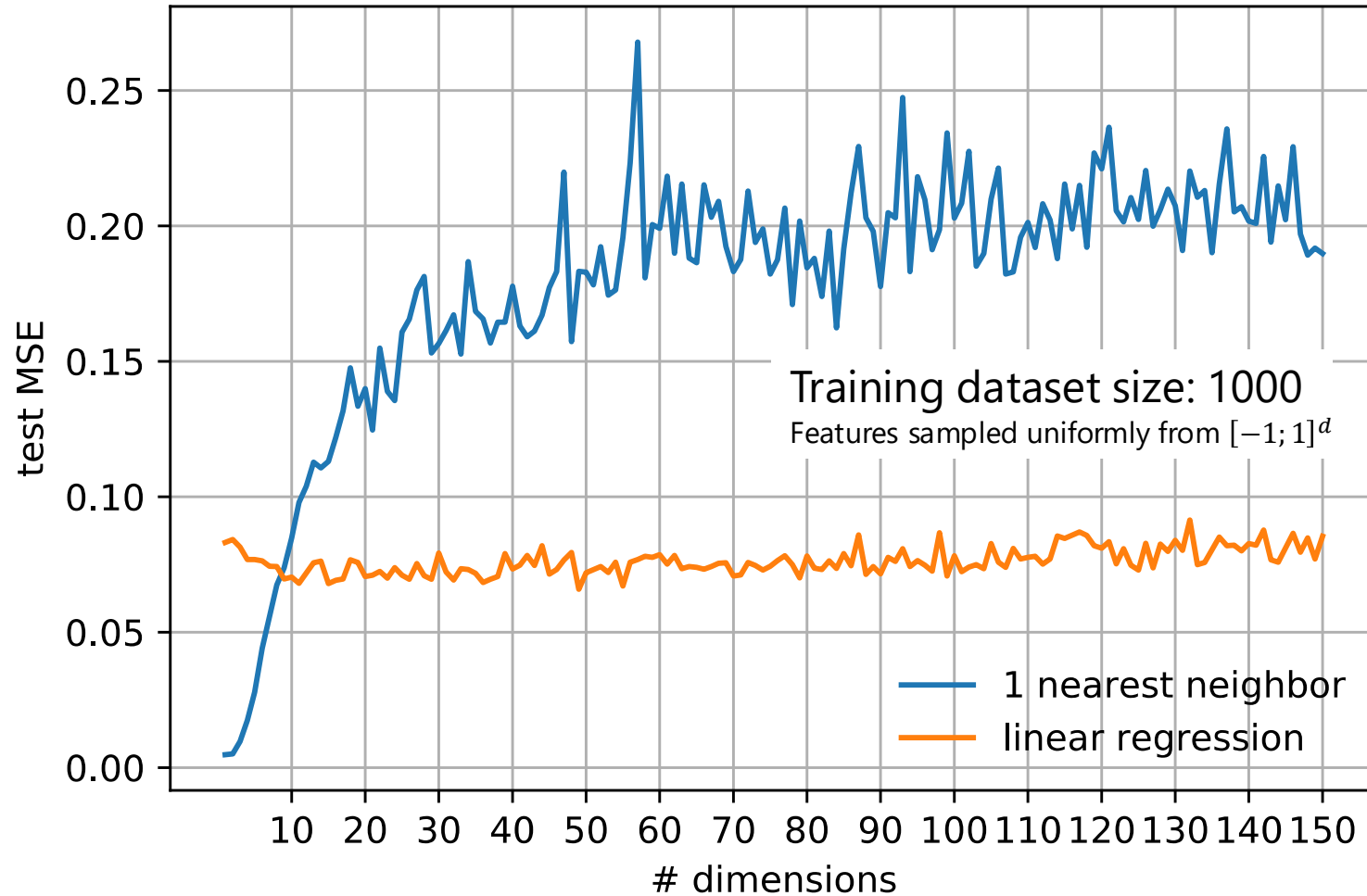
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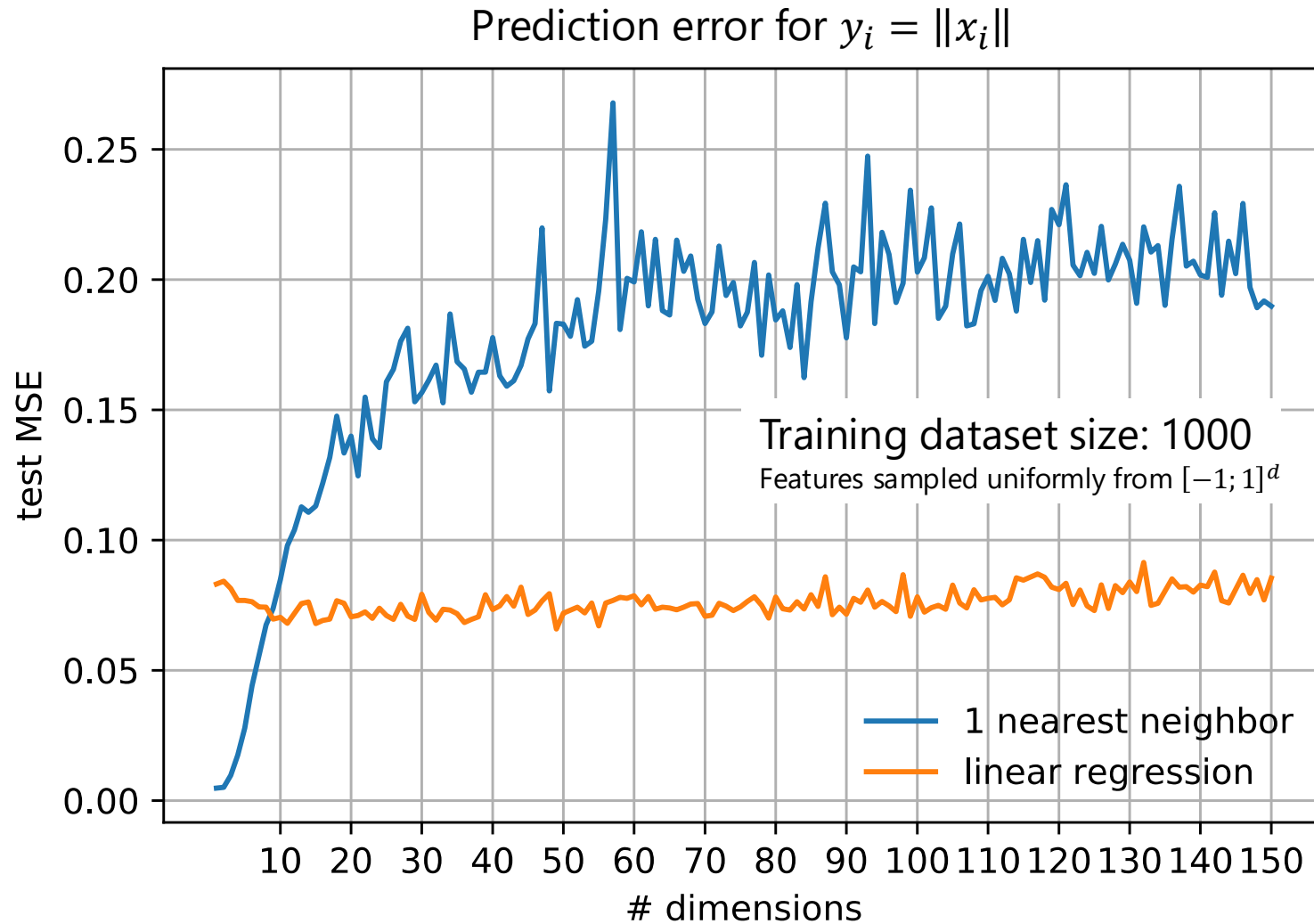
For this example, both assumptions are correct, but one is **stronger** than the other

Example: kNN(k = 1) VS Linear Regression

Prediction error for $y_i = \|x_i\|$

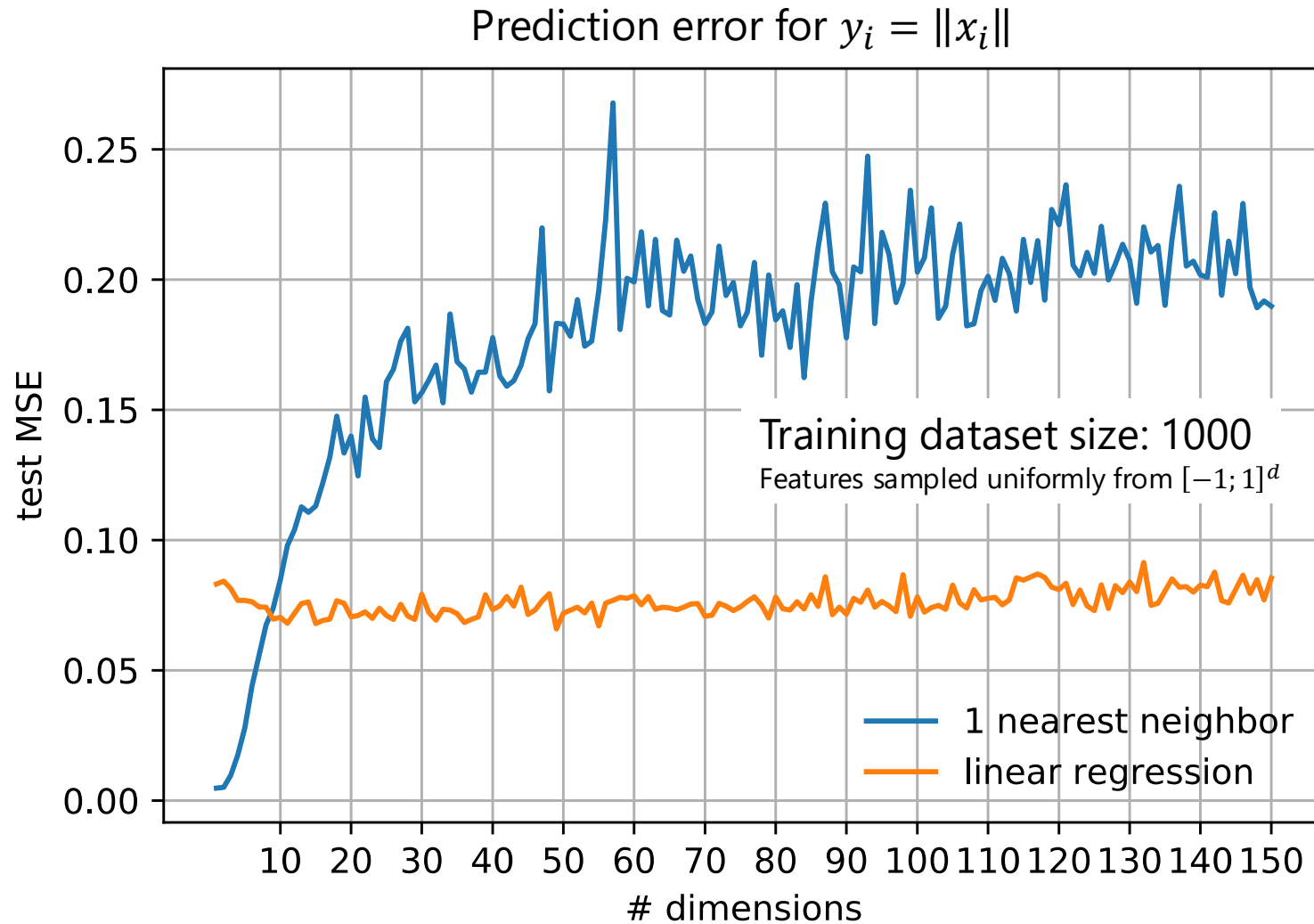


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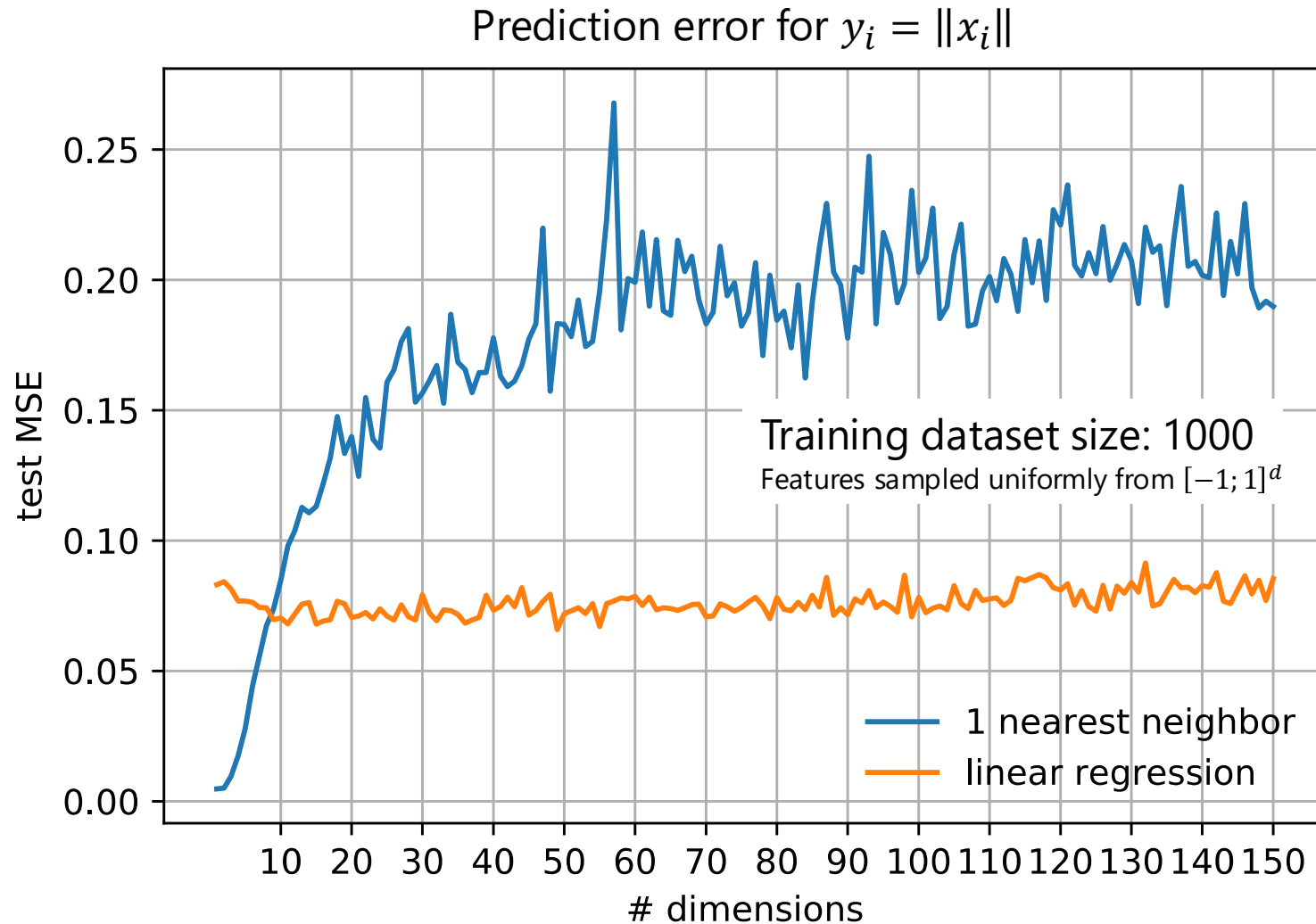


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Imposing assumptions about the data **restricts the space of possible solutions**

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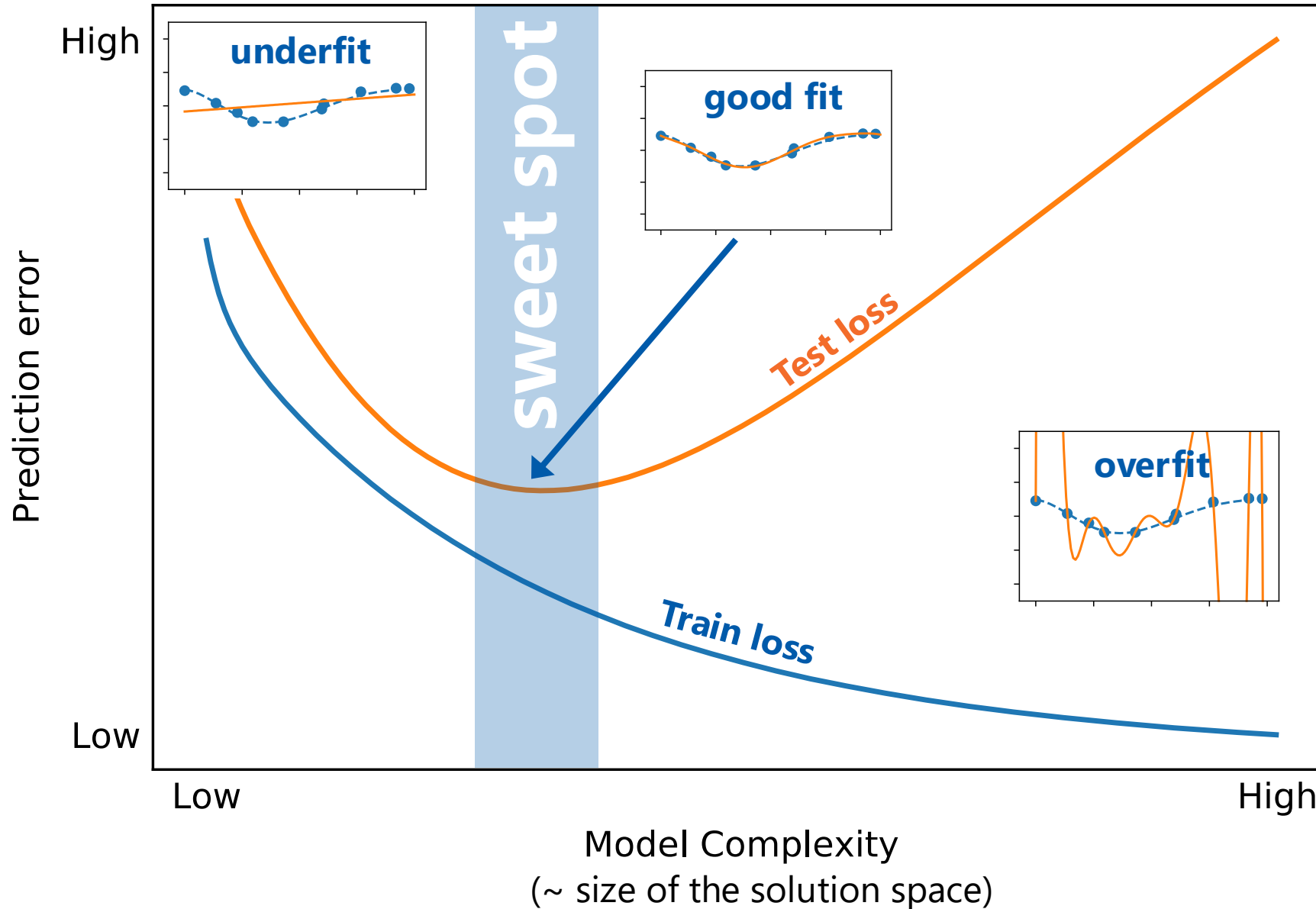
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Imposing assumptions about the data **restricts the space of possible solutions**

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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 - ▶ Use test data to detect underfitting and overfitting
-
- ▶ Food for thought: how can Linear Regression model be used to fit a n-th degree polynomial?

Thank you!



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