



Machine Learning

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2021

Content

1. The Big Picture

2. Supervised Learning

- Linear Regression, Logistic Regression, Support Vector Machines, Trees, Random Forests, Boosting, Artificial Neural Networks

3. Unsupervised Learning

- Principal Component Analysis, K-means, Mean Shift

Supervised Learning

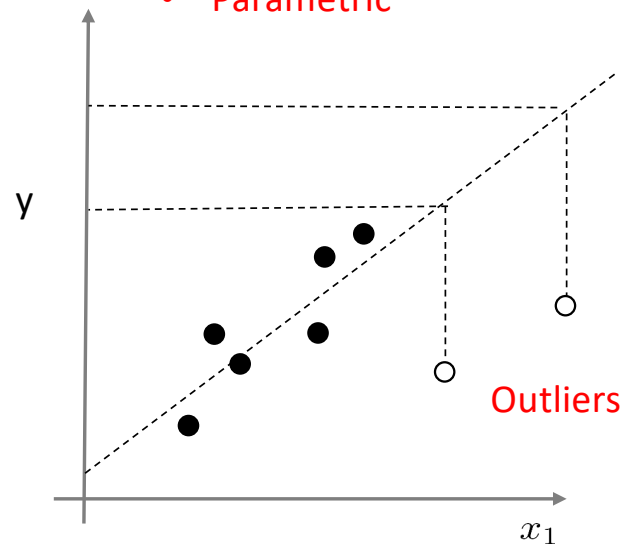
- Linear Regression
- Logistic Regression
- Support Vector Machines
- **Trees (Decision and Regression)**
- **Random Forests**
- **Boosting**
- Artificial Neural Networks

Classification and Regression Trees (CART)

Regression

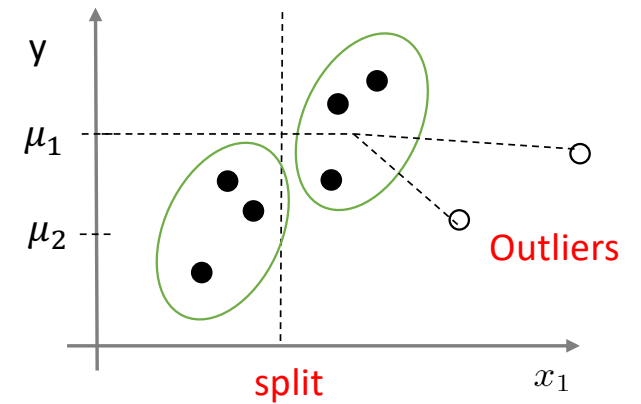
Linear regression

- Linear models
- Parametric



Regression trees

- Non Linear model
- Non-Parametric

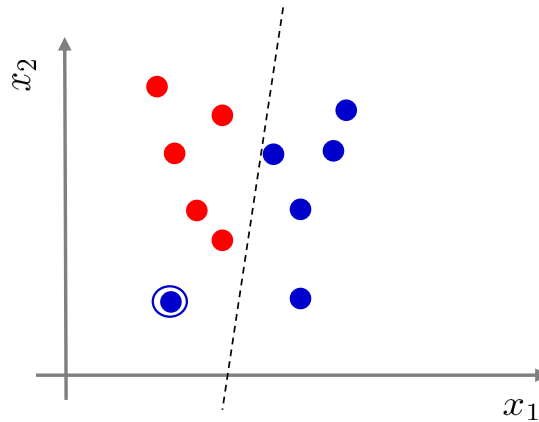


Classification and Regression Trees (CART)

Logistic regression

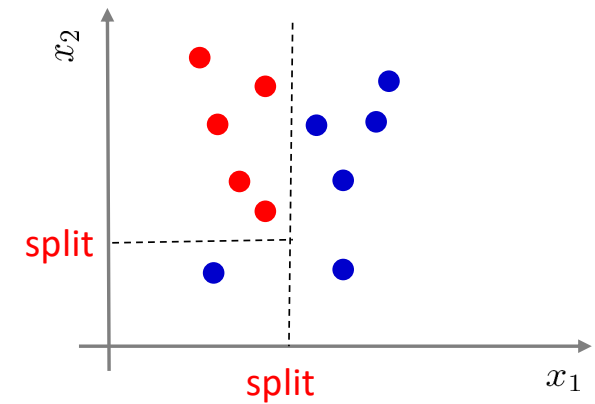
- Linear models
- Parametric

Classification



Classification trees

- Non Linear model
- Non-Parametric



Classification Trees (aka Decision Trees)

Example of Restaurant Data

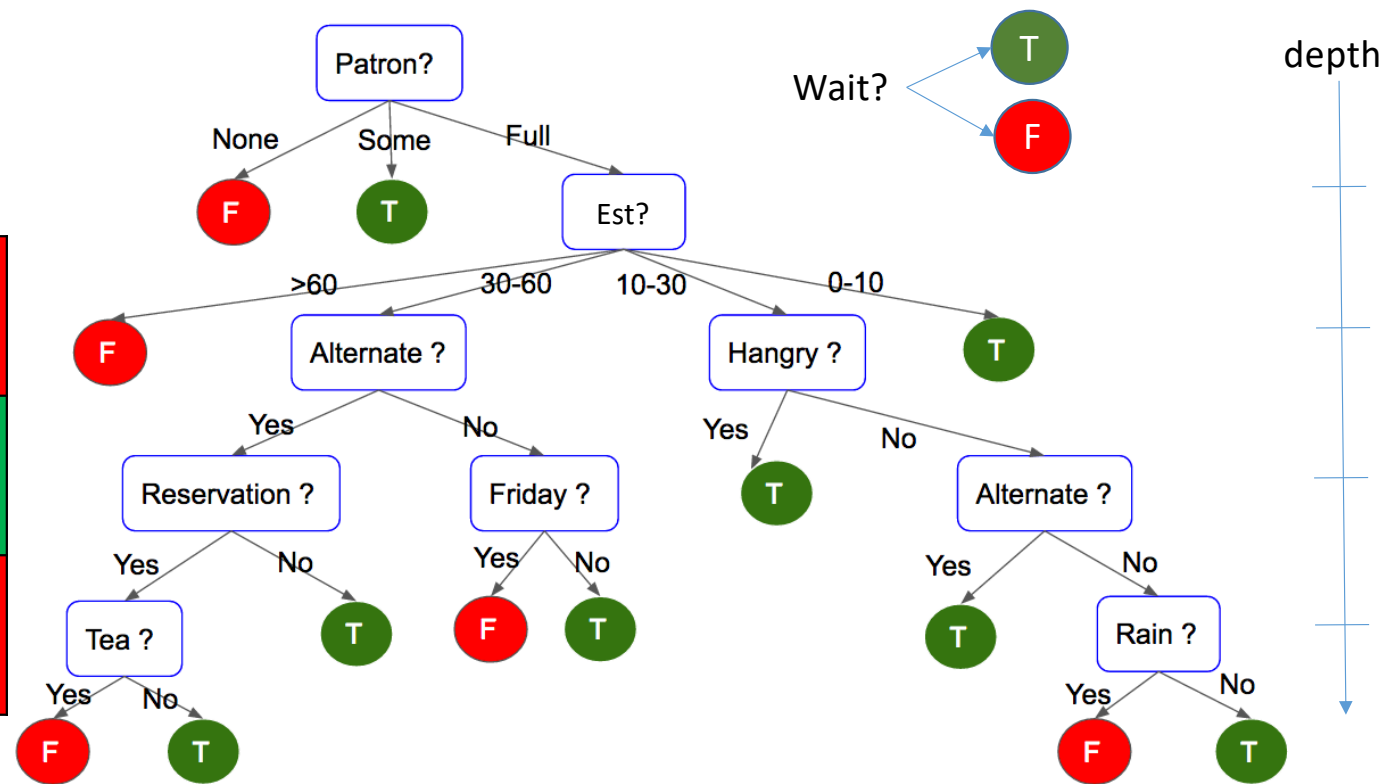
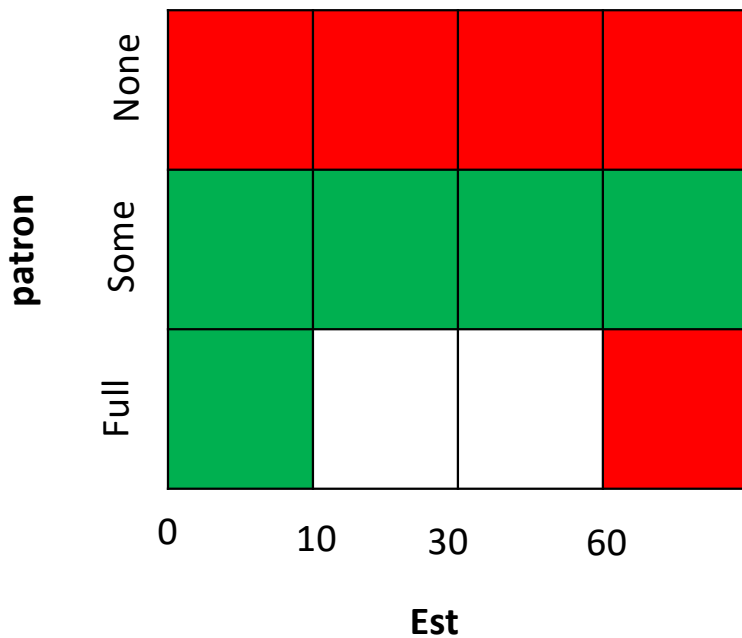
X	F										Y
Client	Alt	Tea	Fri	Hun	Patron	Price	Rain	Res	Type	Est	Wait
1	T	F	F	T	Some	\$\$\$	F	T	Moroccan	0-10	T
2	T	F	F	T	Full	\$	F	F	Chinese	30-60	F
3	F	T	F	F	Some	\$	F	F	Burger	0-10	T
4	T	F	T	T	Full	\$	F	F	Chinese	10-30	T
5	T	F	T	F	Full	\$\$\$	F	T	Moroccan	>60	F
6	F	T	F	T	Some	\$\$	T	T	Italian	0-10	T
7	F	T	F	F	None	\$	T	F	Burger	0-10	F
8	F	F	F	T	Some	\$\$	T	T	Chinese	0-10	T
9	F	T	T	F	Full	\$	T	F	Burger	>60	F
10	T	T	T	T	Full	\$\$\$	F	T	Italian	10-30	F
11	F	F	F	F	None	\$	F	F	Chinese	0-10	F
12	T	T	T	T	Full	\$	F	F	Burger	30-60	T

- Alt: is there any other alternative?
- Fri: is it Friday?
- Hun: is the client hungry?
- Patron: how many people are in the restaurant?
- Res: Restaurant
- Est: wait estimate

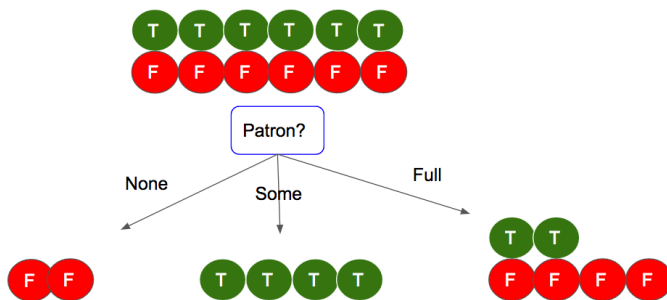
Most of the features are
Discrete (=categorical, =qualitative)

Classification Trees (aka Decision Trees)

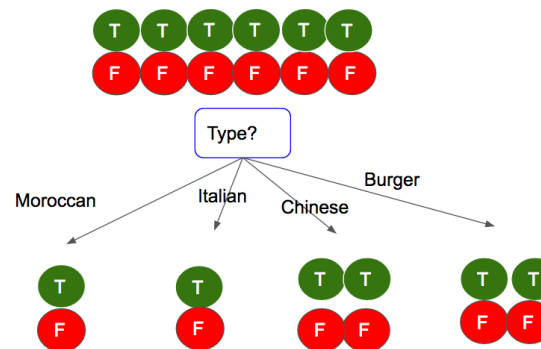
Pick one feature at a time,
and make a binary decision



DT: Which feature to split with first?



More informative
Less impurity



Less informative
More impurity

Split with the feature
F that **maximizes** the
Information Gain

$$I(F) = H(S) - EH(F)$$

Information
Gain

Parent
entropy

Expected
entropy

S: subset = {p positives and n negatives}

F: Feature

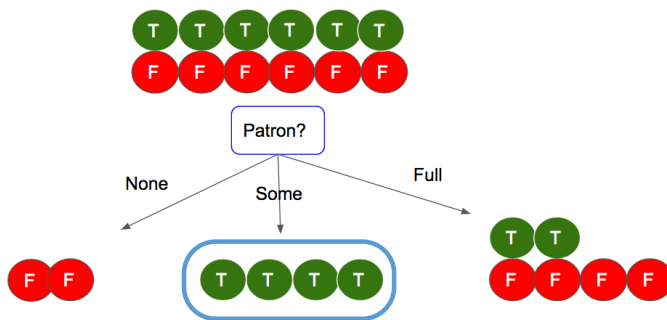
Entropy

$$H(S) = - \sum_c p_c \log_2(p_c)$$

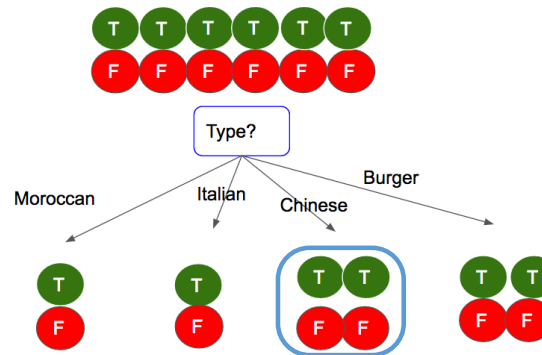
Python: `np.log2()`

p_c : probability of examples in class c
 S : subset of data examples

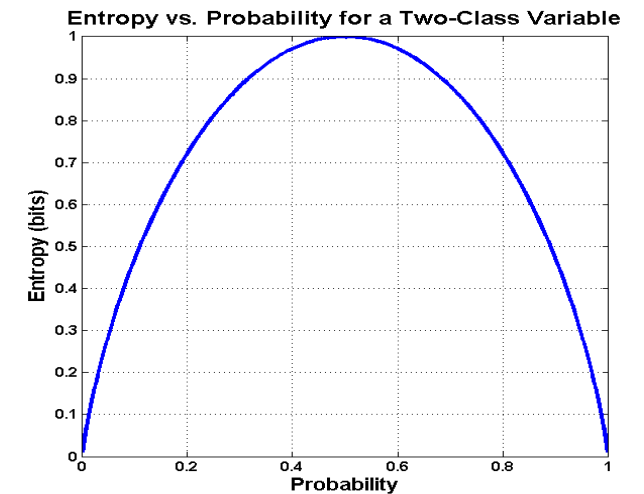
Interpretation: Measure of the **impurity** in a **subset** of examples



All examples in the **same** class
Entropy = 0



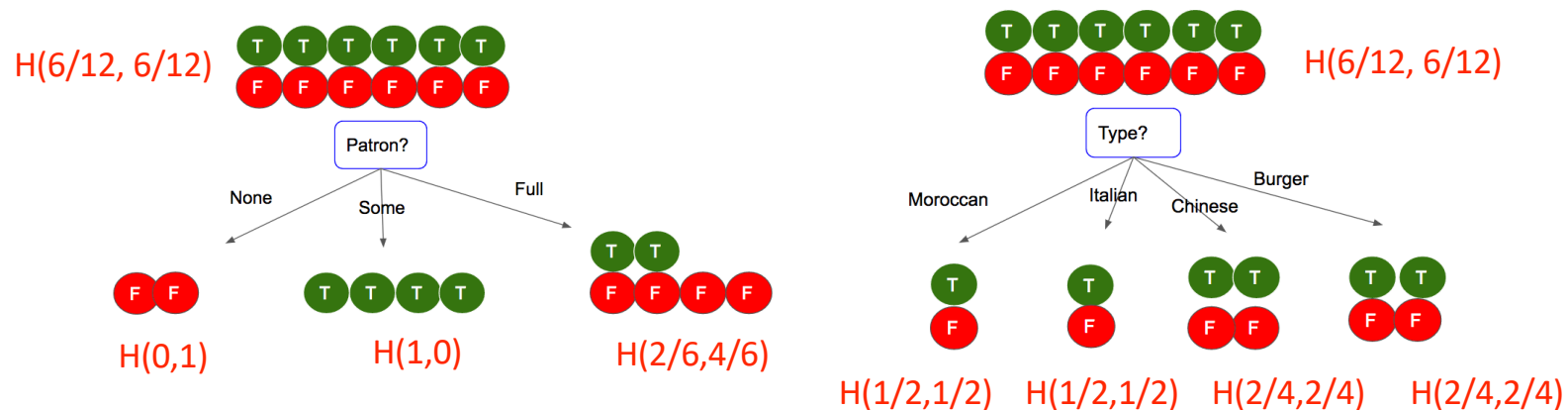
All examples **evenly split** between classes
Entropy = 1



Entropy (binary classification)

$$H\left(\frac{p}{p+n}, \frac{n}{p+n}\right) = -\frac{p}{p+n} \log\left(\frac{p}{p+n}\right) - \frac{n}{p+n} \log\left(\frac{n}{p+n}\right)$$

p: positive
n: negative

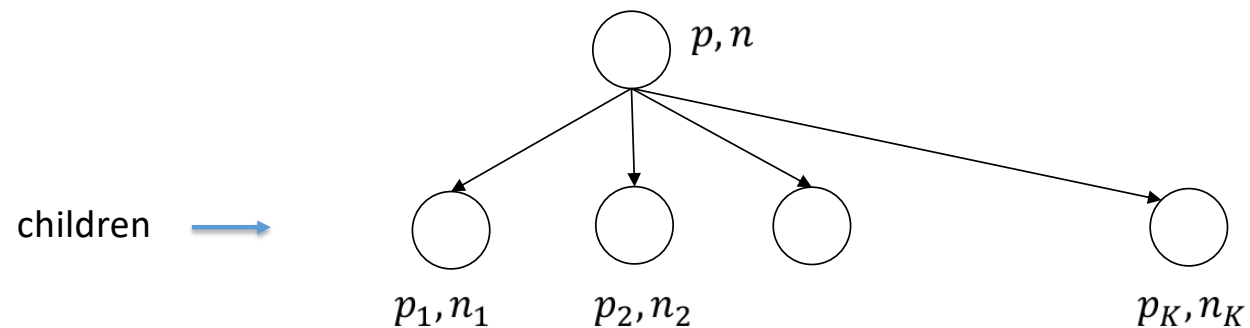


Expected Entropy

$$EH(F) = \sum_{i=1}^K \frac{p_i + n_i}{p + n} H\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$$

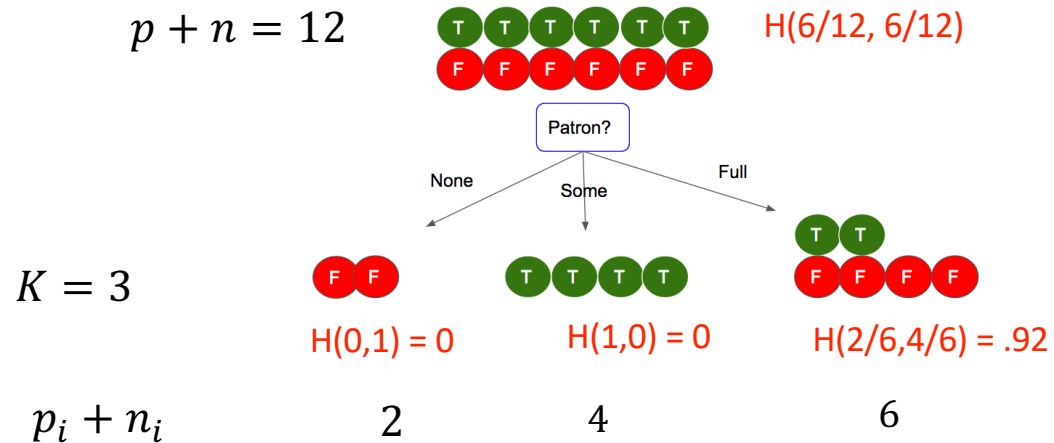
K = number of splits (regions) with Feature **F**
= number of **children nodes**

Expectation Entropy = weighted average of **children** entropy



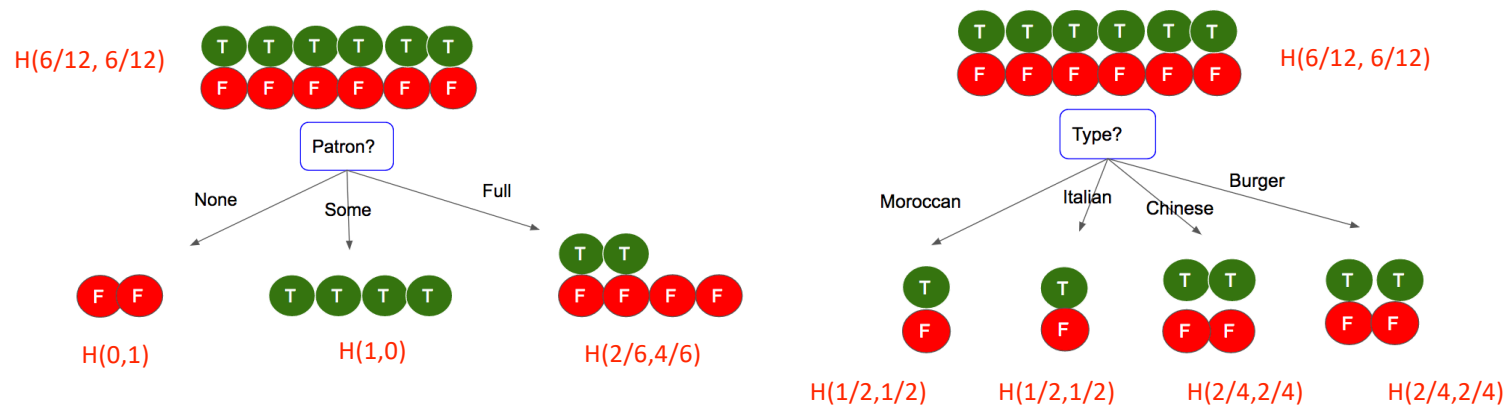
Expected Entropy (Example)

$$EH(F) = \sum_{i=1}^K \frac{p_i + n_i}{p + n} H\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$$



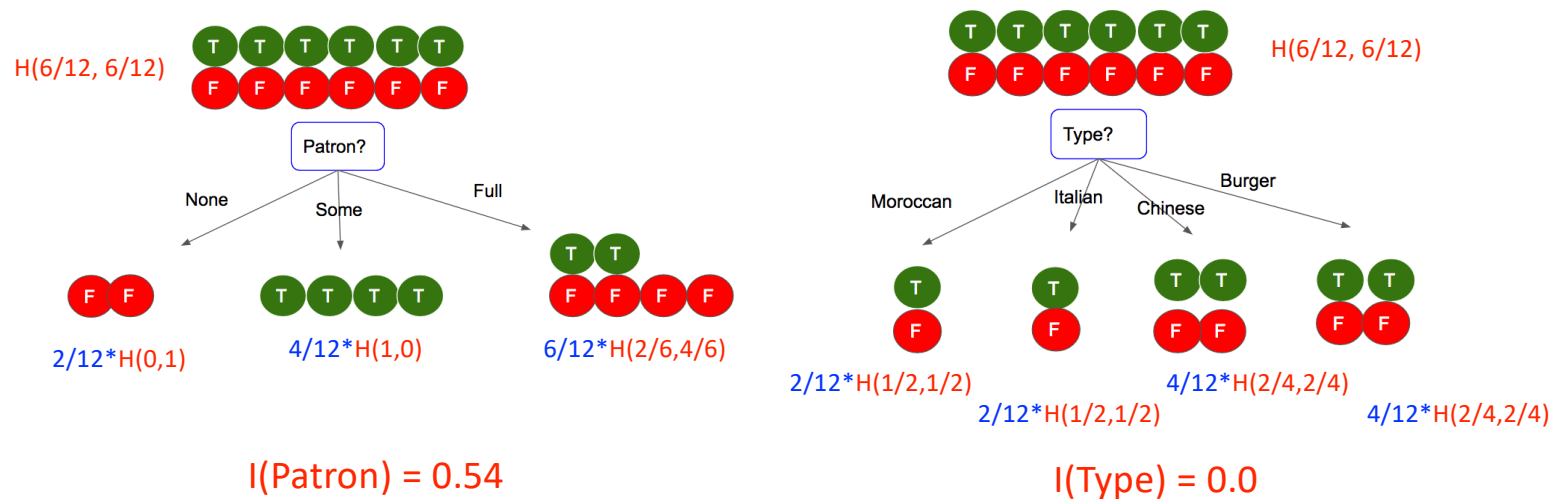
Information Gain

$$I(F) = H\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - EH(F)$$



Information Gain

$$I(F) = H\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - EH(F)$$



Other impurity measures

- p_c : probability of examples in class c
- S : subset of data examples

- **CART** algorithm uses the **Entropy**

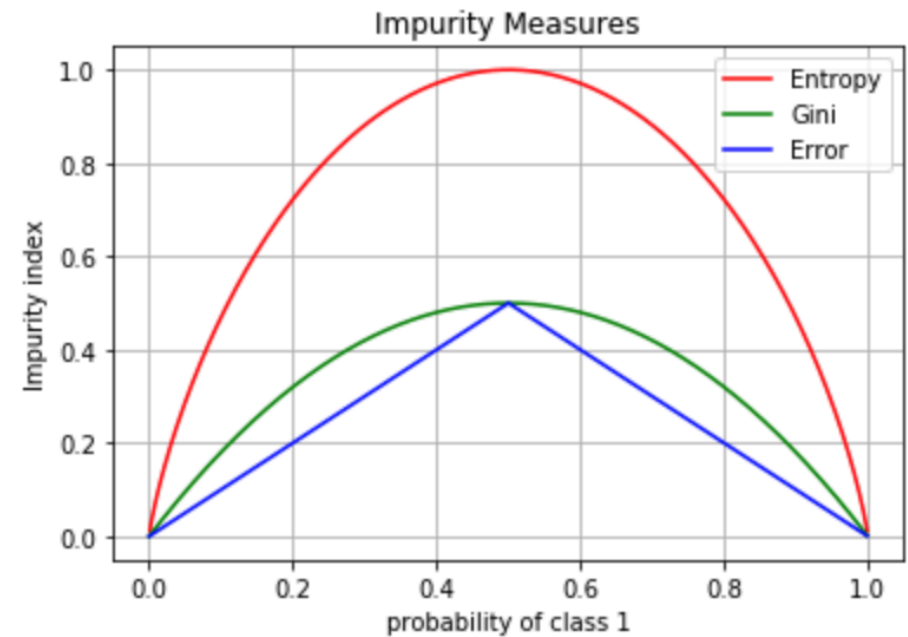
$$H(S) = - \sum_c p_c \log_2(p_c)$$

- Iterative **Dichotomiser ID3** and **C4.5** algorithms use **Gini Index**

$$G(S) = 1 - \sum_c p_c^2$$

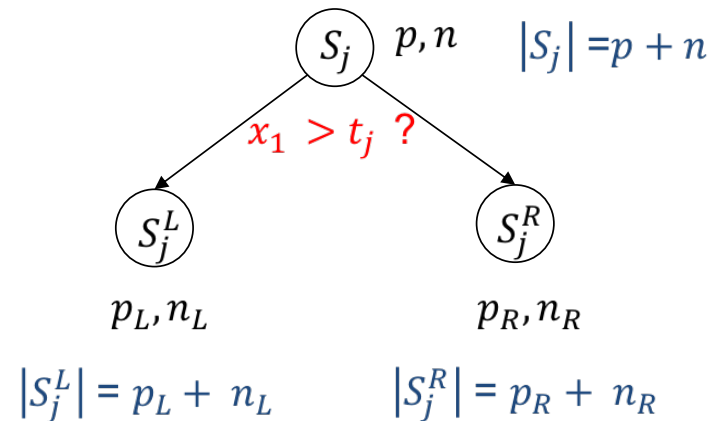
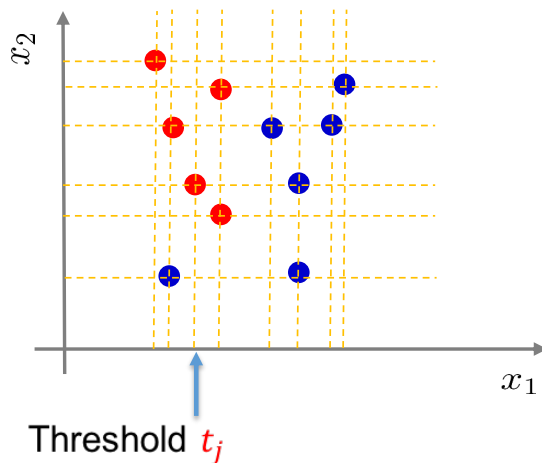
- One could also use the **Class Error**

$$E(S) = 1 - \max_c(p_c)$$



What if a feature is continuous (quantitative)?

$$I_j = H(S_j) - \sum_{i \in \{L,R\}} \frac{|S_j^i|}{|S_j|} H(S_j^i)$$



Note: Doing so, trees are almost **Binary**! Even if a feature is categorical (qualitative)

Decision Trees

- **Advantages**

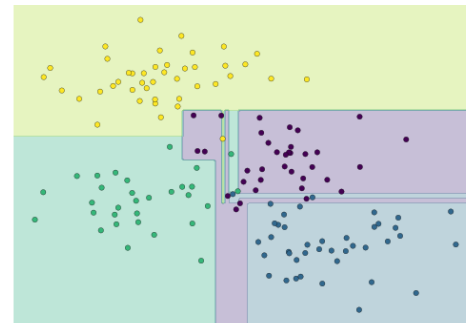
- Easy to interpret
- Deals with non linearity
- Handle qualitative features without the need to create fictive ones (one hot vector)
- Provide most important features (in terms of information gain)

Decision Trees

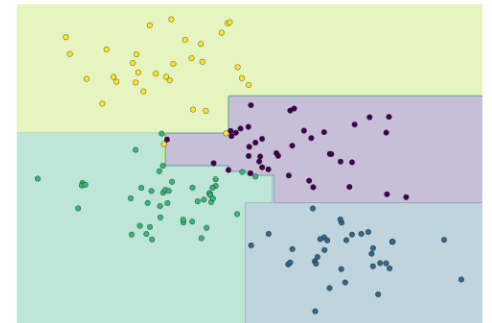
- **Disadvantages**

- Trees leads to **overfitting** (**high variance**): little change in little number of examples affect the whole tree.

DT on Data1



DT on Data2 = half of Data1



Decision Trees

- **Disadvantages**

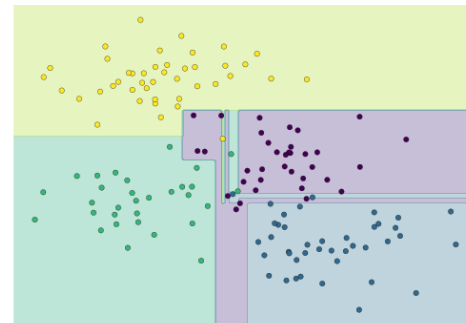
- Trees leads to **overfitting** (**high variance**): little change in little number of examples affect the whole tree.

- **Solution: Ensemble Methods**

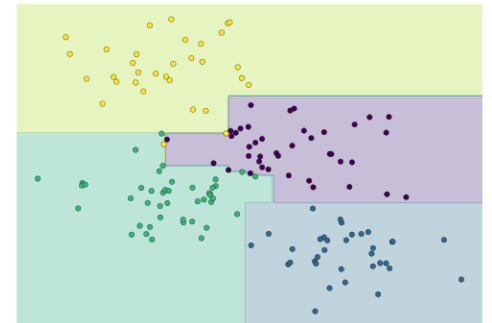
- **Bagging: Random Forest** (Leo Breiman 2001) consists of combining multiple **independent weak trees** to reduce variance.
- **Boosting** to reduce bias



DT on Data1



DT on Data2 = half of Data1



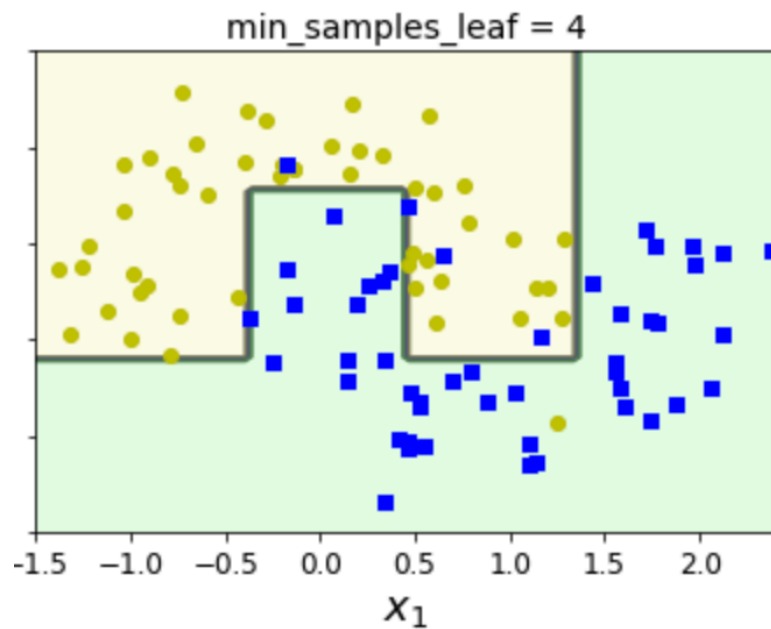
A tree **alone** will overfit.

However, it is clear that **in some places**, the two trees **together** produce consistent results

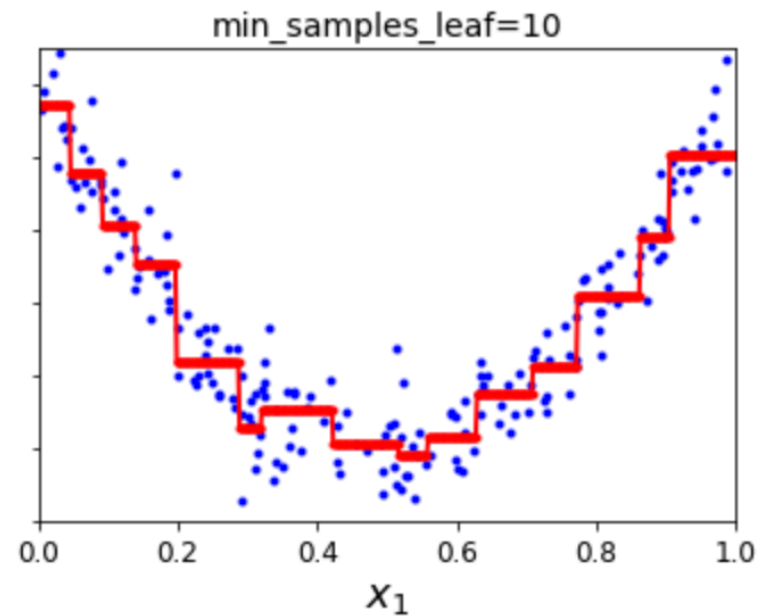
This idea comes from Bootstrapping (**Brad Efron 1979**): Given a set of **m** independent observations o_1, \dots, o_m , each with variance σ^2 , the variance of the mean **o** of the observations is given by σ^2/m .

Classification And Regression Trees

Classification (Decision) Trees



Regression Trees



Supervised Learning

- Linear Regression
- Logistic Regression
- Support Vector Machines
- Trees (Decision and Regression)
- **Random Forests**
- Boosting
- Artificial Neural Networks

Random Forest

Bagging

Bootstrap Aggregating

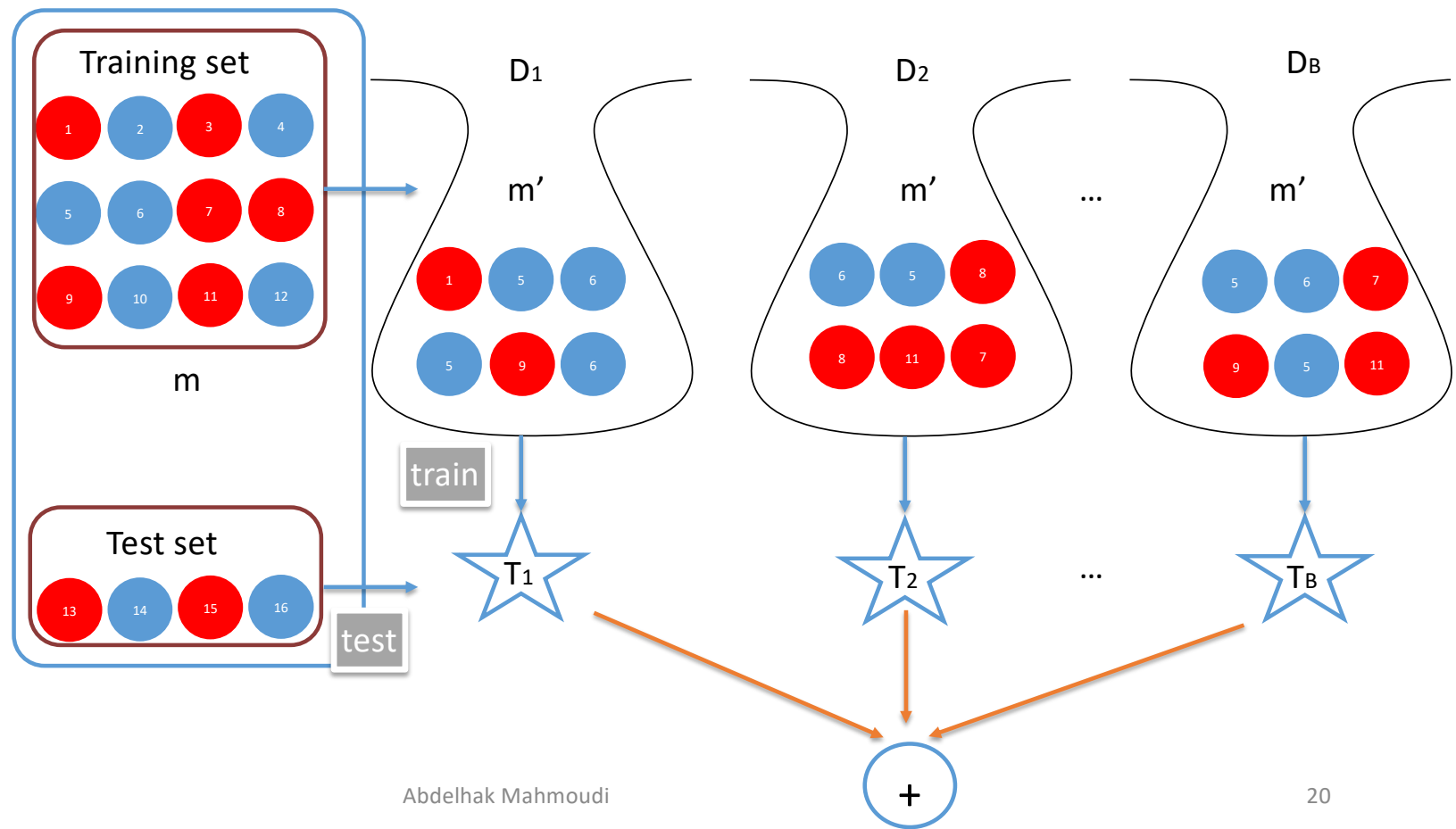
Training

Pick m' examples with replacement and train B trees

Testing

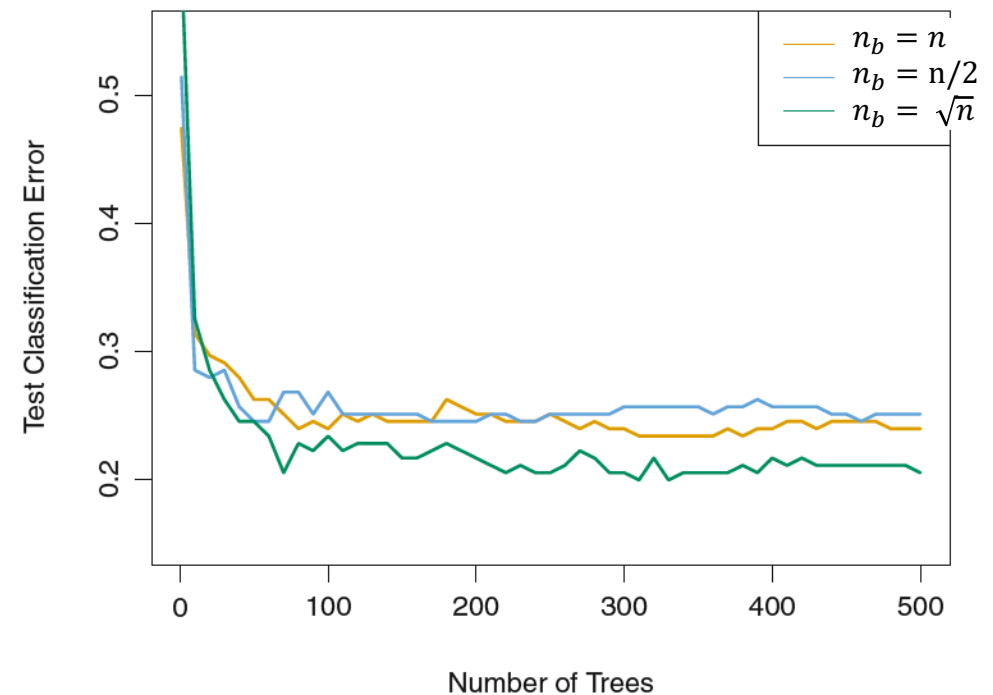
Regression: mean errors of all the B trees

Classification: vote



Random Forest

- **Problem:** Bagged trees will look quite similar to each other, so averaging them will not lead to much reduction of variance!
- **Solution:** Random Forest constructs multiple trees where each tree uses n_b random features from the n initial features (generally $n_b = \sqrt{n}$)
- $n_b = n \rightarrow$ Bagging case



Random Forest

- Both training and **prediction are very fast**, because of the simplicity of the underlying decision trees.
- Tasks can be straightforwardly **parallelized**, because the individual trees are entirely independent entities.
- The multiple trees allow for a **probabilistic** classification: a majority vote among estimators gives an estimate of the probability
- RF is a **Nonparametric** model, extremely flexible, and can thus perform well on tasks that are under-fit by other models.

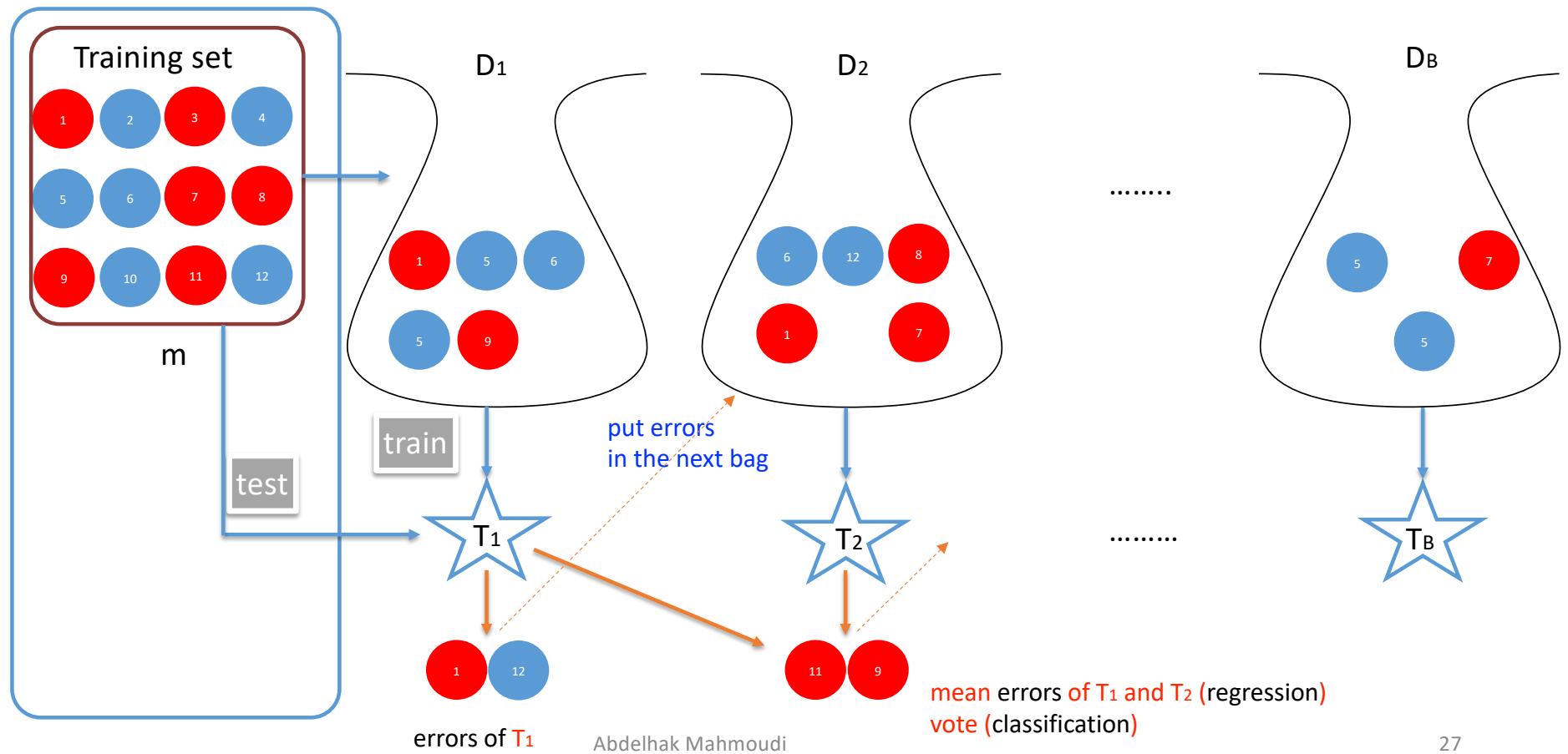
Random Forest

- Hyper-Parameters Tuning
 - d: Depth of the trees
 - B: number of Bags (Estimators)

Supervised Learning

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- Trees (Decision and Regression)
- Random Forests
- **Boosting**
- Artificial Neural Networks

Boosting



Boosting

- **Outperforms** RF
- **Smaller Trees** (depth = 1) are sufficient because the growth of a particular tree takes into account **preceding** trees.
- Smaller trees can aid in **interpretability**.
- **Boosting** (Freund & Schapire 1990)
- **Adaboost** (**A**daptive **B**oosting), 1996

