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- Decision trees
- Ensemble methods
- Bagging
- Random forests
- Boosting

Machine learning – Block 2

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Autumn 2023

This week's lecture

- Trees
- Bagging
- Random Forest
- Boosting (Trees)

Assignment 1

Short evaluation.

1. Research ammanuens positions ()
2. Master Thesis projects (deadline friday)

Section 1

Decision trees

Decision trees: basic idea

- A popular method that can be used for both classification and regression is decision trees.

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Decision trees: basic idea

- A popular method that can be used for both classification and regression is decision trees.
- Have you ever played the game "20 questions"?
- Decision trees is more or less that game!
- In the case of classification, the idea is to classify the new observation by
  1. Asking a questions
  2. Based on the previous answer, ask new question
  3. Questions are asked until a conclusion is reached

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Decision trees: basic idea

Name	Body temp	Gives birth	Legs	Class
Human	warm-blooded	yes	yes	mammal
Whale	warm-blooded	yes	no	mammal
Cat	warm-blooded	yes	yes	mammal
Cow	warm-blooded	yes	yes	mammal
Python	cold-blooded	no	no	reptile
Komodo dragon	cold-blooded	no	yes	reptile
Turtle	cold-blooded	no	yes	reptile
Salmon	cold-blooded	no	no	fish
Eel	cold-blooded	no	no	fish
Pigeon	warm-blooded	no	yes	bird
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Classify Komodo dragon with a decision tree:

1. Does it give live birth?

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Classify Komodo dragon with a decision tree:

1. Does it give live birth? (No!)
2. Is it warm-blooded?

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Classify Komodo dragon with a decision tree:

1. Does it give live birth? (No!)
2. Is it warm-blooded? (No!)
3. Does it have legs?

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Classify Komodo dragon with a decision tree:

1. Does it give live birth? (No!)
2. Is it warm-blooded? (No!)
3. Does it have legs? (Yes!) $\rightarrow$ Reptile

Regression trees: The regions of a tree

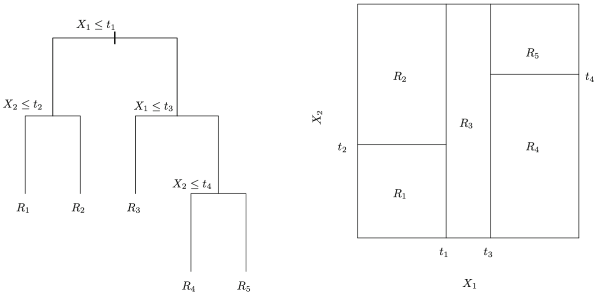

Figure: Regions of a tree (Garreth et al, 2013, Fig. 8.3)

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Regression Trees

$$T(x) = \sum_{m=1}^{M} \gamma_m I(x \in R_m)\,,$$

where M is the total number of regions and $I(x \in R_m)$ is an indicator variable if x_i belongs to region R_m and γ_m is the prediction for region m.

Regression Trees

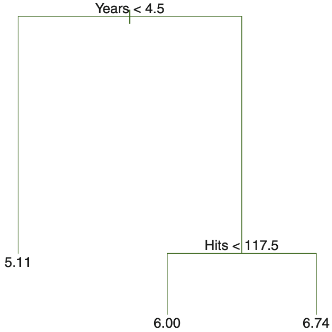

Figure: Regression Tree (Garreth et al, 2013, Fig. 8.1.)

- The `Hitters dataset`: log Salaries of Baseball players.
- The end of the tree contain the observations.

Regression Trees

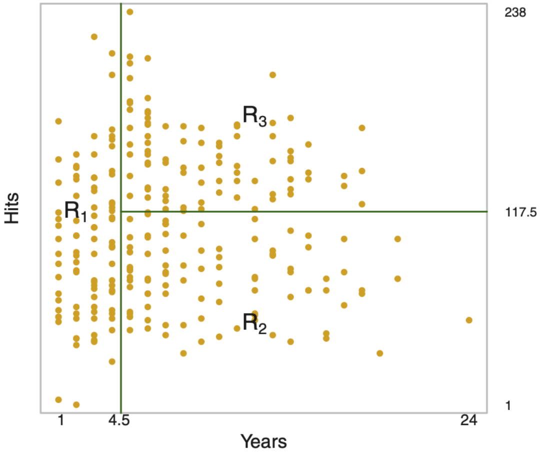

Figure: `Hitters` data and regression tree regions (Garreth et al, 2013, Fig. 8.2.)

Estimating a Decision Tree

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3. Usually we estimate γ_m as the mean of y_i in the region as:

$$\hat{\gamma}_m = \frac{1}{N_m} \sum_{x_i \in R_m}^{N_m} y_i \,,$$

where N_m is the number of observations in region R_m.

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   where N_m is the number of observations in region R_m.
4. Learning R_m exact is generally computationally infeasable so we use a greedy heuristic.

Growing a Decision Tree: Greedy Algorithm

Let $\mathcal{S}$ be the set of all observations $\{1, ..., N\}$ and `S[[m]]` be the set of observation indecies in R_m and `l` is the minimal number of leafs per node.

Input: $\mathcal{S}$, `X`, `y`, `l`

1. `S[[1]]` $= \mathcal{S}$,`M = 1`, `m = 1`
2. `while m <= M` then do:
   - 2.1 `if(size(S[[m]]) >= 2*l)`
     - 2.1.1 `S[[M+1]]`, `S[[M+2]]`, `j[m]`, `s[m]` $=$ `split_tree(X[S[[m]],], y[S[[m]],],l)`
     - 2.1.2 `M = M + 2`
   - 2.2 `else`
     - 2.2.1 compute $\hat{\gamma}$ for `S[[m]]`
   - 2.3 `m = m + 1`

Output: `j`, `s`, γ

Example of a tree: `j = {Years, Hits}`, `s = {4.5, 117.5}`, $\hat{\gamma} = \{122, 317, 245\}$

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How to do a split?

Here we try to compute Eq. (9.12-9.14) in ESL:

$$R_1(j,s) = \{X|X_j \leq s\} \text{ and } R_2(j,s) = \{X|X_j > s\}$$

$$\min_{j,s}\left(\min_{c_1}\sum_{x_i\in R_1(j,s)}(y_i - c_1)^2 + \min_{c_2}\sum_{x_i\in R_2(j,s)}(y_i - c_2)^2\right)$$

Inner minimization is solved by:

$$\hat{c}_m = \frac{1}{N_m}\sum_{x_i\in R_m}^{N_m} y_i\ ,$$

How to do a split? Pseudo-code

Input: $\mathbf{X}, \mathbf{y}, l$

1. $SS = \text{Inf}$ # Store sum of squares in matrix of dim $P \times N_s$
2. $S = \text{Inf}$ # Store split point in matrix of dim $P \times N_s$
3. for $j \in \{1, ..., P\}$ # all features
   3.1 for $k \in \{1, ..., N_s\}$ # all observations in set s
      3.1.1 $s = x_{k,j}$ # Split point (use the value of x)
      3.1.2 if $(|R_1(s,j)| < l$ or $|R_2(s,j)| < l)$ next # Dont create too few leaves
      3.1.3 $\hat{c}_1 = \frac{1}{|R_1(s,j)|} \sum_{x_i \in R_1(s,j)} y_i$
      3.1.4 $\hat{c}_2 = \frac{1}{|R_2(s,j)|} \sum_{x_i \in R_2(s,j)} y_i$
      3.1.5 $SS_{k,j} = \sum_{x_i \in R_1(s,j)} (y_i - c_1)^2 + \sum_{x_i \in R_2(s,j)} (y_i - c_2)^2$ # Compute Sum of Squares
      3.1.6 $S_{k,j} = \text{s}$
4. $k_{final}, j_{final} = \min_{k,j} SS$
5. $s_{final} = S_{k_{final}, j_{final}}$
6. return $R_1(s_{final}, j_{final}), R_2(s_{final}, j_{final}), s_{final}, j_{final}$

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Decision trees: Classification Trees

- How do we do if we have a classification tree?

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- The Gini is maximized when all classes have the same number of observations at t.
- One criterion for splitting could be to minimize the Gini in the next level of the tree. That way we will get "purer" nodes.

Important concepts in trees

- Tree depth: the length of the longest path from the root to a leaf (i.e. greatest number of questions that the tree can ask).

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- Overfitting (high variance)
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The solution to this is

- Pruning: forcing the tree to be smaller by adding a stopping condition, e.g. a maximum depth or minimal leaf size.
- But decision trees are quite bad predition models...

Section 2

Ensemble methods

Wisdom of the crowd

Simulated example (Prize academy, see ESL):

1. 50 members vote in 10 categories, each with 4 nominations.

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1. 50 members vote in 10 categories, each with 4 nominations.
2. For any category, only 15 voters have some knowledge ($p > 0.25$)
3. For each category, the 15 experts are chosen at random from the 50.

Wisdom of the crowd

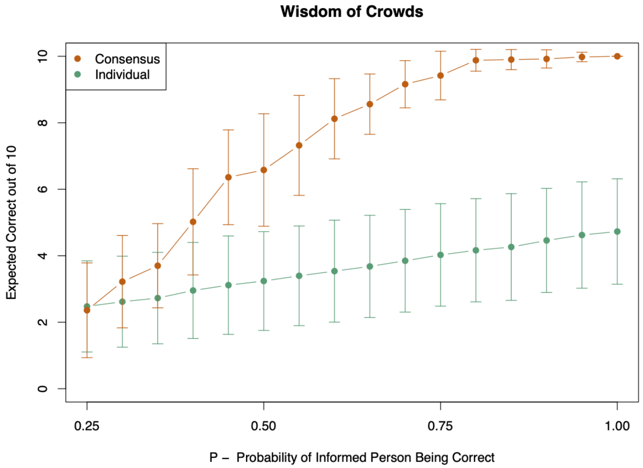

Figure: Simulated Award Voting, Fig. 8.11 (ESL)

General idea of ensembles

The idea of an ensemble is simple: If it difficult to find one really good model perhaps we can find several weaker models and combine their predictions.

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General idea of ensembles

The idea of an ensemble is simple: If it difficult to find one really good model perhaps we can find several weaker models and combine their predictions.

A simple example: Say you have one outcome Y and 4 covariates X_1, X_2, X_3, X_4. The goal is to predict Y. A possible ensemble would be to fit

$$\begin{aligned} y &= \alpha_1 + \beta_1 X_1 + \epsilon_1 \\ y &= \alpha_2 + \beta_2 X_2 + \epsilon_2 \\ y &= \alpha_3 + \beta_3 X_3 + \epsilon_3 \\ y &= \alpha_4 + \beta_4 X_4 + \epsilon_4 \end{aligned}$$

and then use the mean of their predictions

$$\hat{y}_{ensemble} = \frac{1}{4}\sum_{i=1}^{4} \hat{y} = \frac{1}{4}\sum_{i=1}^{4} (\hat{\alpha}_i + \hat{\beta}_i X_i) \tag{1}$$

Two key parts of an ensemble

1. The prediction models (sometimes called ‘learners’)
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   - A single model in an ensemble can be a simple or a complex model
   - Often the ensemble contains many simple models.
2. The weighting of each prediction in the final ensemble prediction
   - Many different algorithms for weighting together the predictions from many models
   - Models/learners with better predictive power can be given larger weights in the final prediction

Ensambles of decision trees

- A common type of ensembles is ensembles of decision trees.
- We will focus on this case, but note that any type of model can be included in an ensemble in principle.

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Bagging and Boosting

Remember, the error of a prediction/classification can be decomposed as

$$error = bias^2 + variance + bayeserror. \quad (2)$$

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- Shallow models/weak learners (with few parameters) tend to have small variance and large bias

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- Complex models/strong learners (with many parameters) tend to have small bias and large variance (tend to be overfitted)
- Shallow models/weak learners (with few parameters) tend to have small variance and large bias

Bagging: Ensemble methods that aim to decrease the variance of complex/strong learners with low bias and large variance

Boosting: Ensemble methods that aim to decrease the bias of shallow/weak learners with low variance and large bias

Section 3

Bagging

Bagging (Bootstrap AGGregating)

- Train several deep trees and combine their results
- Use bootstrap to train different trees

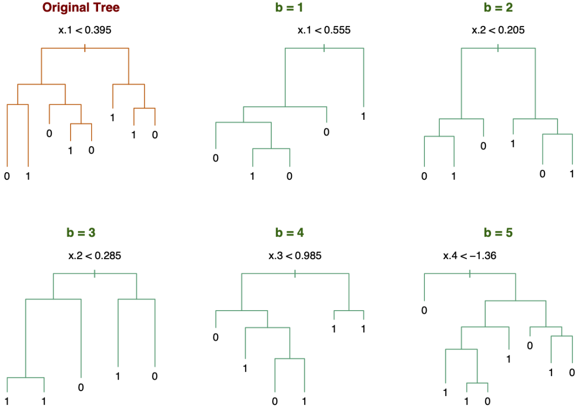

Figure: Bagging trees, Fig. 8.9 (ESL)

Bagging (Bootstrap AGGregating)

1. Draw, *with replacement*, a random sample of N units from the original sample
2. Fit a prediction model (e.g., a deep decision tree)
3. Repeat steps 1-2 B times
4. Weight together the predictions from the B models into a final ensemble prediction as

$$\hat{f}_{\text{bag}}(x_i) = \frac{1}{B}\sum_b \hat{f}^b(x_i)$$

Section 4

Random forests

Random Forest

A random forest is a bagging ensemble method, but with one extra step. Consider a sample of N units and K observed covariates/features

Random forest algorithm:

1. Draw, *with replacement*, a random sample of N units from the original sample
2. **Draw, without replacement, a random subset of k covariates/features**
3. Fit a prediction model (e.g., a decision tree)
4. Repeat step 1-3 B times
5. Weight together the predictions from the B models into a final ensemble prediction

It is common to use $k = \sqrt{K}$ (rounded down) for classification and $k = K/3$ for regression. But these are only rules of thumb: k is a *tuning parameter*.

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Random Forest, variance reduction

- Consider each tree to be an i.i.d. random variable with variance σ^2.
- The average of these trees then have variance

$$\frac{1}{B}\sigma^2.$$

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Random Forest, variance reduction

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- The second term will vanish with increasing B leaving just the first term left: a function of the correlation between the trees
- The remaining part of the variance is minimized by only consider a subset of the covariates when constructing trees - reducing the correlation between them.

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Bagging vs. random forest

- In bagging, the trees are often highly correlated
  - If some covariates are strong predictors of the outcome (in the training data), many trees in the 'bag' will us the same covariates in their decisions

Bagging vs. random forest

- In bagging, the trees are often highly correlated
  - If some covariates are strong predictors of the outcome (in the training data), many trees in the 'bag' will us the same covariates in their decisions
- In a random forest, the trees are less similar/correlated since all covariates are not available when each tree is constructed.
- A random forest (with many trees) uses the predictive ability of all covariates rather than just a few $\rightarrow$ improves out of sample performance.

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Section 5

Boosting

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Boosting

1. In boosting, models/trees are trained sequentially

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Boosting

1. In boosting, models/trees are trained sequentially
2. Each new model tries to target weak spots of the previous models in the ensemble to improve the performance of the ensemble

Boosting

1. Fit a prediction model/classifier (e.g., a decision tree) using the original sample
   - Give the misclassified observations higher weights
2. Draw, *with replacement*,*with probability proportional to the weights*, a random sample of N units from the original sample
3. Fit a prediction model/classifier (e.g., a *shallow* decision tree) using the new sample
4. Update the weights of each observation according to the average misclassification of the trained classifiers
5. Repeat step 2-4 B times
6. Weight together the predictions from the B models into a final ensemble prediction, giving larger weights to classifiers with smaller errors

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Boosting

For boosting to work well, the updates of the weights must be chosen in some clever way. One successful method is *gradient descent*.

We will not focus more on the particular algorithms. For now, we are satisfied with understanding the concept of boosting:

Train a bunch of classifiers sequentially. Force each new classifier to train more on data that the previous classifiers had problems with classifying by giving those samples a higher probability to be sampled.

XGBoost

1. State of the Art method

XGBoost

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2. Use gradient boosting trees with regularization

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XGBoost

1. State of the Art method
2. Use gradient boosting trees with regularization
3. Is scalable to very large data