CSE 480/680

1/13/26

Lecture 13

K-NN regression

Real-valued $f(x)$ for classification

Test error/Training error

Bias and Variance (in K-NN)

Posted

L I-1 NN

L II Linear

Math Refresh

Fri @ OH

Prediction problems by the type of output ✓

K-NN

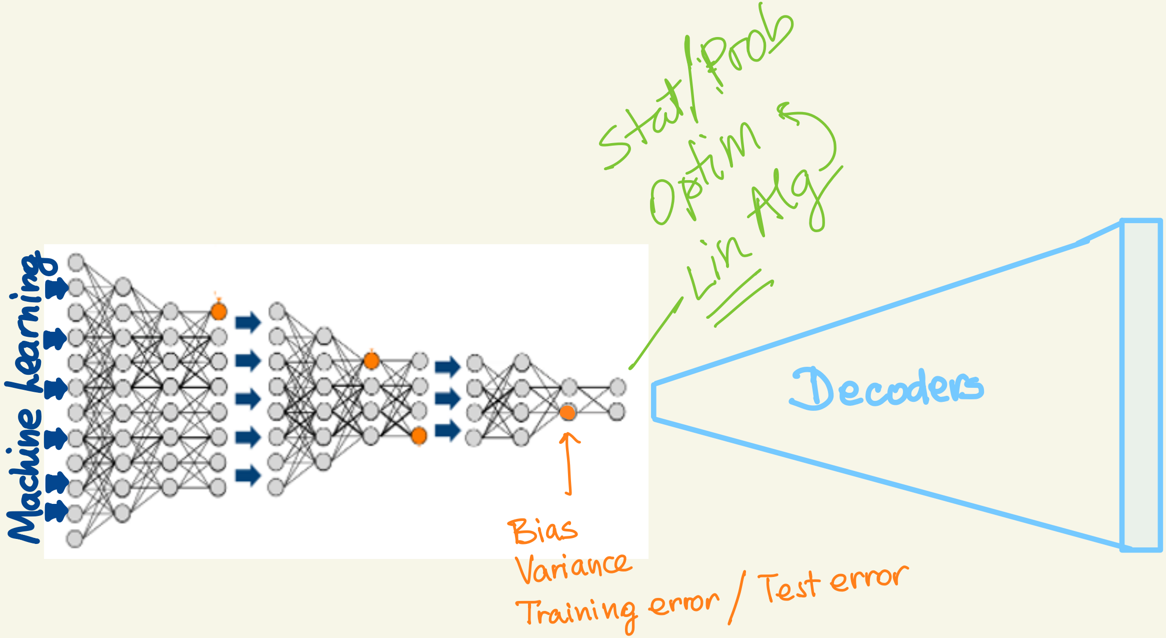
The Nearest-Neighbor and ~~kernel predictors~~

Bias-Var Tradeoff

Some concepts in Classification → $f(x) \in \mathbb{R}$

— " — " → Test/Train error

Reading HTF Ch.: 2.3.2 Nearest neighbor, 6.1–3. Kernel regression, 6.6.2 kernel classifiers,, Murphy Ch.: , Bach Ch.:


Machine learning
Stat/Prob
Optim
Lin Alg
Decoders
Bias
Variance
Training error / Test error

Predictors

- K-Nearest-Neighbor

Algorithms

Concepts

- Decision Region, Dec. Boundary

The Nearest-Neighbor predictor

- **1-Nearest Neighbor** The label of a point x is assigned as follows:
  1. find the example x^i that is nearest to x in $\mathcal{D}$ (in Euclidean distance)
  2. assign x the label y^i, i.e.

$$\hat{y}(x) = y^i$$

- **K-Nearest Neighbor** (with $K = 3, 5$ or larger)
  1. find the K nearest neighbors of x in $\mathcal{D}$: $x^{i_1, \ldots i_K}$
  2. - for classification $f(x) =$ the most frequent label among the K neighbors (well suited for multiclass)
     - for regression $f(x) = \frac{1}{K} \sum_{i \text{ neighbor of } x} y^i =$ mean of neighbors' labels

avg of the K neighbors

1. Find K exampels nearest to x

2. $\hat{y}(x) = \text{avg}\{y^{(1)}, \ldots y^{(k)}\}$ $x^{(1)}, \ldots x^{(k)} \in X^{1:n}$

kth neighbor

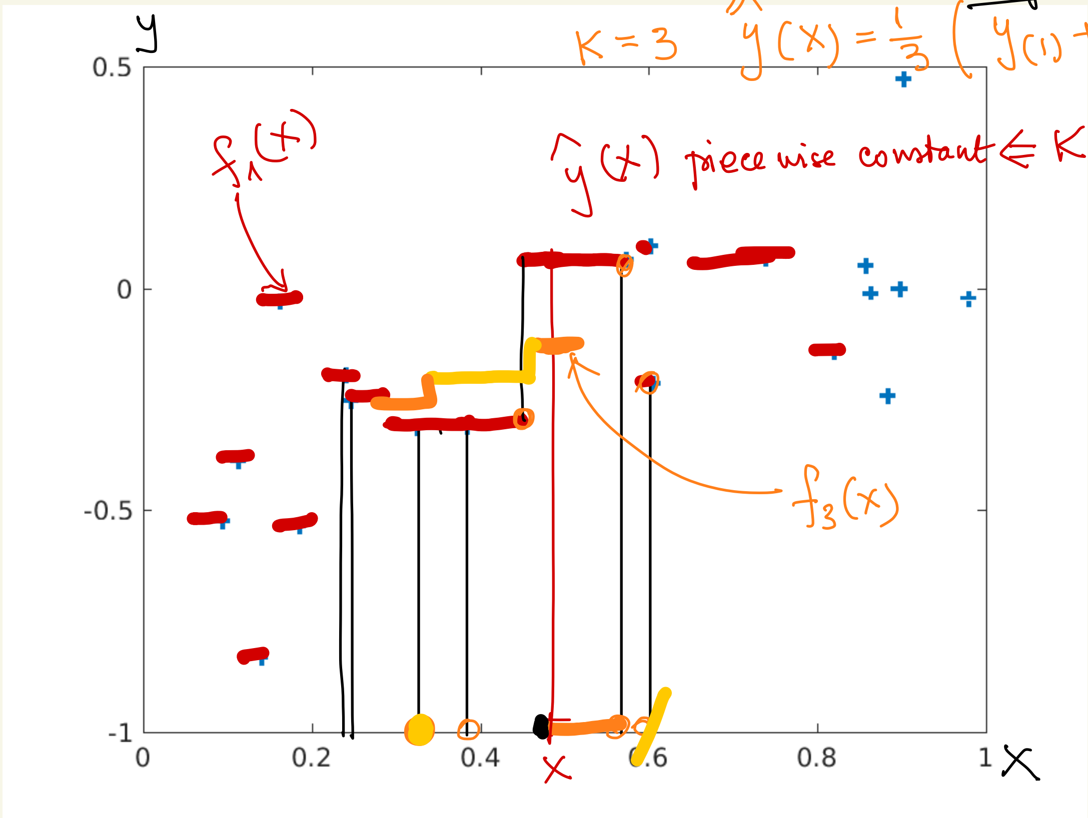
- No parameters to estimate!
- No training!
- But all data must be stored (also called memory-based learning)

$y^{(k)} = y^i$ iff $x^{(k)} = x^i$

Regression

$K=3 \qquad \hat{y}(x) = \frac{1}{3}\left(y_{(1)} + y_{(2)} + y_{(3)}\right)$

2nd neighbor of x



$f_K(x)$ = K-NN predictor

$\hat{y}(x) = ?$

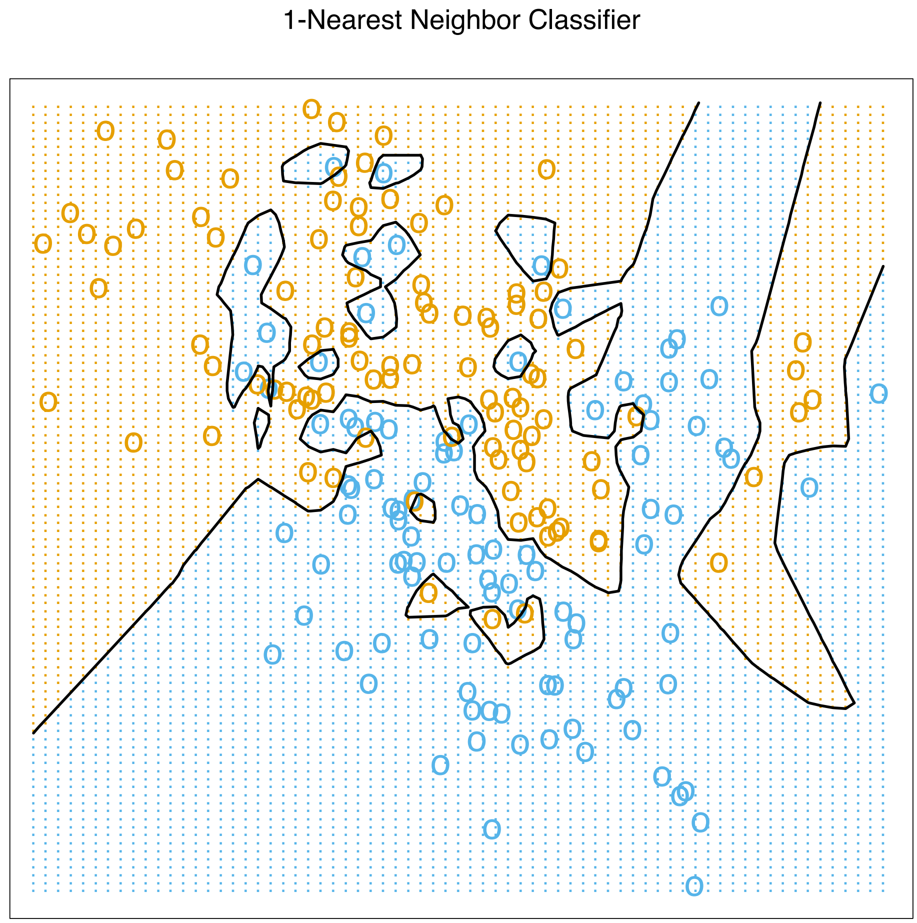
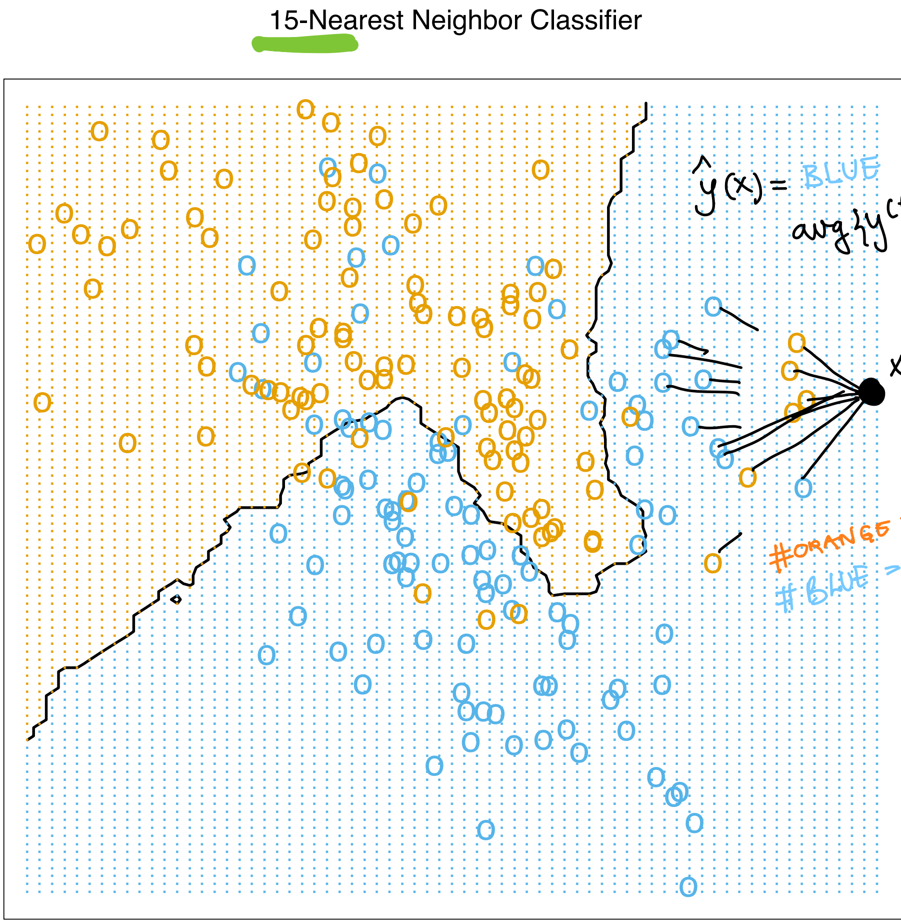


FIGURE 2.3. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$)*, and then predicted by* 1*-nearest-neighbor classification.*

K = 15

Real-valued classifier



$$\hat{y}(x) = \text{BLUE} = \text{sign}\Big(\underbrace{\operatorname*{avg}_{k=1:K}\{y^{(k)}\}}_{f(x)\in\mathbb{R}}\Big)$$

$$\text{avg}\{y^{(k)}\} = \frac{9-6}{15} = +0.2$$

$> 0 \Rightarrow$ BLUE

$< 0 \Rightarrow$ ORANGE

x

#ORANGE = 6 = −1

#BLUE = 9 = +1

FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable* (BLUE $= 0$, ORANGE $= 1$) *and then fit by* 15*-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the* 15*-nearest neighbors.*

Classifiers with real-valued output

Binary classification

- Since $y \in \{\pm 1\}$, naturally $f : \mathbf{X} \rightarrow \{\pm 1\}$
- But sometimes we prefer a classifier $f : \mathbf{X} \rightarrow \mathbb{R}$ (from a predictor class $\mathcal{F}$ of real-valued functions)
- In this case, the prediction $\hat{y}$ is usually

$$\boxed{\hat{y} \;=\; \operatorname{sgn}(f(x))} \tag{7}$$

This is sometimes known as the sign trick.

Examples of real-valued classifiers

- Logistic Regression
- Naive Bayes

in both of the above, $f(x) = P[Y = 1|X = x] \in [0, 1]$. Hence

$$\hat{y} \;=\; \operatorname{sgn}\left(f(x) - \frac{1}{2}\right) \tag{8}$$

- Support Vector Machines
- Kernel classifiers
- Neural Networks

Sign trick

> The *sign* function $\operatorname{sgn}(y) = y/|y|$ if $y \neq 0$ and 0 iff $y = 0$ turns a real valued variable Y into a discrete-valued one.

Why real valued f?

- for statistical models $f(x) = P[Y = 1 \mid X = x]$ Example: Logistic regression
- for non-statistical models, $|f(x)|$ measures **confidence** in prediction $\hat{y}$, with $|f(x)| \approx 0$ meaning low confidence. Example: SVM
- if f is differentiable[1], the gradient ∇f is used in **learning algorithms** Examples: Logistic Regression, neural networks, some forms of linear regression such as Lasso

f(x) correct $\Updownarrow$

The margin (assuming $y \in \{\pm 1\}$)

- The **margin** of a classifier f at point $x \in \mathbf{X}$ is defined as

$$z = yf(x). \quad (9)$$

> 0 $y > 0,\ f(x) > 0$

$y = -,\ f(x) < 0$

Wrong High confi?

- Note that $\mathrm{sgn}(z) = y\hat{y}$.

0 z

LOW CONFI High confi

- If $z > 0$, $\hat{y} = y$ and $f(x)$ is correct
- If $z \gg 0$, then $f(x)$ is correct, and classifier has high confidence
- If $z < 0$, then $f(x)$ is incorrect, and $|z|$ measures "how wrong" is f on this x
- Note also that $z \approx 0$ means that the classification $\hat{y}$ is not robust, whether correct or not

[1] and ∇f not 0 almost everywhere

Real valued multi-way classifiers

- We train m classifier $f_{1:m}:\mathbf{X}\rightarrow\mathbb{R}$. Then (typically)

$$\hat{y} \;=\; \operatorname*{argmax}_{c=1:m} f_{1:m}(x). \tag{10}$$

- $\hat{y}=y$ means the classifier is correct
- the training can be done
  - independently for each f_c, $c=1:m$ (e.g. generative classifiers – in Lecture II)
  - or at the same time (e.g. neural networks, SVM)

- The **margin** is defined as

$$z(x) \;=\; f_y - \max_{c\neq y} f_c(x) \tag{11}$$

In other words
- if $\hat{y}=y$ (correct), then $z=f_{\text{true}}-f_{\text{nextbest}} > 0$
- if $\hat{y}\neq y$ (mistake), then $z=f_{\text{true}}-f_{\hat{y}} < 0$ (since $f_{\hat{y}}(x)$ is the max of $f_c(x)$)

Lecture Notes I-2 – Examples of Predictors. Nearest Neighbor and Kernel Predictors. Bias and Variance

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Reading HTF Ch.: 2.1–5,2.9, 7.1–4 bias-variance tradeoff, Murphy Ch.: 1., 8.6[1], Bach Ch.:

[1] Neither textbook is close to these notes except in a few places; take them as alternative perspectives or related reading

Training and testing error

- Let $\mathcal{D} = \{(x^1, y^1), (x^2, y^2), \dots (x^n, y^n)\}$ be the training set and let the K-NN classifier from $\mathcal{D}$ be f_K
- How "good" is f_K?
- **Training error** $= \frac{1}{n}\#(\text{errors of } f_K \text{ on } \mathcal{D}) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{[f_K(x^i) \neq y^i]}$ $\in [0,1]$

$$\mathbf{1}_{[\text{expression}]} = \begin{cases} 1 & \text{expression TRUE} \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

indicator

Training and testing error

- Let $\mathcal{D} = \{(x^1, y^1), (x^2, y^2), \dots (x^n, y^n)\}$ be the training set and let the K-NN classifier from $\mathcal{D}$ be f_K
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- **Test error** $Pr[\underbrace{f_K(x) \neq y}_{\text{error}}]$ ← User cares about this

Training and testing error

f

- Let $\mathcal{D} = \{(x^1, y^1), (x^2, y^2), \ldots (x^n, y^n)\}$ be the training set and let the K-NN classifier from $\mathcal{D}$ be f_K
- How "good" is f_K?
- **Training error** $= \frac{1}{n}\#(\text{errors of } f_K \text{ on } \mathcal{D}) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{[f_K(x^i) \neq y^i]}$
- **Test error** $Pr[f_K(x) \neq y]$ for new points $(x, y) \sim P_{XY}$ Want
- We approximate the test error by using a **test set** $\mathcal{D}^{\text{test}} = \{(\tilde{x}^1, \tilde{y}^1), (\tilde{x}^2, \tilde{y}^2), \ldots (\tilde{x}^{n'}, \tilde{y}^{n'})\}$ from the same P_{XY}.
- Thus, in practice, **Test error**$= \frac{1}{n'}\#(\text{errors of } f_K \text{ on } \mathcal{D}^{\text{test}}) = \frac{1}{n'}\sum_{i=1}^{n'} \mathbf{1}_{[f_K(\tilde{x}^i) \neq \tilde{y}^i]}$

ALGO

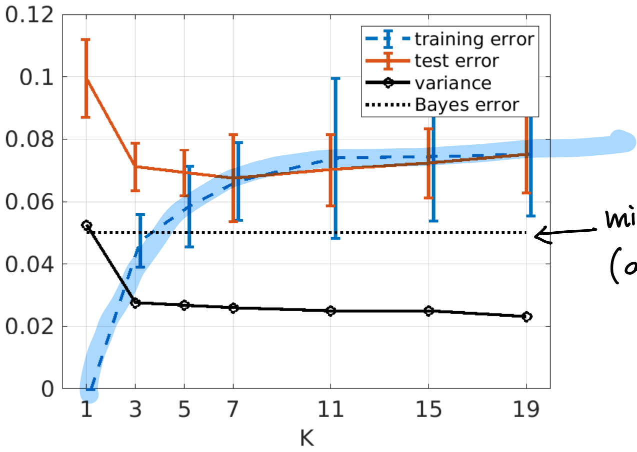
$\underset{\text{test}}{n'} \neq \underset{\text{train}}{n}$

THEORY

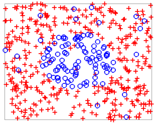
Training and testing error for K-NN

$n = 200$

$n' = 500$



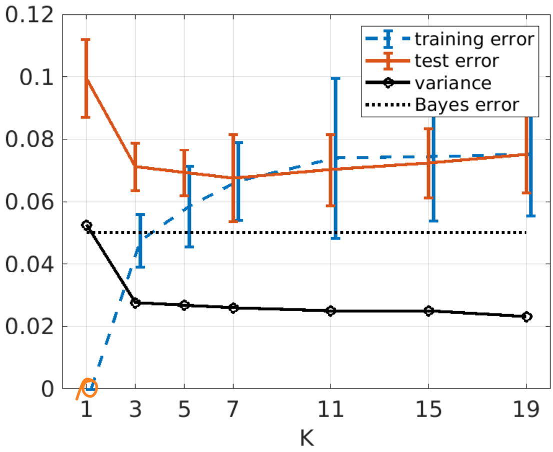
min possible error 5%
(also called Bayes error)

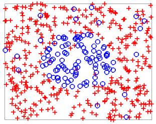


Ignore the "variance" and "Bayes error" for now

Training and testing error for K-NN

$K^* = 7$

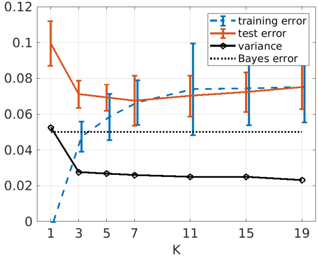


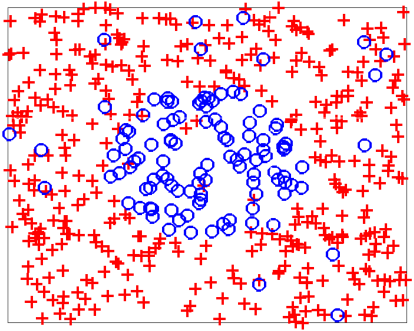


Ignore the "variance" and "Bayes error" for now

- So, what's happening? For $K = 1$, training error=0 but test error is large
- As K increases, test error decreases at first, then increases again

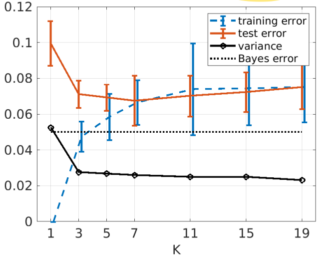
The case $K = 1$: Variance

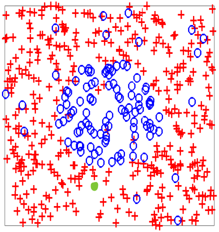




- $\mathcal{D} \sim P_{XY} \Rightarrow \mathcal{D}$ is **random**

The case $K = 1$: Variance





K-NN classifier

→ for any x $f_K(x)$ is a r.v

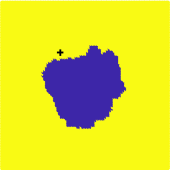
← $f_1(x)$ for 2 different $\mathcal{D}$'s from the same distribution

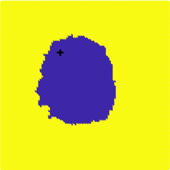
($K = 1$)

- $\mathcal{D} \sim P_{XY} \Rightarrow \mathcal{D}$ is **random**
- Hence any function f_K we estimate from $\mathcal{D}$ is also random
- Formally, for any fixed x, $f_K(x)$ is a random variable, hence it has a variance.
- In this course, we do not explicitly calculate the variance, but we want to know what increases or decreases it.

The case of K large: Bias

($K = 11$)

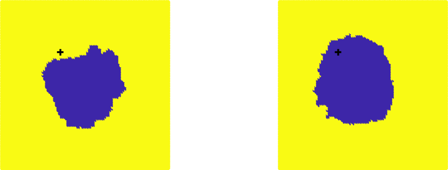




$f_{11}(x)$ for two different $\mathcal{D}$'s from same P_{XY}

The case of K large: Bias

($K = 11$)



- **Bias** means to let one's own prior beliefs override the evidence.
- 1) In data science/ML/statistics **every model/prediction** is a combination of **prior belief** and data ⇒ Bias necessary
- **prior** = before seeing the data
- 2) (usually) **prior belief** = prior **knowledge**, e.g. from previous experiments ⇒ Bias useful, complements data
- Bias can take many forms – in this course you will encounter several
- We do not explicitly calculate bias, but we want to identify where it is coming from, and what increases/decreases it
- One way to look for bias: if a predictor f cannot exactly/accurately predict a training set, "whatever is causing this" is bias.

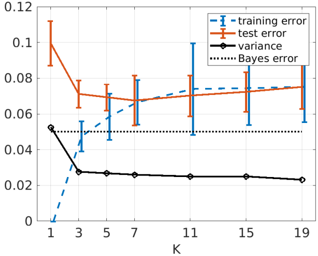
The Bias-Variance trade-off

data ⇒ randomness

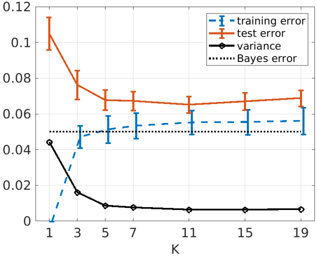
- When bias ↗, variance ↘

believe ↘ data

- When data set size n ↗, variance ↘



n=200



n = 2000