

Lecture 16 - 29/10/24

Recall:

- Bagging
 - Random Forest
 - Boosting
 - Stacking
- One kind of ensemble mainly aims to **reduce variance!**
- Another one aims to **reduce bias!**

Bagging

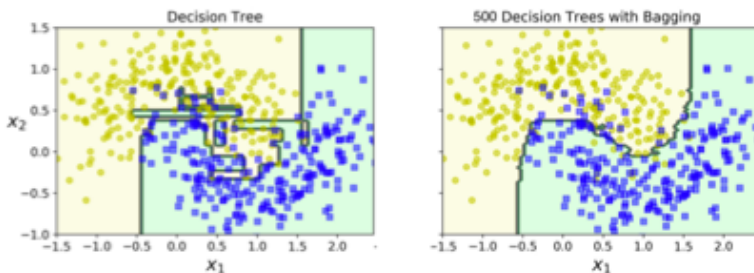
- **MEANING** → **Bootstrap Aggregation**
- **Principle:**
 - Make **bootstrapped subsets** of the training data
 - Train a **separate model on each subset**.
 - Given that samples come from same dataset, **not truly indep.**
- **Prediction:**
 - **Combination of predictions of all models**
- **Final Step:**
 - Typically use **hard voting** to combine predictions for classifications.
 - Typically use **averaging** for regression.
- **Scenario:**
 - I have a classifier which has **high variance prob.**
 - It has **low bias**.
 - I have **computational power available**

NOTE:

CREATING DIVERSITY
IN THE DATA,
INTRODUCES DIVERSITY
IN THE MODELS

try Bagging!!!

An example of Decision Tree (left) vs. a bagging ensemble of 500 trees (right)



WE CAN SEE HOW WE PROVIDE A GREAT
way to **AVOID OVERFITTING**

- **Validation:**
 - **Out-of-Bag evaluation**
 - We know that in **bagging** we use **bootstrapped data** → **Sampling with replacement**
 - **Not all datapoints will be in a given bag!**
 - **≠ datapoint are incl./excl. in ≠ bags.**
 - On **avg 37%** are **out-of-bag samples** if bags are the same size as dataset
 - Out of Bag samples **will be used for validation!**
 - **✓ data point** in original set we **combine pred** where it wasn't sampled

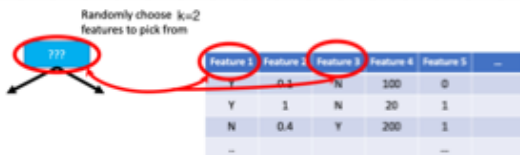
- VARIATION ERROR IS THE AVG ERROR ACROSS THESE COMBINED MODELS.
- THE COB PREDICTION ERROR IS AN UNBIASED ESTIMATION OF THE TEST ERROR.
- THIS METHOD CAN REPLACE CROSS-VALIDATION.

• ADVANTAGES:

- EASY TO IMPLEMENT
- TRAINING IN PARALLEL
- PRED IS AVG OR VOTE
- REDUCES VARIANCE
- OUT-OF-BAG VALIDATION

Random Forest

- ESSENTIALLY A BAGGING DECISION TREE WITH MODIFIED SPLITTING CRITERION
- PROCESS:
 - MAKE BOOTSTRAPPED DATA SETS FROM TRAINING SET
 - \forall DATASET, TRAIN A FULL DECISION TREE WITH MODIFIED SPLIT STRATEGY:
 - BEFORE FINDING EACH SPLIT:
 - * RANDOMLY CHOOSE K FEATURES
 - * ONLY CONSIDER THOSE FEATURE OR SPLIT
 - OUTPUT OF RANDOM FOREST IS THE AGGREGATED OUTPUT OF ALL TREES



$m=2$



Random Forest ARE NICE BECAUSE:

- ONLY FEW HYPER-PARAMETERS:
 - m = # of bootstrapped datasets.
 - k = # of randomly selected features.
- BASED ON DECISION TREES WHICH AVOID HARD PROCESS.
- AVERAGE DEPTH ESTIMATES FEATURE IMPORTANCE!

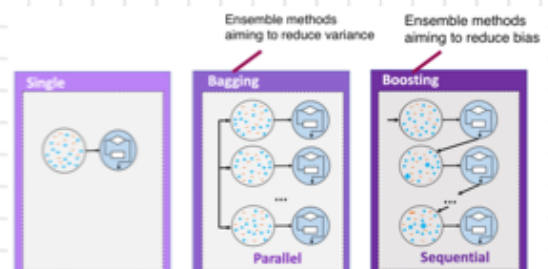
Extra Trees

- MEANING \rightarrow EXTREMELY RANDOMIZED TREES
- UNLIKE BAGGING & RANDOM FOREST, THEY FIT EACH D.T. ON WHOLE DATASET. ~~BOOTSTRAP~~
- UNLIKE RANDOM FOREST, THEY ALSO PICKS A RANDOM CUT-POINT AT EACH OF THE K FEATURES.
- LIKE RANDOM FOREST, THEY ALSO RANDOMLY SAMPLES K FEATURES TO FIND THE GOOD SPLIT.

* WE KNOW THAT BAGGING & ASSOCIATED METHODS \rightarrow REDUCE VARIANCE

* WHAT ABOUT REDUCING BIAS THAT?

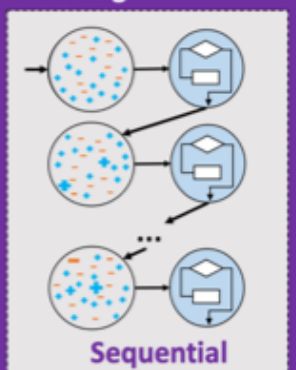
USE BOOSTING!!!



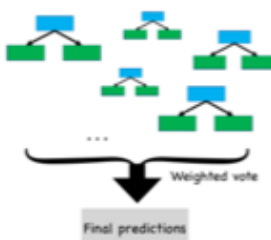
BOOSTING

- **SEQUENCE OF WEAK LEARNERS** COMBINED INTO A STRONG LEARNER
- **STEPS:**
 - TRAIN A WEAK LEARNER
 - GET TRAINING ERROR
 - TRAIN NEXT WEAK LEARNER BASED ON THAT ERROR
 - ...
 - **FINAL PREDICTIONS:** A COMBINATION OF ALL TRAINED WEAK LEARNERS.
- **VARIOUS BOOSTING METHODS EXIST** → AdaBoost, Gradient Boosting...

Boosting



AdaBoost



AFTER MAKING EACH TREE, THE ERRORS:

- INFLUENCE WEIGHTS OF NEXT TRAINING.
- DETERMINE WEIGHT OF TREE IN FINAL.

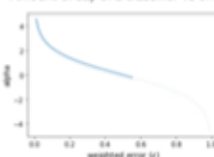
AdaBoost Training

Start with equal weights for all the training samples, e.g., $w_i^{(1)} = \frac{1}{N}$

For $c = 1, \dots, M$ iterations (trees):

- Train a model $h_c(x)$ based on the weighted training samples
- Calculate the total error on the training set: $\epsilon_c = \sum_{i: h_c(x_i) \neq y_i} w_i^{(c)}$
- Based on the total error, calculate the model's amount of say: $\alpha_c = \ln\left(\frac{1 - \epsilon_c}{\epsilon_c}\right)$
- Update the samples' weights:
 - Increase for misclassified samples: $w_i^{(c)} = w_i^{(c)} e^{\alpha_c}$
 - Unchanged for correct classifications: $w_i^{(c)} = w_i^{(c)}$
- Normalize all weights so they sum up to 1: $w_i^{(c+1)} = \frac{w_i^{(c)}}{\sum_{j=1}^n w_j^{(c)}}$

Amount of say of a classifier vs error



Some implementations add a hyper-parameter (learning rate) here to avoid overfitting

Some implementations also decrease the weights of correctly classified samples and then normalize

TWO TYPES OF WEIGHTS:

- w_i = TRAINING SAMPLE
- α_c = V MODEL

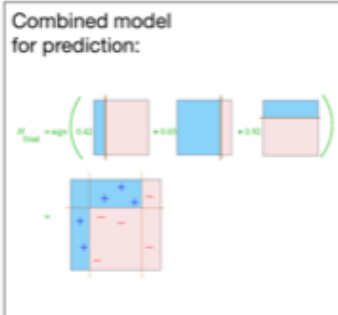
PREDICTION:

$$\text{SIGN}\left(\sum_{c=1}^M \alpha_c h_c(x)\right)$$

+1 or -1

WEAK LEARNERS = STUMPS

Example AdaBoost with decision stumps as base classifier



We said "Train a model $h_c(x)$ based on the weighted training samples" But how do we incorporate the weights into the training process?

Think about it!



WE CAN INCORPORATE THE WEIGHTS INTO THE ASSESSMENT OF SPOTS.

A DATAPOINT IS NO MORE WORTH 1 UNIT, IT COUNTS AS ITS WEIGHT w_i IN IMPURITY CALCULATION.

$$b + \text{THEIR WEIGHTED AVG} = p_1 \phi(h_1) + p_2 \phi(h_2)$$

$$p_k = \sum_{i: y_i = k} w_i$$

GRADIENT BOOSTING

- Commonly used for BOTH REGRESSION & CLASSIFICATION.

Gradient Boost:
small steps on the right direction

- Sequential algorithm like AdaBoost
- Use of treess (max-depth=3) as weak learner is common

• **Training:**

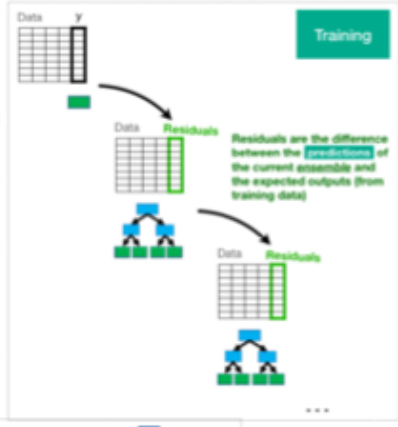
- Start with a single leaf (initial prediction, e.g., the average of all labels)
- use the current **ensemble** to predict the training data and compute the residuals
- Fit a new tree to the residuals

Side note: Stochastic gradient boosting is a variation of the method that only uses a subset of data in each iteration

Prediction:

$$\text{Predictions} = \text{Initial Prediction} + \text{Learning rate} \times \text{Tree 1} + \text{Learning rate} \times \text{Tree 2} + \dots$$

learning rate (often 0.1) must be used to avoid overfitting



BAGGING VS BOOSTING

BAGGING

- Usually HELPS DECREASING VARIANCE
- Not much effect with stable models
- Easy to PARALLELIZE

BOOSTING

- HELPS DECREASING BIAS
- Doesn't solve OVERFITTING
- Sometimes HURTS PERFORMANCE
- CANNOT BE FULLY PARALLELIZED

Bottom line: IT DEPENDS!!

STACKING

- Instead of voting for a better → **RAW META-LEARNER**.

ONE OF OUR CHOICE

SEVERAL GBT PREDICTIONS OF INDIVIDUAL MODELS AS INPUT & EXPECTED LABELS FOR DATA SAMPLES AS OUTPUT.

