Machine Learning Days, EPFL

YYYYXYYYYY

Ensemble Techniques: "Unity is strength"

Jessica Lanini EPFL, Lausanne January, 2020



Ensemble Techniques: "Unity is strength"

Machine Learning Days, EPFL

YYXYYXYYYYY

What to expect from the workshop:

[13:30-14:30] Theory of ensemble techniques

What ensemble techniques are

Different types of ensemble techniques: overview

Background: Decision Tree

Random Forest

AdaBoost

[14:30- 14:45] Q&A

[14:45-15:00] Introduction to the Mini-Project: Predicting Daily Bike Rentals

[15-17] Mini-Project: Predicting Daily Bike Rentals

Analysis and Data Preparation

Definition of useful functions (e.g. cross-validation)

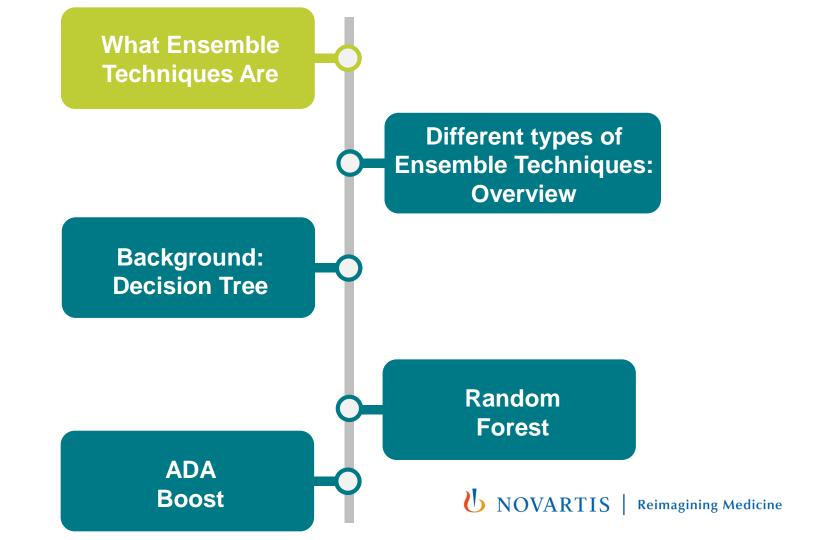
Models evaluation

Analysis of features importance

Robustness Analysis

Hyperparameters Optimization



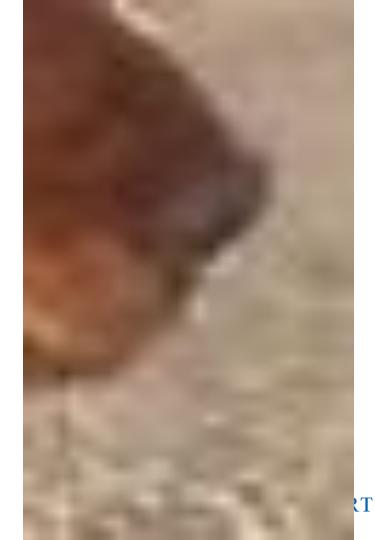


QUIZ!!!

What does the image represent?







Reimagining Medicine









ARTIS | Reimagining Medicine

QUIZ!!!

What does the image represent?

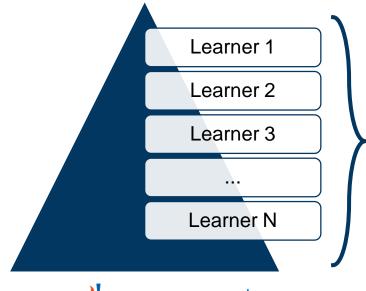


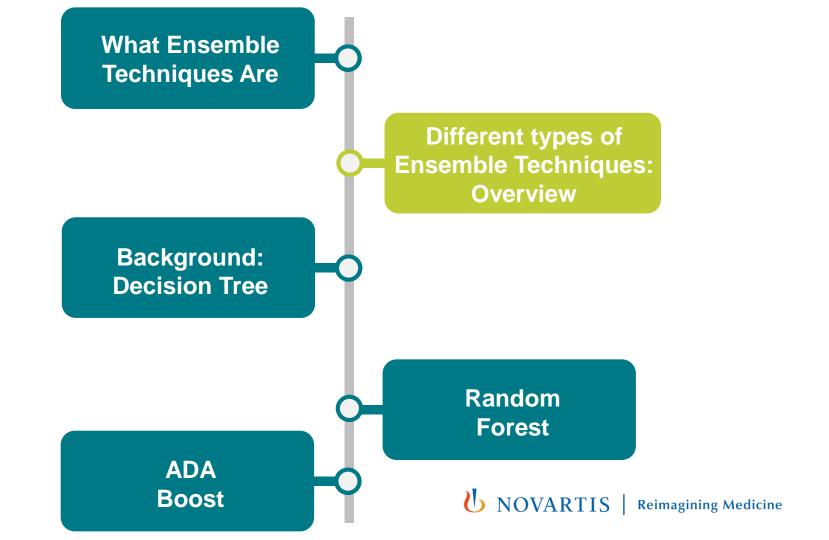


What Ensemble Techniques Are

Techniques that use multiple learning algorithms to obtain better <u>predictive</u> <u>performance</u> than could be obtained from any of the constituent learning algorithms alone.' [Wikipedia]

- Idea:
 - Train multiple `weak' learner
 - Combine their prediction
 - Voting
 - Averaging
 - Weighted Averaging

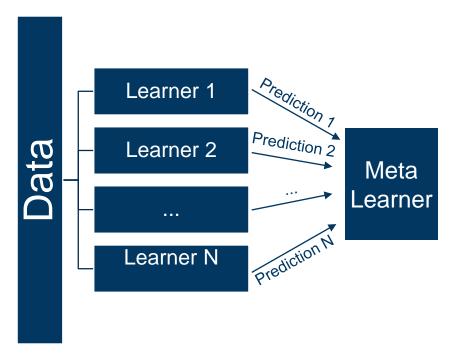




Types of Ensemble Techniques: Overview

Stacking

- N learners
- Same training set
- Meta Learner/Blender–takes previouspredictions

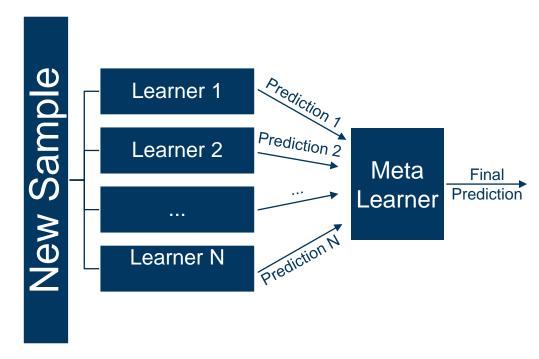




Types of Ensemble Techniques: Overview

Stacking

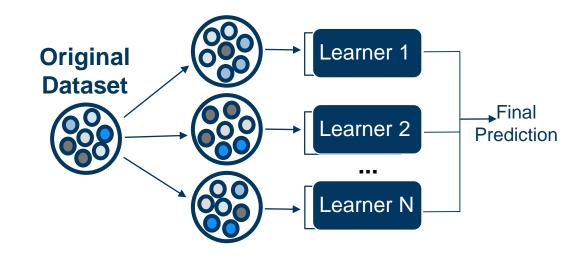
- N learners
- Same training set
- Meta Learner/Blender
 - takes previous predictions
- New sample



Types of Ensemble Techniques: Overview

Bagging

- Random sampling with replacement of the training set (bootstrap)
- Train *n* learners in parallel
- Combine predictions
- Reduce variance

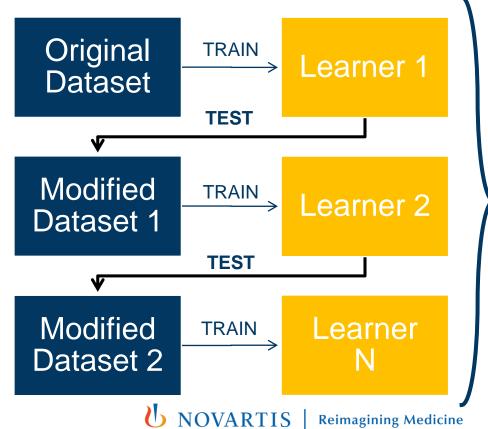


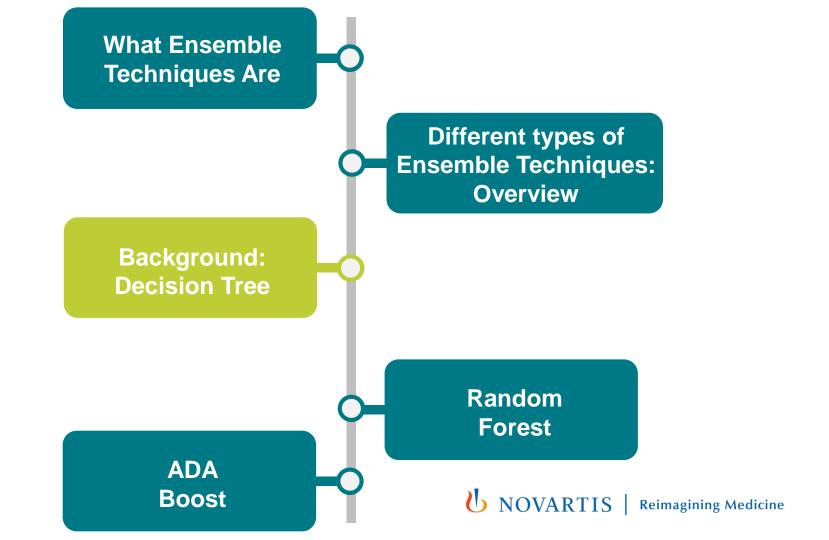
Types of Ensemble Techniques:

Overview

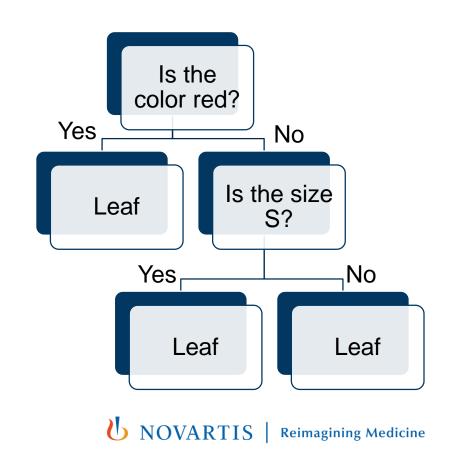
Boosting

- Weak learners are trained in series
- Train set changes according to the error of the previous learner
- Final prediction depends on the learner's amount of saying
- Reduce bias





- Non-parametric supervised learning method
- Different types:
 - ID3
 - C4.5
 - C5.0
 - CART
 - Classification and Regression Tree
 - Procedure to decide which question to ask and when



Color	Size	Discount	Label
Red	М	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	М	40%	Shirt
Green	L	50%	Skirt



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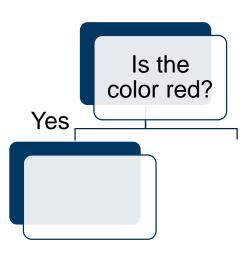


- All nodes receive a list of samples
 - Root receives the entire training set
- True/False question about one of the features

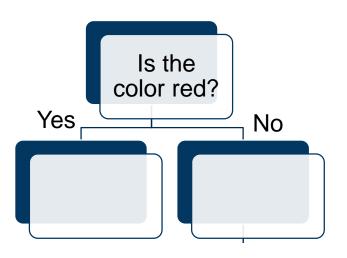
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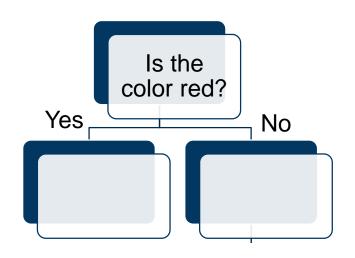


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- All nodes receive a list of samples
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- The data are split according to the answer at each sample

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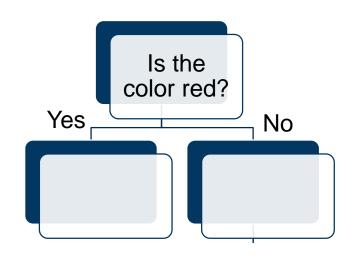


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- True/False question about one of the features
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- Goal: unmix label

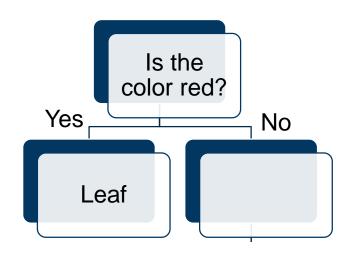


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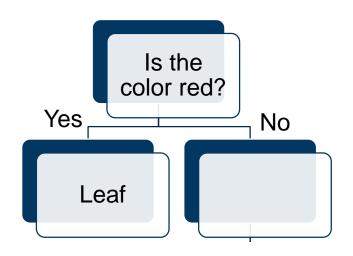
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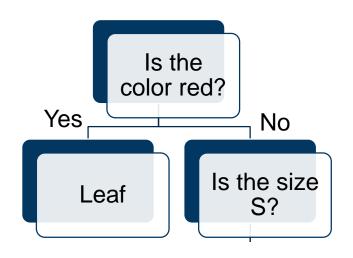
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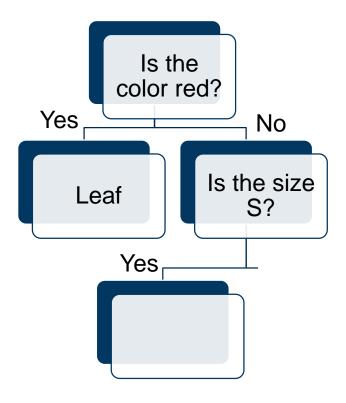


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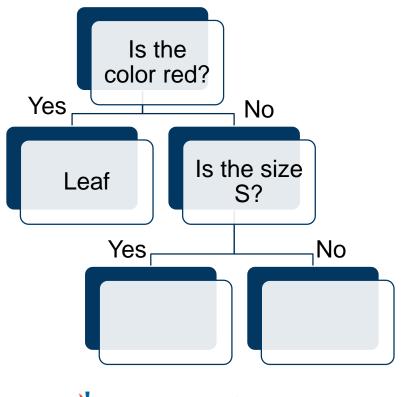
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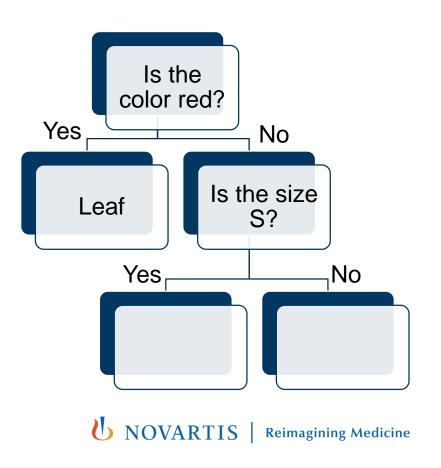




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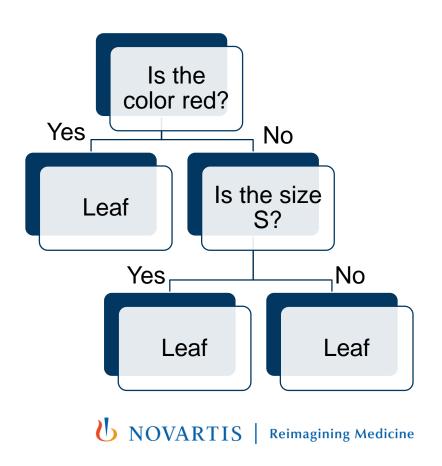
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Which question to ask and when

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- Which question to ask and when
 - Gini impurity (or Entropy)
 - Information Gain

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Gini Impurity

 quantifies the amount of uncertainty

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- quantifies the amount of uncertainty
- **•** [0,1]

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- quantifies the amount of uncertainty
- **•** [0,1]

$$G = \sum_{i=1}^C p(i)*(1-p(i))$$

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Shirt
$$G_1 = \frac{3}{5} \cdot \left(1 - \frac{3}{5}\right) + \frac{1}{5} \cdot \left(1 - \frac{1}{5}\right) + \frac{1}{5} \cdot \left(1 - \frac{1}{5}\right)$$

$$=\frac{14}{25}$$



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$$=\frac{14}{25}$$



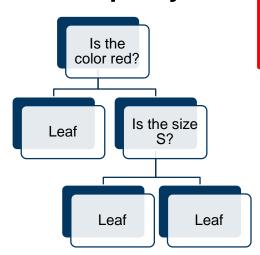
Skirt

- quantifies the amount of uncertainty
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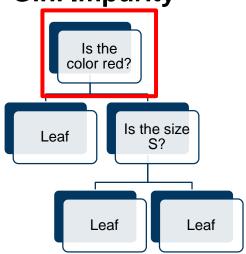
$$G_1 = \frac{14}{25}$$



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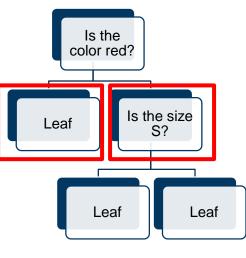


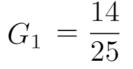
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Is the color Red?

Gini Impurity





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Is the color Red?



Color	Size	Discount	Label
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) T			



Gini Impurity

Is the color Red?

$$G_{2,1} = 1 \cdot (1-1) = 0$$



Color	Size	Discount	Label	
Yellow	S	20%	Jeans	
Green	L	50%	Skirt	
U NOVARTIS Reimagining Medicine				

 $G_{2,2} = \left[\frac{1}{2} \cdot \left(1 - \frac{1}{2}\right)\right] \cdot 2 = \frac{1}{2}$

- Which question to ask and when
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Information Gain



Information Gain

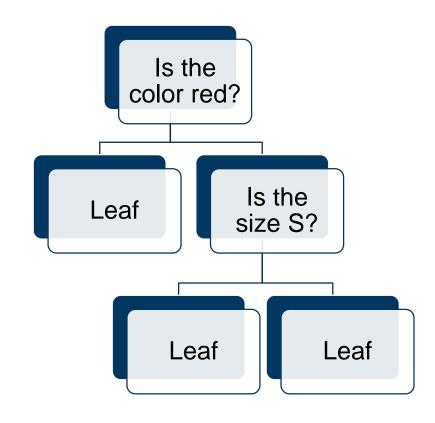
Information Gain

$$IG_i^j = G_i - G_j$$



Information Gain

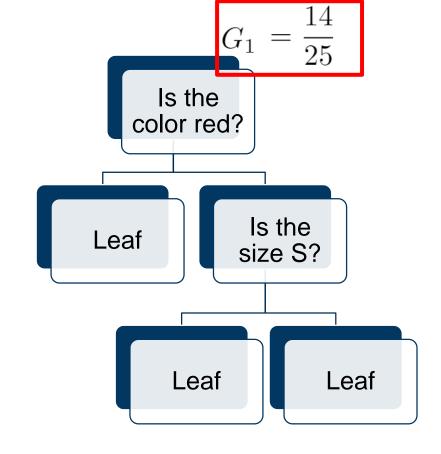
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Information Gain

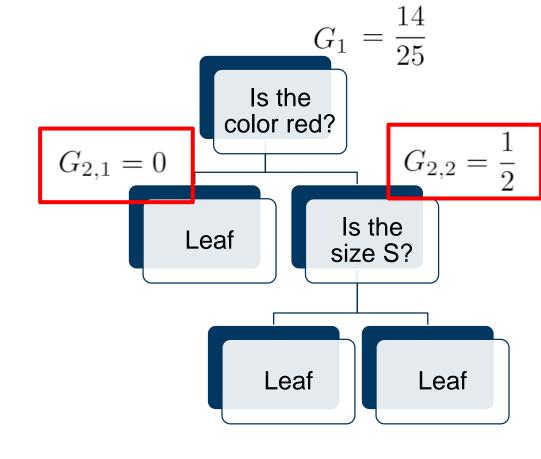
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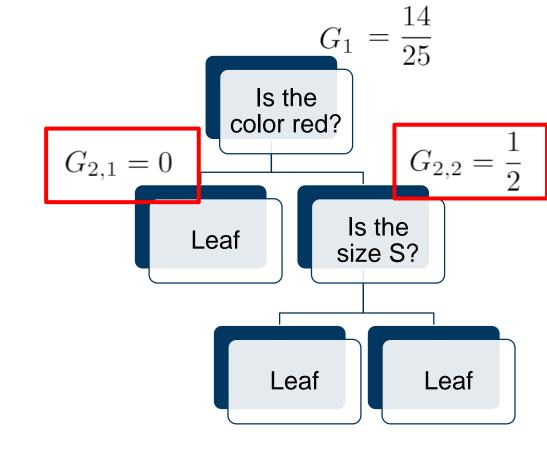
$$IG_i^j = G_i - G_j$$





Information Gain

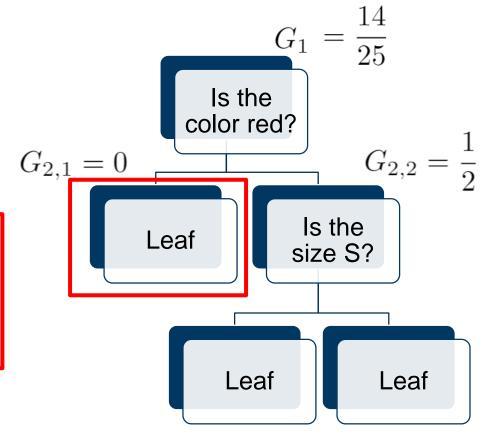
$$IG_i^j = G_i - \boxed{G_j}$$





Information Gain

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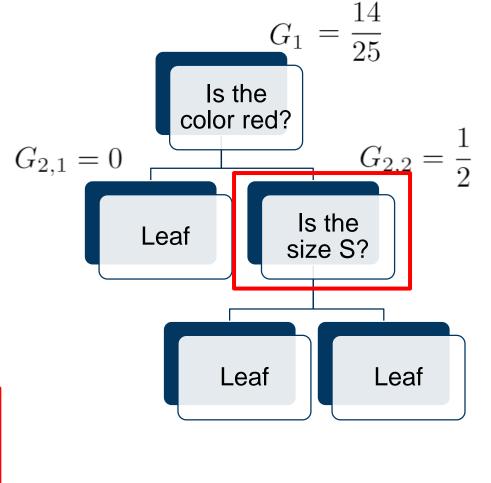




Information Gain

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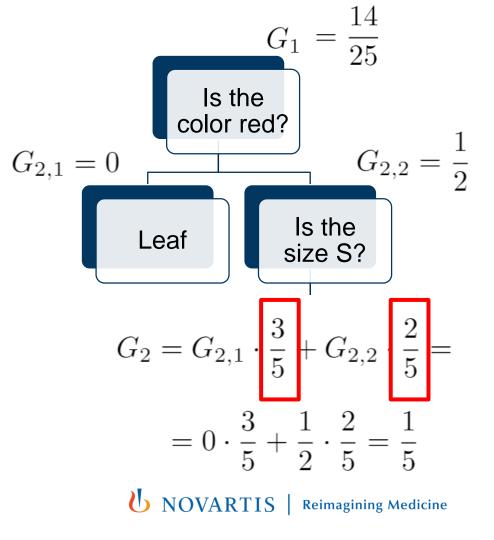




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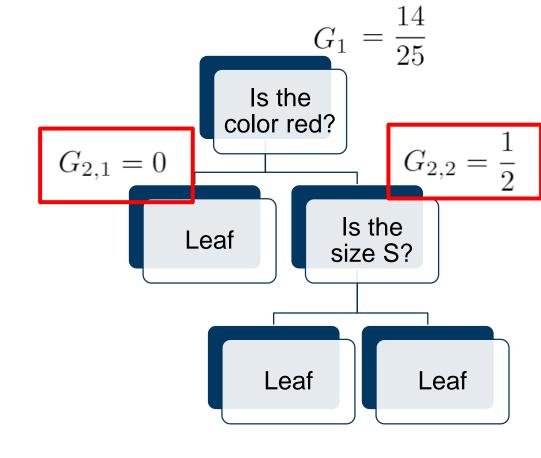
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Information Gain

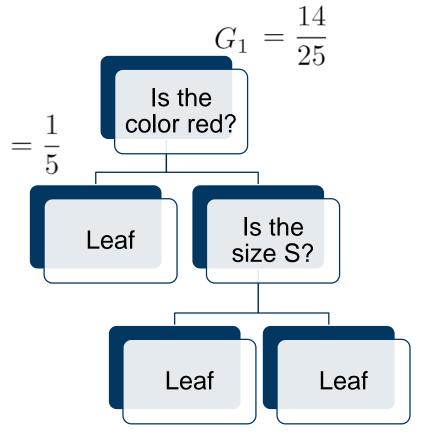
$$IG_i^j = G_i - G_j$$





Information Gain

$$IG_i^j = G_i - G_j = \frac{14}{25} - \frac{1}{5} = \frac{9}{25}$$



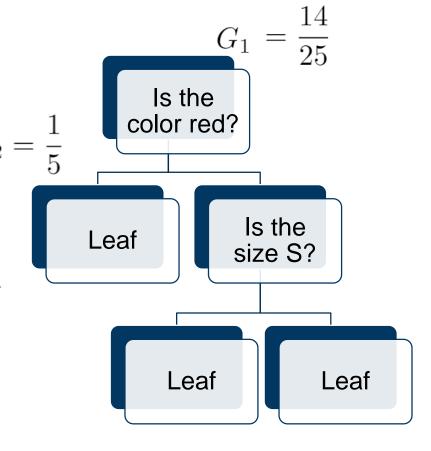


Information Gain

 How much a question reduce the uncertainties

$$IG_i^j = G_i - G_j = \frac{14}{25} - \frac{1}{5} = \frac{9}{25}$$

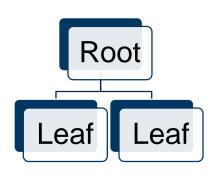
 NB: the best feature to split is the one that maximizes the IG

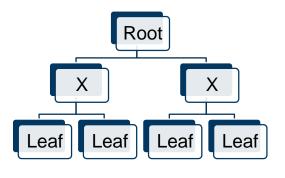


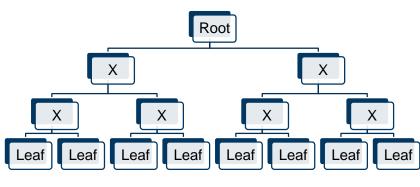


Hyperparameters

Max depth







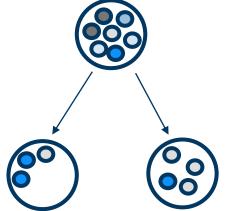
$$Depth = 1$$

Depth =
$$2$$

Depth
$$= 3$$

Hyperparameters

- Max depth
- Minimum number of samples to split



Minimum number of samples to split = 6

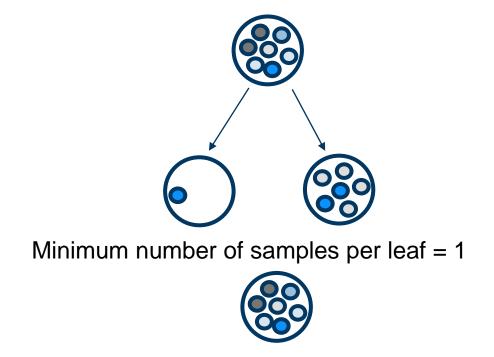


Minimum number of samples to split = 8



Hyperparameters

- Max depth
- Minimum number of samples to split
- Minimum number of samples per leaf



No Split!!!!

Minimum number of samples per leaf = 7

PROS

- Simple to understand and interpret
- No need for complex data preparation
- Handle numerical and Categorical Data
- No assumption on the data



PROS

- Simple to understand and interpret
- No need for complex data preparation
- Handle numerical and Categorical Data
- No assumption on the data

CONS

- Sensitive to small data perturbation
- Not incremental
- No guarantee to return the globally optimal solution
- Sensitive to unbalanced dataset
- Overfitting
 - Pruning
 - Ensemble Methods



- Scikit-Learn
 - What is it?
 - Decision Tree for Classification

Decision Tree for <u>Regression</u>

```
from sklearn import tree

clf = tree.DecisionTreeClassifier()

clf = clf.fit(X, Y)

clf.predict([[2., 2.]]) or

clf.predict_proba([[2., 2.]])

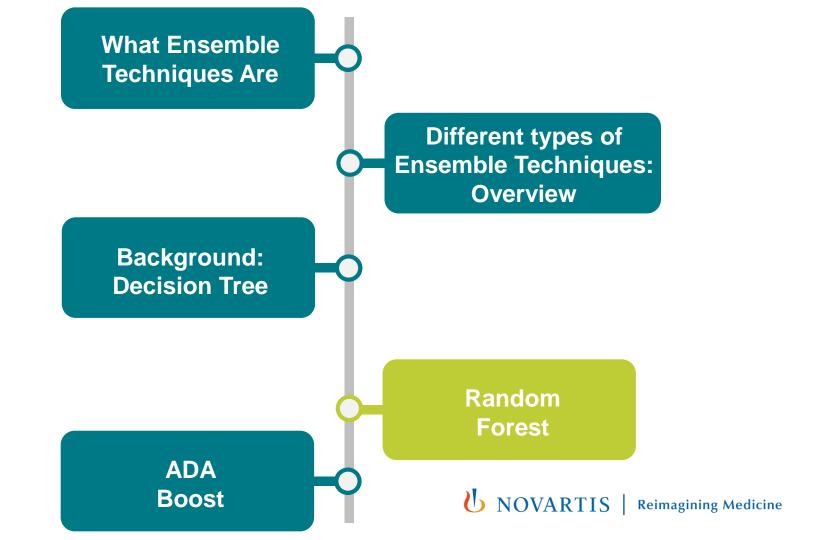
tree.plot_tree(clf)
```

```
from sklearn import tree

clf = tree.DecisionTreeRegressor()

clf = clf.fit(X, Y)

clf.predict([[2., 2.]])
```



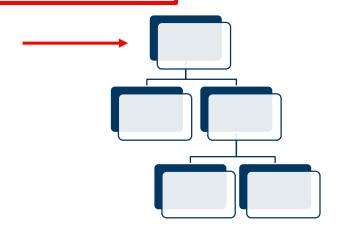
- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness





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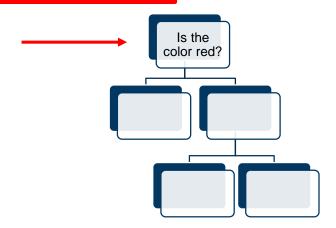
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- Boosting method
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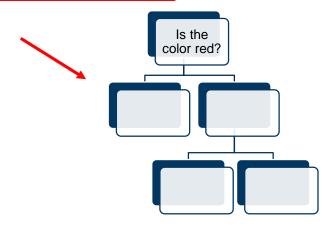
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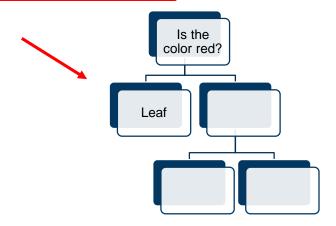
Color	Size	Discount	Label
Red	M	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	M	40%	Shirt
Green	L	50%	Skirt





- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness

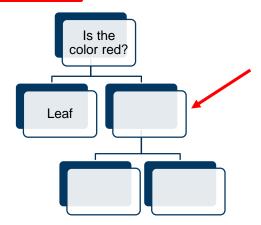
Color	Size	Discount	Label
Red	M	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	M	40%	Shirt
Green	L	50%	Skirt





- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness

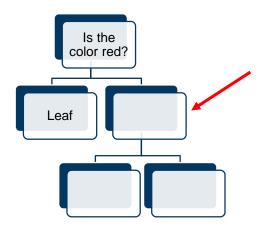
Color	Size	Discount	Label
Red	М	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	М	40%	Shirt
Green	L	50%	Skirt





- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness

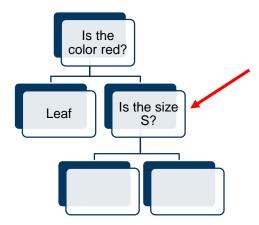
Size	Discount	Label
S	20%	Jeans
L	50%	Skirt





- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness

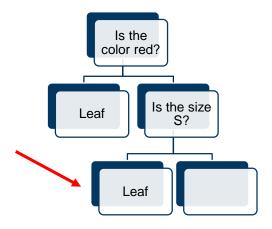
Size	Discour	t Label
S	20%	Jeans
L	50%	Skirt





- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness

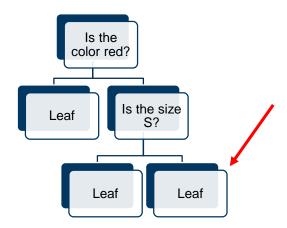
Size	Discount	Label
S	20%	Jeans
L	50%	Skirt





- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness

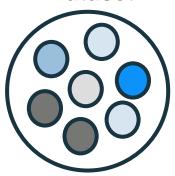
Size Discount		Label
S	20%	Jeans
L	50%	Skirt



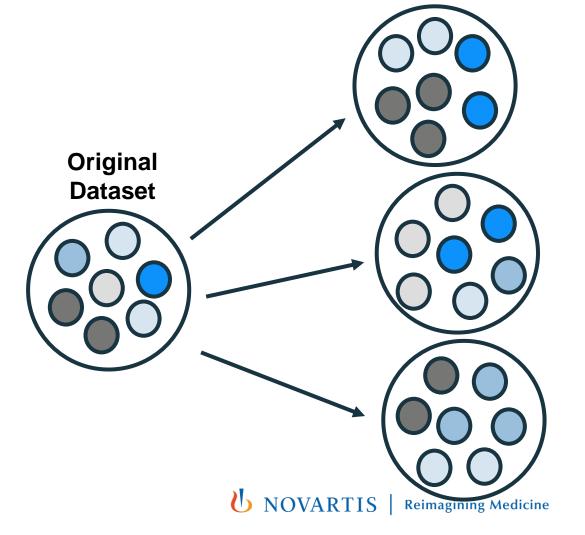


- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness
 - Bagging (Bootstrap Aggregation)

Original Dataset



- Boosting method
 - Regression
 - Classification
- Weak Learner': decision tree
- Ensuring Models Diversity
 - Feature randomness
 - Bagging (Bootstrap Aggregation)



- Pseudo-code:
 - Create a "bootstrapped" dataset

Color	Size	Discount	Label
Red	M	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	М	40%	Shirt
Green	L	50%	Skirt



- Pseudo-code:
 - Create a "bootstrapped" dataset

Color	Size	Discount	Label
Red	M	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	M	40%	Shirt
Green	L	50%	Skirt





- Pseudo-code:
 - Create a "bootstrapped" dataset

Color	Size	Discount	Label
Red	M	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	M	40%	Shirt
Green	L	50%	Skirt

x2

- Pseudo-code:
 - Create a "bootstrapped" dataset

Color	Size	Discount	Label
Red	М	50%	Shirt
Red	S	50%	Shirt
Red	М	40%	Shirt
Green	L	50%	Skirt
Green	L	50%	Skirt

Color	Size	Discount	Label
Red	M	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Red	M	40%	Shirt
Green	L	50%	Skirt



x2

- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set

Color	Size	Discount	Label
Red	М	50%	Shirt
Red	S	50%	Shirt
Red	М	40%	Shirt
Green	L	50%	Skirt
Green	L	50%	Skirt

- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set
 - Compute the best feature where to split

Color	Size	Discount	Label
Red	М	50%	Shirt
Red	S	50%	Shirt
Red	М	40%	Shirt
Green	L	50%	Skirt
Green	L	50%	Skirt

- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set
 - Compute the best feature where to split

Color	Size	Discount	Label
Red	М	50%	Shirt
Red	S	50%	Shirt
Red	М	40%	Shirt
Green	L	50%	Skirt
Green	L	50%	Skirt

Is the color red?



- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set
 - Compute the best feature where to split
 - Split dataset

Color	Size	Discount	Label
Red	M	50%	Shirt
Red	S	50%	Shirt
Red	M	40%	Shirt

yes

Is the color red?

- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set
 - Compute the best feature where to split
 - Split dataset

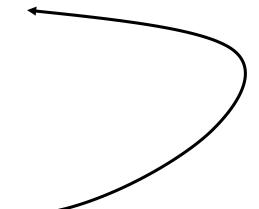
Color	Size	Discount	Label	
Red	M	50%	Shirt	
Red	S	50%	Shirt	
Red	М	40%	Shirt	
	Is the	yes color red?	6	
Color	Size	Discount	Label	
Green	L	50%	Skirt	
Green	L	50%	Skirt	



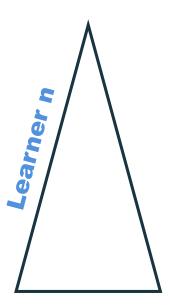
- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set
 - Compute the best feature where to split
 - Split dataset
 - If not stop condition:



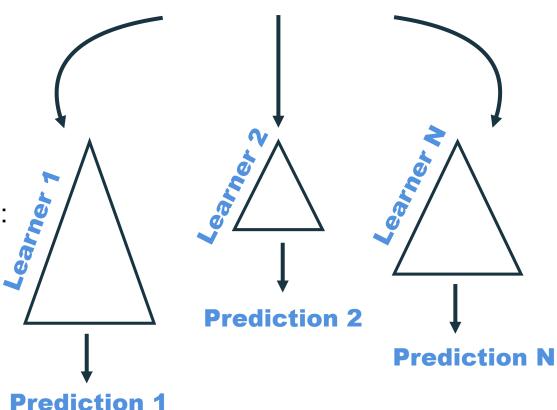
- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set
 - Compute the best feature where to split
 - Split dataset
 - If not stop condition:
 - Repeat



- Pseudo-code:
 - Create a "bootstrapped" dataset
 - Randomly select a subset of the features set
 - Compute the best feature where to split
 - Split dataset
 - If not stop condition:
 - Repeat



- Check Performances
 - New samples
 - Averaging
 - Voting
 - Hyperparameter optimisation:
 - Grid search
 - Random search
 - Etc...



Test set



- Hyperparameters:
 - Number of learners
 - Max depth
 - Minimum number of samples to split
 - Minimum number of samples per leaf



PROS:

- Very popular in practice
- Easy to implement
- Parallelizes easily
- Robustness

CONS:

- Very High number of trees
- Computation process slower

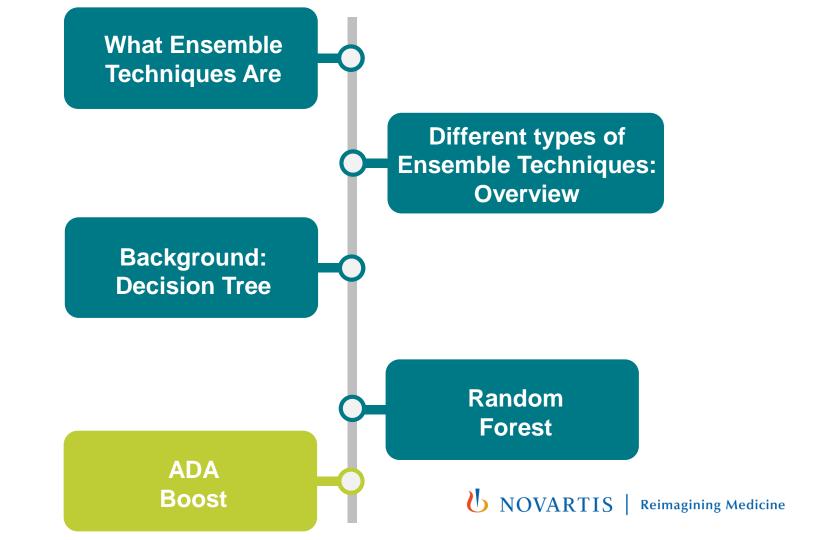
Scikit-Learn

Random Forest for <u>Classification</u>

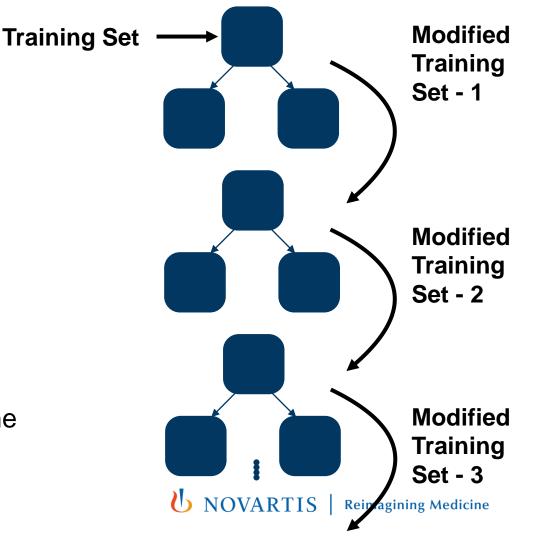
Random Forest for <u>Regression</u>

```
from sklearn.ensemble import
RandomForestClassifier
clf=RandomForestClassifier(n_estimators = 100,
random_state=0)
clf = clf.fit(X, Y)
clf.predict([[2., 2.]]) or
clf.predict_proba([[2., 2.]])
```

```
from sklearn.ensemble import
RandomForestRegressor
clf=RandomForestRegressor(n_estimators = 100, random_state=0)
clf = clf.fit(X, Y)
clf.predict([[2., 2.]])
NOVARTIS Reimagining Medicine
```



- Boosting method
 - Regression
 - Classification
- `Weak Learner': stump
- Boosting
 - Weak learners are trained in series
 - Errors made by one stumps influence the input dataset of the next stump



Pseudocode:



- Pseudocode:
 - Assign to each sample the same weight

Is this a Shirt?

Color	Size	Discount	Label
Red	М	50%	Shirt
Yellow	S	20%	Jeans
Red	S	50%	Shirt
Green	М	40%	Shirt
Red	L	50%	Jeans

- Pseudocode:
 - Assign to each sample the same weight

Is this a Shirt?

Weight	Color	Size	Discount	Label
1/5	Red	М	50%	Shirt
1/5	Yellow	S	20%	Jeans
1/5	Red	S	50%	Shirt
1/5	Green	М	40%	Shirt
1/5	Red	L	50%	Jeans

Is this a Shirt?

Pseudocode:

 Assign to each sample the same weight

 Select feature that gives the best split



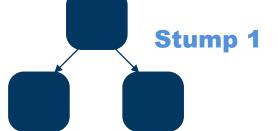
Is it the color red?

Stump 1

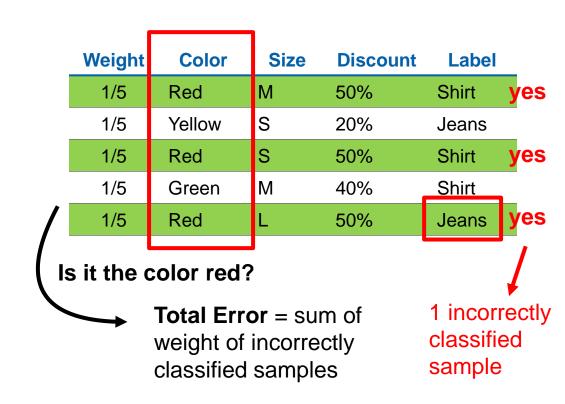
- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has

Is it the color red?

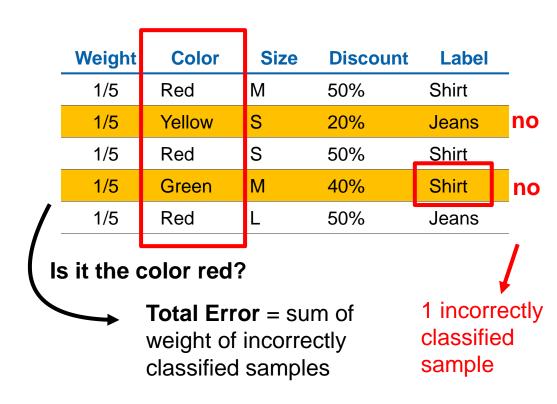
Weight	Color	Size	Discount	Label
1/5	Red	M	50%	Shirt
1/5	Yellow	S	20%	Jeans
1/5	Red	S	50%	Shirt
1/5	Green	M	40%	Shirt
1/5	Red	L	50%	Jeans



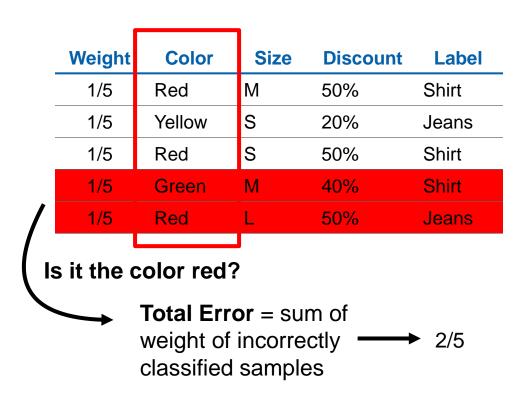
- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error



- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error



- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error



- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error

Weight	Color	Size	Discount	Label
1/5	Red	М	50%	Shirt
1/5	Yellow	S	20%	Jeans
1/5	Red	S	50%	Shirt
1/5	Green	М	40%	Shirt
1/5	Red	L	50%	Jeans

Amount of say =

$$Amount of Say = \frac{1}{2}log(\frac{1 - Total Error}{Total Error})$$



- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error

Weight	Color	Size	Discount	Label
1/5	Red	М	50%	Shirt
1/5	Yellow	S	20%	Jeans
1/5	Red	S	50%	Shirt
1/5	Green	М	40%	Shirt
1/5	Red	L	50%	Jeans

Amount of say =

$$Amount of Say = \frac{1}{2}log(\frac{1 - Total Error}{Total Error})$$
 2/5

- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error

Weight	Color	Size	Discount	Label
1/5	Red	M	50%	Shirt
1/5	Yellow	S	20%	Jeans
1/5	Red	S	50%	Shirt
1/5	Green	М	40%	Shirt
1/5	Red	L	50%	Jeans

Amount of say =

$$Amount of Say = \frac{1}{2}log(\frac{1 - TotalError}{TotalError}) \longrightarrow 0.088$$



- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error
 - Change the sample weights

Weight	Color	Size	Discount	Label
1/5	Red	М	50%	Shirt
1/5	Yellow	S	20%	Jeans
1/5	Red	S	50%	Shirt
1/5	Green	М	40%	Shirt
1/5	Red	L	50%	Jenas

- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error
 - Change the sample weights

Weight	Color	Size	Discount	Label
1/5	Red	М	50%	Shirt
1/5	Yellow	S	20%	Jeans
1/5	Red	S	50%	Shirt
0.218	Green	М	40%	Shirt
0.218	Red	L	50%	Jeans

 $NewSampleWeight = SampleWeight \cdot e^{Amount of Say}$



- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error
 - Change the sample weights

Weight	Color	Size	Discount	Label
0.183	Red	М	50%	Shirt
0.183	Yellow	S	20%	Jeans
0.183	Red	S	50%	Shirt
0.218	Green	М	40%	Shirt
0.218	Red	L	50%	Jeans

 $NewSampleWeight = SampleWeight \cdot e^{Amount of Say}$

- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error
 - Change the sample weights
 - Normalize the weights

Weight	Color	Size	Discount	Label
0.185	Red	М	50%	Shirt
0.185	Yellow	S	20%	Jeans
0.185	Red	S	50%	Shirt
0.221	Green	M	40%	Shirt
0.221	Red	L	50%	Jeans

- Pseudocode:
 - Assign to each sample the same weight
 - Select feature that gives the best split
 - Determine how much to say the stump has
 - Compute the total error
 - Change the sample weights
 - Normalize the weights
 - Create a new dataset
 considering the sample weight

	Weight	Color	Size	Discount	Label
Ī	0.185	Red	М	50%	Shirt
	0.185	Yellow	S	20%	Jeans
_	0.185	Red	S	50%	Shirt
	0.221	Green	М	40%	Shirt
	0.221	Red	L	50%	Jeans
	Weight	Color	Size	Discount	Label
_	Weight 0.221	Color Red	Size L	Discount 50%	Label Jeans
·					
	0.221	Red	L	50%	Jeans
	0.221	Red Red	L L	50% 50%	Jeans Jeans

Is the answer yes or not?

A.S =

0.3

A.S =

A.S =

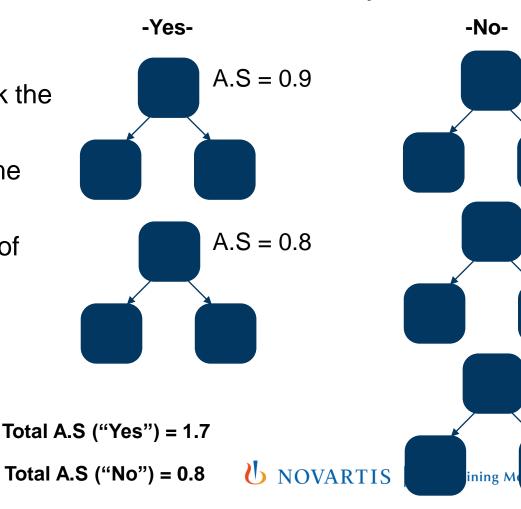
0.1

0.4

Adaboost

- Given a new sample, check the answer of each stump
- Group stumps with the same answer
- Compute the total Amount of Say

-Yes-



PROS:

- Easy to implement
- Improve accuracy of the weak learners
- Not prone to overfitting

CONS:

- Sensitive to noise data
- Affected by outliers

Scikit-Learn

Adaboost for <u>Classification</u>

Adaboost for <u>Regression</u>

```
from sklearn.ensemble import
AdaBoostClassifier
clf=AdaBoostClassifier(n_estimators = 100,
random_state=0)
clf = clf.fit(X, Y)
clf.predict([[2., 2.]]) or
clf.predict_proba([[2., 2.]])
```

```
from sklearn.ensemble import
AdaBoostRegressor
clf=AdaBoostRegressor(n_estimators = 100,
random_state=0)
clf = clf.fit(X, Y)
clf.predict([[2., 2.]])
NOVARTIS Reimagining Medicine
```

References

- [1] Scikit-learn: Machine Learning in Python, Pedregosa et al., JMLR 12, pp. 2825-2830, 2011.
- [2] https://www.kdnuggets.com/2019/01/ensemble-learning-5-main-approaches.html
- [3] Géron, Aurélien. *Hands-on machine learning with Scikit-Learn and TensorFlow: concepts, tools, and techniques to build intelligent systems.* "O'Reilly Media, Inc.", 2017.
- [4] https://www.datacamp.com/community/tutorials/adaboost-classifier-python
- [5] https://julienbeaulieu.gitbook.io/wiki/sciences/machine-learning/decision-trees
- [6] https://julienbeaulieu.gitbook.io/wiki/sciences/machine-learning/decision-trees
- [7] https://dev.to/nexttech/classification-and-regression-analysis-with-decision-trees-jgp
- [8] https://www.kdnuggets.com/2019/01/ensemble-learning-5-main-approaches.html
- [9] https://medium.com/ml-research-lab/bagging-ensemble-meta-algorithm-for-reducing-variance-c98fffa5489f
- [10] https://www.kdnuggets.com/2019/01/ensemble-learning-5-main-approaches.html

Thank you

YYYYXYYYYY



Mini-Project: Predicting Daily Bike Rentals

The project will be structured as follows:

- 1) Analysis and Data Preparation
- 2) Definition of useful functions (e.g. for cross-validation, test/train split, computation of metrics of interest etc.)
- 3) Models Evaluation
- 4) Analysis of features importance
- 5) Robustness Analysis
- 6) Hyperparameter Optimization

Test/Train split

- Big mistake: train and test the model on the same data
 - The model memorize the data
 - The model may not able to generalize (overfitting)
- Good practice: hold out part of the original data as test set
- A common split is 80% 20%
- Main problem: dependency on the specific train-test split

Original Dataset

Train Set

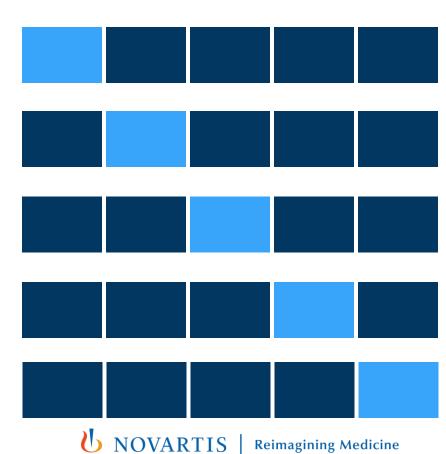
Test Set



K-fold Cross Validation

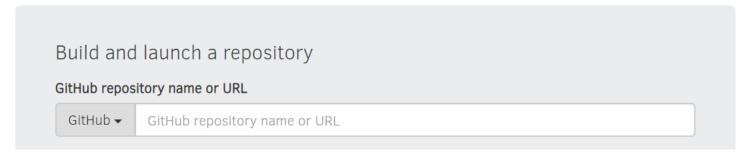
- Statistical method to estimate model performances on unseen data
- Used to select and compare different models
- Main idea:
 - Split dataset into k sets
 - Use the k-1 folds to train the model
 - Use the remaining kth fold to validate the model
 - Repeat the procedure for each kth set
 - Average the performances

Original Dataset



Setup your environment

- Go to: https://mybinder.org/
- Copy my github repository link (<u>https://github.com/Jlanini/AMLD_2020</u>) in this section:



Launch!

