Machine Learning
Lecture 5: Decision trees

Harbour.Space University
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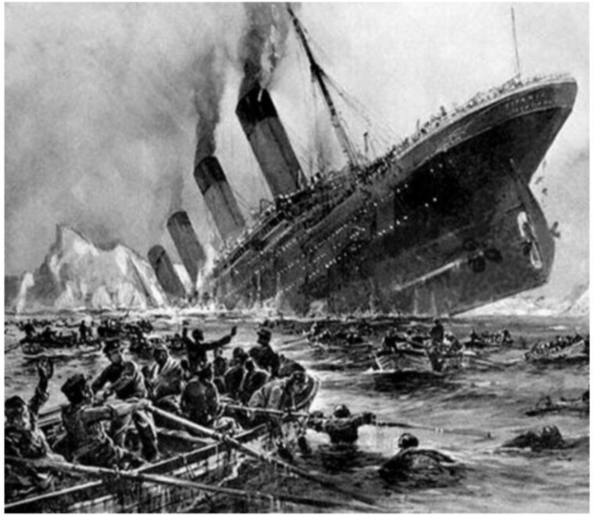
Outline

1. Decision tree definition
2. Decision trees in classification and regression
3. Constructing decision tree
4. Information criterions
5. Pruning
6. Boostrap
7. Random Forest

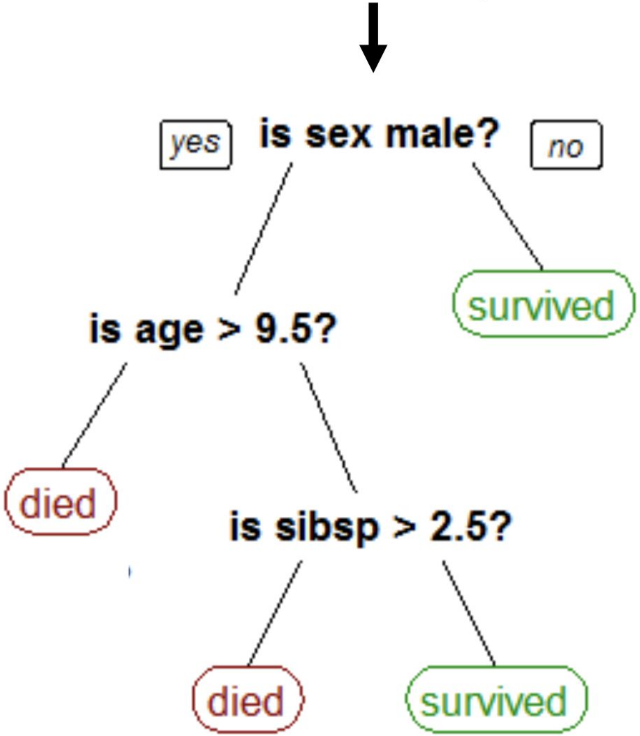
The dataset



- Titanic Dataset - the “Hello world” dataset in ML
- Target is binary: survived or not
- A lot of great tutorials with this dataset
  - E.g. challenge on Kaggle
- You will meet it in Lab 1

Decision tree

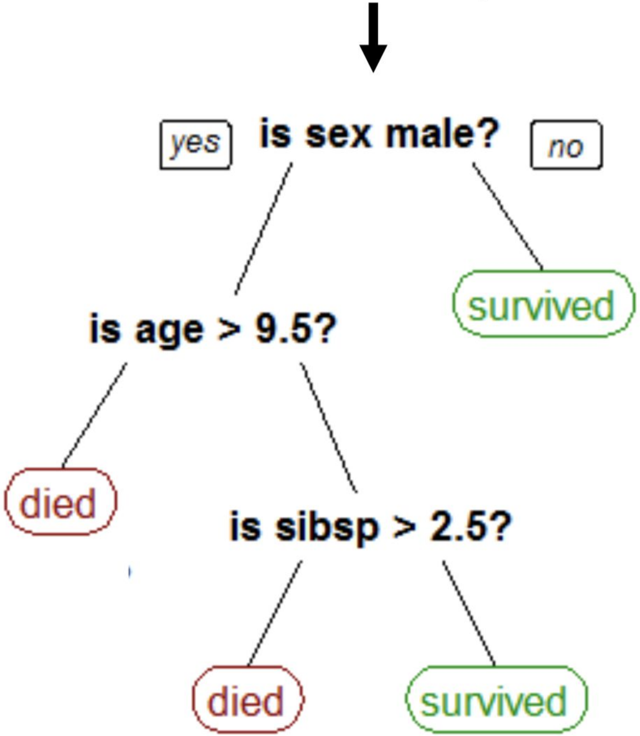
$$x = (9, \quad male, \quad 3)$$



Decision tree

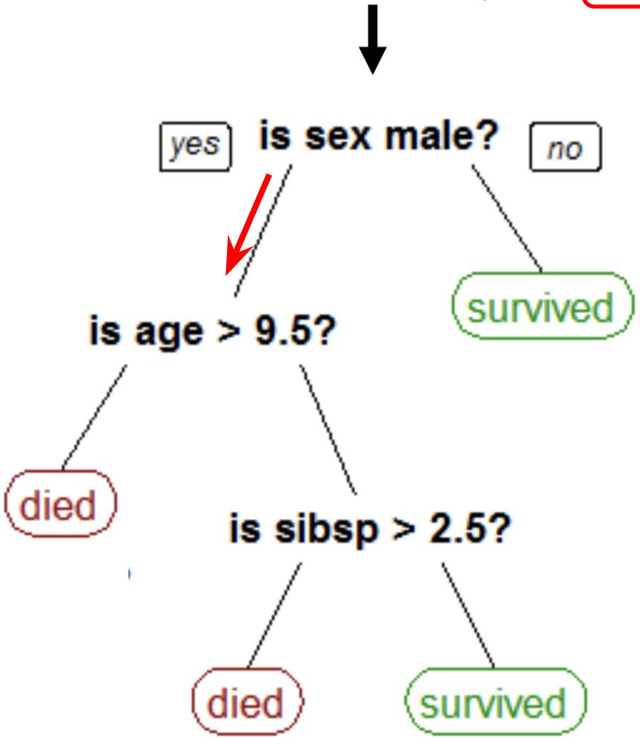
age sex sibsp

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



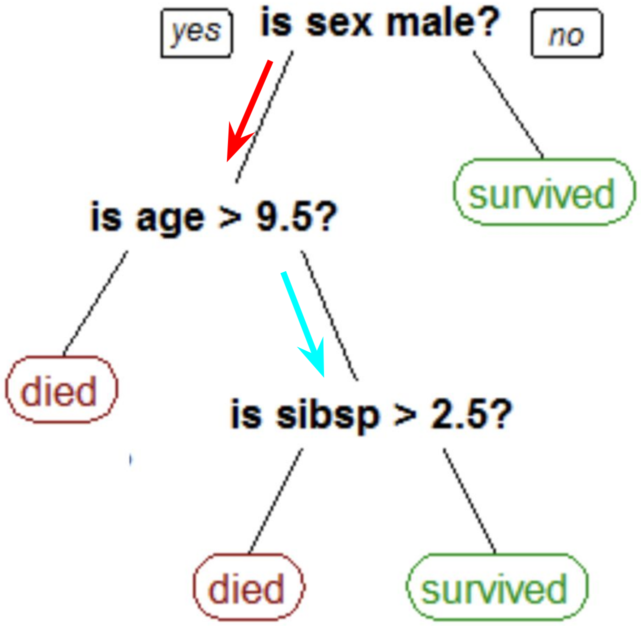
Decision tree

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

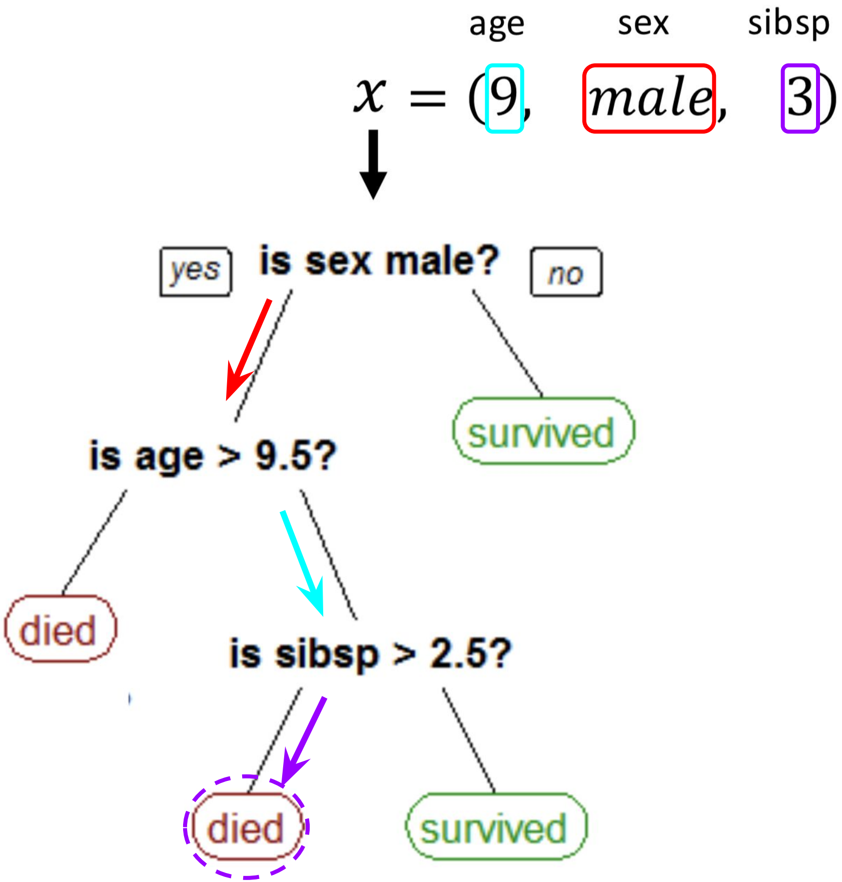


Decision tree

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



Decision tree



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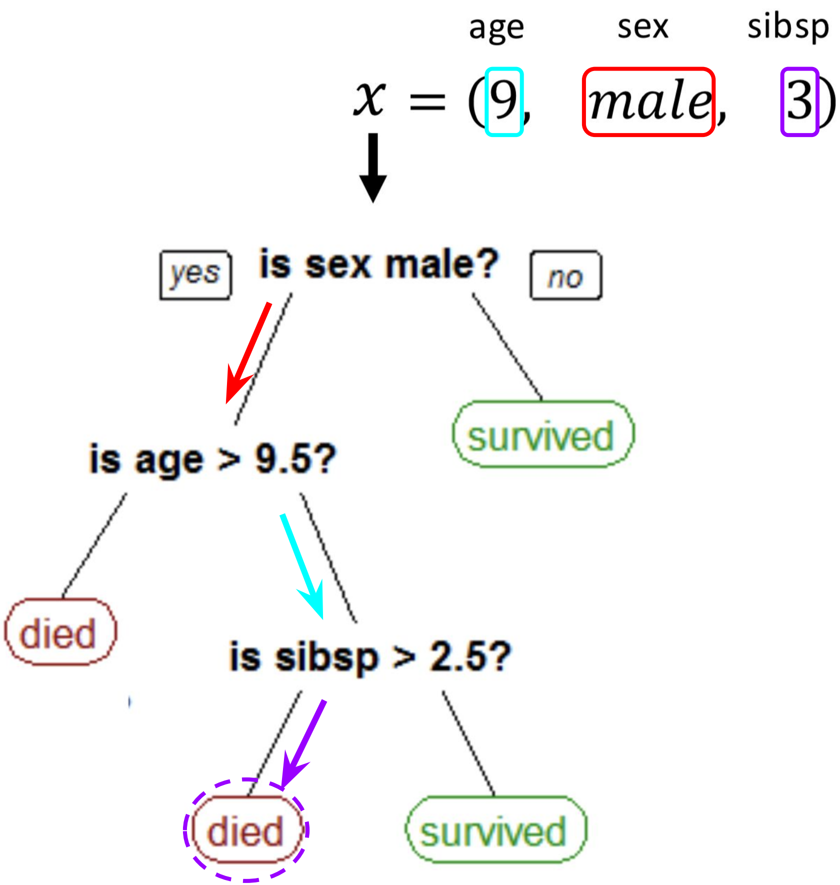
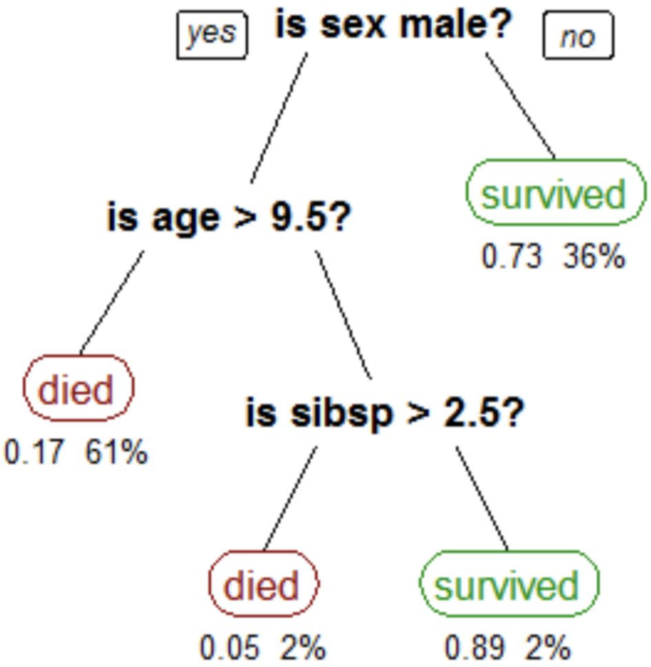
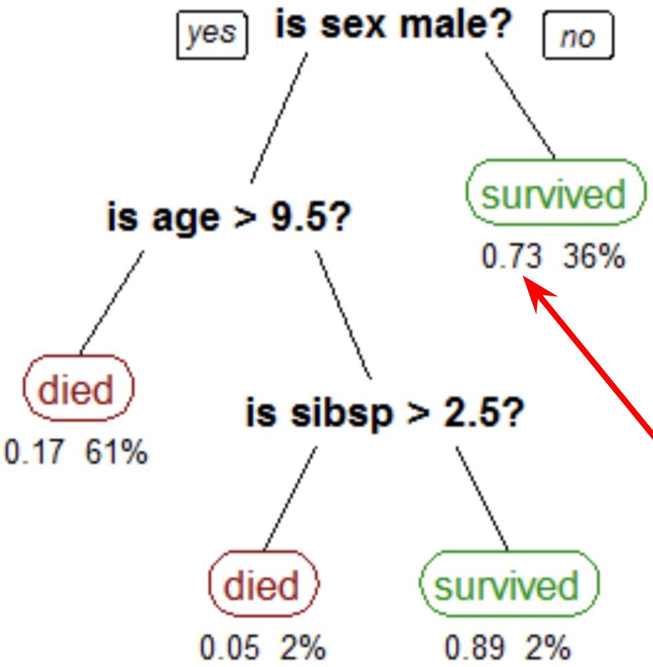


$$y = died$$

Decision tree in classification

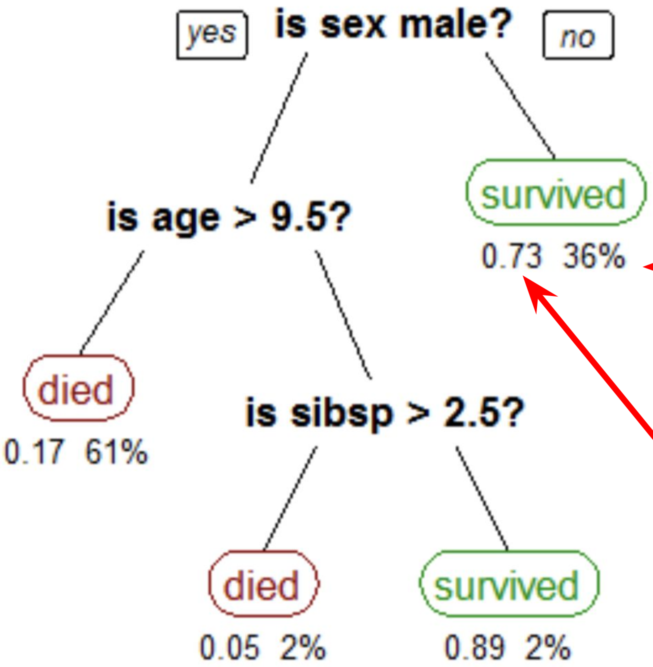


Decision tree in classification



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

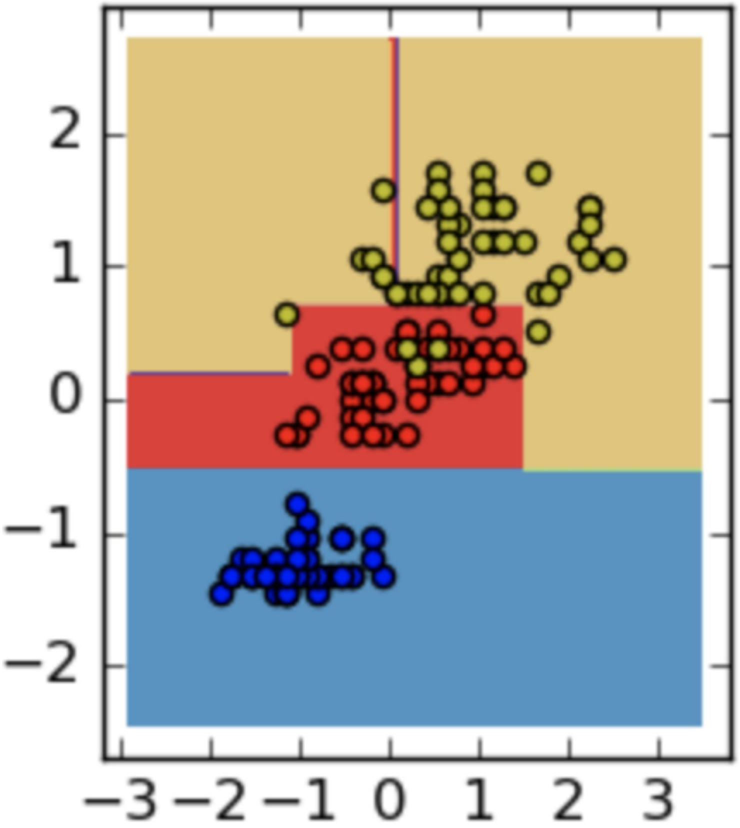
Decision tree in classification



Part of dataset in this leaf

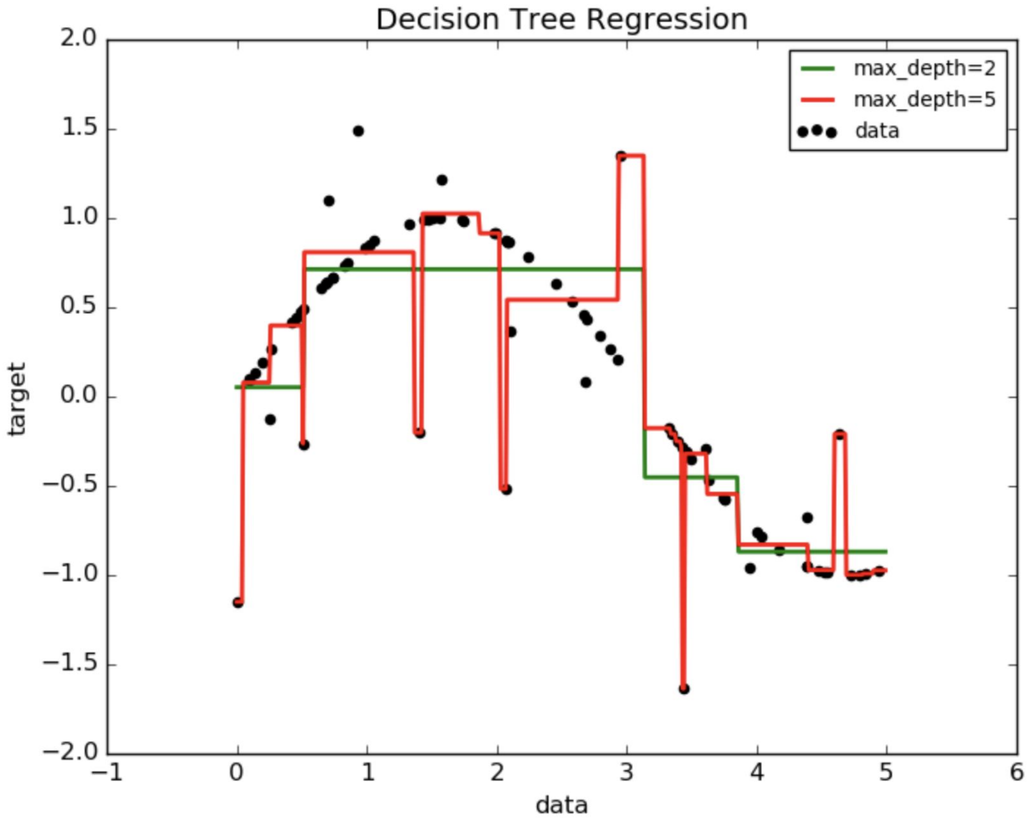
Part of survived passengers
= part of objects of 1st class

Decision tree in classification



Classification problem with 3 classes and 2 features.

Decision tree in regression



Green - decision tree of depth 2

Red - decision tree of depth 5

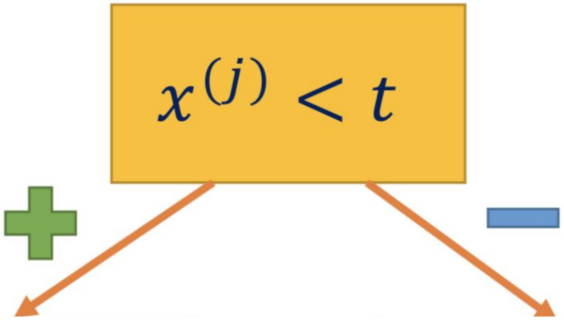
Every leaf corresponds to some constant.

Constructing decision trees

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

1. Make a split

Constructing decision trees



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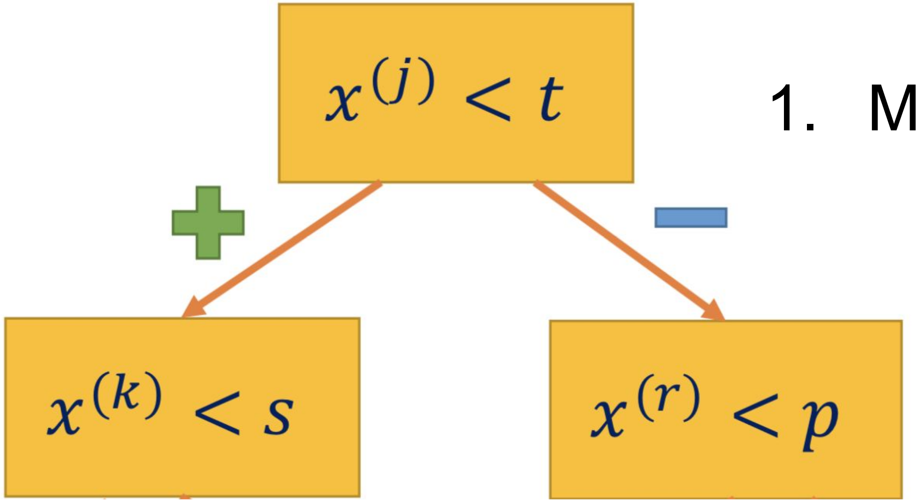
Constructing decision trees



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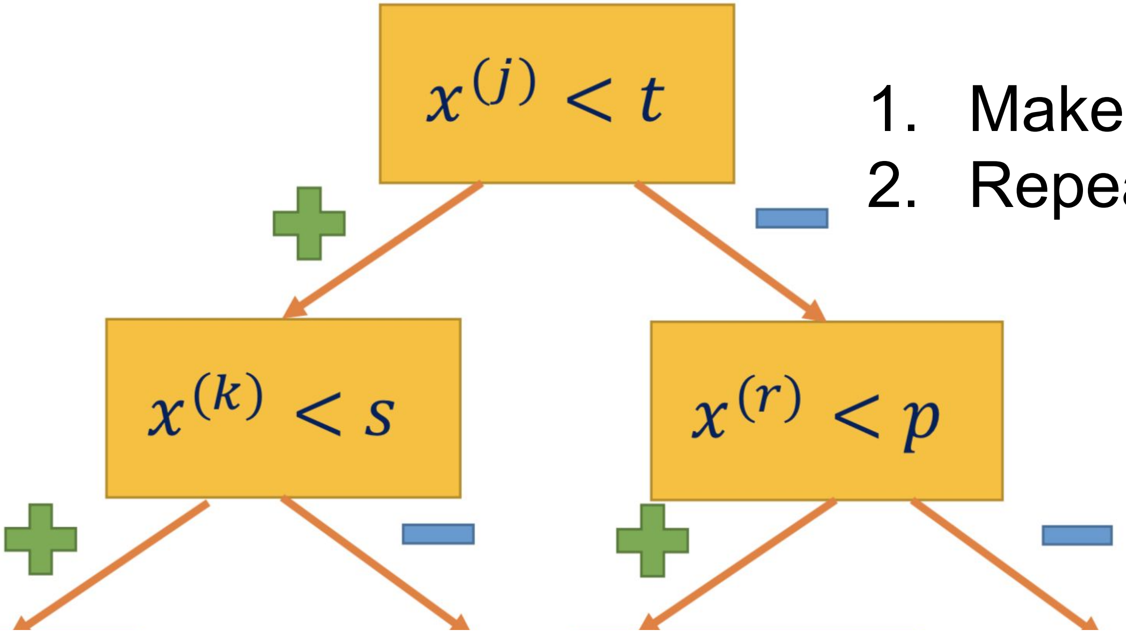
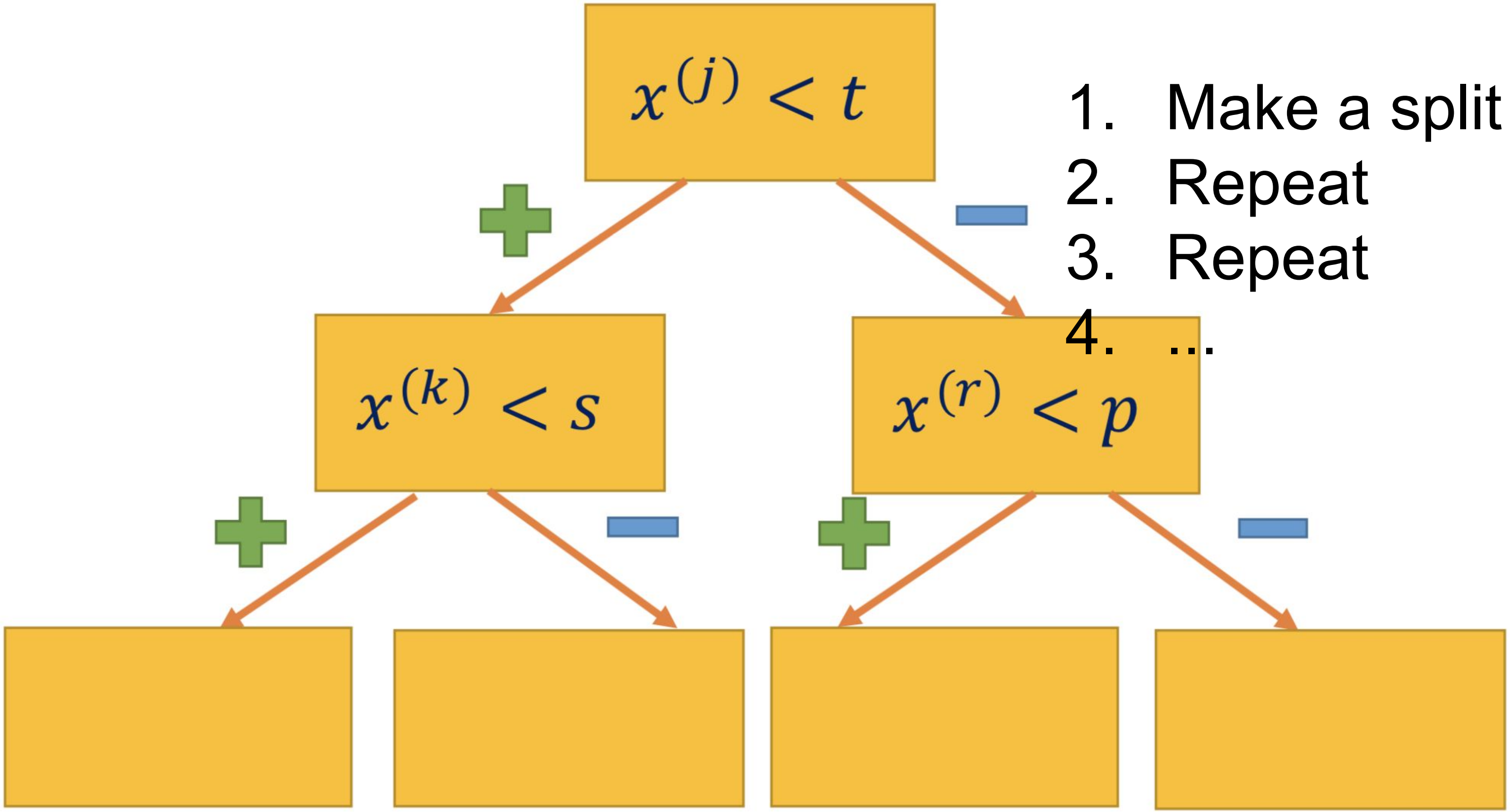


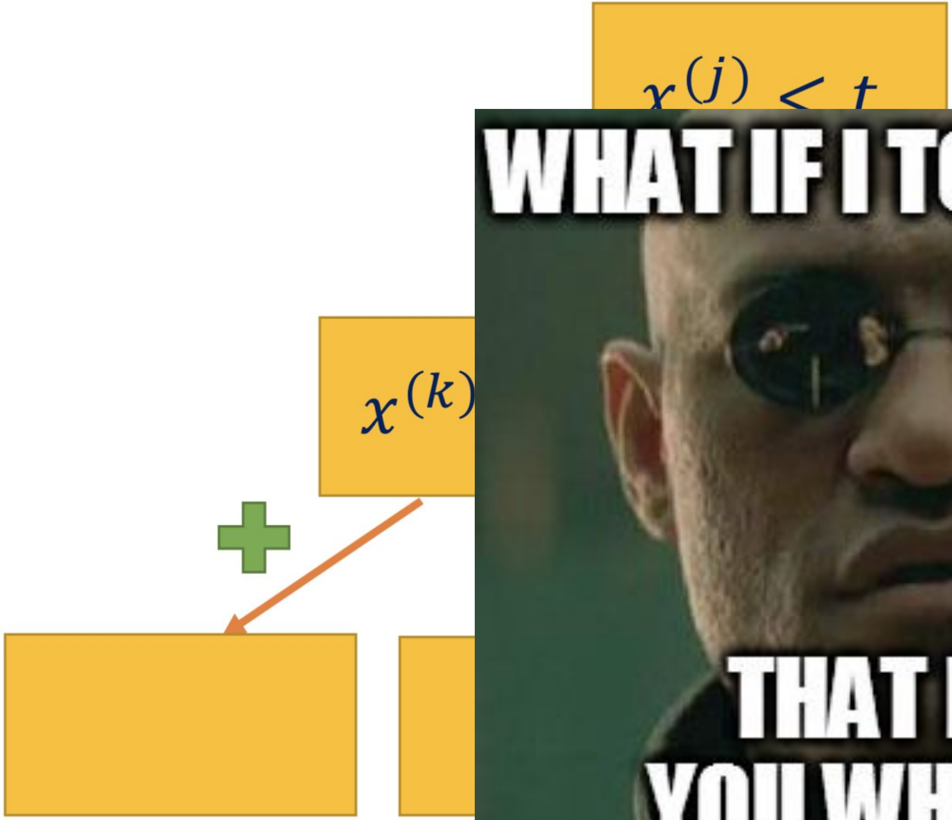
1. Make a split
2. Repeat

Constructing decision trees



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

Constructing decision trees



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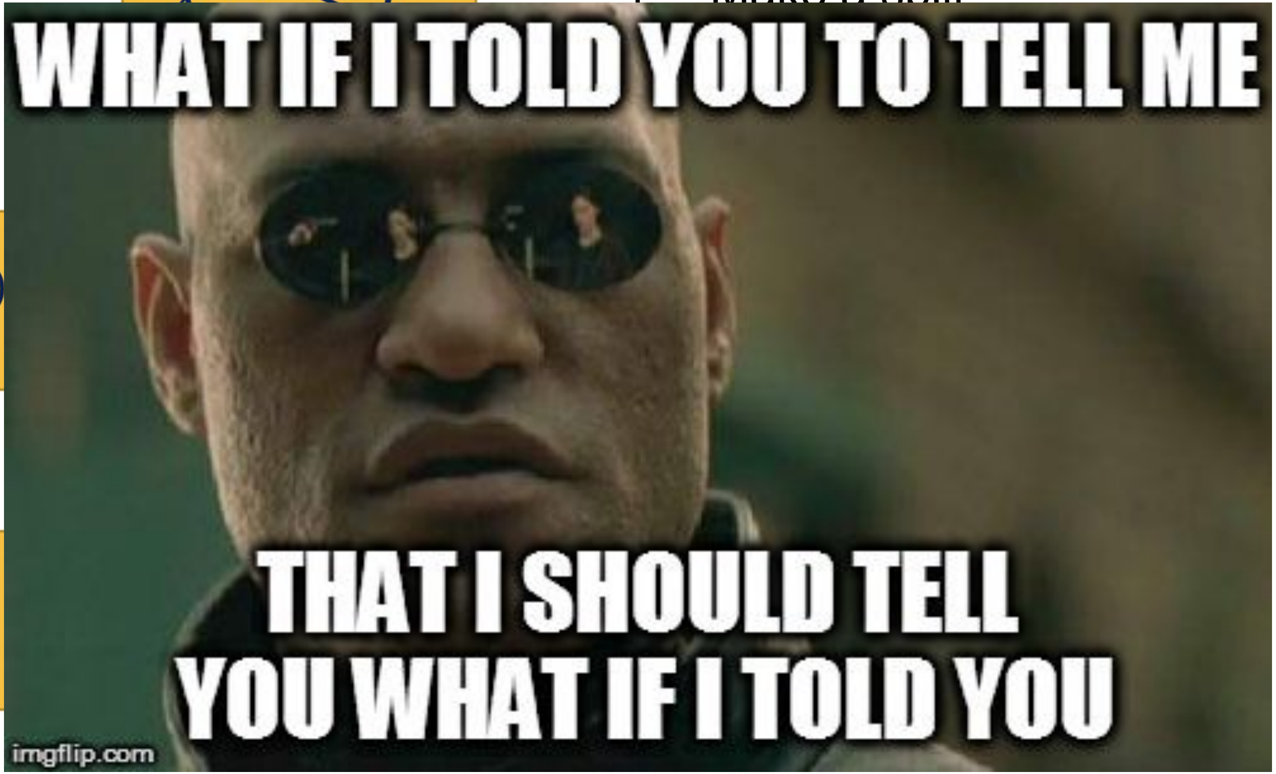

How to split data properly?

Q

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

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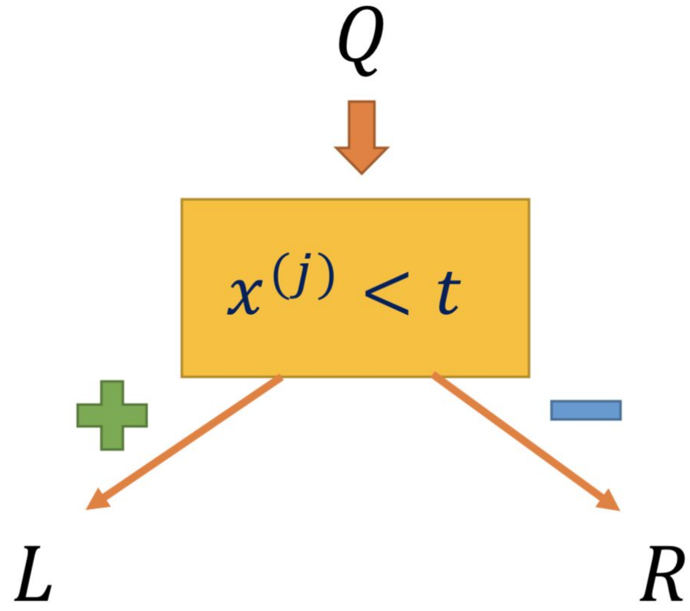

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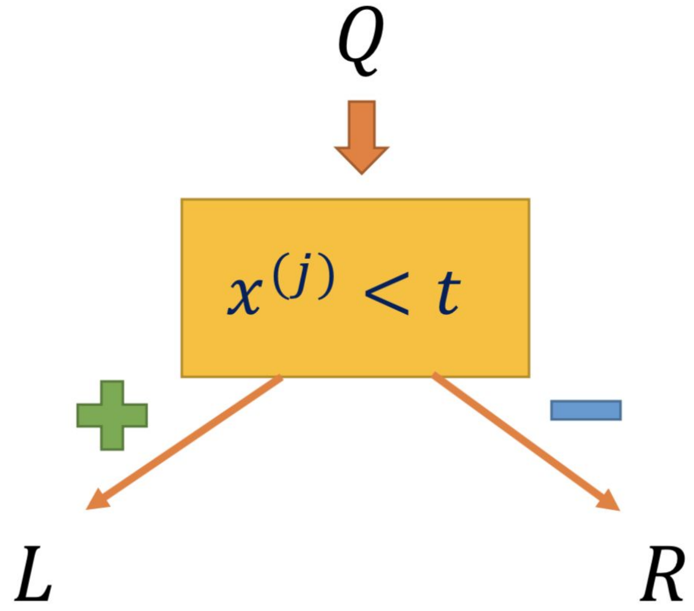
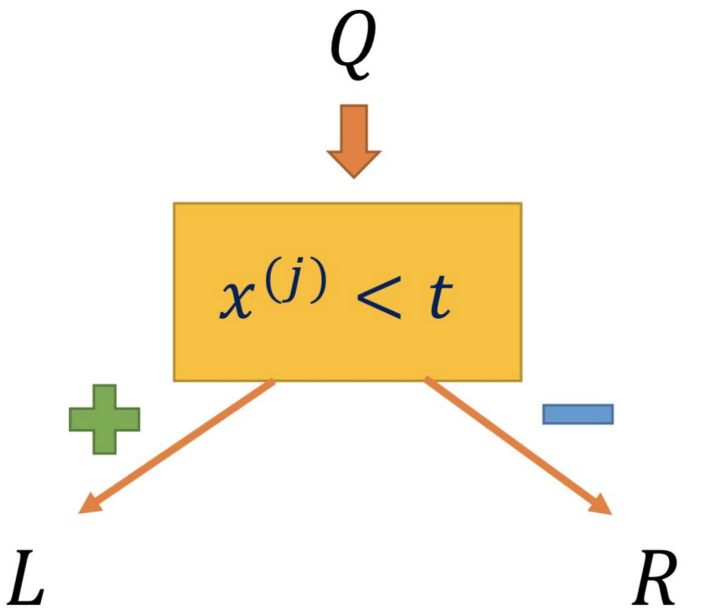


$$G(j,t) = \frac{|L|}{|Q|} H(L) + \frac{|R|}{|Q|} H(R)$$

How to split data properly?



What is H()?

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

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

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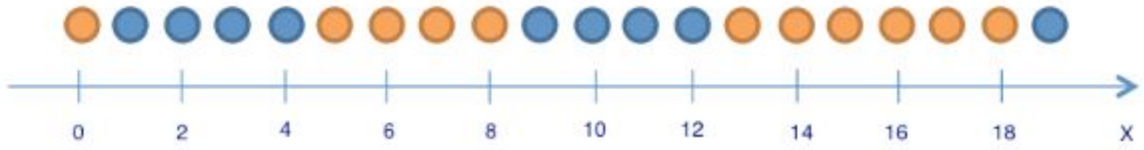

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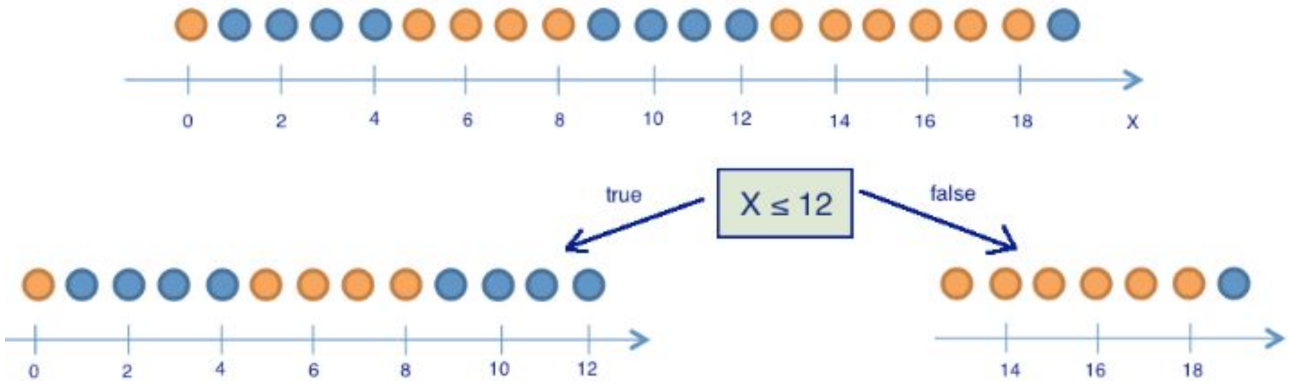
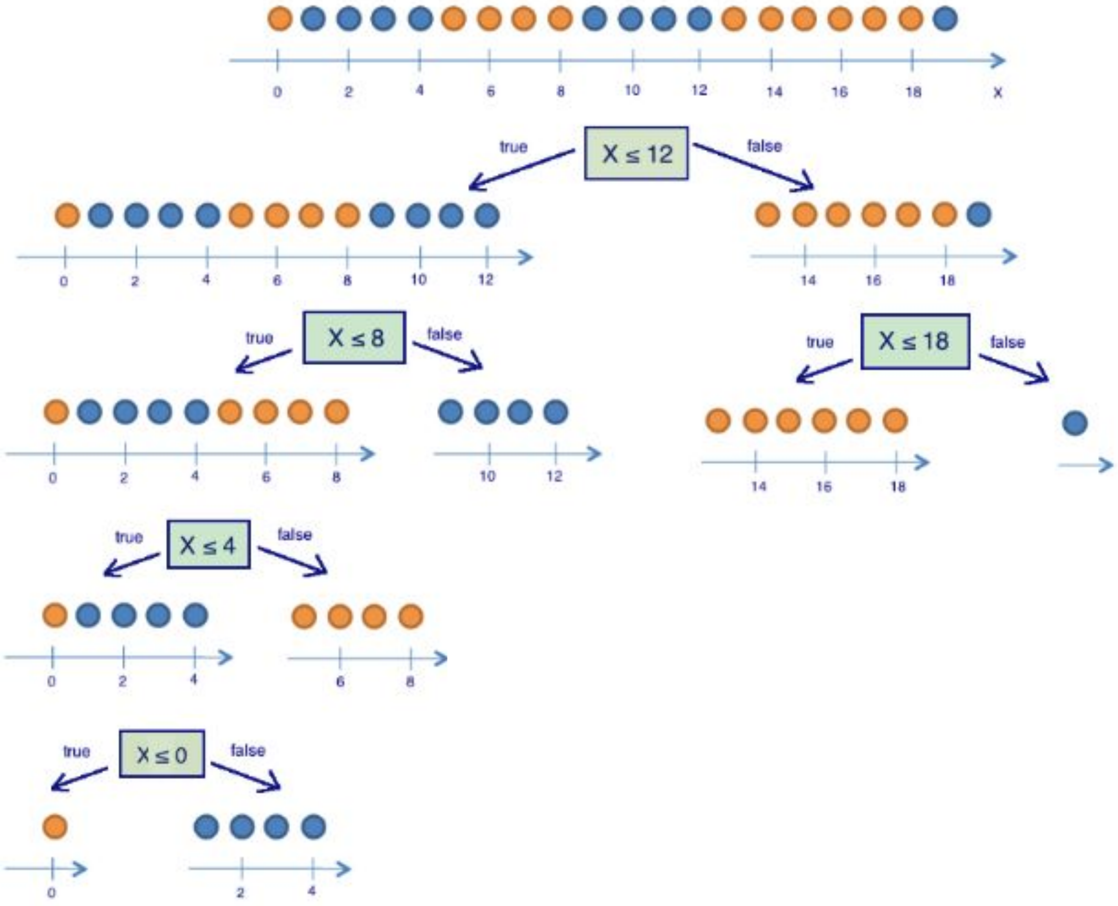


Information criteria: Entropy



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

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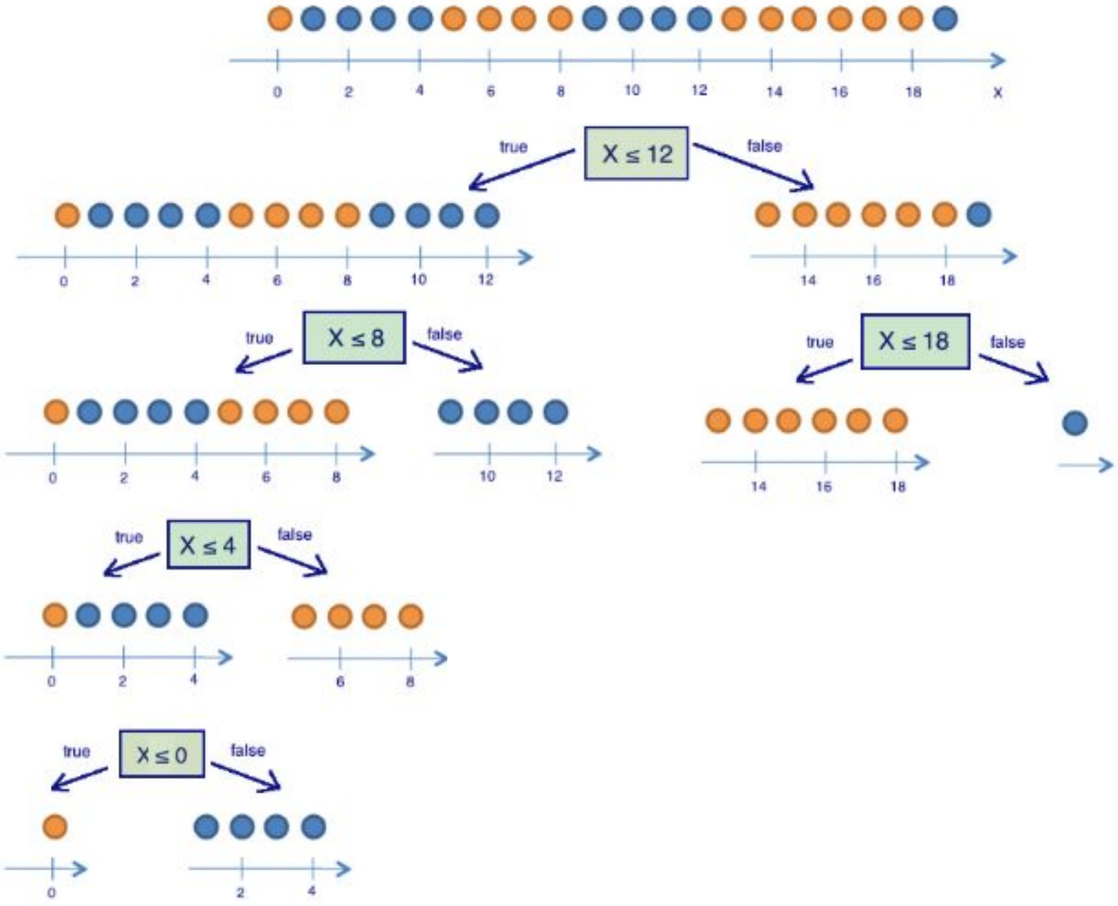

$$S = -\sum_k p_k \log_2 p_k$$

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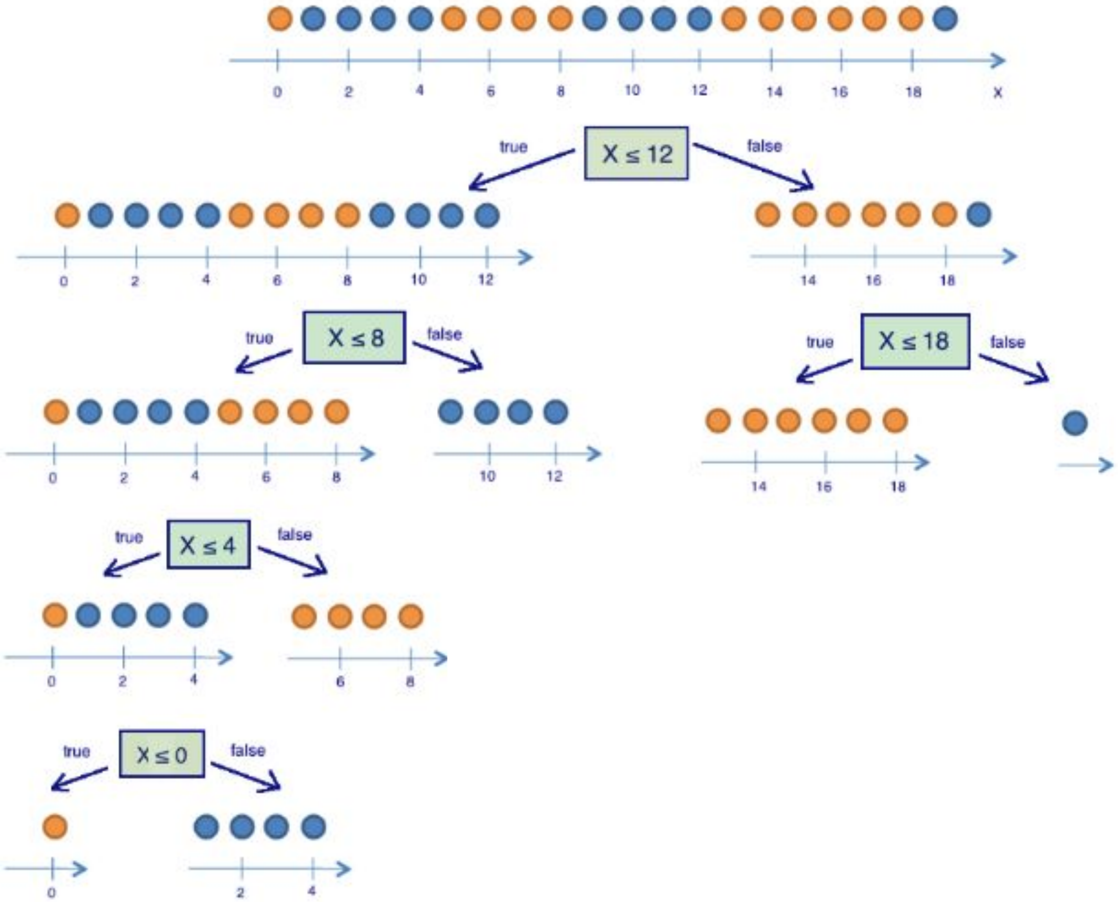
Information criteria: Entropy



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

In binary case N = 2

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

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Information criteria: Gini impurity

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

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Information criteria: Gini impurity

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

In binary case N = 2

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

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

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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?

Information criteria

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

1. Mean squared error

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

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

Pruning

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

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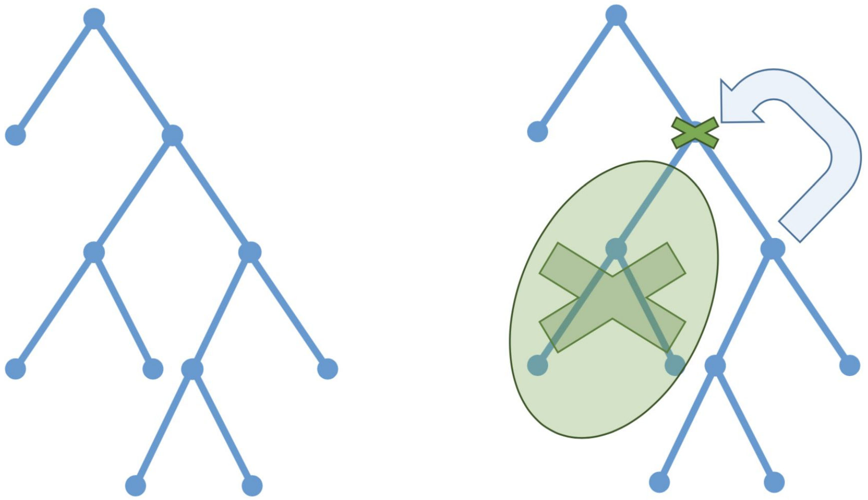

Pruning

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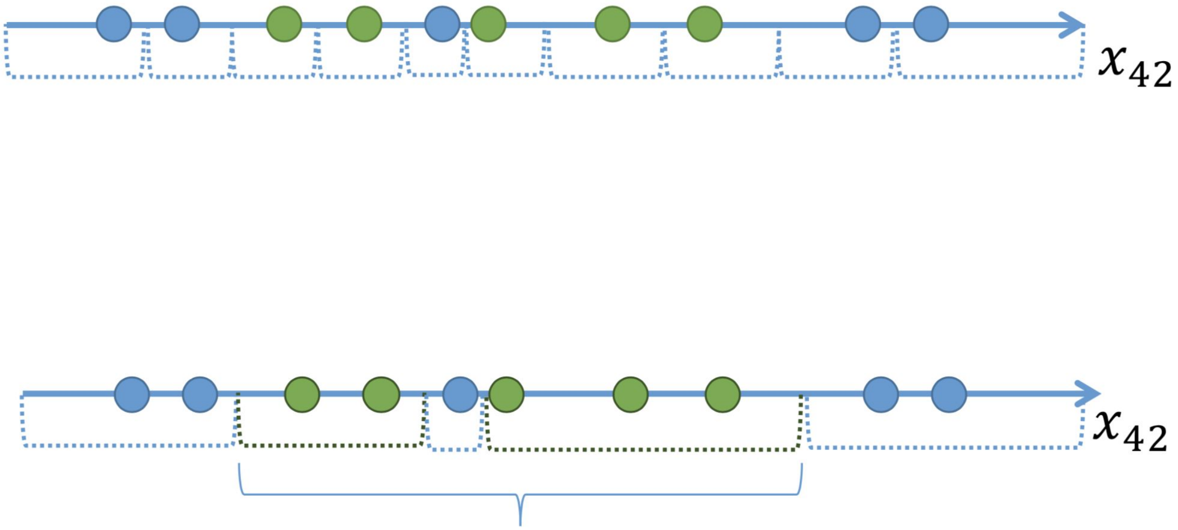
Actually, it is the main trick in CART tree construction algorithm.

Binarisation

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



How the trees are actually constructed

- ID-3
- C4.5
- C5.0
- CART
- etc.

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

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:

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

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

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

Error decreased by N times!

Bootstrap

Consider the errors ~~unbiased and uncorrelated~~:

Because this is a lie

$$\mathbb{E}_x \varepsilon_j(x) = 0;$$
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The final model averages all predictions:

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

$$E_N = \mathbb{E}_x\left(\frac{1}{N}\sum_{j=1}^{n} b_j(x) - y(x)\right)^2 =$$
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$$\boxed{= \frac{1}{N}E_1.}$$

Error decreased by N times!

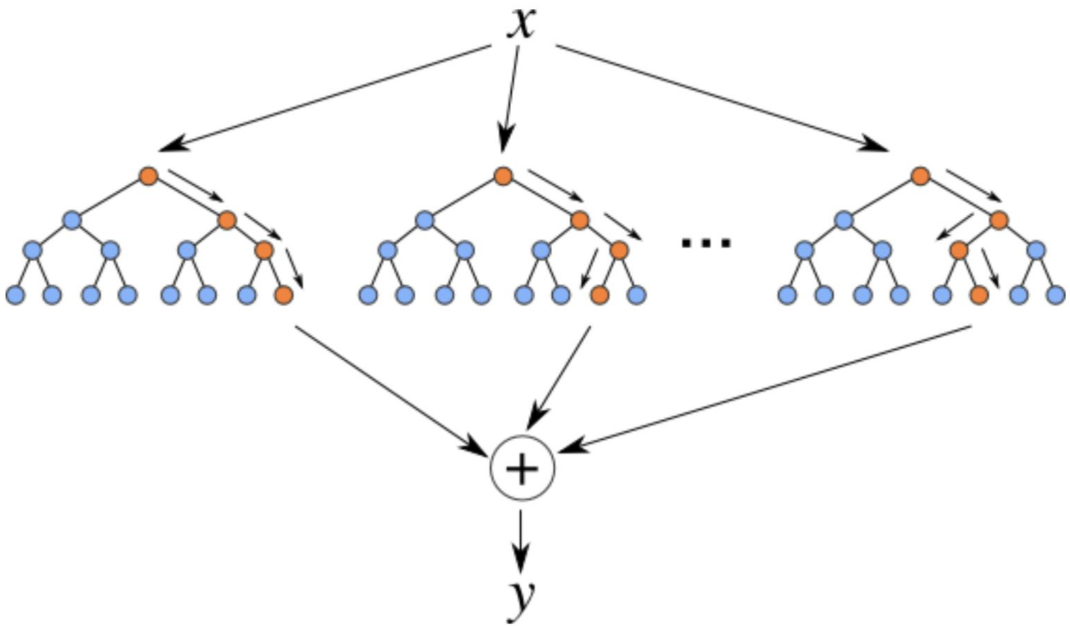
Bagging = Bootstrap aggregating

Decreases the variance if the basic algorithms are not correlated.

RSM - Random Subspace Method

Same approach, but with features.

Bagging + RSM = Random Forest



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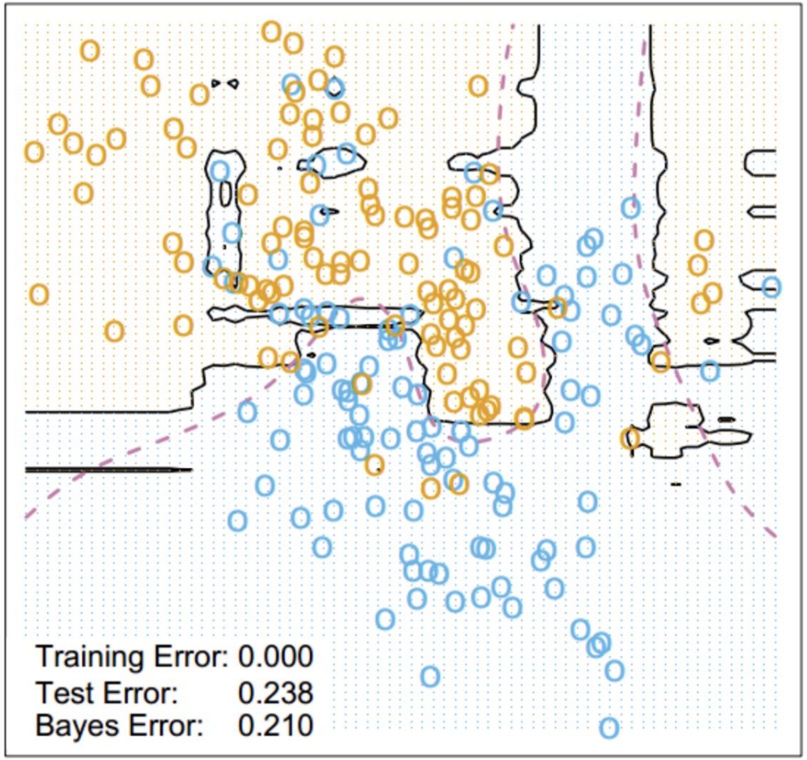
$$\mathrm{OOB} = \sum_{i=1}^{\ell} L\left(y_i, \frac{1}{\sum_{n=1}^{N}[x_i \notin X_n]} \sum_{n=1}^{N} [x_i \notin X_n] b_n(x_i)\right)$$

Random Forest Classifier



3−Nearest Neighbors