



UPPSALA
UNIVERSITET

Machine learning – Block 2

Måns Magnusson
Department of Statistics, Uppsala University

Autumn 2022



UPPSALA
UNIVERSITET

This week's lecture

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

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



UPPSALA
UNIVERSITET

Assignment 1

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

Short evaluation.

1. Assignment 1: Still needs to be reduced? What to remove?
2. More math?
3. Research ammanuens positions (deadline wednesday)
4. Master Thesis projects (deadline friday)



UPPSALA
UNIVERSITET

Decision trees: basic idea

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

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



UPPSALA
UNIVERSITET

Decision trees: basic idea

- **Decision trees**
 - Ensemble methods
 - Bagging
 - Random forests
 - Boosting
- A popular method that can be used for both classification and regression is **decision trees**.
 - Have you ever played the game "20 questions"?



UPPSALA
UNIVERSITET

Decision trees: basic idea

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

- 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!



Decision trees: basic idea

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

- 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



Decision trees: basic idea

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

- 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



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

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
Penguin	warm-blooded	no	yes	bird



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

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
Penguin	warm-blooded	no	yes	bird

Classify **Komodo dragon** with a decision tree:

1. Does it give live birth?



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

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
Penguin	warm-blooded	no	yes	bird

Classify **Komodo dragon** with a decision tree:

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



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

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
Penguin	warm-blooded	no	yes	bird

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?



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

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
Penguin	warm-blooded	no	yes	bird

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!**) → **Reptile**



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

Regression trees: The regions of a tree

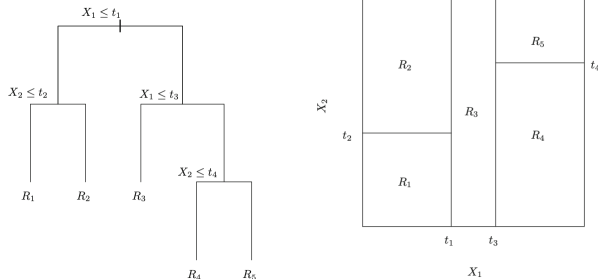


Figure: Regions of a tree (Garreth et al, 2013, Fig. 8.3)



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

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

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 .



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

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.



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

Regression Trees

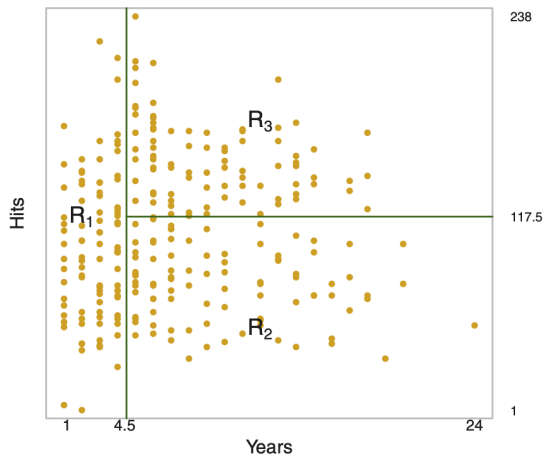


Figure: Hitters data and regression tree regions (Garreth et al, 2013, Fig. 8.2.)



UPPSALA
UNIVERSITET

Estimating a Decision Tree

1. A tree has two groups of parameters $\Theta = (\gamma, R)$ that we need to learn.

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



Estimating a Decision Tree

1. A tree has two groups of parameters $\Theta = (\gamma, R)$ that we need to learn.
2. We want a tree that minimize $L(\theta) = \sum_i^N (y_i - T_{\Theta}(x_i))^2$, here the squared loss

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



Estimating a Decision Tree

1. A tree has two groups of parameters $\Theta = (\gamma, R)$ that we need to learn.
2. We want a tree that minimize $L(\theta) = \sum_i^N (y_i - T_{\Theta}(x_i))^2$, here the squared loss
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 .



Estimating a Decision Tree

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

1. A tree has two groups of parameters $\Theta = (\gamma, R)$ that we need to learn.
2. We want a tree that minimize $L(\theta) = \sum_i^N (y_i - T_{\Theta}(x_i))^2$, here the squared loss
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 .

4. Learning R_m exact is generally computationally infeasible so we use a **greedy** heuristic.



Growing a Decision Tree: Greedy Algorithm

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

Input: $\mathcal{S}, X, y, 1$

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

Output: j, s, γ

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



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:

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



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

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 $j \in \{1, \dots, P\}$ # all features
 - 3.1 for $k \in \{1, \dots, N_s\}$ # all observations in set s
 - 3.1.1 $s = x_{k,j}$ # Split point (use the value of x)
 - 3.1.2 if $(|R_1(s,j)| < l \text{ or } |R_2(s,j)| < l)$ 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 $S_{k,j} = s$
4. $k_{final}, j_{final} = \min_{k,j} SS$
5. $s_{final} = S_{k_{final}, j_{final}}$
6. return $R_1(s_{final}, j_{final}), R_2(s_{final}, j_{final}), s_{final}, j_{final}$



UPPSALA
UNIVERSITET

Decision trees: Classification Trees

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

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



UPPSALA
UNIVERSITET

Decision trees: Classification Trees

- How do we do if we have a classification tree?
- We just change the loss function $L(\theta)$.

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



Decision trees: Classification Trees

- How do we do if we have a classification tree?
- We just change the loss function $L(\theta)$.
- Let $p(j|t)$ be the fraction of observations in class j at the node t and let J be the number of classes.

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



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

Decision trees: Classification Trees

- How do we do if we have a classification tree?
- We just change the loss function $L(\theta)$.
- Let $p(j|t)$ be the fraction of observations in class j at the node t and let J be the number of classes.
- The **Gini** for node t is defined as

$$Gini(t) = 1 - \sum_{j=1}^J p(j|t)^2$$



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

Decision trees: Classification Trees

- How do we do if we have a classification tree?
- We just change the loss function $L(\theta)$.
- Let $p(j|t)$ be the fraction of observations in class j at the node t and let J be the number of classes.
- The **Gini** for node t is defined as

$$Gini(t) = 1 - \sum_{j=1}^J p(j|t)^2$$

- Gini is a measure of "impurity". If all observations belong to the same class, then

$$Gini(t) = 1 - 1^2 - 0 - \dots - 0 = 0.$$



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

Decision trees: Classification Trees

- How do we do if we have a classification tree?
- We just change the loss function $L(\theta)$.
- Let $p(j|t)$ be the fraction of observations in class j at the node t and let J be the number of classes.
- The **Gini** for node t is defined as

$$Gini(t) = 1 - \sum_{j=1}^J p(j|t)^2$$

- Gini is a measure of "impurity". If all observations belong to the same class, then

$$Gini(t) = 1 - 1^2 - 0 - \dots - 0 = 0.$$

- The Gini is maximized when all classes have the same number of observations at t .



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

Decision trees: Classification Trees

- How do we do if we have a classification tree?
- We just change the loss function $L(\theta)$.
- Let $p(j|t)$ be the fraction of observations in class j at the node t and let J be the number of classes.
- The **Gini** for node t is defined as

$$Gini(t) = 1 - \sum_{j=1}^J p(j|t)^2$$

- Gini is a measure of "impurity". If all observations belong to the same class, then

$$Gini(t) = 1 - 1^2 - 0 - \dots - 0 = 0.$$

- 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).

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



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).
- **Leaf size:** the number of observations in a leaf.

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



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

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).
- **Leaf size:** the number of observations in a leaf.

Decision trees can become quite large, which may lead to:

- Overfitting (high variance)
- Difficulties interpreting the tree



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

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).
- **Leaf size:** the number of observations in a leaf.

Decision trees can become quite large, which may lead to:

- Overfitting (high variance)
- Difficulties interpreting the tree

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.



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

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).
- **Leaf size:** the number of observations in a leaf.

Decision trees can become quite large, which may lead to:

- Overfitting (high variance)
- Difficulties interpreting the tree

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 prediction models...



UPPSALA
UNIVERSITET

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**.

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



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

$$y = \alpha_1 + \beta_1 X_1 + \epsilon_1$$

$$y = \alpha_2 + \beta_2 X_2 + \epsilon_2$$

$$y = \alpha_3 + \beta_3 X_3 + \epsilon_3$$

$$y = \alpha_4 + \beta_4 X_4 + \epsilon_4$$

and then use the mean of their predictions

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



UPPSALA
UNIVERSITET

Two key parts of an ensemble

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

1. The prediction models (sometimes called 'learners')
 - A single model in an ensemble can be a simple or a complex model
 - Often the ensemble contains many simple models.



Two key parts of an ensemble

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

1. The **prediction models** (sometimes called 'learners')
 - 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



Ensembles of decision trees

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

- 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.



Bagging and Boosting

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

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

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



Bagging and Boosting

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

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

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

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



Bagging and Boosting

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

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

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

- **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 and Boosting

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

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

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

- **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



Bagging (Bootstrap AGGregating)

Consider a sample of N units.

Bagging algorithm:

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



Bagging (Bootstrap AGGregating)

Consider a sample of N units.

Bagging algorithm:

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

Train several deep trees and combine their results by weighting together their predictions



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*.



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

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

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



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

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

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

- Trees constructed from the same set of covariates will be correlated and therefore **not independent**.
- The variance of the average of these correlated trees then becomes

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$



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

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

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

- Trees constructed from the same set of covariates will be correlated and therefore **not independent**.
- The variance of the average of these correlated trees then becomes

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$

- The second term will **vanish with increasing B** leaving just the first term left: a function of the **correlation between the trees**



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

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

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

- Trees constructed from the same set of covariates will be correlated and therefore **not independent**.
- The variance of the average of these correlated trees then becomes

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$

- 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.



Differences between bagging and random forest:

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

- 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 use 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.

This means that a random forest (with many trees) uses the predictive ability of all covariates rather than just a few, which usually improves out of sample performance.



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

Boosting

In boosting, models are trained sequentially where 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



- Decision trees
- Ensemble methods
- Bagging
- Random forests
- **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.



UPPSALA
UNIVERSITET

XGBoost

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

1. State of the Art method



UPPSALA
UNIVERSITET

XGBoost

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

1. State of the Art method
2. Use gradient boosting trees with regularization



UPPSALA
UNIVERSITET

XGBoost

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

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