Basic concepts

Lecture 1a

Course leader: Oleg Sysoev

Course topics

Block 1

- Basic concepts in machine learning. Software for ML. Classification and regression
- Dimensionality reduction and model selection
- Kernel methods (SVM) and neural networks

Block 2

- Mixture models and ensemble methods

Course organization

- 1 topic= 3-4 lectures (campus) +1 lab (2h* 3, campus)+seminar (zoom)

- Course given as
  - 732A99 (9 ECTS): Block 1+Block 2
  - 732A68 (9 ECTS): Block 1+Block 2
  - TDDE01 (6 ECTS): Block 1

- **Labs**
  - Sign-up at LISAM, **exactly 3 persons**! (otherwise group may be split)
  - Takes around 8h , group report
  - Published a day in advance – try doing before attending the first lab session!
  - **Statement of Contribution:** describe clearly how each member contributed to the group report (what exactly was done by each person). Without it lab is automatically failed.
  - Offline short question answering on LISAM
  - Deadlines
  - To pass exam, **each student needs to have experience of solving all lab tasks** → make sure to try all tasks before the exam!
  - Submission via LISAM

Course organization

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

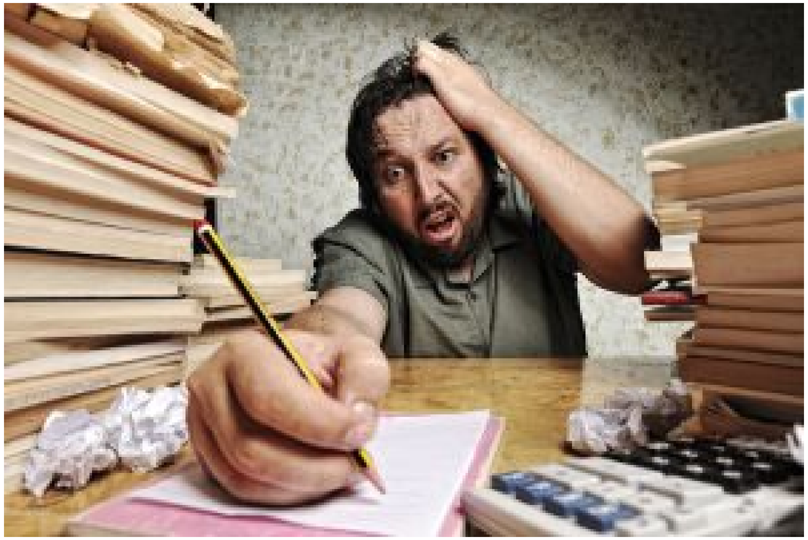
- Tutorials
  - Topic 1 and 2 block 1 have tutorials = basic exercises with answers. Go through **before** the respective lab!

- Seminars
  - Obligatory attendance of all seminars
  - Zoom
  - Speaker and opponent groups
  - Discussion of the latest lab
  - Presentation schedule will be published on LISAM (Seminars.PDF)

Course organization

- Examination
  - laboratory part + computer-based exam

- Lecture 1b is ’Basic Statistics’



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- Lecture 1c is ’Introduction to R’

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**.

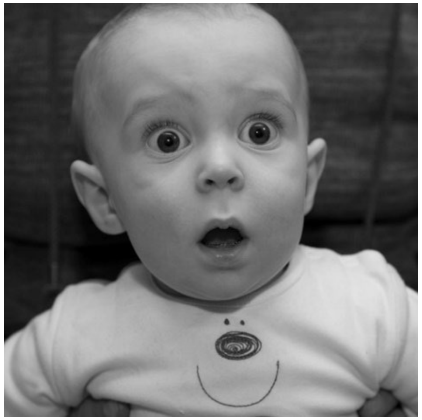
- ML often uses **statistical (probabilistic) models for analyzing data** .
  - Data mining and knowledge discovery tend to use less rigorous, but often effective, algorithms.
  - ML is not a discovery of a hidden information (Data Mining)

- 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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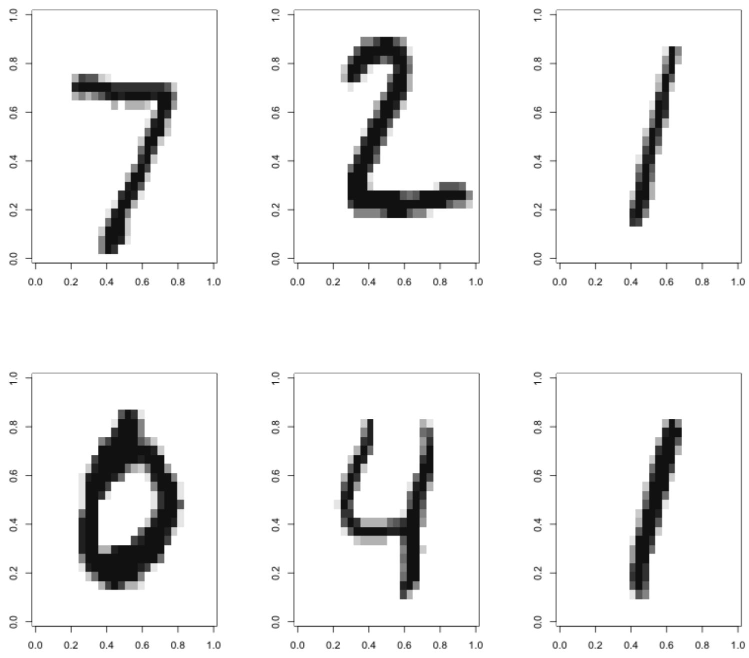
The currency exchange rate tomorrow will be 10.41!

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 classification with LASSO regularization
- Support vector machines
- Neural Networks (deep?)

Example: classifying hadwritten digits

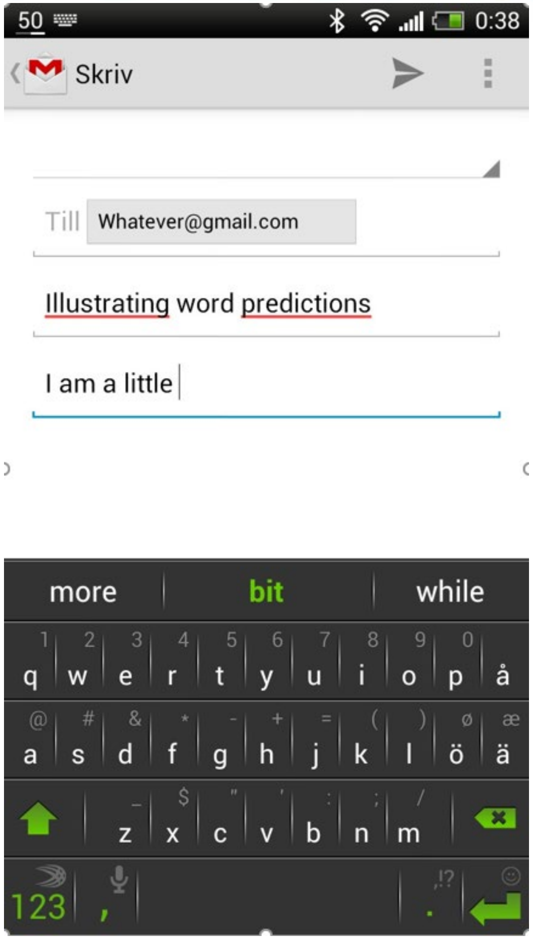
- Confusion matrix

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

- Markov Model of the sentence and Bayes theorem:

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

- Intuition:
  - $p(person|intelligent) = 0.1$
  - $p(tree|intelligent) = 0.0001$

Highest P(?|Donald) ?

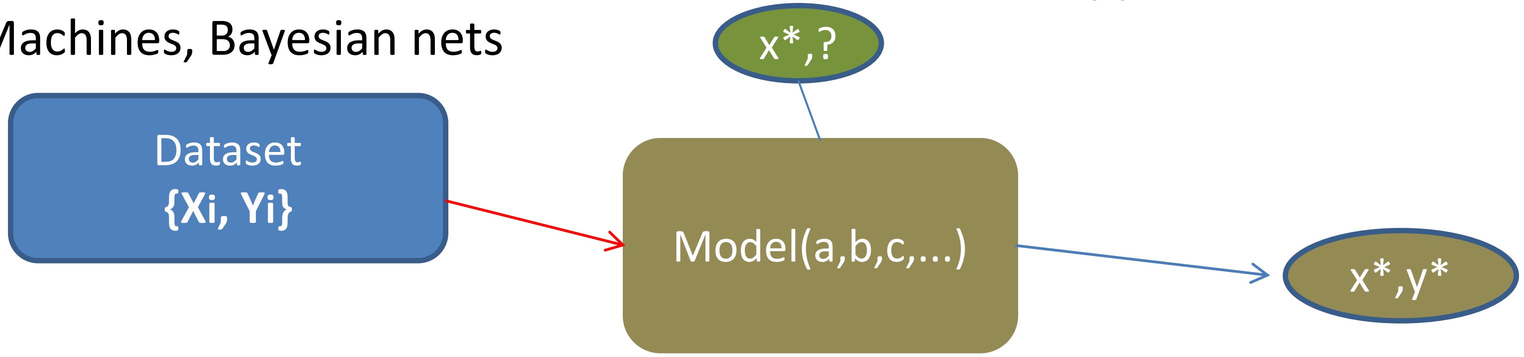
- Probability for sentence depends only on $p(w_n|w_{n-1})$
- How to compute ? Investigate a lot of data!

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

- 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 (generalize beyond seen training data)
  - **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. (ex. ChatGPT)

- **Transfer learning:** use knowledge from some domain to train better models in a similar domain

Basic ML ingridients

- **Data** T: observations (cases)
  - Features $x_1, .. x_p$
  - Targets $y_1, \ldots, y_r$

Case	x_1	x_2	y
1			
2			
…			

- **Mathematical Model** $P(x|\, w_1, \ldots w_k)$ or $P(y|x, w_1, \ldots w_k)$
  - Example: Linear regression $\mathrm{p}(y|x, w_o, w_1, \sigma^2) = N(w_0 + w_1 x, \sigma^2)$
- **Learning algorithm** (data→get parameters $\hat{w}$ or $p(w|D)$)
  - Maximum likelihood, Bayesian estimation…
- **Prediction** of new data x_* by using the fitted model

Types of data sets

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

X	Y
1.1	M
2.3	F

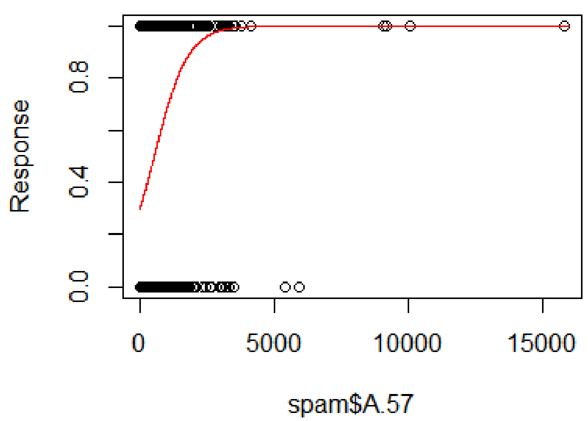
- **Test data** (test set T*): used for predictions
  - Supervised learning: estimate $p(y_*)$ or $\widehat{y_*}$ for new $\boldsymbol{x}_*$

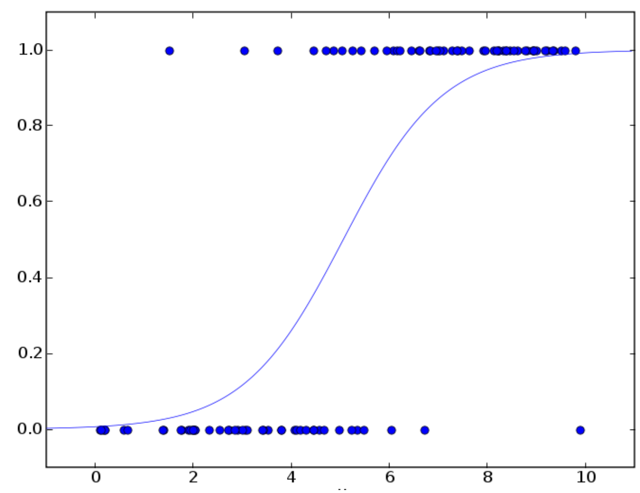
X	Y
1.3	?
2.9	?

Logistic regression

- **Data** $y_i \in \{Spam, Not\ Spam\}, x_i = \#of\ a\ word$
- **Model**: $p(y = Spam|w, x) = \frac{1}{1+e^{-w_0-w_1x}}$
- **Learning algorithm**: maximum likelihood
- **Prediction** : $p(spam) = p(Y = spam|x_*)$

We can also make point predictions
-how?





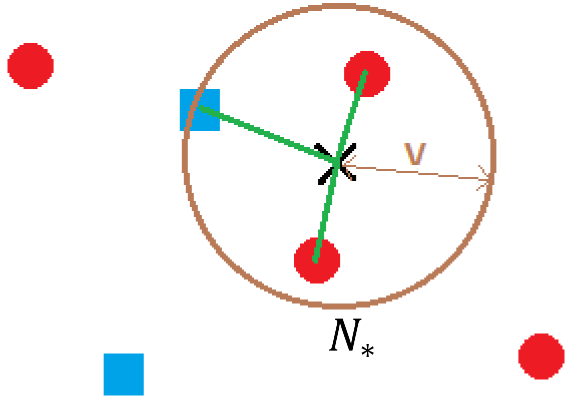
K-nearest neighbor model

- Can be classification or regression

- Basic idea:
  - For given x_*, find K nearest observations
  - Classification: majority voting
  - Regression: compute mean

- K is called **hyperparameter**

3-NN method



K-nearest neighbor algorithm

Data: Training data $\{\mathbf{x}_i, y_i\}_{i=1}^n$ and test input $\mathbf{x}_\star$
Result: Predicted test output $\widehat{y}(\mathbf{x}_\star)$

1 Compute the distances $\|\mathbf{x}_i - \mathbf{x}_\star\|_2$ for all training data points $i = 1, \ldots, n$
2 Let $\mathcal{N}_\star = \{i : \mathbf{x}_i$ is one of the k data points closest to $\mathbf{x}_\star\}$
3 Compute the prediction $\widehat{y}(\mathbf{x}_\star)$ as

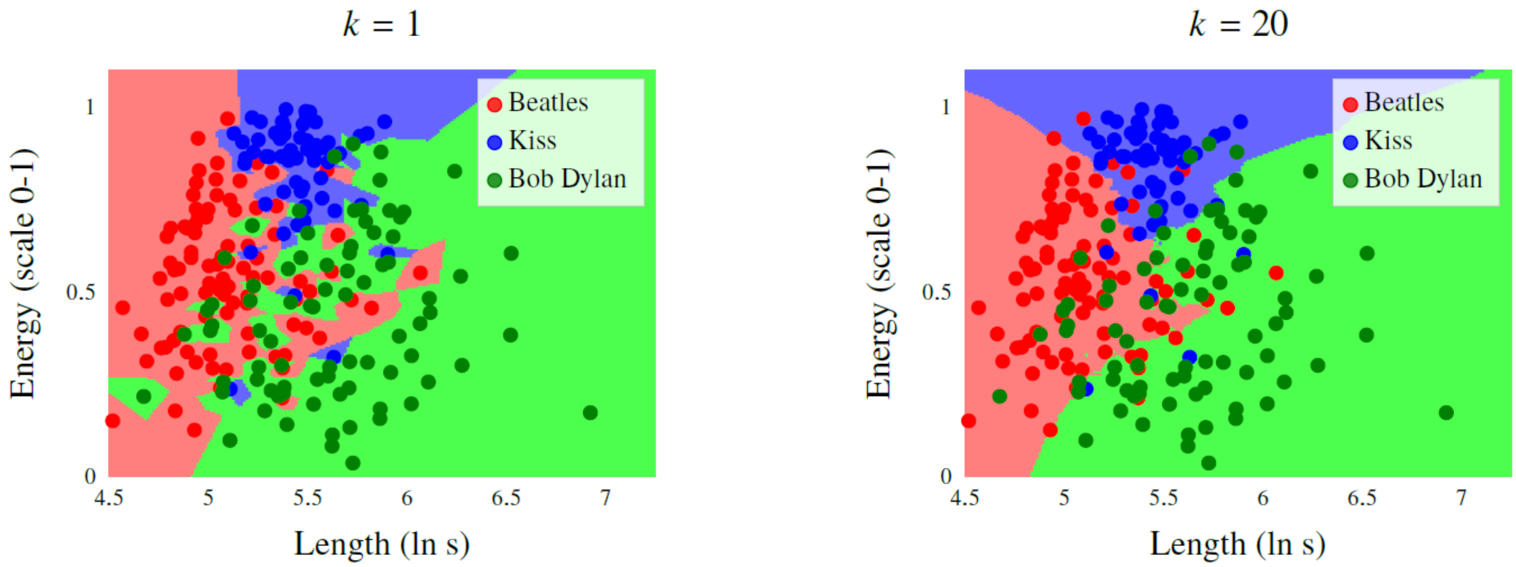
$$\widehat{y}(\mathbf{x}_\star) = \begin{cases} \text{Average}\{y_j : j \in \mathcal{N}_\star\} & \text{(Regression problems)} \\ \text{MajorityVote}\{y_j : j \in \mathcal{N}_\star\} & \text{(Classification problems)} \end{cases}$$

K-nearest neighbor model

- **Data** $\mathrm{T} = \{(\boldsymbol{x}_i, y_i), i = 1, \dots, n\}$
- **Model**: W same size as T
- **Learning algorithm**: Set W=T, compute distances in W
- **Prediction**:
  - $y_* = \frac{1}{|N_*|} \sum_{i \in N_*} y_i$
  - $y_* = MajorityVote_{j \in N_*}(y_j)$

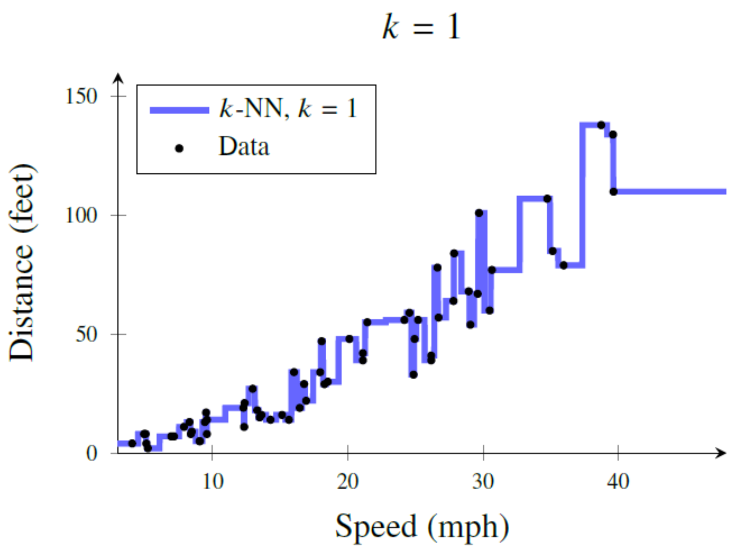
K-nearest neigbor example

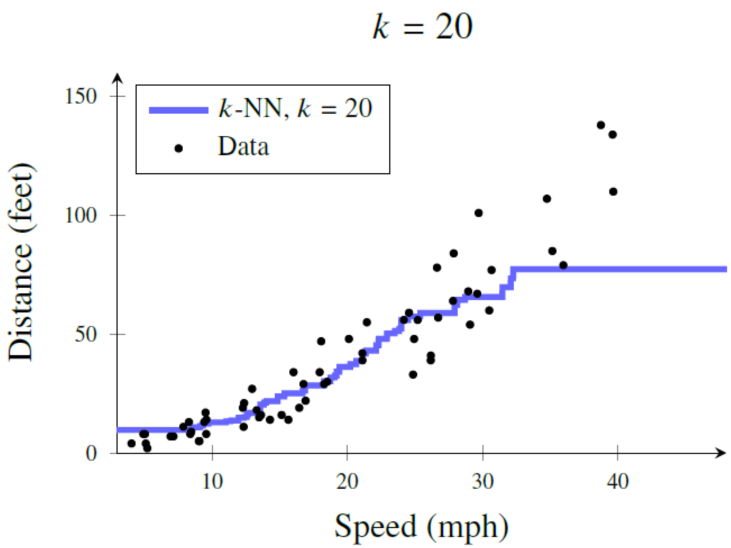
- Classification
  - Music data, x1=song length, x2=a signal processing characteristic



K-nearest neighbor example

- Regression
  - Car data: x1 speed when brake signal given, x2 distance until full stop

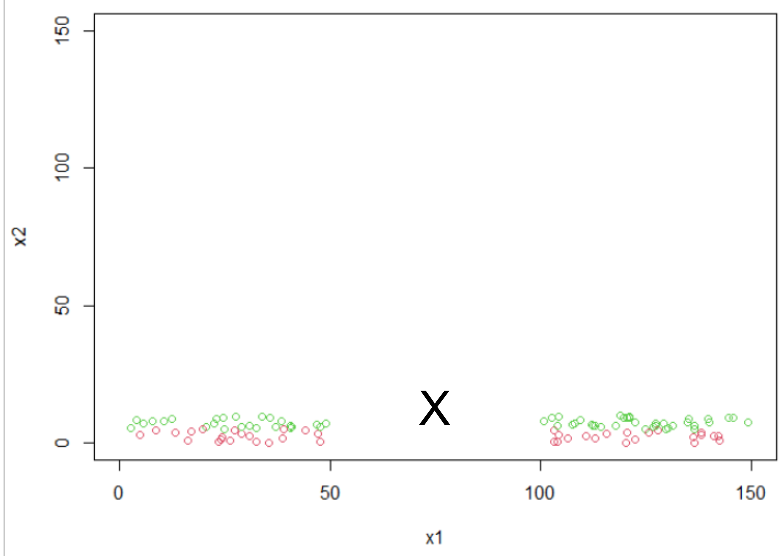


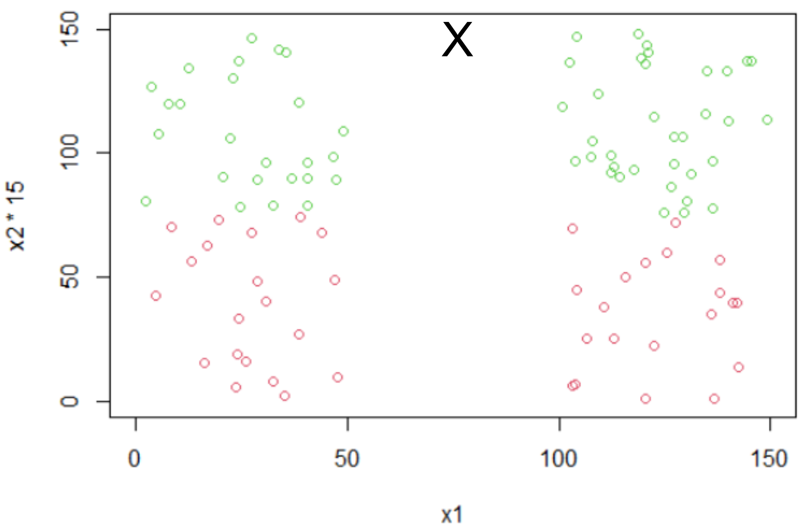


How to choose K?

K-nearest neighbor model

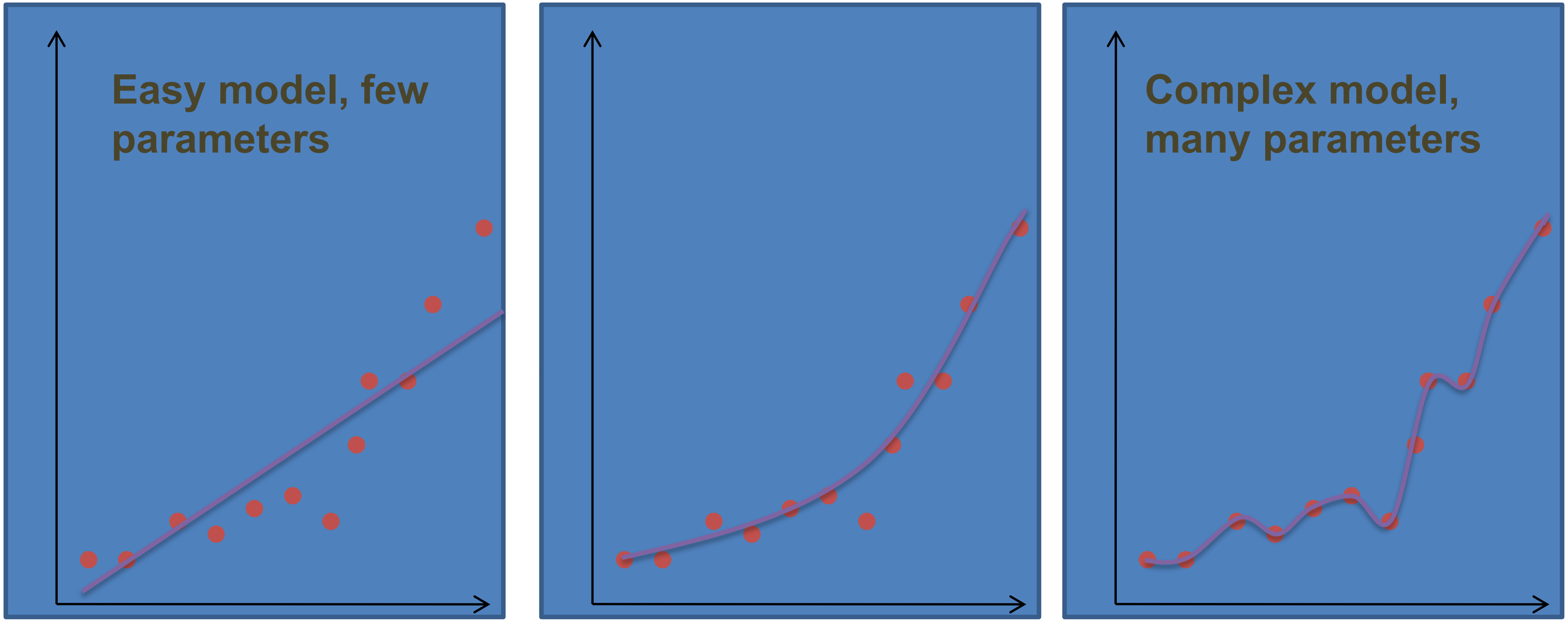
- **Feature preprocessing**: scaling
  - Important, for ex when defining distance
  - Usual preprocessing: $x'_{ij} = \frac{x_{ij} - mean(x_{ij}|\ i=1,\ldots n)}{std(x_{ij}|i=1,\ldots n)}$





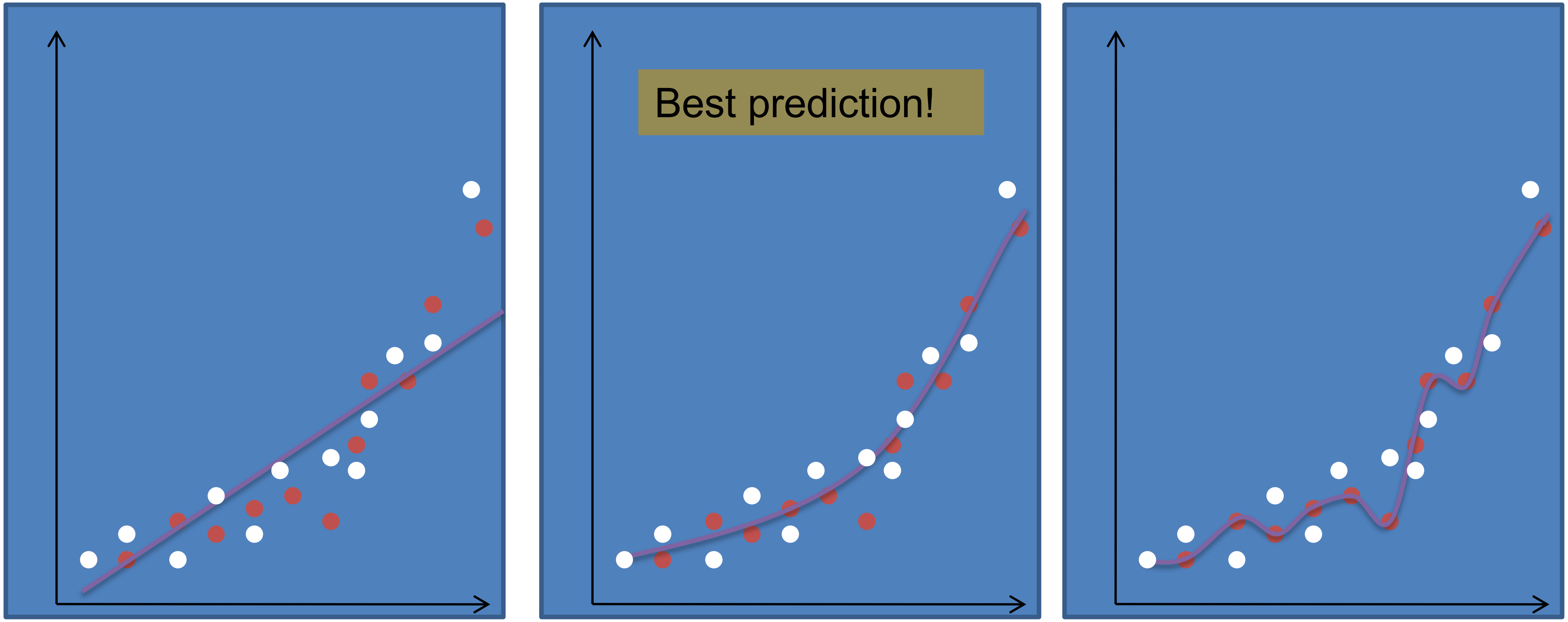
Overfitting

- Which model feels appropriate?



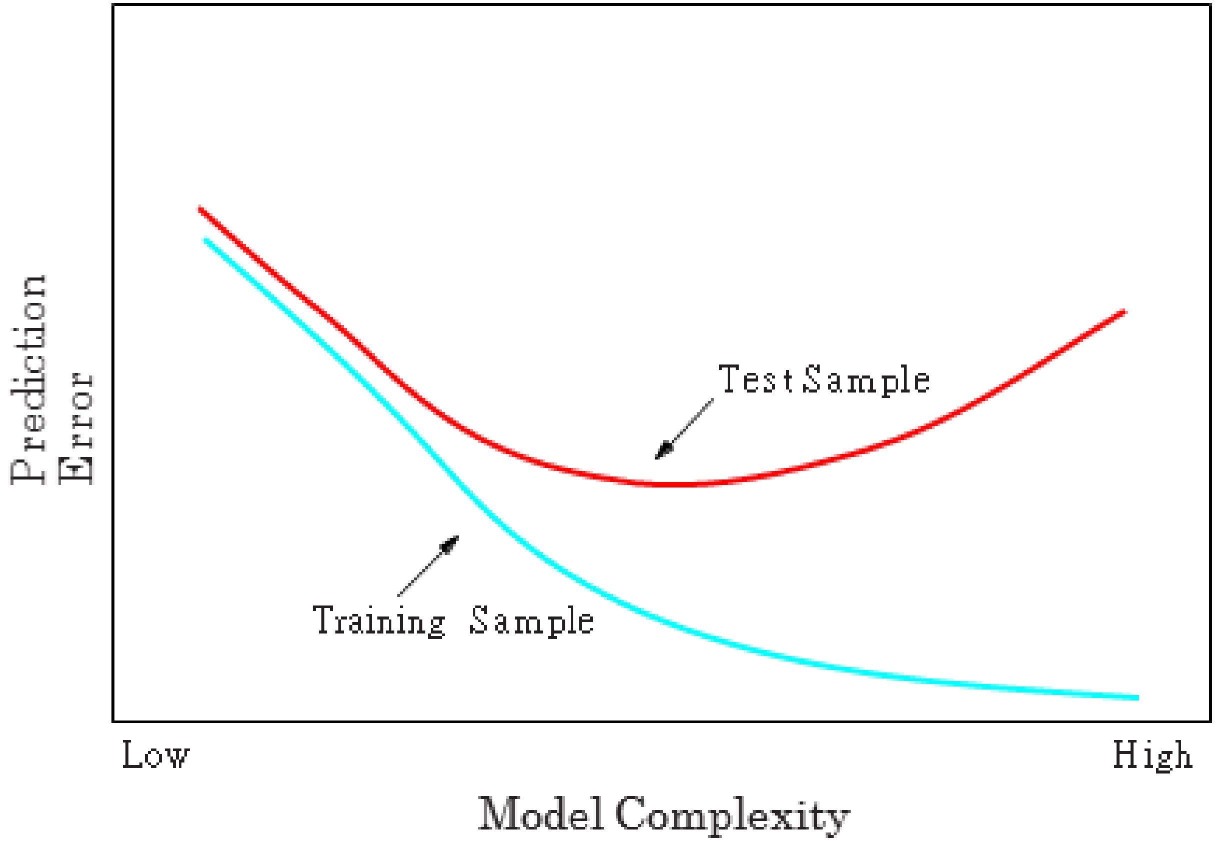
Overfitting

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 estimated 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

Holdout method

Divide into training, validation and test sets

Training	Validation	Test

- Choose proportions in some way
- Test set is used to test a performance on a new data

Holdout in R

- How to partition into train/test?
  - Use set.seed(12345) in the labs to get identical results

```
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.7))
train=data[id,]
test=data[-id,]
```

- How to partition into train/valid/test?

```
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.4))
train=data[id,]

id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.3))
valid=data[id2,]

id3=setdiff(id1,id2)
test=data[id3,]
```

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**

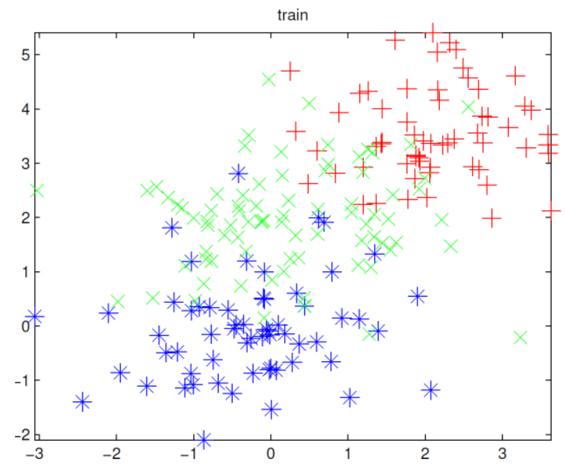
$$R(Y,\hat{Y}) = \frac{1}{N}\sum_{i=1}^{N} I(Y_i \neq \hat{Y}_i)$$

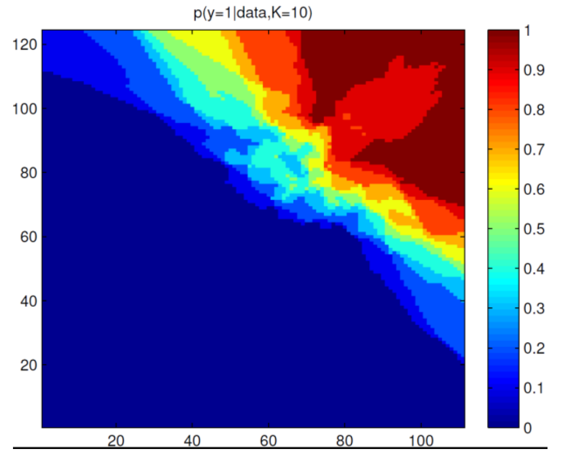
- Classification, cross-entropy for M classes $C_1, \dots, C_M$:

$$R(Y,\hat{p}(Y)) = -\sum_{i=1}^{N}\sum_{m=1}^{M} I(Y_i = C_m)\log\hat{p}(Y_i = C_m)$$

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) changes with training data
    - Example: K-NN classifier

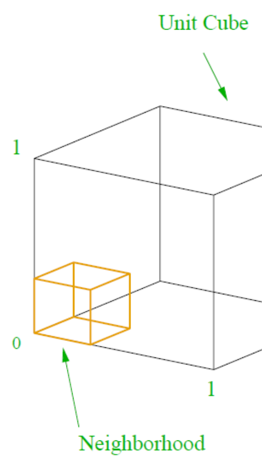


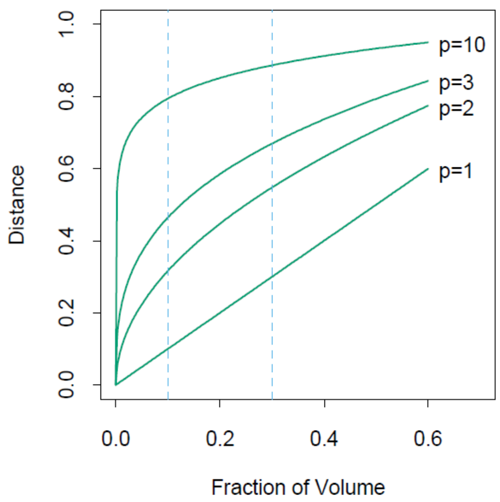


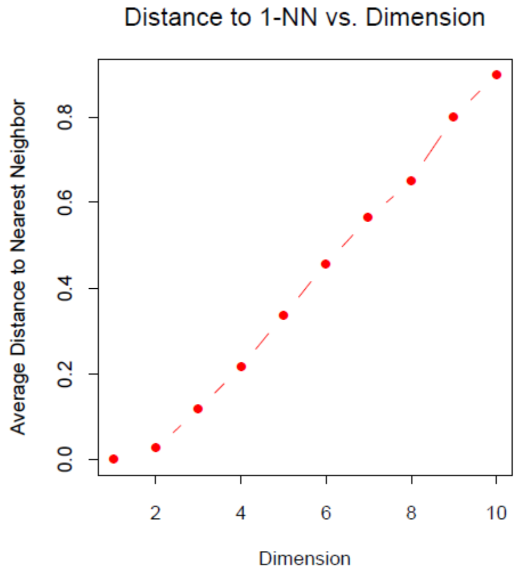
Curse of dimensionality

- Given data T:
  - 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 x's should lead to small change in y → interpolation