Machine Learning course

Lecture 5: Decision trees and Ensembles

Harbour.Space
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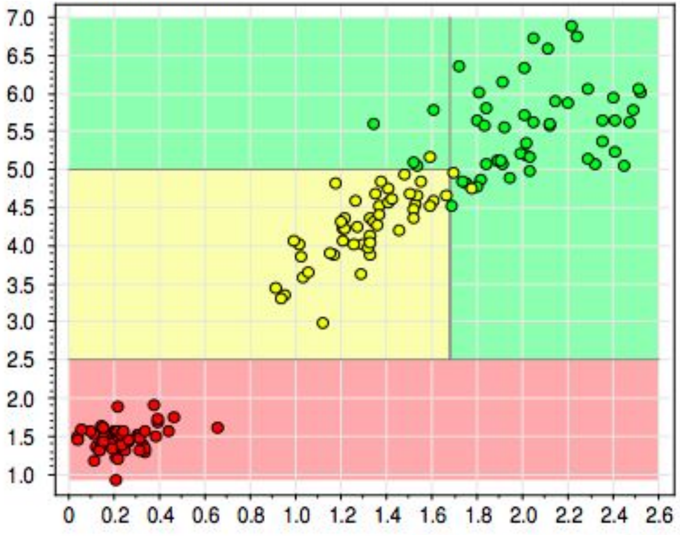
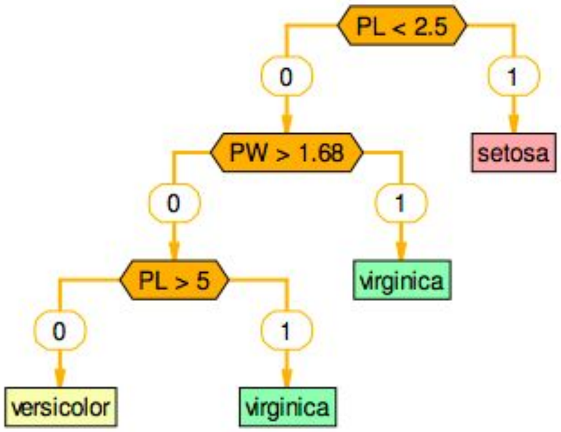
Outline

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. Bootstrap and Bagging (optional)
7. Random Forest (optional)

Decision Tree: intuition

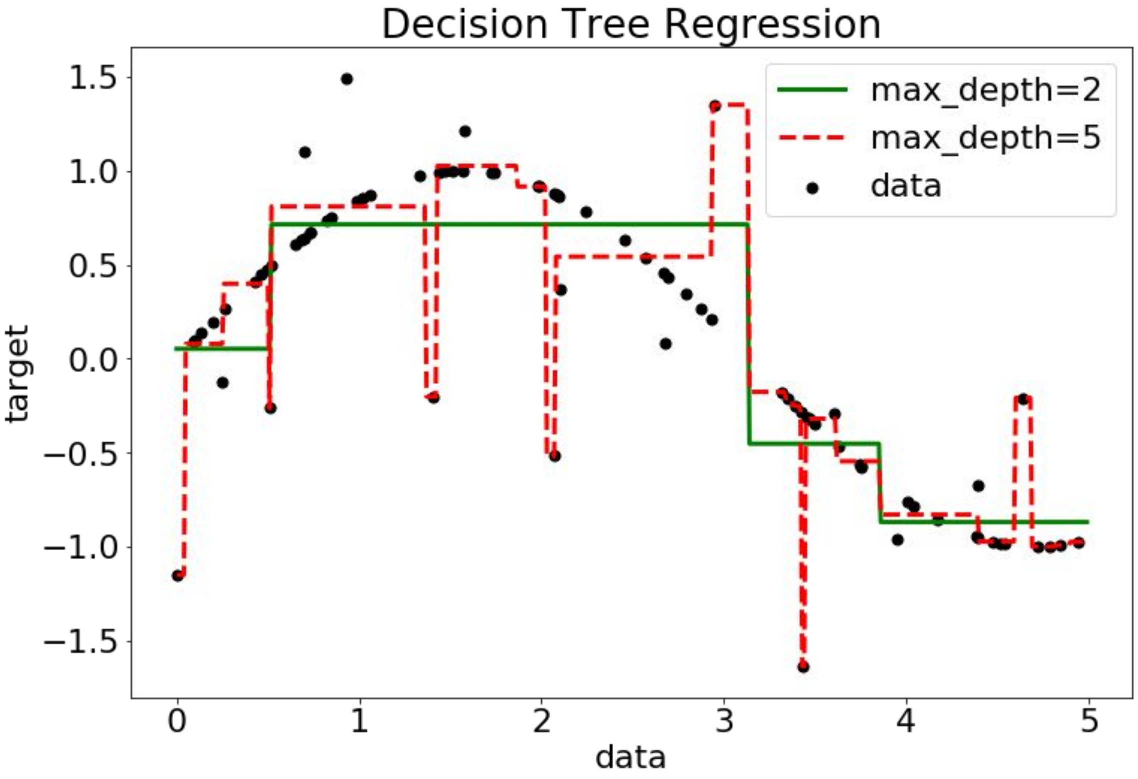
Decision tree for Iris data set





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

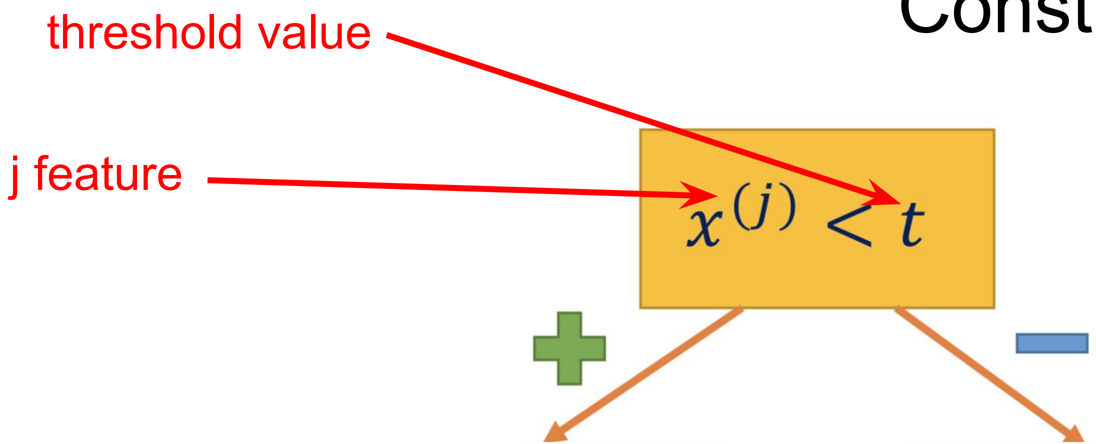
threshold value

j feature

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

1. Make a split

Constructing decision trees



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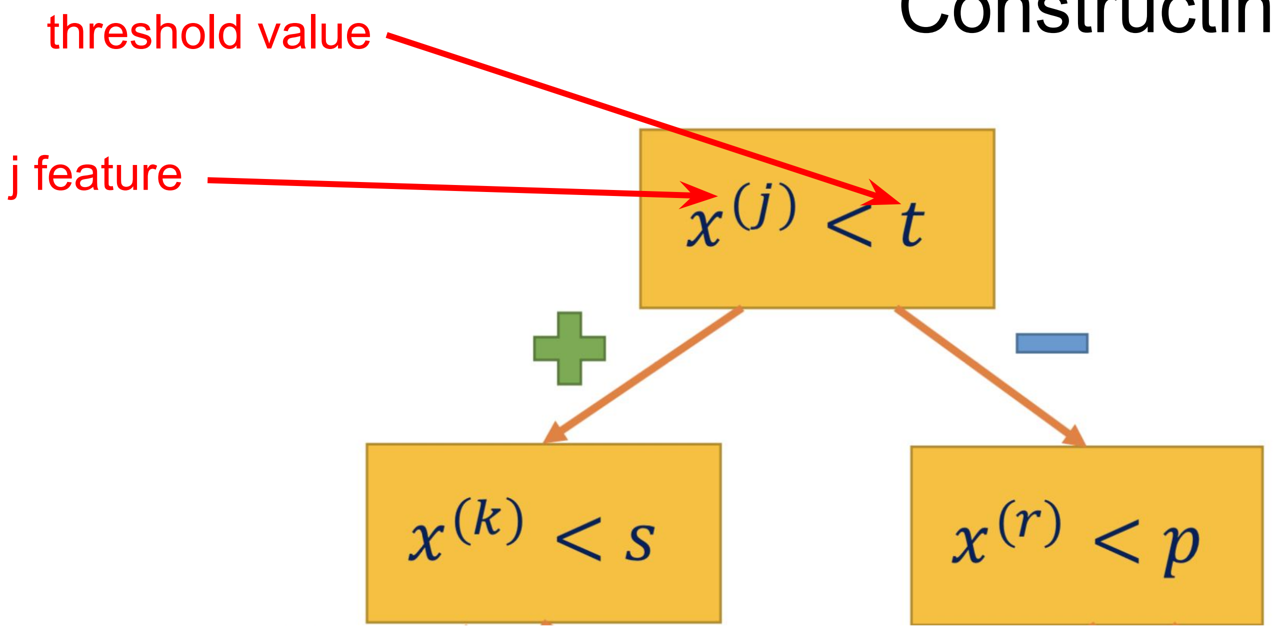
Constructing decision trees



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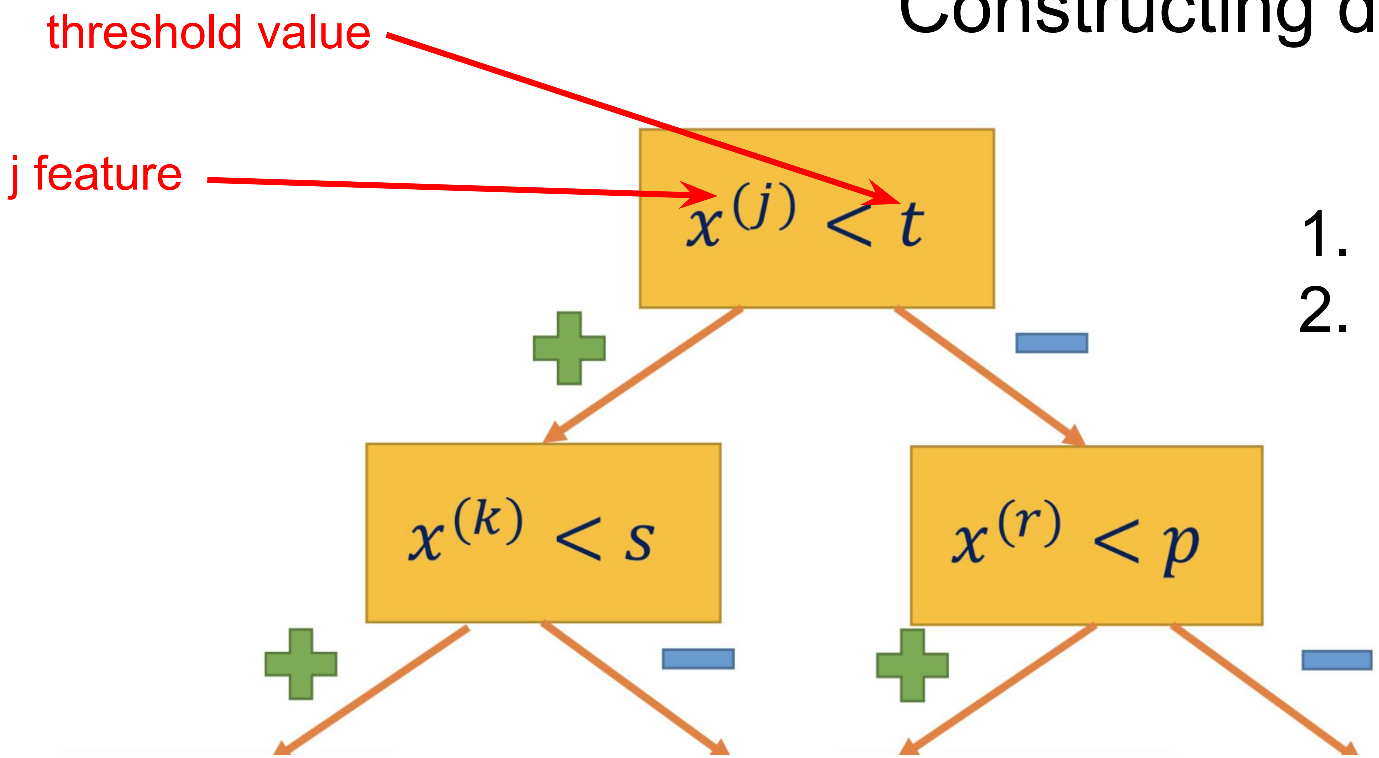
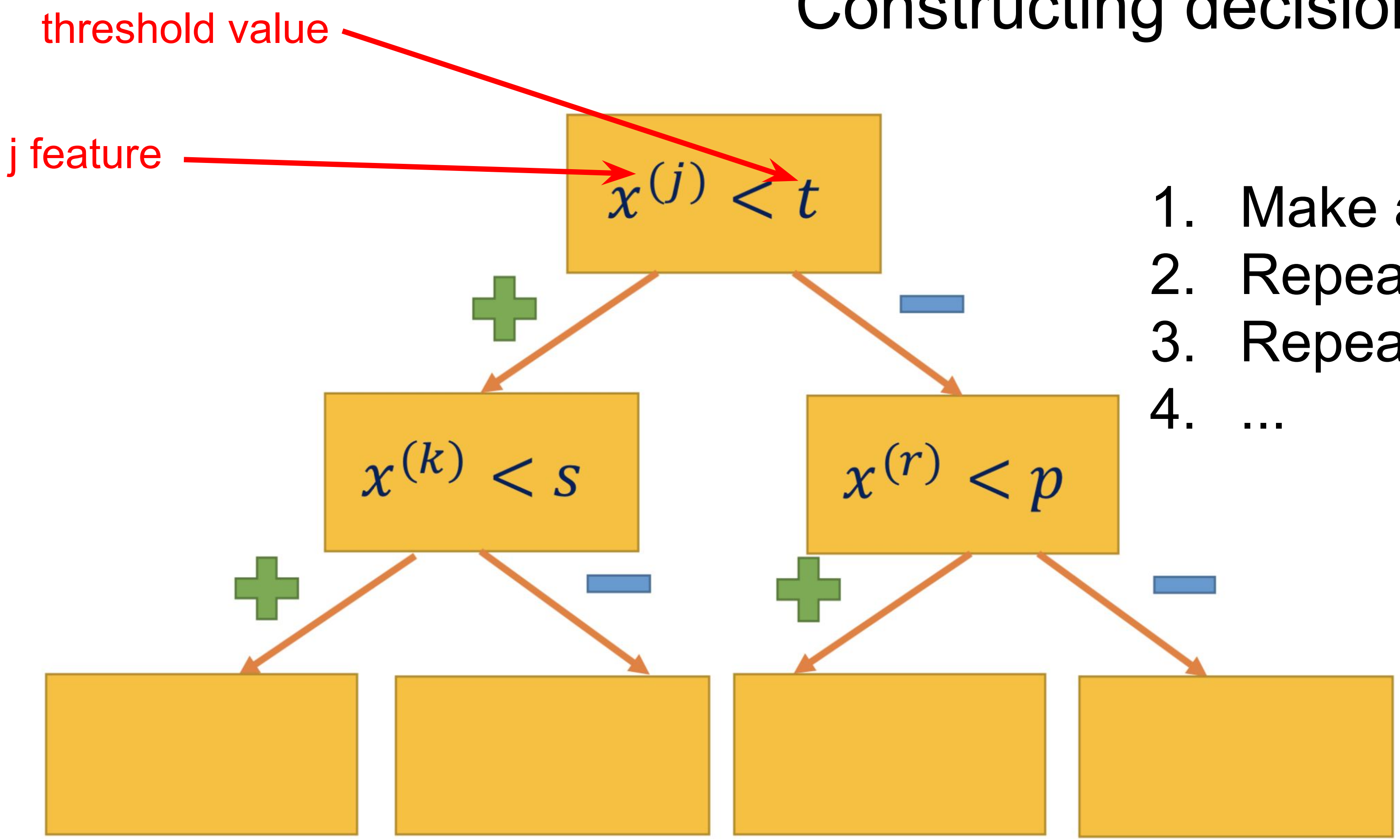
Constructing decision trees



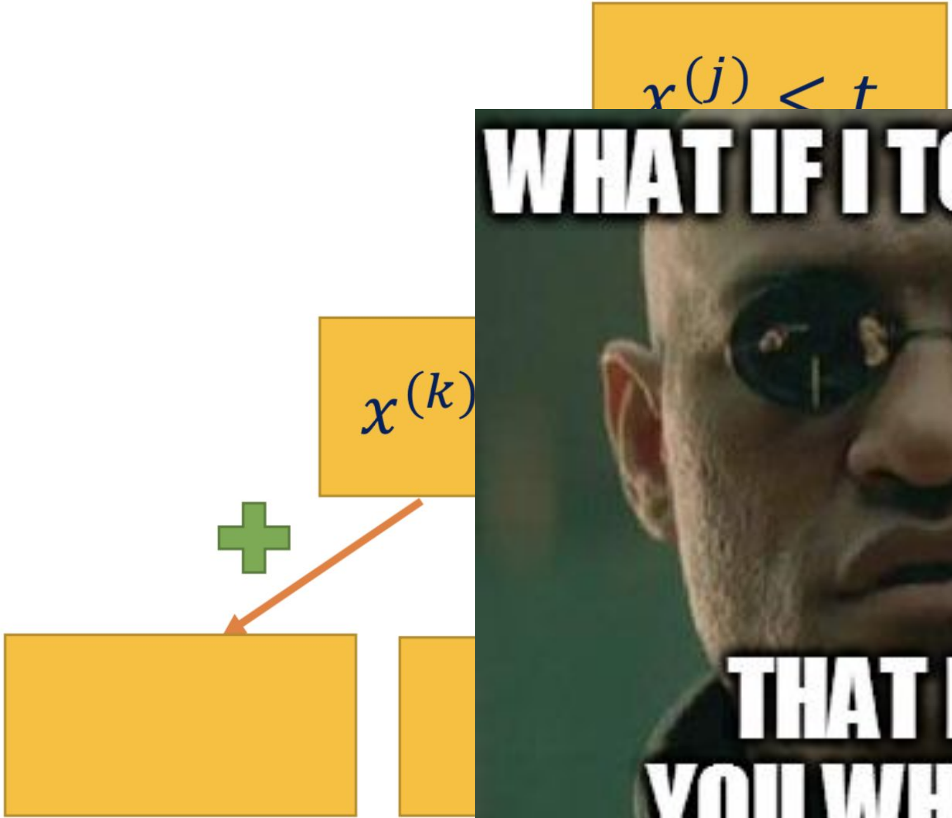
1. Make a split
2. Repeat

Constructing decision trees



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

Constructing decision trees



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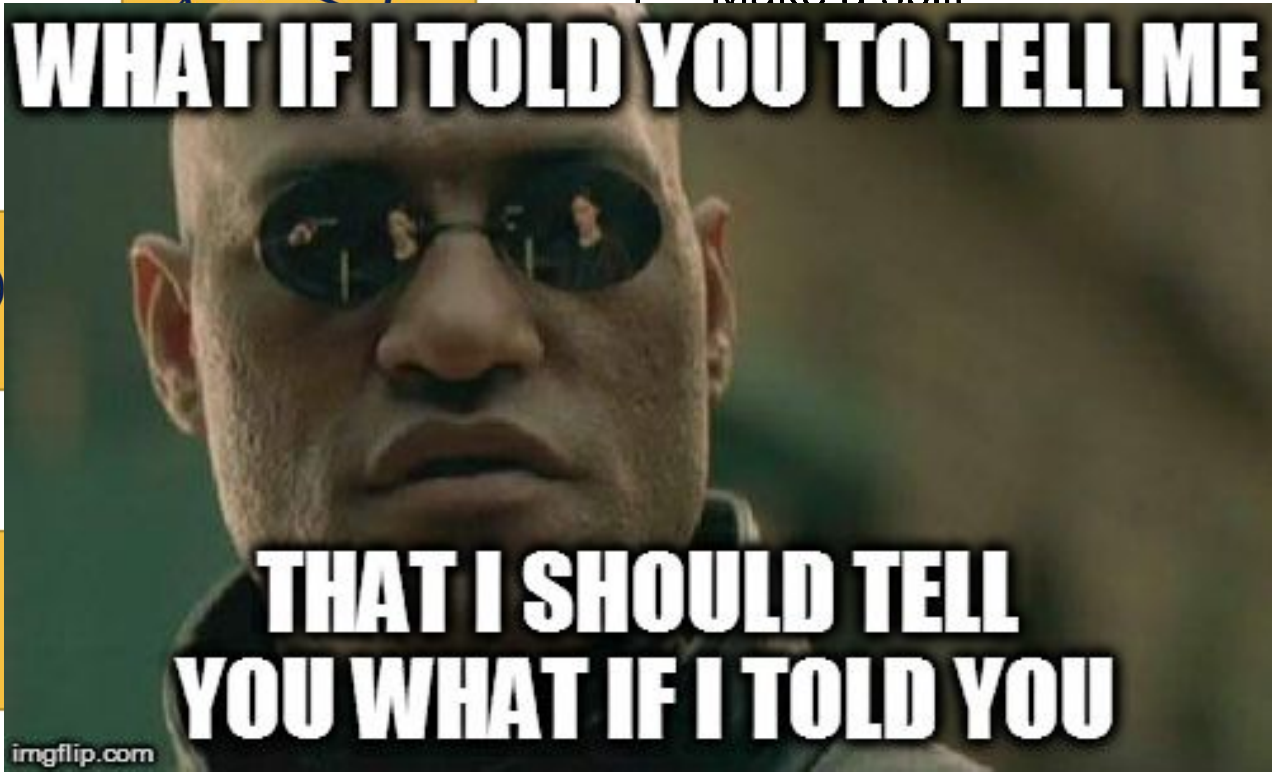
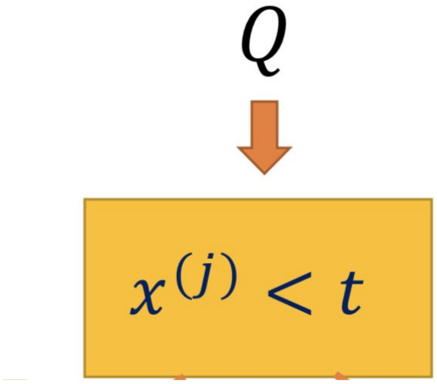


How to split data properly?



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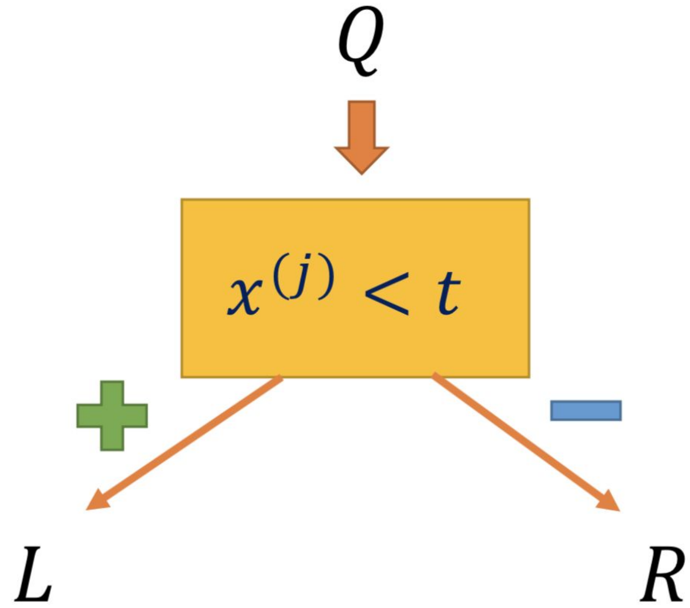

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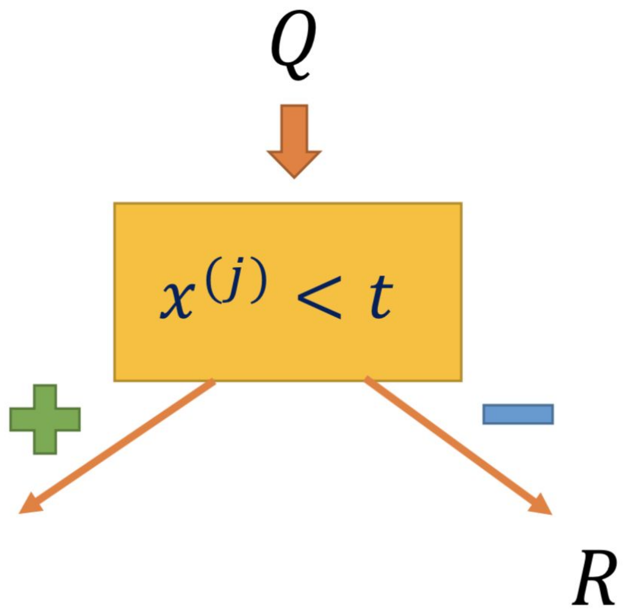
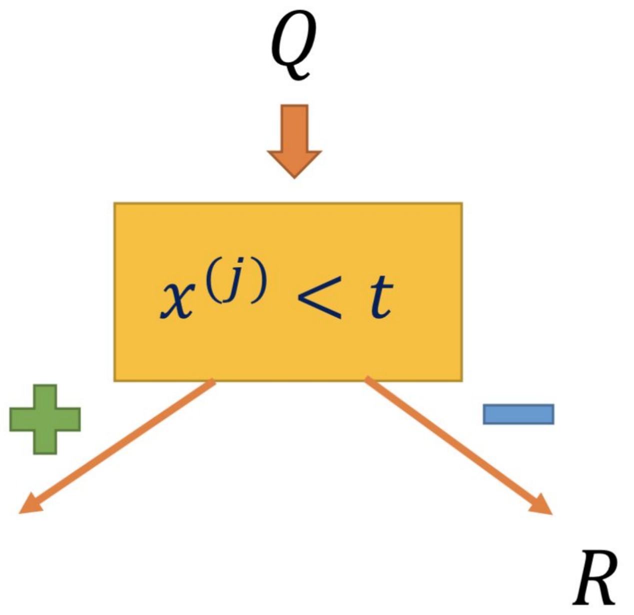


$$G(j,t) = \frac{|L|}{|Q|}H(L) + \frac{|R|}{|Q|}H(R)$$

How to split data properly?

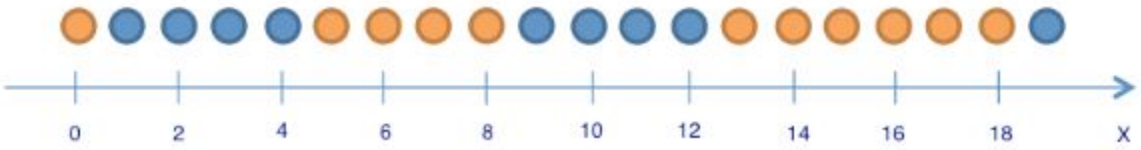


What is H()?

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

Information criteria

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



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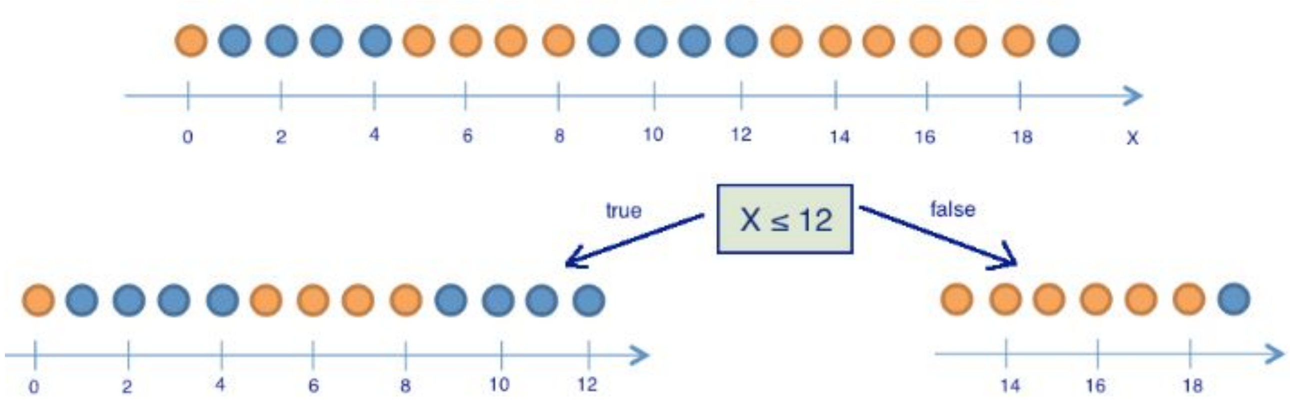

Information criteria

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

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:

$$H(R) = 1 - \sum_k (p_k)^2$$

H(R) is measure of “heterogeneity” of our data.
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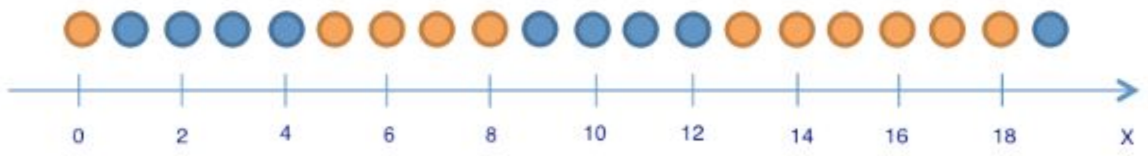

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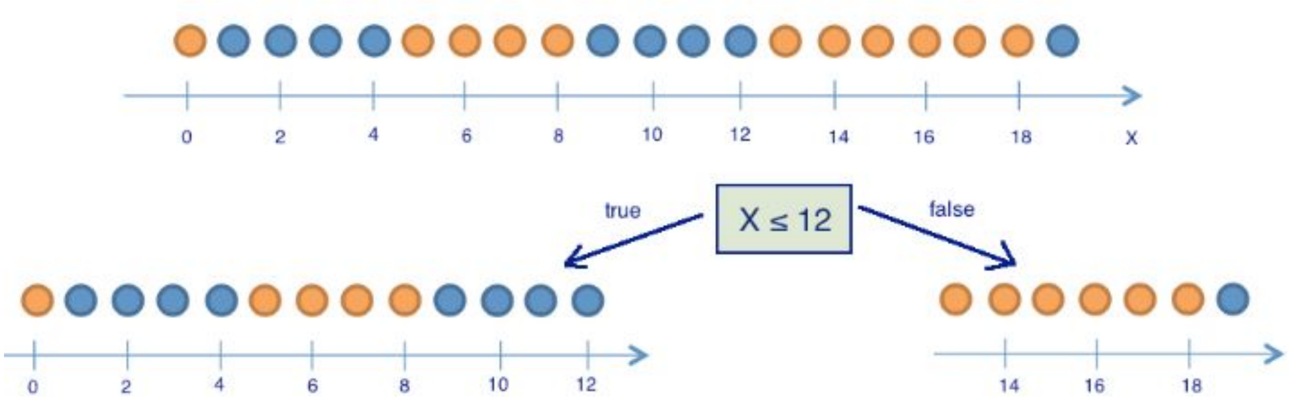

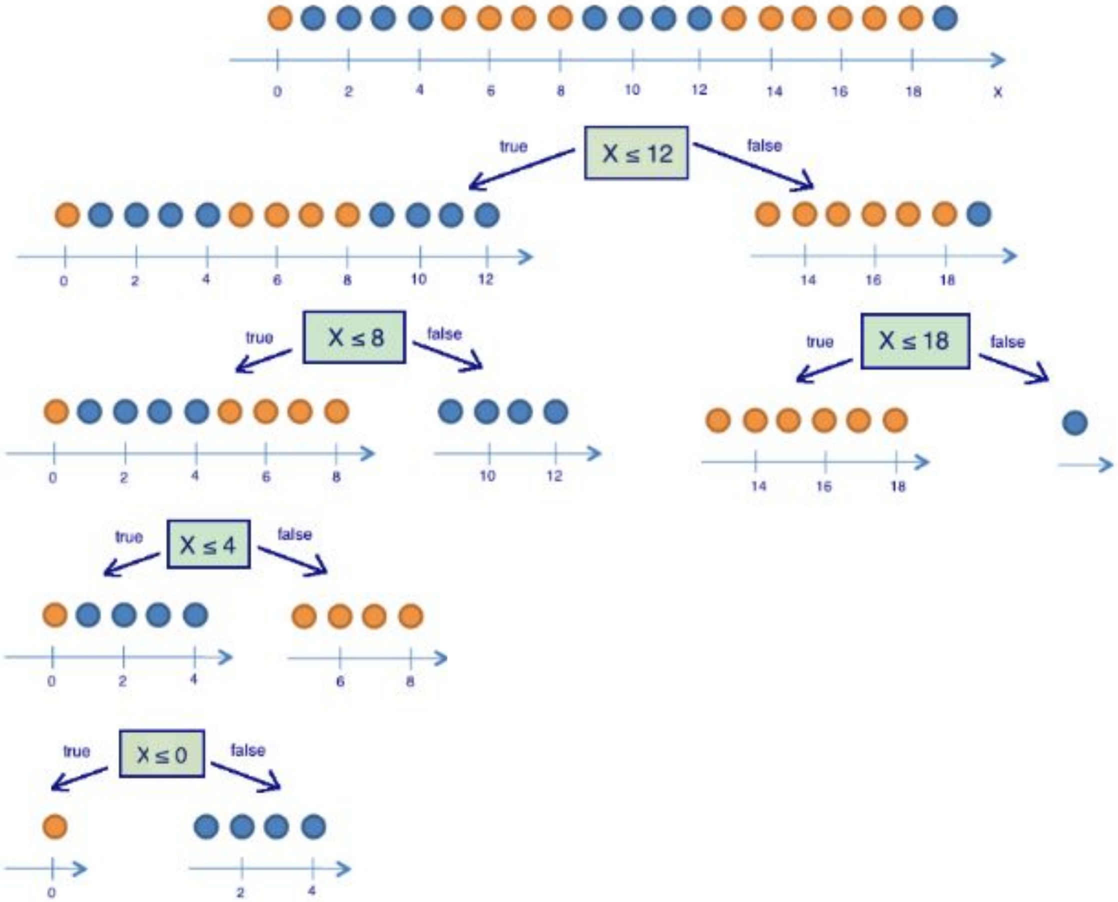

Information criteria: Entropy

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

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:

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

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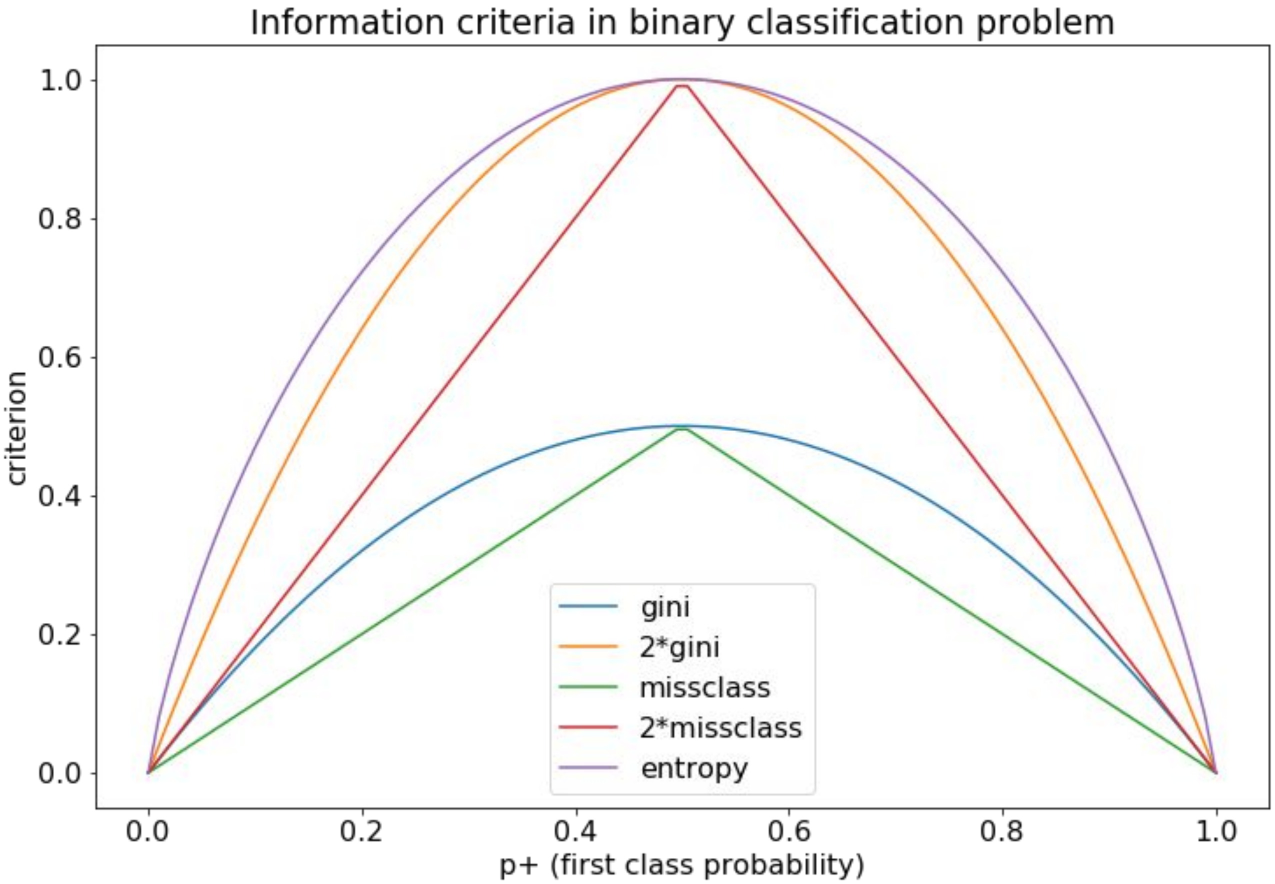
Information criteria



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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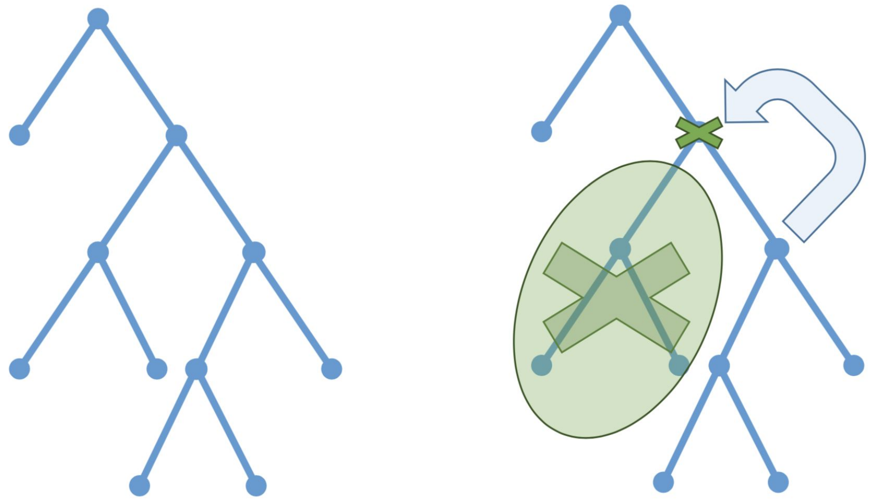
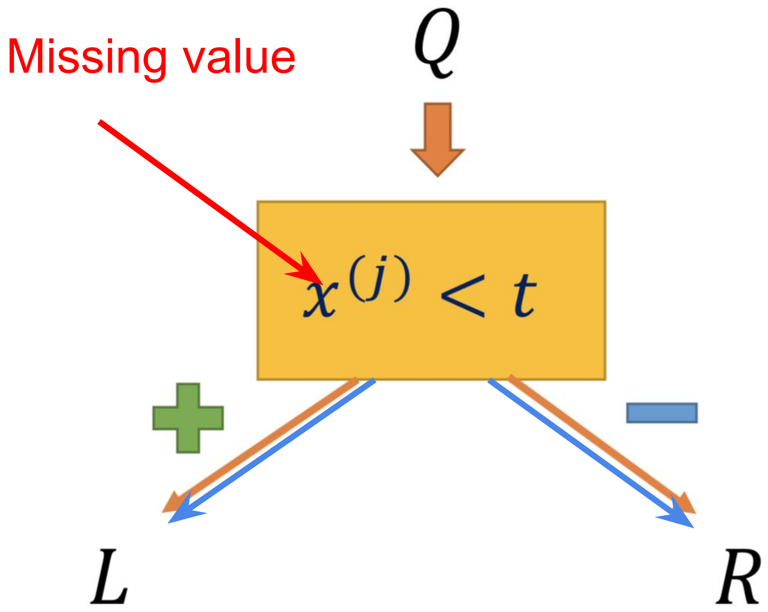


Special highlights

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:

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

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

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

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

Error decreased by N times!

Bagging = Bootstrap aggregating

Decreases the variance if the basic algorithms are not correlated.

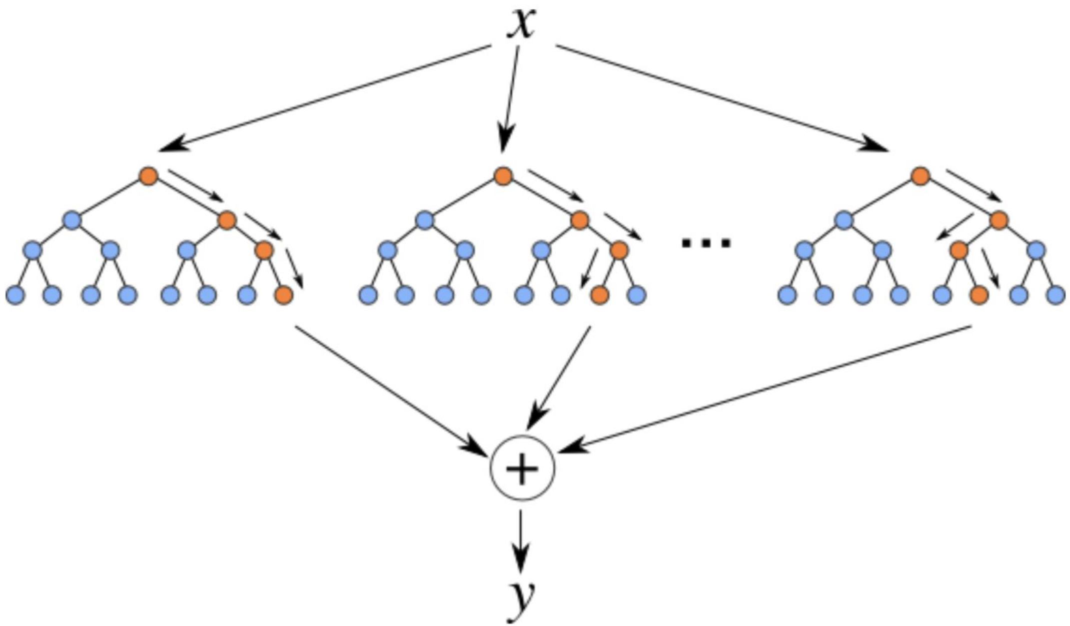
Random Forest

RSM - Random Subspace Method

Same approach, but with features.

Random Forest

Bagging + RSM = Random Forest

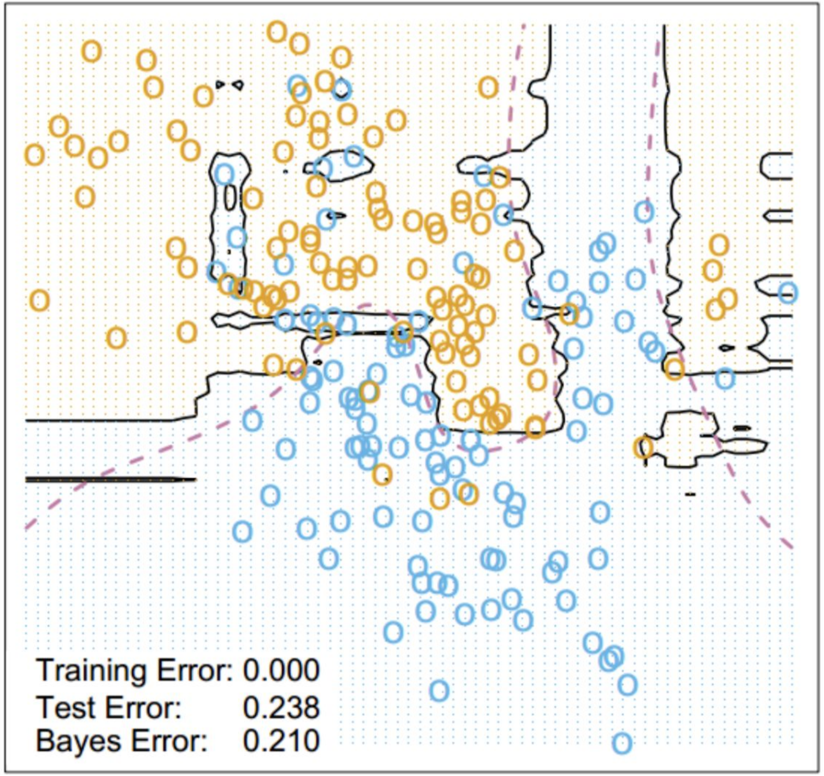


Random Forest

- 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