

# Information Service Engineering

# Lecture 11: Basic Machine Learning - 2



Leibniz Institute for Information Infrastructure

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FIZ Karlsruhe - Leibniz Institute for Information Infrastructure

AIFB - Karlsruhe Institute of Technology

Summer Semester 2021

### 4.1 A Brief History of AI

### 4.2 Introduction to Machine Learning

### 4.3 Main Challenges of Machine Learning

### 4.4 Machine Learning Workflow

### 4.5 Basic ML Algorithms 1 - k-Means Clustering

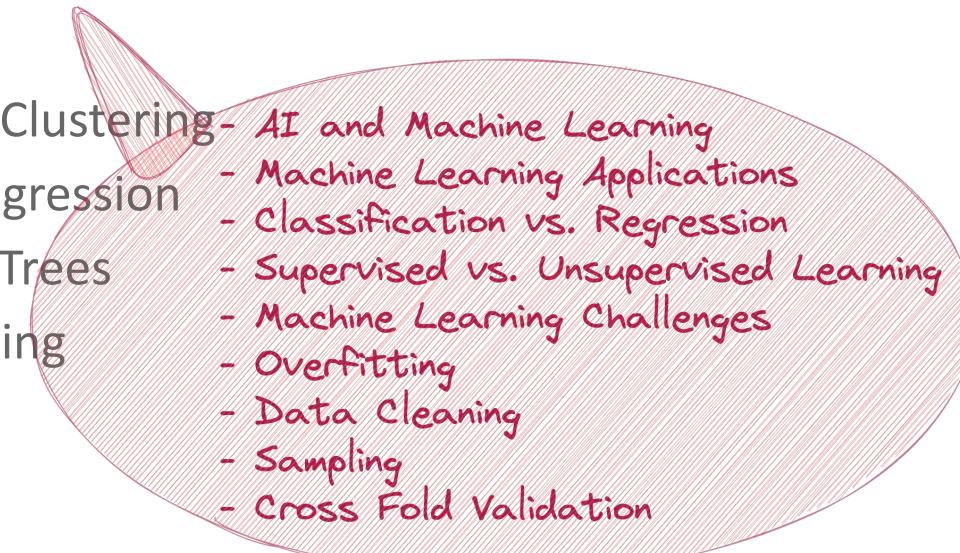
### 4.6 Basic ML Algorithms 2 - Linear Regression

### 4.7 Basic ML Algorithms 3 - Decision Trees

### 4.8 Neural Networks and Deep Learning

### 4.9 Word Embeddings

### 4.10 Knowledge Graph Embeddings

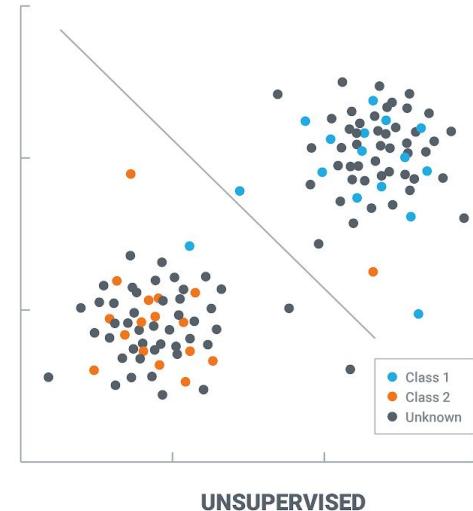


## 4. Basic Machine Learning

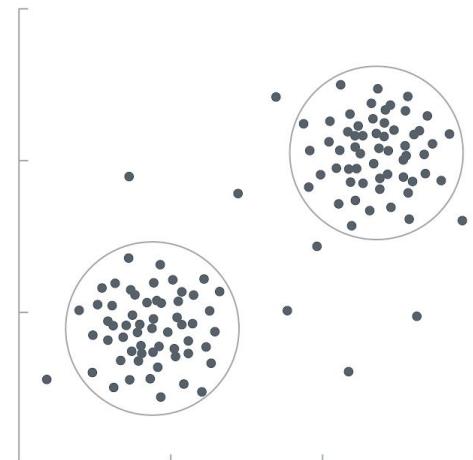
- 4.1 A Brief History of AI
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# Supervised and Unsupervised Learning

- In **supervised learning** aka **predictive analytics**, data consists of observations  $(x_i, y_i)$ ,  $x_i \in \mathbb{R}^p$ ,  $i = 1, \dots, n$
- Such data is called **labeled data**, and the  $y_i$  are thought of as the labels for the data.

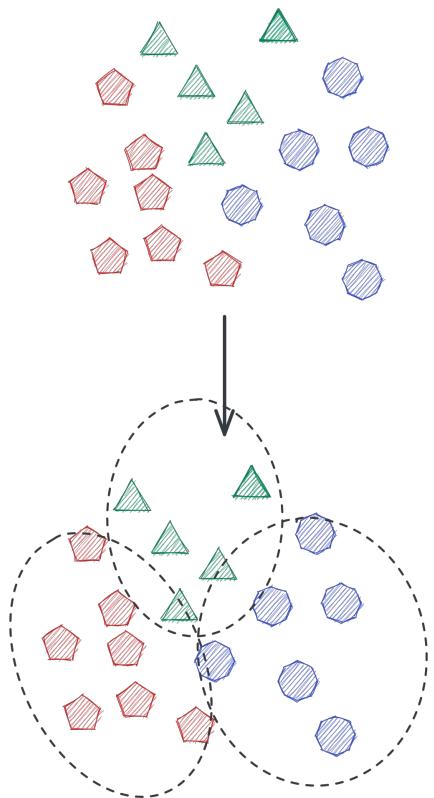


- In **unsupervised learning**, we just look at data  $x_i \in \mathbb{R}^p$ ,  $i = 1, \dots, n$  to detect patterns.
- This is called **unlabeled data**.
- Even if we have labels  $y_i$ , we may still wish to temporarily ignore the  $y_i$  and conduct unsupervised learning on the inputs  $x_i$ .



# Examples for Unsupervised Learning Tasks

- Identify similar groups of **online shoppers** based on their browsing and purchasing history.
- Identify similar groups of **music listeners** or **movie viewers** based on their ratings or recent listening/viewing patterns.
- Identify similar groups of patients based on their medical records.
- Determine how to **place sensors, broadcasting towers, law enforcement, or emergency-care centers** to guarantee that desired coverage criteria are met.

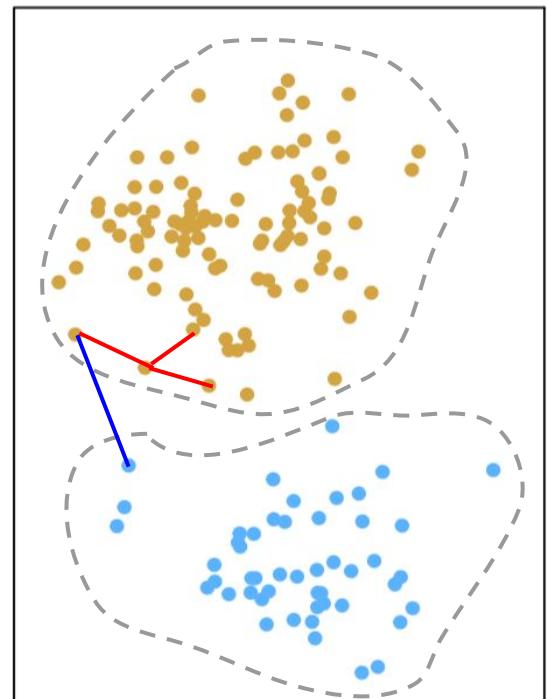


# Unsupervised Learning

- If there are no labels, how do we know if results are meaningful?
  - Experts might interpret the result (**external evaluation**).
- However, we need **Unsupervised Learning**, because:
  - Labeling large datasets is very costly.
  - We may have no idea what/how many classes there are (data mining).
  - We may want to use **clustering** to gain some insight into the structure of the data before designing a classifier.

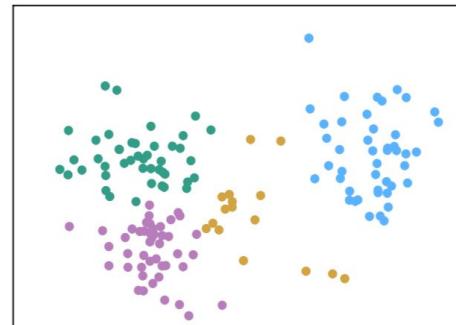
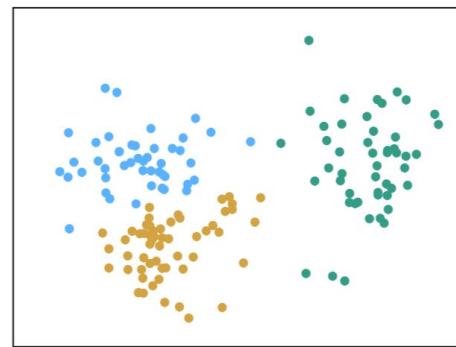
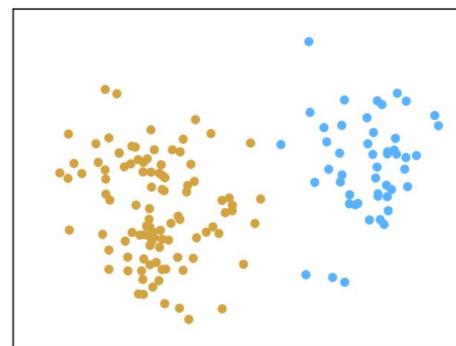
# Clustering

- What is a good clustering?
  - **Internal distances** (within the cluster) should be **small**.
  - **External distances** (inter-cluster) should be **large**.
- Clustering is a way to discover new categories.



# Clustering

- A **clustering** is a partition  $\{C_1, \dots, C_k\}$ , where each  $C_k$  denotes a subset of the observations.
- Each observation belongs to one and only one of the clusters.
- To denote that the  $i^{\text{th}}$  observation is in the  $k^{\text{th}}$  cluster, we write  $i \in C_k$ .



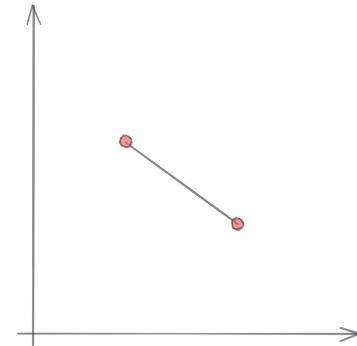
# Clustering - What does 'Similarity' mean?

- To start with, we need a **proximity measure**:
  - **Similarity measure**  
 $s(x_i, x_k)$ : large, if  $x_i$  and  $x_k$  are similar
  - **Dissimilarity measure** (distance)  
 $d(x_i, x_k)$ : small, if  $x_i$  and  $x_k$  are similar

# Distance Measures

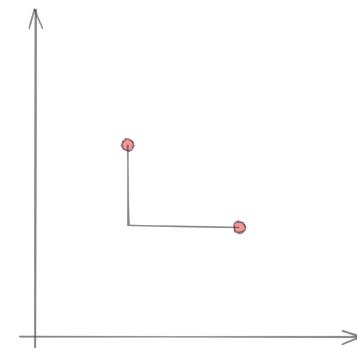
- **Euclidean distance:**  $d(x_i, x_j) = \sqrt{\sum_{k=1}^d (x_i^{(k)} - x_j^{(k)})^2}$

- translation invariant



- **Manhattan distance:**  $d(x_i, x_j) = \sum_{k=1}^d |x_i^{(k)} - x_j^{(k)}|$

- less complex to compute



# k-Means Clustering

- **Main idea:**  
A good clustering is one for which the **within-cluster variation** is as small as possible.
- The **within-cluster variation**  $WCV(C_k)$  for cluster  $C_k$  is some measure of the amount by which the observations within each class differ from one another.
- **Goal:** Find  $C_1, \dots, C_K$  that minimize  $\sum_{k=1}^K WCV(C_k)$ .

“Partition the observations into  $K$  clusters such that the  $wCV$  summed up over all  $K$  clusters is as small as possible.”

# k-Means Clustering

- **Determine within-cluster variation**

- **Goal:** Find  $C_1, \dots, C_K$  that minimize  $\sum_{k=1}^K WCV(C_k)$ .
- Use Euclidean distance:  $WCV(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^p (x_{ij} - x_{i'j})^2$ ,  
where  $|C_k|$  denotes the number of observations in cluster  $k$ .
- The total number of clusters  $K$  is a fixed parameter.

# k-Means Clustering

- WCV( $C_k$ ) can be rewritten:

$$\begin{aligned} WCV(C_k) &= \frac{1}{|C_k|} \sum_{i,i' \in C_k} \|(x_i - x_{i'})\|_2^2 \\ &= 2 \sum_{i \in C_k} \|x_i - \bar{x}_k\|^2 \end{aligned}$$

- with  $\bar{x}_k = \frac{1}{|C_k|} \sum_{i \in C_k} x_i$  is just the **average of all the points in Cluster  $C_k$  (Cluster Centroid or Cluster Center)**.

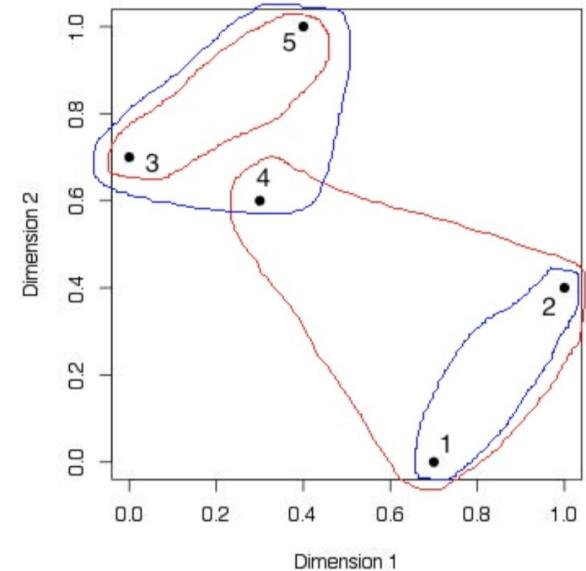
# k-Means Clustering

- Simple Example

- n=5 and K =2
- distance matrix

	1	2	3	4	5
1	0	0.25	0.98	0.52	1.09
2	0.25	0	1.09	0.53	0.72
3	0.98	1.09	0	0.10	0.25
4	0.52	0.53	0.10	0	0.17
5	1.09	0.72	0.25	0.17	0

- Red clustering:  $\sum WCV(C_k) = (0.25 + 0.53 + 0.52)/3 + 0.25/2 = 0.56$
- Blue clustering:  $\sum WCV(C_k) = 0.25/2 + (0.10 + 0.17 + 0.25)/3 = 0.30$

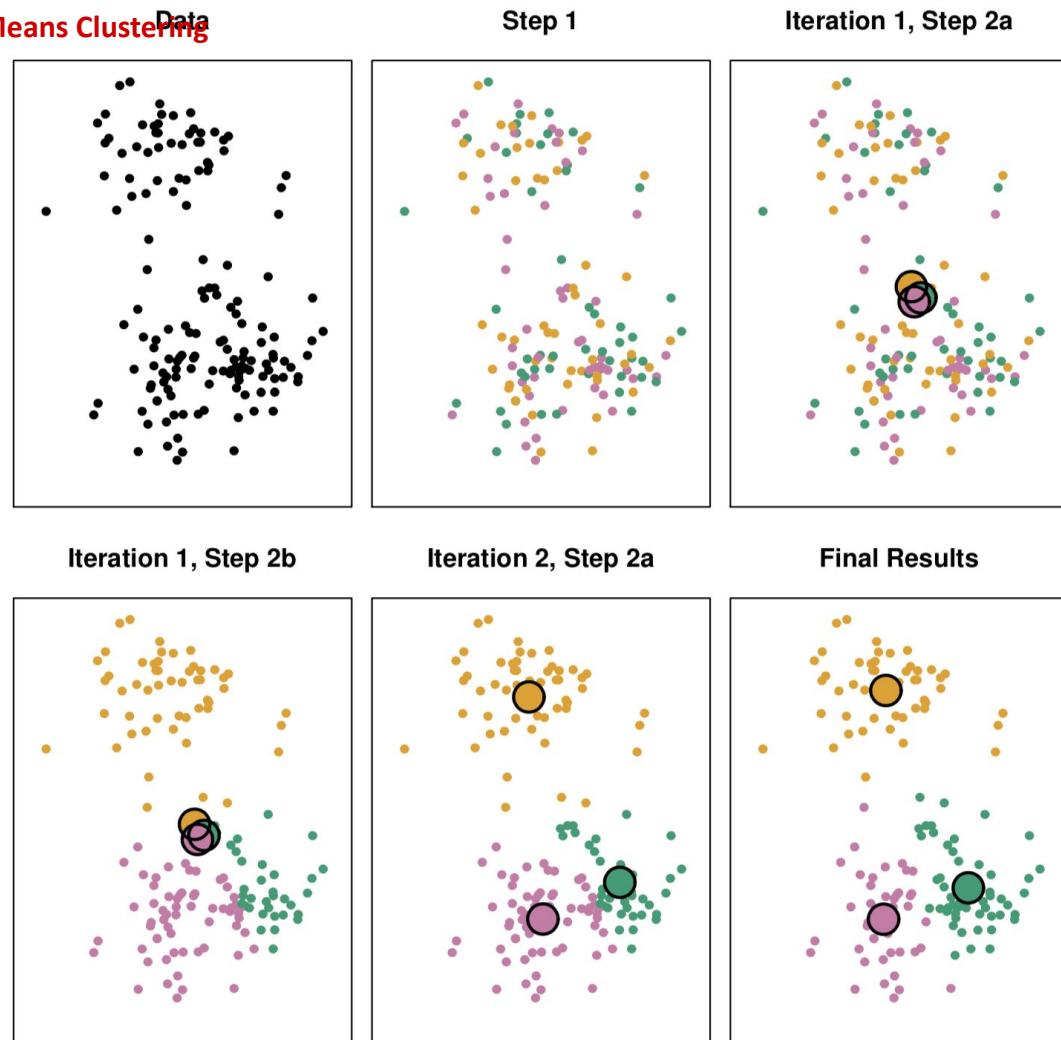


# k-Means Algorithm

1. Start by **randomly** partitioning the observations into **K clusters**.
2. Until the clusters stop changing, repeat:
  - a. For each cluster, compute the **cluster centroid**.
  - b. Assign each observation to the cluster whose centroid is the closest.

# k-Means Algorithm

- Example: K=3



# k-Means Summary

- It is infeasible to actually optimize  $WCV(C_k)$  in practice, but K-means provides a so-called **local optimum** of this objective.
- The achieved result depends both on K, and also on the random initialization.
- It is a good idea to try different random starts and pick the best result among them.
- There is a method called **K-means++** that improves how the clusters are initialized.

# k-Means Clustering Hands On

 11 - ISE2021 - k-Means Example.ipynb 

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## Basic Machine Learning - k-Means Examples

This is the colab notebook example for lecture 11 Basic Machine Learning 2, chapter 4.5 Basic ML Algorithms 1 - k-Means Clustering, of AIFB/KIT Lecture "Information Service Engineering" Summer Semester 2021.

In this colab notebook you will learn how to make use of the [SciKit Learn](#) library for applying machine learning algorithms, in particular the k-means clustering, [matplotlib](#) to draw diagrams, [numpy](#) to manage multi-dimensional arrays.

*Please make a copy of this notebook to try out your own adaptions via "File -> Save Copy in Drive"*

## k-Means Clustering

Clustering algorithms seek to learn, from the properties of the data, an optimal division or discrete labeling of groups of points.

Many clustering algorithms are available in [Scikit-Learn](#). This colab notebook will give you an example how to use *k-means clustering*, which is implemented in `sklearn.cluster.KMeans`.

As usual we start with importing required libraries.

```
[ ] %matplotlib inline
import matplotlib.pyplot as plt
import seaborn as sns; sns.set() # for plot styling
import numpy as np
```

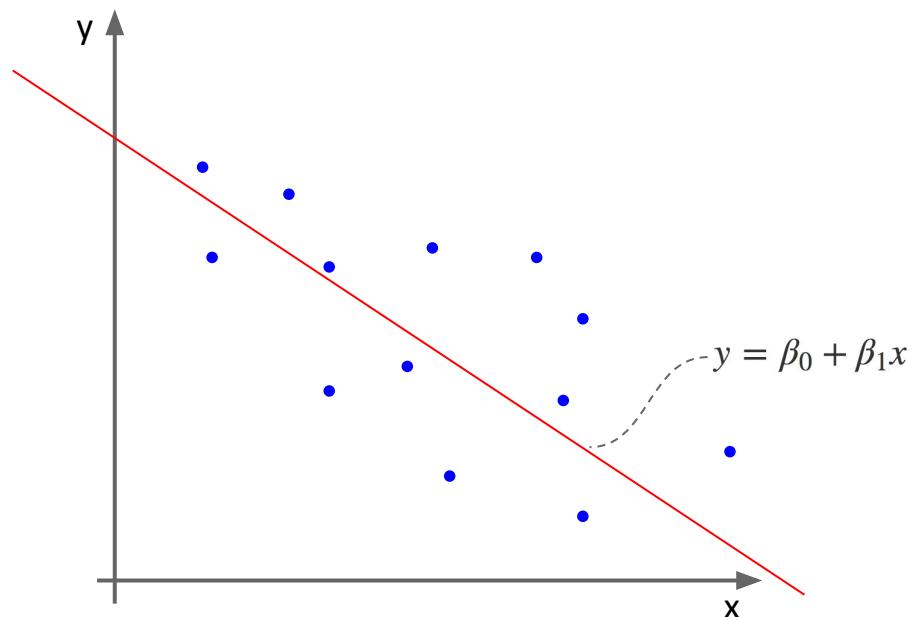
[k-Means Clustering Python Colab Notebook](#)

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# Linear Regression

- With **Linear Regression** we aim to fit a line to a scattering of data.



# Linear Regression

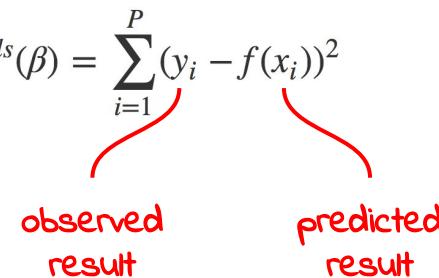
- Notation:

- Input vector  $x \in \mathbb{R}^N$
- Output vector  $y \in \mathbb{R}$
- Parameters  $\beta = (\beta_0, \beta_1, \dots, \beta_N)^\top \in \mathbb{R}^{N+1}$

- Linear model:  $f(x) = \beta_0 + \sum_{j=1}^N \beta_j x_j$

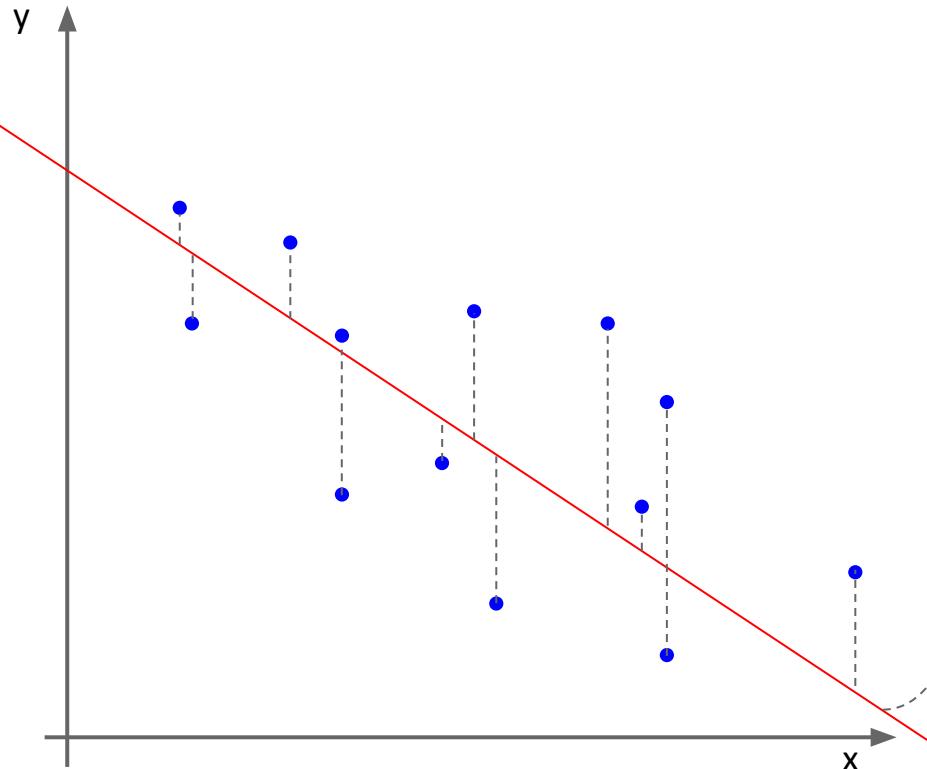
- Given training data  $D = \{(x_i, y_i)\}_{i=1}^P$

- We define the least squares costs (or "loss")  $L^{ls}(\beta) = \sum_{i=1}^P (y_i - f(x_i))^2$



observed result      predicted result

# Linear Regression



- Try to find the line (hyperplane) that fits best to the given data by **minimizing its distance between the data and the line**.
- The **Least Squares Cost ( $L^{ls}(\beta)$ )** framework aims at recovering the line (hyperplane) that **minimized** the total squared length of the error.

$$L^{ls}(\beta) = \sum_{i=1}^P (y_i - f(x_i))^2$$

$$f(x) = \beta_0 + \sum_{j=1}^N \beta_j x_j$$

# Linear Regression

- **Find optimal parameters  $\beta$**

- Augment input vector with a 1 in front:  $\mathbf{x} = (1, x) = (1, x_1, x_2, \dots, x_N)^\top \in \mathbb{R}^{N+1}$

$$\beta = (\beta_0, \beta_1, \dots, \beta_N)^\top \in \mathbb{R}^{N+1}$$

$$f(x) = \beta_0 + \sum_{j=1}^N \beta_j x_j = \mathbf{x}^\top \beta$$

- Simplified linear model:

$$L^{ls}(\beta) = \sum_{i=1}^P (y_i - \mathbf{x}^\top \beta)^2 = \|y - \mathbf{X}\beta\|^2$$

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_P^\top \end{pmatrix} = \begin{pmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,N} \\ \vdots & & & & \vdots \\ 1 & x_{1P,1} & x_{1P,2} & \dots & x_{1P,N} \end{pmatrix}, y = \begin{pmatrix} y_1 \\ \vdots \\ y_P \end{pmatrix}$$

# Linear Regression

- Find optimal parameters  $\beta$

- Rewrite LSC:

$$L^{ls}(\beta) = \sum_{i=1}^P (y_i - \mathbf{x}^\top \beta)^2 = \|y - \mathbf{X}\beta\|^2$$

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_P^\top \end{pmatrix} = \begin{pmatrix} 1 & x_{1,1} & x_{1,2} & \dots & x_{1,N} \\ \vdots & & & & \vdots \\ 1 & x_{1P,1} & x_{P,2} & \dots & x_{P,N} \end{pmatrix}, \quad y = \begin{pmatrix} y_1 \\ \vdots \\ y_P \end{pmatrix}$$

- Compute optimum by setting the gradient to zero:

$$0_P^\top = \frac{\partial L^{ls}(\beta)}{\partial \beta} = -2(y - \mathbf{X}\beta)^\top \mathbf{X}$$

$$\Leftrightarrow 0_P = \mathbf{X}^\top \mathbf{X}\beta - \mathbf{X}^\top y$$

$$\Leftrightarrow \hat{\beta}^{ls} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top y$$

via chain rule:

$$f(x) = u(v(x)) \Rightarrow f'(x) = u'(v(x))v'(x)$$

# Example - Berlin Climate Data

## Climate Dataset

- **Date** year-mm-dd
- **AverageTemperature** average surface temperature
- **AverageTemperatureUncertainty** uncertainty of measurement
- **City** city of measurement
- **Country** country of measurement
- **Latitude** latitude
- **Longitude** longitude

### New:

- **Year** extracted from date
- **12MonthAvgTemperature** 12 month average of the temperature



## Berlin Average Temperatures 1753-2013

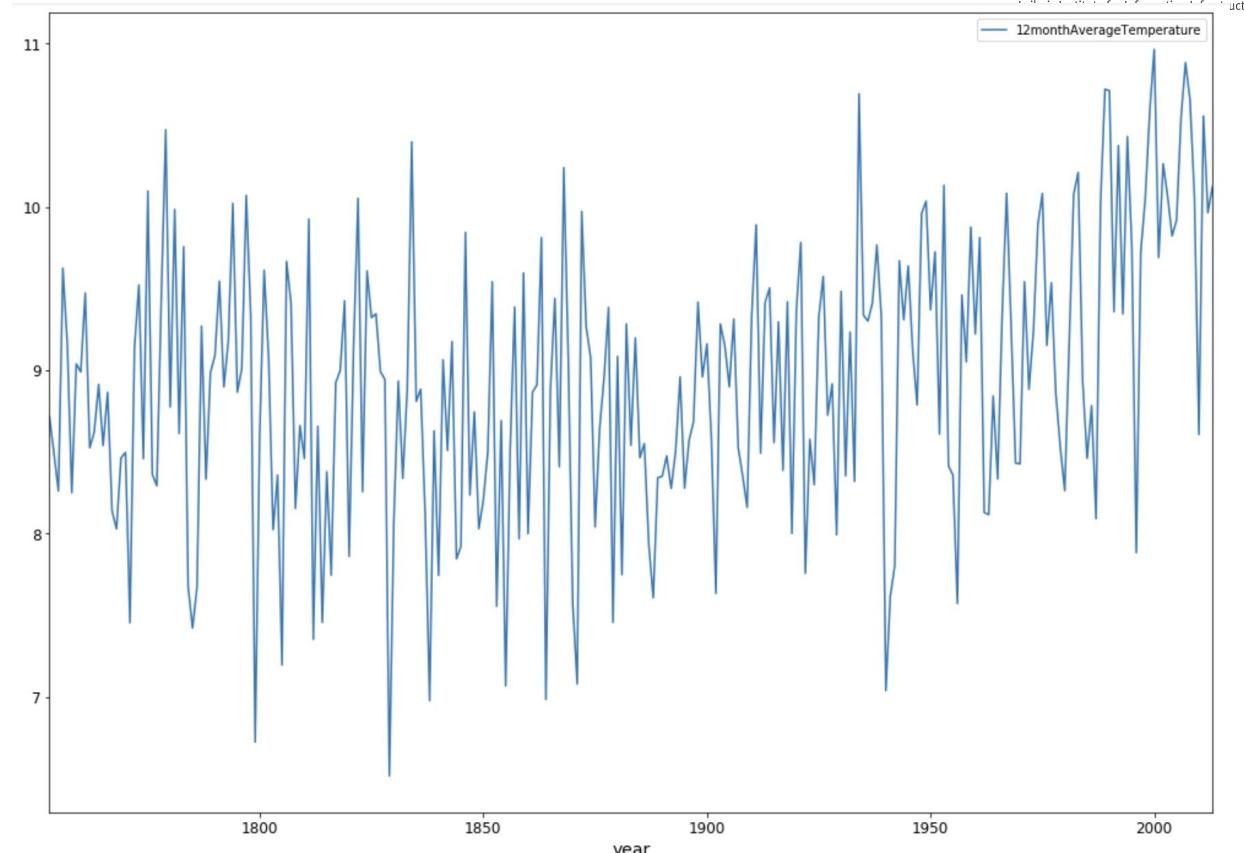
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	A	B	C	D	E	F	G	H	I	J	K
1	date	year	12monthAverag	AverageTemper	AverageTemper	City	Country	Latitude	Longitude		
2	1753-01-01	1753	8.715666667	-2.452	7.998	Berlin	Germany	52.24N	13.14E		
3	1754-01-01	1754	8.492833333	-1.341	2.212	Berlin	Germany	52.24N	13.14E		
4	1755-01-01	1755	8.261083333	-6.032	6.072	Berlin	Germany	52.24N	13.14E		
5	1756-01-01	1756	9.624833333	2.619	6.38	Berlin	Germany	52.24N	13.14E		
6	1757-01-01	1757	9.153666667	-1.883	4.262	Berlin	Germany	52.24N	13.14E		
7	1758-01-01	1758	8.250833333	-4.598	1.266	Berlin	Germany	52.24N	13.14E		
8	1759-01-01	1759	9.03925	2.143	7.459	Berlin	Germany	52.24N	13.14E		
9	1760-01-01	1760	8.989166667	-2.831	5.388	Berlin	Germany	52.24N	13.14E		
10	1761-01-01	1761	9.47275	-0.742	8.045	Berlin	Germany	52.24N	13.14E		
11	1762-01-01	1762	8.52625	1.105	3.177	Berlin	Germany	52.24N	13.14E		
12	1763-01-01	1763	8.619916667	-5.068	6.828	Berlin	Germany	52.24N	13.14E		
13	1764-01-01	1764	8.913666667	1.933	5.876	Berlin	Germany	52.24N	13.14E		
14	1765-01-01	1765	8.539666667	0.679	11.287	Berlin	Germany	52.24N	13.14E		
15	1766-01-01	1766	8.865166667	-2.678	7.946	Berlin	Germany	52.24N	13.14E		
16	1767-01-01	1767	8.138416667	-8.253	7.235	Berlin	Germany	52.24N	13.14E		
17	1768-01-01	1768	8.02925	-5.705	13.971	Berlin	Germany	52.24N	13.14E		
18	1769-01-01	1769	8.463583333	0.72	7.133	Berlin	Germany	52.24N	13.14E		
19	1770-01-01	1770	8.4975	-1.689	8.09	Berlin	Germany	52.24N	13.14E		
20	1771-01-01	1771	7.454	-2.867	8.727	Berlin	Germany	52.24N	13.14E		
21	1772-01-01	1772	9.13475	-0.944	9.804	Berlin	Germany	52.24N	13.14E		
22	1773-01-01	1773	9.522083333	1.64	2.79	Berlin	Germany	52.24N	13.14E		
23	1774-01-01	1774	8.458666667	-1.993	9.485	Berlin	Germany	52.24N	13.14E		
24	1775-01-01	1775	10.09666667	-0.523	5.569	Berlin	Germany	52.24N	13.14E		
25	1776-01-01	1776	8.363	-8.336	6.452	Berlin	Germany	52.24N	13.14E		

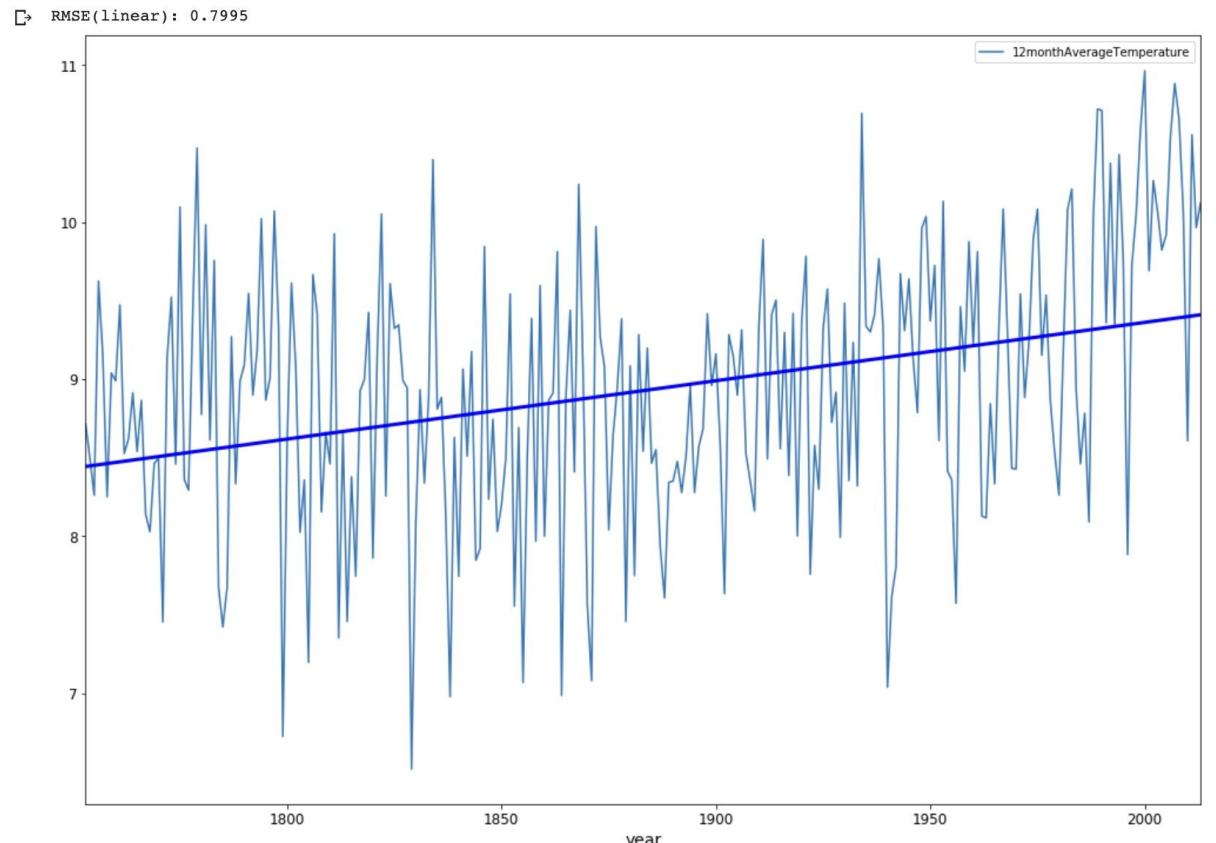
# Example - Berlin Climate Data

- There might be a correlation between the **year** of a measurement and the **temperature**.



# Example Berlin Climate Data

- The linear regression prediction might underfit the data.
- There might be a **non linear correlation**.
- The **temperature** might also be dependent on other factors, such as e.g. **latitude**, etc.



# Root Mean Square Error (RMSE)

- A popular measure for the achieved quality of the prediction is the **Root Mean Square Error RMSE**:

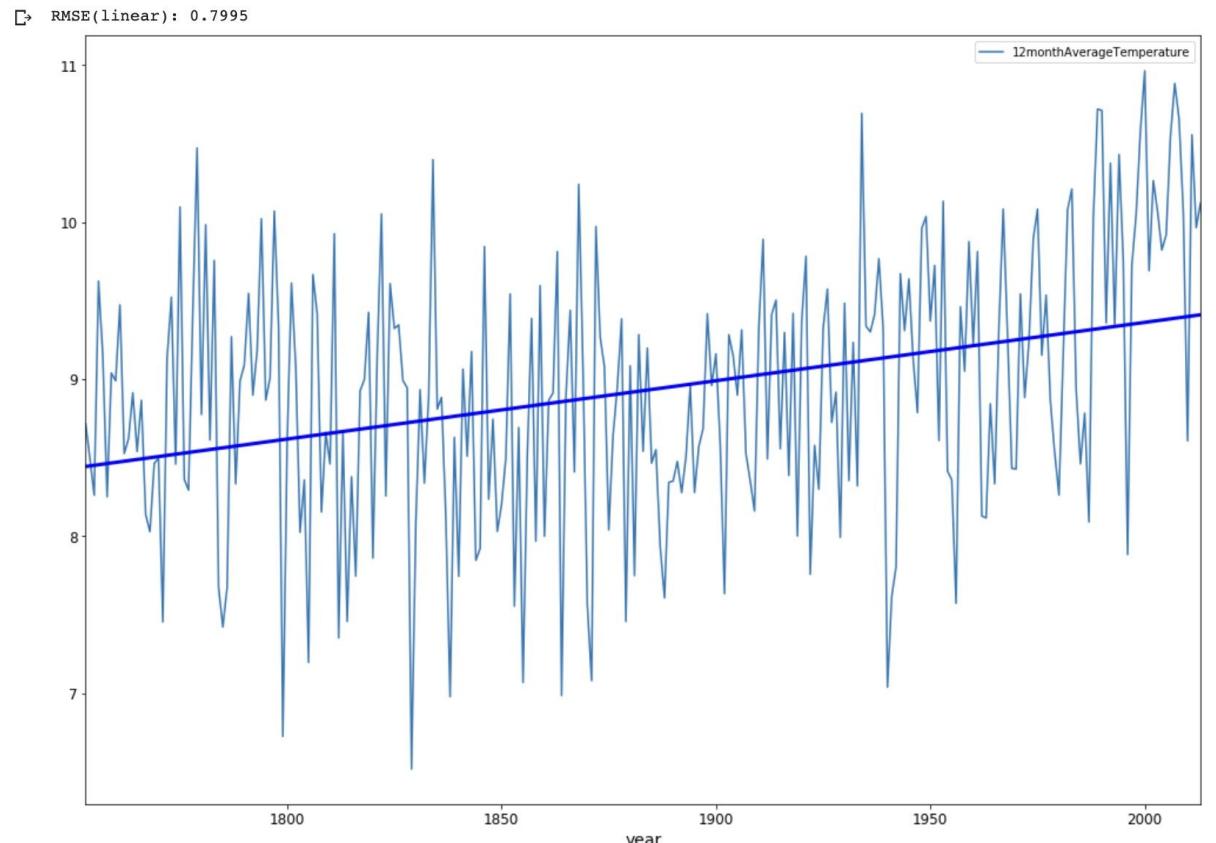
$$RMSE(\mathbf{X}, h) = \sqrt{\frac{1}{m} \sum_{i=1}^m (h(\mathbf{x}_i^\top) - y_i)^2}$$

with  $m$  ... number of dataset instances  
 $\mathbf{x}_i^\top$  ... feature vector for  $i$ th instance  
 $y_i$  ... label (desired output) of  $i$ th instance  
 $h$  ... hypothesis (prediction function)

$$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1^\top \\ \vdots \\ \mathbf{x}_P^\top \end{pmatrix}$$

# Example Berlin Climate Data

- The linear regression prediction might underfit the data.
- There might be a **non linear correlation**.
- The **temperature** might also be dependent on other factors, such as e.g. **latitude**, etc.
- **RMSE=0.7995**



# Non Linear (Polynomial) Regression

- Replace the inputs  $x_i \in \mathbb{R}^d$  by some **non-linear features**  $\phi(x_i) \in \mathbb{R}^k$

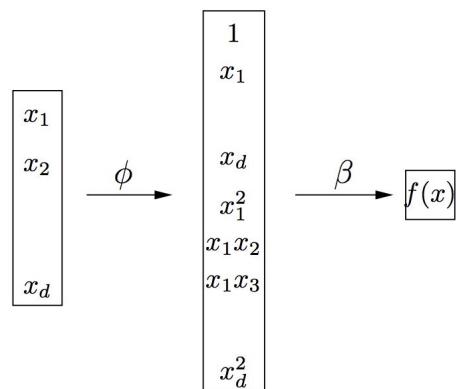
- The optimal  $\beta$  is the same  $\hat{\beta}^{ls} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$  but with  $\mathbf{X} = \begin{pmatrix} \phi(x)_1^\top \\ \vdots \\ \phi(x)_P^\top \end{pmatrix} \in \mathbb{R}^{n \times k}$
- **What are “features”?**

- a) Features are an arbitrary set of basis functions.
- b) Any function linear in  $\beta$  can be written as  $f(x) = \phi(x)^\top \beta$   
for some  $\phi$  - which we denote as “**features**”.

# Non Linear (Polynomial) Regression

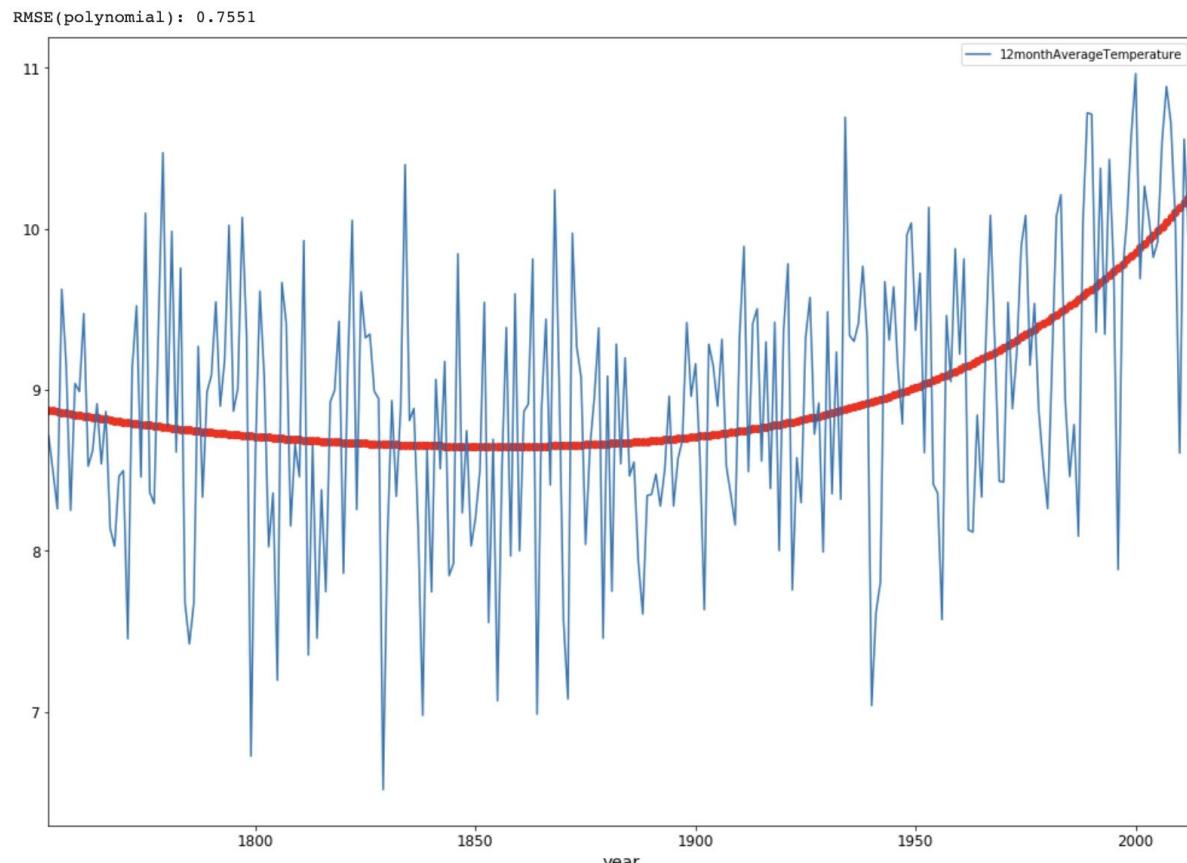
- Linear features:  $\phi(x) = (1, x_1, \dots, x_N) \in \mathbb{R}^{1+N}$
- Quadratic features  $\phi(x) = (1, x_1, \dots, x_N, x_1^2, x_1x_2, x_1x_3, \dots, x_n^2) \in \mathbb{R}^{1+N+\frac{N(N+1)}{2}}$

$$x \quad \phi(x) \quad f(x) = \phi(x)^\top \beta$$



# Example - Berlin Climate Data

- We might also try a **non linear (polynomial) regression**.
- Here degree=8, **RMSE = 0.7551**



# Berlin Climate Change Regression in a Notebook

11 - ISE 2021 - ClimateData Regression HandsOn 
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## Basic Machine Learning - Linear Regression Examples

This is the colab notebook example for lecture 11 Basic Machine Learning 2, chapter 4.6 Basic ML Algorithms 2 - Linear Regression, of AIFB/KIT Lecture "Information Service Engineering" Summer Semester 2021.

In this colab notebook you will learn how to make use of the [SciKit Learn](#) library for applying machine learning algorithms, in particular linear and polynomial regression, [matplotlib](#) for data visualization, [pandas](#) for data analysis, [numpy](#) to manage multi-dimensional arrays.

*Please make a copy of this notebook to try out your own adaptions via "File -> Save Copy in Drive"*

### Set Up

```
[ ] # Common imports
import numpy as np
import pandas as pd

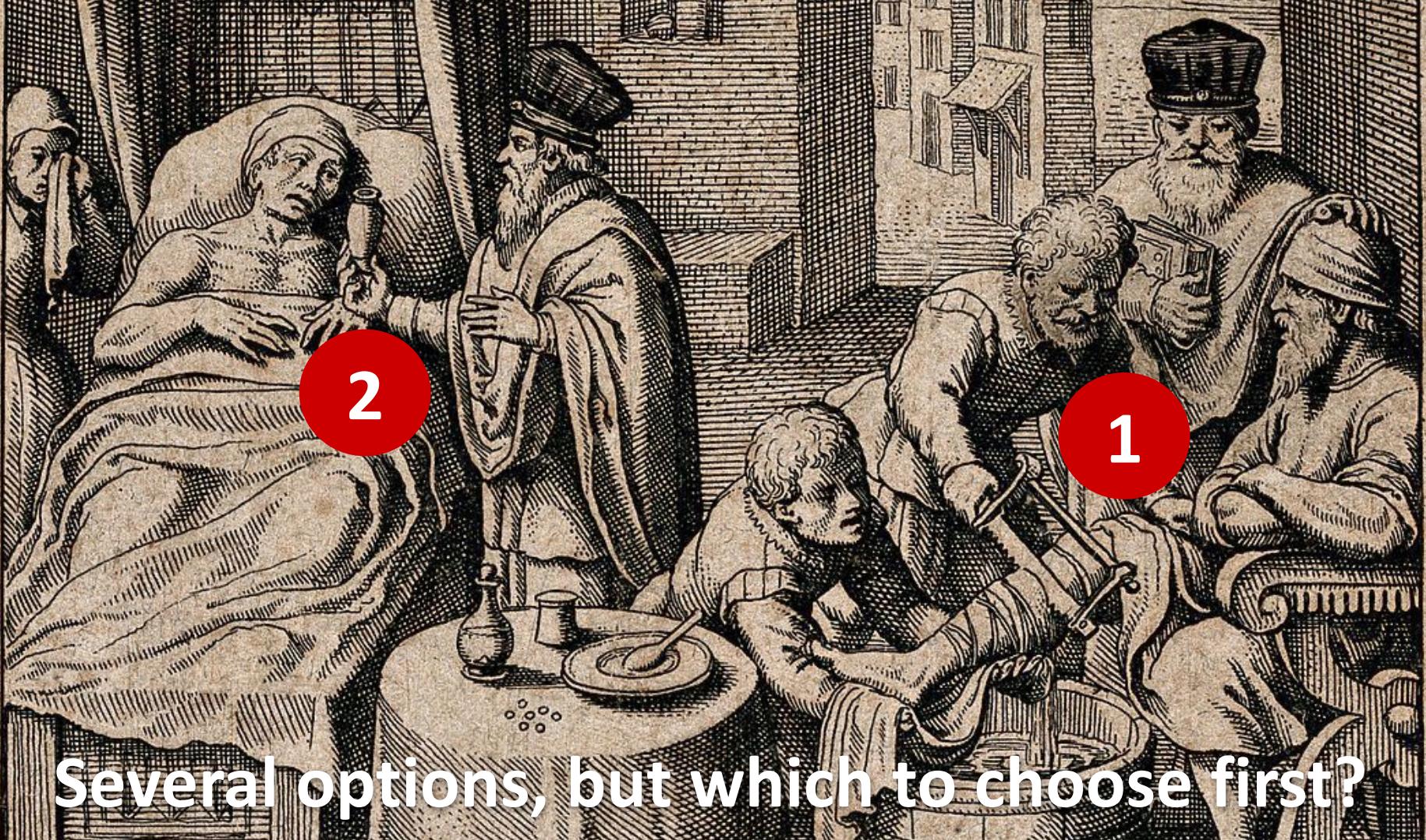
# To plot pretty figures
%matplotlib inline
import matplotlib
import matplotlib.pyplot as plt
plt.rcParams['axes.labelsize'] = 14
plt.rcParams['xtick.labelsize'] = 12
plt.rcParams['ytick.labelsize'] = 12
```

### Get the Data

[Linear Regression Python Colab Notebook](#)

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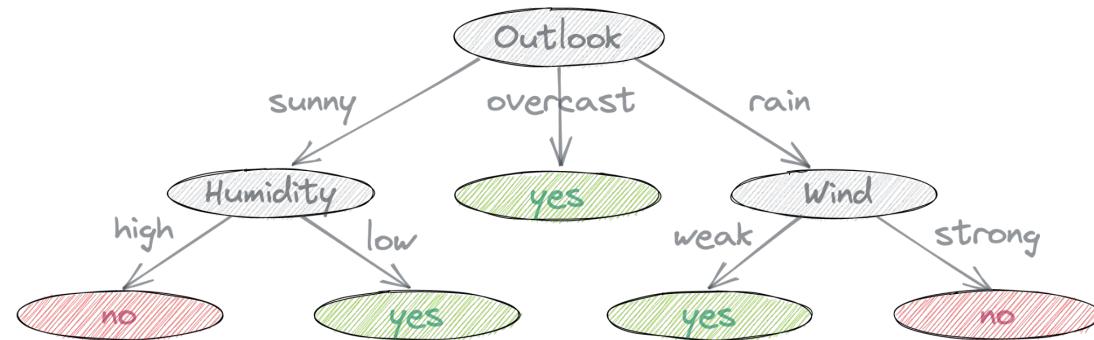
Several options, but which to choose first?

# Decision Trees

- In many classification or regression problems,  
we expect **all attribute values present at the same time.**
- However...
  - sometimes **new attributes occur only over time,**
  - sometimes it is more efficient,  
**first to check the most promising attributes only.**

# Should We Play Tennis?

- Depends on
  - Outlook
  - Wind
  - Temperature
  - Humidity
  - ...
- Internal node: test attribute  $X_i$
- Branch: selects value for  $X_i$
- Leaf node: predict  $Y$
- Given: a set of possible instances: **<Humidity=low, Wind=weak, Outlook=rain, Temp=high>**



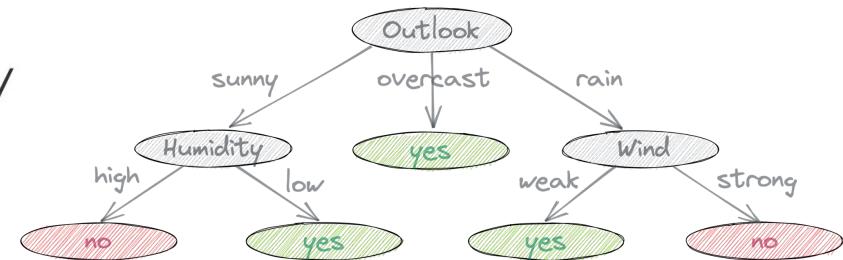
# Decision Tree Learning

- **Problem Setting:**
  - Set of possible instances  $X$ ,
  - each instance  $x \in X$  is a feature vector  $x = \langle x_1, x_2, \dots, x_n \rangle$ .
- Unknown **target function**  $f = X \rightarrow Y$ 
  - $Y$  is discrete valued.
- Set of **function hypotheses**  $H = \{h \mid h : X \rightarrow Y\}$ 
  - each hypothesis  $h$  is a decision tree.
- **Input:**
  - Training examples  $\{\langle x^{(i)}, y^{(i)} \rangle\}$  of unknown target function  $f$ .
- **Output:**
  - Hypothesis  $h \in H$  that best approximates target function  $f$ .

# Decision Tree Learning

- In general, decision trees represent a **disjunction of conjunctions** of constraints on the attribute values of instances.
- The given decision tree corresponds to:

$$\begin{aligned}
 & (\text{outlook} = \text{sunny} \wedge \text{humidity} = \text{low}) \vee \\
 & (\text{outlook} = \text{overcast}) \vee \\
 & (\text{outlook} = \text{rain} \wedge \text{wind} = \text{weak})
 \end{aligned}$$



- Decision Trees can represent any function.

# Decision Tree Learning

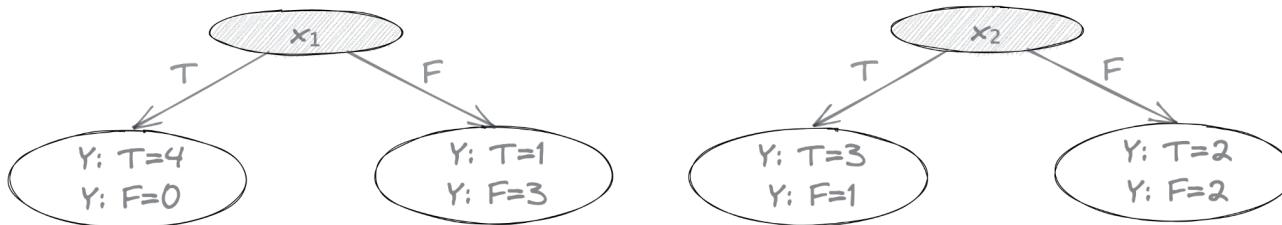
- Constructing a decision tree is easy:
  - Given  **$n$  features**, there are  **$n!$  possible decision trees**.
- Unfortunately, a decision tree can grow very large.
  - Given  **$n$  features** with  **$m$  possible choices**,
  - then a decision tree might grow up to size  **$m^n$** .
- The **size of a decision tree** depends on the **order of its features**.
- **Learning algorithm** tries to determine a good ordering.
- Learning the simplest (smallest) decision tree is an **NP complete problem** (if you are interested, check: Hyafil & Rivest'76).

# Decision Tree Learning - ID3 Algorithm

- Resort to a **greedy heuristic**:
  - Start from an empty decision tree,
  - split on next “best” attribute,
  - recurse.
- What is the best attribute?
- We use **information theory** to guide us.

# Decision Tree Learning - ID3 Algorithm

- Which attribute is better to split on,  $X_1$  or  $X_2$ ?



- **Idea:** Use counts at leaves to define probability distributions, so we can measure uncertainty.

$X_1$	$X_2$	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F
F	T	F
F	F	F

# Decision Tree Learning - ID3 Algorithm

## Entropy

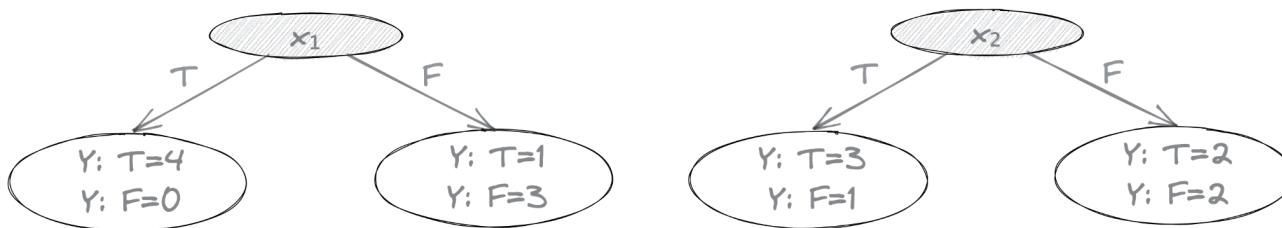
- The **Information Content (Entropy)**  $H$  of a feature variable  $x$  with  $n$  possible feature values is based on its relative frequency of occurrence (probability):

$$H(x) = - \sum_{i=1}^n p_i \cdot \log_2(p_i)$$

- The unit to measure information content is **bit** (*binary digit, basic indissoluble information unit*).

# Decision Tree Learning - ID3 Algorithm

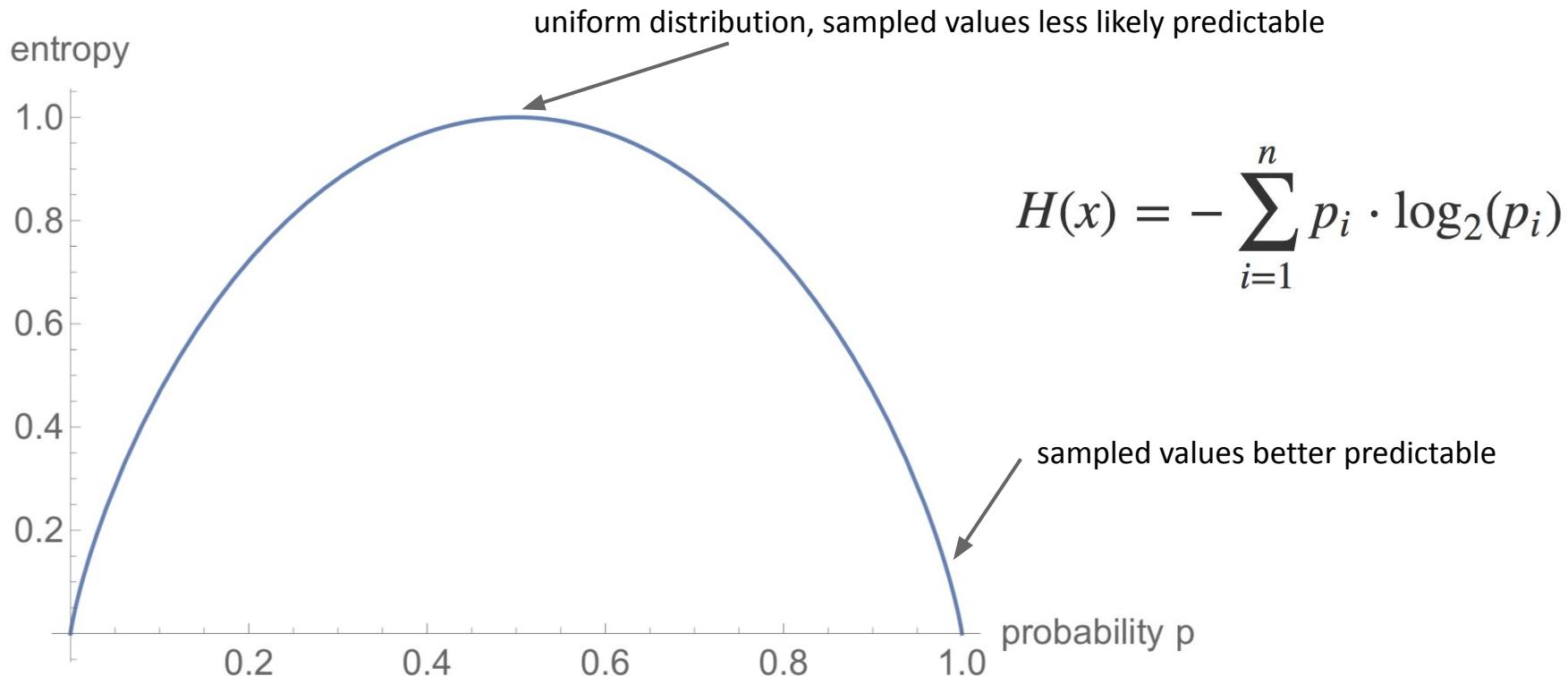
- Which attribute is better to split on,  $X_1$  or  $X_2$ ?



- Entropy of Y:** [T=5, F=3]  $H(Y) = -\frac{5}{8} \log_2(\frac{5}{8}) - \frac{3}{8} \log_2(\frac{3}{8}) = 0.95$  bit

$X_1$	$X_2$	Y
T	T	T
T	F	T
T	T	T
T	F	T
F	T	T
F	F	F
F	T	F
F	F	F

# Decision Tree Learning - ID3 Algorithm



# Decision Tree Learning - ID3 Algorithm

## Information Gain

- The **Information Gain** of a feature  $Y$  due to a feature  $X$  is a measure of the effectiveness of a feature in classifying the training data.
- It is simply the **expected reduction in entropy** caused by partitioning the examples according to this feature:

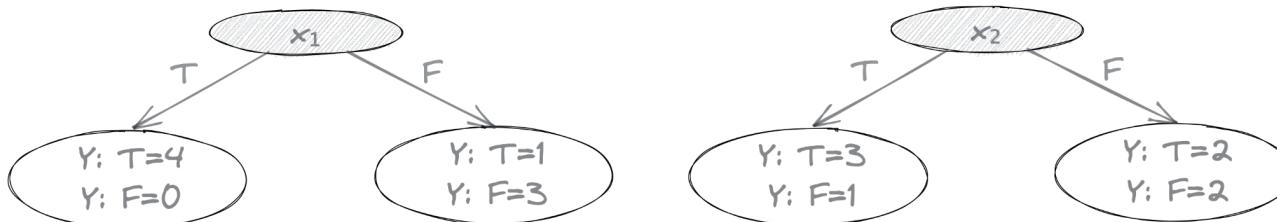
$$\begin{aligned} IG(Y|X) &= H(Y) - H(Y|X) \\ &= H(Y) - \sum_{x \in X} \frac{|Y_x|}{|Y|} H(Y_x) \end{aligned}$$

- Where  $x$  are all possible values of feature  $X$ , and  $Y_x$  the subset of all instances in  $Y$  with  $X=x$

# Decision Tree Learning - ID3 Algorithm

- Which attribute is better to split on,  $X_1$  or  $X_2$ ?

$$IG(Y|X) = H(Y) - \sum_{x \in X} \frac{|Y_x|}{|Y|} H(Y_x)$$

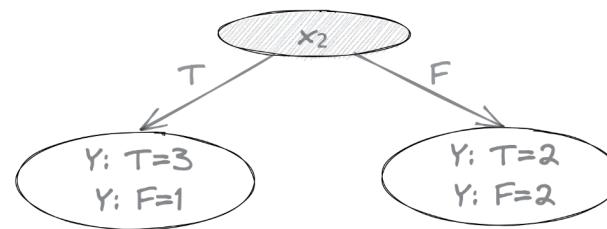
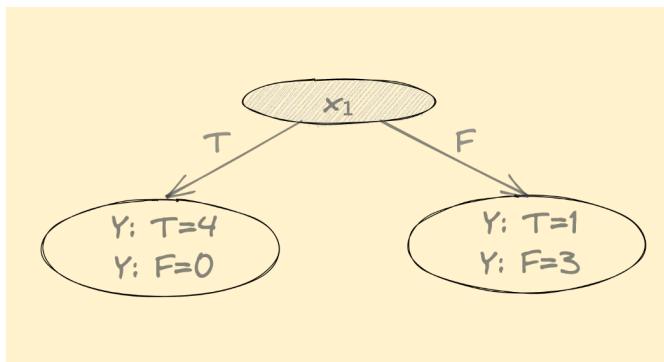


- $IG(Y|X_1) = 0.95 - (4/8 H(X_1=\text{True}) + 4/8 H(X_1=\text{False})) = 0.95 - (0 + 0.4) = \mathbf{0.55}$   
 $IG(Y|X_2) = 0.95 - (4/8 H(X_2=\text{True}) + 4/8 H(X_2=\text{False})) = 0.95 - (0.4 + 0.5) = \mathbf{0.05}$

# Decision Tree Learning - ID3 Algorithm

- Which attribute is better to split on,  $X_1$  or  $X_2$ ?

$$IG(Y|X) = H(Y) - \sum_{x \in X} \frac{|Y_x|}{|Y|} H(Y_x)$$



- $IG(Y|X_1) = 0.95 - (4/8 H(X_1=True) + 4/8 H(X_1=False)) = 0.95 - (0 + 0.4) = \textcolor{red}{0.55}$   
 $IG(Y|X_2) = 0.95 - (4/8 H(X_2=True) + 4/8 H(X_2=False)) = 0.95 - (0.4 + 0.5) = \textcolor{red}{0.05}$

# Decision Tree Learning - ID3 Algorithm

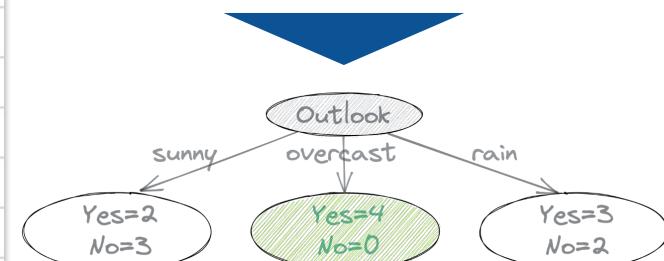
- ID3 **greedy heuristic**:
  1. Start from an empty decision tree.
  2. Split on next “best” attribute,  
i.e. the attribute with the **next highest information gain**.
  3. Recurse.



# ID3 Algorithm - Example

Outlook	Temperature	Humidity	Wind	PlayTennis
sunny	hot	high	weak	no
sunny	hot	high	strong	no
overcast	hot	high	weak	yes
rain	mild	high	weak	yes
rain	cool	low	weak	yes
rain	cool	low	strong	no
overcast	cool	low	strong	yes
sunny	mild	high	weak	no
sunny	cool	low	weak	yes
rain	mild	low	weak	yes
sunny	mild	low	strong	yes
overcast	mild	high	strong	yes
overcast	hot	low	weak	yes
rain	mild	high	strong	no

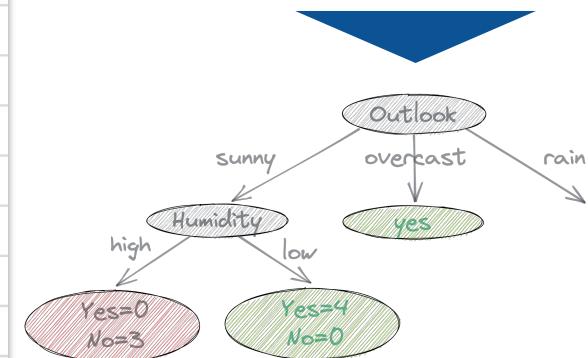
$$\begin{aligned} \text{IG(PlayTennis, Outlook)} &= 0.246 \\ \text{IG(PlayTennis, Humidity)} &= 0.151 \\ \text{IG(PlayTennis, Wind)} &= 0.048 \\ \text{IG(PlayTennis, Temperature)} &= 0.029 \end{aligned}$$



# ID3 Algorithm - Example

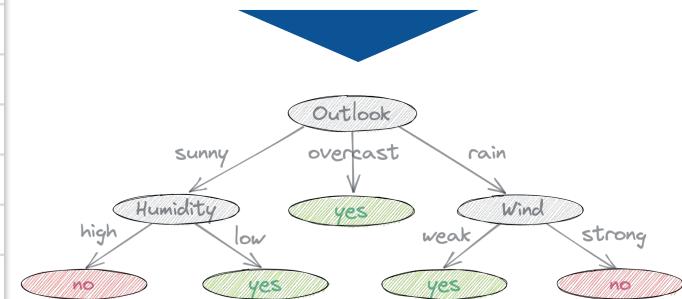
Outlook	Temperature	Humidity	Wind	PlayTennis
sunny	hot	high	weak	no
sunny	hot	high	strong	no
overcast	hot	high	weak	yes
rain	mild	high	weak	yes
rain	cool	low	weak	yes
rain	cool	low	strong	no
overcast	cool	low	strong	yes
sunny	mild	high	weak	no
sunny	cool	low	weak	yes
rain	mild	low	weak	yes
sunny	mild	low	strong	yes
overcast	mild	high	strong	yes
overcast	hot	low	weak	yes
rain	mild	high	strong	no

$$\begin{aligned} \text{IG(Outlook, Humidity)} &= 0.97 \\ \text{IG(Outlook, Wind)} &= 0.57 \\ \text{IG(Outlook, Temperature)} &= 0.019 \end{aligned}$$



# ID3 Algorithm - Example

Outlook	Temperature	Humidity	Wind	PlayTennis
sunny	hot	high	weak	no
sunny	hot	high	strong	no
overcast	hot	high	weak	yes
rain	mild	high	weak	yes
rain	cool	low	weak	yes
rain	cool	low	strong	no
overcast	cool	low	strong	yes
sunny	mild	high	weak	no
sunny	cool	low	weak	yes
rain	mild	low	weak	yes
sunny	mild	low	strong	yes
overcast	mild	high	strong	yes
overcast	hot	low	weak	yes
rain	mild	high	strong	no



# Decision Trees - Pros and Cons

- **Simple to understand** and interpret.
  - Able to handle both **numerical and categorical data**.
  - Requires **little data preparation**.
  - Uses a **white box model**.
  - Possible to **validate a model using statistical tests**.
  - Performs well with **large datasets**.
  - **Mirrors human decision making** more closely than other approaches.
  - **BEWARE:** Decision Tree models easily overfit.
- DT Learning Algorithms:
    - **ID3** (Iterative Dichotomiser 3)
    - **C4.5** (successor of ID3)
    - **CART** (Classification And Regression Tree)
    - **CHAID** (CHi-squared Automatic Interaction Detector). Performs multi-level splits when computing classification trees.
    - **MARS**: extends decision trees to handle numerical data better.

# Decision Trees Hands On Example

CO 11 - ISE2021 - Decision Trees Example.ipynb 

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+ Code + Text RAM  Disk 

**Basic Machine Learning - Decision Trees Examples**

This is the colab notebook example for lecture 11 Basic Machine Learning 2, chapter 4.7 Basic ML Algorithms 3 - Decision Trees, of AIFB/KIT Lecture "Information Service Engineering" Summer Semester 2021.

In this colab notebook you will learn how to make use of the [SciKit Learn](#) library for applying machine learning algorithms, in particular the decision trees and random forest classifier, [matplotlib](#) and [seaborn](#) for data visualization, [pandas](#) to analyze and manipulate data.

*Please make a copy of this notebook to try out your own adaptions via "File -> Save Copy in Drive"*

```
[2]
# Common imports
from sklearn.model_selection import train_test_split
from sklearn import tree
from sklearn.metrics import accuracy_score,confusion_matrix

# for data analysis and manipulation
import pandas as pd

# To plot pretty figures
%matplotlib inline
import matplotlib
import matplotlib.pyplot as plt
import seaborn as sns
plt.rcParams['axes.labelsize'] = 10
plt.rcParams['xtick.labelsize'] = 10
plt.rcParams['ytick.labelsize'] = 10
```

[Decision Tree Python Colab Notebook](#)

We will load a dataset with **weather observations**, including the information whether it has rained or not. We will use this dataset to train a **decision tree classifier** that predicts - based on the available weather data - **whether it will rain the next day or not**.

## 4. Basic Machine Learning

- 4.1 A Brief History of AI
- 4.2 Introduction to Machine Learning
- 4.3 Main Challenges of Machine Learning
- 4.4 Machine Learning Workflow
- 4.5 Basic ML Algorithms 1 - k-Means Clustering
- 4.6 Basic ML Algorithms 2 - Linear Regression
- 4.7 Basic ML Algorithms 3 - Decision Trees
- 4.8 Neural Networks and Deep Learning
- 4.9 Word Embeddings
- 4.10 Knowledge Graph Embeddings

# 4. Basic Machine Learning - 2

## Bibliography

- S. Marsland, ***Machine Learning, An Algorithmic Perspective***, 2nd. ed., Chapman & Hall / CRC Press, 2015
  - Chap. 14.1 (k-Means Algorithm)
  - Chap. 3.5 (Linear Regression)
  - Chap. 12 (Decision Trees)

(The book should also be available on the Web as pdf, just keep looking...)

## 4. Basic Machine Learning - 2

### Syllabus Questions

- What's the difference between supervised and unsupervised ML?
- Explain the basic concept of k-Means Clustering.
- Explain the concept of Linear Regression.
- What kind of problems can be solved via Linear Regression?
- Explain the difference between Linear, Multilinear, and Polynomial Regression.
- When are Decision Trees preferred over Linear (Multilinear or Polynomial) Regression?
- Explain the concept of Information Gain.
- What are the Pros and Cons of Decision Trees?