# Basic concepts

Lecture 1a

Course leader: Oleg Sysoev

# Course topics

## Block 1

- Basic concepts in machine learning. Software for ML.
- Regression, regularization and model selection
- Classification methods
- Dimensionality reduction and uncertainty estimation
- Support vector machines and kernel methods
- Neural networks and deep learning

## Block 2

- Splines and additive models. High-dimensional problems
- Mixture models and online learning. Ensemble methods

# Course organization

- 1 topic= 4-5 lectures +1 lab (2h* 3)+seminar

- Course given as
  - 732A99 (9 ECTS): Block 1+Block2
  - 732A68 (9 ECTS): Block 1+Block2
  - TDDE01 (6 ECTS): Block 1

- **Labs**
  - SU rooms used
  - Take around 8h
  - Individual and group reports
  - Sharing only ideas in the group, not text or codes
  - Bring your own laptop if you have – limited amount of computers in the rooms
  - Deadlines
  - Individual Special tasks (optional)– if you solve all of them and get at least 14 points at the exam, you get 2 points more.
  - Submission via LISAM

# Course organization

- Lectures
  - Available as PowerPoint or PDF, normally at LISAM

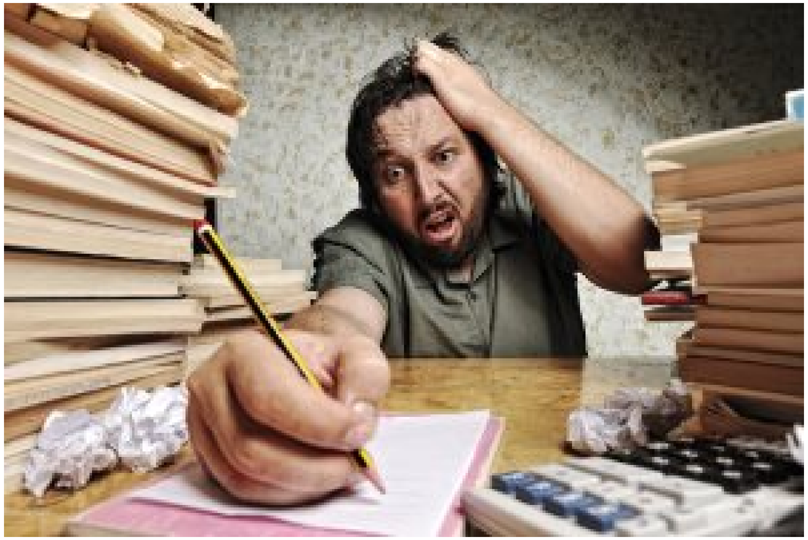
- Seminars
  - Speaker and opponent groups
  - Is a laboratory part, obligatory attendance for speakers and opponents
  - Discussion of the latest lab.
    - Note: lab assignments are slighlty different for TDDDE01/732A99 but all kinds of assignments may appear at the exam!
  - Define your group (3 persons) today or tomorrow
    - TDDE01: https://docs.google.com/spreadsheets/d/1jnIbeYR-U7b8fILpWLtmNNkYGYll2LiBtI5aw6MWusE/edit?usp=sharing
    - 732A99/732A68: https://docs.google.com/spreadsheets/d/1nTxRMhUiZGspMY9BGos4XWwO2CMhcFoyB4QrJciHDLg/edit?usp=sharing
    - Doctoral students: not needed, individual submission only
    - **Difficult to find a group? Put your name in some cell…**

# Course organization

- Examination
  - TDDE01, 732A99: laboratory part + computer-based exam

- Doctoral students:
  - Follow 723A99, get 6hp
  - Course **does take** its time (40-60% of full time)!
  - Examination: individual lab submission
  - Seminars not obligatory, but highly recommended

- Lecture 1c is ’Introduction to R’



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# What is Machine Learning ?

- *Machine learning is a subfield of* ***computer science*** *that evolved from the study of* ***pattern recognition*** *and computational learning theory in* ***artificial intelligence****.*

- *Machine learning explores the study and construction of* ***algorithms*** *that can* ***learn*** *from and make* ***predictions*** *on* ***data****. Such algorithms operate by building a model from example inputs in order to make data-driven predictions or* ***decisions****, rather than following strictly static program instructions.*

Wikipedia (Oct 15, 2016).

# Machine Learning and Statistics

- ML=**intersection** of **computer science**, **statistics** and **artificial intelligence**.
  - Related: **data mining**, **knowledge discovery** and **data science**.

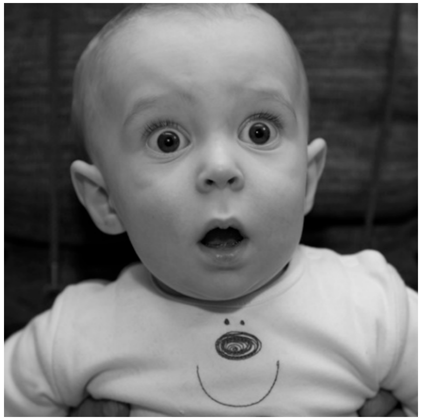
- ML uses mainly **statistical (probabilistic) models for analyzing data** .
  - Data mining and knowledge discovery tend to use less rigorous, but often effective, algorithms.
  - ML is not a discovery of a hidden information (Data Mining)

- ML vs Statistics: ML has a **heavier focus on prediction** , and lesser on interpretation.

- ML applications often involve large sets →**computational complexity** of algorithms is important.
  - Statistics often does not care about runtime

# Why probability models?

- Probability models and statistical inference provide a **framework**
- A principled **way to think** about any problem in machine learning
  - Probabilistic model →Estimation →Prediction
- Probabilistic models **quantify uncertainties**.
  - Deterministic answers may often be inappropriate



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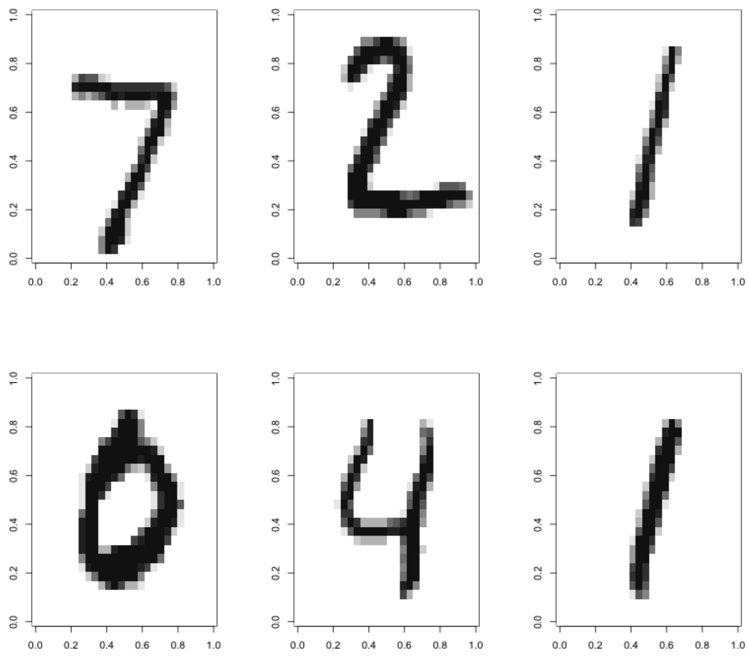
*The currency exchange rate tomorrow will be 10.41!*

# Why probability models?

*As robotics is now moving into the open world, the issue of* ***uncertainty*** *has become a major stumbling block for the design of capable robot systems. Managing uncertainty is possibly the most important step towards robust real-world robot systems.*

*from the book Probabilistic Robotics by Thrun et al.*

# Example: classifying hadwritten digits



# Example: classifying hadwritten digits

**Training** data: 60000 images.

**Test** data: 10000 images.

**Features**: intensities (0-255, scaled to 0-1) in the $28 \times 28 = 784$ pixels as features.

**Methods:**

- Multinomial regression with LASSO prior
- Support vector machines
- Neural Networks (deep?)

# Example: classifying hadwritten digits

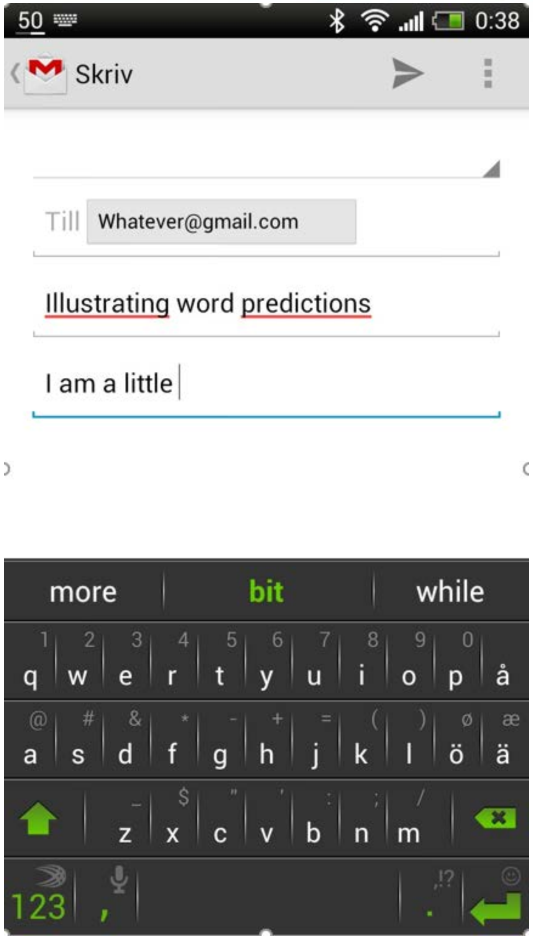
- Confusion matrix

PREDICTION

TRUTH

| | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 966 | 0 | 8 | 1 | 1 | 7 | 9 | 2 | 4 | 6 |
| 1 | 0 | 1121 | 1 | 1 | 0 | 2 | 3 | 13 | 7 | 7 |
| 2 | 2 | 2 | 957 | 13 | 5 | 4 | 4 | 21 | 7 | 0 |
| 3 | 0 | 2 | 9 | 947 | 0 | 29 | 1 | 3 | 12 | 10 |
| 4 | 0 | 0 | 12 | 1 | 940 | 5 | 5 | 9 | 8 | 32 |
| 5 | 6 | 1 | 3 | 19 | 1 | 816 | 9 | 1 | 24 | 9 |
| 6 | 4 | 4 | 13 | 1 | 7 | 12 | 926 | 0 | 10 | 1 |
| 7 | 1 | 0 | 9 | 10 | 2 | 2 | 0 | 954 | 5 | 13 |
| 8 | 1 | 4 | 17 | 11 | 2 | 10 | 1 | 3 | 892 | 4 |
| 9 | 0 | 1 | 3 | 6 | 24 | 5 | 0 | 22 | 5 | 927 |

# Example: smartfone typing predictions



# Example: smartfone typing predictions

- Assume a simple (Markov) model of a sentence:

$$p(w_1, \dots, w_n) = p(w_1)p(w_2|w_1)\dots p(w_n|w_{n-1})$$

- Intuition:
  - $p(person|crazy) = 0.1$
  - $p(horse|crazy) = 0.0001$

Highest P(?|Donald) ?

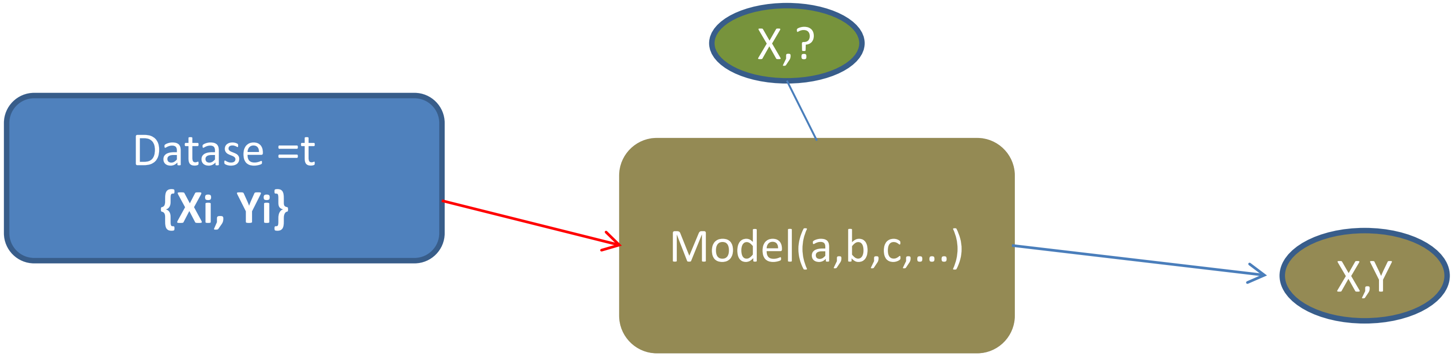
- Probability for sentence depends only on $p(w_n|w_{n-1})$
- How to compute ? Investigate a lot of data!

$$p(w_k|w_{k-1}) = \frac{\#\ cases\ w_k\ follows\ w_{k-1}}{\#\ cases\ w_k}$$

- In practice, more advanced model used
  - Neural networks for ex.

# Types of learning

- **Supervised learning** (classification, regression)
  - Compute parameters from data
  - Given features of a new object, predict target
  - **Classification** (Y=categorical), **Regression** (Y=continuous)
- Most of ML models: Neural Nets, Decision Trees, Support Vector Machines, Bayesian nets



# Types of learning

- Unsupervised learning (→Data Mining)
  - No target
  - Aim is to extract interesting information about
    - Relations of parameters to each other
    - Grouping of objects

Ex: clustering, density estimation, association analysis

X1<-> X2<-> X3…

# Types of learning

- **Semi-supervised**: targets are known only for some observations.

- **Active learning**. Strategies for deciding which observations to label

- **Reinforcement learning**. Find suitable actions to maximize the reward. True targets are discovered by trial and error.

# Basic ML ingridients

- **Data** $D$: observations (cases)
  - Features $X_1, .. X_p$
  - Targets $Y_1, \dots, Y_r$

| Case | $X_1$ | $X_2$ | $Y$ |
|---|---|---|---|
| 1 | | | |
| 2 | | | |
| … | | | |

- **Model** $P(x|\, w_1, \dots w_k)$ or $P(y|x, w_1, \dots w_k)$
  - Example: Linear regression $p(y|x, w) = N(w_0 + w_1 x, \sigma^2)$

- **Learning procedure** (data→get parameters $\hat{w}$ or $p(w|D)$ )
  - Maximum likelihood, MAP, Bayes rule…

- **Prediction** of new data $X^{new}$ by using the fitted model

# Types of data sets

- **Training data** (training set D): used for fitting the model
  - Supervised learning: $w_i$ in $P(y|\boldsymbol{x}, w_1, \dots w_k)$ estimated using D

| X | Y |
|---|---|
| 1.1 | M |
| 2.3 | F |

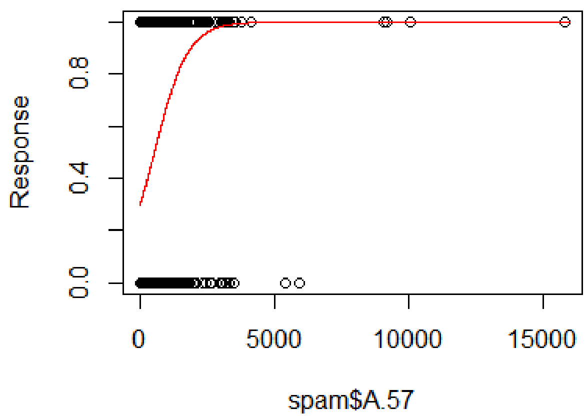
- **Test data** (test set T): used for predictions
  - Supervised learning: estimate $p(Y)$ or $\hat{Y}$ for new $\boldsymbol{x}$

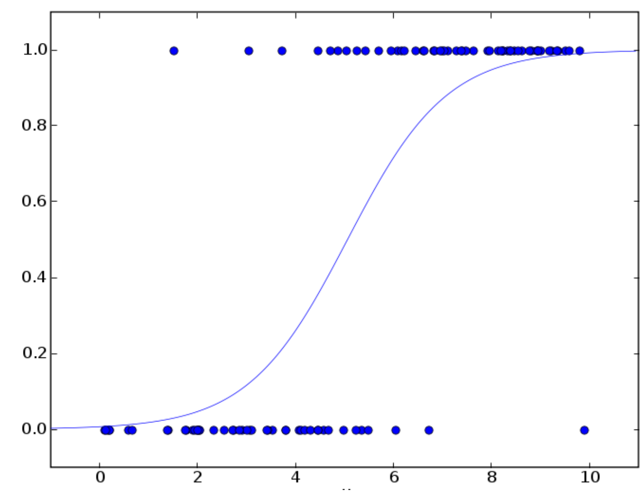
| X | Y |
|---|---|
| 1.3 | ? |
| 2.9 | ? |

# Logistic regression

- Data $Y_i \in \{Spam, Not\ Spam\}, X_i = \#of\ a\ word$
- Model: $p(Y = Spam|w, x) = \frac{1}{1+e^{-w_0-w_1 X}}$
- Fitting: maximum likelihood
- Prediction : $p(spam) = p(Y = spam|x)$

We can also make point predictions
-how?



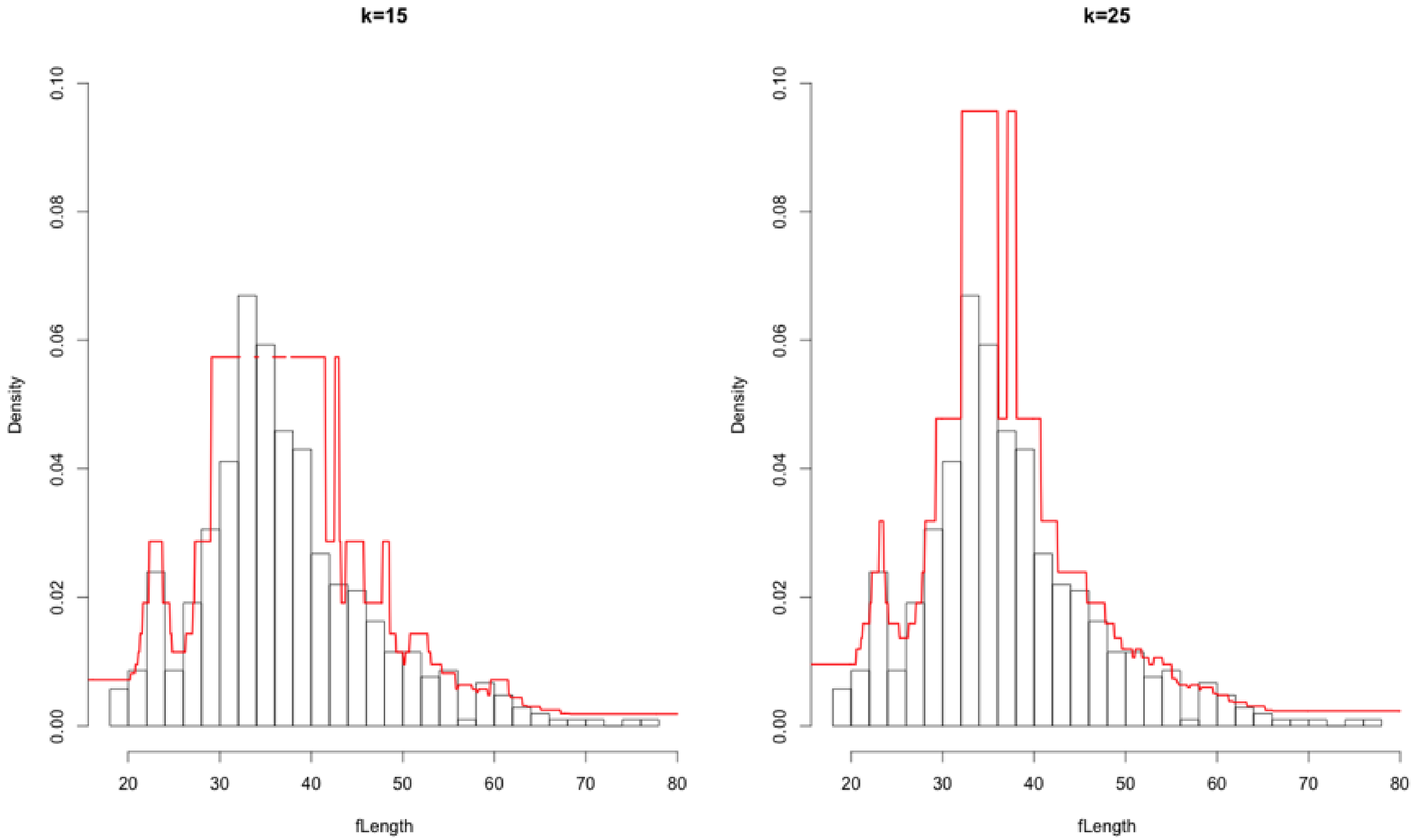



# K-nearest neighbor density estimation

- Data: Fish length $X_1, \dots X_N$
- Model $p(x|K) = \frac{K}{N \cdot \Delta}$
  - $K$: #neighbors in training data
  - $\Delta$: length of the interval containing $K$ neighbors

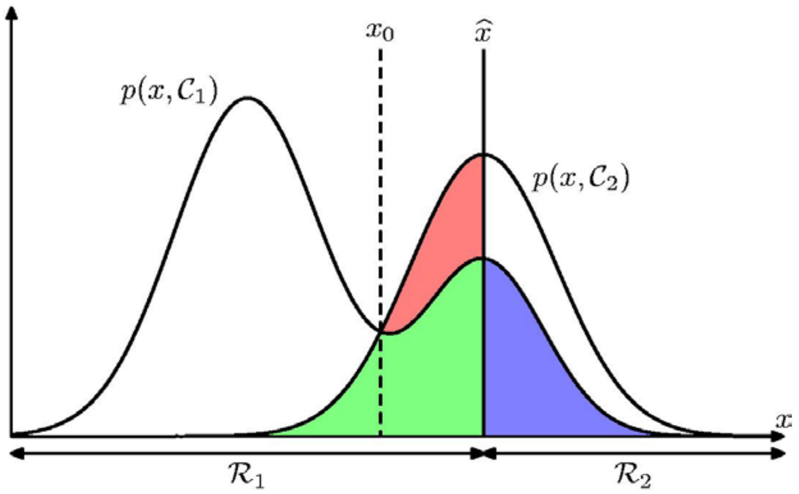
- Learning: Fix some $K$ or find an appropriate $K$
- Prediction: predict $p(x|K)$

# K-nearest neighbor density estimation



# K-nearest neighbor density estimation

- Why estimating a density can be interesting:
  1. Estimate **class-conditional densities** $p(x|y = C_i)$
  2. Predict



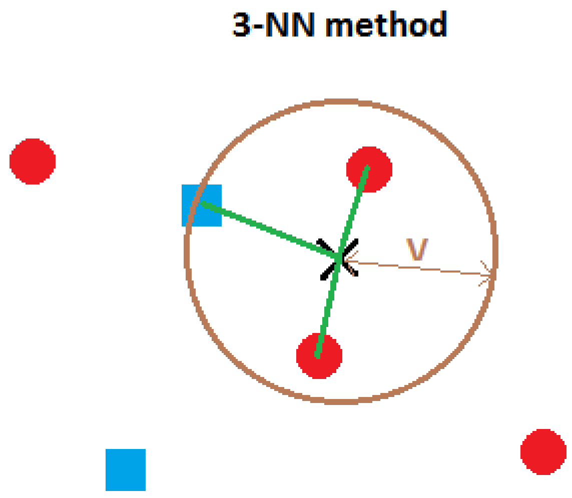
# K-nearest neighbor classification

- Given $N$ observations $(\boldsymbol{X}_j, Y_j)$
  - $Y_j = C_i$, where $C_1, \dots C_m$ are possible class values

- Model assumptions
  - Apply K-NN density estimation:

$$p(X = x | Y = C_i) = \frac{K_i}{N_i V}, p(C_i) = \frac{N_i}{N}$$

  - $V$: volume of the sphere
  - $K_i$: #obs from training data of $Y = C_i$ in the sphere
  - $N_i$: #obs from training data of $Y = C_i$



# Bayesian classification

- Prediction $\hat{Y}(\boldsymbol{x}) = C_l$

$$l = \arg \max_{i \in \{1,\ldots,m\}} p(C_i|\boldsymbol{x})$$

- Bayes theorem

$$p(C_i|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|C_i)p(C_i)}{p(\boldsymbol{x})}$$

- We get

$$p(C_i|x) \propto \frac{K_i}{K}$$

# K-nearest neighbor classification

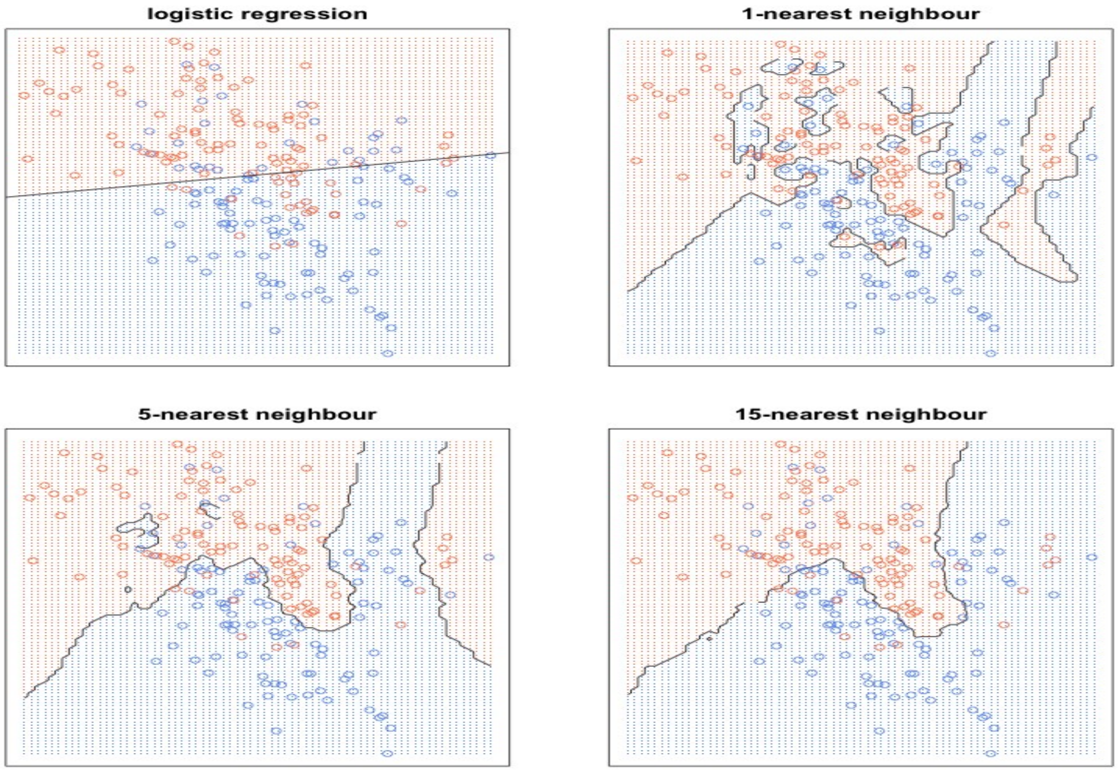
## Algorithm

1. Given training set $D$,number $K$, and test set $T$
2. For each $x \in T$
   1. For each $i = 1, \dots M$
      1. $p'(C_i|x) = \frac{K_i}{K}$
   2. Compute $l = \arg \max_{i \in \{1,\dots,m\}} p'(C_i|\boldsymbol{x})$
   3. Predict $\hat{Y}(x) = C_l$

**Majority voting**: prediction for $x$ is defined by majority voting of $K$ neighbors

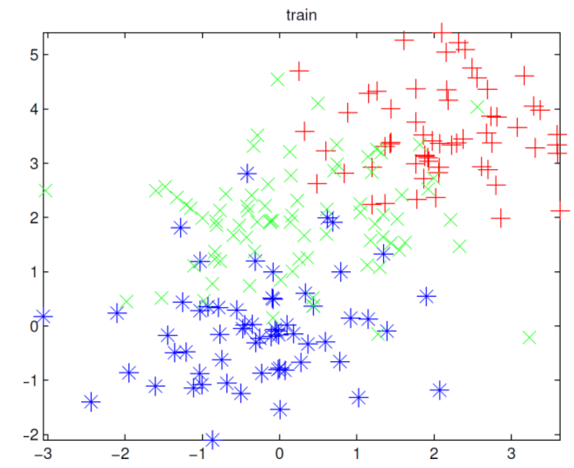
# K-nearest neigbor example

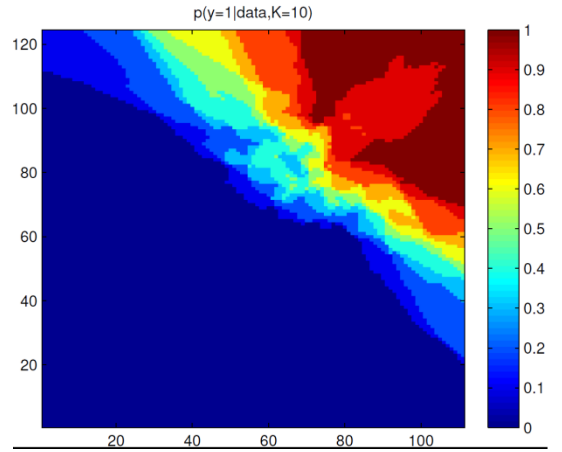
Why classification results are so different for K-NN?



# Model types

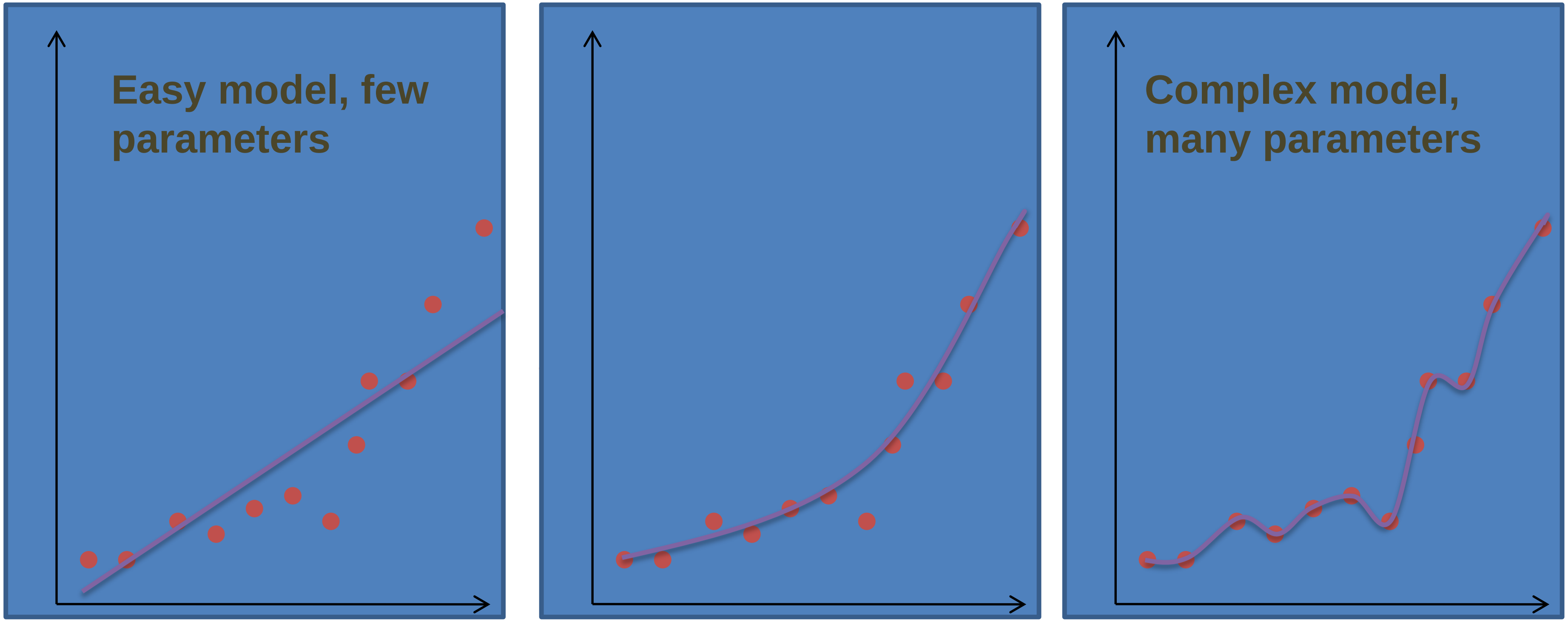
- Parametric models
  - Have certain number of parameters independently of the size of training data
  - Assumption about of the data distribution
  - Ex: logistic regression
- Nonparametric models
  - Number of parameters (complexity) grows with training data
    - Example: K-NN classifier



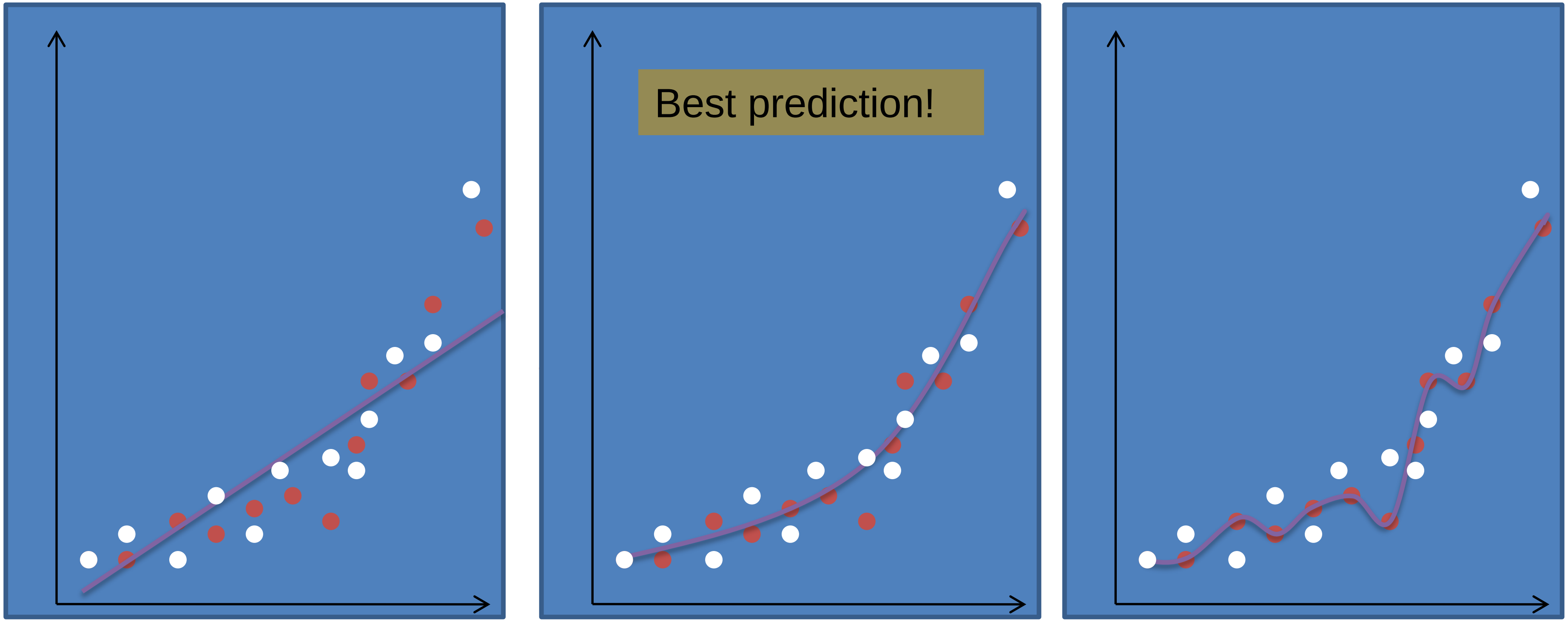
# Overfitting

- Which model feels appropriate?



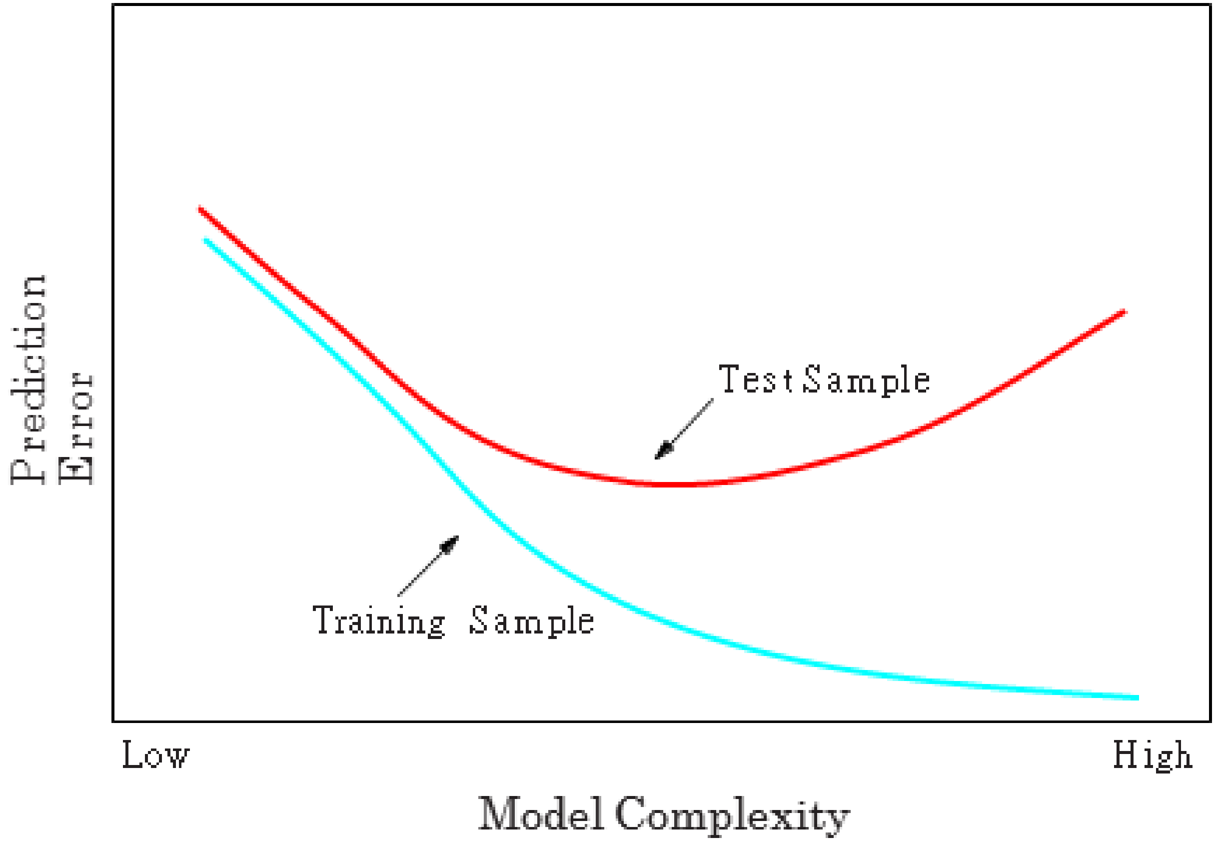
# Overfitting

Now new data from the same process



# Overfitting

- Observed:



# Model selection

- Given several models $M_1, \ldots M_m$
- Divide data set into **training** and **test** data

| Training | Test |
| --- | --- |

- Fit models $M_i$ to training data→get parameter values
- Use fitted models to predict test data and compare **test errors** $R(M_1), \ldots R(M_m)$
- Model with lowest prediction error is best

Comment:

- Approach works well for moderate/large data

# Typical error functions

- Regression, **MSE** :

$$R(Y,\hat{Y}) = \frac{1}{N}\sum_{i=1}^{N}(Y_i - \hat{Y}_i)^2$$

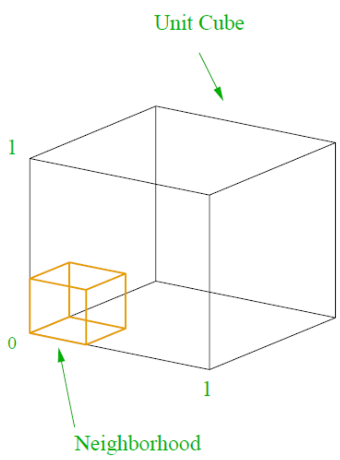
- Classification, **misclassification rate**

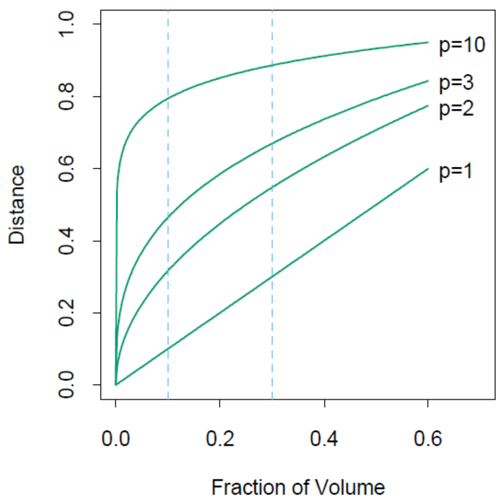
$$R(Y,\hat{Y}) = \frac{1}{N}\sum_{i=1}^{N} I(Y_i \neq \hat{Y}_i)$$

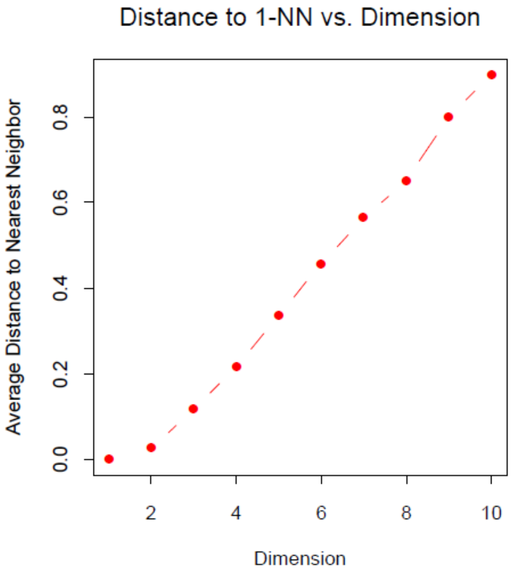
# Curse of dimensionality

- Given data $D$:
  - Features $X_1, .. X_p$
  - Targets $Y_1, \dots, Y_r$
- When $p$ increases models using ”proximity” measures work badly
- Curse of dimensionality: A point has no ”near neighbors” in high dimensions → using class labels of a neighbor can be misleadning
  - Distance-based methods affected

# Curse of dimensionality



# Curse of dimensionality

- Hopeless? No!

- Real data normally has much lower effective dimension
  - Dimensionality reduction techniques

- Smoothness assumption
  - small change in one of Xs should lead to small change in Y→interpolation