Introduction to Machine Learning Lecture 5: Decision trees and Random Forests

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Nikolay Karpachev

Outline

- Decision tree
 - Definition
 - Constructing decision tree
 - Information criteria
 - Pruning
- 2. Composition methods
 - Bootstrap
 - Random subspace method
- 3. Random Forest

Classification (regression) models so far

- Linear classification / linear regression
 - Very efficient
 - Achieve reasonably good quality
 - Can capture only linear dependencies

- Naive bayes model
 - Very simple
 - Feature independence assumption does not hold in real data

Decision Tree: intuition

<u>Decision tree</u> is a logic-based classifier that is able to capture nonlinear dependencies

x = (9, male, 3)Example: Titanic dataset is sex male? survived is age > 9.5? died is sibsp > 2.5? survived died

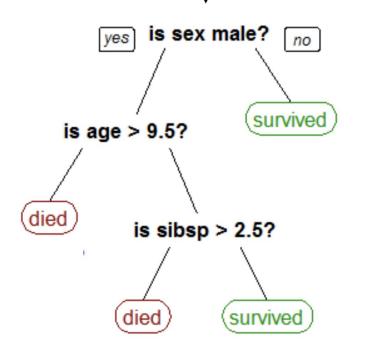
Example: Titanic dataset

$$x = (9, male, 3)$$

sex

age

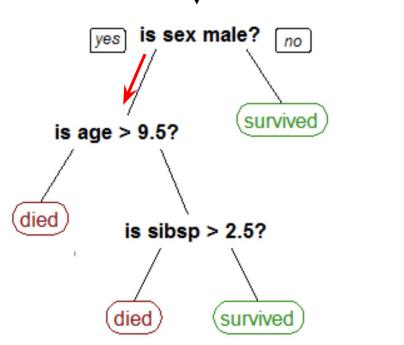
sibsp



Example: Titanic dataset

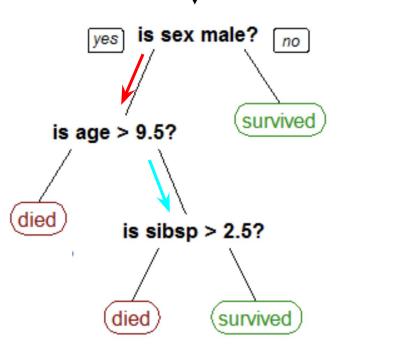
$$x = (9, male, 3)$$

sex



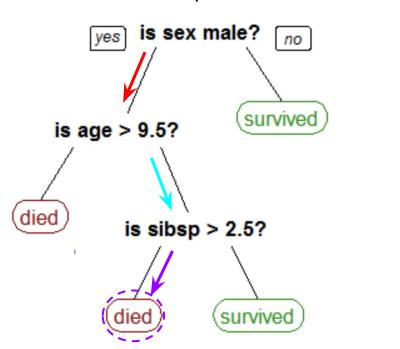
Example: Titanic dataset

$$x = (9, male, 3)$$



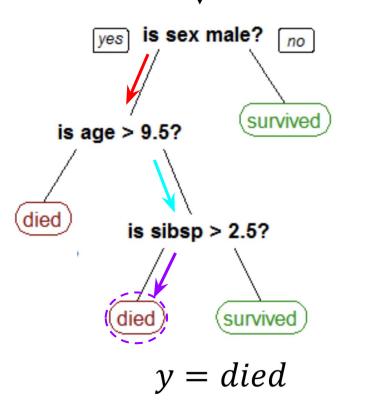
Example: Titanic dataset

$$x = (9, male, 3)$$



Example: Titanic dataset

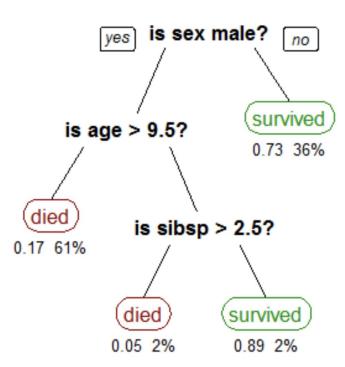
$$x = (9, male, 3)$$



Decision tree in classification

Example: Titanic

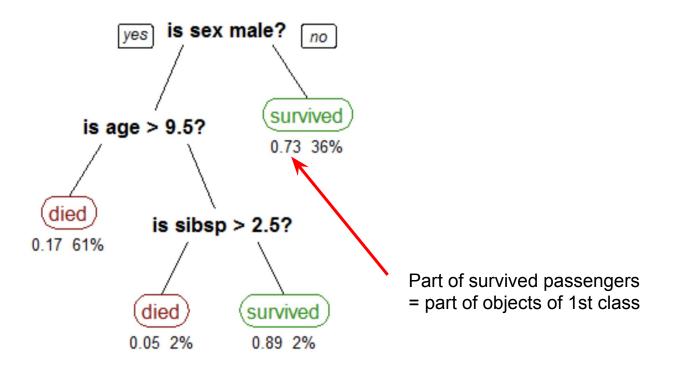
dataset



Decision tree in classification

Example: Titanic

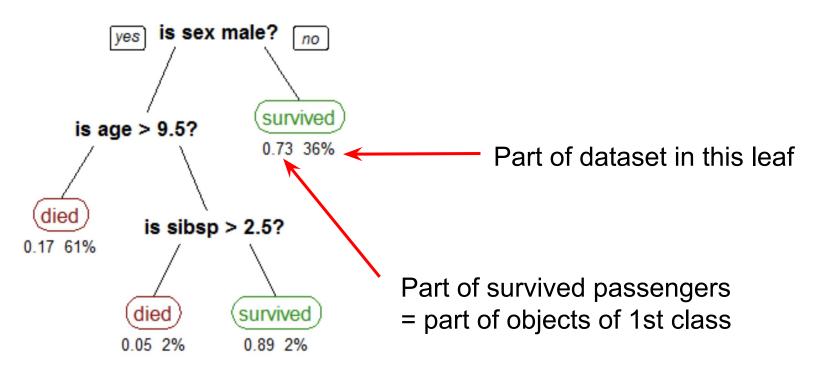
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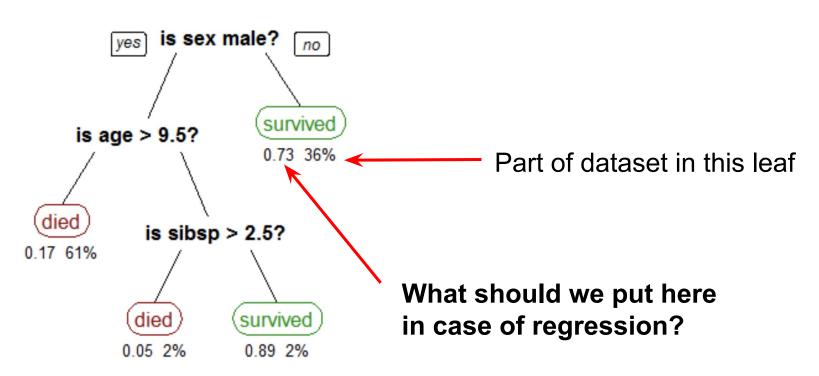
Decision tree in classification

Example: Titanic

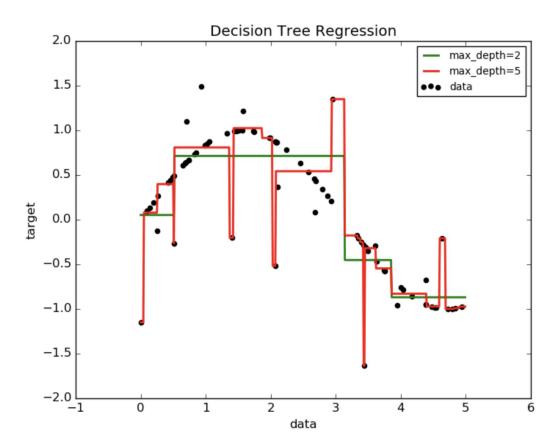
dataset



Decision tree in regression



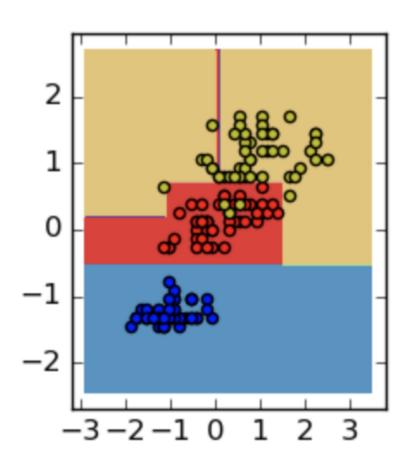
Decision tree in regression



Green - decision tree of depth 2
Red - decision tree of depth 5

Every leaf corresponds to some constant.

Decision tree surface

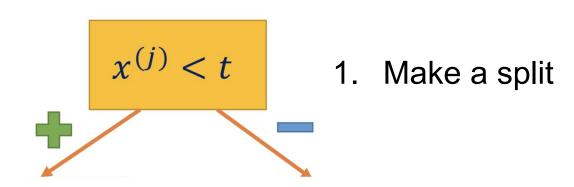


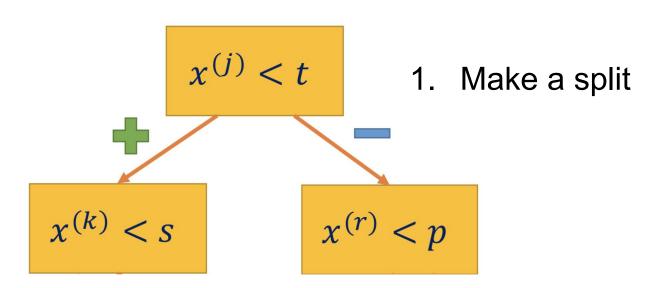
Classification problem with 3 classes and 2 features.

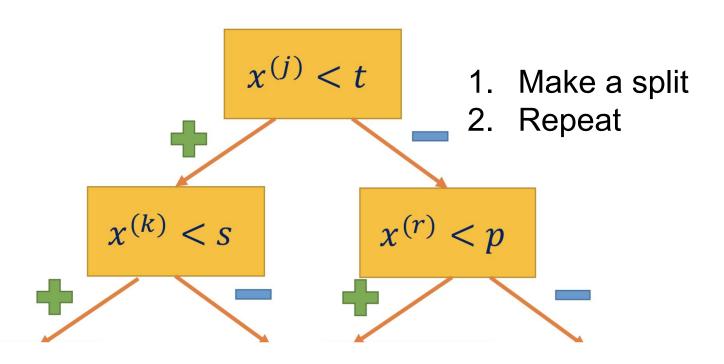
Decision Tree construction procedure

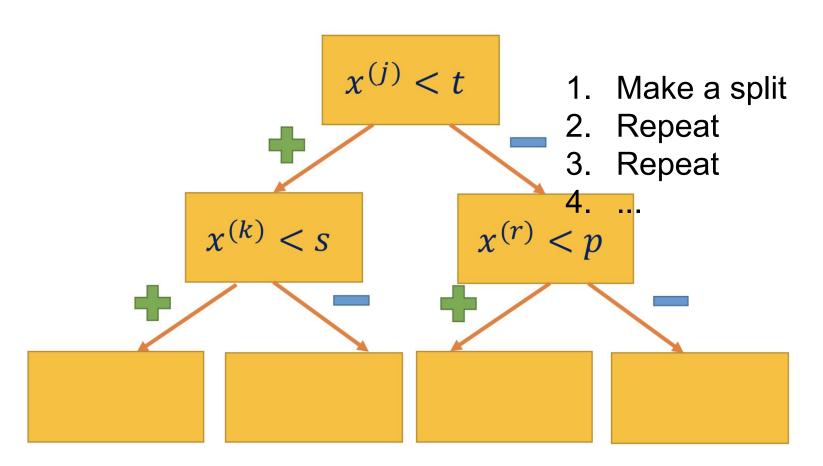
 $x^{(j)} < t$

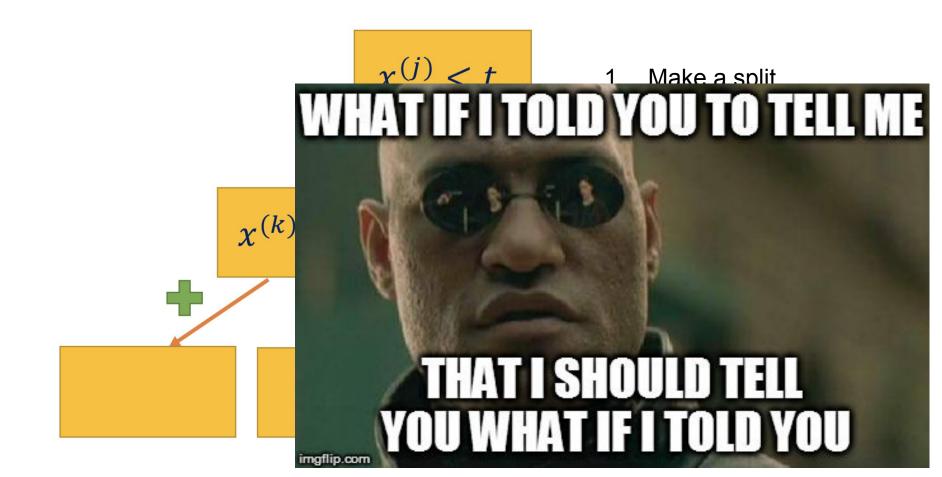
1. Make a split

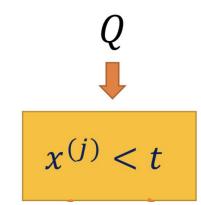


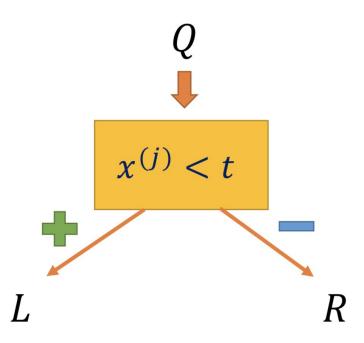


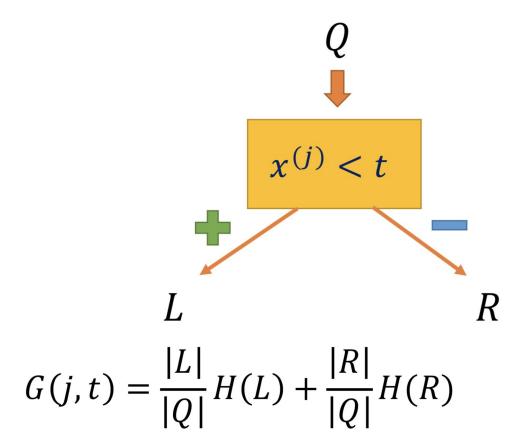


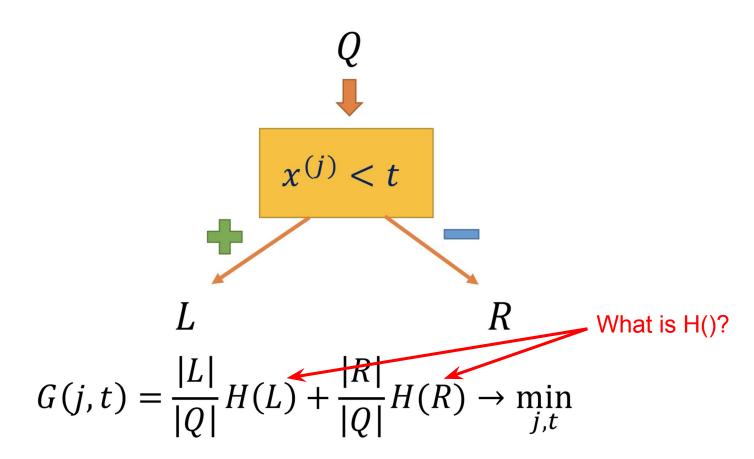












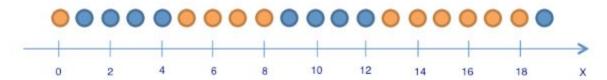
H(R) is measure of "heterogeneity" of our data. Consider binary classification problem:

1. Misclassification criteria:
$$H(R) = 1 - \max\{p_0, p_1\}$$

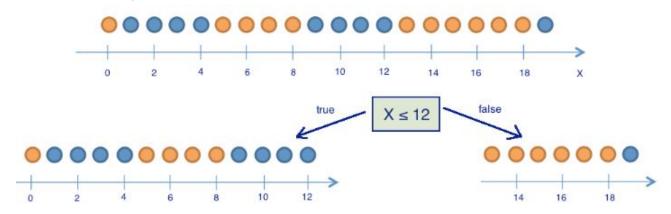
2. Entropy criteria:
$$H(R) = -p_0 \log_2 p_0 - p_1 \log_2 p_1$$

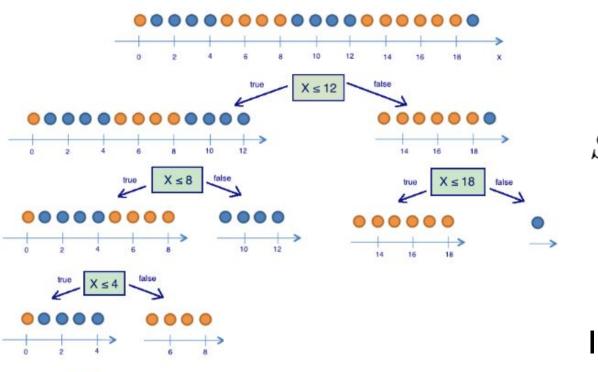
3. Gini impurity:
$$H(R) = 1 - p_0^2 - p_1^2 = 1 - 2p_0p_1$$

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H(R) is measure of "heterogeneity" of our data. Consider binary classification problem:





Information criteria: Entropy $S = -\sum p_k \log_2 p_k$

In binary case N = 2

$$S = -p_{+} \log_{2} p_{+} - p_{-} \log_{2} p_{-} = -p_{+} \log_{2} p_{+} - (1 - p_{+}) \log_{2} (1 - p_{+})$$

Information criteria: Gini impurity

$$G = 1 - \sum_{k} (p_k)^2$$

In binary case N = 2

$$G = 1 - p_+^2 - p_-^2 = 1 - p_+^2 - (1 - p_+)^2 = 2p_+(1 - p_+)$$

H(R) is measure of "heterogeneity" of our data. Consider multiclass classification problem:

1. Misclassification criteria:
$$H(R) = 1 - \max_k \{p_k\}$$

2. Entropy criteria:
$$H(R) = -\sum_k p_k \log_2 p_k$$

3. Gini impurity:
$$H(R) = 1 - \sum_{k} (p_k)^2$$

H(R) is measure of "heterogeneity" of our data. Consider regression problem:

1. Mean squared error

$$H(R) = \min_{c} \frac{1}{|R|} \sum_{(x_i, y_i) \in R} (y_i - c)^2$$

What is the constant?

$$c^* = \frac{1}{|R|} \sum_{y_i \in R} y_i$$

Time for your questions and a coffee break

Decision Tree can build a very complex dependency

In fact, it can perfectly fit the training data

Trivia: how can we construct such a tree?

Decision Tree can build a very complex dependency

In fact, it can perfectly fit the training data

Just create a very deep tree with one object per leaf. Training error = 0

Thus, decision trees are very prone to overfitting!

General idea: let's make the decision rule more simple and smooth

Two main approaches:

- Stopping criteria
 - Create new rules until stopping criterion is satisfied
 - The criterion controls the complexity
- Pruning
 - Simplify constructed tree

Stopping criteria

Maximum tree depth

- Maximum tree depth
- Minimal number of objects inside a leaf

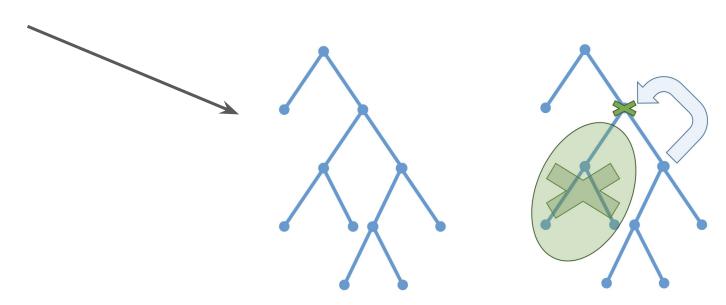
- Maximum tree depth
- Minimal number of objects inside a leaf
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- Maximum tree depth
- Minimal number of objects inside a leaf
- Maximum number of leaves
- Stop if all the objects in the leaf share the same class
- Stop when quality metric stops increasing by x% after the split

Pruning

- Post-pruning:
 - Simplify constructed tree.



Compositions of decision trees (ensembles)

Compositions

- Decision trees are prone to overfitting
- At the same time, they capture complex dependencies

Main idea:

- Let's train multiple decision trees that differ in some training properties
- Then their predictions' average will be the final answer

Consider dataset X containing N objects.

Pick I objects with return from X and repeat in N times to get N datasets.

Error of model trained on Xj:
$$\varepsilon_j(x) = b_j(x) - y(x), \qquad j = 1, \ldots, N,$$

Then
$$\mathbb{E}_x(b_j(x)-y(x))^2=\mathbb{E}_x\varepsilon_j^2(x)$$
.

The mean error of N models:
$$E_1 = \frac{1}{N} \sum_{i=1}^N \mathbb{E}_x \varepsilon_j^2(x)$$
.

Consider the errors unbiased and uncorrelated:

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$

 $\mathbb{E}_x \varepsilon_i(x) \varepsilon_j(x) = 0, \quad i \neq j.$

 $a(x) = \frac{1}{N} \sum_{j=1}^{N} b_j(x).$

Error decreased by N times!

$$E_N = \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^n b_j(x) - y(x) \right)^2 =$$

$$E_N = \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^N b_j(x) - y(x) \right)$$
$$= \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^N \varepsilon_j(x) \right)^2 =$$

$$\mathcal{L}_x\left(\frac{1}{N}\right)$$

$$x \left(\frac{1}{N} \sum_{j=1}^{N} x_j \right)$$

$$\sum_{j=1}^{n} b_j(x) - y(x)$$

$$-y(x)$$

 $= \frac{1}{N^2} \mathbb{E}_x \left(\sum_{j=1}^N \varepsilon_j^2(x) + \sum_{i \neq j} \varepsilon_i(x) \varepsilon_j(x) \right) =$

$$y(x)$$
 =

$$\mathbb{E}_{x}\varepsilon_{x}(x)=0$$

$$\mathbb{E}_x \varepsilon_i(x) = 0$$
:

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$

Consider the errors unbiased and uncor

$$\mathbb{E}_x \varepsilon_i(x) = 0;$$
 This is a lie

$$E_{\sigma\varepsilon_i}(x)\varepsilon_i(x) = 0, \quad i \neq i$$

$$\mathbb{E}_{x} \varepsilon_{i}(x) \varepsilon_{j}(x) = 0, \quad i \neq j.$$

$$\mathbb{E}_x \varepsilon_i(x) \varepsilon_j(x) = 0, \quad i \neq j.$$

The final model averages all predictions:

$$a(x) = \frac{1}{N} \sum_{j=1}^{N} b_j(x).$$

$$N \stackrel{\sum}{\underset{j=1}{\sum}} J (\gamma)$$

$$j=1$$
Error decreased by N times!

$$E_N = \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^n b_j(x) - y(x) \right)^2 =$$

$$= \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^N \varepsilon_j(x) \right)^2 =$$

$$= \frac{1}{N^2} \mathbb{E}_x \left(\sum_{j=1}^N \varepsilon_j^2(x) + \sum_{i \neq j} \varepsilon_i(x) \varepsilon_j(x) \right) =$$

$$E_1$$
.

Bagging = Bootstrap aggregating

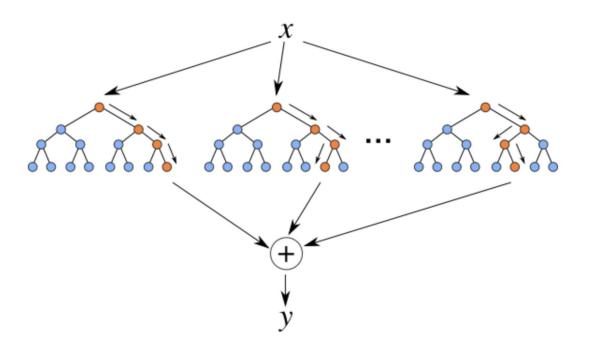
Decreases the error if the basic algorithms are not correlated.

RSM - Random Subspace Method

Same approach, but with features.

Random Forest

Bagging + RSM = Random Forest



Random Forest

Training procedure:

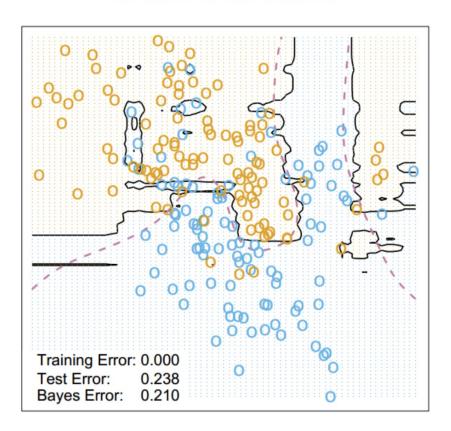
- Create N bootstrap samples from the data
- For each sample, train a decision tree with RSM
- Average the trees' answers for the ensemble prediction

Random Forest

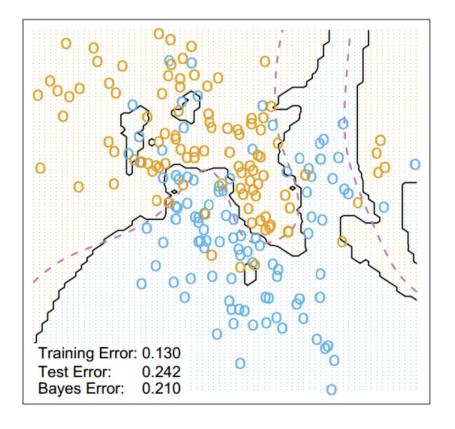
- One of the greatest "universal" models.
- There are some modifications: Extremely Randomized Trees, Isolation Forest, etc.
- Allows to use train data for validation: OOB

OOB =
$$\sum_{i=1}^{\ell} L\left(y_i, \frac{1}{\sum_{n=1}^{N} [x_i \notin X_n]} \sum_{n=1}^{N} [x_i \notin X_n] b_n(x_i)\right)$$

Random Forest Classifier



3-Nearest Neighbors



Thanks for your attention