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

Harbour.Space University
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Outline

1. Decision tree
    - Definition
    - Constructing decision tree
    - Information criterions
    - 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

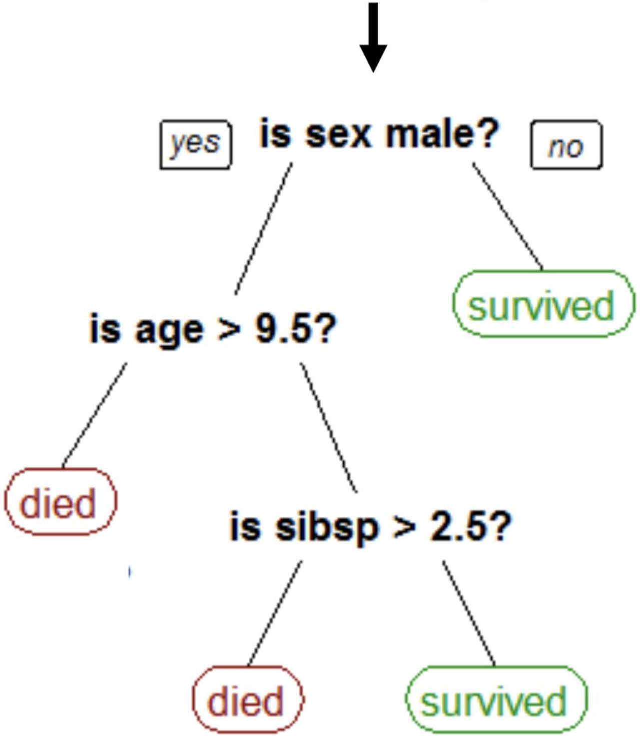
Decision tree

Decision tree is a logic-based classifier that is able to capture nonlinear dependencies

Decision tree

Example: Titanic dataset

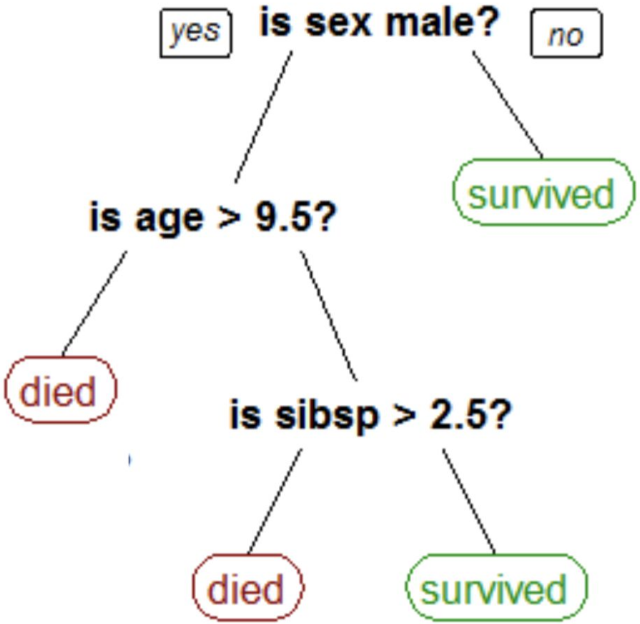
$$x = (9, \quad male, \quad 3)$$



Decision tree

Example: Titanic dataset

$$\begin{array}{cccc} & \text{age} & \text{sex} & \text{sibsp} \\ x = (& 9, & male, & 3) \end{array}$$



Decision tree

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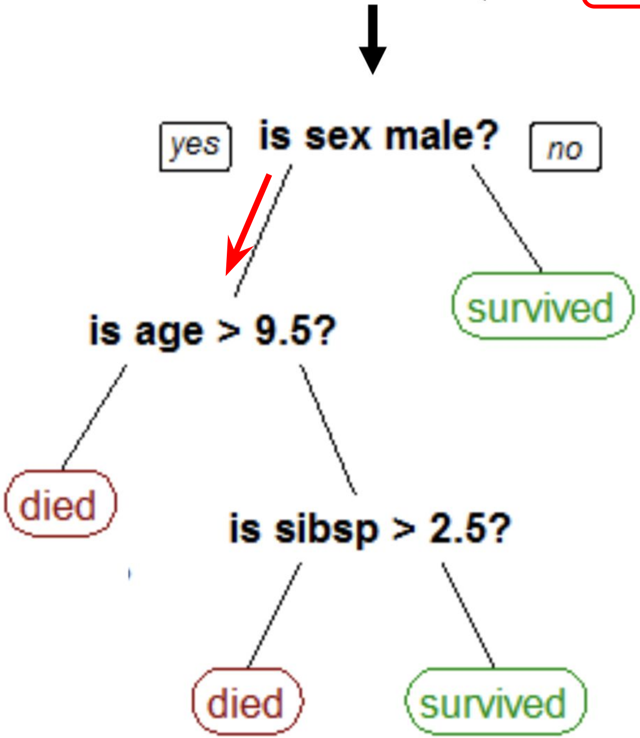

Decision tree

Example: Titanic dataset

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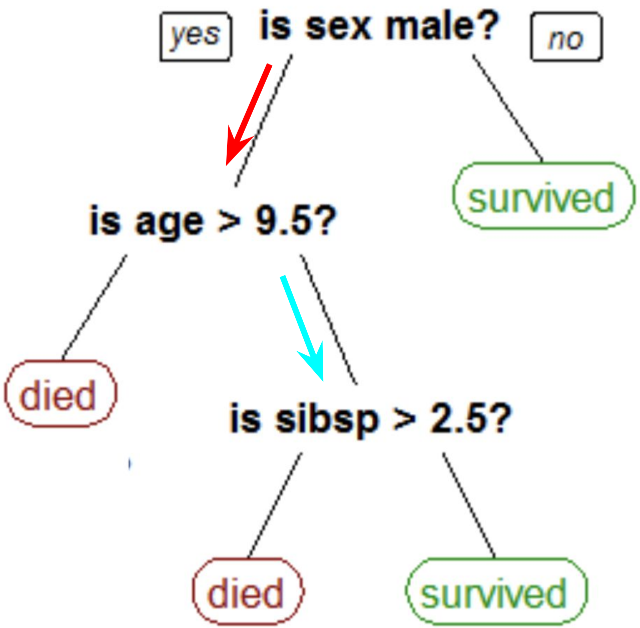
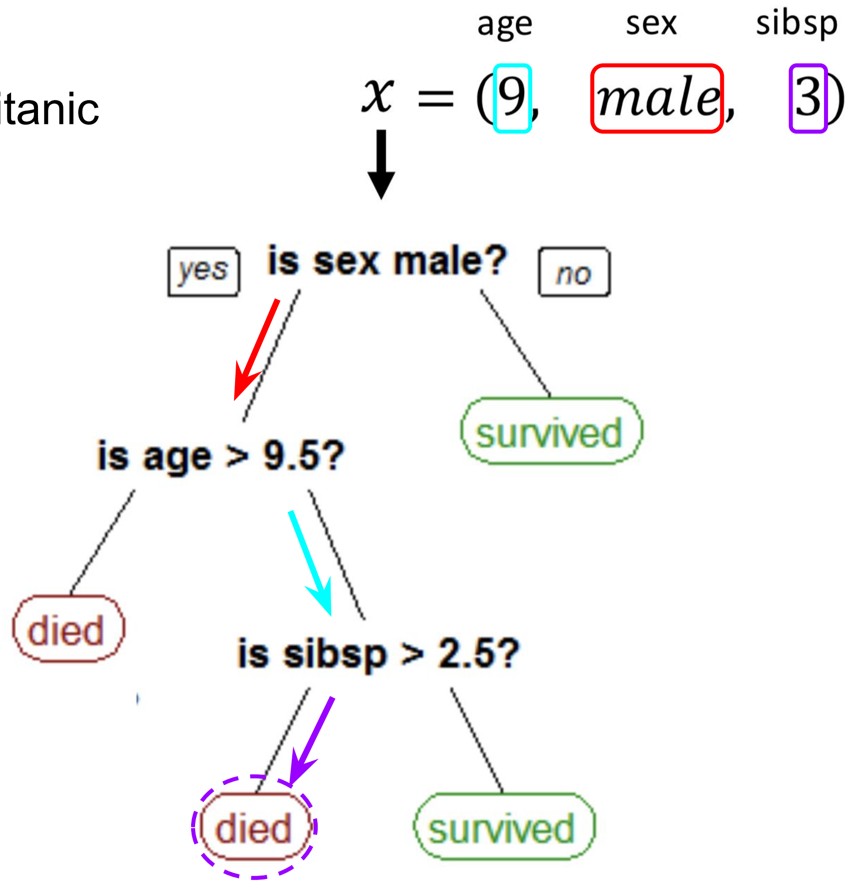


Decision tree

Example: Titanic dataset



Decision tree

Example: Titanic dataset

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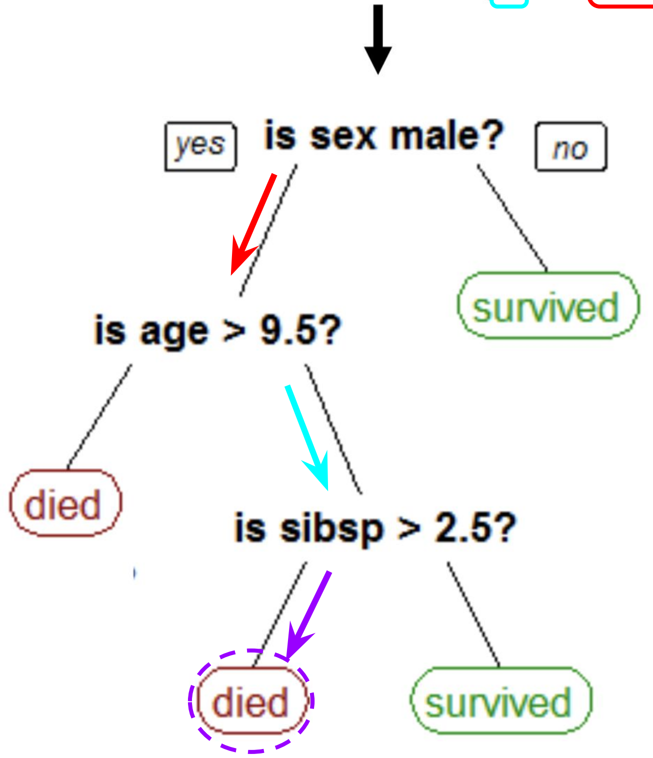
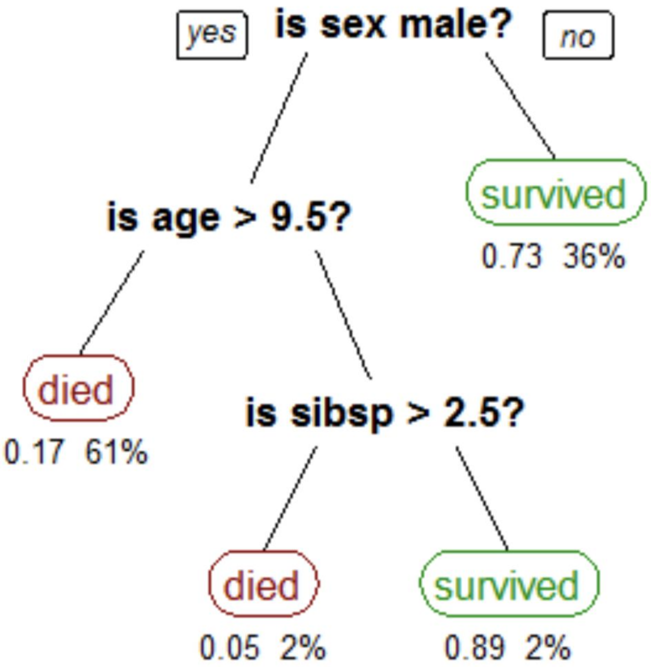


$$y = died$$

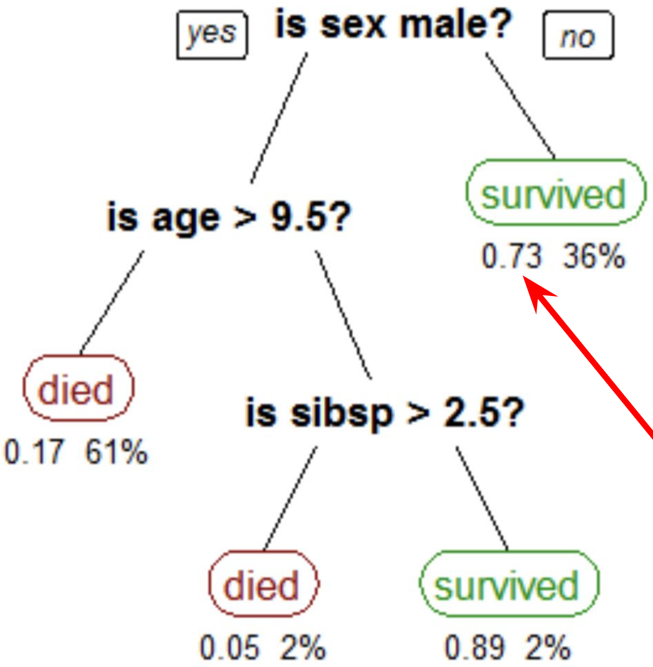
Decision tree in classification

Example: Titanic dataset



Decision tree in classification

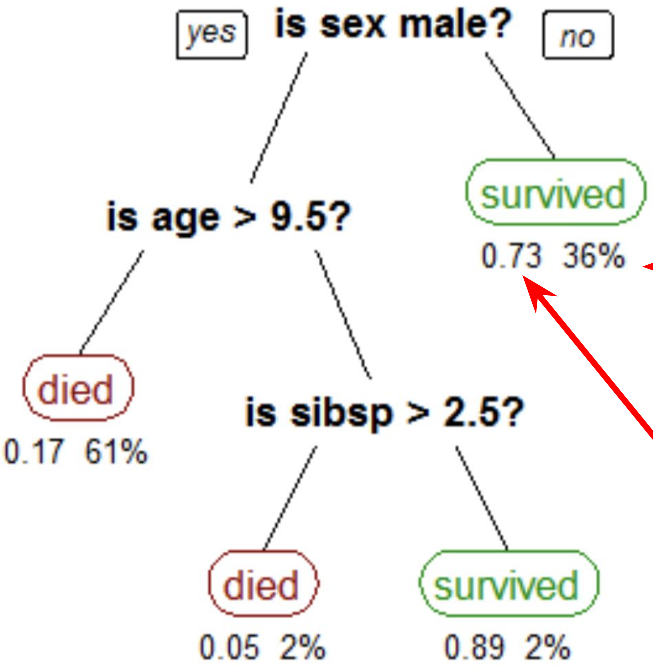
Example: Titanic dataset



Part of survived passengers
= part of objects of 1st class

Decision tree in classification

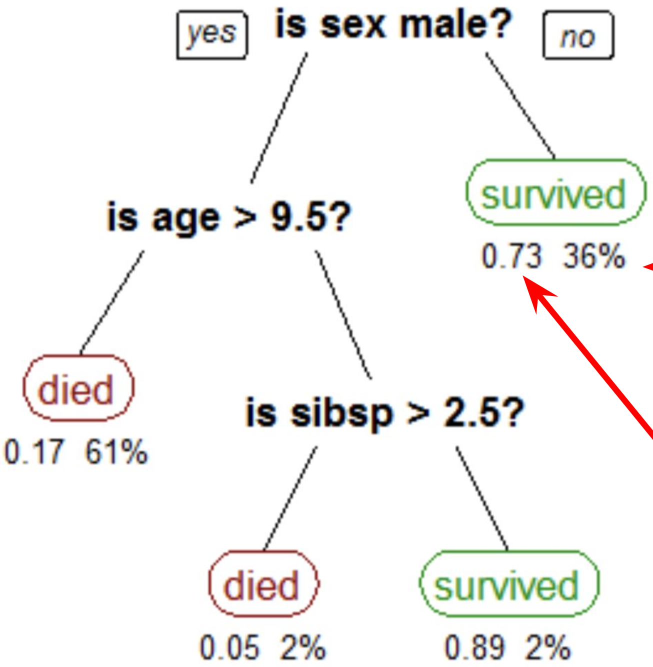
Example: Titanic dataset



Part of dataset in this leaf

Part of survived passengers
= part of objects of 1st class

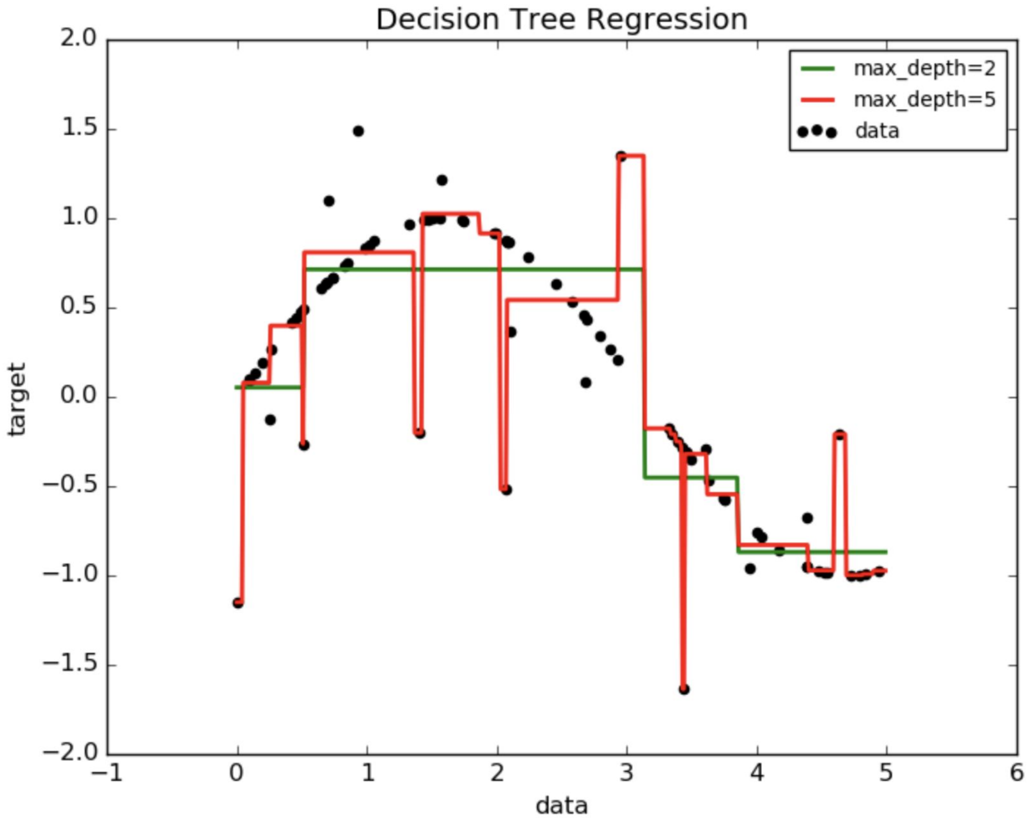
Decision tree in regression



Part of dataset in this leaf

What should we put here in case of regression?

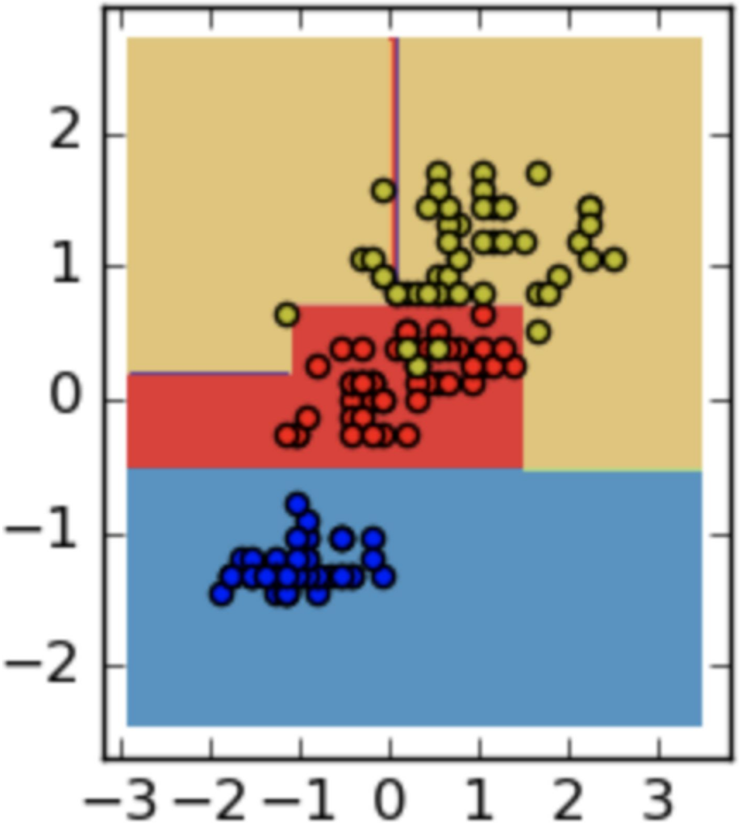
Decision tree in regression



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

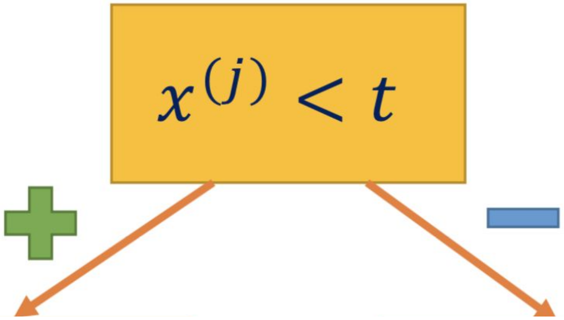
construction procedure

Constructing decision trees

$$\boxed{x^{(j)} < t}$$

1. Make a split

Constructing decision trees



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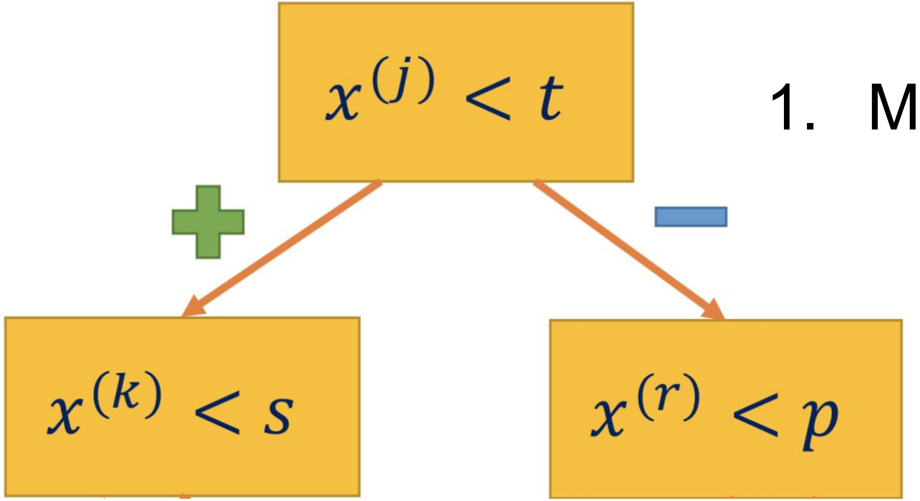
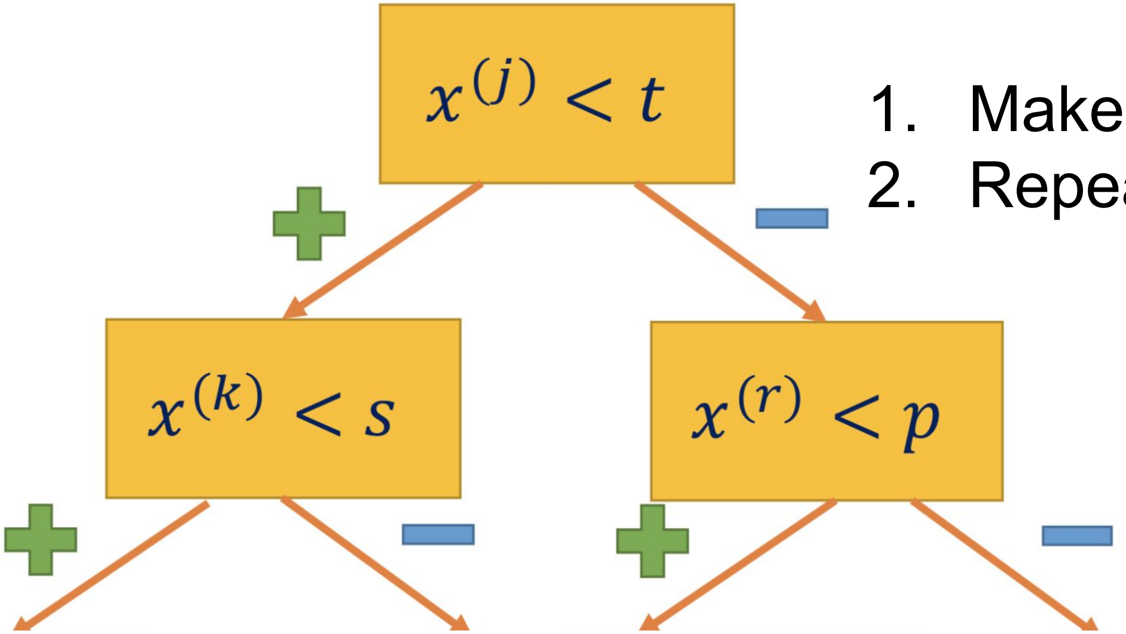
Constructing decision trees



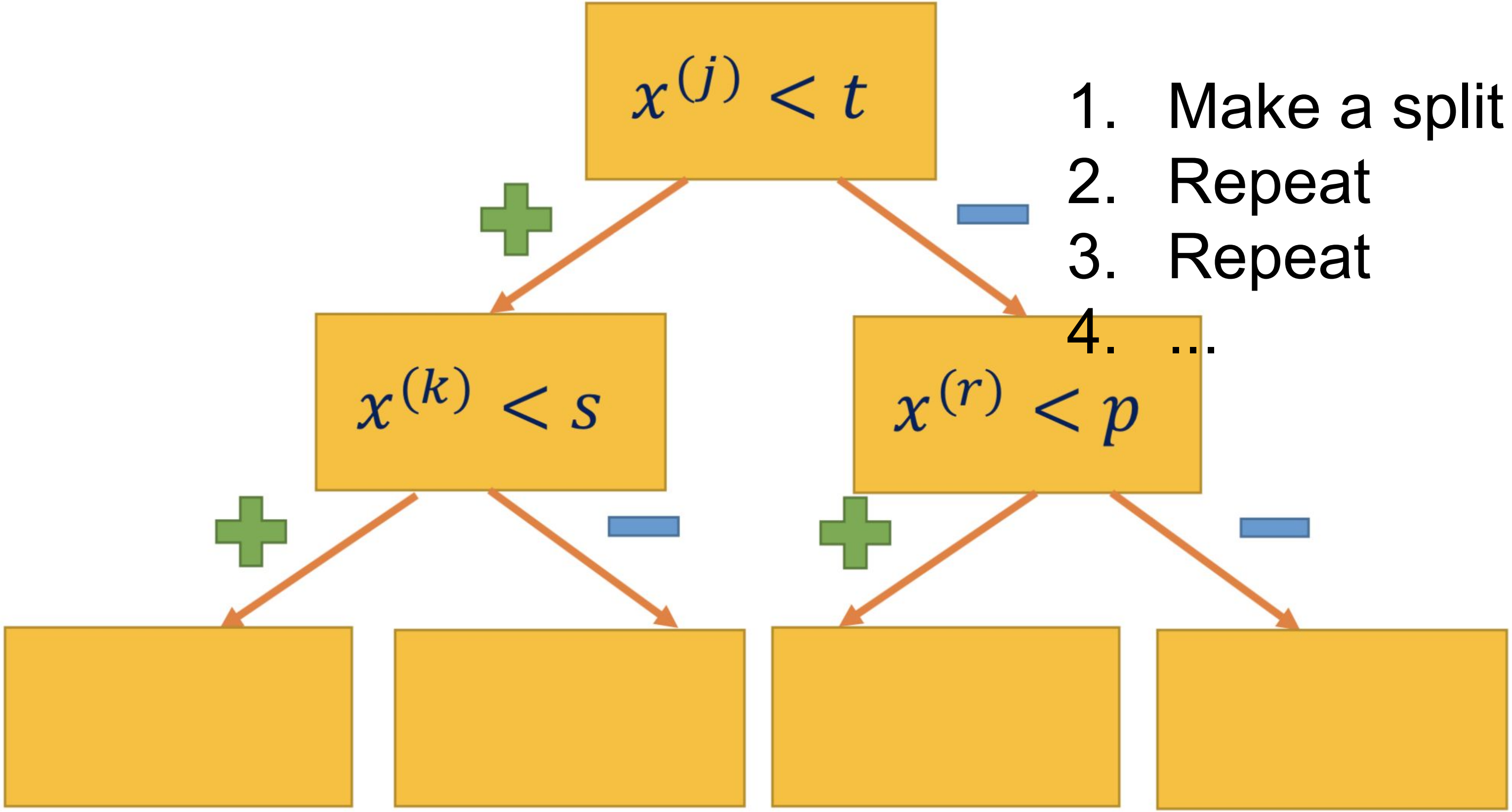
1. Make a split

Constructing decision trees



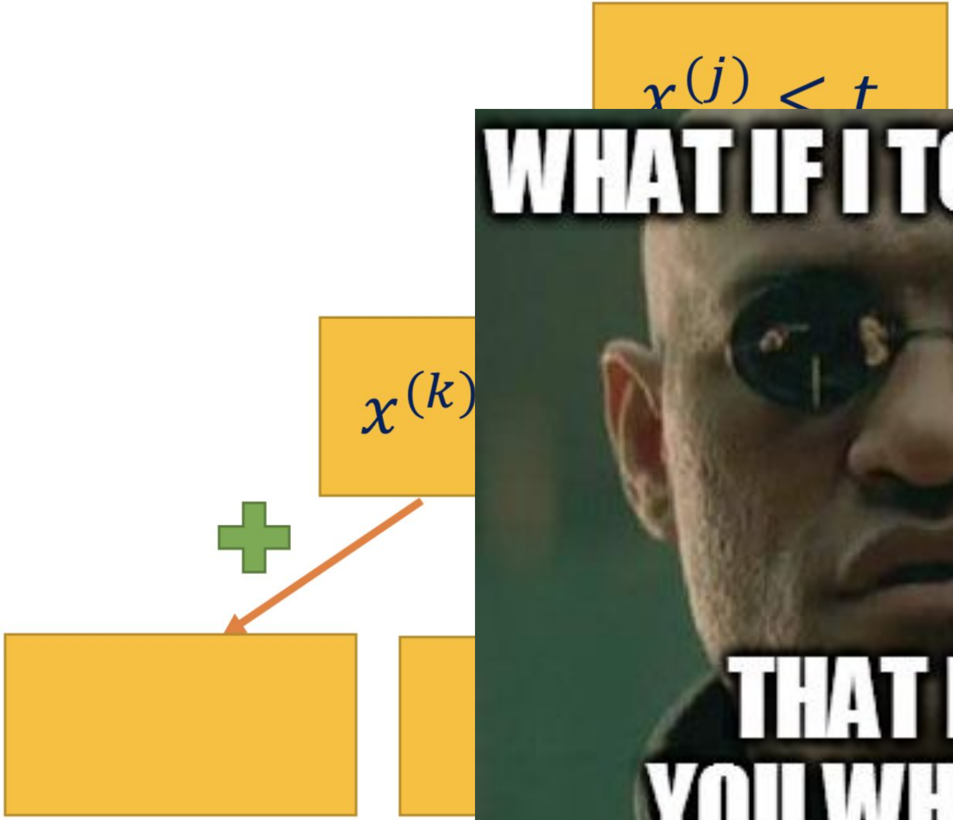
1. Make a split
2. Repeat

Constructing decision trees



1. Make a split
2. Repeat
3. Repeat
4. ...

Constructing decision trees



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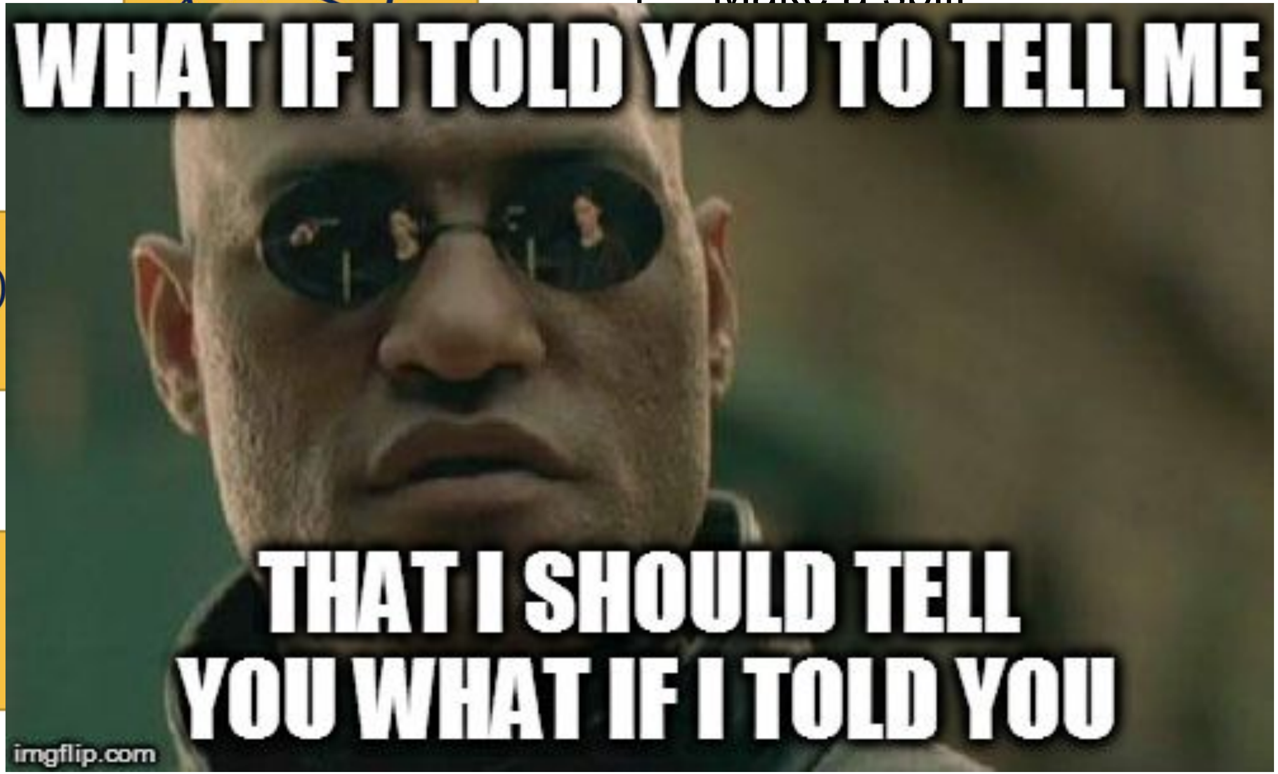
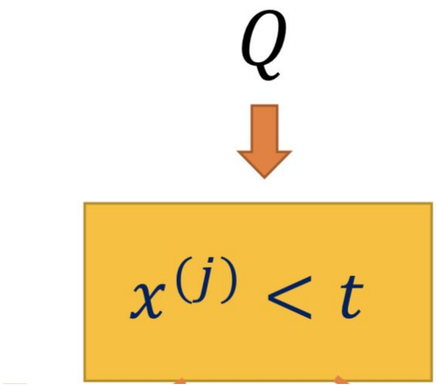


How to split data properly?



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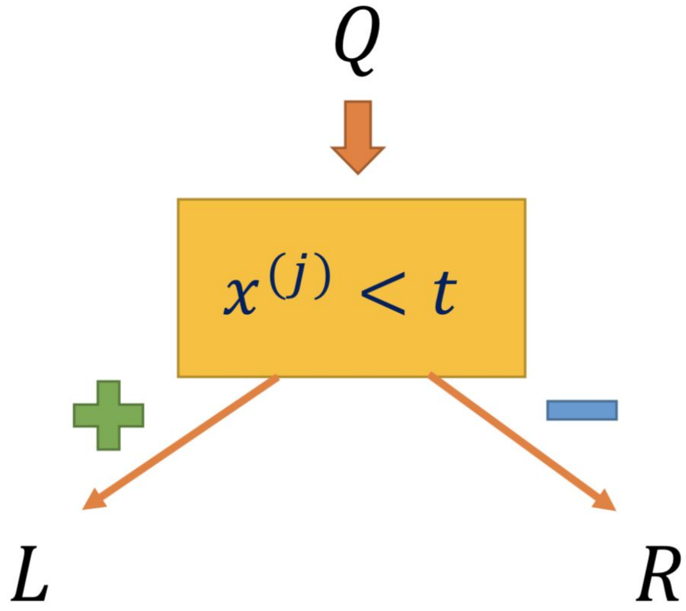

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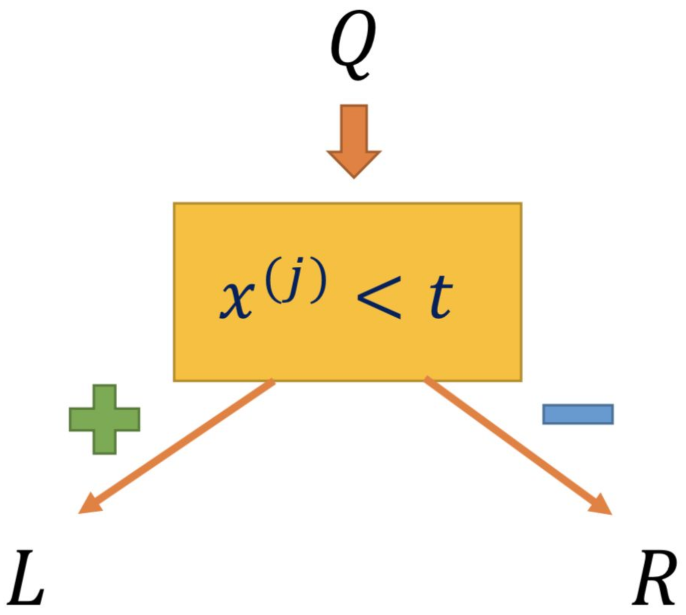
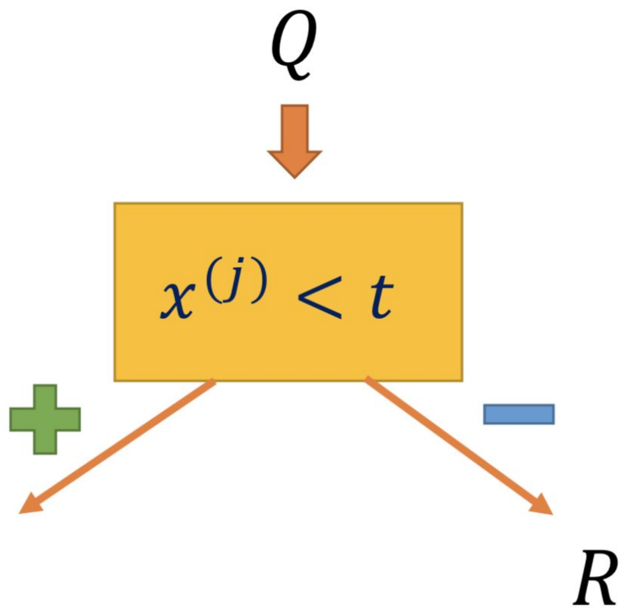


$$G(j,t) = \frac{|L|}{|Q|}H(L) + \frac{|R|}{|Q|}H(R)$$

How to split data properly?



What is H()?

$$G(j,t) = \frac{|L|}{|Q|} H(L) + \frac{|R|}{|Q|} H(R) \to \min_{j,t}$$

Information criteria

Information criteria

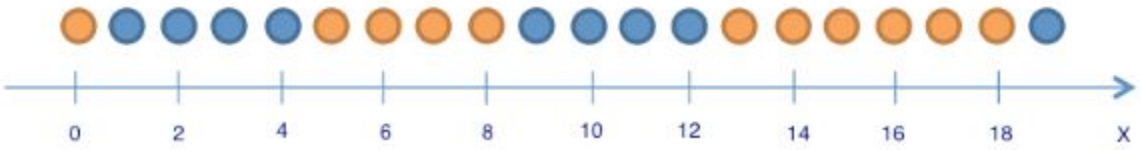
H(R) is measure of “heterogeneity” of our data.
Consider binary classification problem:

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: $$H(R) = 1 - p_0^2 - p_1^2 = 1 - 2p_0p_1$$

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



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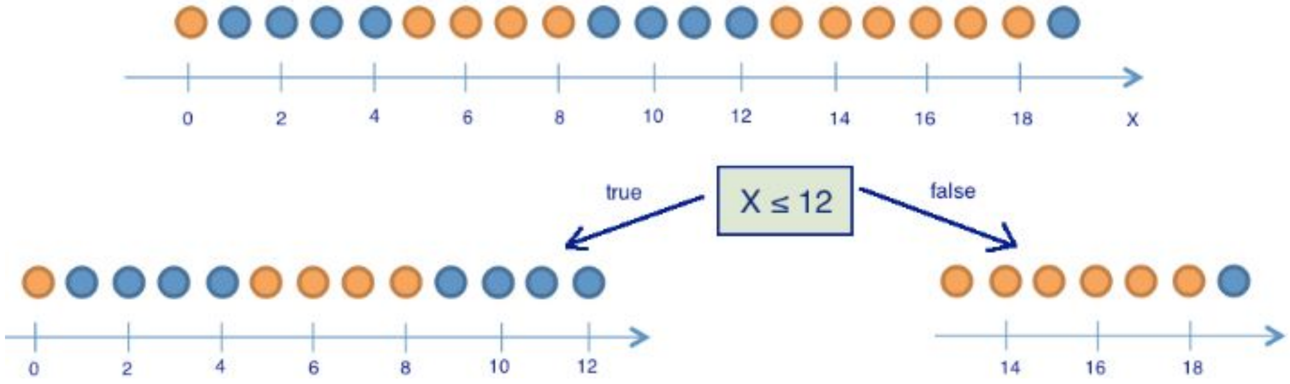
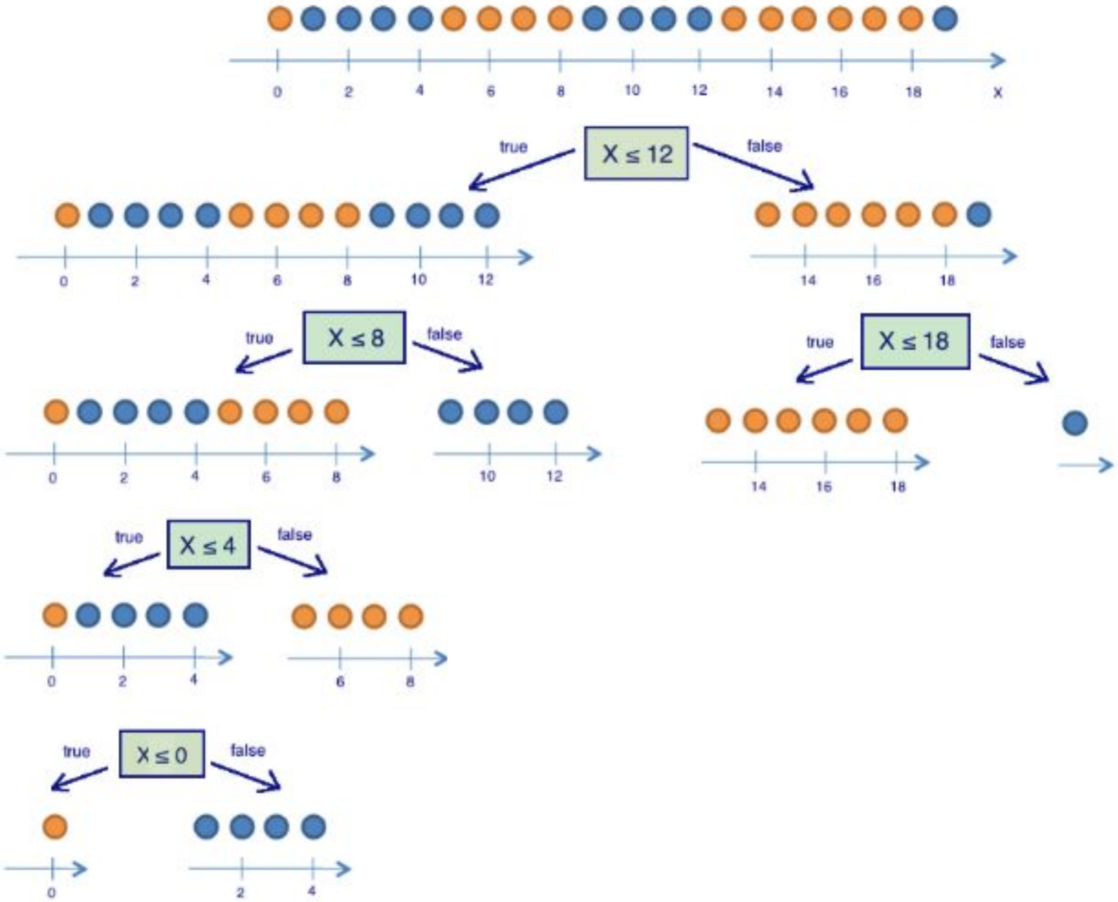


Information criteria: Entropy



$$S = -\sum_k p_k \log_2 p_k$$

In binary case N = 2

$$S = -p_+ \log_2 p_+ - p_- \log_2 p_- = -p_+ \log_2 p_+ - (1 - p_+) \log_2 (1 - p_+)$$

source: https://habr.com/ru/company/ods/blog/322534/

Information criteria: Gini impurity

$$G = 1 - \sum_k (p_k)^2$$

In binary case N = 2

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

source: https://habr.com/ru/company/ods/blog/322534/

Information criteria

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

Regularization for decision trees

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?

Regularization for decision trees

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!

Regularization for decision trees

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

Regularization for decision trees

Stopping criteria

- Maximum tree depth

Regularization for decision trees

Stopping criteria

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

Regularization for decision trees

Stopping criteria

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

Regularization for decision trees

Stopping criteria

- 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

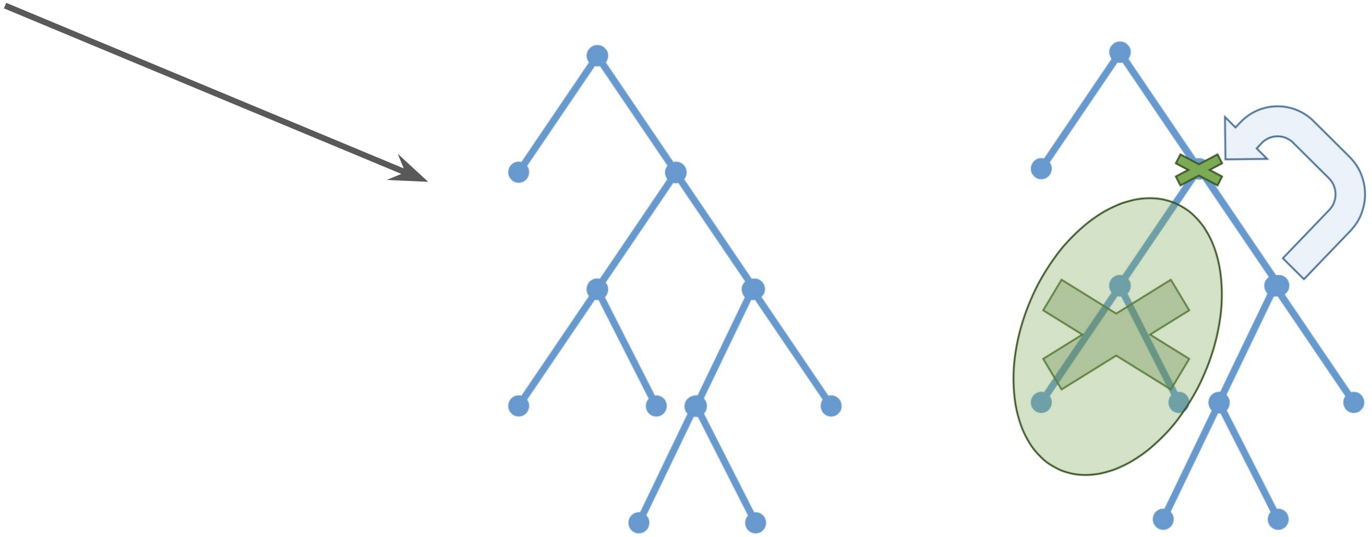
Regularization for decision trees

Stopping criteria

- 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

Bootstrap

Bootstrap

Consider dataset X containing N objects.

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

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

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

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

Bootstrap

Consider the errors unbiased and uncorrelated:

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

$$E_N = \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^{n} b_j(x) - y(x) \right)^2 =$$
$$= \mathbb{E}_x \left(\frac{1}{N} \sum_{j=1}^{N} \varepsilon_j(x) \right)^2 =$$
$$= \frac{1}{N^2} \mathbb{E}_x \left(\sum_{j=1}^{N} \varepsilon_j^2(x) + \underbrace{\sum_{i \neq j} \varepsilon_i(x)\varepsilon_j(x)}_{=0} \right) =$$
$$\boxed{= \frac{1}{N} E_1.}$$

The final model averages all predictions:

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

Error decreased by N times!

Bootstrap

Consider the errors ~~unbiased and uncorrelated~~:

This is a lie

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

The final model averages all predictions:

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

$$E_N = \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{n} b_j(x) - y(x)\right)^2 =$$
$$= \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{N} \varepsilon_j(x)\right)^2 =$$
$$= \frac{1}{N^2}\mathbb{E}_x\left(\sum_{j=1}^{N} \varepsilon_j^2(x) + \underbrace{\sum_{i\neq j} \varepsilon_i(x)\varepsilon_j(x)}_{=0}\right) =$$
$$\boxed{= \frac{1}{N}E_1.}$$

Error decreased by N times!

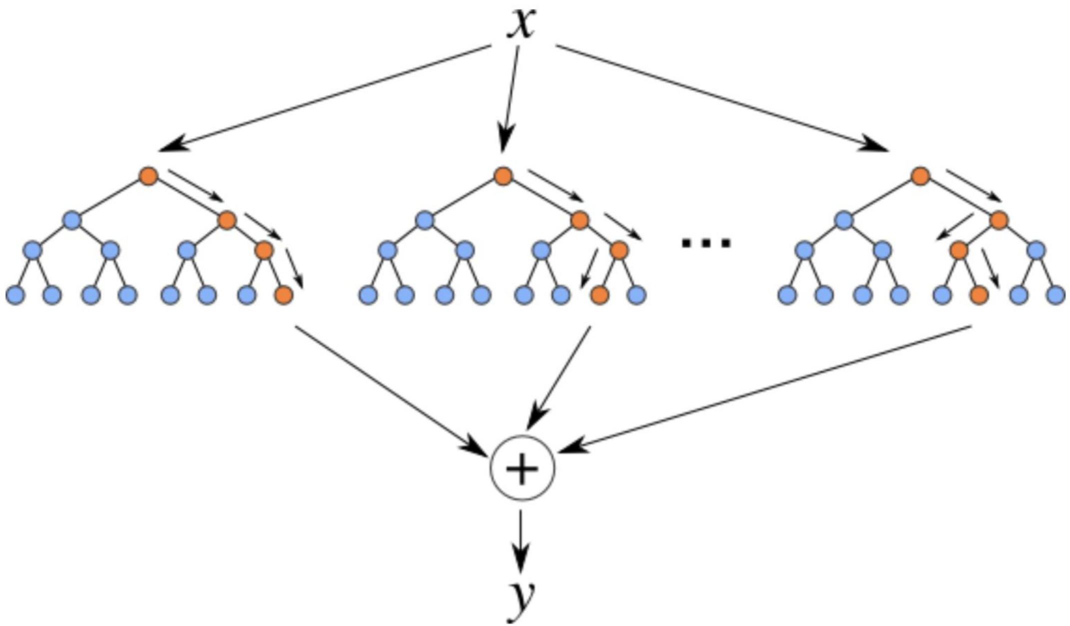
Bagging = Bootstrap aggregating

Decreases the error if the basic algorithms are not correlated.

RSM - Random Subspace Method

Same approach, but with features.

Bagging + RSM = Random Forest



Random Forest

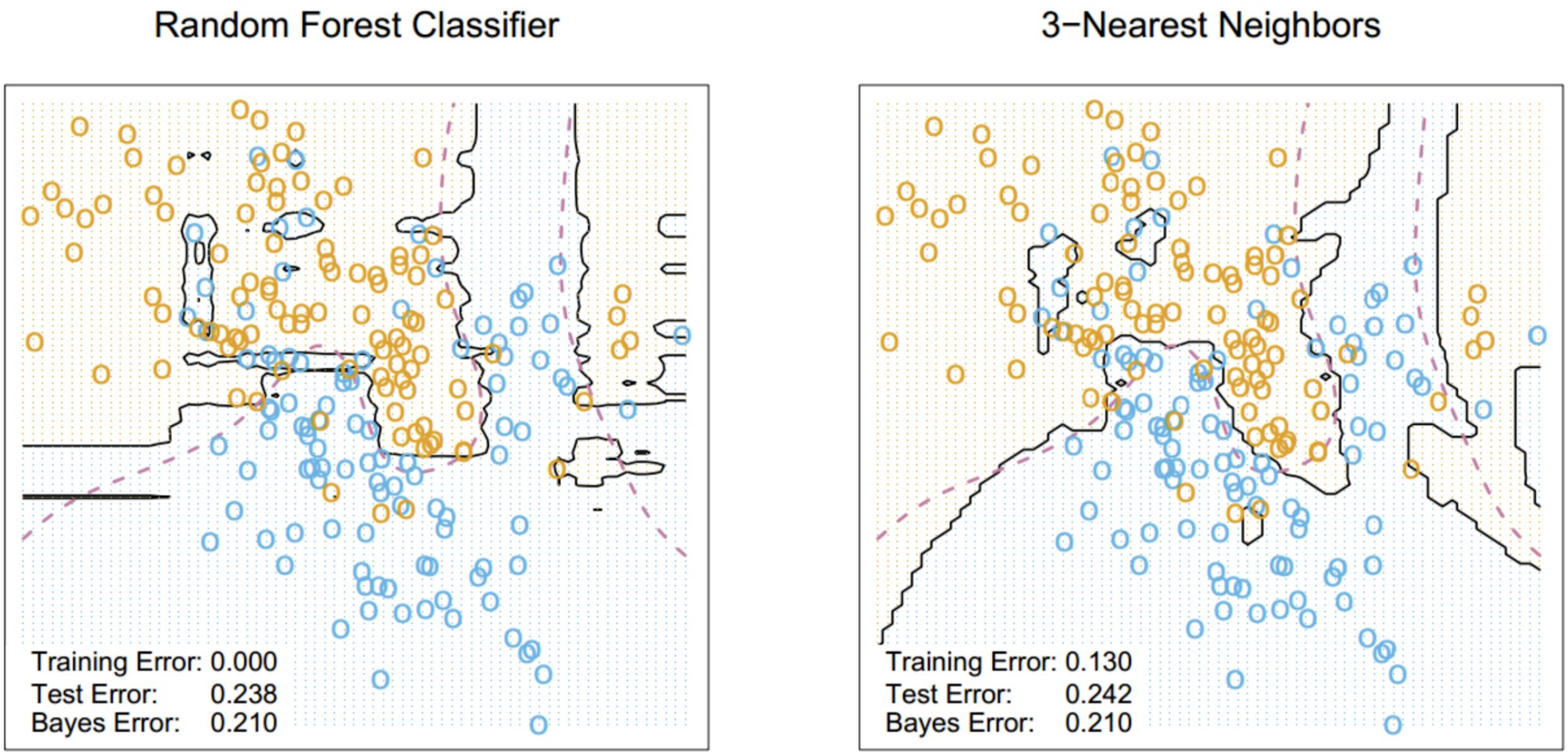
Training procedure:

- 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

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


Random Forest Classifier
Training Error: 0.000
Test Error: 0.238
Bayes Error: 0.210
3−Nearest Neighbors
Training Error: 0.130
Test Error: 0.242
Bayes Error: 0.210

Thanks for your attention