

# 6<sup>th</sup> Summer School on INtelligent signal processing for FrontlEr Research and Industry

30<sup>th</sup> August 2021, University Autónoma de Madrid



## Introduction to Machine Learning and Deep Learning (Part I)

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Universidad Autónoma  
de Madrid



- What is Machine Learning?
- Performance evaluation
- Examples of Machine Learning algorithms
- Ensembles
- Conclusions

- **Arthur Lee Samuel (1901-1990)**  
Pioneer of artificial intelligence research  
[IEEE Computer Pioneer Award](#) 1987

**“Field of study that gives computers the ability to learn from data without being explicitly programmed”**



Source: <https://history-computer.com/people/arthur-samuel-biography-history-and-inventions/>

“Field of study that gives computers the **ability** to learn from data without being explicitly programmed”

- Looking for a function to mimic human brain decisions...

### –Speech Recognition

$$f\left( \text{[Waveform]} \right) = \text{“How are you”}$$

### –Image recognition

$$f\left( \text{[Cat Image]} \right) = \text{“Cat”}$$

### –Playing Go

$$f\left( \text{[Go Board]} \right) = \text{“5-5” (next move)}$$

“Field of study that gives computers the ability to learn from **data** without being explicitly programmed”

- It can be any **unprocessed digital signal** of any nature like a fact, value, text, sound or picture
- It can have temporal dependency (**time-series**)
- Often transformed to **Numerical and Categorical** types
  
- Organized as **Datasets**, which are collections of data instances that all share a common attribute
- Requires **annotations** of attributes for each data instance of the dataset **to measure efficiency**

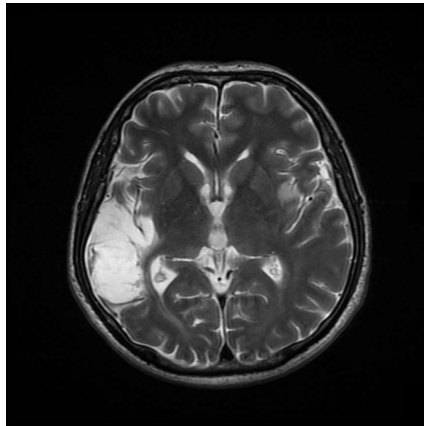
“Field of study that gives computers the ability to **learn** from data without being explicitly programmed”

- **Learning problems** in Machine Learning

**Algorithm employs data annotations?**

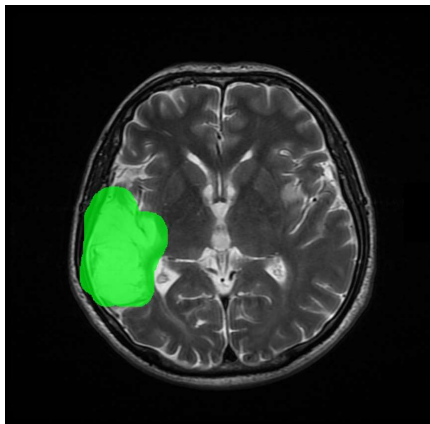
		Supervised learning	Unsupervised learning
Type of signals	Discrete	Classification or categorization	Clustering
	Continuous	Regression	Dimensionality reduction

- The **accuracy of ML algorithms** must be evaluated to choose the best one for each specific task

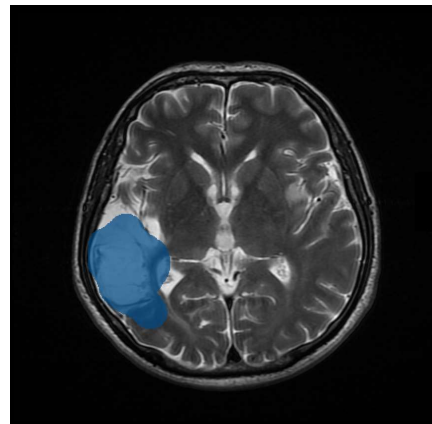


### Task

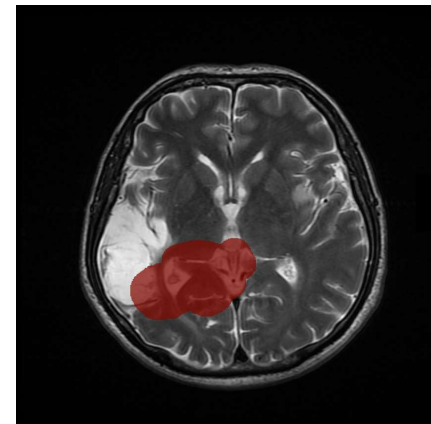
Brain Tumor Segmentation in MRI images  
(i.e. identify which image pixels are tumor)



ML algorithm #1



ML algorithm #2



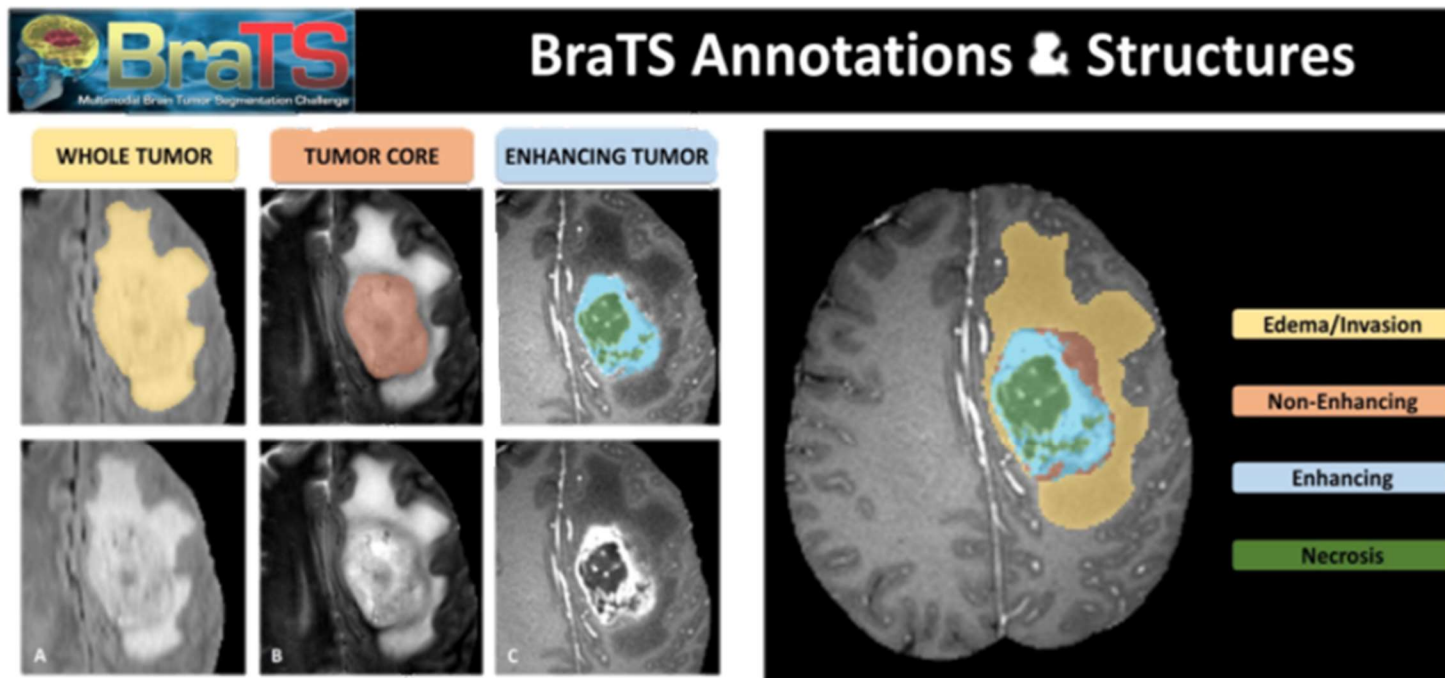
ML algorithm #3

**Which one  
is the best?**

Example created with <https://htmlsegmentation.s3.eu-north-1.amazonaws.com/index.html>

- Three key elements

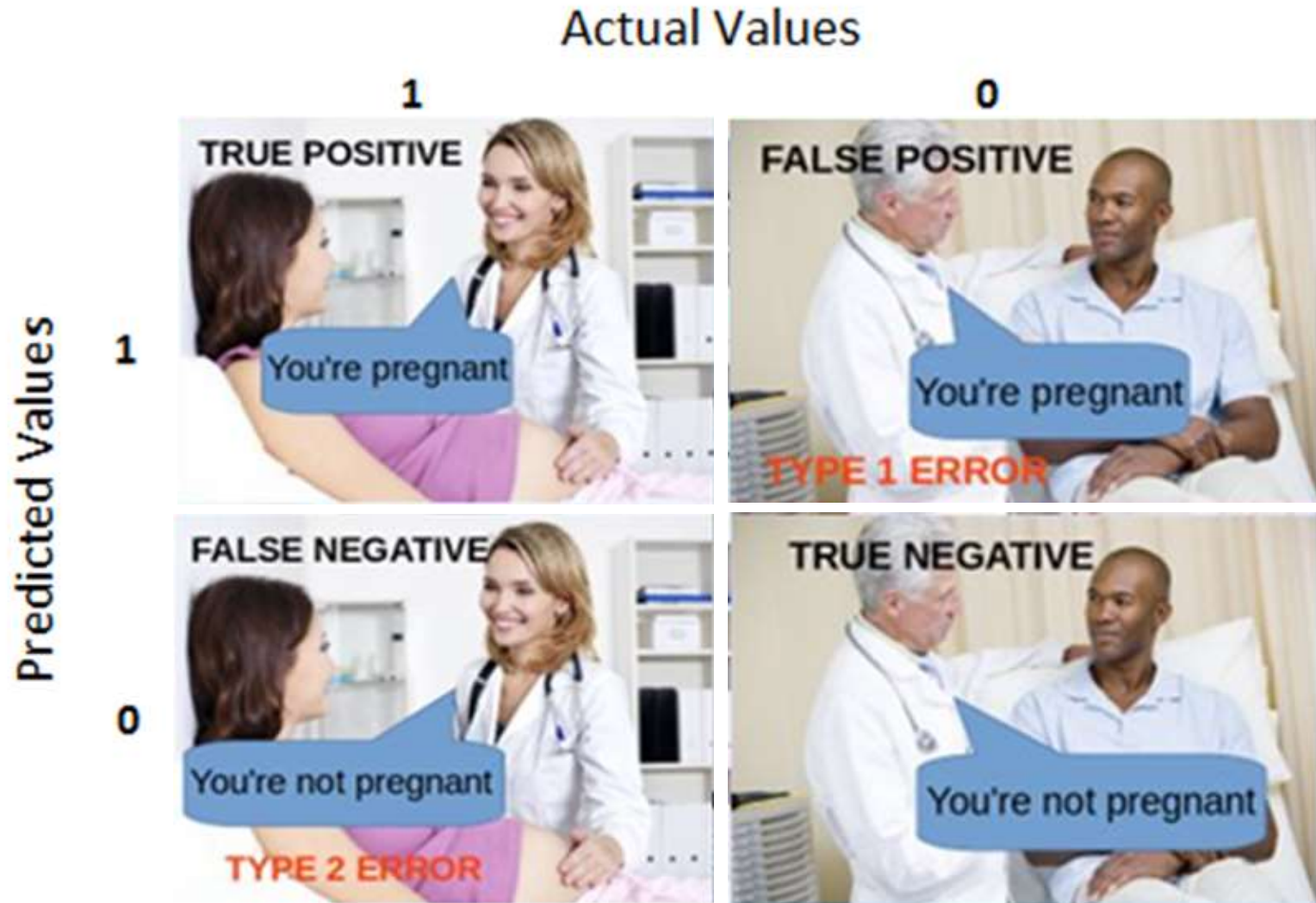
- **Result**: prediction of the algorithm (e.g. category, scalar value,...)
- **Ground-truth**: the **knowledge of the truth** for the specific task. (e.g. ideal expected result for the category, scalar value,...)
- **Metric**: function to compute similarity between result and ground-truth



Source: <https://www.med.upenn.edu/cbica/brats2020/data.html>



- **Metrics for binary classifier evaluation**  
(can be also applied to classify data instances into multiple classes)



Source: <http://www.info.univ-angers.fr/>

- Classification **accuracy** and **error**

$$\text{Accuracy} = \frac{TP+T}{TP+TN+FP+F}$$

$$= \frac{\# \text{ correct predictions}}{\# \text{ total predictions}}$$

$$\text{Error rate} = \frac{FP+F}{TP+TN+FP+FN}$$

$$= \frac{\# \text{ wrong predictions}}{\# \text{ total predictions}}$$

- **Confusion matrix**

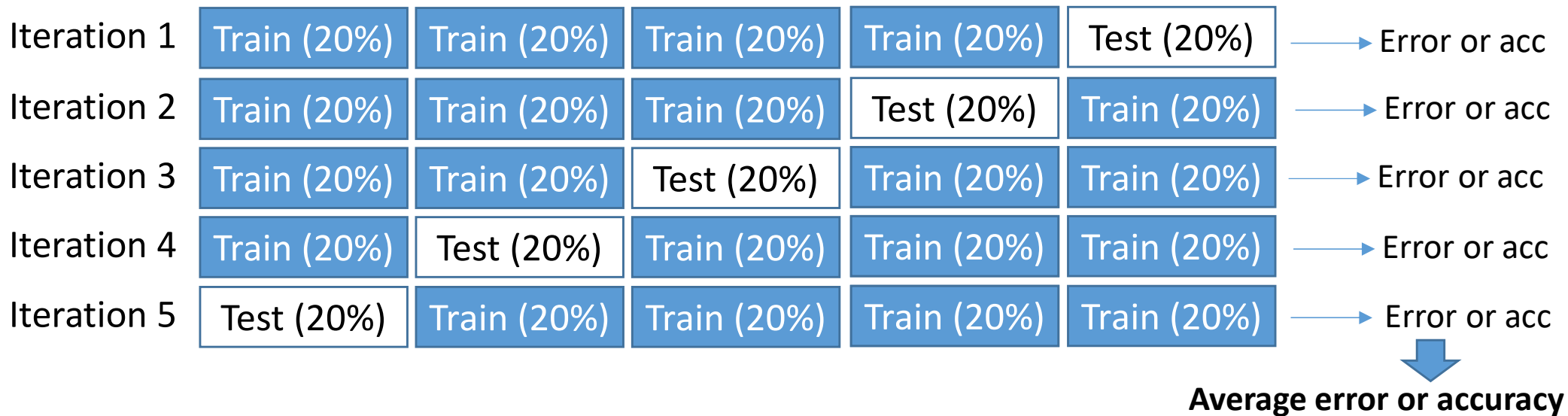
- Performance visualization and summary of results
- Diagonal are correct predictions
- Allows to focus on errors

	Predicted class	
Actual class	Cat	Dog
Cat	6	2
Dog	1	3

Extended description at  
[https://en.wikipedia.org/wiki/Confusion\\_matrix](https://en.wikipedia.org/wiki/Confusion_matrix)

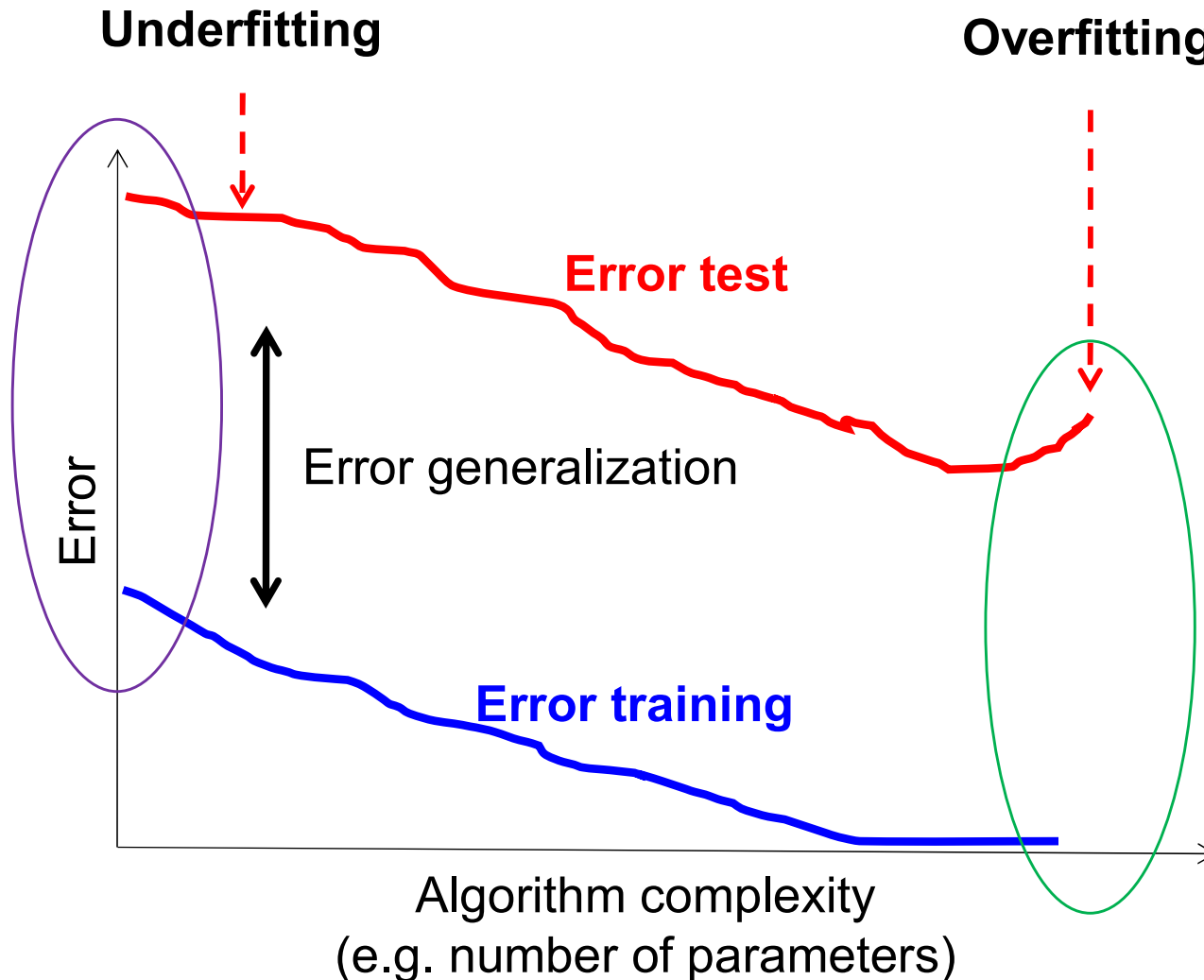
- *Many more metrics... (see suggested readings)*

- If dataset is large (i.e. millions of samples), **split in two sets**:
  - **Train** (85-98%): algorithm fitting (i.e. adjust) parameters for best performance
  - **Test** (15-2%): validate the algorithm trained with different data
- If dataset is not large (i.e. thousands of samples), then dataset is **randomly split into “k” folds** (often k=5 so 20% each)



- Moreover, a **validation set** is often added to add fairness in evaluation
  - **Train set** used for algorithm fitting (resulting in a learned model)
  - **Validation set** used to estimate prediction error for selecting the best model
  - **Test set** used to assess the generalization error of the final chosen model

- Error generalization: algorithm complexity for a given dataset



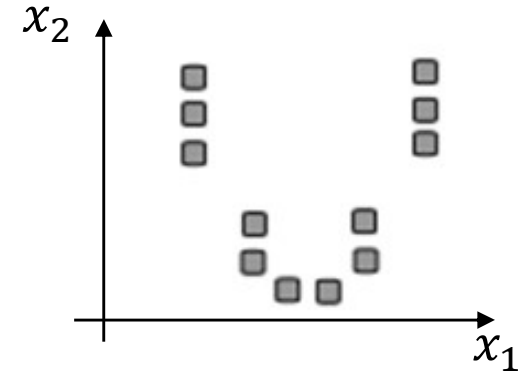
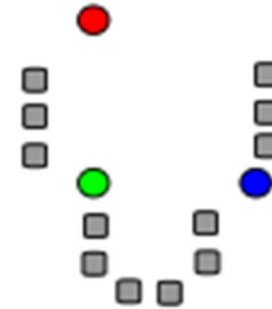
Adapted from D. Hoiem



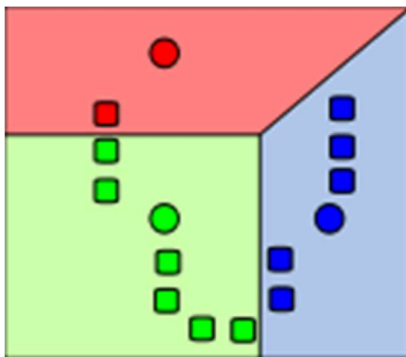
Source: <https://www.deepmarketer.com/blog/2017/1/30/machine-learning-algorithm-taxonomy>

- Unsupervised learning: K-means<sup>1</sup>
  - Iterative algorithm for clustering

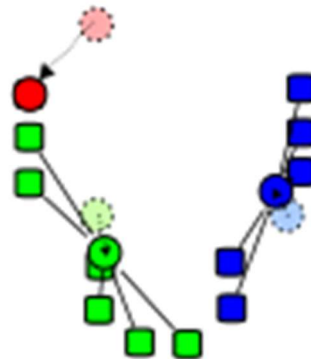
**Step 1: Select the number of clusters and set randomly a cluster center (i.e. representative)**



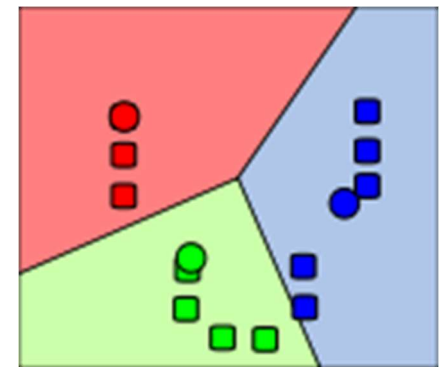
**Step 2:** associate each data to clusters by minimum distance with cluster centers



**Step 3:** update cluster centers with the mean of new data associated to each cluster in step 1



**Step 4:** repeat step 2 and 3 until convergence of cluster centers



<sup>1</sup>Lloyd, Stuart P. "Least Squares Quantization in PCM."

IEEE Transactions on Information Theory. Vol. 28, 1982, pp. 129–137.

Credit images: <https://en.wikipedia.org/>

- Supervised learning: Support Vector Machines<sup>1</sup>

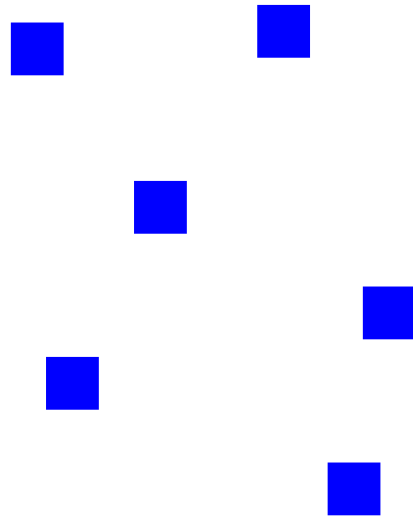
A linear classifier learns a linear function to determine the classification boundaries

Training data sample  $i$ th

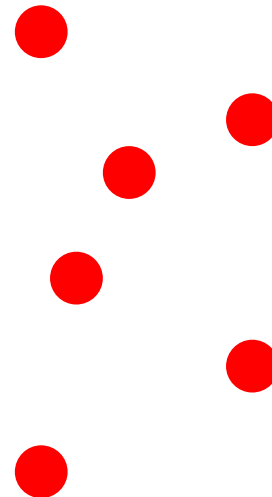
$$\hat{y}^i = f(\vec{\omega} \cdot \vec{x}^i) = f\left(\sum_{j=0}^{N_d} \omega_j \cdot x_j^i\right)$$

Algorithm params

Training data  
for class A



Training data  
for class B



<sup>1</sup>C. Burges, "A Tutorial on Support Vector Machines for Pattern Recognition", Data Mining and Knowledge Discovery, 1998

- Supervised learning: Support Vector Machines

- Defines a hyperplane  $\vec{\omega} \cdot \vec{x}^i - \vec{b} = 0$  for binary classification

$$\hat{y}^i = \text{sgn}(\vec{\omega} \cdot \vec{x}^i + \vec{b})$$

$$\hat{y}^i = \text{sgn}\left(\sum_{j=1}^{N_d} \omega_j \cdot x_j^i + \vec{b}\right)$$

- Prediction

- Class **x** (+1) if  $\vec{\omega} \cdot \vec{x}^i - \vec{b} > 0$

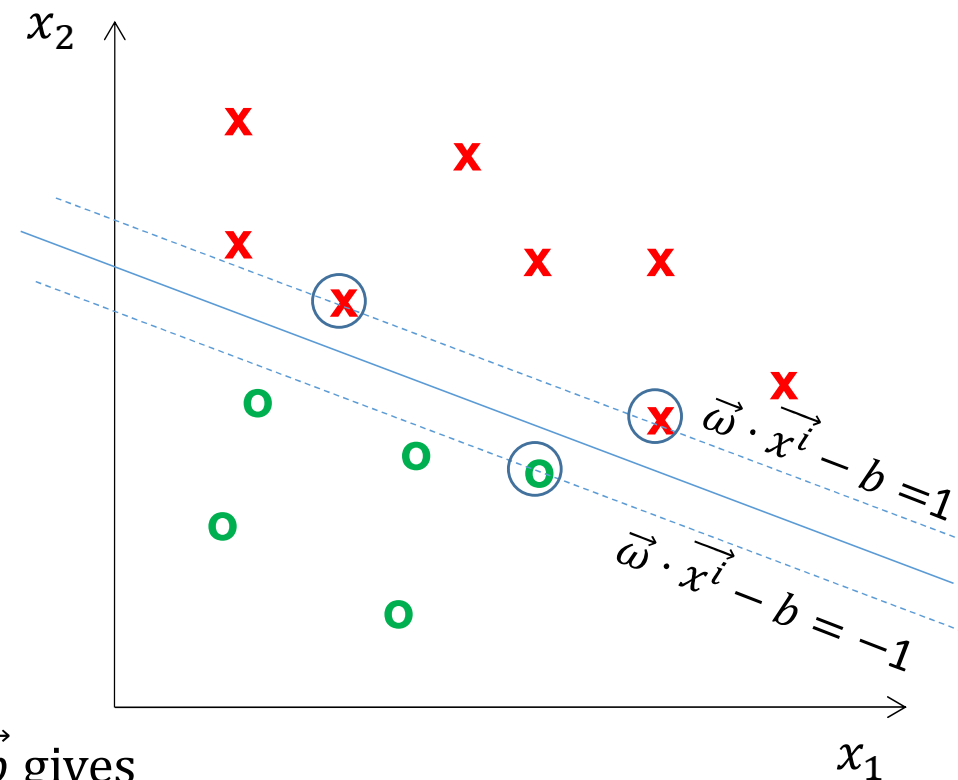
- Class **o** (-1) if  $\vec{\omega} \cdot \vec{x}^i - \vec{b} < 0$

- Training

- minimize  $\|\vec{\omega}\|$  subject to  $\vec{\omega} \cdot \vec{x}^i - \vec{b}$  gives

- the correct classification  $y^i$  for all data samples  $\vec{x}^i$

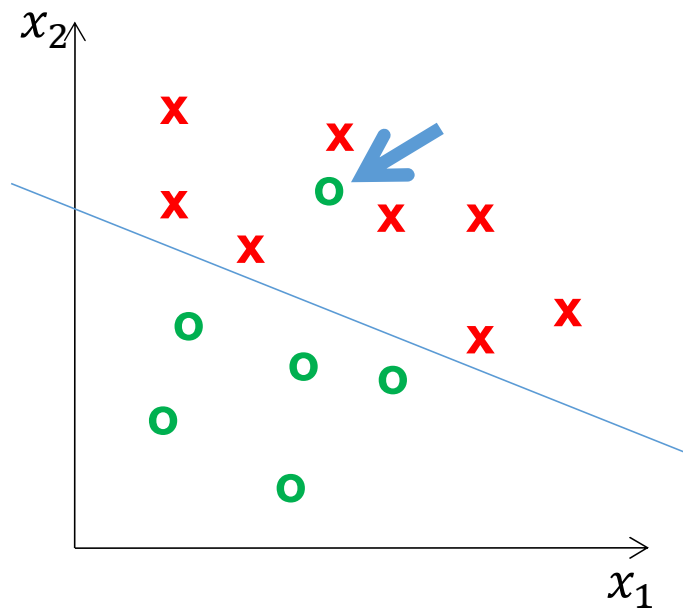
- Optimal solution  $\vec{\omega}_{opt} = \sum_k \alpha^k y^k \vec{x}^k$





- Supervised learning: Support Vector Machines

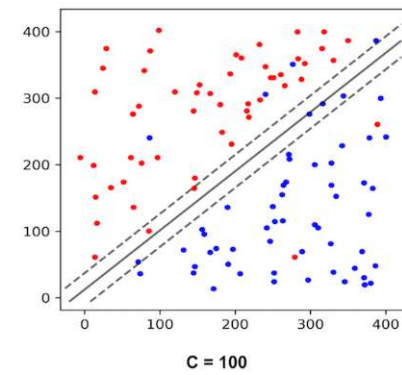
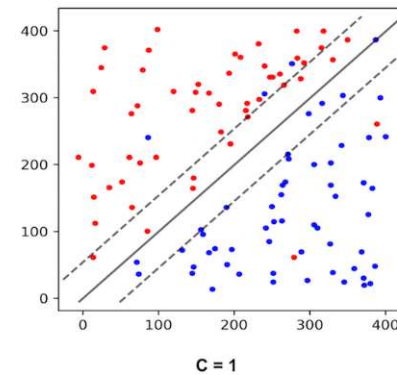
What if data is non-linear?



Option A



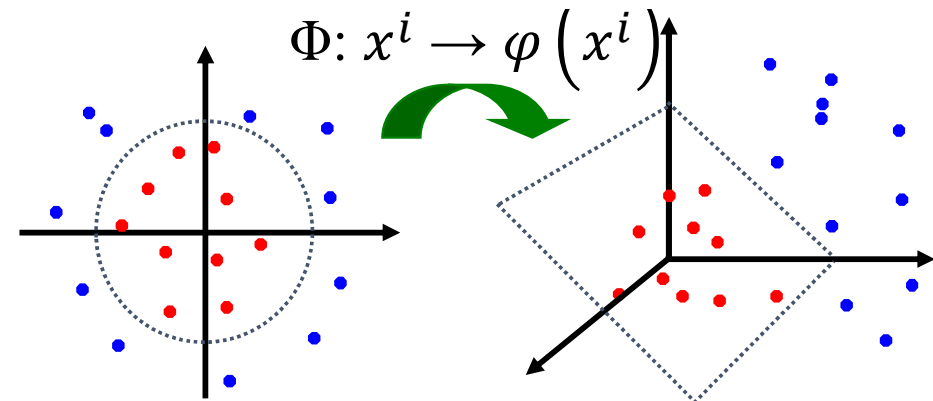
Employ a linear SVM and tolerate errors (i.e. add a C regularization term)



Option B



Map data instances to a higher dimensional space where data is linearly separable



Credit images: <https://www.learnopencv.com/svm-using-scikit-learn-in-python/>  
& Andrew Moore

- Decision Trees<sup>1</sup>:

- Very popular algorithm due to their intelligibility and simplicity

- **Classification or regression**

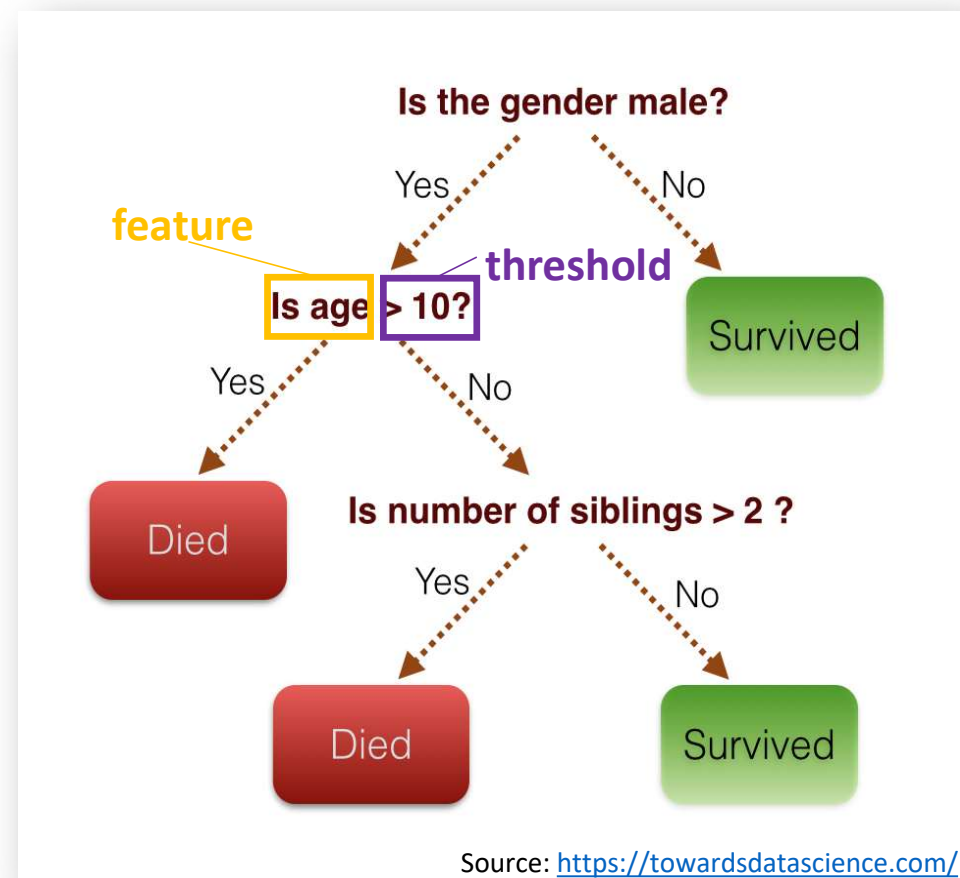
- Structure:

- Root Node
- Intermediate Nodes
- **Leaf nodes → predictions**

- Tree structure built sequentially by:

- Splitting data into subsets (i.e. for each available feature)
- Measuring feature performance
- Finding the optimal threshold

### Survival of passengers on the Titanic



<sup>1</sup>X. Wu et al. "Top 10 algorithms in data mining". Knowledge and information systems, 14(1), 1-37. 2008.

- Combine **multiple algorithms** applied to the same data to get one high-accuracy meta-algorithm
  - “No Free Lunch” Theorem - No single algorithm wins all the time!

Weather forecast for 7-days (sun or storm?)

Reality (ground-truth)	M	T	W	T	F	S	S
ML algo 1		X		X			X
ML algo 2	X			X			X
ML algo 3			X		X	X	
ML algo 4			X		X		
ML algo 5		X				X	
Combine							

Example based on Dr. Carla P. Gomes

- When combining multiple **independent** and **diverse predictions** which are at least **more accurate than random** guessing, random errors cancel each other, **correct predictions are reinforced**.
- Often **weak learners** are employed in the ensemble (**low-accuracy but very fast time** for training and prediction)

Weather forecast for 7-days (sun or storm?)

Reality (ground-truth)	M	T	W	T	F	S	S
ML algo 1	☁️	☁️ X	☀️	☁️ X	☁️	☀️	☁️ X
ML algo 2	☁️ X	☀️	☀️	☁️ X	☁️	☀️	☁️ X
ML algo 3	☁️	☀️	☁️ X	☁️	☁️ X	☁️ X	☀️
ML algo 4	☁️	☀️	☁️ X	☁️	☁️ X	☀️	☀️
ML algo 5	☁️	☁️ X	☀️	☁️	☁️	☁️ X	☀️
Combine	☁️	☀️	☀️	☁️	☁️	☀️	☀️

Each **classifier has 70% accuracy** for the task and it is independent to other classifiers

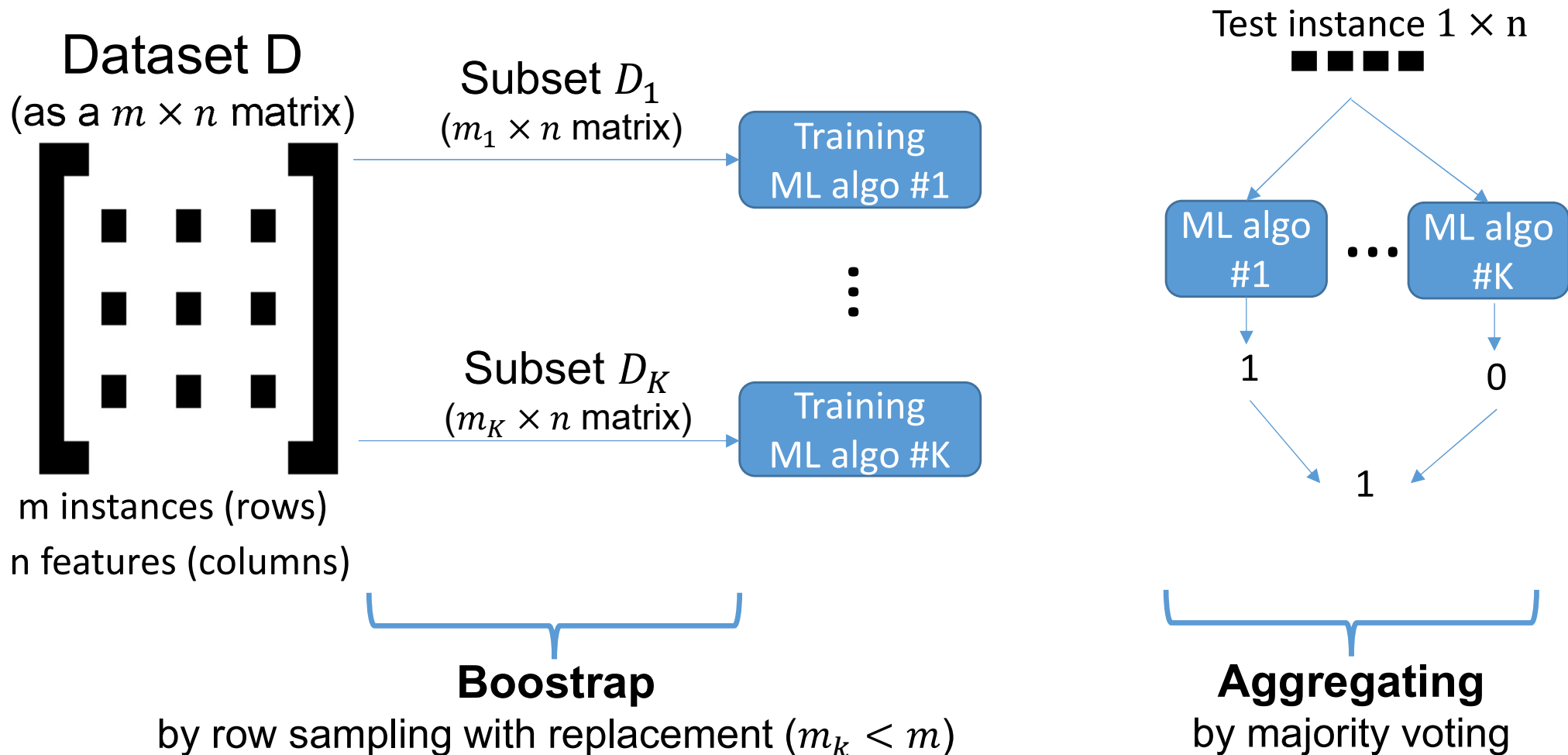
### Majority vote accuracy

- 5 classifiers - **83.7% accuracy**
- 101 classifiers - **99.9% accuracy**

Hint: Probability that  $k$  out of  $n$  independent trials of a random experiment are successful, with success probability  $p$  is  $\binom{n}{k} p^k (1 - p)^{n-k}$

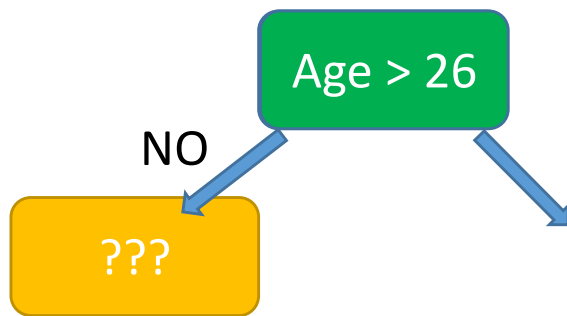
- Two main design choices
  - **Combining strategies:** averaging, majority vote, stacking,...
  - **Learning paradigm:** bagging, boosting,....

**Goal:** **reduce the variance** (i.e. low test accuracy) of combining weak learners by **parallel training** each algorithm with a subset composed of **random selection of data instances**



- Random Forest<sup>1</sup>

- **Widely used** ensemble method that employs **decision trees**.
- However, **decision trees alone tend to overfit** when becoming deep (overfitting  $\equiv$  high variance  $\equiv$  high train accuracy and low test accuracy)
- To overcome this limitation, **features are randomly selected for each node of the tree**, so to avoid dependency on “dominant” features

Decision Tree  $DT_1$ 

For each intermediate node, take remaining features and repeat the random selection & choosing the best feature

Subset  $D_1$   
( $m_1 \times n$  matrix)

#children	Age	Commute time	Salary	Change job?
0	27	30min	32K	No
2	30	15min	35k	No
0	22	30min	20k	Yes
1	27	15min	25k	Yes
1	26	15min	25k	Yes

<sup>1</sup>L. Breiman. “Random Forests”, Machine Learning 45 (1): 5-32. ,Springer, 2001

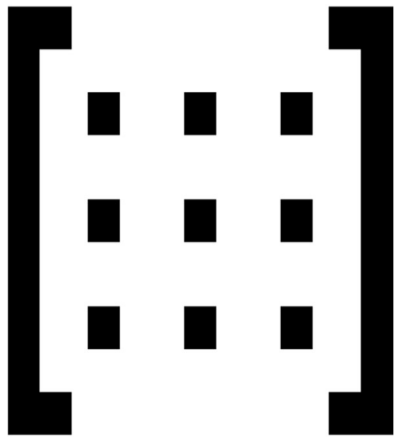
**Goal:** learn a **cascade of algorithms** (weak learners), where each algorithm attempts to **correct the previous errors**

Bagging / Random Forest	Boosting / Adaboost <sup>1</sup>
<ul style="list-style-type: none"><li>- All data samples have equal weight</li><li>- Parallel algorithms</li><li>- All algorithms have equal say</li><li>- Fully grown trees (each tree may have different depth)</li></ul>	<ul style="list-style-type: none"><li>- Data samples have adaptive weights</li><li>- Sequential algorithms</li><li>- All algorithms have different say</li><li>- Weak learners: stumps (trees with one node and two leaves)</li></ul>

<sup>1</sup>Y. Freund & R. Schapire. "A decision-theoretic generalization of on-line learning and an application to boosting". *Journal of Computer and System Sciences*. 55: 119–139, 1997

- Adaboost<sup>1</sup>

Dataset D  
(as a  $m \times n$  matrix)



m instances (rows)  
n features (columns)

We have weights associated to each data instance

### Test stage

**Execution:** apply all the algorithms in the ensemble for each data instance.

**Get overall "say":** accumulate the "say" or importance of classifiers for the predictions

**Final prediction:** prediction with the highest accumulated importance or "say"

### Training stage

#### Initialization:

- Set equal weights to all data instances
- Define the number of algorithms

...

#### Recursively do for each ML algorithm $i$ th

##### 1. Training

- Randomly select a subset of data based on data instance weights
- Train ML algorithm  $i$ th
- Evaluate accuracy using subset

##### 2. Update

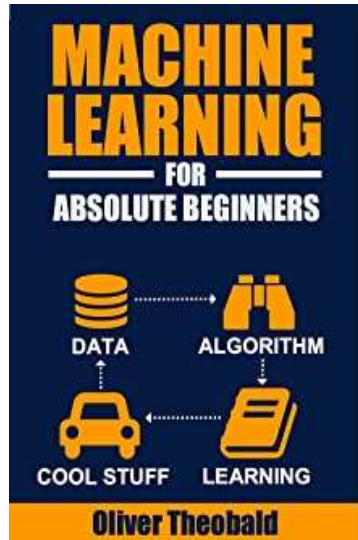
- Compute "say" for algorithm  $i$ th proportional to its accuracy
- Update weights of data instances
  - Increase weight if incorrect
  - Decrease weight if correct

<sup>1</sup>Y. Freund & R. Schapire. "A decision-theoretic generalization of on-line learning and an application to boosting". *Journal of Computer and System Sciences*. 55: 119–139, 1997



- Machine Learning requires to **prepare raw data** in order to remove noise, errors or impose requirements of algorithms
  - Data cleaning & annotation, Feature selection & transforms, ...
- Must **understand the type of ML algorithms needed** to solve a particular problem (it may be a mix of different types)
- Most of the **training strategies oriented to avoid overfitting** (i.e. high train accuracy but low test accuracy)
- Finding best algorithms/ensembles may involve running multiple times with different settings (**hyperparameter tuning**)

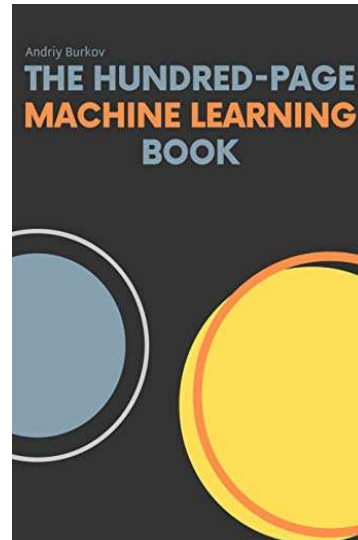
Beginner



2nd Ed 2021

<https://amzn.to/2TUhHXW>

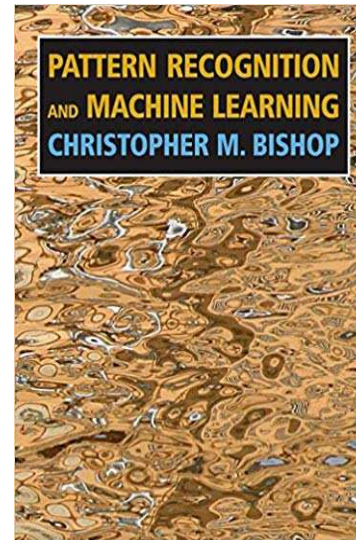
Intermediate



2019,

<https://bit.ly/2TRmtW4>

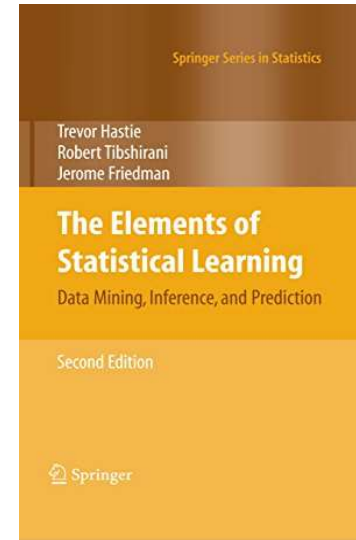
Intermediate



2006

<https://bit.ly/2V7wz5W>

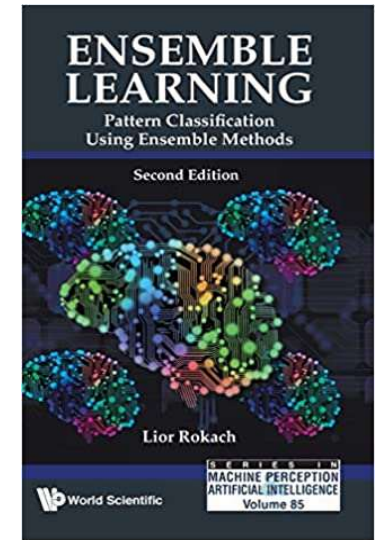
Expert



2009

<https://bit.ly/3jhvPTw>

Expert



2nd Ed 2019

<https://amzn.to/3io2R57>

- As for practical work, please do check tutorials and up-to-date examples available for popular ML & DL frameworks (TensorFlow, PyTorch, scikit-learn, Spark ML, Torch, Keras,...)

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ANY QUESTIONS?