Machine Learning Course
basic track

Lecture 6: Decision trees and Ensembles

MIPT, Moscow
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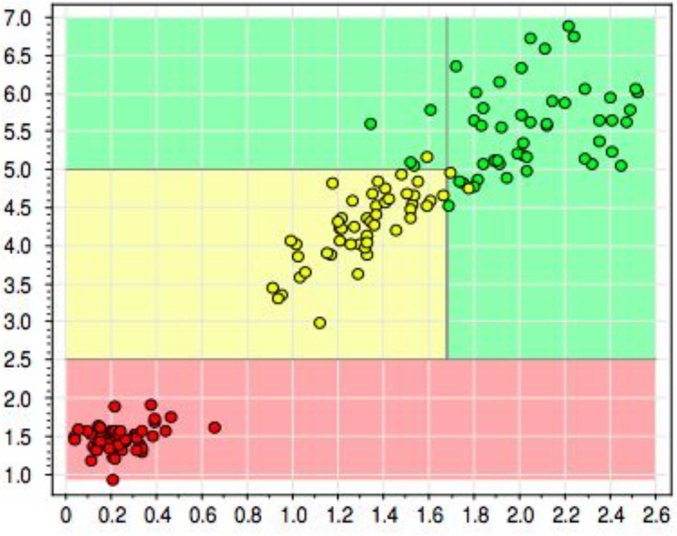
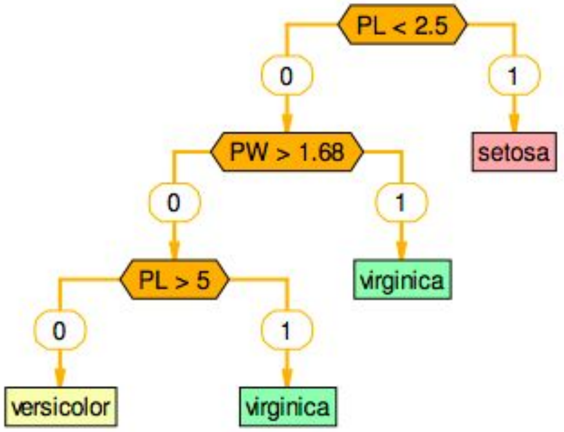
Outline

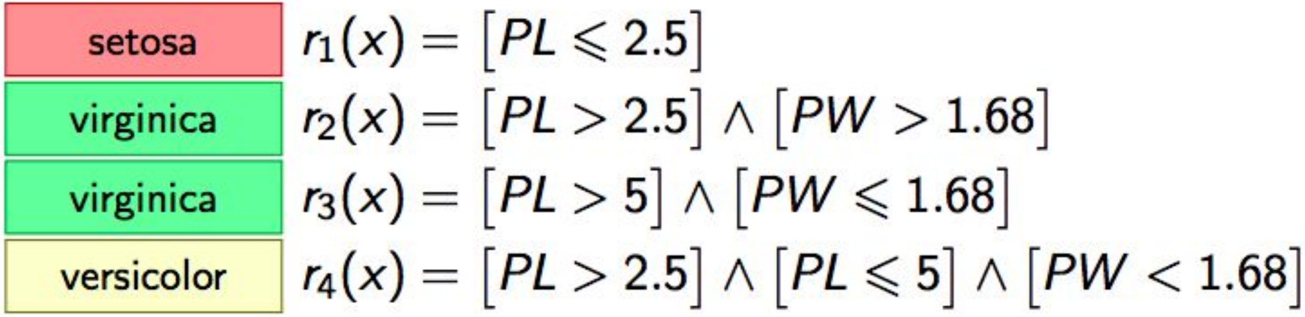
1. Decision tree: intuition
2. Decision tree construction procedure
3. Information criteria
4. Pruning
5. Decision trees special highlights
   - Decision tree as linear model
   - Dealing with missing data
   - Categorical features
6. Boostrap and Bagging
7. Random Forest

Decision Tree: intuition

Decision tree for Iris data set

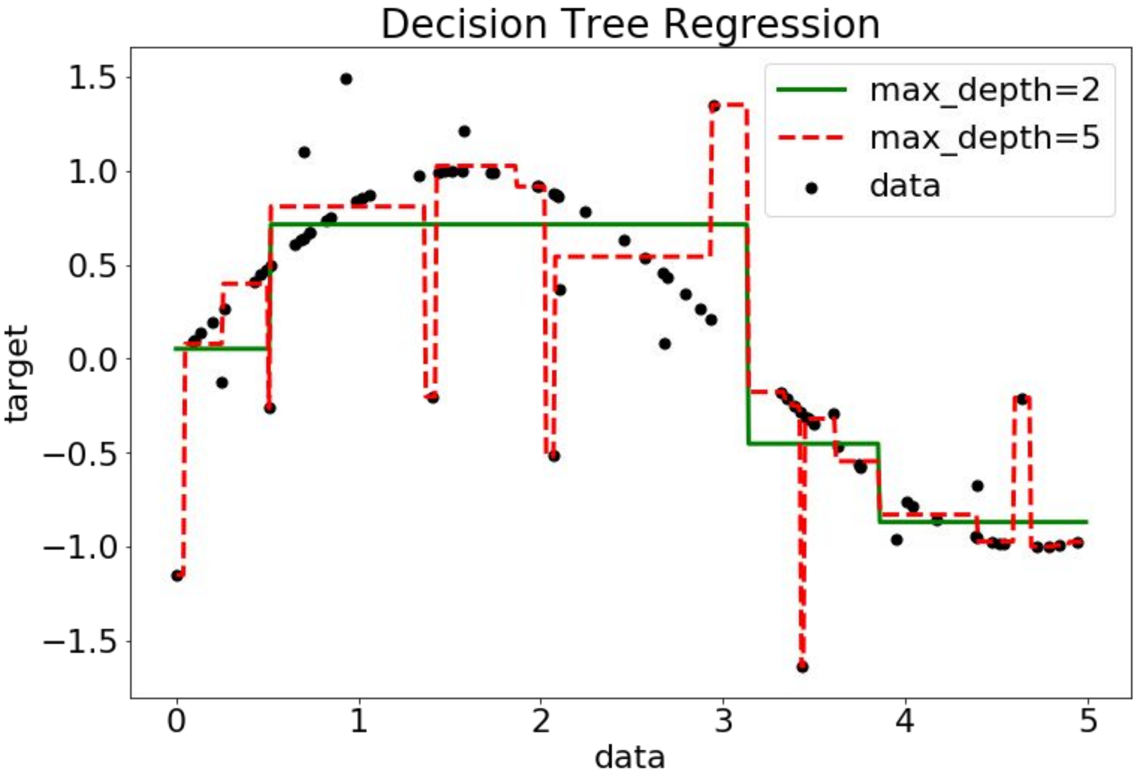






🟥 setosa	$r_1(x) = [PL \leqslant 2.5]$
🟩 virginica	$r_2(x) = [PL > 2.5] \wedge [PW > 1.68]$
🟩 virginica	$r_3(x) = [PL > 5] \wedge [PW \leqslant 1.68]$
🟨 versicolor	$r_4(x) = [PL > 2.5] \wedge [PL \leqslant 5] \wedge [PW < 1.68]$

Decision tree in regression



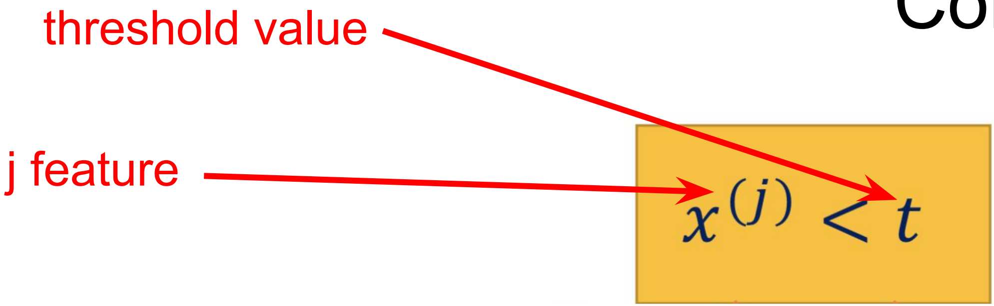
Green - decision tree of depth 2
Red - decision tree of depth 5

Every leaf corresponds to some constant.

Decision Tree

construction procedure

Constructing decision trees



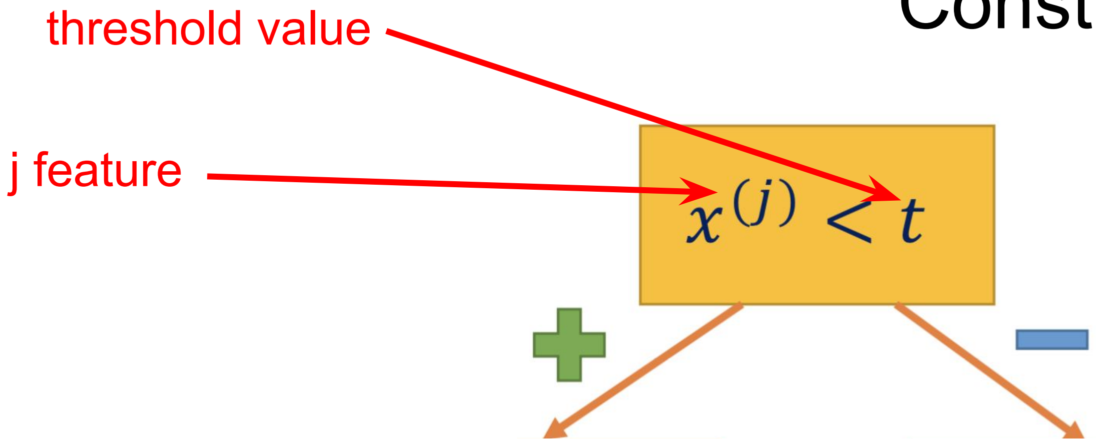
threshold value

j feature

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

1. Make a split

Constructing decision trees



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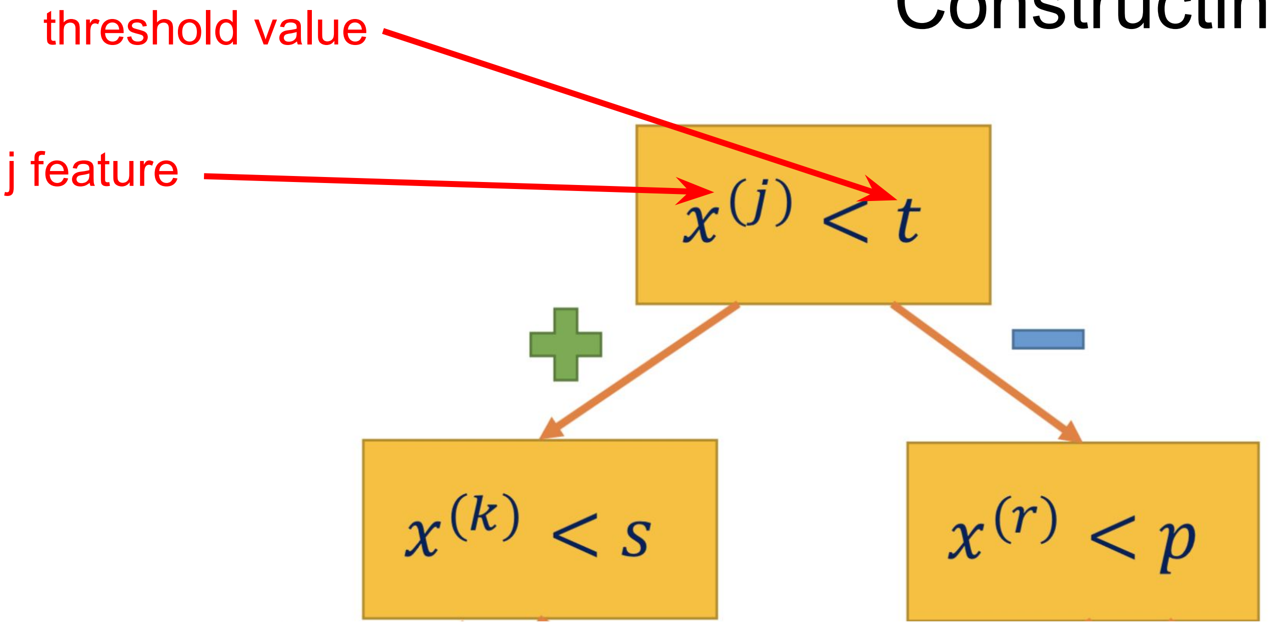
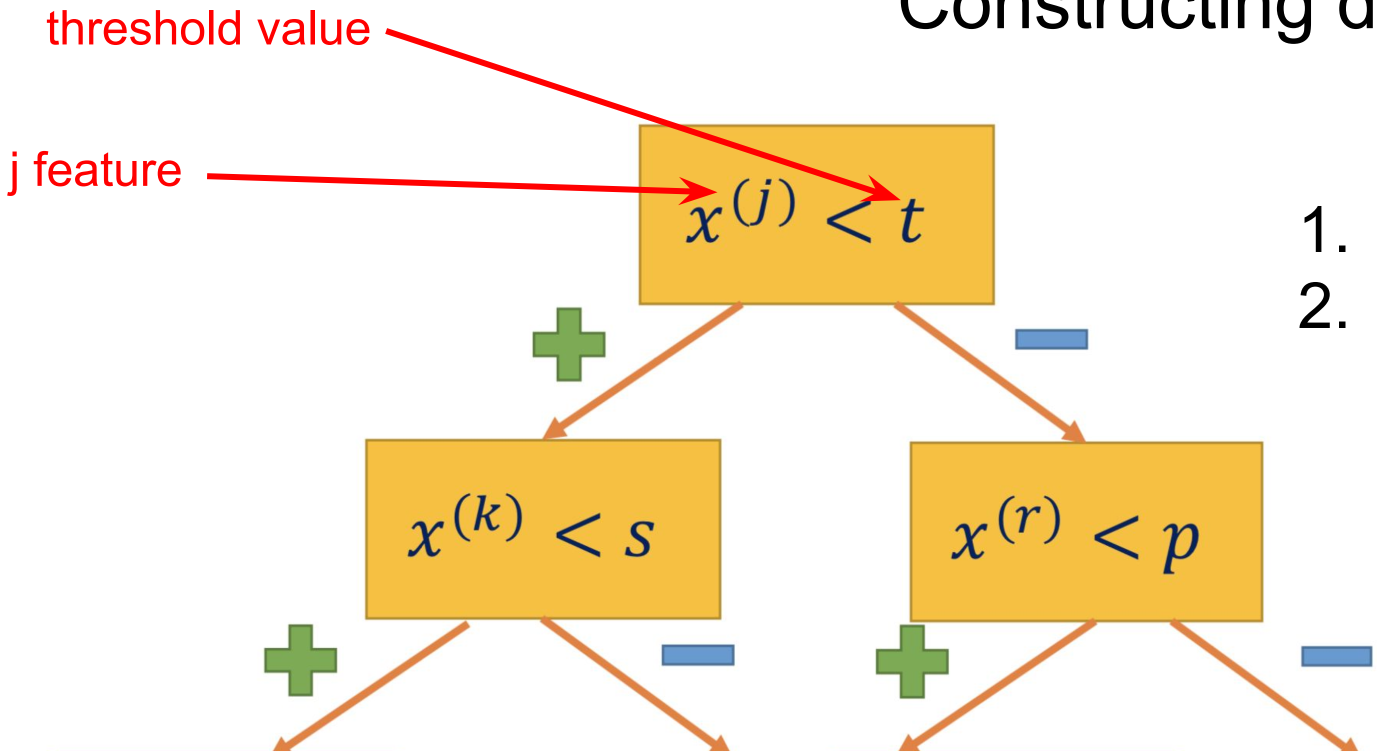


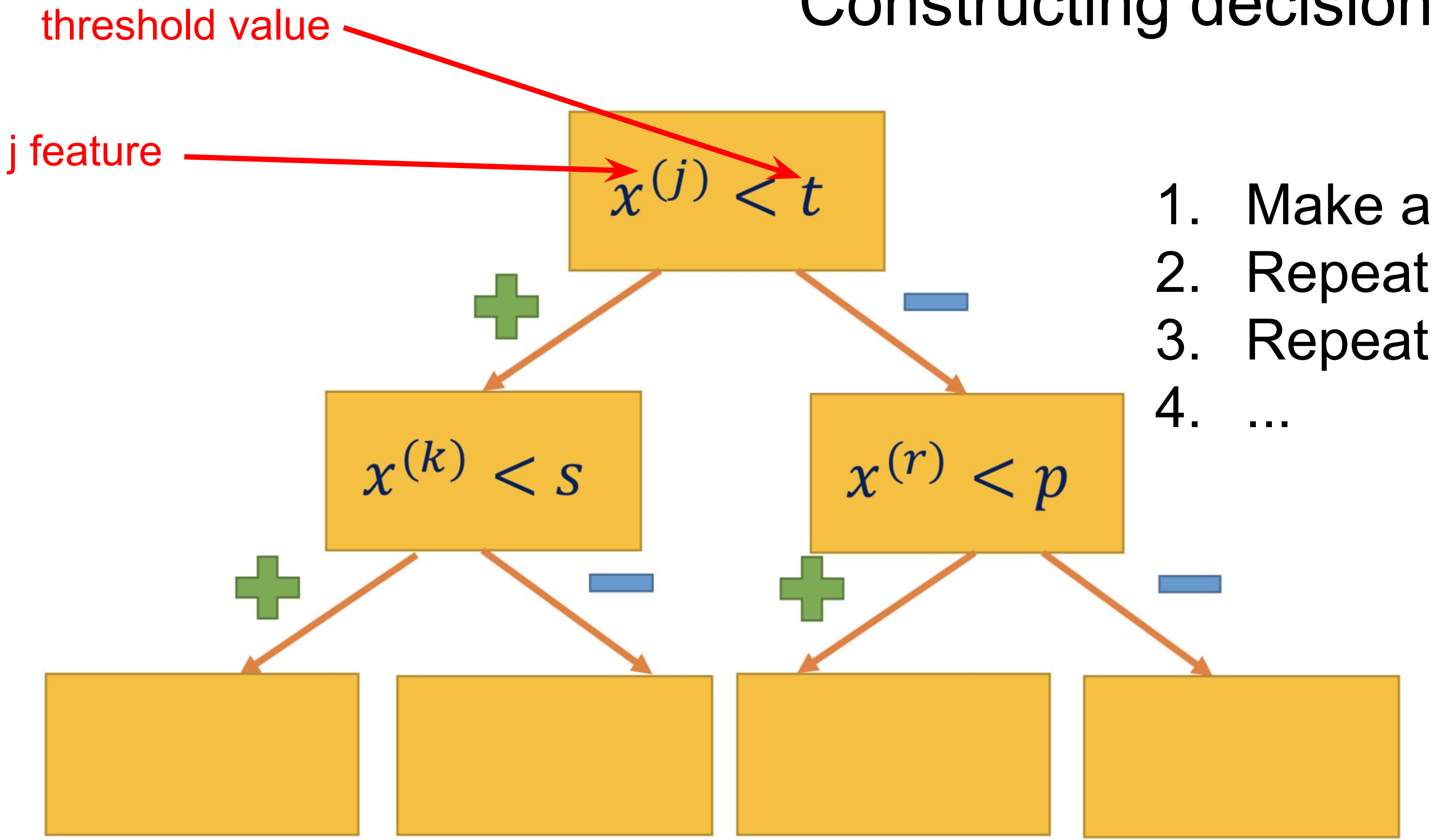
1. Make a split

Constructing decision trees



1. Make a split
2. Repeat

Constructing decision trees

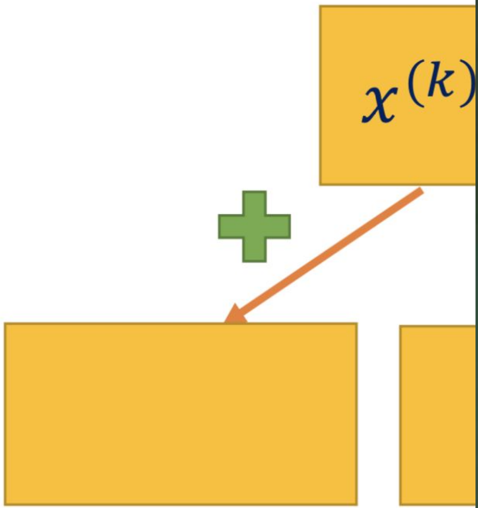


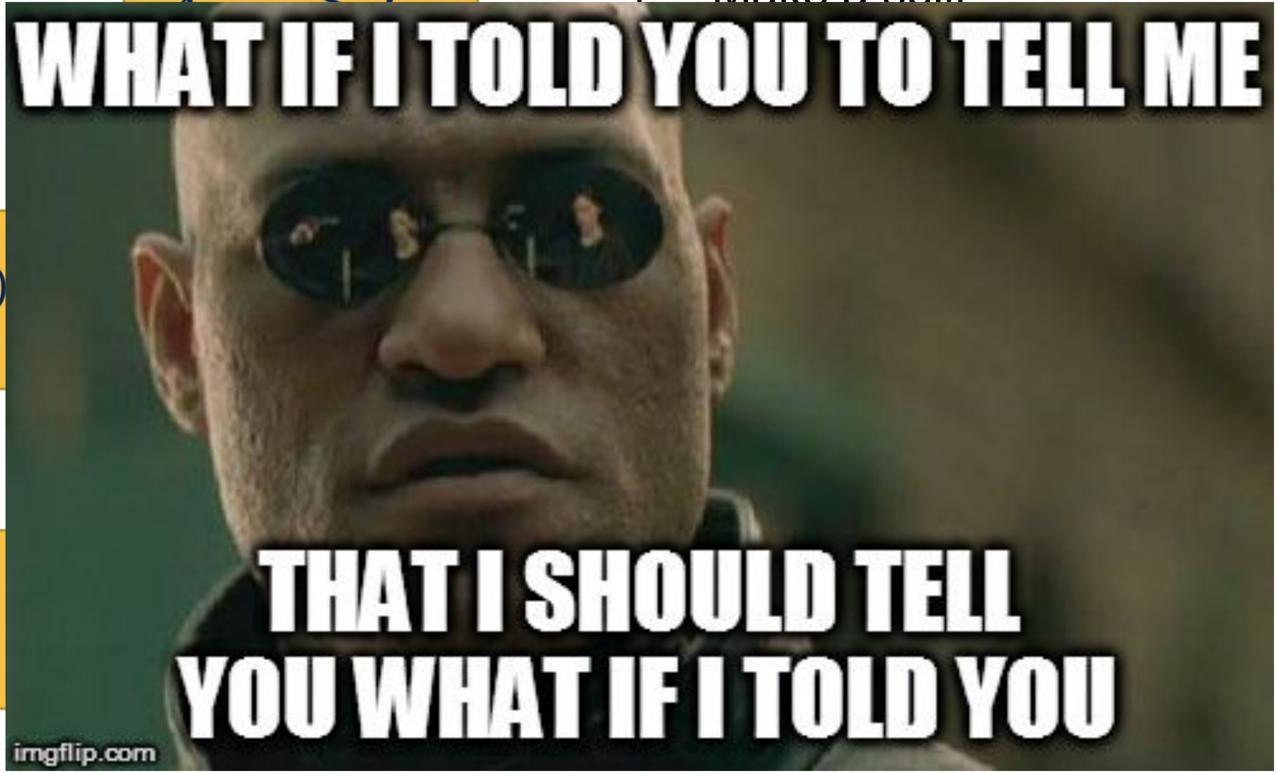
1. Make a split
2. Repeat
3. Repeat
4. ...

Constructing decision trees

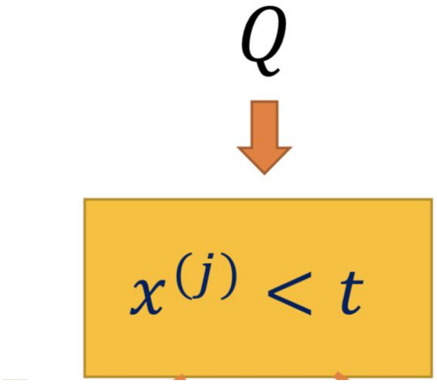
$x^{(j)} < t$

1. Make a split





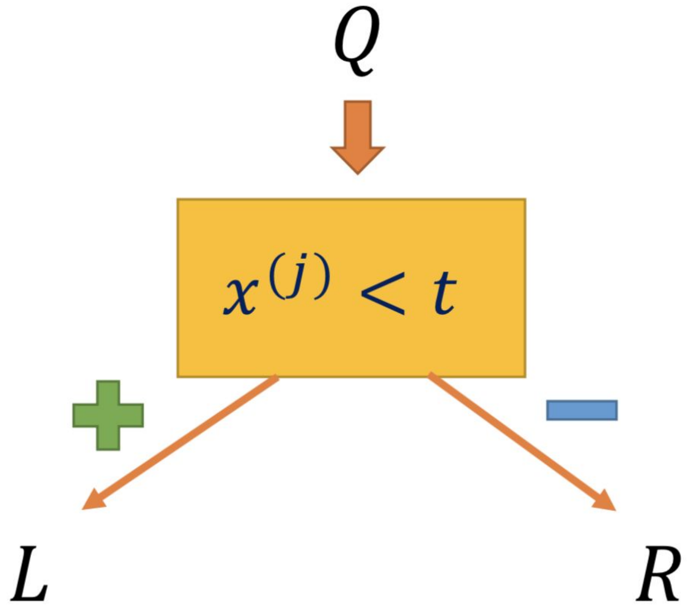
How to split data properly?



Q

$x^{(j)} < t$

How to split data properly?



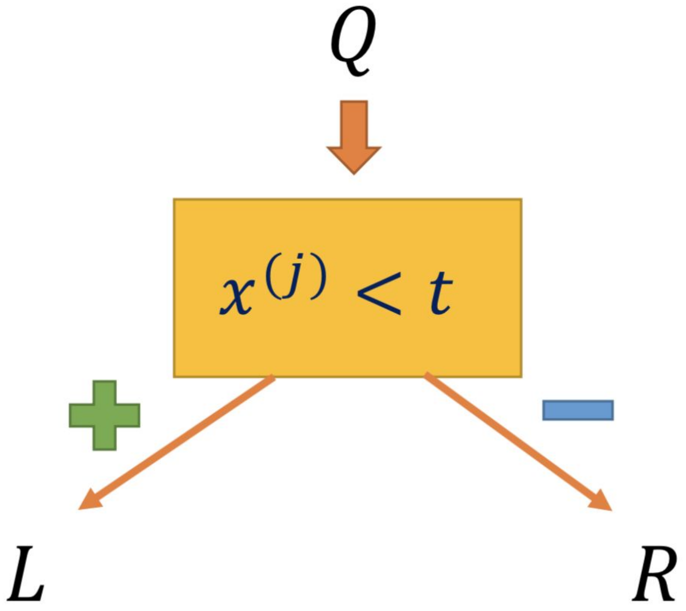
Q

$x^{(j)} < t$

+ L

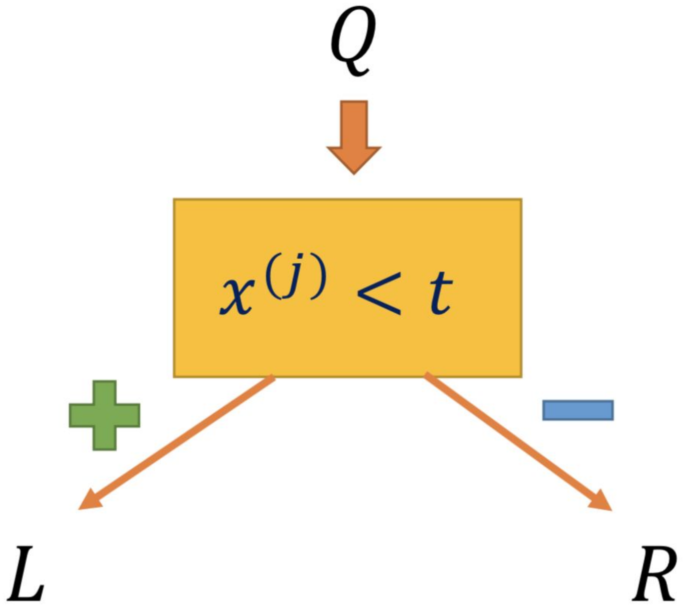
− R

How to split data properly?



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

How to split data properly?



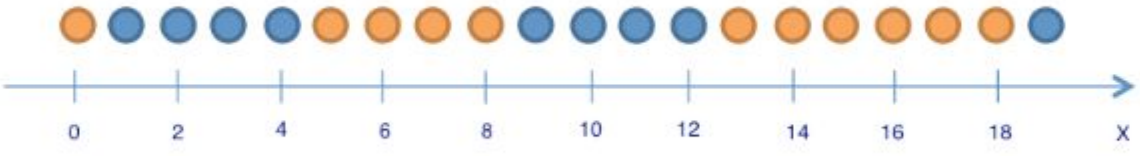
$$G(j,t) = \frac{|L|}{|Q|} H(L) + \frac{|R|}{|Q|} H(R) \rightarrow \min_{j,t}$$

What is H()?

Information criteria

Information criteria

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



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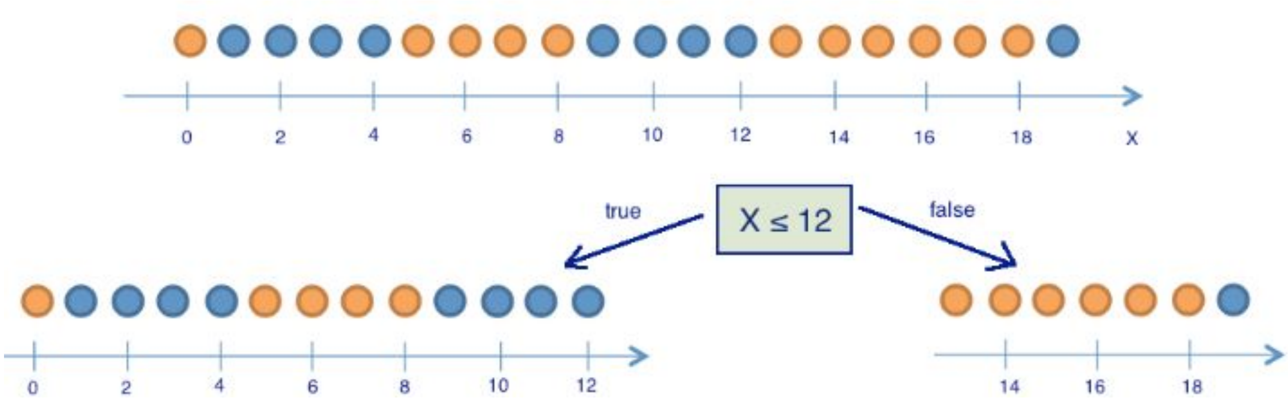


Information criteria

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

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

1. Entropy criteria: $H(R) = -p_0 \log p_0 - p_1 \log p_1$

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

Information criteria

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

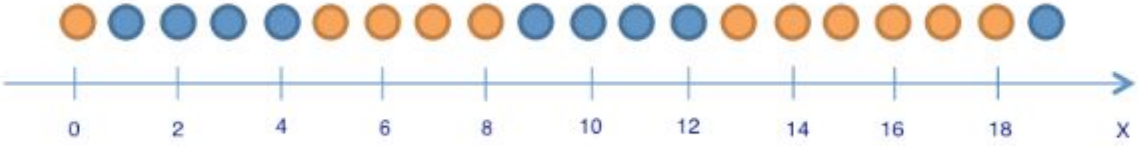
Obvious way: Misclassification criteria: $H(R) = 1 - \max_{k}\{p_k\}$

1. Entropy criteria: $$H(R) = -\sum_{k=0}^{K} p_k \log p_k$$

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

Information criteria

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



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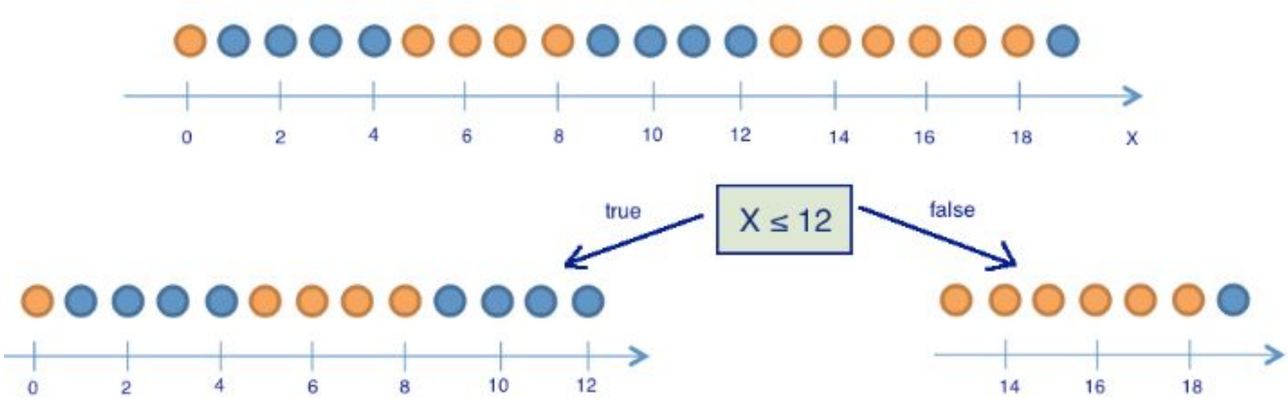

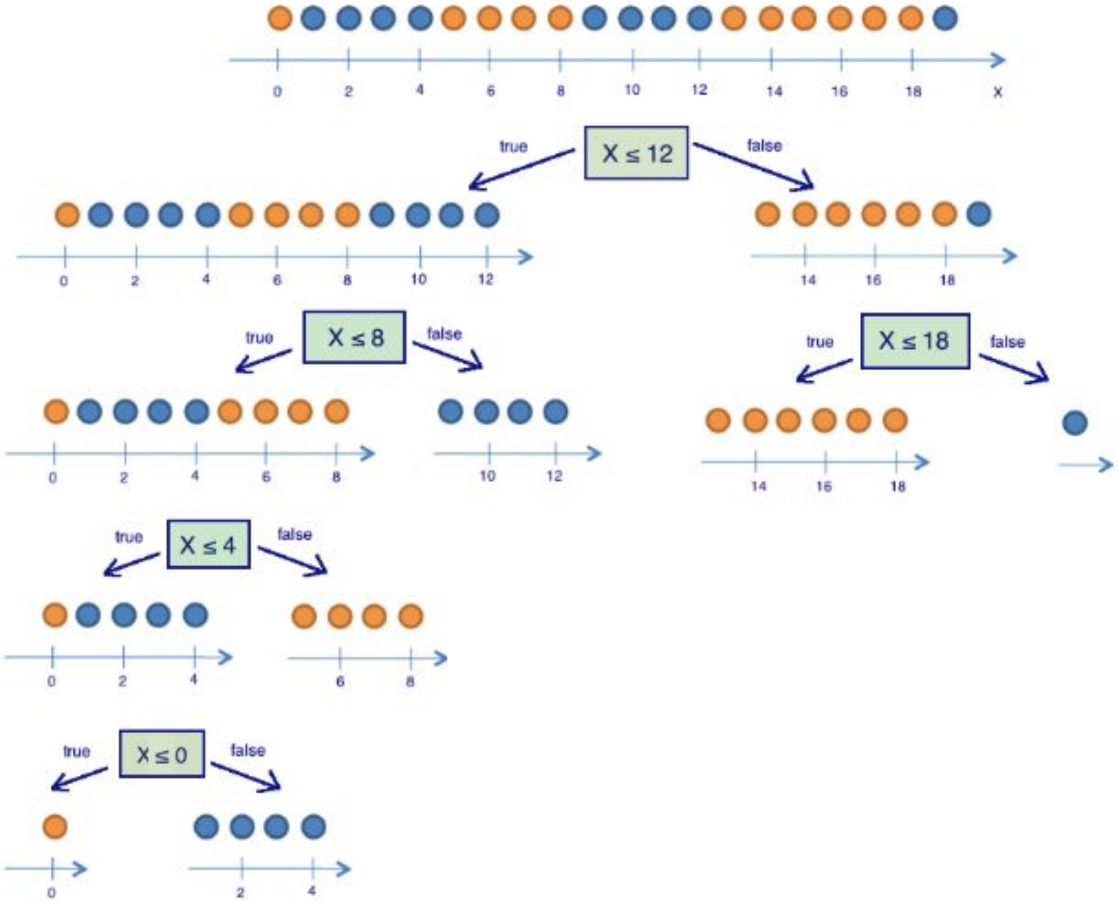

Information criteria: Entropy

$$S = -M \sum_{k=0}^{K} p_k \log p_k$$

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:

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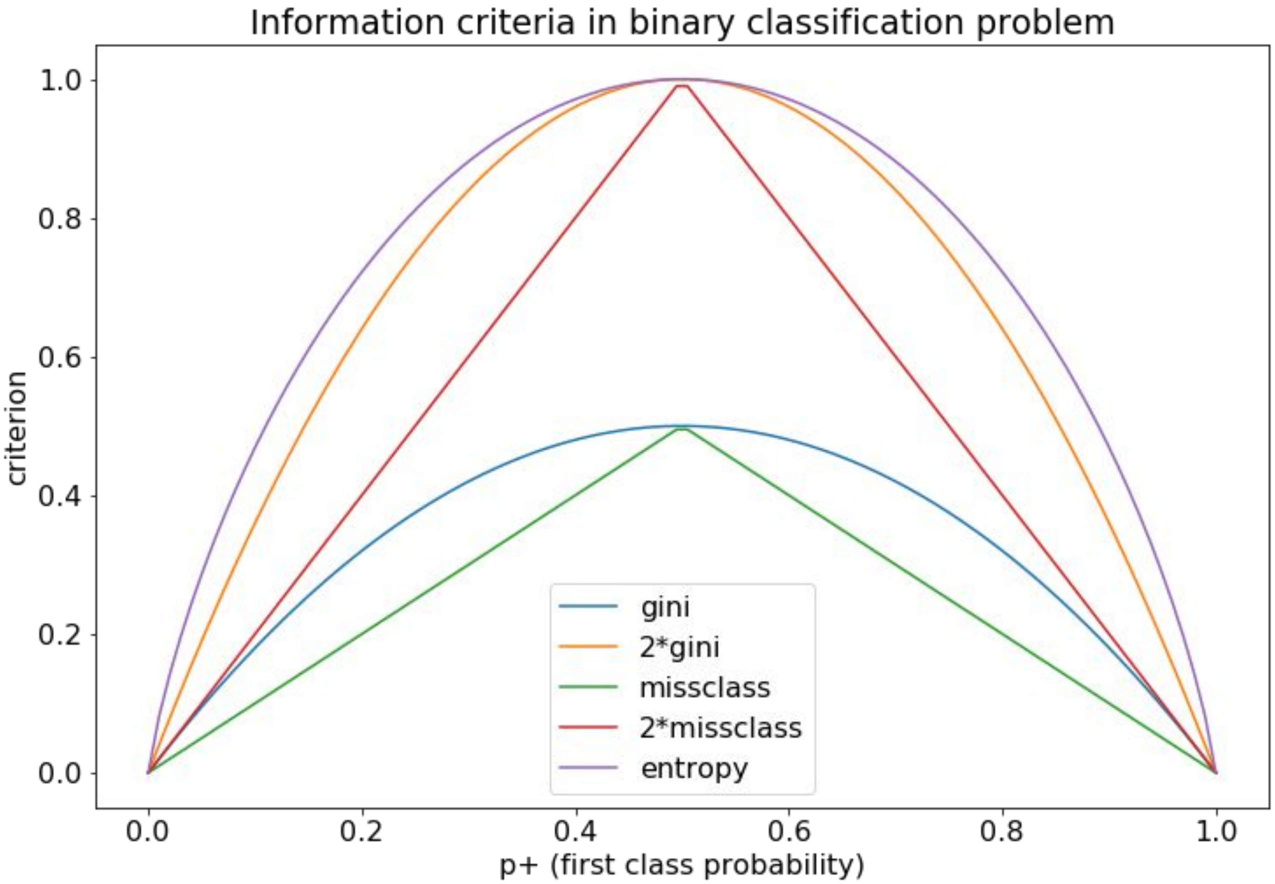
Information criteria



Information criteria

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?

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

Pruning

Pruning

- Pre-pruning:
    - Constrain the tree before construction.
- Post-pruning:
    - Simplify constructed tree.

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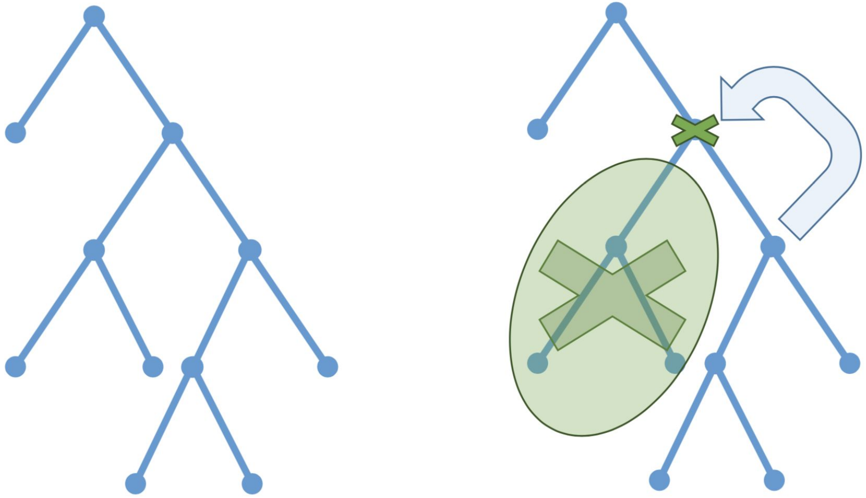
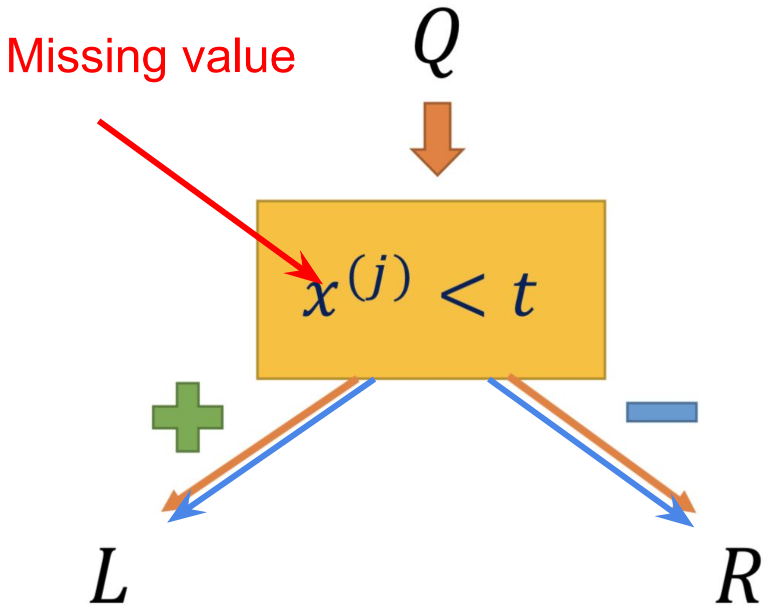


Special highlights

Missing values in Decision Trees

- If the value is missing, one might use both sub-trees and average their predictions



$$\hat{y} = \frac{|L|}{|Q|}\hat{y}_L + \frac{|R|}{|Q|}\hat{y}_R$$

Decision Trees as Linear models

Let J be the subspace of the original feature space, corresponding to the leaf of the tree.

Prediction takes form

$$\hat{y} = \sum_{j} w_j [x \in J_j]$$

Construction algorithms: overview

- ID-3
  - Entropy criteria; Stops when no more gain available
- C4.5
  - Normalised entropy criteria; Stops depending on leaf size; Incorporates pruning
- C5.0
  - Some updates on C4.5
- CART
  - Gini criteria; Cost-complexity Pruning; Surrogate predicates for missing data;
- etc.

Bootstrap and Bagging

Bootstrap

Consider dataset X containing m objects.

Pick m 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: $E_1 = \frac{1}{N} \sum_{j=1}^{N} \mathbb{E}_x \varepsilon_j^2(x).$

Bootstrap

Consider the errors unbiased and uncorrelated:

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

The final model averages all predictions:

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

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

Error decreased by N times!

$$\boxed{= \frac{1}{N}E_1.}$$

Bootstrap

Consider the errors ~~unbiased and uncorrelated~~:

This is a lie

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

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

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

$$= \frac{1}{N^2} \mathbb{E}_x \left(\sum_{j=1}^{N} \varepsilon_j^2(x) + \underbrace{\sum_{i \neq j} \varepsilon_i(x) \varepsilon_j(x)}_{=0} \right) =$$

Error decreased by N times!

$$\boxed{= \frac{1}{N} E_1.}$$

Bagging = Bootstrap aggregating

Decreases the variance if the basic algorithms are not correlated.

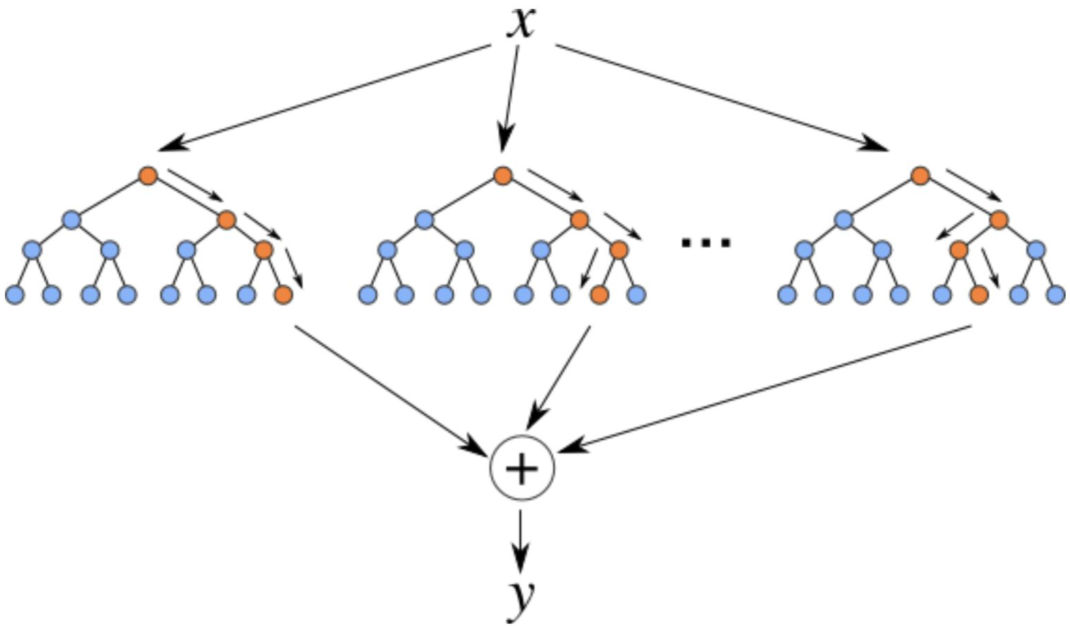
Random Forest

RSM - Random Subspace Method

Same approach, but with features.

Random Forest

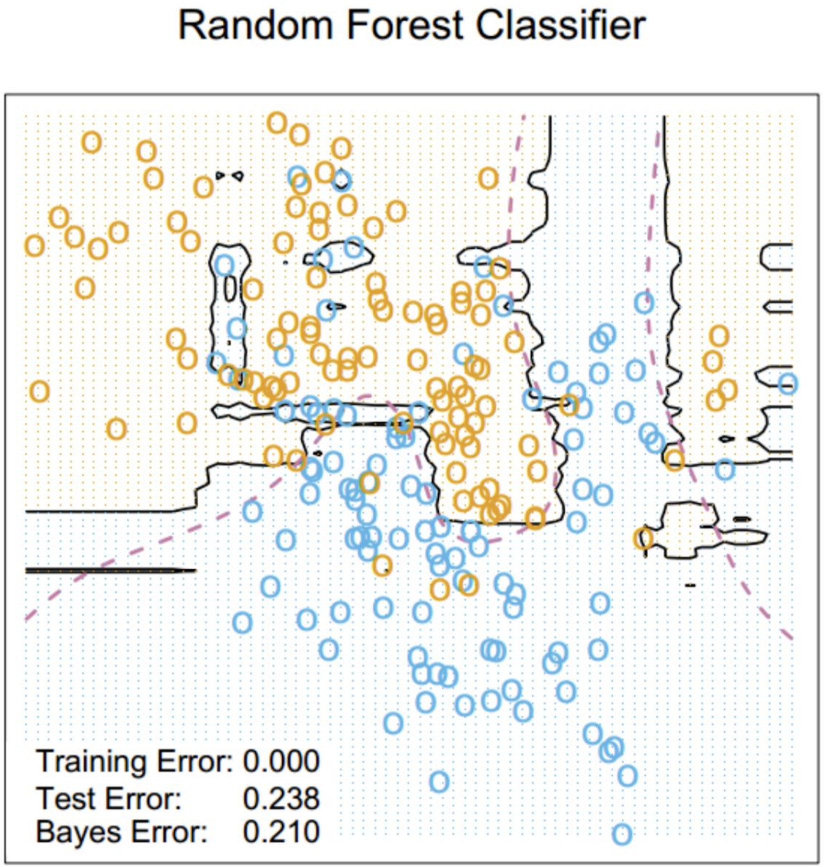
Bagging + RSM = Random Forest



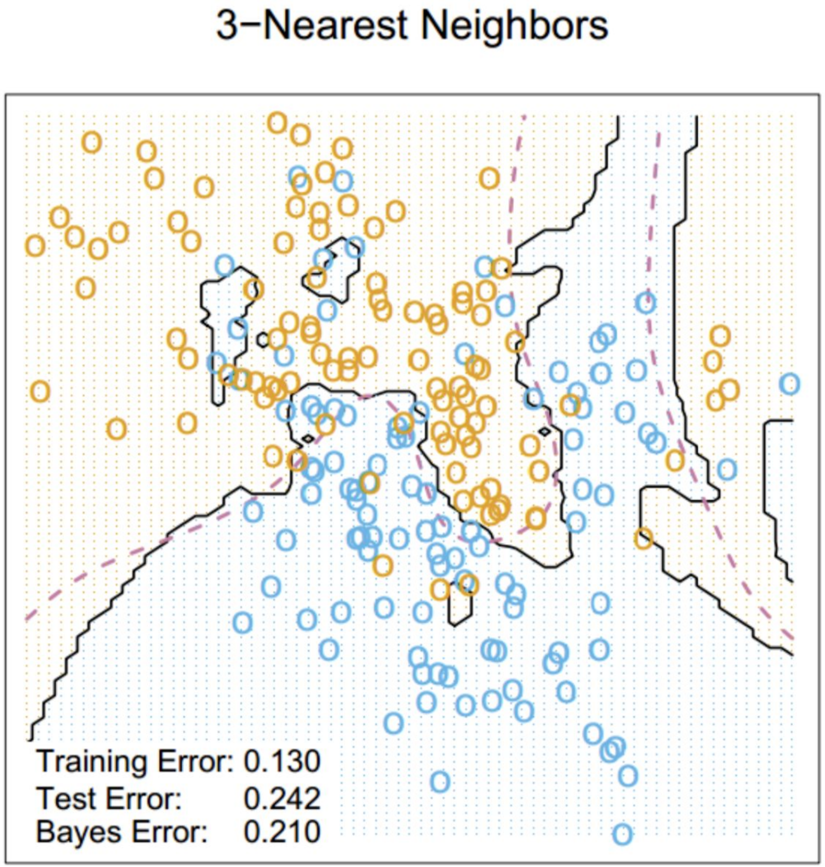
Random Forest

- 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

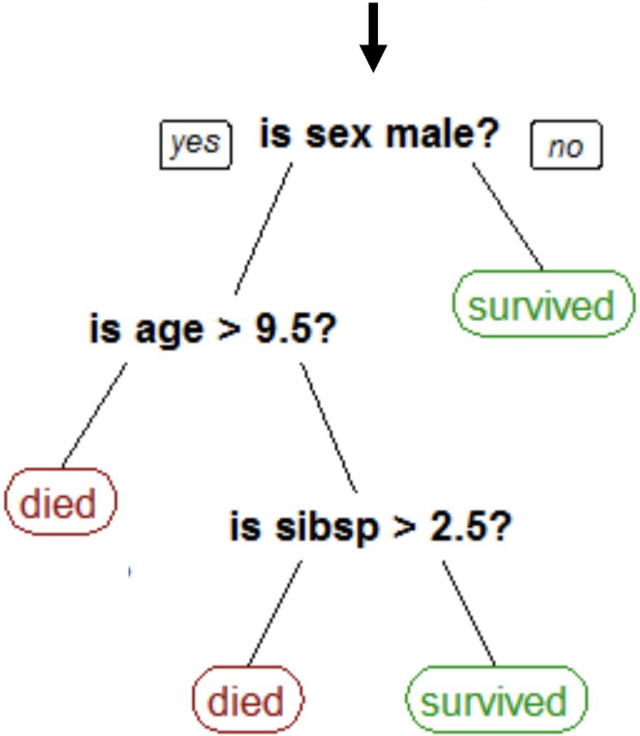


3−Nearest Neighbors

Backlog

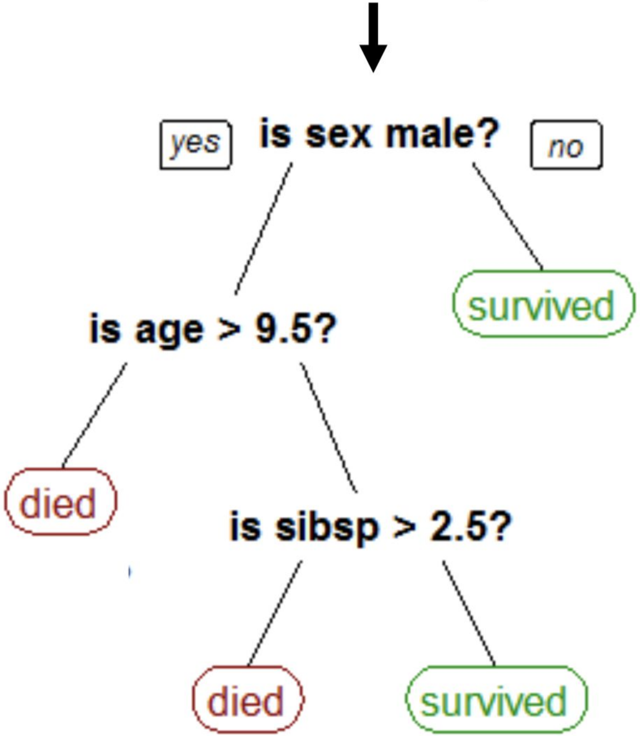
Decision tree

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



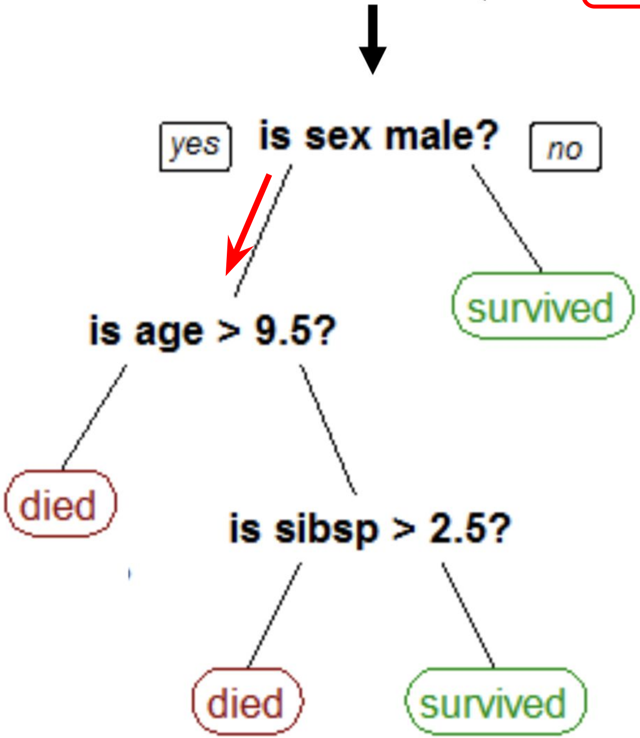
Decision tree

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



Decision tree

$$x = (\overset{\text{age}}{9}, \overset{\text{sex}}{\boxed{male}}, \overset{\text{sibsp}}{3})$$



Decision tree

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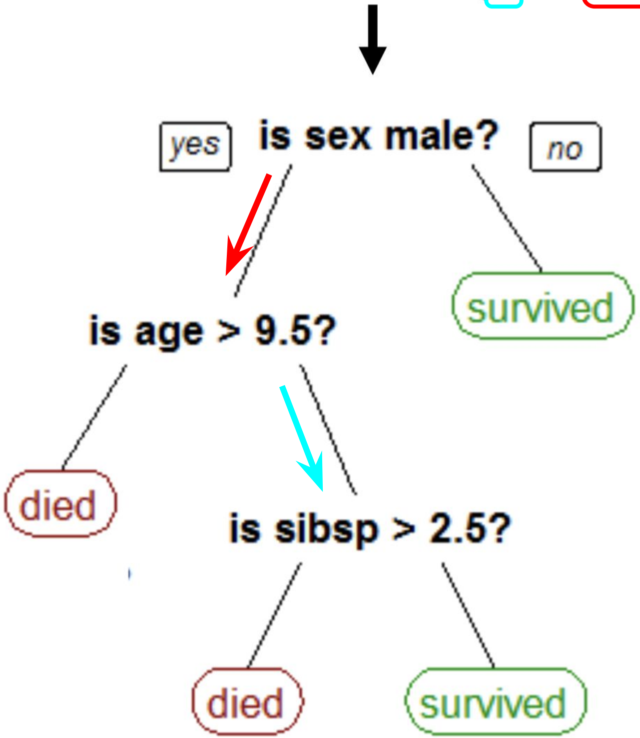


yes

is sex male?

no

is age > 9.5?

survived

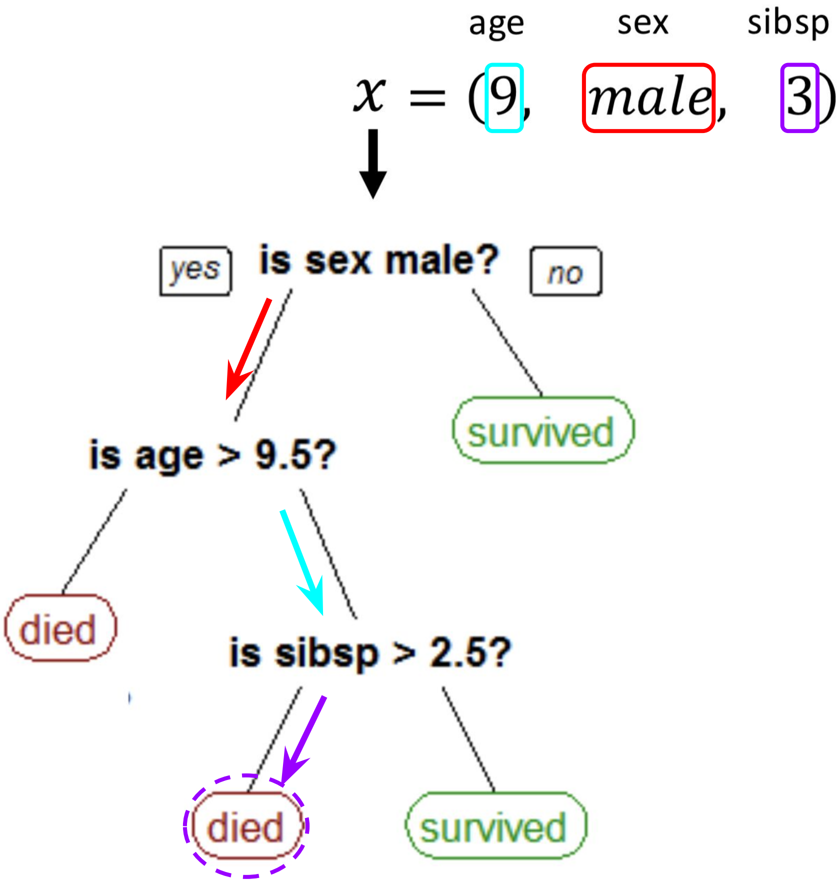
died

is sibsp > 2.5?

died

survived

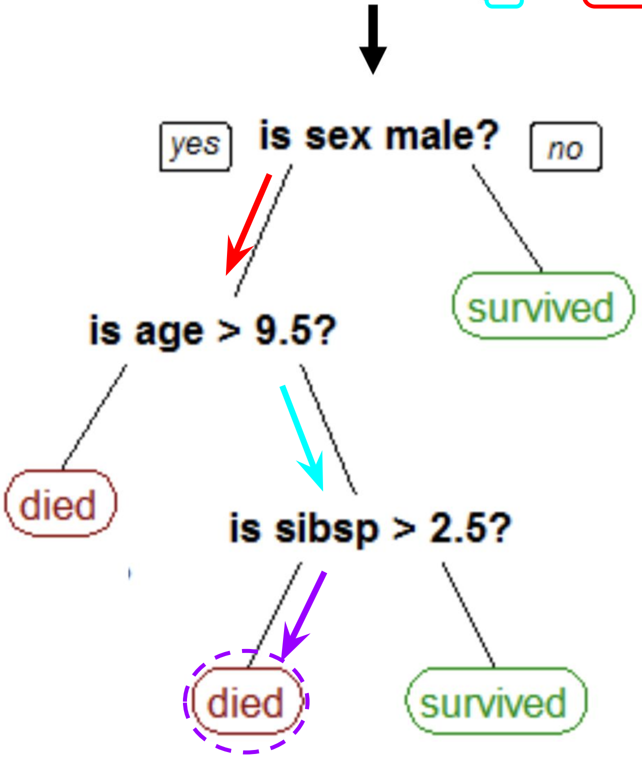
Decision tree



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

Decision tree

$$x = (\overset{\text{age}}{\boxed{9}}, \overset{\text{sex}}{\boxed{male}}, \overset{\text{sibsp}}{\boxed{3}})$$



yes

is sex male?

no

survived

is age > 9.5?

died

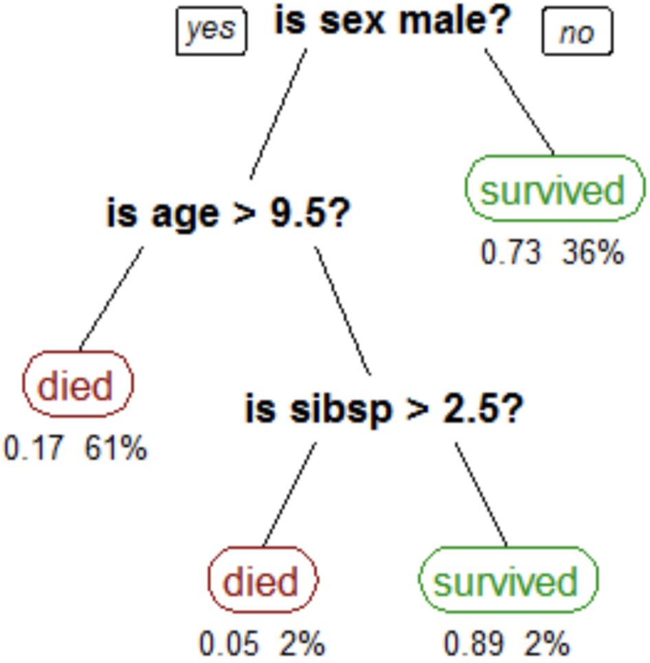
is sibsp > 2.5?

died

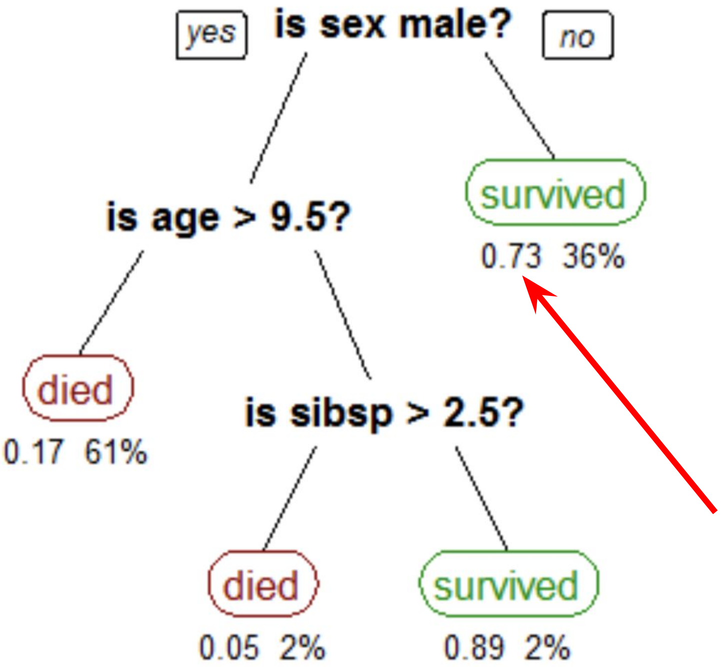
survived

$$y = died$$

Decision tree in classification

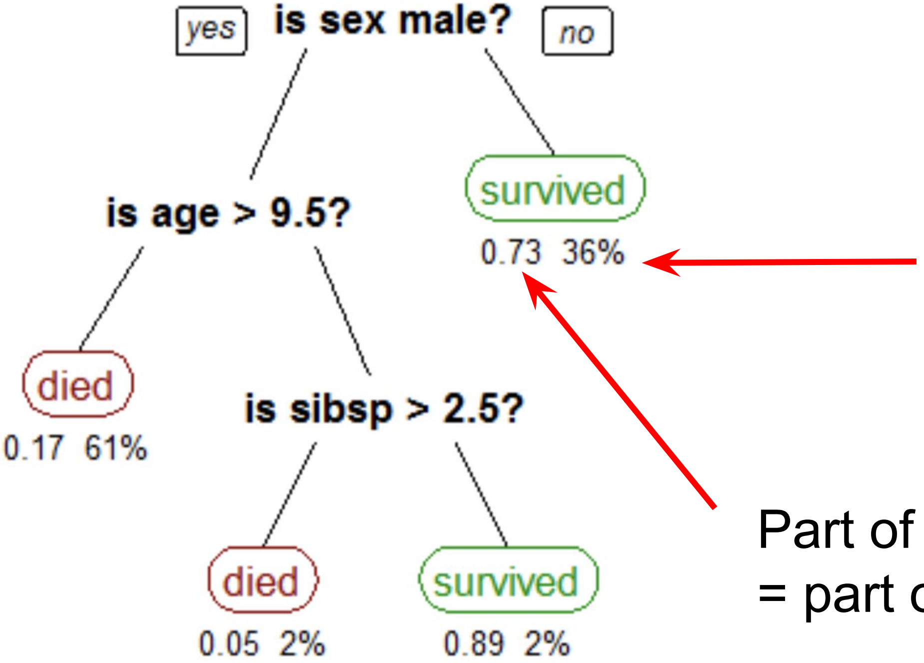


Decision tree in classification



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

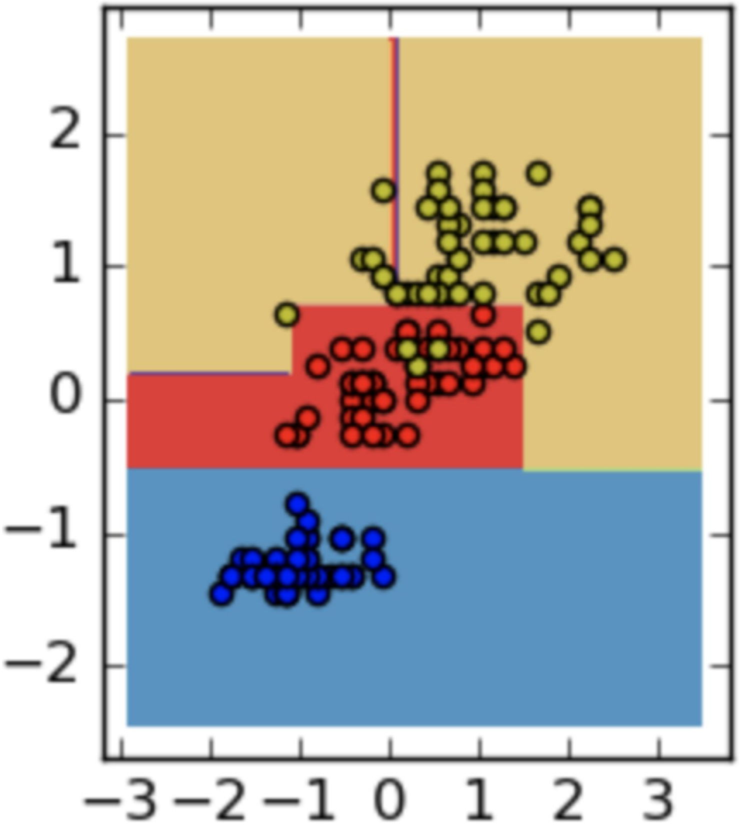
Decision tree in classification



Part of dataset in this leaf

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

Decision tree in classification



Classification problem with 3 classes and 2 features.

Pruning

- Pre-pruning:
    - Constrain the tree before construction.
- Post-pruning:
    - Simplify constructed tree.

Actually, it is the main trick in CART tree construction algorithm.

Binarisation

Idea: instead selecting one threshold define several for one feature.