Decision Trees

Classification and Regression Trees, impurity functions, solution properties

Machine Learning and Data Mining, 2021

Artem Maevskiy

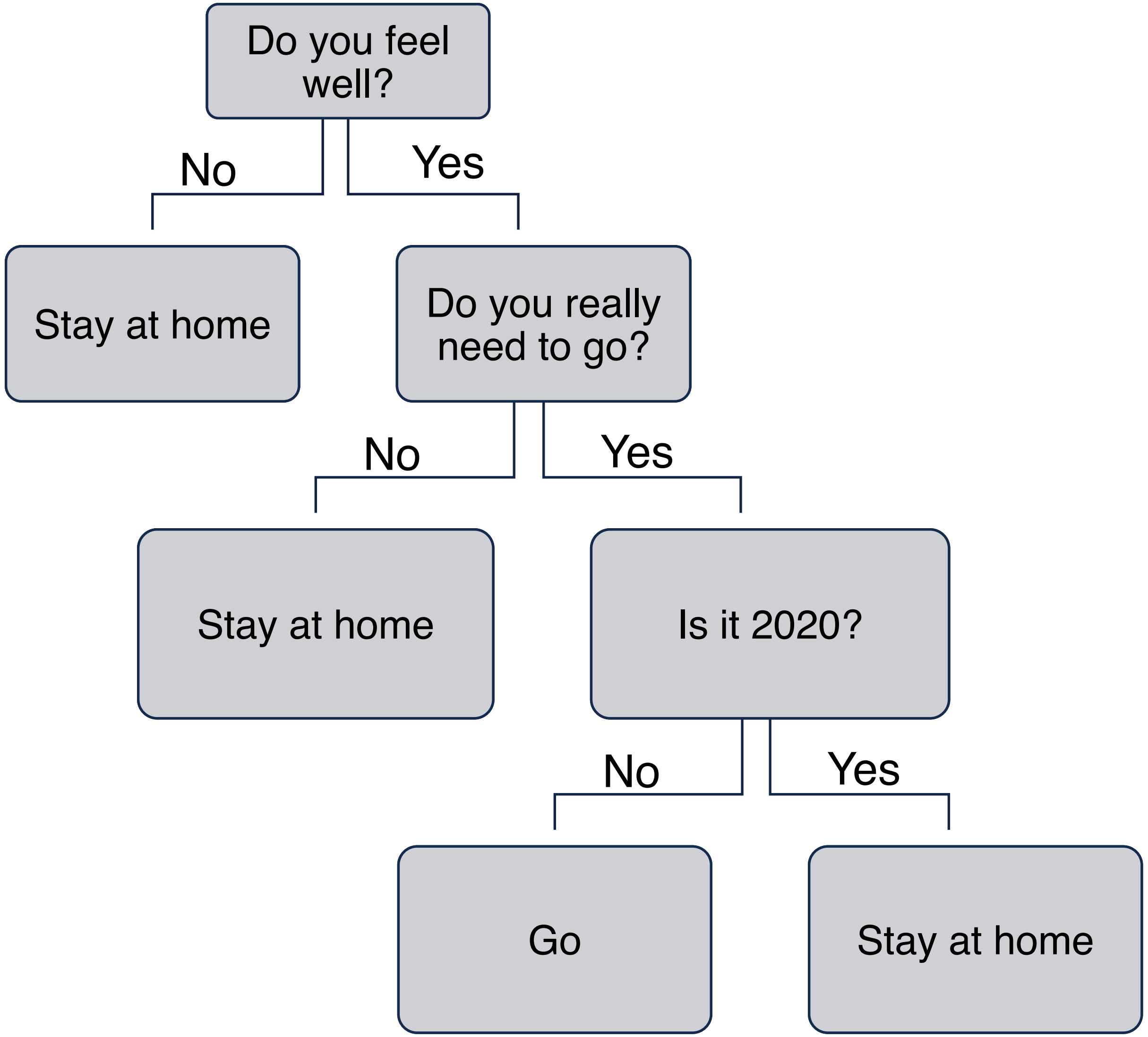
National Research University Higher School of Economics

LAMBDA • HSE

October 13, 2021

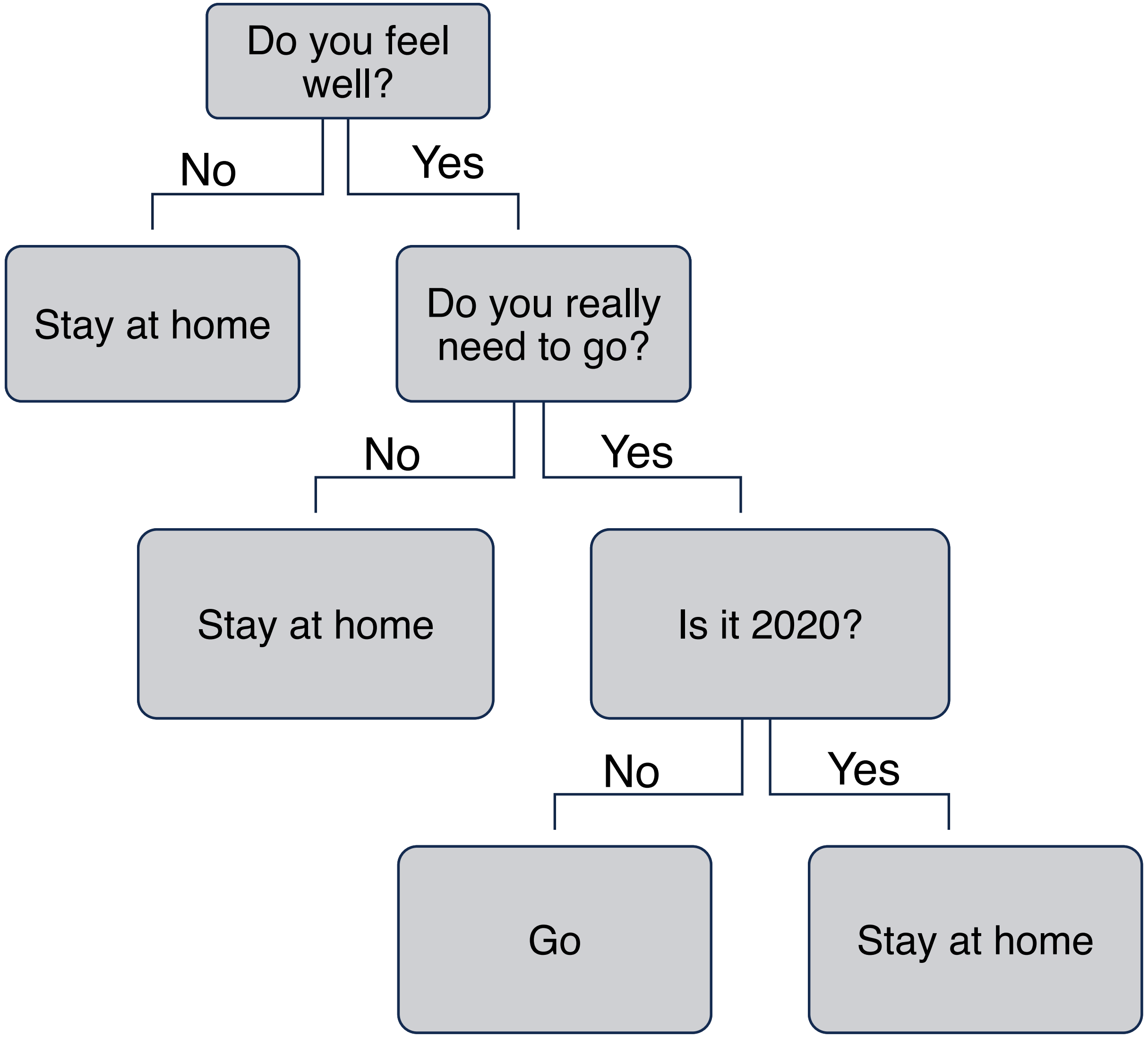
Basics

“Should you go to work?” chart



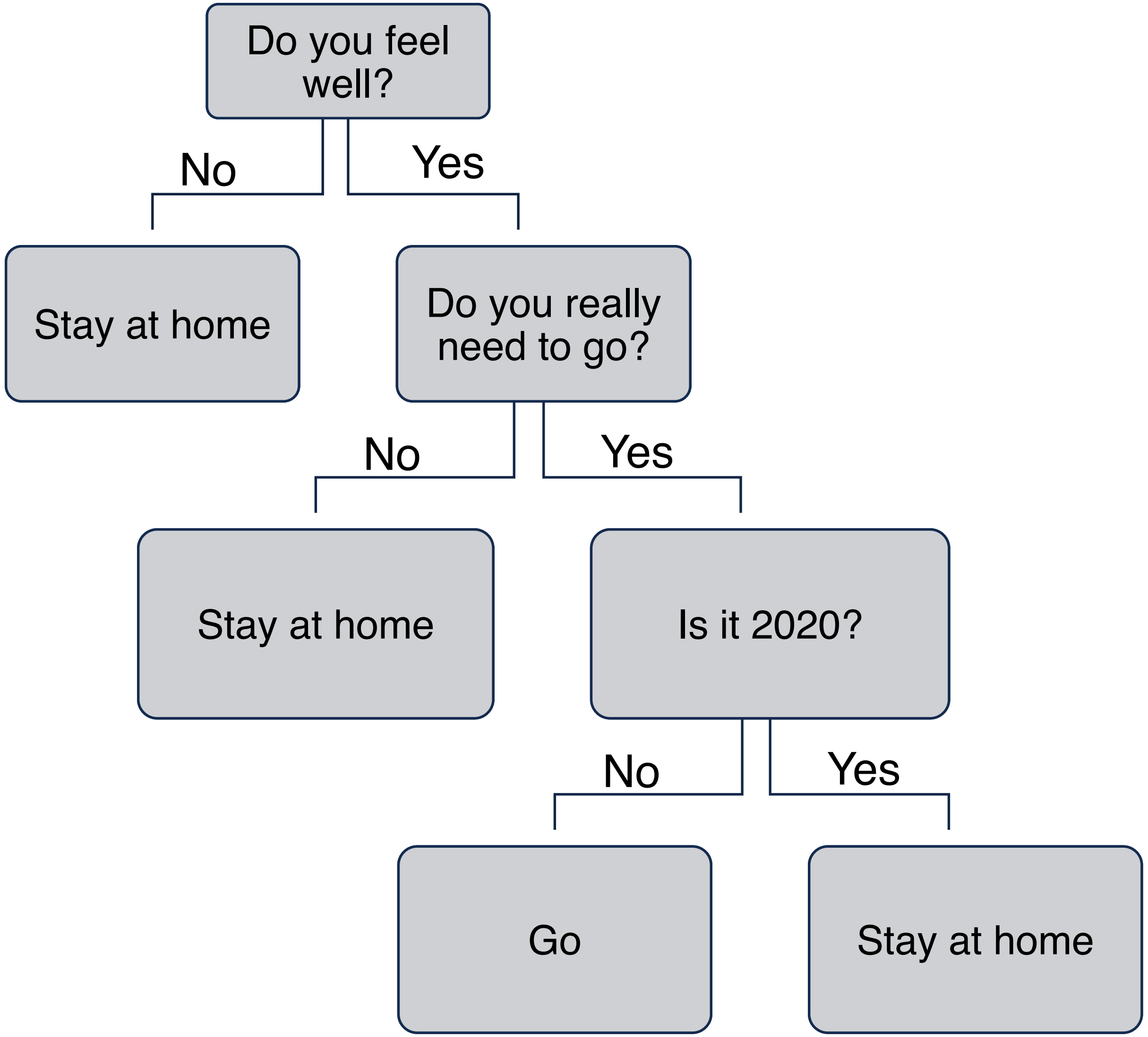
“Should you go to work?” chart

- Directed graph



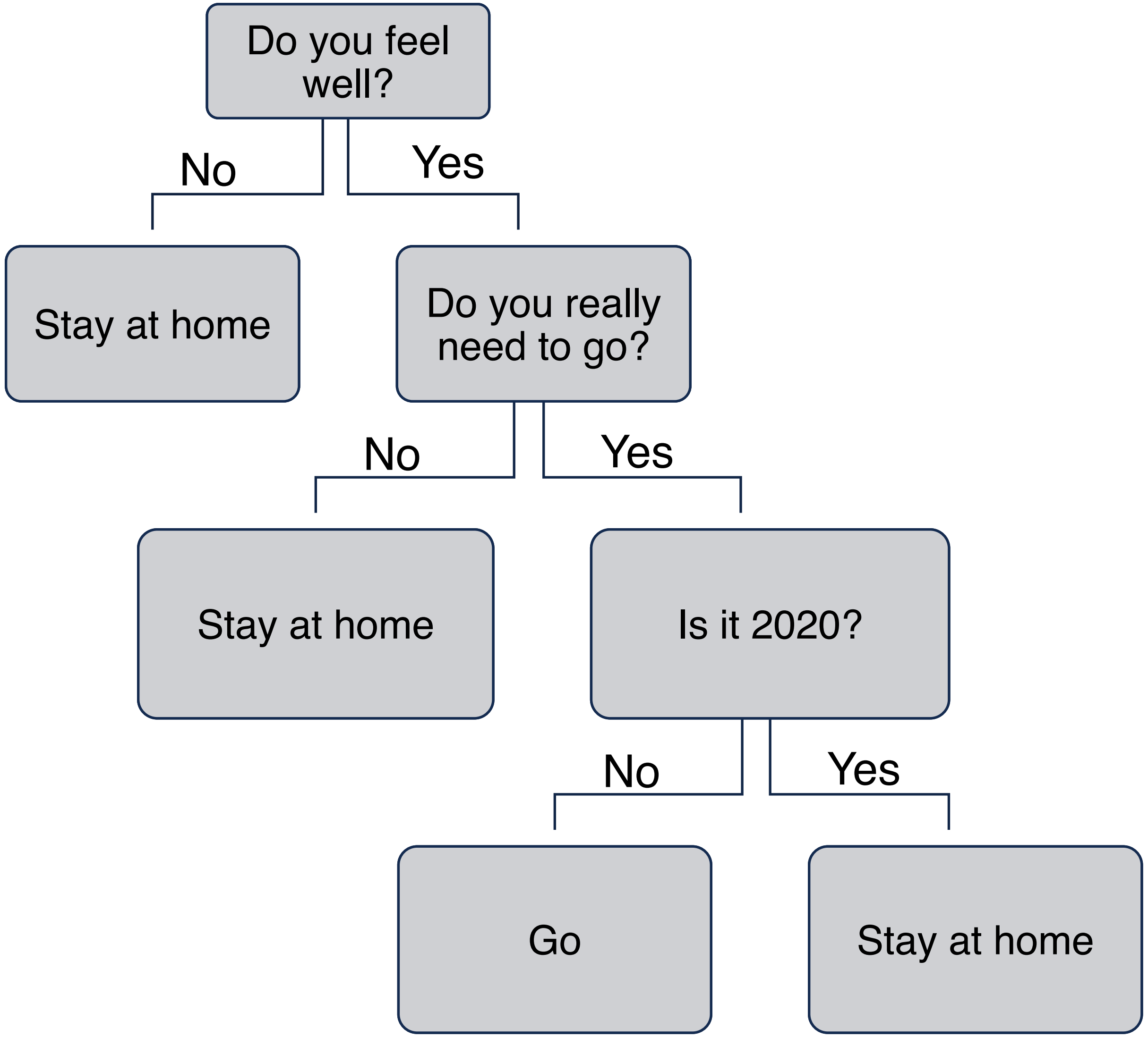
“Should you go to work?” chart

- Directed graph
- No loops



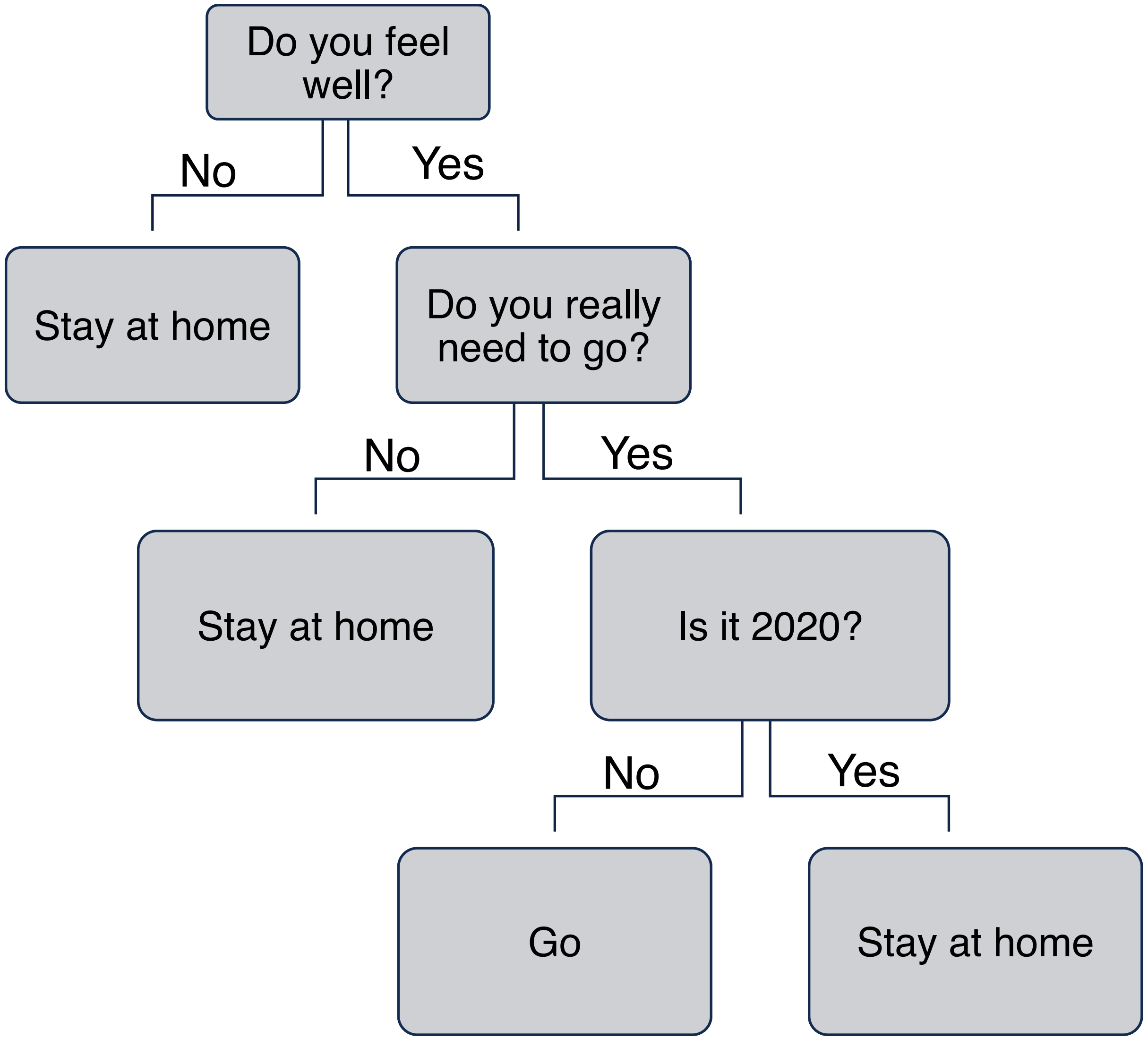
“Should you go to work?” chart

- Directed graph
- No loops
- Single root node



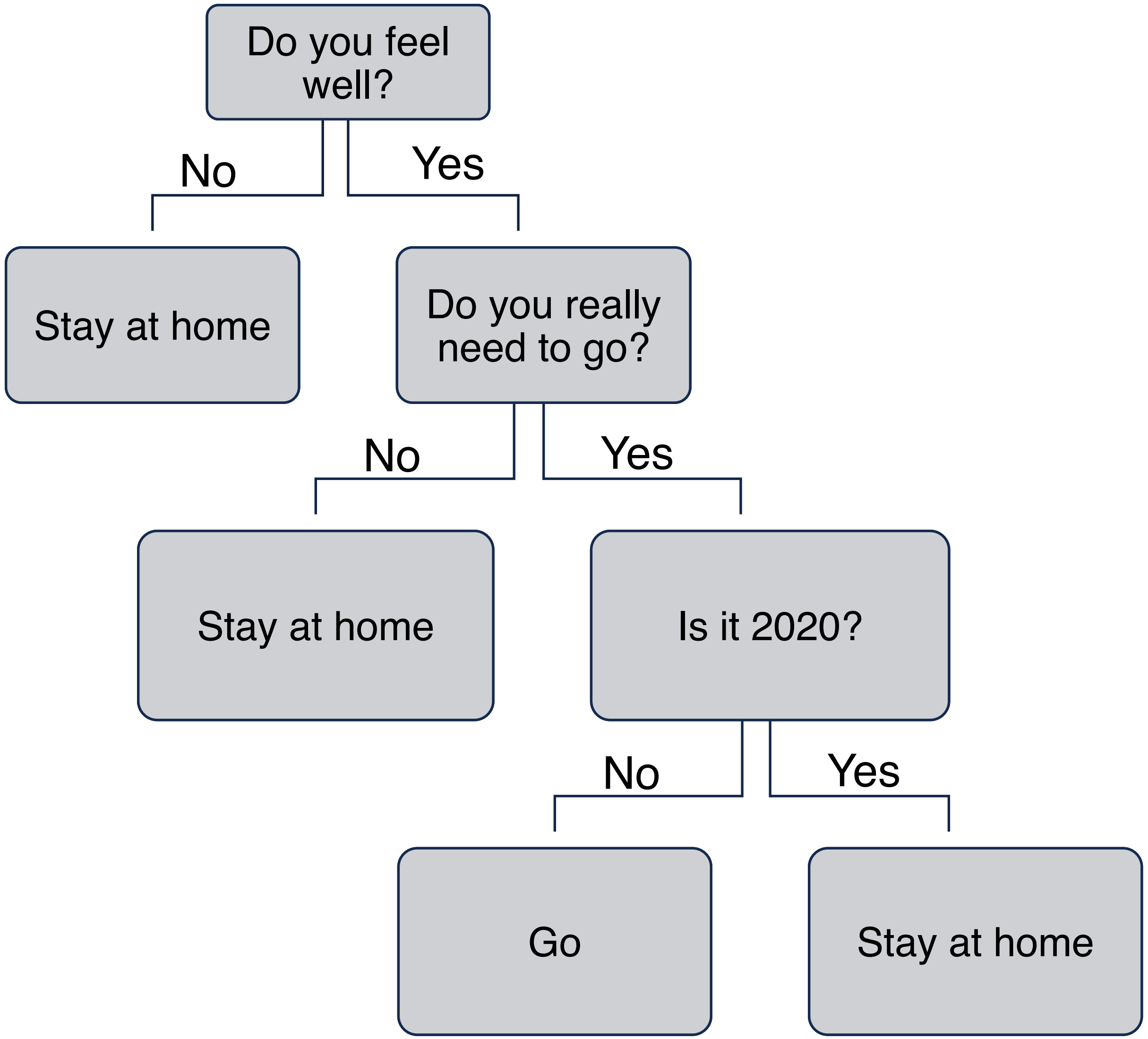
“Should you go to work?” chart

- Directed graph
- No loops
- Single root node
- Each node has:
  - either 0 child nodes (**terminal node**, “leaf”)

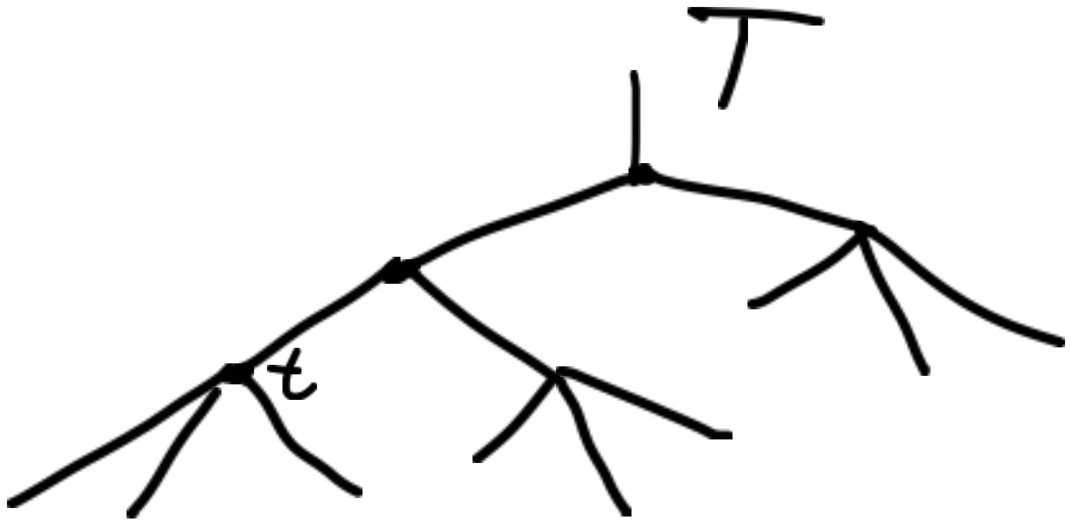


"Should you go to work?" chart

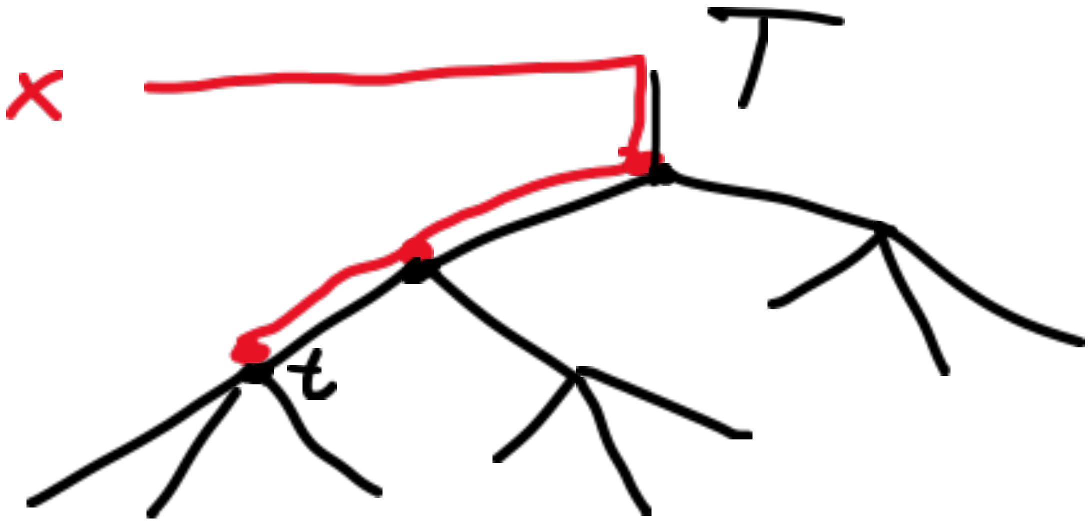
- Directed graph
- No loops
- Single root node
- Each node has:
  - either 0 child nodes (**terminal node**, "leaf")
  - or ≥2 child nodes (**internal node**)
    - 2 nodes for binary trees



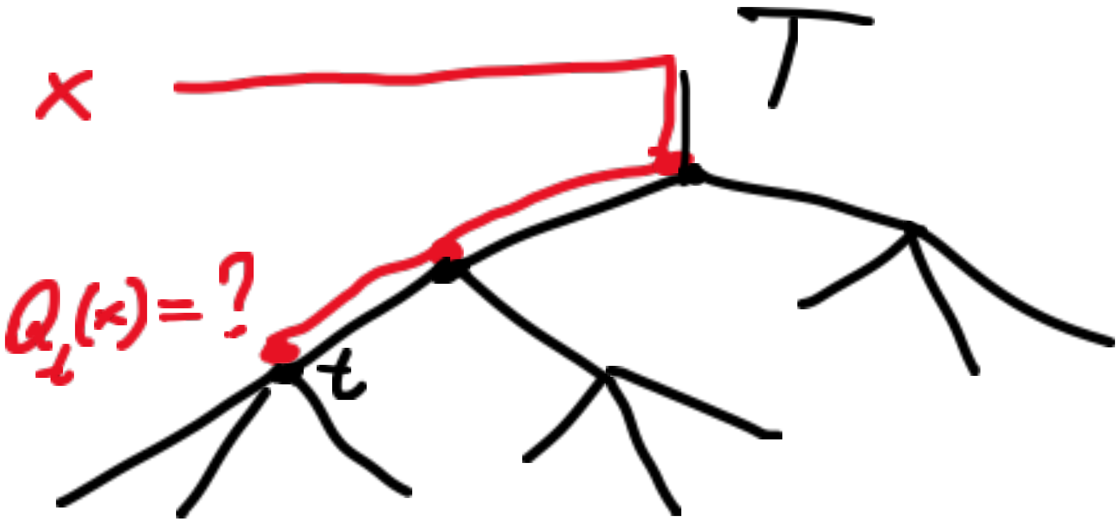
Defining a tree (general approach)



Defining a tree (general approach)

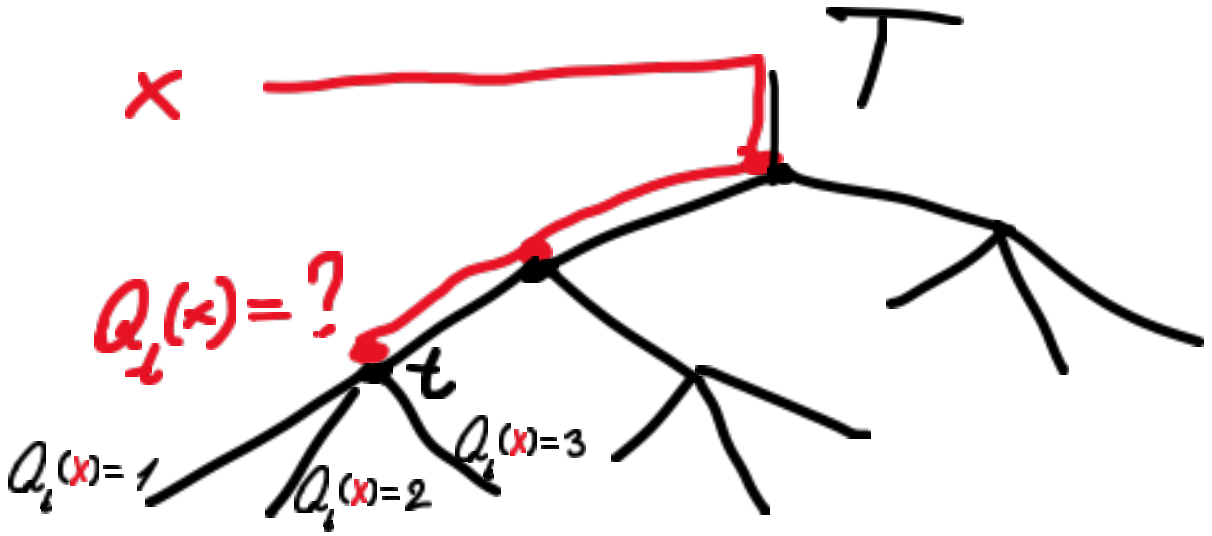


Defining a tree (general approach)



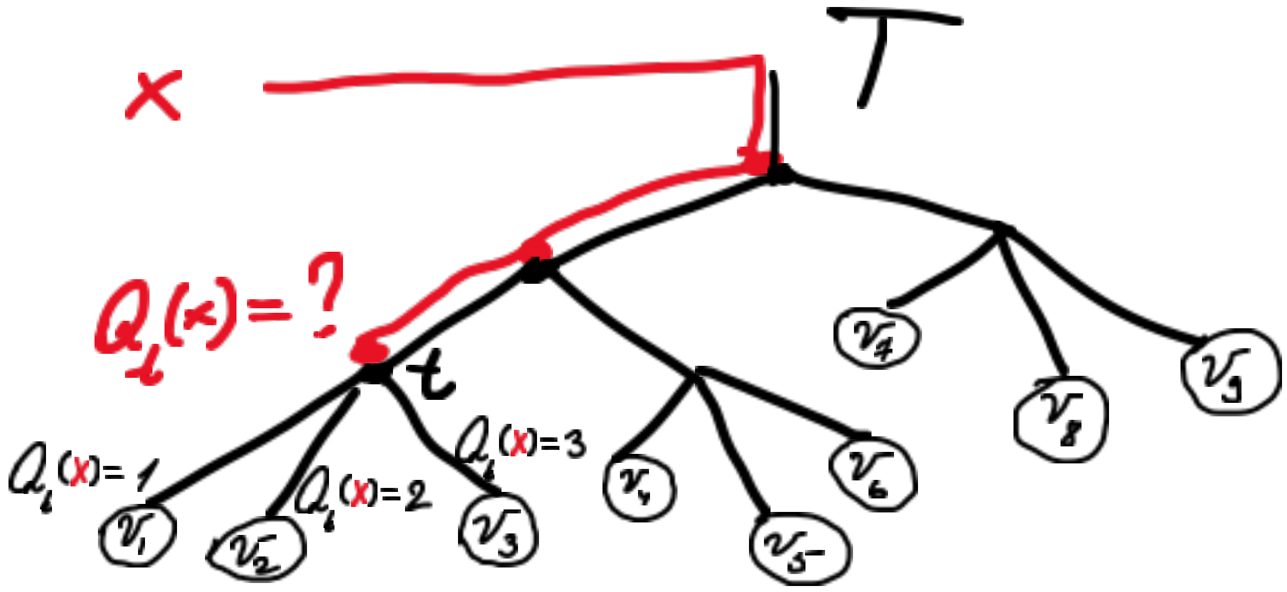
- For each node $t \in T$ define a check function $Q_t(x)$

Defining a tree (general approach)



- For each node $t \in T$ define a check function $Q_t(x)$
- For each child node of t assign a set of unique values of $Q_t(x)$

Defining a tree (general approach)



- For each node $t \in T$ define a check function $Q_t(x)$
- For each child node of t assign a set of unique values of $Q_t(x)$
- Assign each terminal node i a prediction value v_i

Classification and Regression Trees (CART)

CART

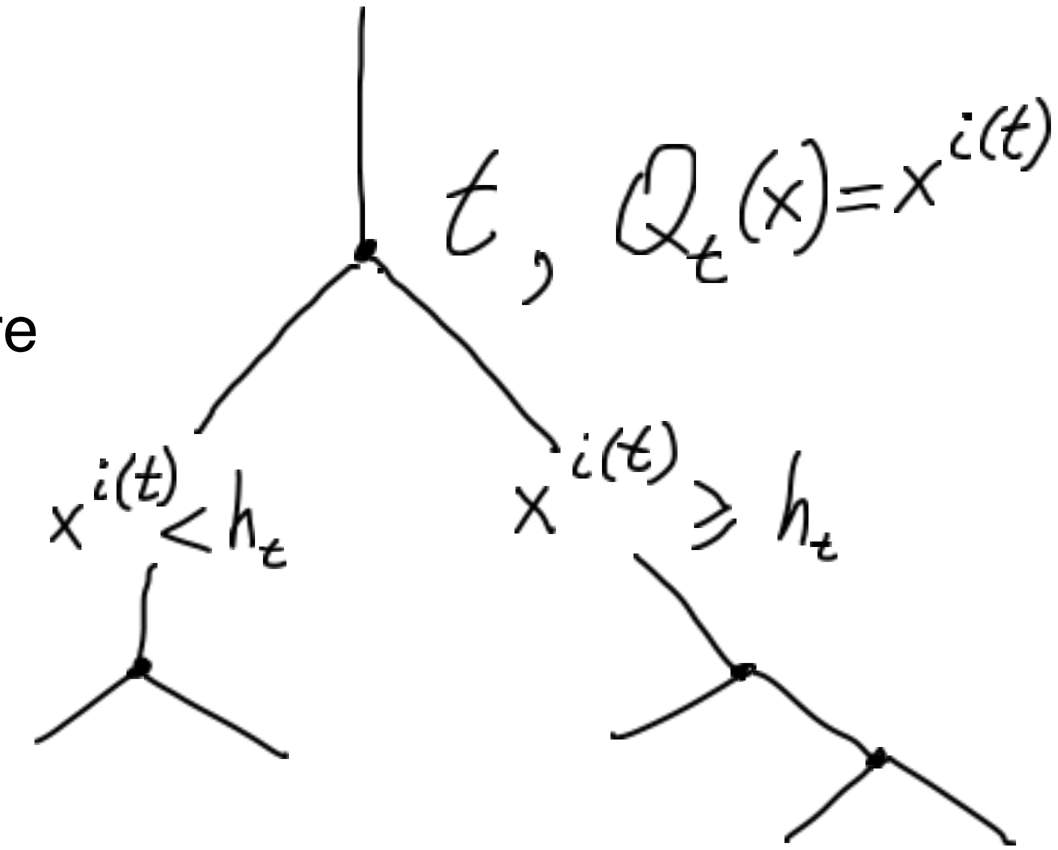
Binary trees

Check function:

$Q_t(x) = x^{i(t)}$ — pick a single (i-th) feature

Child nodes:

Left or right depending on whether $Q_t(x) \geq h_t$



Finding the best tree is not trivial. In practice a **greedy algorithm** is used.

Growing a tree

Given a dataset $D = \left\{ (x_1, y_1), \ldots (x_N, y_N) \right\}$, and **impurity function** $I(D)$

Start from a single root node t_0, all data residing in it: $D_{t_0} = D$

https://pixabay.com/users/openclipart-vectors-30363/

Growing a tree

Given a dataset $D = \left\{ (x_1, y_1), \ldots (x_N, y_N) \right\}$, and **impurity function** $I(D)$

Start from a single root node t_0, all data residing in it: $D_{t_0} = D$

While stop condition not met, repeat for each leaf node t:

https://pixabay.com/users/openclipart-vectors-30363/

Growing a tree

Given a dataset $D = \left\{ \left(x_1, y_1\right), \ldots \left(x_N, y_N\right) \right\}$, and **impurity function** $I(D)$

Start from a single root node t_0, all data residing in it: $D_{t_0} = D$

While stop condition not met, repeat for each leaf node t:

Find feature i and element $\left(x_k, y_k\right) \in D_t$, such that for the two subsets

$$D_{t^{\text{left}}} = \left\{ \left(x, y\right) \mid \left(x, y\right) \in D_t,\ x^i < x_k^i \right\},$$

$$D_{t^{\text{right}}} = \left\{ \left(x, y\right) \mid \left(x, y\right) \in D_t,\ x^i \geq x_k^i \right\}$$

the decrease of impurity:

$$\left|D_t\right| \cdot \Delta I_t = \left|D_t\right| \cdot I\left(D_t\right) - \left(\left|D_{t^{\text{right}}}\right| \cdot I\left(D_{t^{\text{right}}}\right) + \left|D_{t^{\text{left}}}\right| \cdot I\left(D_{t^{\text{left}}}\right)\right) > 0$$

is maximized (over k and i).

https://pixabay.com/users/openclipart-vectors-30363/

Growing a tree

Given a dataset $D = \left\{ \left(x_1, y_1\right), \ldots \left(x_N, y_N\right) \right\}$, and **impurity function** $I(D)$

Start from a single root node t_0, all data residing in it: $D_{t_0} = D$

While stop condition not met, repeat for each leaf node t:

Find feature i and element $\left(x_k, y_k\right) \in D_t$, such that for the two subsets

$D_{t^{\text{left}}} = \left\{ \left(x, y\right) \mid \left(x, y\right) \in D_t,\ x^i < x_k^i \right\}$,

$D_{t^{\text{right}}} = \left\{ \left(x, y\right) \mid \left(x, y\right) \in D_t,\ x^i \geq x_k^i \right\}$

the decrease of impurity:

$$\left| D_t \right| \cdot \Delta I_t = \left| D_t \right| \cdot I\left(D_t\right) - \left(\left| D_{t^{\text{right}}} \right| \cdot I\left(D_{t^{\text{right}}}\right) + \left| D_{t^{\text{left}}} \right| \cdot I\left(D_{t^{\text{left}}}\right) \right) > 0$$

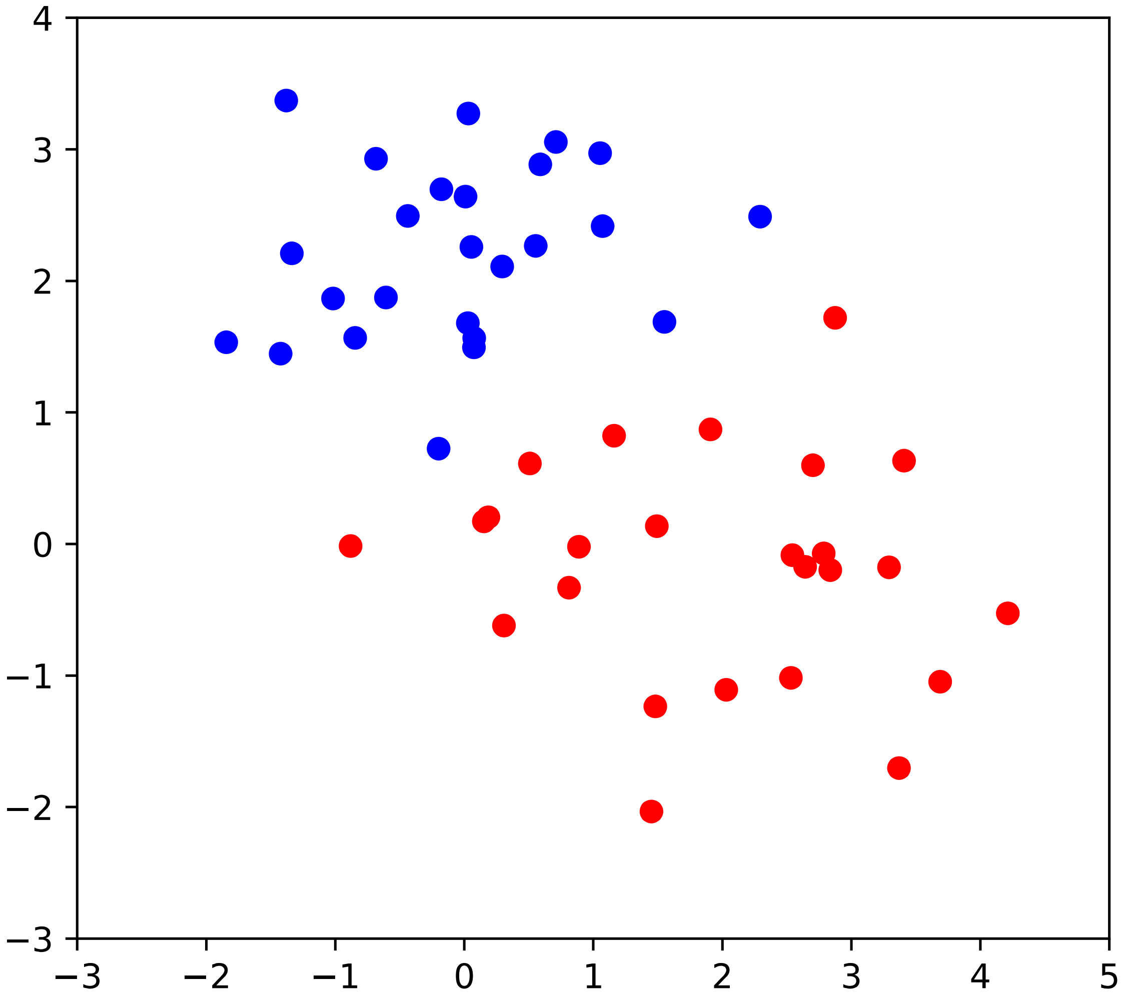
is maximized (over k and i).

Set the check function $Q_t(x) = x^i$, and threshold $h_t = x_k^i$,

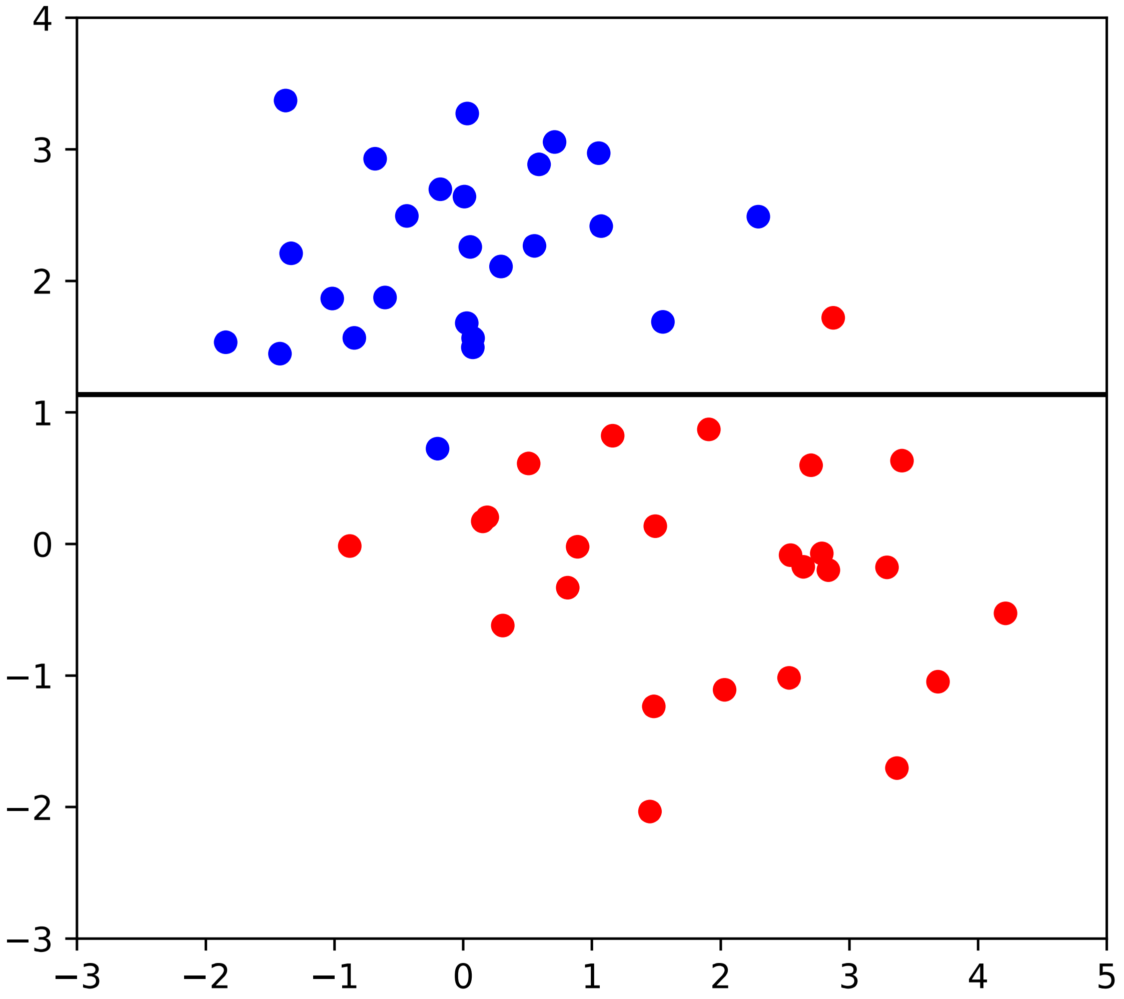
attach the two new corresponding child nodes t^{left} and t^{right} to t.

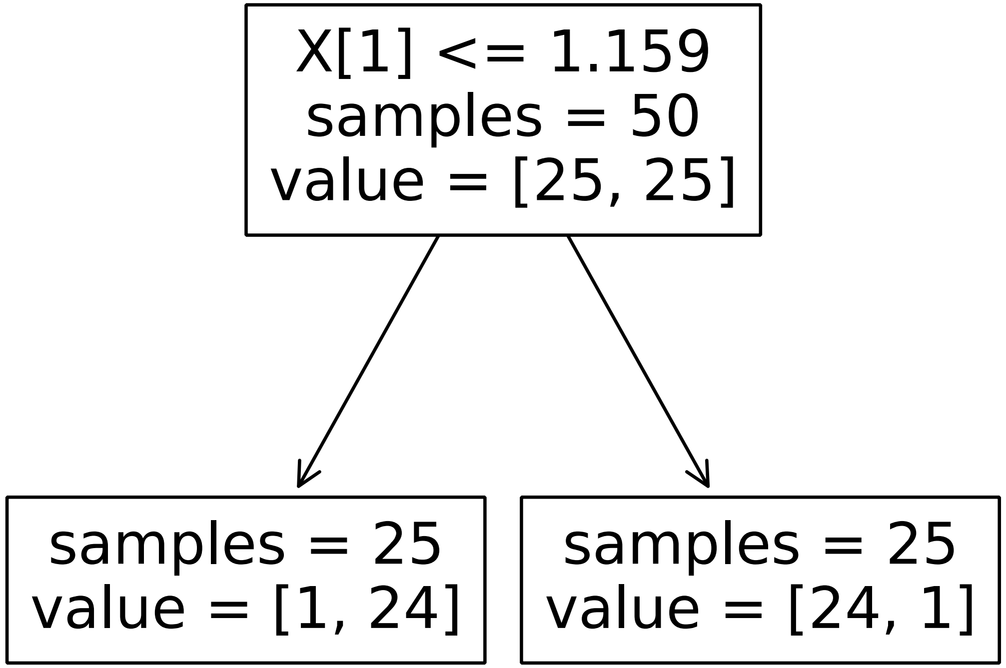
https://pixabay.com/users/openclipart-vectors-30363/

Growing a tree

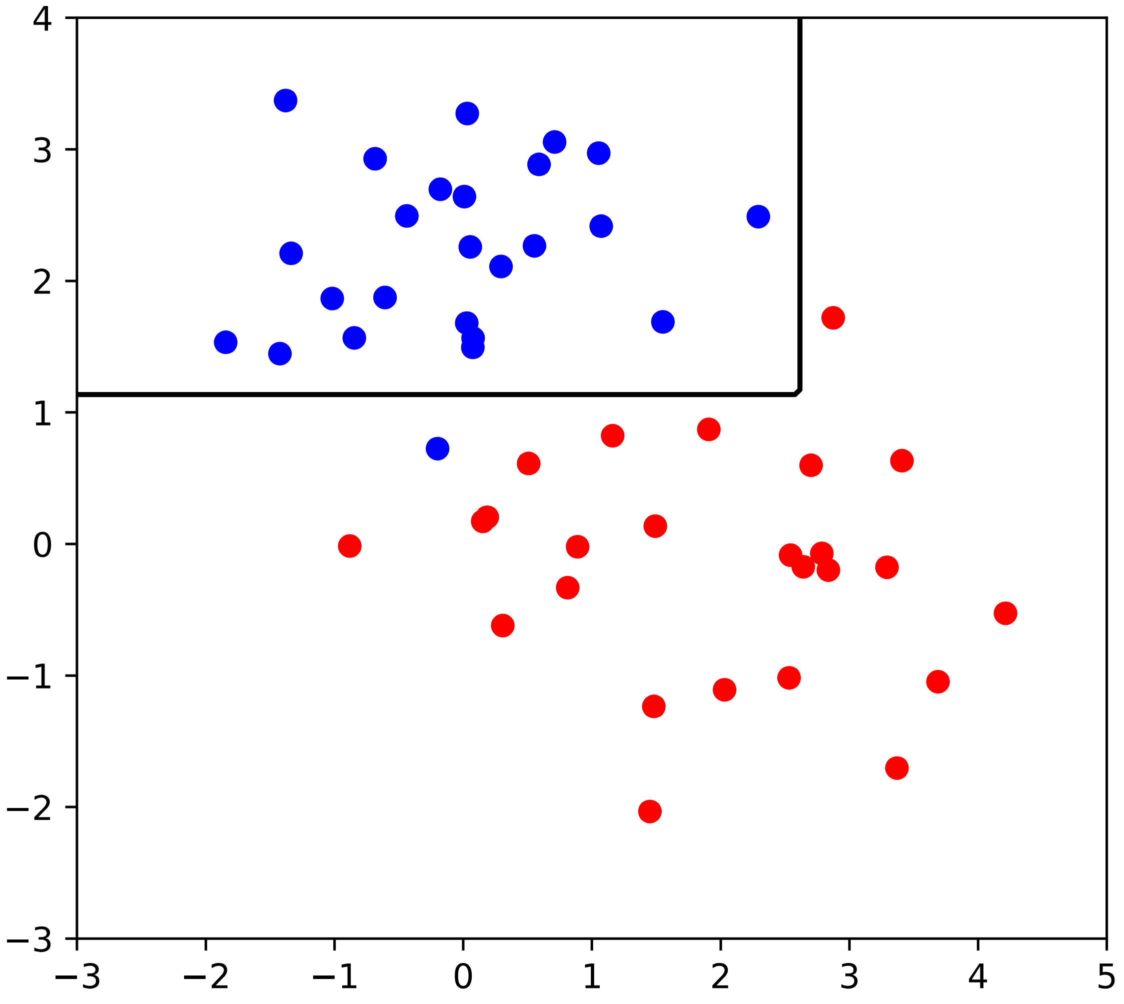


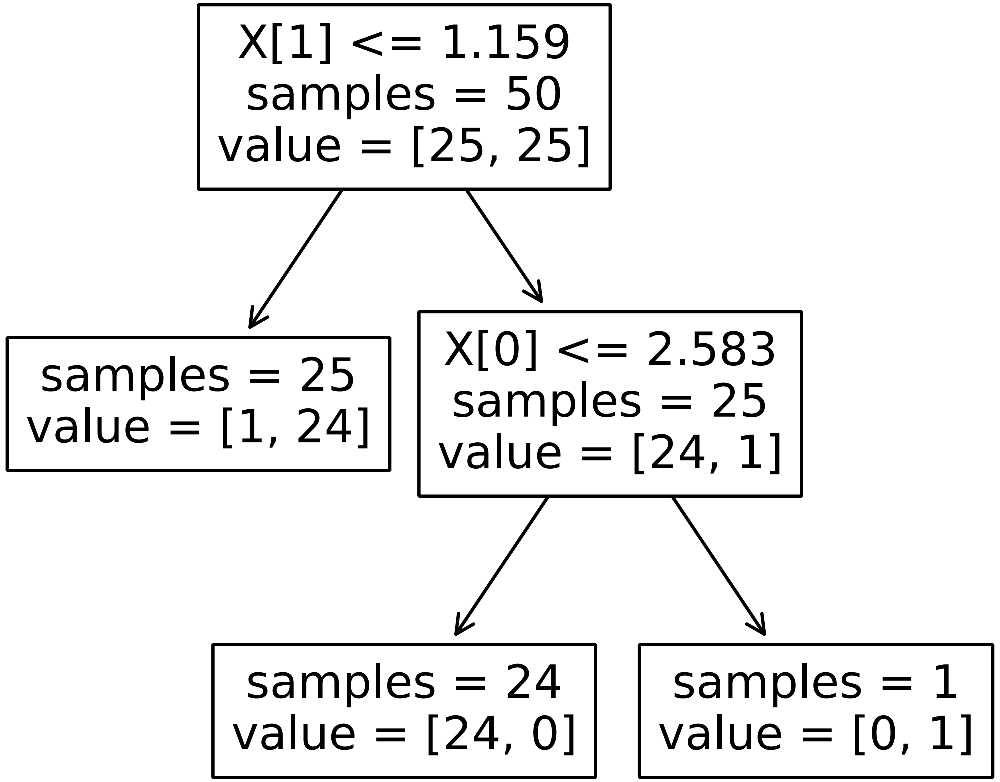
Growing a tree



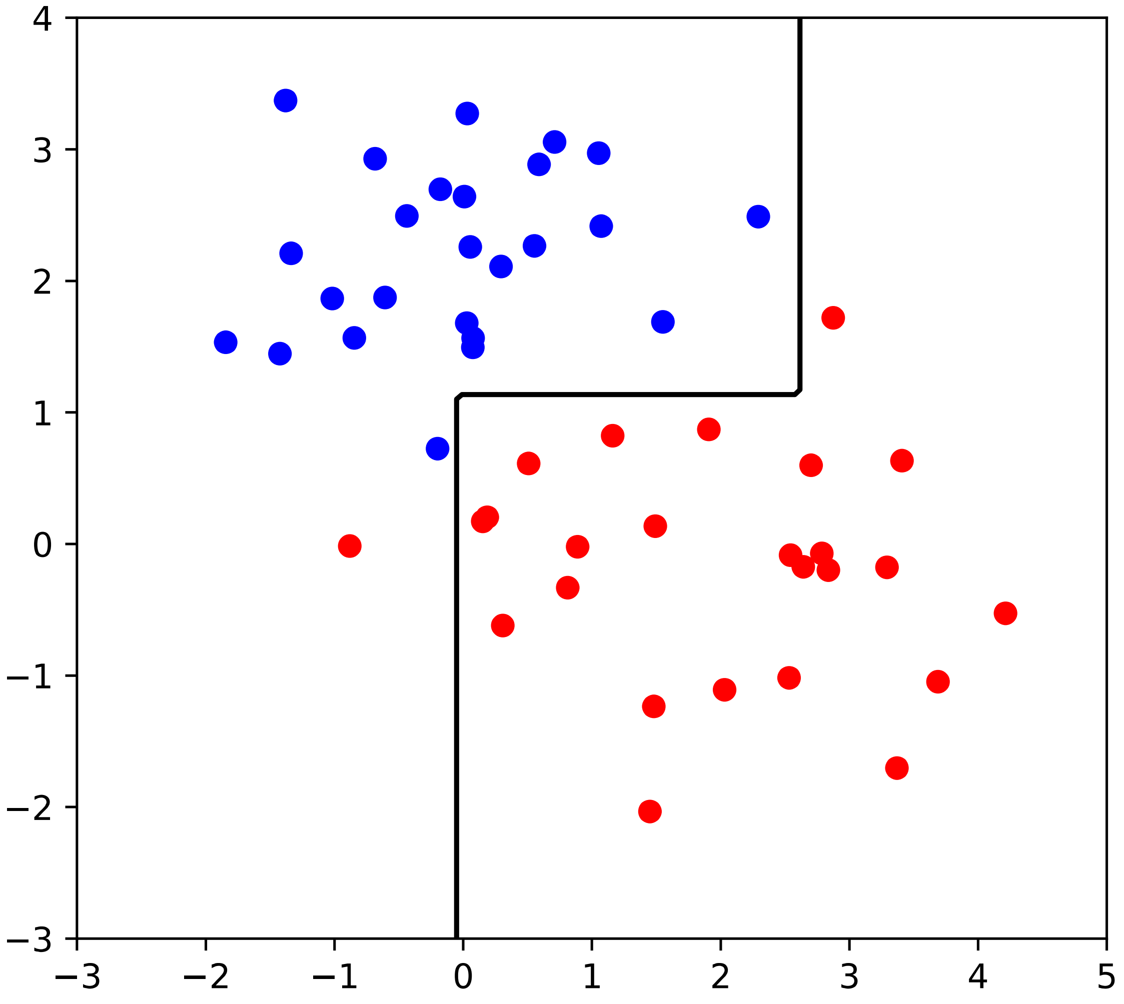


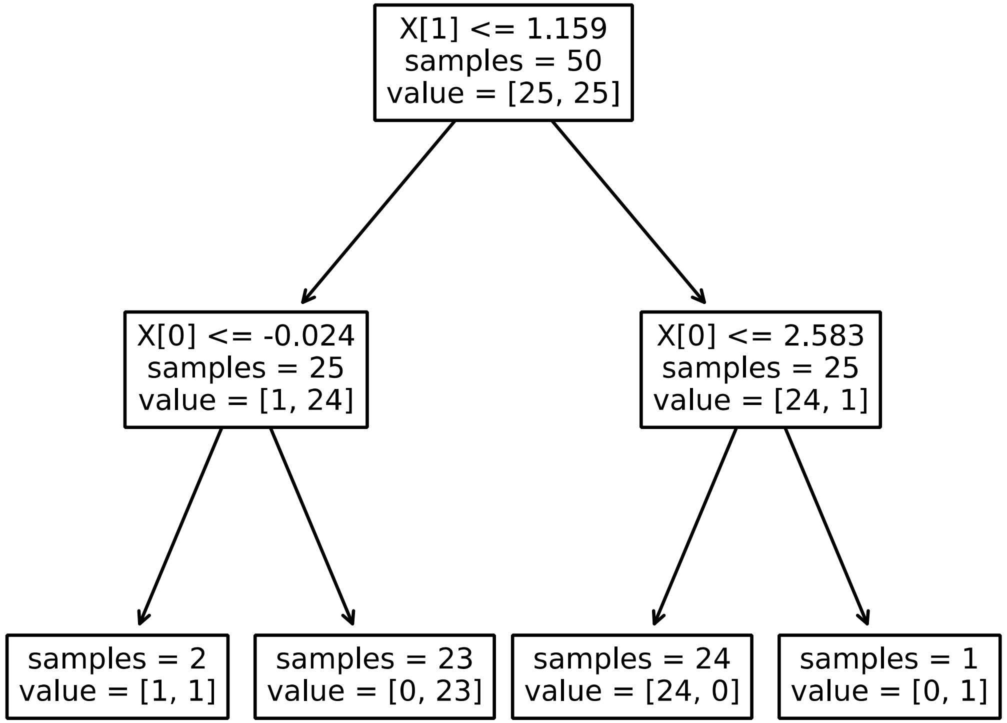
Growing a tree



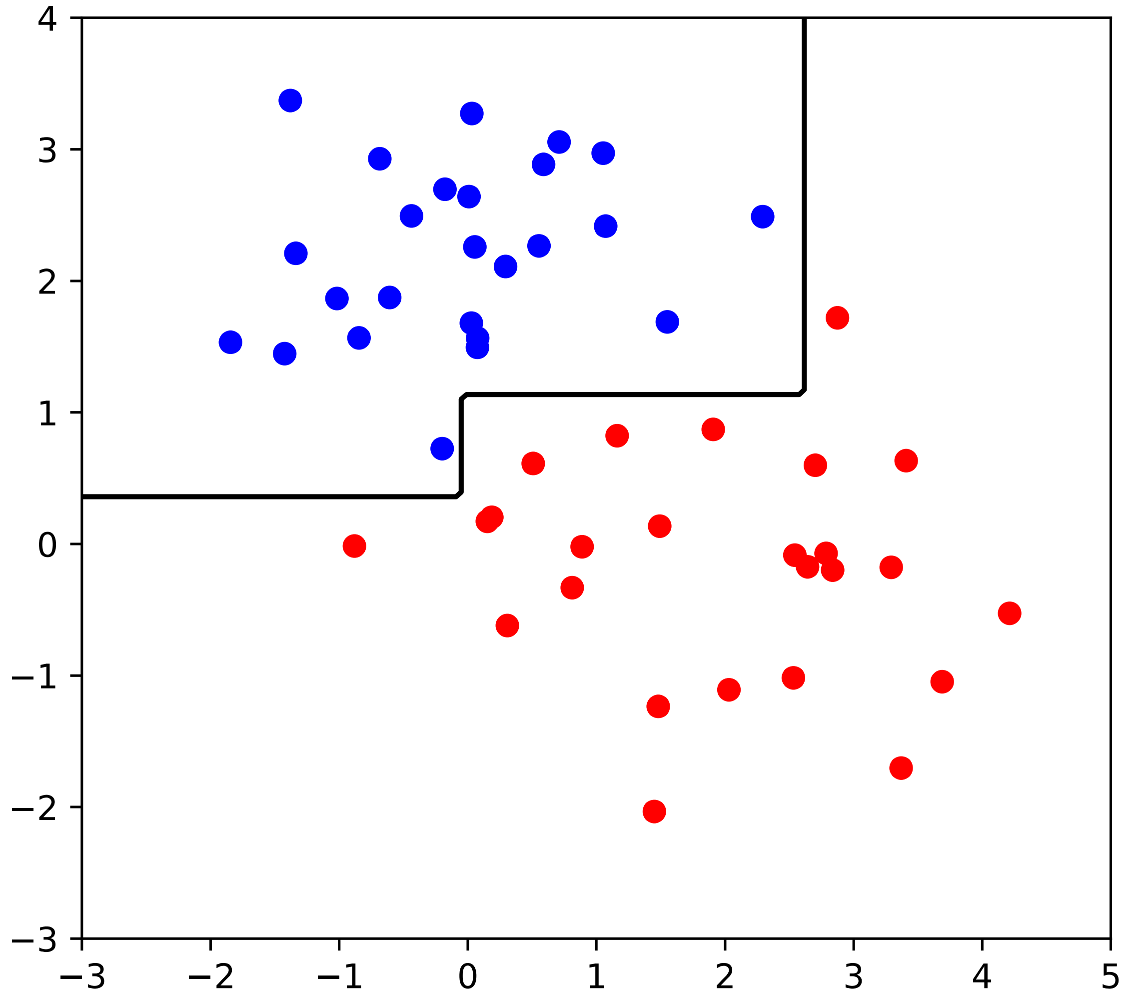


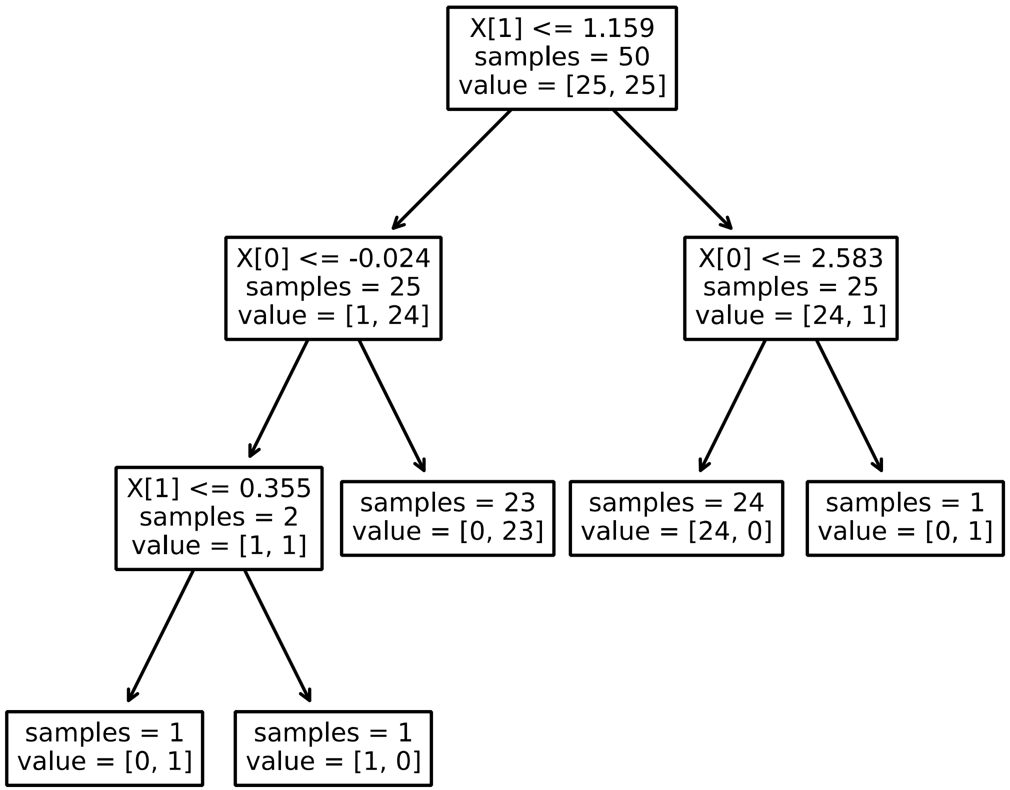
Growing a tree





Growing a tree





Impurity measures

Regression

mean target

MSE: $$I(D_t) = \frac{1}{|D_t|} \sum_{(x,y)\in D_t} \left(y - \mu_{D_t}\right)^2$$

MAE: $$I(D_t) = \frac{1}{|D_t|} \sum_{(x,y)\in D_t} \left|y - m_{D_t}\right|$$

median target

Impurity measures

What about classification?

Define class probabilities:

$$p_j = \frac{1}{|D_t|} \sum_{(x,y) \in D_t} \mathbb{I}[y = j]$$

Then, impurity function $\phi(D_t) = \phi(p_1, \ldots, p_C)$ should satisfy:

Impurity measures

What about classification?

Define class probabilities:

$$p_j = \frac{1}{|D_t|} \sum_{(x,y)\in D_t} \mathbb{I}[y = j]$$

Then, impurity function $\phi(D_t) = \phi(p_1, \ldots, p_C)$ should satisfy:

- ϕ is defined for $p_j \geq 0$ and $\sum_j p_j = 1$
- ϕ is maximized when all $p_j = 1/C$
- ϕ is minimized when a single $p_j = 1$, while others $p_i = 0,\ i \neq j$
- ϕ is symmetric wrt its arguments

Impurity measures

Classification

Probability of an error when predicting randomly with prior class probabilities p_i

Gini criterion:

$$I(D_t) = \sum_{i=1}^{C} p_i(1 - p_i) = 1 - \sum_{i=1}^{C} p_i^2$$

Entropy:

$$I(D_t) = -\sum_{i=1}^{C} p_i \log p_i$$

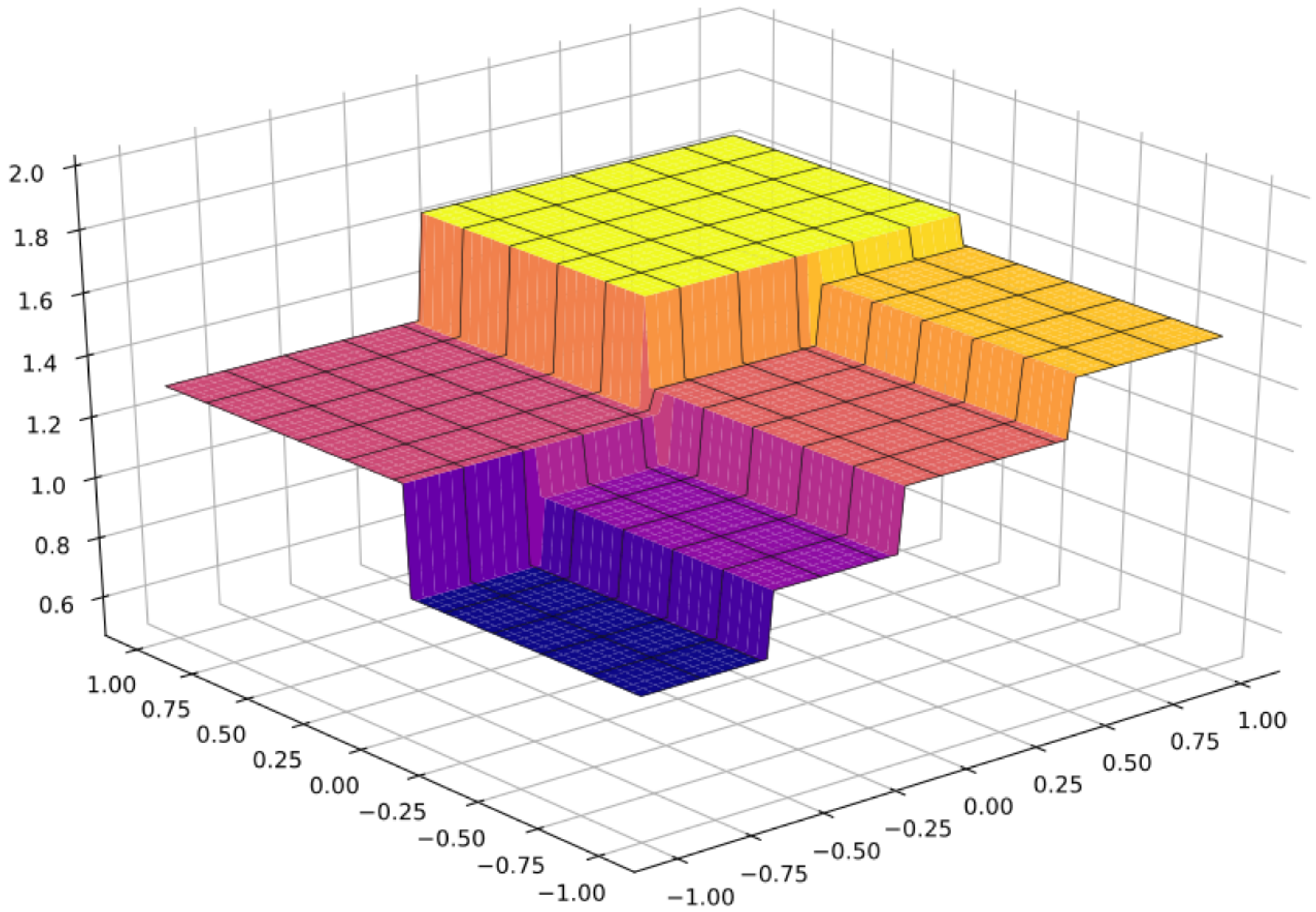
Shortest possible expected message length for the alphabet distributed under p_i

Stopping criteria

- Maximum tree depth
- Maximum number of leaves
- Minimum number of samples in node to make a split
- Minimum number of samples in a leaf
- Minimum impurity gain
- You name it…

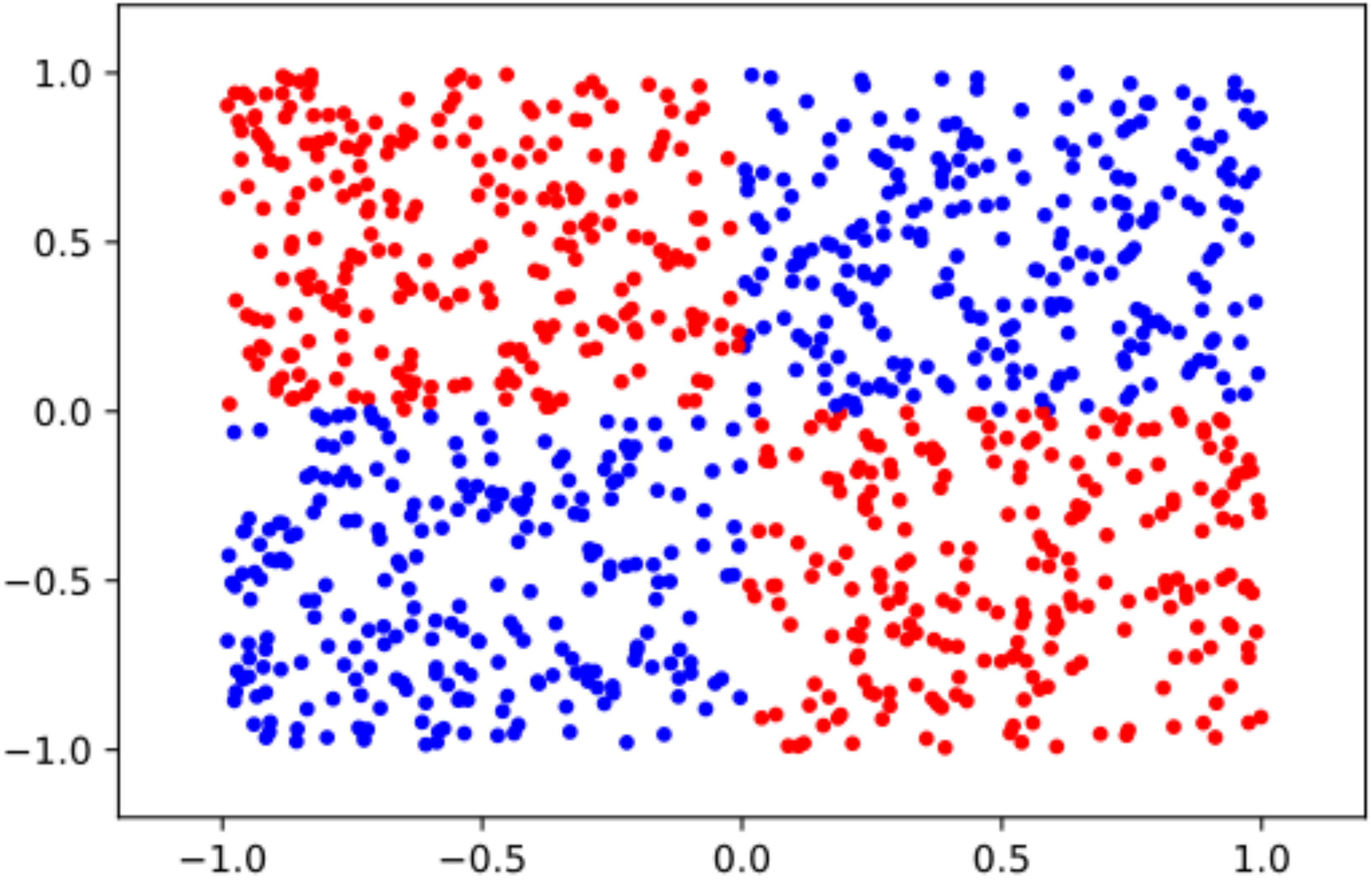
Solution properties

Prediction function



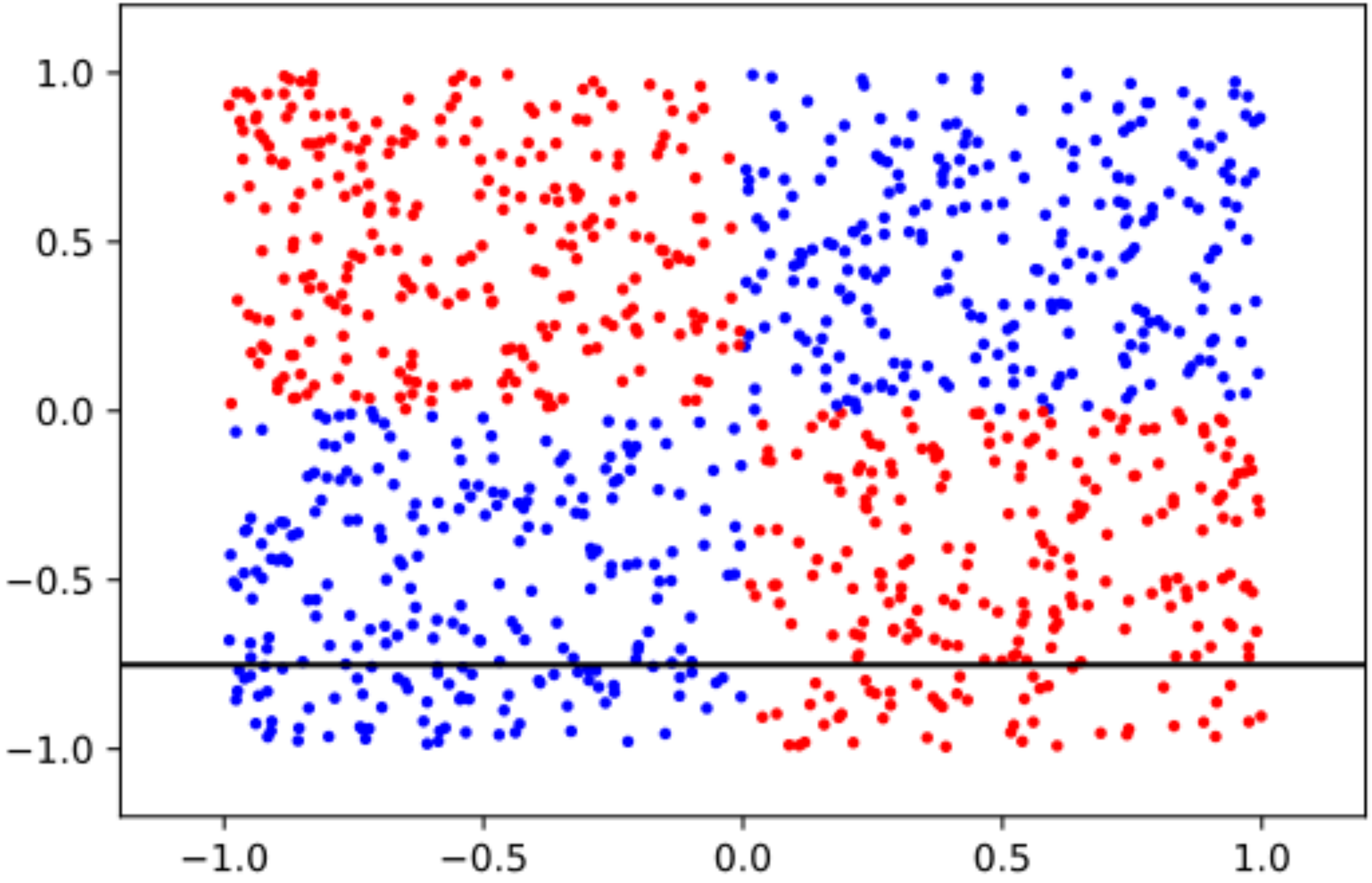
- Decision boundaries always **orthogonal to feature axes**
- Resulting function is a **piecewise constant**

XOR example



The greedy algorithm does not necessarily lead to the optimal solution!

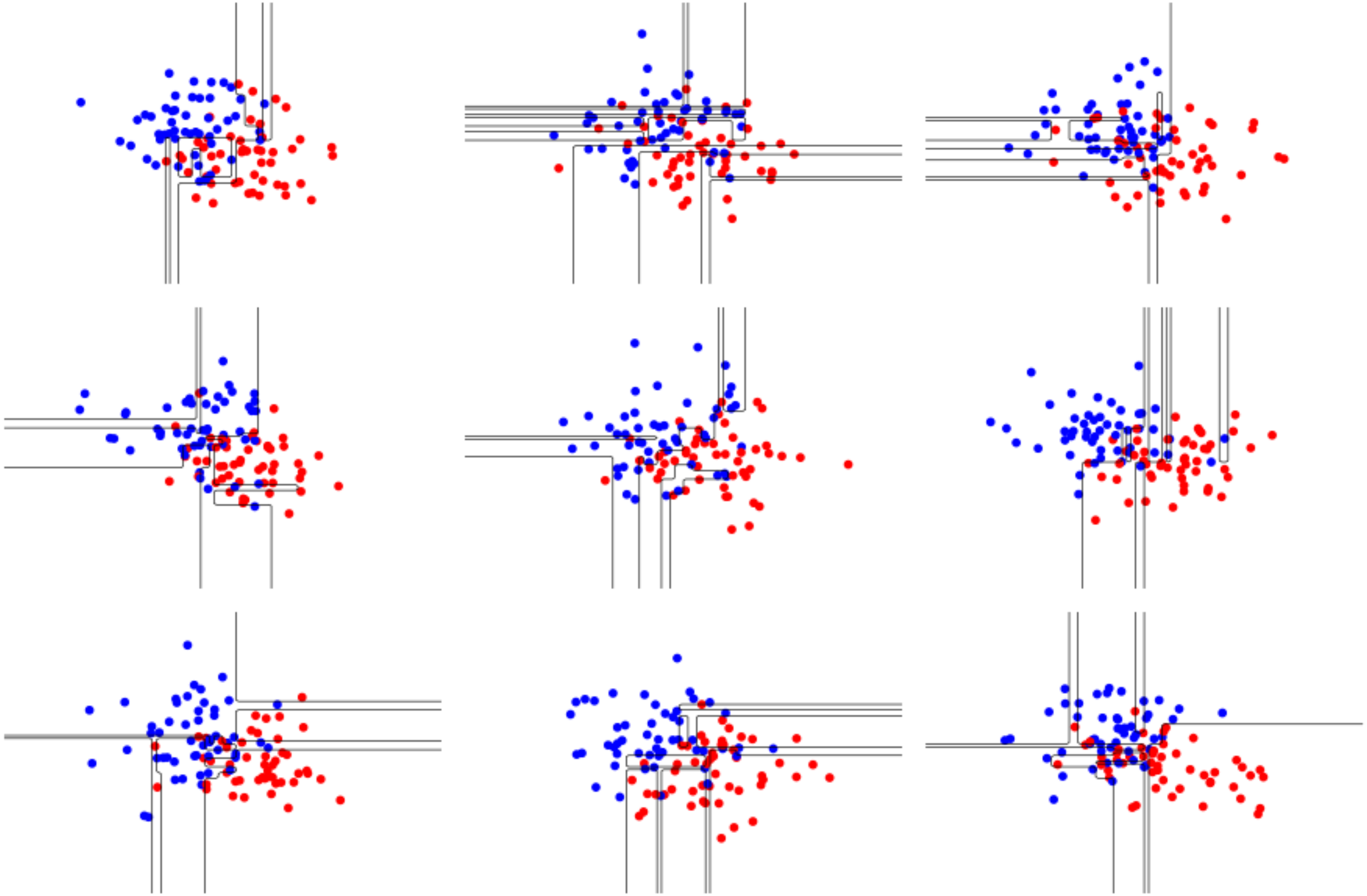
XOR example



The greedy algorithm does not necessarily lead to the optimal solution!

High Variance

- Without a stopping criterion the tree will grow until every object is classified correctly
- Can be regularized by a stopping criterion or with **pruning**



Cost-Complexity Pruning

Original algorithm optimizes the sample-weighted impurity in the terminal nodes of the tree T:

$$R(T) = \sum_{t \in \mathrm{leaves}(T)} \left| D_t \right| \cdot I\left(D_t\right)$$

Can modify this objective by adding a regularizer proportional to the **number of terminal nodes** $\left|T\right|$:

$$R_\alpha(T) = R(T) + \alpha \left| T \right|$$

Idea: build a full tree under $R(T)$, then remove some of the nodes to optimize $R_\alpha(T)$.

Cost-Complexity Pruning

Let T_t be the subtree tree whose root node is t $\in T$

T_t will be pruned out if:

$$R(T_t) + \alpha \left| T_t \right| > R(t) + \alpha$$

or in other words if:

$$\alpha > \alpha_{\text{eff}}(t) = \frac{R(t) - R(T_t)}{\left| T_t \right| - 1}$$

Categorical features

- Ordinal → label encoding (preserving the order!)
- Nominal → order the categories with:
  - positive class probability (binary classification)
  - target mean/median (regression)
  - (make sure the categories are **well populated** to avoid overfitting!)

Thank you!

amaevskij@hse.ru

SiLiKhon

Artem Maevskiy