# ML4 – improving weak learners

## Machine Learning – Tools and applications for policy – Lecture 5

Iman van Lelyveld – Michiel Nijhuis

DNB Data Science Hub

# ML4 – improving weak learners

1. How to grow a decision tree? How to split?
   - Decision trees, purity measures
2. Can Ensemble Classifiers improve weak learners?
   - Bagging, boosting, AdaBoost, XGBoost
3. Can we use forests in other ways?
   - Isolation forests

# Outline



ML4 – improving weak learners
- Trees
- Forests – Ensemble Classifiers
- Bootstrapping aka Bagging
- Boosting
- Isolation forest

# Knowledge clips

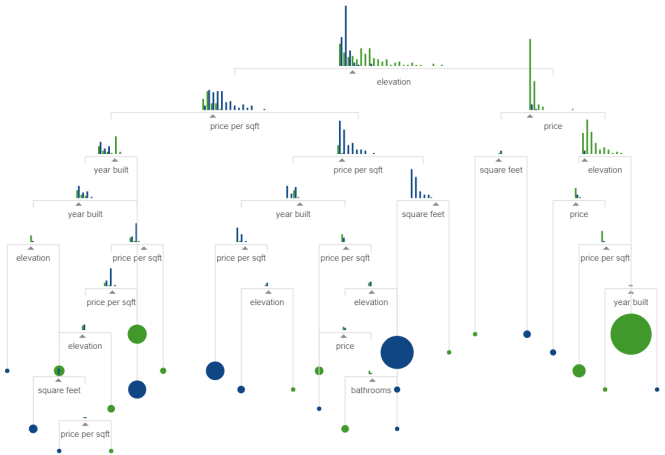


- Decision Tree Classifier from Scratch (Josh Gordon) (link)
- ADAboost clearly explained (Josh Starmer) (link)
- XGBoost from Start to Finish (Josh Starmer) (link)

  An extensive webinar where the XGBoost discussion starts at 36.32. The intro is nice to see how to handle data (labeling, missing values, ...)

# Decision tree






Source: r2d3

DataScience Hub

# Decision trees



- A decision tree is a learning algorithm that constructs a set of decisions based on training data.
- Decision trees are popular because:
  - They are naturally non-linear, so you can use them to solve complex problems
  - They are easy to visualize
  - How they work is easily explained
  - They can be used for regression (predict a number) and classification (predict a class)
- Drawback: classification at each step only use 'local' information

# How to get maximum information gain at each junction?



- At each split we create as much clarity (i.e. information) as possible. The split should make classifying the resulting 'children' easier. Formally (for two-way splits):

$$InformationGain(D_{\mathbf{par}ent}, \mathbf{f}eature) = I(D_{par}) - \frac{N_{left}}{N_{par}} I(D_{left}) - \frac{N_{right}}{N_{par}} I(D_{right})$$

- What could be the **I**mpurity measure?

| | | |
|---|---|---|
| Gini | $I_{\mathbf{Gini}}$ | $= 1 - \sum_{i=1}^{c} p(i\|t)^2$ |
| Entropy | $I_{\mathbf{ent}ropy}$ | $= -\sum_{i=1}^{c} p(i\|t) log_2 p(i\|t)$ |
| Classification error | $I_{\mathbf{clas}sification}$ | $= 1 - max\{p(i\|t)\}$ |

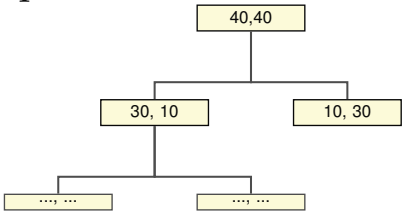
  where $p(i|t)$ is the probability that you get it right in 'child' $t$

- $I_{\mathbf{Gini}}$ and $I_{\mathbf{ent}ropy}$ are minimal if homogeneous and maximal if perfectly mixed

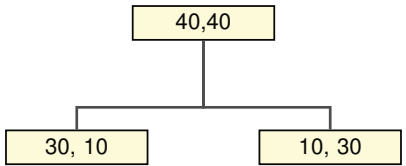
# Splitting with Classification Error: $1 - max\{p(i|t)\}$



## Split scenario A (class 0/1)




$$I_{\mathbf{clas}}(D_{par}) = 1 - 0.5 = 0.5$$
$$I_{\mathbf{clas}}(D_{left}) = 1 - \frac{30}{40} = 0.25$$
$$I_{\mathbf{clas}}(D_{right}) = 1 - \frac{30}{40} = 0.25$$
$$IG_{\mathbf{clas}} = 0.5 - \frac{40}{80}0.25 - \frac{40}{80}0.25 = 0.25$$



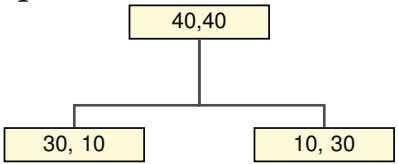

$$I_{\mathbf{clas}}(D_{left}) = 1 - \frac{40}{60} = \frac{20}{60}$$
$$I_{\mathbf{clas}}(D_{right}) = 1 - \frac{20}{20} = 0$$
$$IG_{\mathbf{clas}} = 0.5 - \frac{60}{80}\frac{20}{60} - 0 = 0.25$$

## Split scenario B

DataScience Hub

# Splitting with Gini: $1 - \sum_{i=1}^{c} p(i|t)^2$

## Split scenario A (class 0/1)



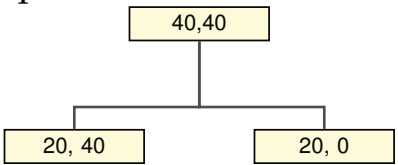

$I_{\text{Gini}}(D_{par})$ = 1 - $(0.5^2 + 0.5^2)$ = 0.5

$I_{\text{Gini}}(D_{left})$ = 1 - $(\frac{10}{40}^2 + \frac{30}{40}^2)$ = $\frac{30}{80}$

$I_{\text{Gini}}(D_{right})$ = 1 - $(\frac{30}{40}^2 + \frac{10}{40}^2)$ = $\frac{30}{80}$

$IG_{\text{Gini}}$ = 0.5 - $\frac{40}{80}\frac{30}{80}$ - $\frac{40}{80}\frac{30}{80}$ = 0.125

## Split scenario B




$I_{\text{Gini}}(D_{left})$ = 1 - $(\frac{20}{60}^2 + \frac{40}{60}^2)$ = $\frac{4}{9}$

$I_{\text{Gini}}(D_{right})$ = 1 - $(1^2 - 0)$ = 0

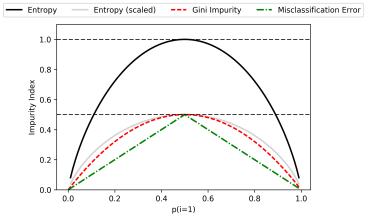
$IG_{\text{Gini}}$ = 0.5 - $\frac{60}{80}\frac{4}{9}$ - 0 = 0.16

# Information gain – wrap up



- The Entropy criterion also prefers Scenario B over A
- Differences between the $I$ criteria are small

  Gini often faster but tends to put most frequent class in 1 branch
- Choice of stopping criteria much more important
  - e.g. until no leaf contains more than $x$ observations
- Overfitting can be reduced by Cost complexity pruning: adding a cost to leafy tree. Not implemented in SKLearn library.
- Alternatives:
  - Set maximum depth of tree
  - Set maximum number of leaf nodes
  - Set minimum number of samples per split




DataScience Hub

# Is a linear classifier better than a tree?

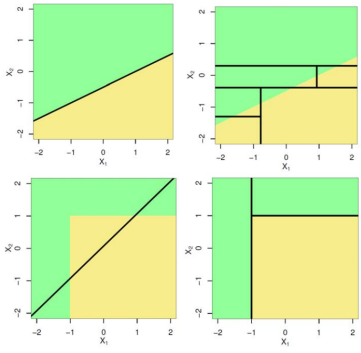


Case 1: linear Data Generating Process (DGP)

- A linear regression (left) is a better fit than a tree (right).

Case 2: non-linear DGP

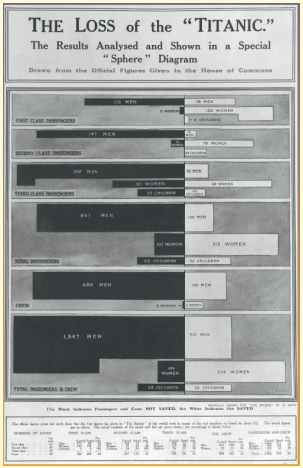
- A tree (right) is a better fit than a linear regression (left).



# Exploring classification with Titanic data



- Following the sinking of the Titanic there was an inquest that documented many features on the passengers
- G.Bron's chart of "The Loss of the 'Titanic"', from The Sphere, 4 May 1912, is the first attempt to show proportions of features (Friendly et al. (2019))
- The data has led to numerous ML flavored analyses (See here, here,here, and here). These are valuable resources to get to grips with classification trees
- A nice example using temperature data is here
- See Jake van der Plas's Notebook which can be found here



# Outline



ML4 – improving weak learners
- Trees
- Forests – Ensemble Classifiers
- Bootstrapping aka Bagging
- Boosting
- Isolation forest

# Learning with ensembles



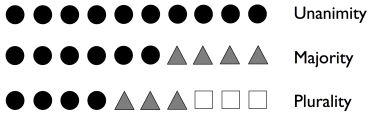
*... the interests of truth require a diversity of opinions.* *(Mill (1859))*

- What if we can learn from the wisdom of crowds? That is, can we combine multiple classifiers?
- In a sense we get a "mixture of experts"
- Predictions more accurate and robust
- Simplest approach: majority voting
- We will discuss the intuition of why this might work

# Majority voting

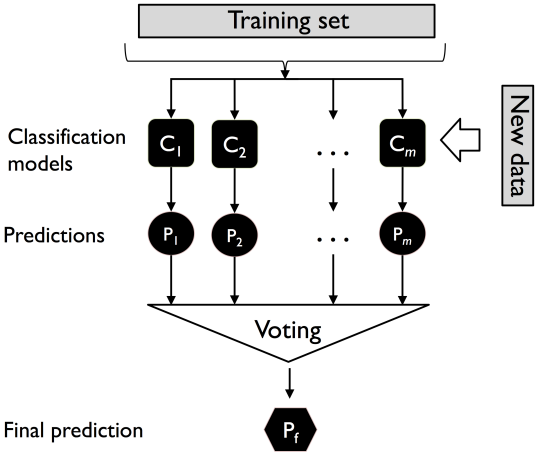


- Majority voting refers to binary setting but can easily generalize to multi-class (e.g. plurality voting)
- Select class label that receives the most votes (mode)
- Train $m$ classifiers $C_1, \ldots, C_m$
- Options:
  1. Build ensemble using different classification algorithms (e.g. SVM, logistic regression, etc.) but same data
  2. Use the same algorithm but fit different subsets of the training set (e.g. random forest)



# General approach





# Combining predictions via majority voting

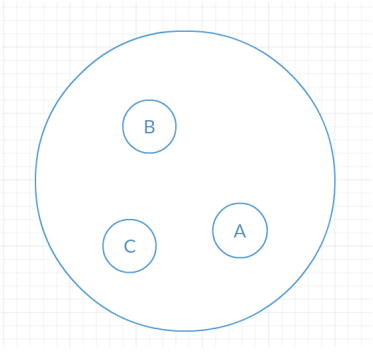


We have predictions of individual classifiers $C_j$ and need to select the final class label $\hat{y}$

$$\hat{y} = mode\{C_1(\mathbf{x}), C_2(\mathbf{x}), \ldots, C_m(\mathbf{x})\}$$

For example, in a binary classification task where $class_1 = -1$ and $class_2 = +1$, we can write the majority vote prediction as follows:

$$C(\mathbf{x}) = sign\left[\sum_j^m C_j(\mathbf{x})\right] = \begin{cases} 1 & \text{if } \sum_j C_j(\mathbf{x}) \geq 0 \\ -1 & \text{otherwise} \end{cases}$$




Rohith Ghandi

# Intuition why ensembles can work better



- If errors $\epsilon$ are more or less independent a combination will reduce the variance
- Assume that all $n$ base classifiers have the same – but independent – error rate $\epsilon$
- The probability of an error of an ensemble can be expressed as a probability mass function of a binomial distribution:

$$P(y \geq k) = \sum_{k}^{n} \binom{n}{k} \epsilon^k (1-\epsilon)^{n-k} = \epsilon_{\text{ensemble}}$$

- Here, $\binom{n}{k}$ is the binomial coefficient and the distribution computes what the probability is of $k$ successes in $n$ trials. In other words, we compute the probability that the prediction of the ensemble is wrong.

# Example



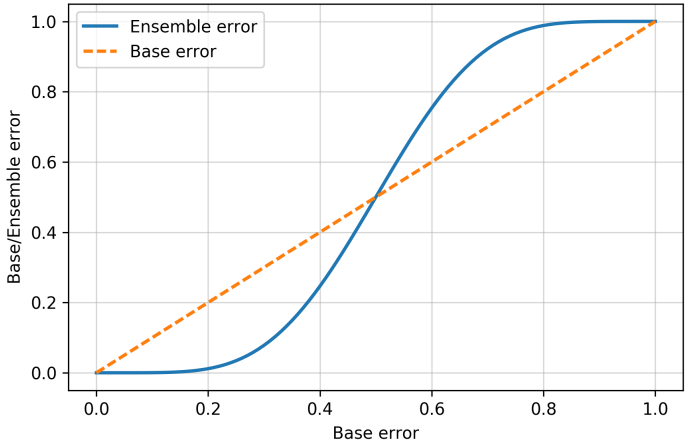
Imagine we have 11 base classifiers ($n = 11$) with individual error rates $\epsilon$ of 0.25 and:

$$P(y \geq k) = \sum_{k=6}^{11} \binom{11}{k} 0.25^k (1 - 0.25)^{11-k} = 0.034$$

So the error rate of the ensemble of $n = 11$ classifiers (0.034) is much lower than the error rate of the individual classifiers (0.25).

# Same reasoning applied to a wider range of error rates





# Voting classifier in scikit-learn



- Simply instantiate several classifiers and make a list
- Pass to sklearn.ensemble.VotingClassifier(...)

```
clf1 = LogisticRegression(random_state=1)
clf2 = RandomForestClassifier(random_state=1)
clf3 = GaussianNB()
estimators=[('lr', clf1), ('rf', clf2), ('gnb', clf3)]
ens_clf = VotingClassifier(estimators)
ens_clf = eclf1.fit(X, y)
```

- If all classifiers can estimate class probabilities, then using soft voting might help. In contrast with hard voting, confident estimators are given more weight

▸ sklearn API link

# Outline



ML4 – improving weak learners
- Trees
- Forests – Ensemble Classifiers
- Bootstrapping aka Bagging
- Boosting
- Isolation forest

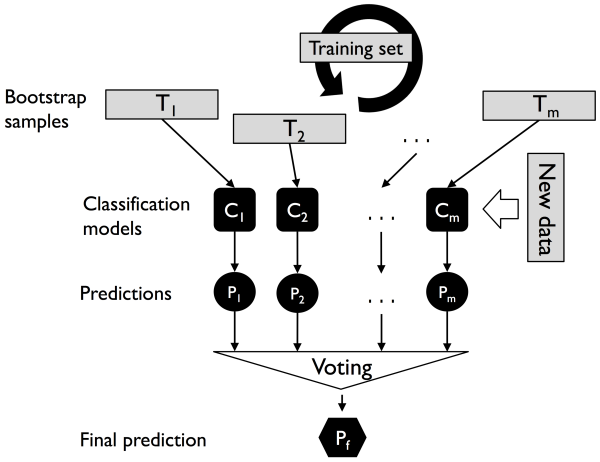
# Bootstrap aggregation (bagging)



- We used the entire training set for the majority vote classifier
- Here we draw random bootstrap samples
  - In statistics, bootstrapping is any test or metric that relies on random sampling with replacement
  - bootstrapping often used as an alternative to statistical inference based on the assumption of a parametric model when that assumption is in doubt
  - Alternatively we can sample *without* replacement: pasting
- The basic idea of bootstrapping is that inference about a population from sample data, can be modeled by resampling with replacement the sample data and performing inference about a sample from resampled data

# Bagging



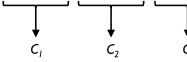

Training set
Bootstrap samples
$T_1$
$T_2$
$T_m$
Classification models
$C_1$
$C_2$
$C_m$
New data
Predictions
$P_1$
$P_2$
$P_m$
Voting
Final prediction
$P_f$

# Bagging example



- Seven training examples
- Sample randomly with replacement
- Use each bootstrap sample to train a classifier $C_j$
- $C_j$ is typically a decision tree
- Random Forests: also use random feature subsets
  - Instantiate a decision tree classifier
  - Make a bagging classifier with decision trees
  - Check that the accuracy is higher for the bagging classifier
- Asses model on out-of-bag (oob) observations (`oob_score=True`)
- Scales nicely because each of the models can be trained separately

| Sample indices | Bagging round 1 | Bagging round 2 | … |
|---|---|---|---|
| 1 | 2 | 7 | … |
| 2 | 2 | 3 | … |
| 3 | 1 | 2 | … |
| 4 | 3 | 1 | … |
| 5 | 7 | 1 | … |
| 6 | 2 | 7 | … |
| 7 | 4 | 7 | … |



# Outline



ML4 – improving weak learners
- Trees
- Forests – Ensemble Classifiers
- Bootstrapping aka Bagging
- Boosting
- Isolation forest

# Boosting



- Basic idea: start with weak learners that have only a slight performance advantage over random guessing (e.g. a decision tree 'stump') and try to boost their performance by focusing on training samples that are hard to classify
- Very simple base classifiers learn from misclassified training examples
- The original boosting algorithm was formulated by Robert Schapire in 1990
- It was later refined into AdaBoost – short for Adaptive Boosting
- AdaBoost used to be the common implementation of boosting. Lately XGBoost is becoming very popular.

# Original boosting algorithm

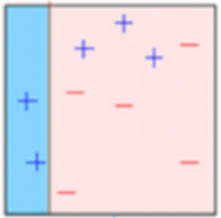


1. Draw a random subset of training samples $d_1$ without replacement from the training set $D$ to train a weak learner $C_1$
2. Draw second random training subset $d_2$ without replacement from the training set and add 50 percent of the samples that were previously misclassified to train a weak learner $C_2$
3. Find the training samples $d_3$ in the training set $D$ on which $C_1$ and $C_2$ disagree to train a third weak learner $C_3$
4. Combine the weak learners $C_1, C_2$, and $C_3$ via majority voting

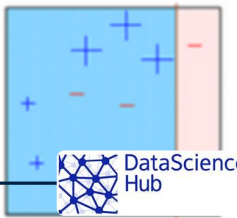
# AdaBoost

- In contrast, AdaBoost uses the complete training set to train the weak learners
- Training samples are re-weighted in each iteration to build a strong classifier
- End goal is to build a strong classifier that learns from the mistakes of the previous weak learners in the ensemble

Learner D1

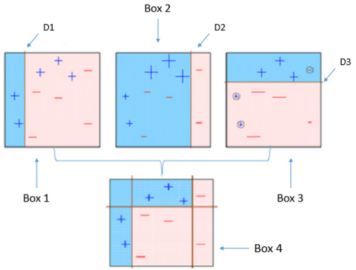


Learner



# AdaBoost

- In contrast, AdaBoost uses the complete training set to train the weak learners
- Training samples are re-weighted in each iteration to build a strong classifier
- End goal is to build a strong classifier that learns from the mistakes of the previous weak learners in the ensemble



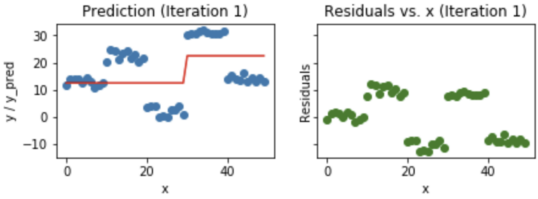

```
# AdaBoost Algorithm
from sklearn.ensemble import
    AdaBoostClassifierclf =
    AdaBoostClassifier()
# n_estimators = 50 (default value)
# base_estimator = DecisionTreeClassifier
    (default value)
clf.fit(x_train,y_train)
clf.predict(x_test)
```

# Gradient boosting

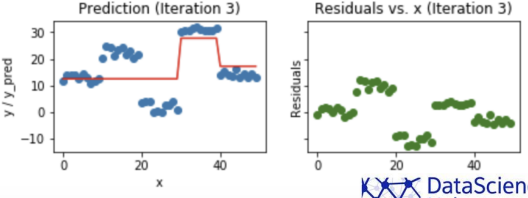


- View boosting problem as an optimization problem, i.e. we take up a loss function and try to optimize it
- New weak learners are added to concentrate on the areas where the existing learners are doing poorly

Iteration 1




Iteration 2



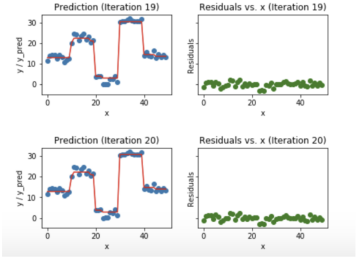

... last round

# Gradient boosting



- View boosting problem as an optimization problem, i.e. we take up a loss function and try to optimize it
- New weak learners are added to concentrate on the areas where the existing learners are performing poorly

```
# Gradient Boosting
from sklearn.ensemble import
    GradientBoostingClassifier
clf = GradientBoostingClassifier()
# n_estimators = 100 (default)
# loss function = deviance(default) used
    in Logistic Regression
clf.fit(x_train, y_train)
clf.predict(x_test)
```



# Best kid on the block: XGBoost



- XGBoost is similar to gradient boosting algorithm, but it has a few smart features
  - Clever penalization of Trees
  - A proportional shrinking of leaf nodes
  - Newton Boosting
  - Extra randomization parameter to reduce correlation between learners

```
# XGBoost
from xgboost import XGBClassifier
clf = XGBClassifier()
# n_estimators = 100 (default)
# max_depth = 3 (default)
clf.fit(x_train, y_train)
clf.predict(x_test)
```

- See the in-depth Webinar by Josh Starmer for a walk through. XGBoost starts at 36.32 but the intro is nice to see how to handle data.

# Forecast combination puzzle



- Ensemble learning is also used a lot in finance/econometric forecasting
  - Bates and Granger (1969), Rapach, Strauss and Zhou (2010), Stock and Watson (2004)
- Puzzle: Many, even sophisticated, models cannot beat a simple mean combination of univariate stock market return forecasts (Jacobsen et al. 2021)
- Especially challenging in streaming applications (Boulegane 2021)

# Outline

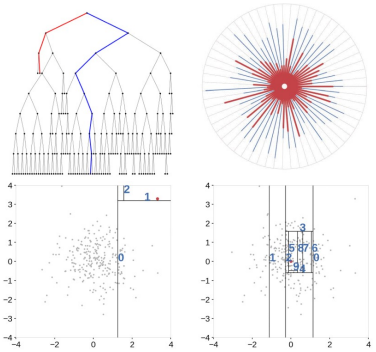


ML4 – improving weak learners
- Trees
- Forests – Ensemble Classifiers
- Bootstrapping aka Bagging
- Boosting
- Isolation forest

# How does an Isolation Forest work?



- 'Isolates' observations by randomly selecting a feature and then randomly selecting a split value (min. < split < max.)
- Since recursive partitioning can be represented by a tree structure, the number of splits required to isolate a sample equals the path length from the root node to the terminating node = Shorter path length), the more likely it is that it is an anomaly
- Can be expressed as an 'outlier score'

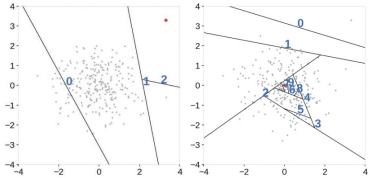


(a) Two normally distrib
clusters

# Extending the Isolation Forest

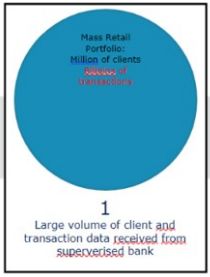


- Extended isolation forest selects random intercept and random slope (Hariri et al. (2021))
- Needs to store less information → faster, especially with many dimensions

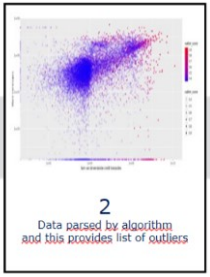


# How DNB applies the outlier detection model for KYC

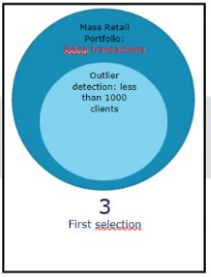




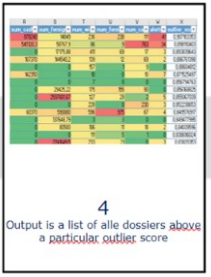

1
Large volume of client and transaction data received from superverised bank



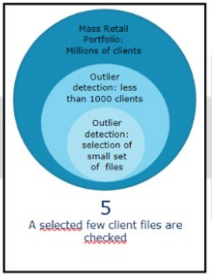
2
Data parsed by algorithm and this provides list of outliers




3
First selection



4
Output is a list of alle dossiers above a particular outlier score



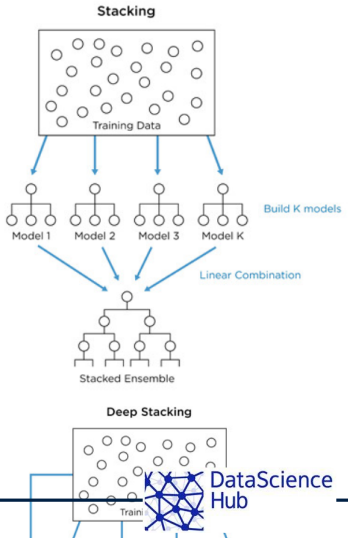

5
A selected few client files are checked

DataScience Hub

# Advanced topic: Stacking and deep stacking



- Stacking combines the outputs from multiple base models into a single score. The base-level models are trained based on a complete dataset, and then their outputs are used as input features to train an ensemble function
- Usually, the ensemble function is a simple linear combination of the base model scores.
- Deep stacking feeds the ensemble outcome(s) into a neural net + the original data



# Stacking steps



1. Split the data into a training and validation set
2. Divide the training set into K folds, for example 10
3. Train a base model (say SVM) on 9 folds and make predictions on the 10th fold
4. Repeat until you have a prediction for each fold
5. Fit the base model on the whole training set
6. Use the model to make predictions on the test set
7. Repeat step 3 – 6 for other base models (for example decision trees)
8. Use predictions from the test set as features to a new model – the meta-model
9. Make final predictions on the test set using the meta model

With regression problems, the values passed to the meta-model are numeric. With classification problems, they are probabilities or class labels.

# Blending



- Blending ≈ stacking, but uses a holdout set from the training set to make predictions. Predictions are done on the holdout set only. Predictions and holdout set are used to build a final model for predictions on the test set. Blending can be seen as stacking, where the meta-model is trained on predictions made by the base model on the hold-out validation set.
- The term blending was introduced by the Netflix Prize in Kaggle.
  - The blended solution achieves a 10-fold performance improvement on Netflix's movie recommendation algorithm.

# Blending (cont.)



- Steps:
  1. Split the data into a test and validation set
  2. Fit base models on the validation set
  3. Make predictions on the validation and test set
  4. Use the validation set and its predictions to build a final model
  5. Make final predictions using this model
- Blending vs stacking:
  - Blending is simpler than stacking and prevents leakage of information in the model. The generalizers and the stackers use different datasets. However, blending uses less data and may lead to overfitting.
  - Cross-validation is more solid on stacking than blending. It iss calculated over more folds, compared to using a small hold-out dataset in blending.

# Summary



In this lecture we covered:

1. How to define a tree, specifically how to split at each node
2. How to combine classifiers: ensemble learning a.k.a. “forests”
3. How ensembles can combine weak learners to come to much stronger learners. In particular AdaBoost and XGBoost
4. How we can use isolation forests for outlier detection

# AdaBoost algorithm



1. Set weight vector $\mathbf{w}$ to uniform weights where $\sum_i w_i = 1$
2. For $j$ in $m$ boosting rounds, do the following:
   1. Train a weighted weak learner $C_j = train(\mathbf{X}, \mathbf{y}, \mathbf{w})$
   2. Predict class labels $\hat{y} = predict(C_j, \mathbf{X})$
   3. Compute the weighted error rate $\epsilon = \mathbf{w} \cdot (\hat{\mathbf{y}} \neq \mathbf{y})$
   4. Compute the coefficient $\alpha_j$ $\alpha_j = 0.5 \log \frac{1-\epsilon}{\epsilon}$
   5. Update the weights $\mathbf{w} := \mathbf{w} \times \exp\big(-\alpha_j \times \hat{\mathbf{y}} \times \mathbf{y}\big)$
   6. Normalize weights to sum to 1 $\mathbf{w} := \mathbf{w} / \sum_i w_i$
3. Compute the final prediction: $\hat{\mathbf{y}} = \Big(\sum_{j=1}^{m} \big(\alpha_j \times predict(C_j, \mathbf{X})\big) > 0\Big)$

# References I




- Boulegane, D. (2021). Machine learning algorithms for dynamic Internet of Things. PhD thesis.
- Friendly, M., Symanzik, J., & Onder, O. (2019). Visualising the Titanic disaster. Significance, 16(1), 14–19.
- Hariri, S., Kind, M. C., & Brunner, R. J. (2021). Extended Isolation Forest. IEEE Transactions on Knowledge and Data Engineering, 33(4), 1479–1489.
- Jacobsen, B., Jiang, F., & Zhang, H. (2021). Ensemble Machine Learning and Stock Return Predictability. Working Paper.
- Mill, J. S. (1859). On Liberty. Cambridge University Press.