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Machine learning – Block 2

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Autumn 2023



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This week's lecture

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

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



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Assignment 1

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

Short evaluation.

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



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- Decision trees
- Ensemble methods
- Bagging
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- Boosting

Section 1

Decision trees



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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**.



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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"?



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Decision trees: basic idea

- Decision trees
- Ensemble methods
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- 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
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- 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
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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 |
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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!**) → **Reptile**



- Decision trees
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Regression trees: The regions of a tree

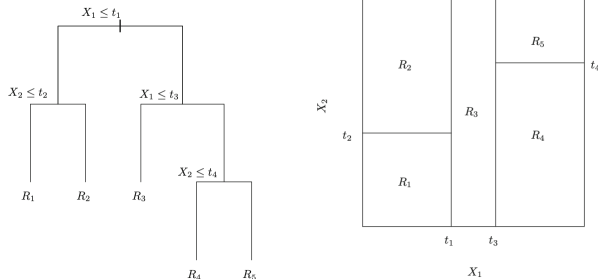


Figure: Regions of a tree (Garreth et al, 2013, Fig. 8.3)



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Regression Trees

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

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 .



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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.



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Regression Trees

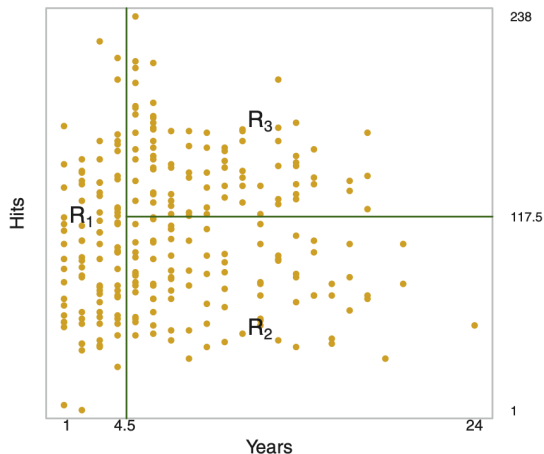


Figure: Hitters data and regression tree regions (Garreth et al, 2013, Fig. 8.2.)



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Estimating a Decision Tree

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

- Decision trees
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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

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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

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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:

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



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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 $R_1(s_{final}, j_{final}), R_2(s_{final}, j_{final}), s_{final}, j_{final}$



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Decision trees: Classification Trees

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

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Decision trees: Classification Trees

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

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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.

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Decision trees: Classification Trees

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- 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

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



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

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



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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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Important concepts in trees

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

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

- Overfitting (high variance)
- Difficulties interpreting the tree



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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.



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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 prediction models...



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- Decision trees
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Section 2

Ensemble methods



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Wisdom of the crowd

- Decision trees
- **Ensemble methods**
- Bagging
- Random forests
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Simulated example (Prize academy, see ESL):

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



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Simulated example (Prize academy, see ESL):

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2. For any category, only 15 voters have some knowledge ($p > 0.25$)



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Simulated example (Prize academy, see ESL):

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.

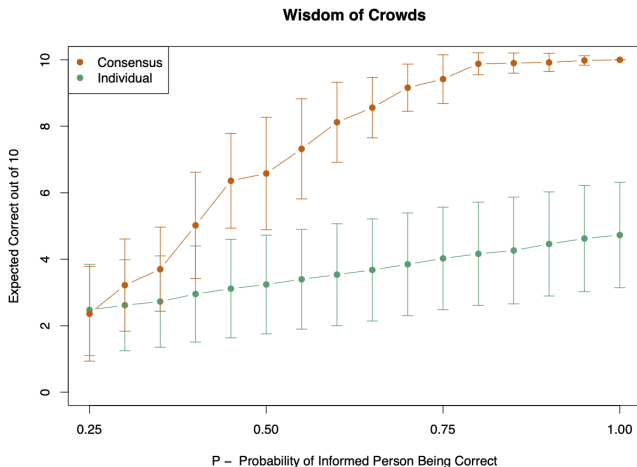


Figure: Simulated Award Voting, Fig. 8.11 (ESL)



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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**.

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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

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

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

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

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

and then use the mean of their predictions

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



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Two key parts of an ensemble

- Decision trees
- Ensemble methods
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- 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

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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

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

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



Bagging and Boosting

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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



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Section 3

Bagging



Bagging (Bootstrap AGGregating)

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

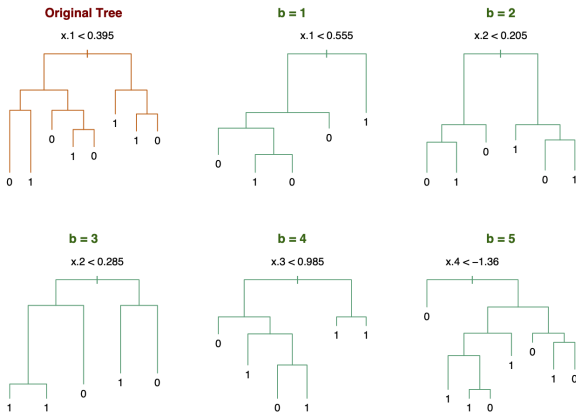


Figure: Bagging trees, Fig. 8.9 (ESL)



Bagging (Bootstrap AGGregating)

- Decision trees
- Ensemble methods
- **Bagging**
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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

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



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Section 4

Random forests



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Random Forest

- Decision trees
- Ensemble methods
- Bagging
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- A bagging ensemble method, but...



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Random Forest

- Decision trees
- Ensemble methods
- Bagging
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- A bagging ensemble method, but...
- Sample of N observations and K covariates/features



- Decision trees
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- A bagging ensemble method, but...
- Sample of N observations and K covariates/features
- 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: Algorithm

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

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



- Decision trees
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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

$$\mathbb{V}(\hat{f}(x)) = \frac{1}{B}\sigma^2.$$



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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

$$\mathbb{V}(\hat{f}(x)) = \frac{1}{B}\sigma^2.$$

- 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

$$\mathbb{V}(\hat{f}(x)) = \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$



Random Forest variance reduction

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

- The variance of the average of correlated trees:

$$\mathbb{V}(\hat{f}(x)) = \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$

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



Random Forest variance reduction

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- The variance of the average of correlated trees:

$$\mathbb{V}(\hat{f}(x)) = \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2.$$

- 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 trees.



Bagging vs. 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



Bagging vs. Random forest

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- In bagging, the trees are often highly correlated
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Bagging vs. Random forest

- Decision trees
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- In bagging, the trees are often highly correlated
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- In a random forest, the trees are less similar/correlated since all covariates are not available when each tree is constructed.
- Intuition: A random forest (with many trees) uses the predictive ability of all covariates rather than just a few → improved out of sample performance.



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

Section 5

Boosting



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Boosting

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

1. In boosting, models/trees are trained sequentially



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Boosting

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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



- Decision trees
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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.



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XGBoost

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

1. State of the Art method



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XGBoost

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



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XGBoost

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