Ensemble Learning

Artificial Intelligence and Machine Learning

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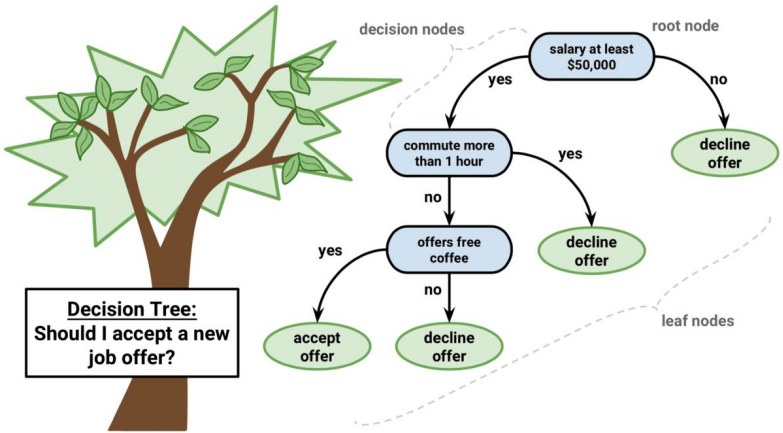
What is a decision tree ?

- Machine learning model with a flowchart-like structure
- Each internal nodes represents a “test” on a feature of our dataset
- Final nodes (leaf) are the predicted class or value
- Available both for classification and regression tasks



Example: Iris dataset

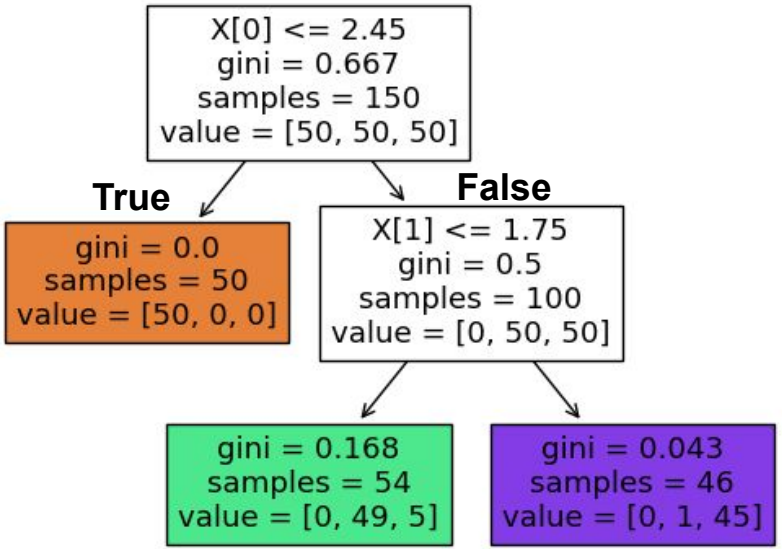
```
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier,plot_tree
import matplotlib.pyplot as plt

iris=load_iris()
X =iris.data[:,2:] #petal length and width
y = iris.target

clf=DecisionTreeClassifier(max_depth=2)
clf.fit(X,y)
plot_tree(clf, filled=True)
plt.show()
```

Iris decision tree

- X[0] : petal length
- X[1]: petal width
- Gini: Impurity metric
  - A node is “pure” if Gini=0
    - If all training instances it applies to belong to the same class

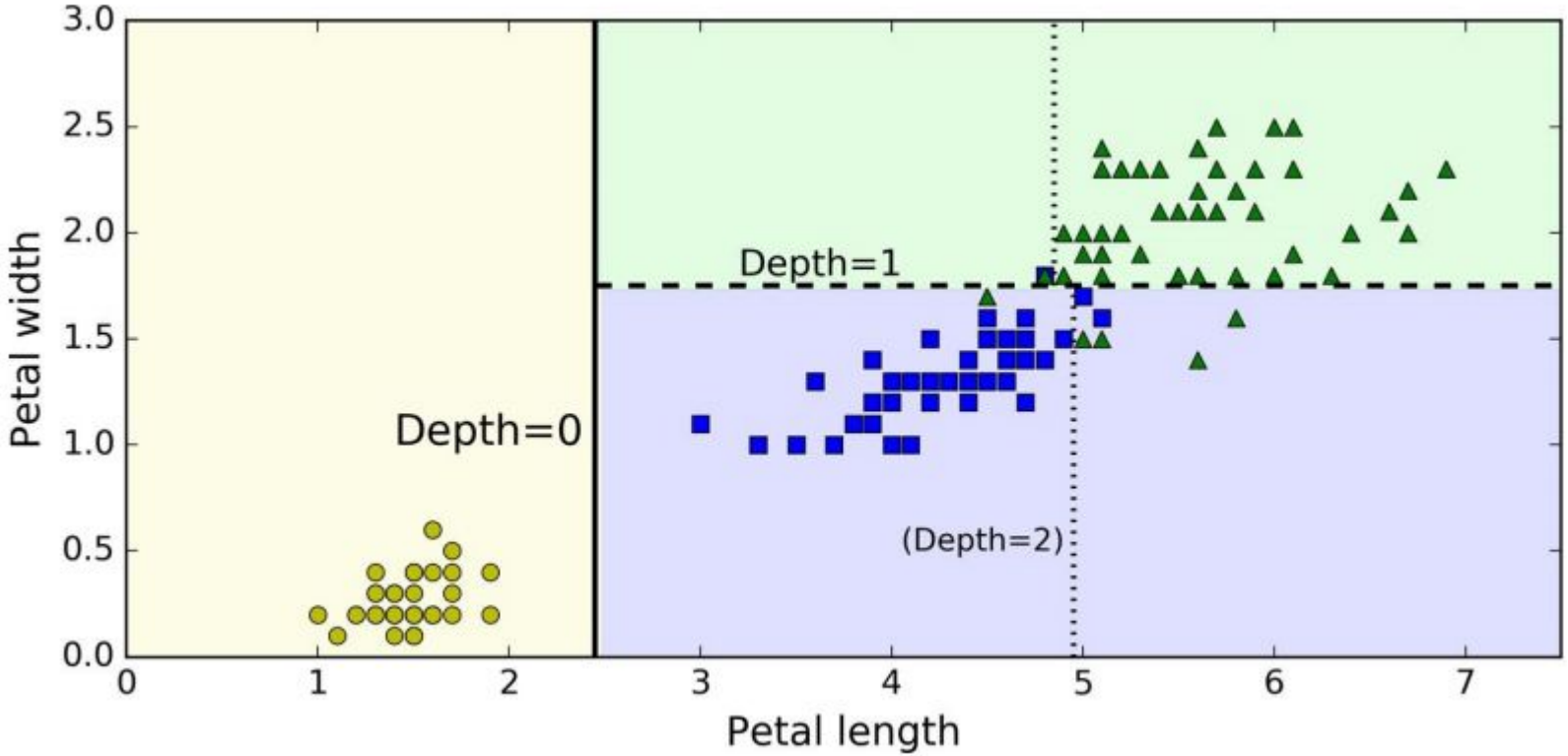
$$G_i = 1 - \sum_{k=1}^{n} p_{i,k}^{\ 2}$$

- $p_{i,k}$ is the ratio of class k instances among the training instances in the i^{th} node.



- Gini for the depth-2 left node is
  $1 - (0/54)^2 - (49/54)^2 - (5/54)^2 = 0.168$
- Ratios corresponds also to output probabilities:
  - 0% for Iris-setosa
  - 90.7% for iris-Versicolor
  - 9,3% for iris-Virginica

Decision boundaries



CART training algorithm

- CART (Classification and Regression Tree algorithm)
- Simple idea:
  a. Splits the training set in two subsets using a single feature k and a threshold t_k (e.g., “petal length <= 2.45”)
  b. To choose k and t_k it looks for the purest subsets (weighted by their size) minimizing a cost function
  c. It stops once it reaches the maximum depth selected as a parameter

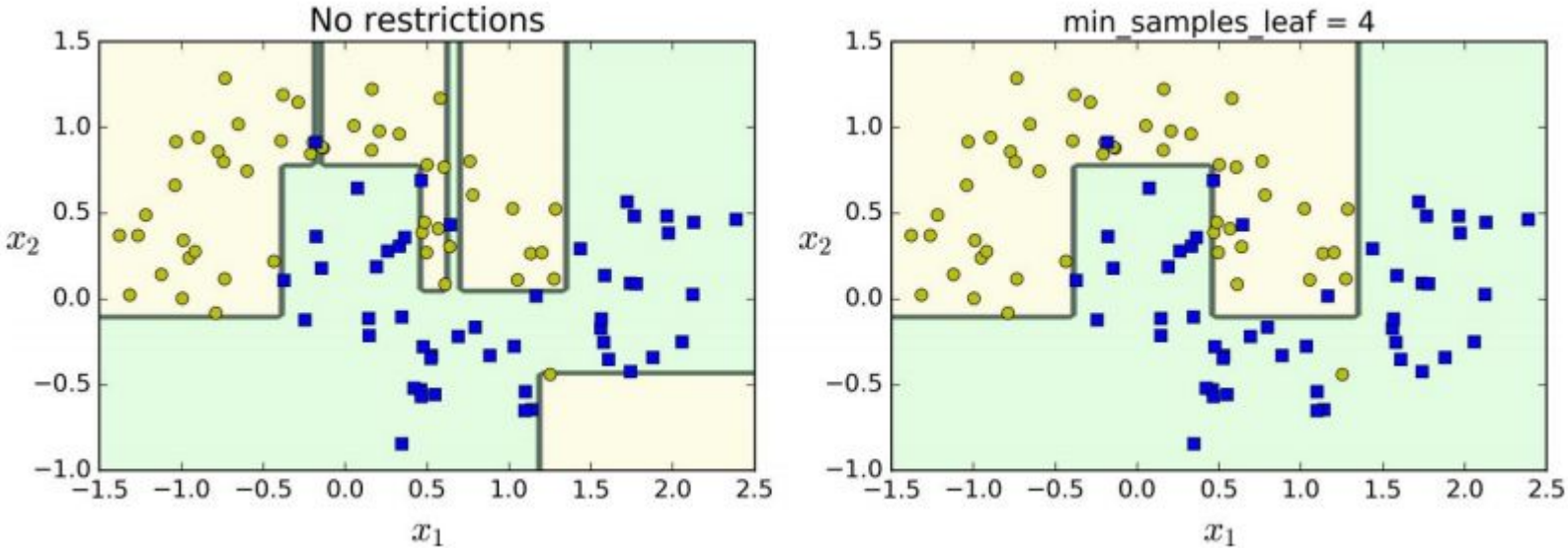
$$J(k, t_k) = \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}}$$

$$\text{where} \begin{cases} G_{\text{left/right}} \text{ measures the impurity of the left/right subset,} \\ m_{\text{left/right}} \text{ is the number of instances in the left/right subset} \end{cases}$$

Problems: Overfitting

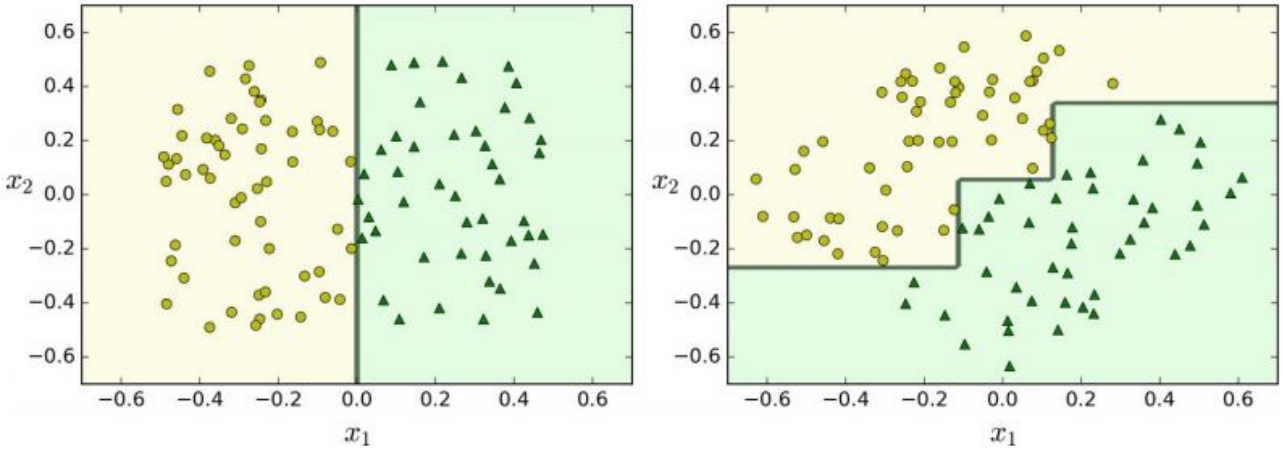
- Decision trees make less assumptions about the training data with respect to linear models
- If left unconstrained the tree structure will adapt itself to the training-set very well !
  - Actually, most of the time it overfits the training-set !
- One solution can be reduce the degree of freedom of the model during the training phase (Regularization)
  - Select a max depth
  - Pruning
  - Select a a minimum number of samples a leaf node must have
  - Select a max feature number that are evaluated for splitting each node

Regularization with min sample leaf



Instability

- A decision tree often finds orthogonal decision boundaries
- Orthogonality makes them sensitive to training set rotation
- A decision tree can fits perfectly a training set but probably will not generalize well in some cases
- An idea to solve this problem is to apply the Principal Component Analysis (PCA) to data in order to have a better orientation of the training data

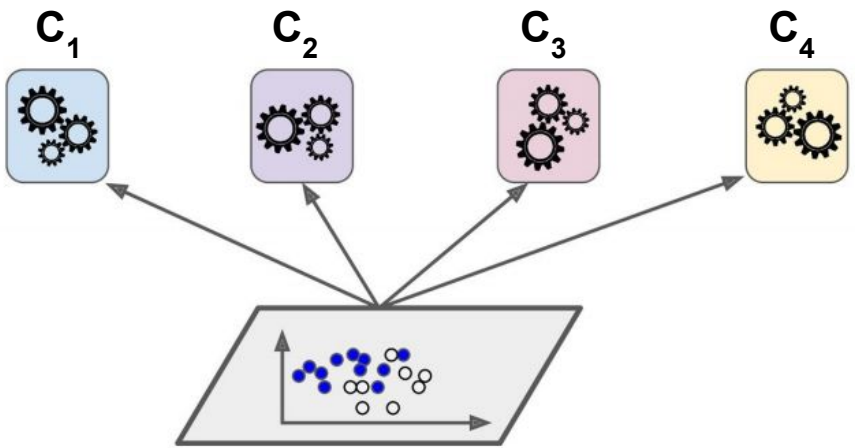


Ensemble learning

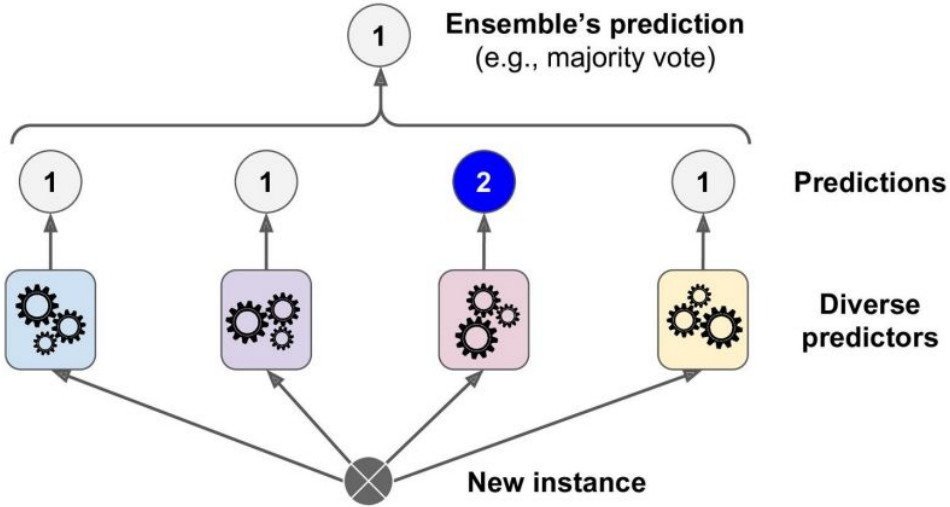
- When you are looking for an answer to a complex problem it is better to ask to different experts and then aggregate their answer (Wisdom of the crowd)

- Key idea: aggregate the predictions of a group of predictors to get better predictions than the best single predictor

Ensemble learning



Training



Test

Why the aggregation is better?

- Suppose you have a slightly biased coin: 51% chance of coming up heads
  - If you toss the coin 1000 times: you will have more or less 510 heads and 490 tails
  - What is the probability of having a majority of heads after 1000 tosses?
    - It is around 73%
    - If 10’000 tosses: the probability is around 95%
    - The more you toss the coin, the higher the probability is

- This is true, when each toss is **independent**
  - The result of each toss does not depend on the others!

Why the aggregation is better?

- N = 1000
- k = n° of heads that in N tosses has to be at least higher than (N/2)+1
- The probability that after N tosses the majority are heads is the sum of the probability of k successes with k in range of (N/2)+1 to N

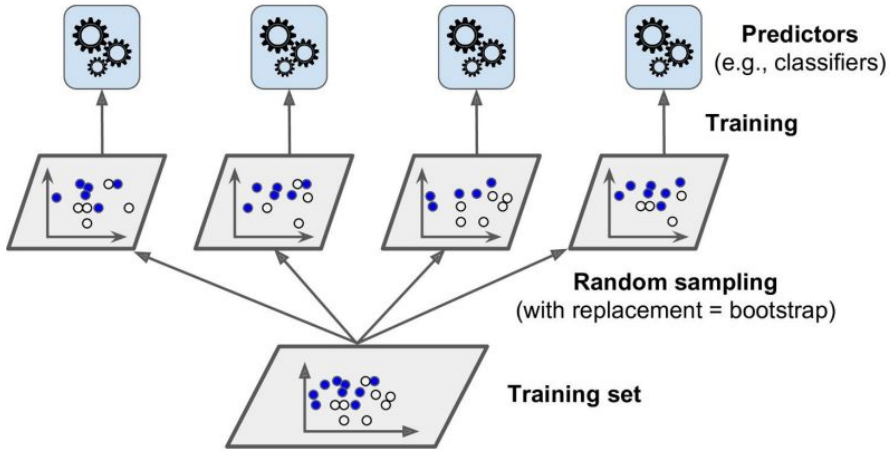
$$\sum_{k=(N/2)+1}^{N} \binom{N}{k} p^k (1-p)^{n-k}$$

Independent predictors

- Similarly, we can build 1000 classifiers that are individually correct only 51% of the time (slightly better than the random guessing -> weak classifier)
- If you predict the majority voted class, you can hope to 73% accuracy
- This is true if **all classifiers are perfectly independent** !
    - They should make uncorrelated errors, otherwise they are likely to make the same type of errors and the majority could be wrong!
    - If all classifiers are trained on the same dataset, are they independent?

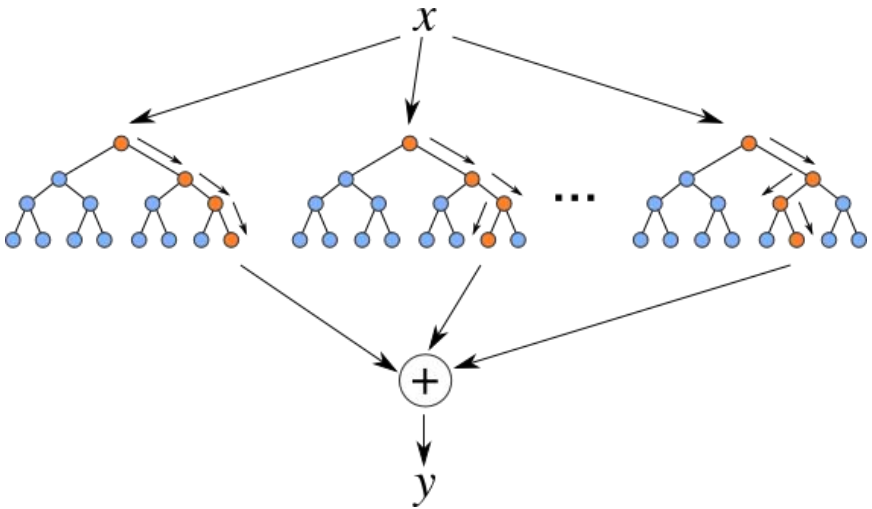
Bootstrap aggregating (Bagging)

- We have only one training-set and we want to use only one algorithm
- We can train the classifiers on different random subsets of the training-set
- When sampling is performed with replacement, this method is called bootstrap
- Each individual predictor has a higher bias than if it were trained on the original dataset, but aggregation reduces both bias and variance



Random forest

- Random forest is a bagging-based model where we make an aggregation of decision trees
- It also sub-samples a fraction of the features when fitting a decision tree to each bootstrap sample



Hard voting classifier

- Another solution to get independent classifiers is to use different algorithms
- Then we can make hard voting

```
from sklearn.linear_model import LogisticRegression
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn import datasets
from sklearn.metrics import accuracy_score
from sklearn.model_selection import train_test_split
from sklearn.ensemble import VotingClassifier

# import data
X, y = datasets.load_breast_cancer(return_X_y=True)
```

Hard voting classifier

```
log_clf = LogisticRegression()
rf_clf= RandomForestClassifier(n_estimators = 10)
svm_clf = SVC()

X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.33, stratify=y)

voting_clf=VotingClassifier(estimators=[('lr',log_clf),('rf',rf_
clf),('svc',svm_clf)], voting='hard')
voting_clf.fit(X_train,y_train)
y_pred= voting_clf.predict(X_test)
print("Voting "+str(accuracy_score(y_test,y_pred)))
```

Hard voting classifier

```
log_clf.fit(X_train,y_train)
y_pred= log_clf.predict(X_test)
print("Logistic "+str(accuracy_score(y_test,y_pred)))

rf_clf.fit(X_train,y_train)
y_pred = rf_clf.predict(X_test)
print("Random forest "+str(accuracy_score(y_test,y_pred)))

svm_clf.fit(X_train,y_train)
y_pred = svm_clf.predict(X_test)
print("Support Vector Machine
"+str(accuracy_score(y_test,y_pred)))
```

Bagging with sklearn

from sklearn.ensemble import BaggingClassifier

```
from sklearn.ensemble import BaggingClassifier
model= BaggingClassifier(n_estimators = 200)
model.fit(X_train,y_train)
```

```
from sklearn.ensemble import RandomForestClassifier
model= RandomForestClassifier(n_estimators = 1000)
model.fit(X_train,y_train)
```

Exercise Breast cancer

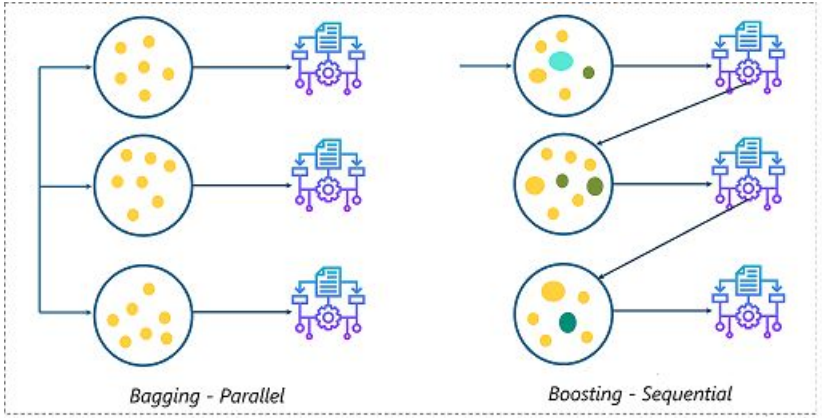
- X, y = datasets.load_breast_cancer(return_X_y=True)

- Split data (70% training and 30% test)
- Train a single decision tree, a bagging classifier with 200 trees and a random forest
- Repeat each training 10 times and consider the average accuracy
- What is the best classifier?
- ADDITIONAL for home: Try to use regularization parameters:
  - https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.BaggingClassifier.html
  - https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
  - https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html

BREAK

Boosting

- Similar to bagging, but now the idea is to train predictors sequentially
- Each predictor tries to correct its predecessor
- Many boosting methods available:
  - Adaptive boosting (AdaBoost)
  - Gradient boosting
  - XGboost (Extreme gradient boosting)

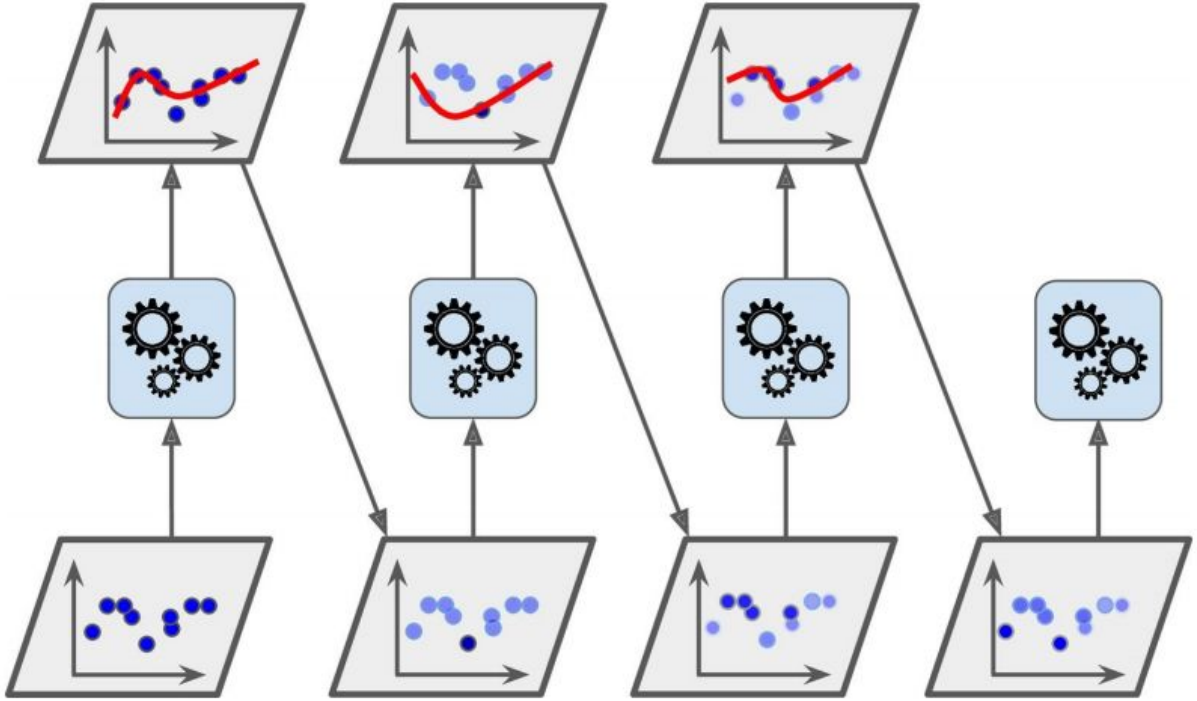


AdaBoost

- To correct a predecessor one way is to pay attention to the training instances that the predecessor under-fitted

- The new predictor will focus more on the hard cases (adaptive)
  a. A first base predictor is trained and used to make predictions on the training-set
  b. The relative weight of misclassified training instances is then increased
  c. A second classifier is trained using the updated weights and so on
  d. To each classifier a weight is assigned
  e. Once all predictors are trained, the ensemble makes predictions like bagging, except that predictors have different weights depending on their accuracy on the training-set

AdaBoost



AdaBoost algorithm

- Each instance weight $\mathbf{w^{(i)}}$ is initially set to 1/m where m is the number of observations
- For each predictor **j** is computed a weighted error-rate $\mathbf{r_j}$

$$r_j = \frac{\sum_{\substack{i=1 \\ \hat{y}_j^{(i)} \neq y^{(i)}}}^{m} w^{(i)}}{\sum_{i=1}^{m} w^{(i)}}$$

where y-hat is the j^{th} predictors' prediction for the i^{th} instance

AdaBoost algorithm

- A predictor's weight α_j is then computed using a learning-rate parameter η
- The more accurate the predictor is, the higher its weight will be.

$$\alpha_j = \eta \log \frac{1 - r_j}{r_j}$$

- After that, the instance weights are updated using the equation below
- All the instance weights are then normalized dividing by the sum of all weights

$$\text{for } i = 1, 2, \cdots, m$$

$$w^{(i)} \leftarrow \begin{cases} w^{(i)} & \text{if } \hat{y}_j^{(i)} = y^{(i)} \\ w^{(i)} \exp(\alpha_j) & \text{if } \hat{y}_j^{(i)} \neq y^{(i)} \end{cases}$$

AdaBoost predictions

- Finally, AdaBoost computes the predictions of all predictors and weights them using α_j
- The predicted class is the one that gets the majority of weighted votes

$$\hat{y}(\mathbf{x}) = \underset{k}{\operatorname{argmax}} \sum_{\substack{j=1 \\ \hat{y}_j(\mathbf{x})=k}}^{N} \alpha_j$$

where N is the number of predictors

Gradient Boosting

- The key idea of GB is additive modelling
  - We can have a final learner $F_L = f_0(x)+f_1(x)+f_2(x)+...+f_{L-1}(x)$
  - Where L is the number of learners we want to use (for example n°of trees)
  - $f_0(x)$ is the first predictor we train on the training-set
  - Each epoch of training we add a new learner that tries to increase the accuracy of the previous one by minimizing a Loss function using gradient descent and not by increasing instances' weight like AdaBoost

Gradient Boosting for Regression (Classification)

- Let's play a game: You are given a dataset in the form of $(x_1,y_1),...,(x_n,y_n)$.
- The task is to fit a model F(x) to minimize the square loss (sum of square difference between y_true and y_pred)
- Suppose your friend wants to helè you and gives you his model F
- You check his model and find the model is good but not perfect because it makes some mistakes:
  - For example: $F(x_1) = 0.5$ while $y_1 = 0.6$
  - $F(x_2) = 1.8$ while $y_2 = 1.7$
- You cannot change the model F or change its parameters but you want to improve it

Gradient Boosting for Regression (Classification)

- We cann an additional model (regression tree for example) **h** to F, so the new prediction will be F(x)+**h**(x)
- You wish to improve the model such that
  - $F(x_1)+h(x_1) = y_1$
  - $F(x_2)+h(x_2) = y_2$
  - $F(x_n)+h(x_n) = y_n$

  - $\mathbf{h}(x_1) = y_1 - F(x_1)$
  - $\mathbf{h}(x_2) = y_2 - F(x_2)$
  - $\mathbf{h}(x_n) = y_n - F(x_n)$

Can any regression tree h achieve this goal perfectly ? Probably not! But some regression might be able to do this approximately

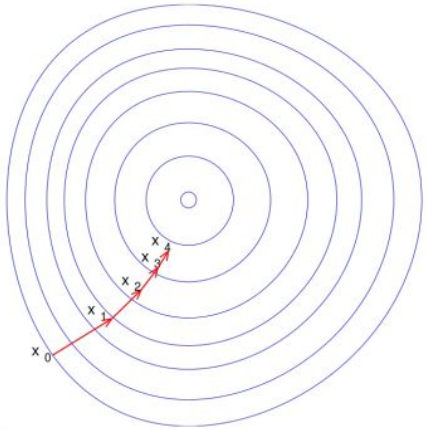
Gradient Boosting for Regression (Classification)

- To get this predictor **h** we can fit a regression tree with a different formulation of the original dataset where the target value to predict will be *y - F(x)*
- $\{x_1,y_1 - F(x_1),...,(x_n,y_n - F(x_n)\}$
- $y_i - F(x_i)$ are usually called residuals
- We want to minimize the entire loss for all training examples (1,...,n)
- To minimize this loss we can use the gradient descent

Gradient Descent

Minimize a function by moving in the opposite direction of the gradient.

$$\theta_i := \theta_i - \rho \frac{\partial J}{\partial \theta_i}$$



Gradient Boosting for Regression (Classification)

- Loss function $L(y, F(x)) = (y - F(x))^2 / 2$
- We want to minimize $J = \sum_i L(y_i, F(x_i))$ by adjusting $F(x_1), F(x_2) \ldots F(x_n)$

$$\frac{\partial J}{\partial F(x_i)} = \frac{\partial \sum_i L(y_i, F(x_i))}{\partial F(x_i)} = \frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} = F(x_i) - y_i$$

- So we can interpret residuals as negative gradients

$$y_i - F(x_i) = -\frac{\partial J}{\partial F(x_i)}$$

Gradient Boosting for Regression (Classification)

- So at the end we can go back to see the predictors at stage m+1 and define it as

$$F_{m+1}(x) = F_m(x) + h(x) = y$$

$$F_{m+1}(x) = F_m(x) - \nabla_m L(y, F_m(x)) = F_m(x) - \left[\frac{\partial L(y, F_m(x))}{\partial F_m(x)}\right]$$

- With a learning-rate equal to 1

Boosting with sklearn

```
from sklearn.ensemble import AdaBoostClassifier
model= AdaBoostClassifier(n_estimators = 200)
model.fit(X_train,y_train)
```

```
from sklearn.ensemble import GradientBoostingClassifier
model= GradientBoostingClassifier(n_estimators = 200)
model.fit(X_train,y_train)
```

```
from xgboost import XGBClassifier
model = XGBClassifier(n_estimators = 200)
model.fit(X_train, y_train)
```

Exercise - Classification

- X, y = datasets.load_breast_cancer(return_X_y=True)
- Train an ensemble model with 200,1000,2000 trees with AdaBoost, GradientBoosting and XGBoost
- Compute the accuracy and the confusion matrix
- Which model performs better ?
- How results change if you increase the test-set size percentage ?
- Try to use regularization parameters

Exercise 2 - Regression

- X, y = datasets.load_boston(return_X_y=True)
- Train an ensemble model with 200,1000,2000 trees with AdaBoost, GradientBoosting and XGBoost
- Compute the rmse
- Which model performs better ?
- How results change if you increase the test-set size percentage ?
- Try to use regularization parameters