Teoria degli Algoritmi

Corso di Laurea Magistrale in Matematica Applicata

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Recap from Last Lectures

- We presented 2 linear models: linear regression and logistic regression
- Those hypotheses work well whenever there exists a linear relationship between the features (input) and the response (output)
- Model's parameter estimation done either analytically (OLS) or iteratively (Gradient Descent)

Tree-based Methods

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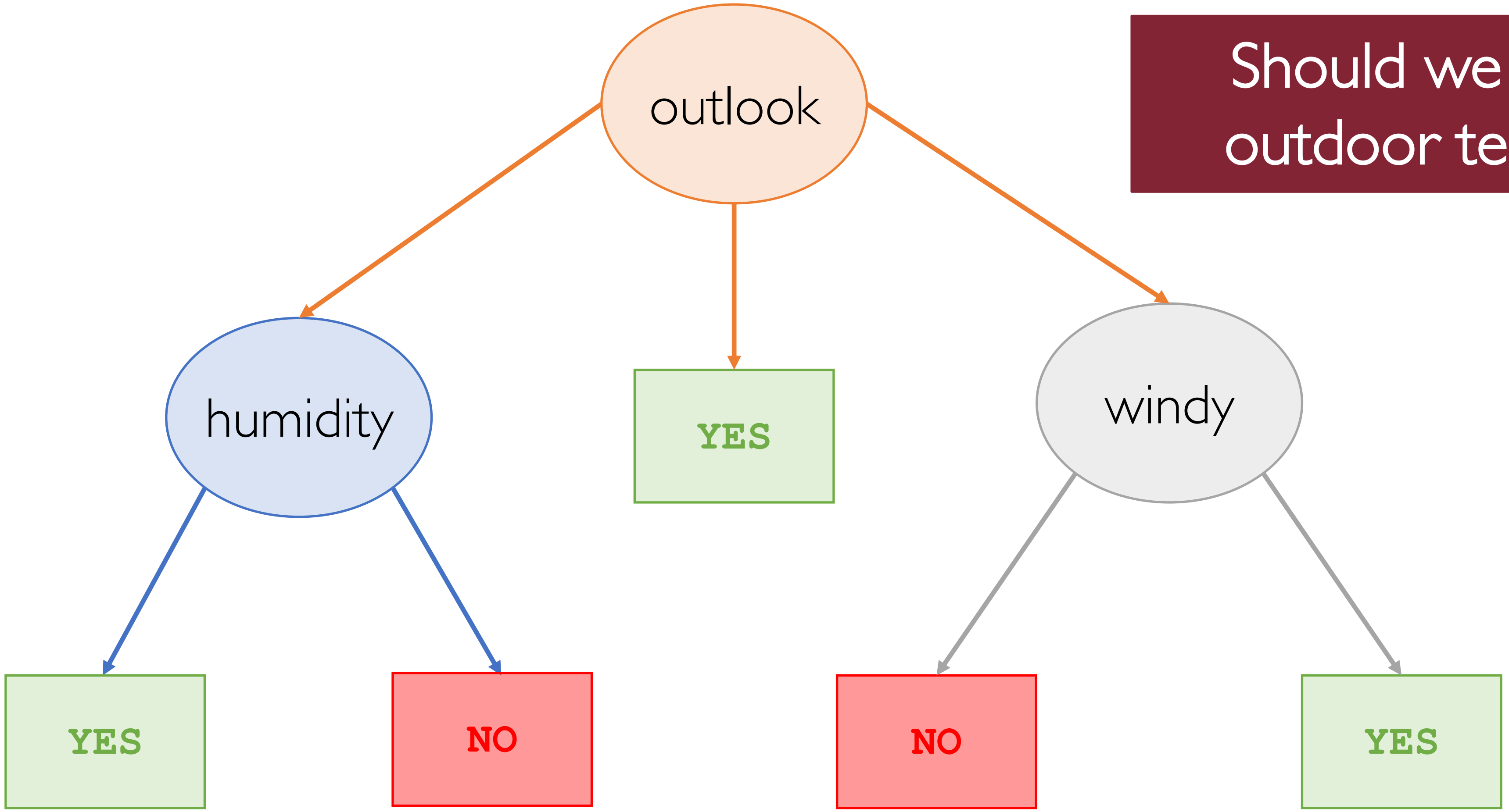
- A prediction is computed by taking the mean (regression) or the mode (classification) of the points in the region which the observation belongs
- The set of splitting rules can be represented as a tree (decision tree)
- Highly human-interpretable models

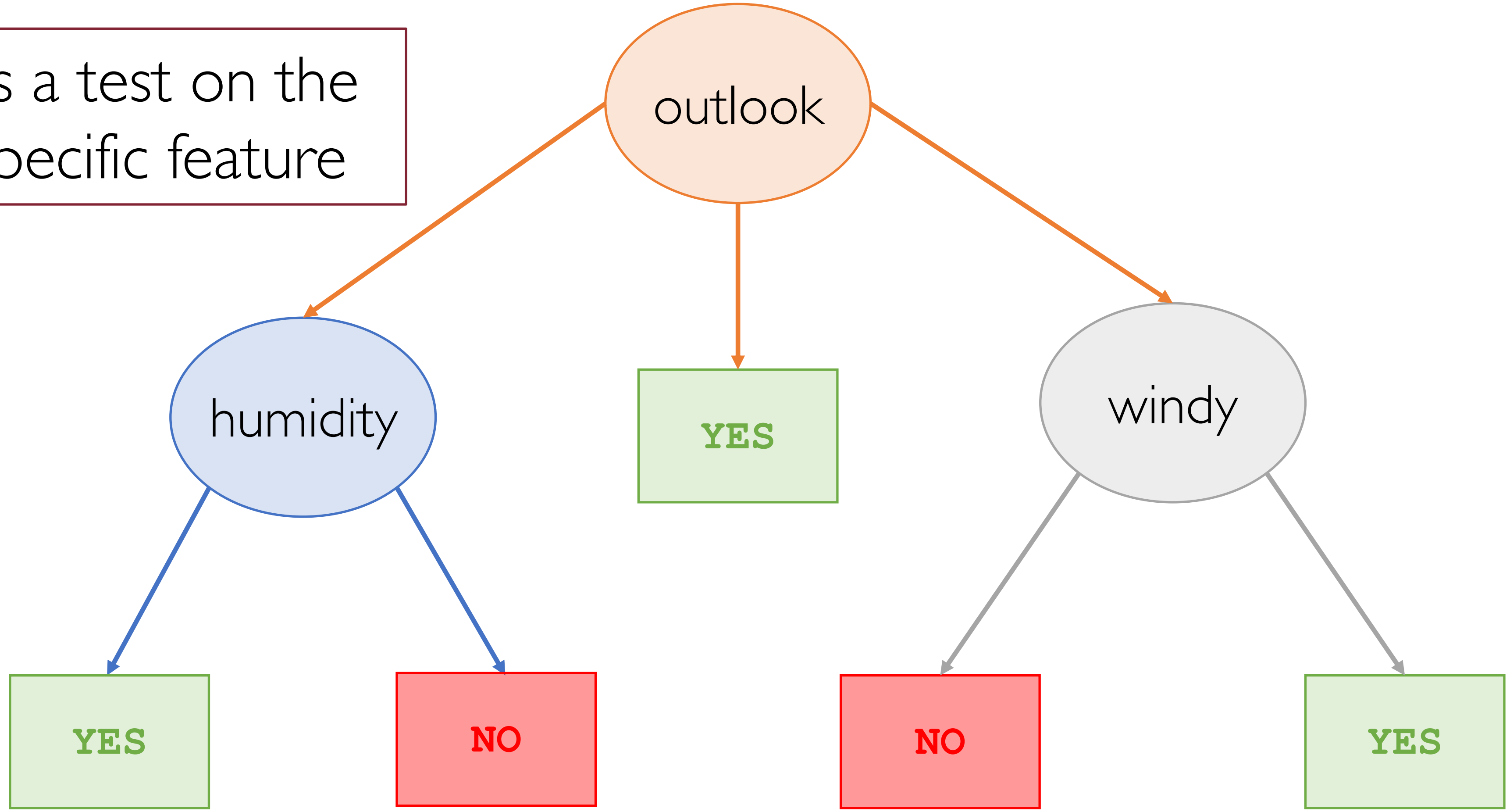
Decision Tree: An Example



Should we play outdoor tennis?

Decision Tree: An Example

Each node is a test on the value of a specific feature



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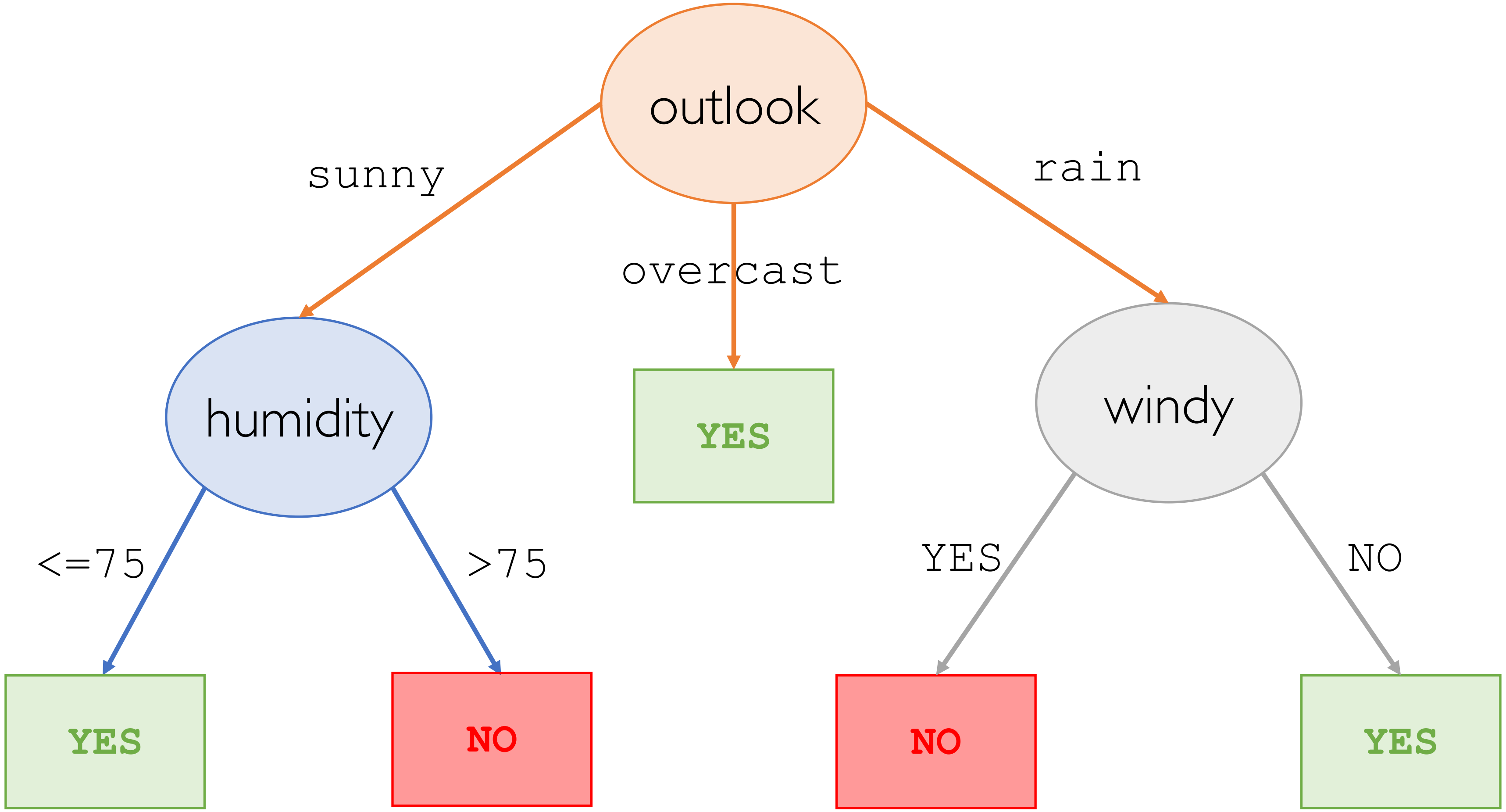

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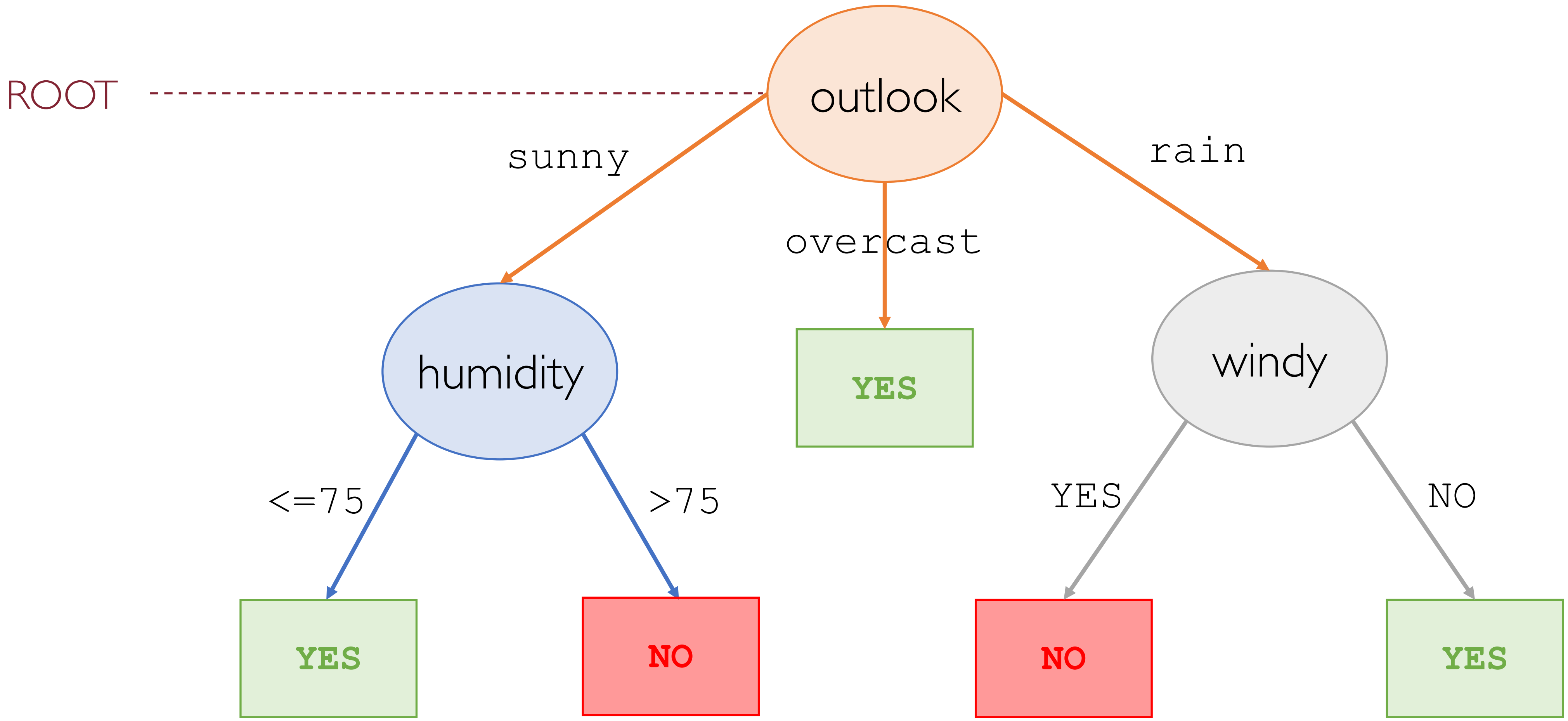

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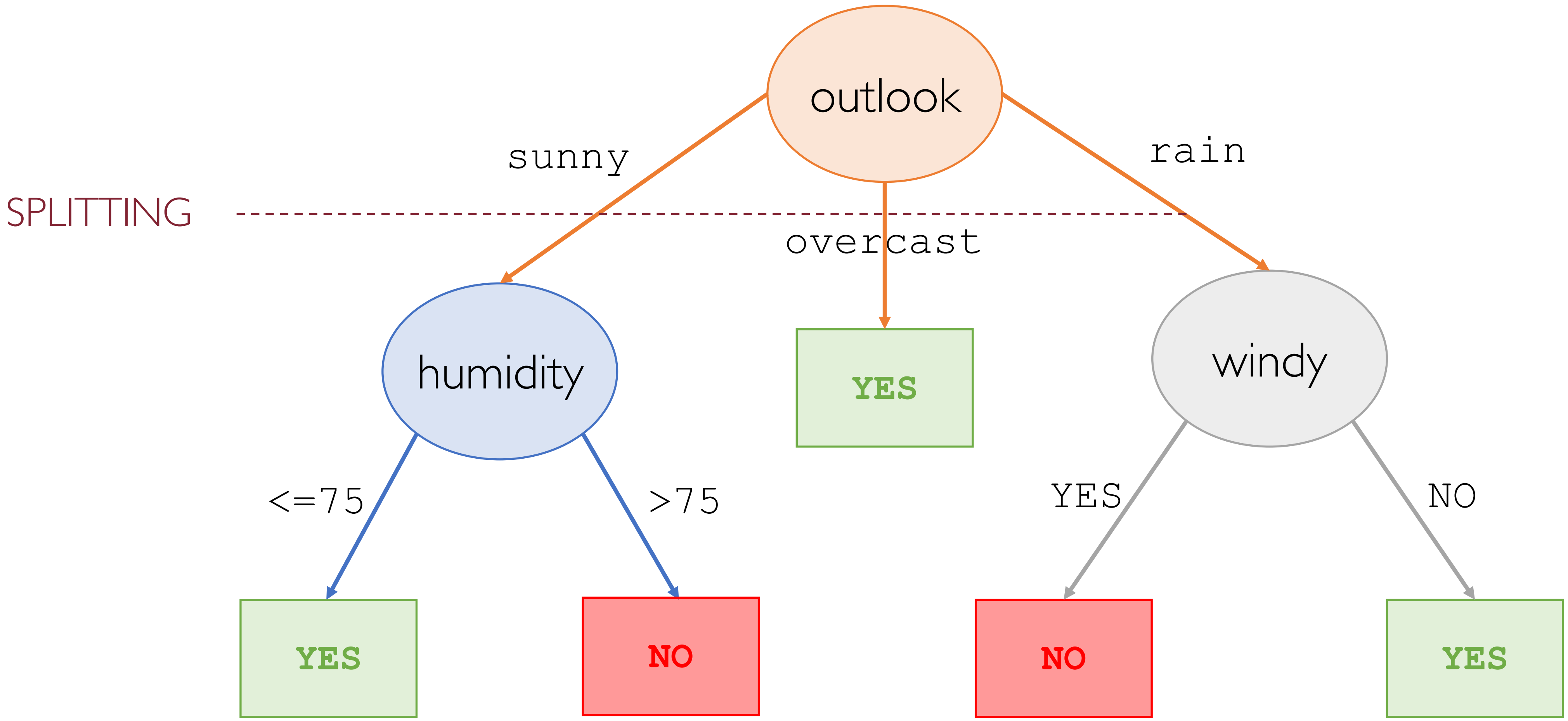

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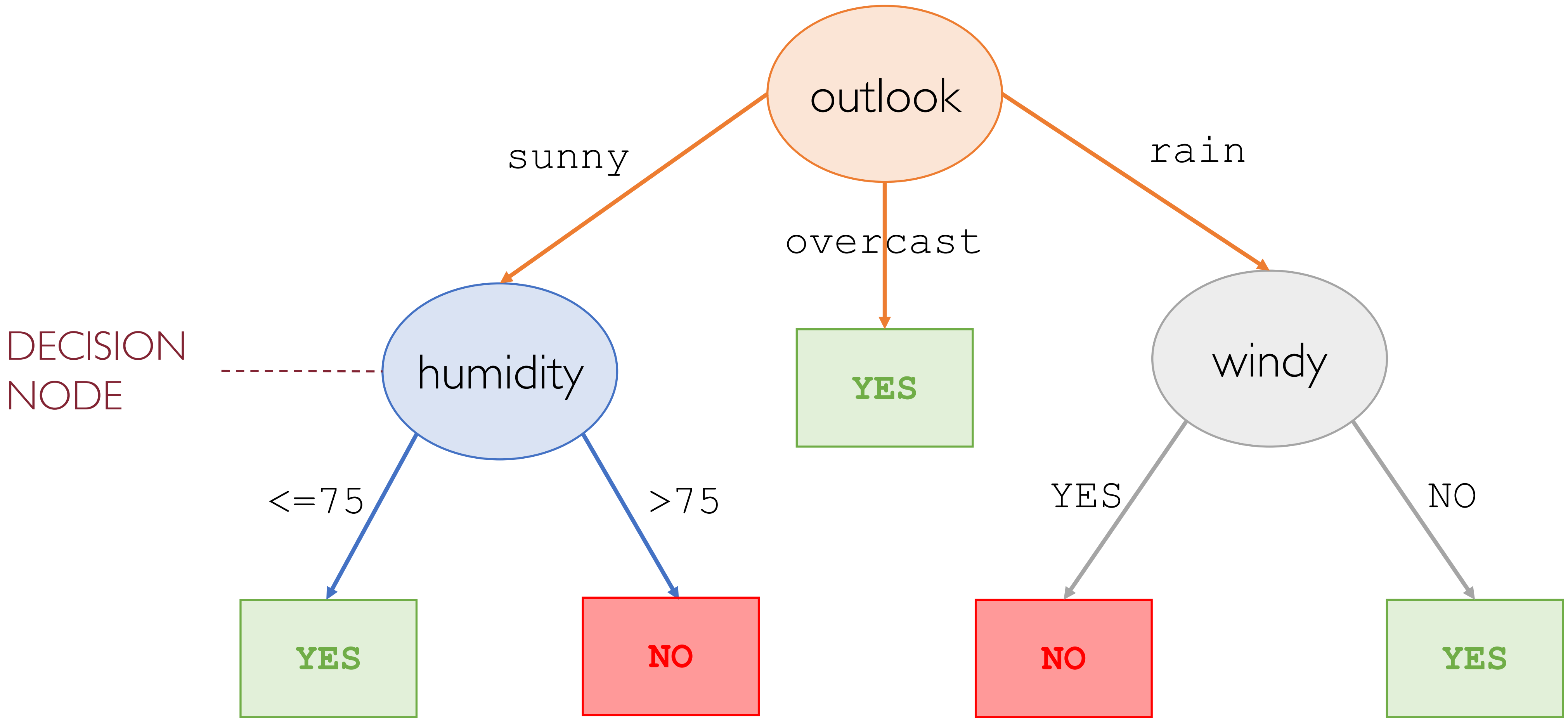

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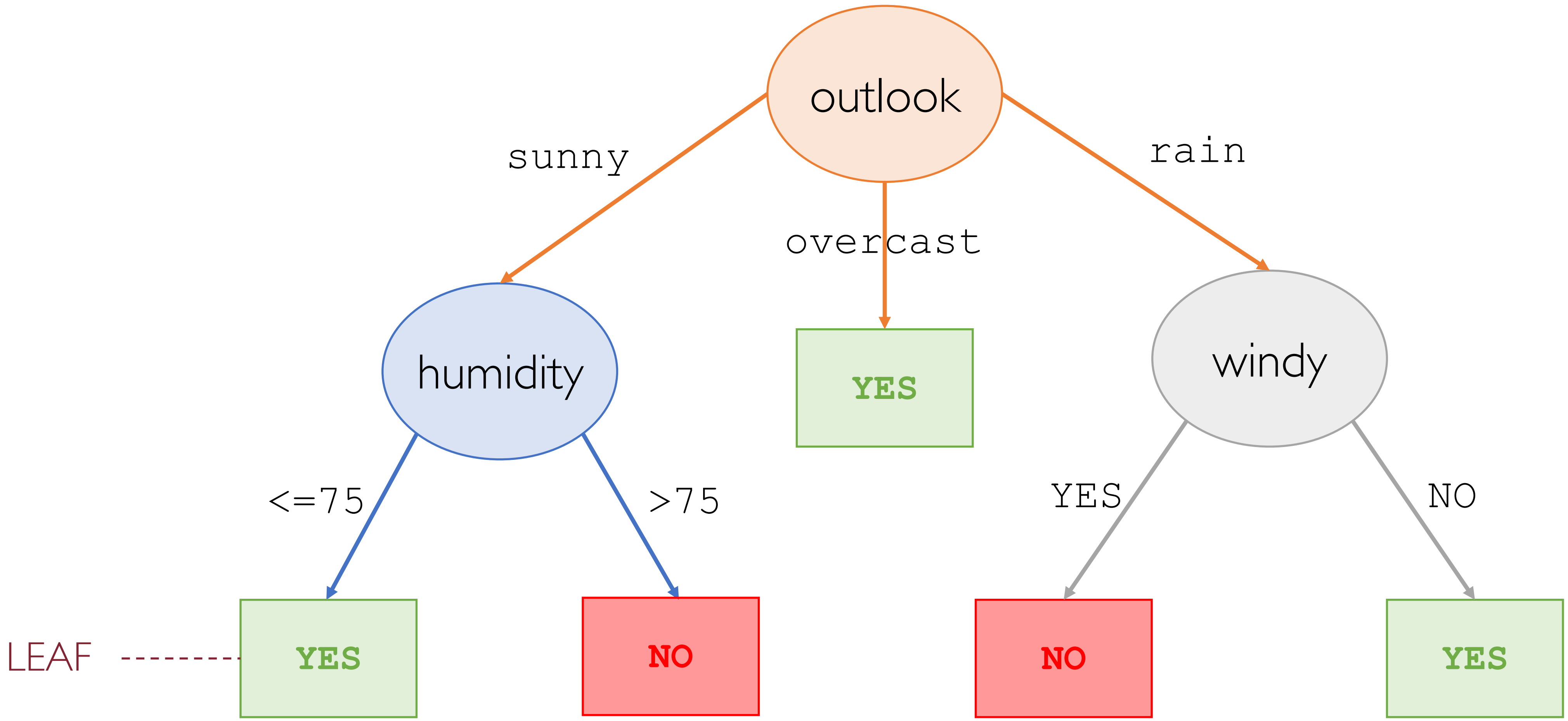

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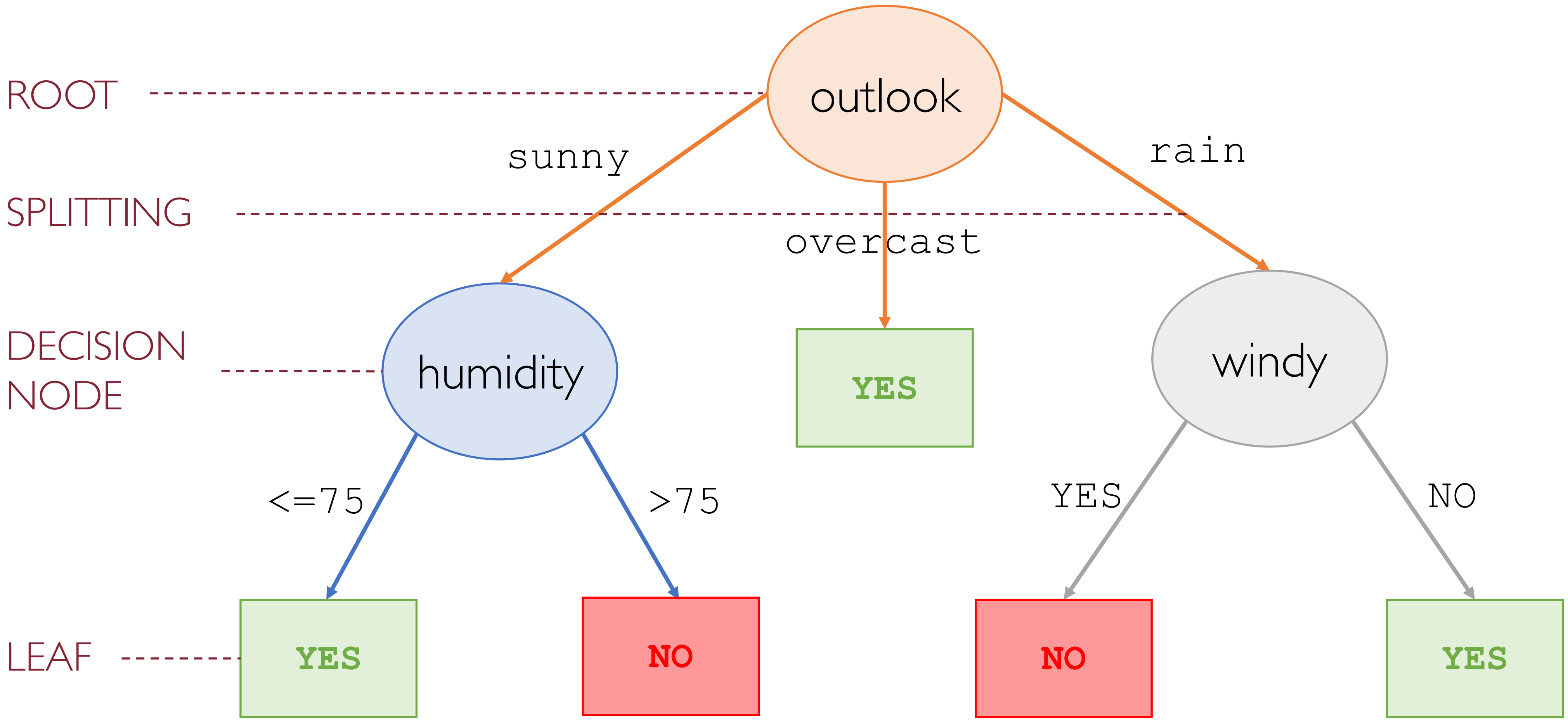
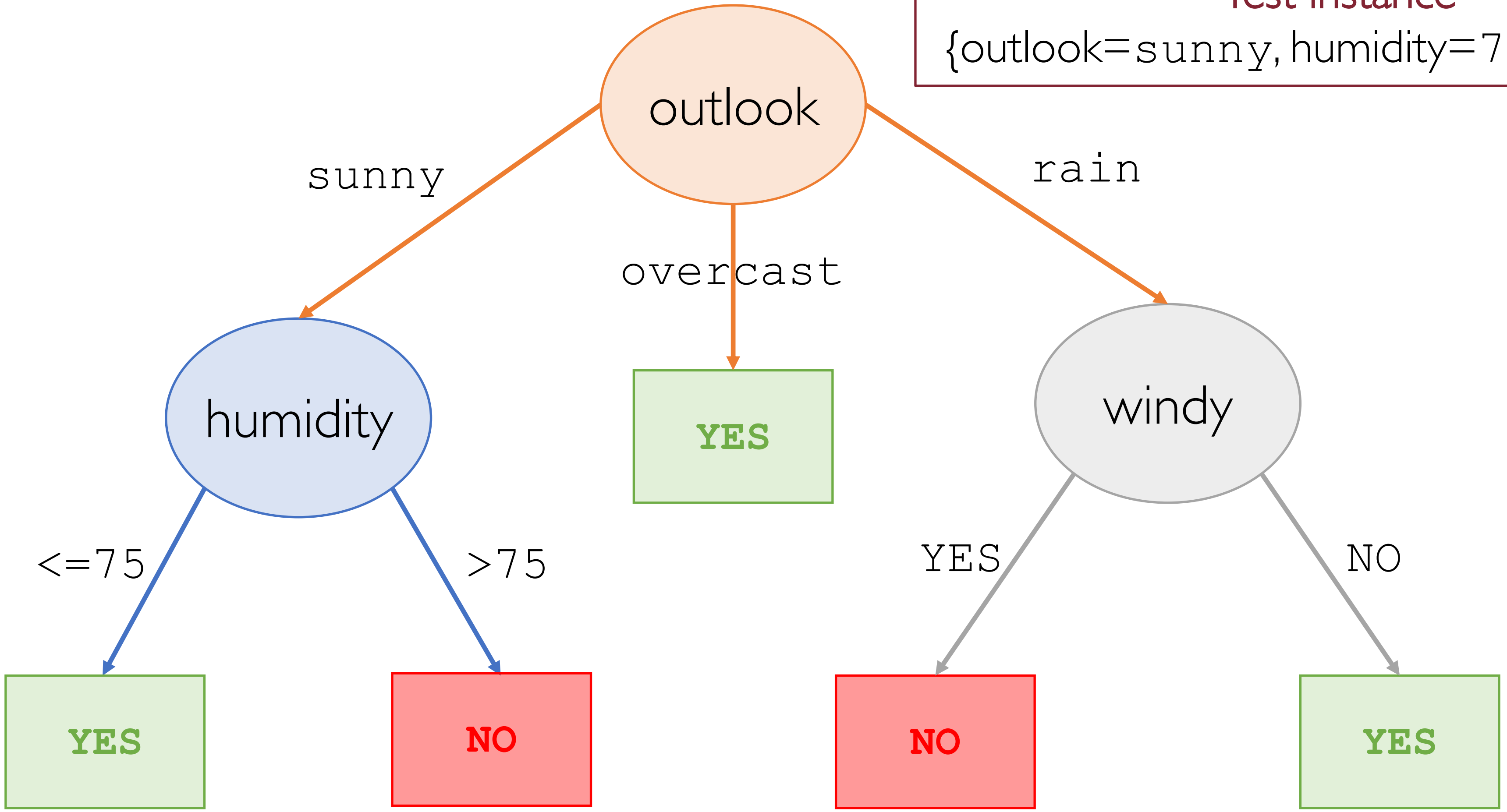


Decision Tree: An Example

Test instance
{outlook=sunny, humidity=72, windy=Y}



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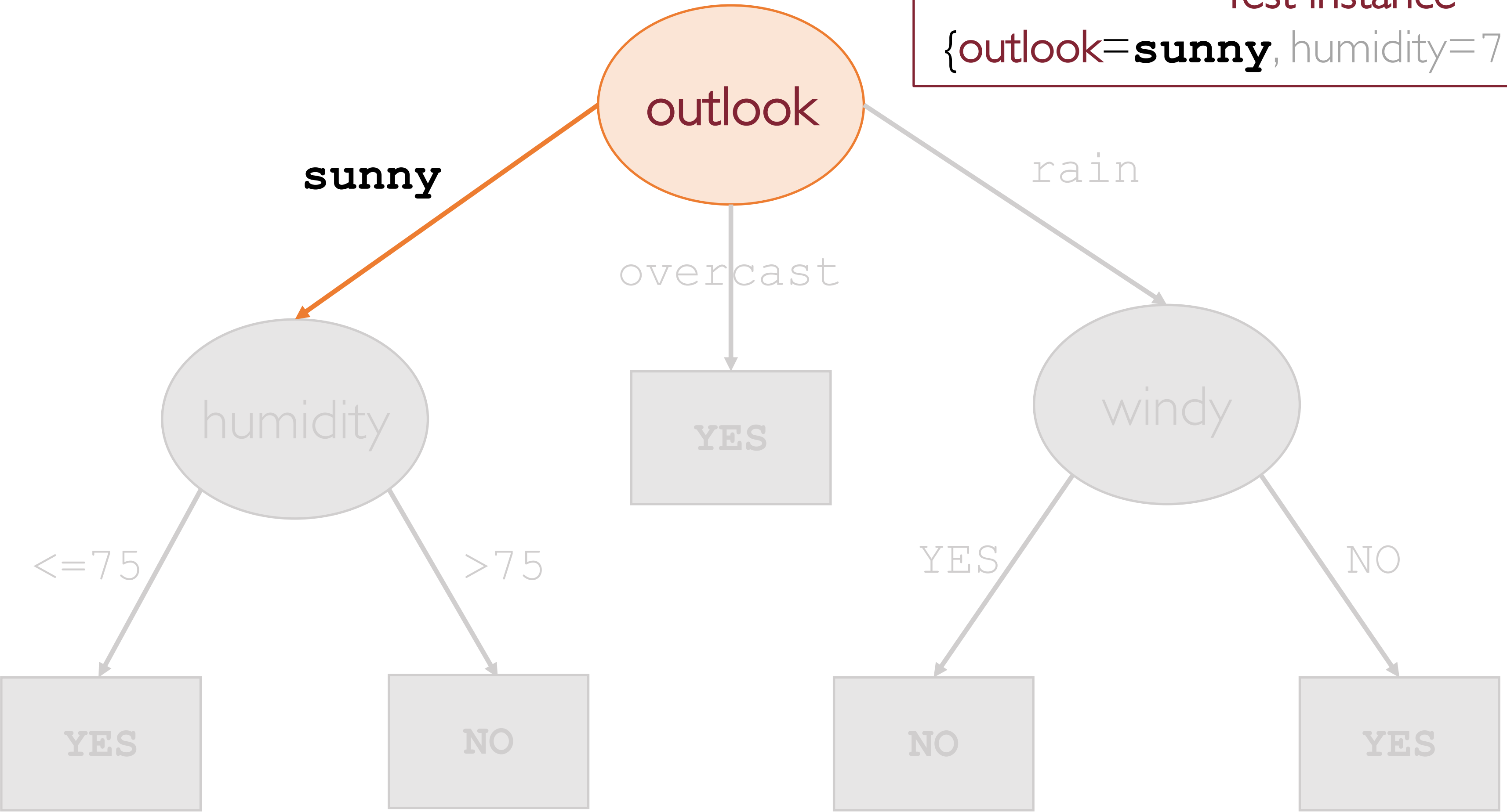

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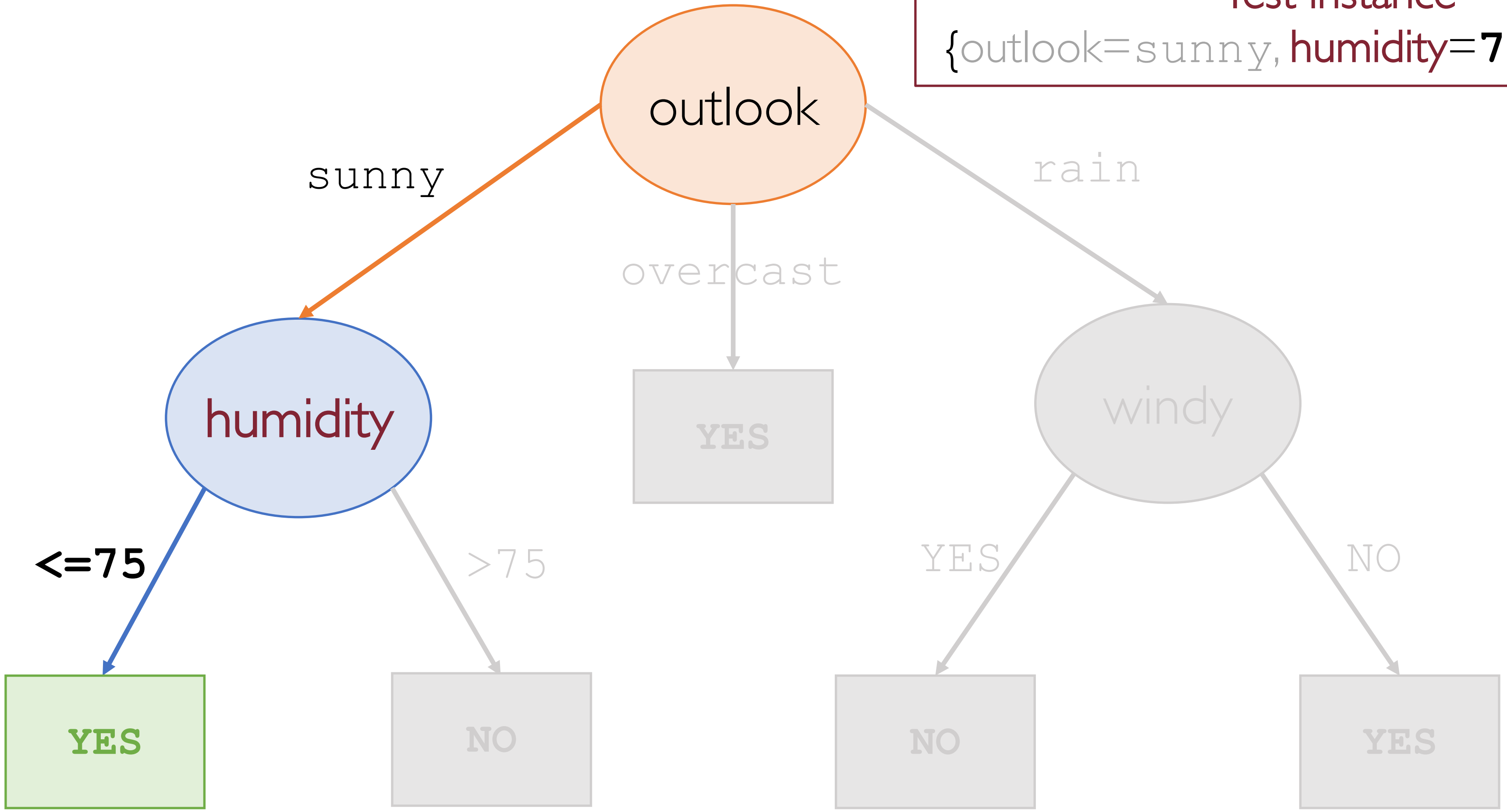

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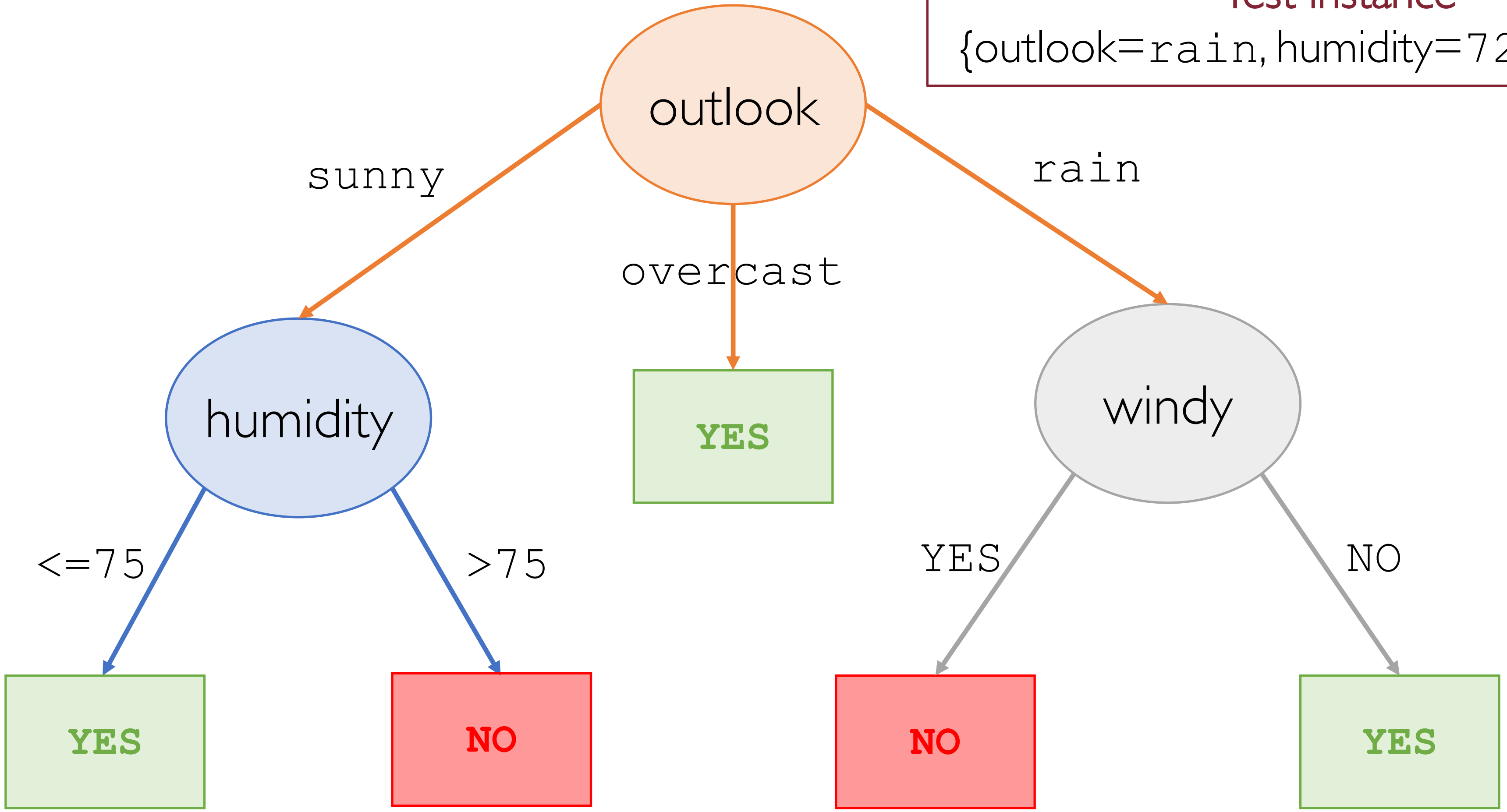

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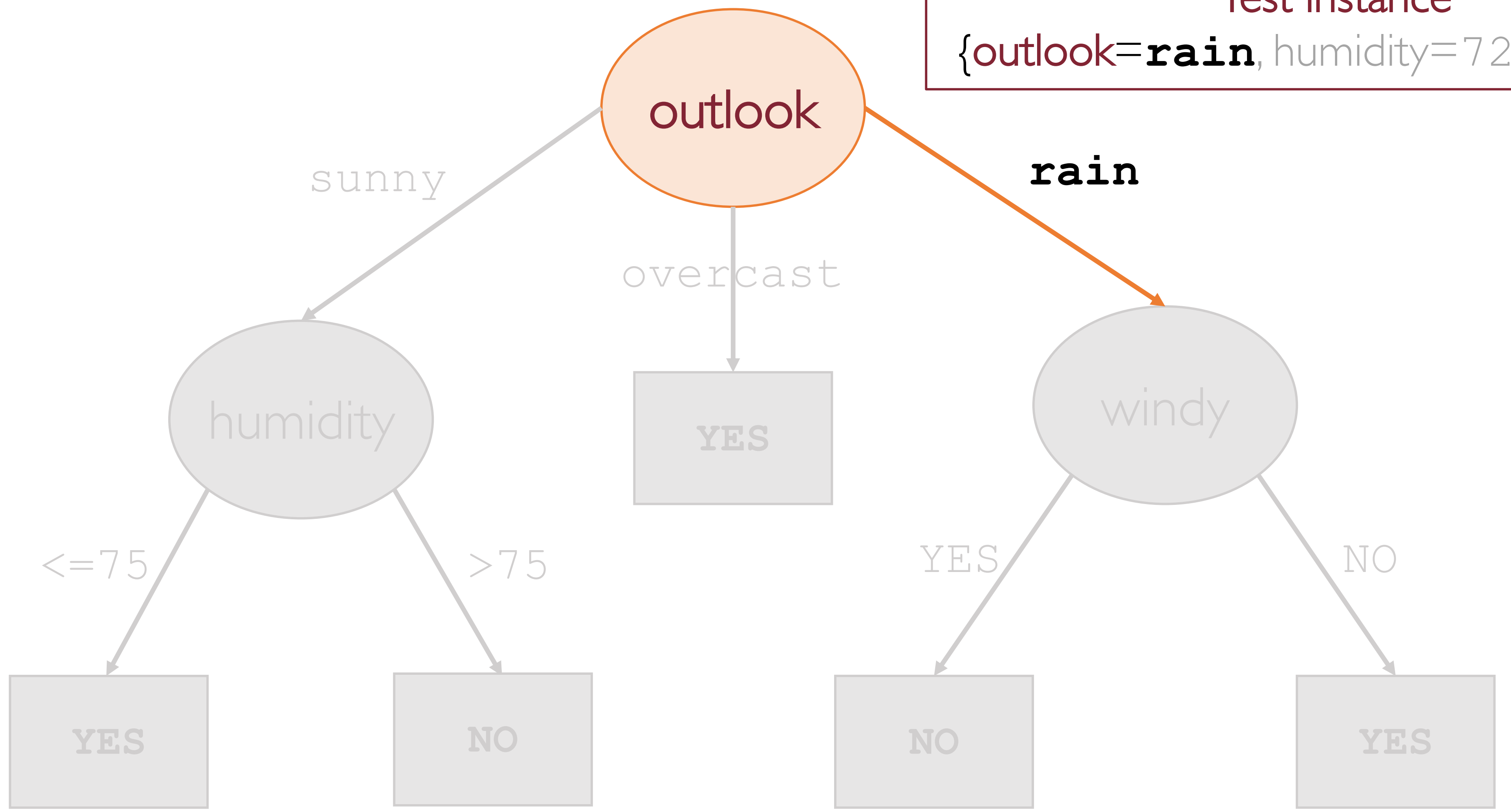

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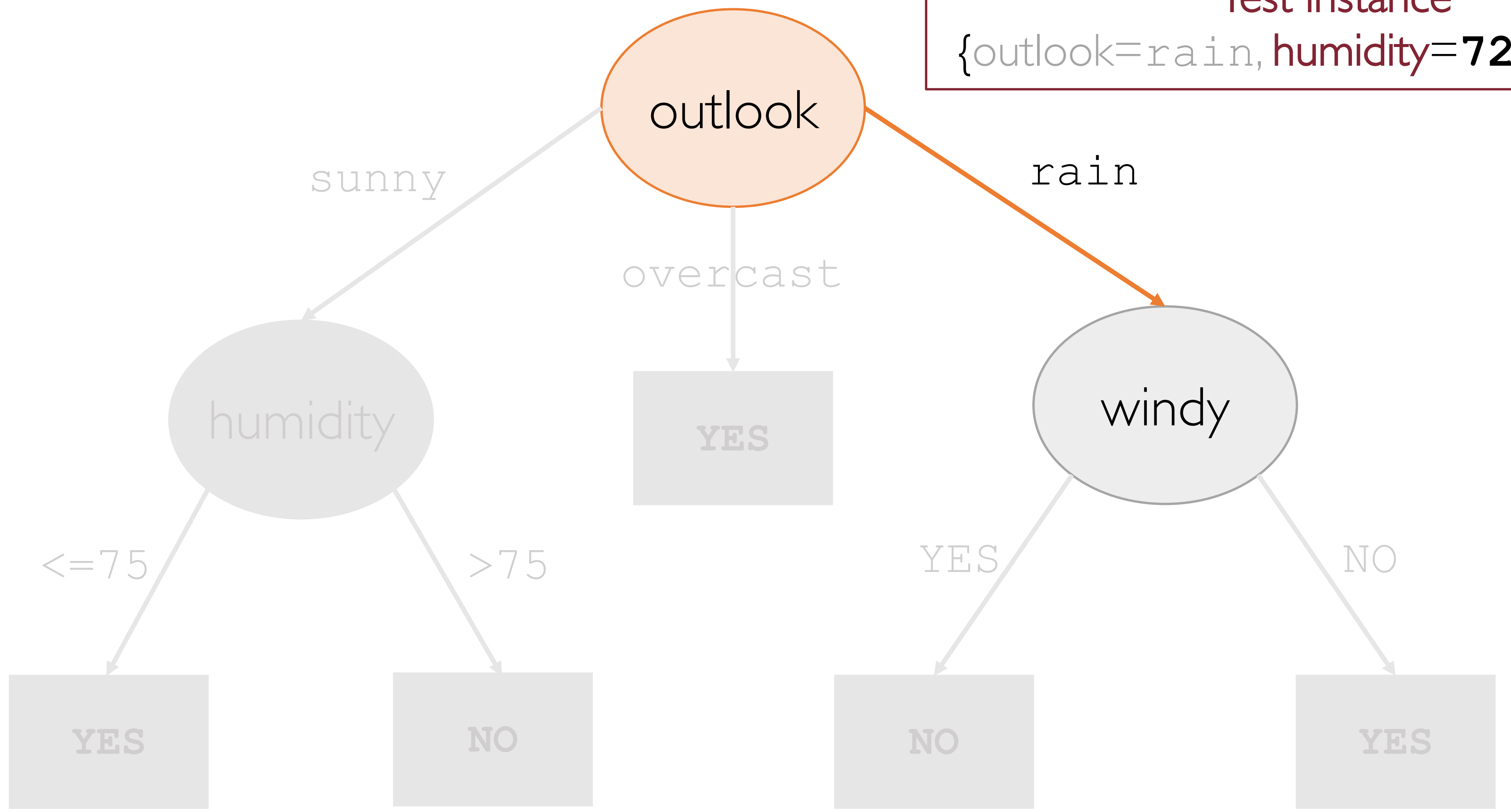

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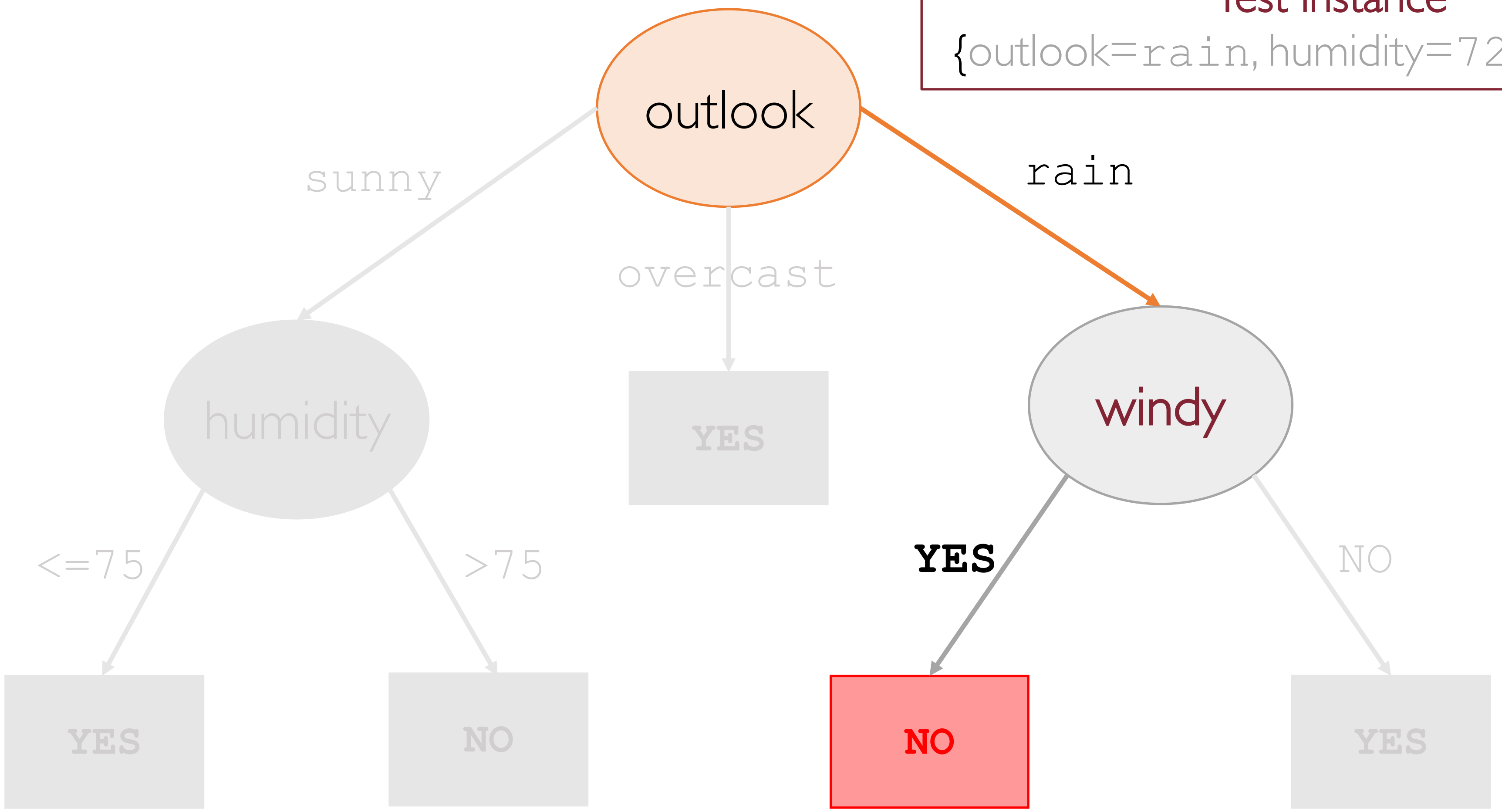

A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$	input feature space
$\mathcal{Y}$	output space
$\quad \mathcal{Y} \subseteq \mathbb{R}$	real-value label (regression)
$\quad \mathcal{Y} = \{1, \ldots, k\}$	discrete-value label (k-ary classification)
$(\mathbf{x}_i, y_i)$	*i*-th labeled instance
$\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,n}) \in \mathcal{X}$	*n*-dimensional feature vector of the *i*-th instance
$y_i \in \mathcal{Y}$	label of the *i*-th instance
$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$	dataset of *m* i.i.d. labeled instances

How Do We Build a Decision Tree?

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- Example:
  - Suppose we split the input feature space in 2 regions: R_1 and R_2 and the response mean as computed from $R_1 = 10$ and $R_2 = 20$
  - For any **x** belonging to R_1 (R_2) will be predicted 10 (20)

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- In theory, partitions could have *any* shape

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The mean computed from observations in R_j

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(e.g., boolean)

One branch for each value

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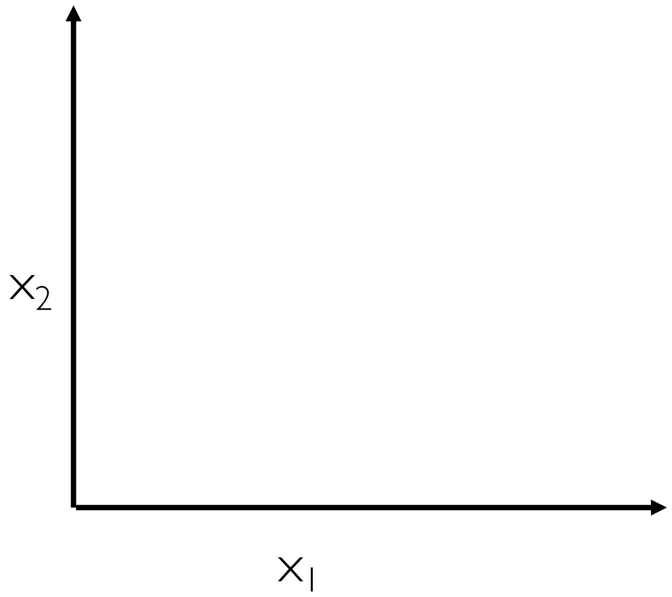

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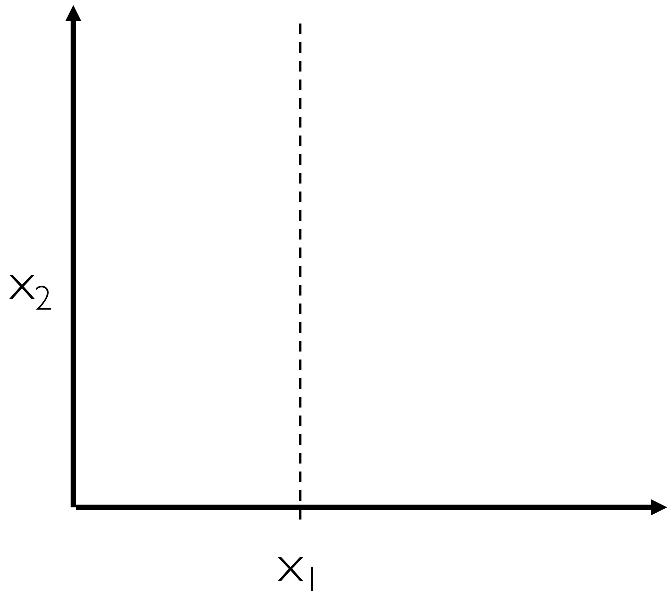

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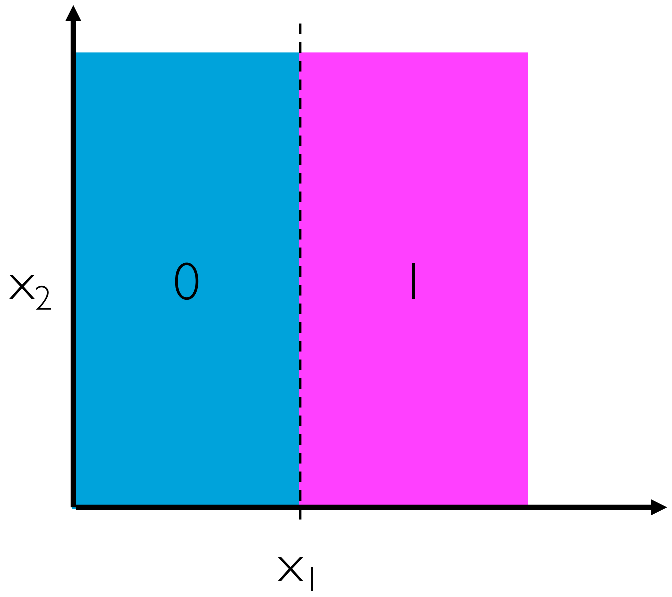

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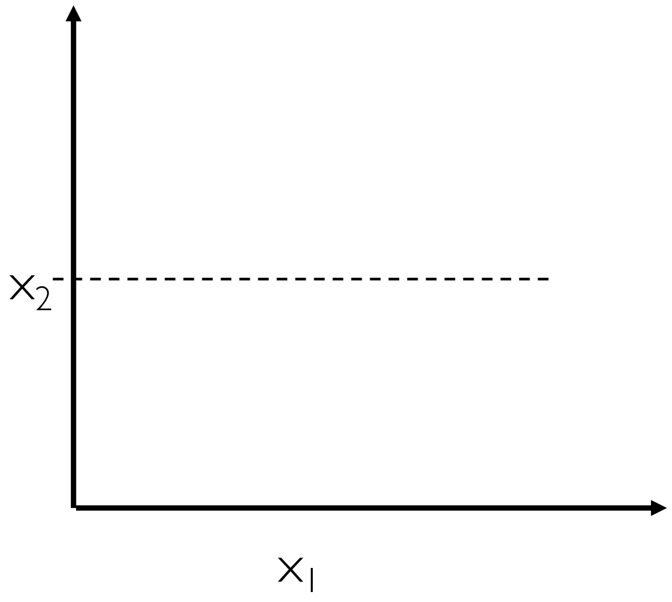

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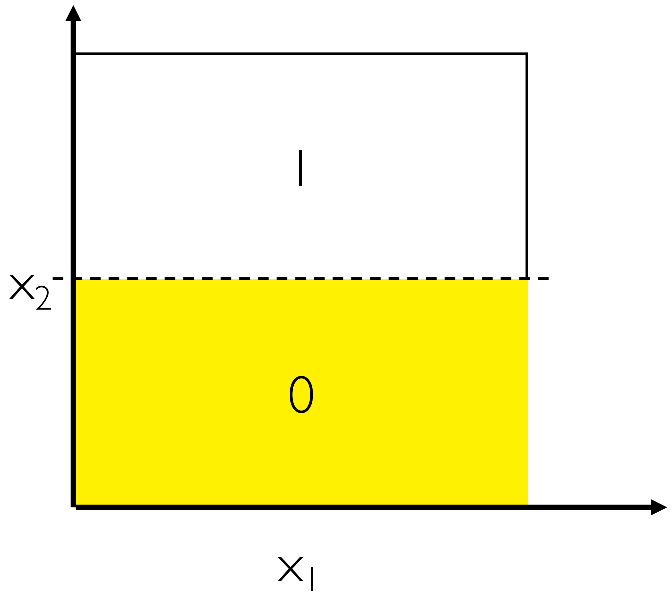

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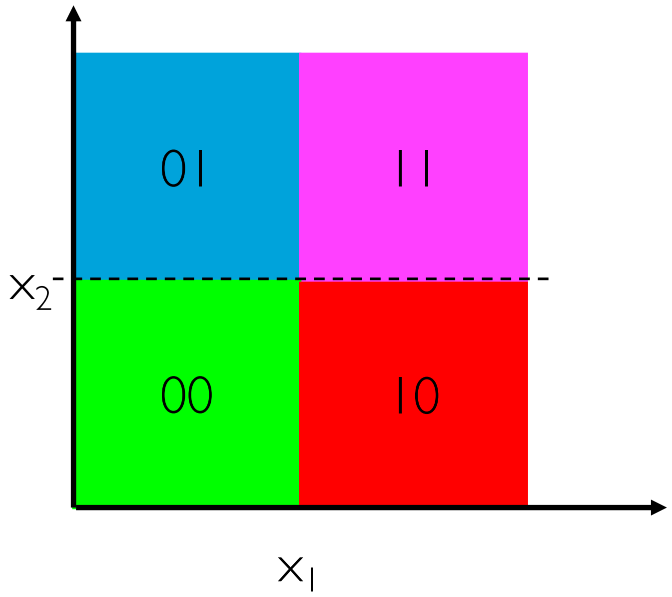

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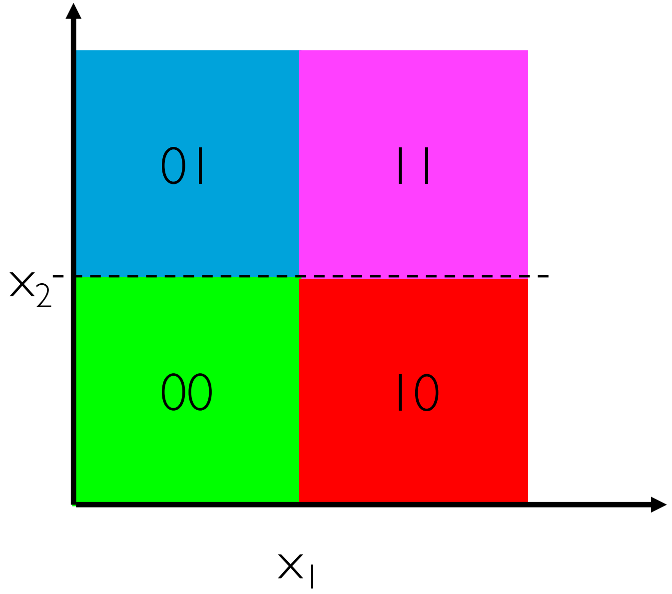

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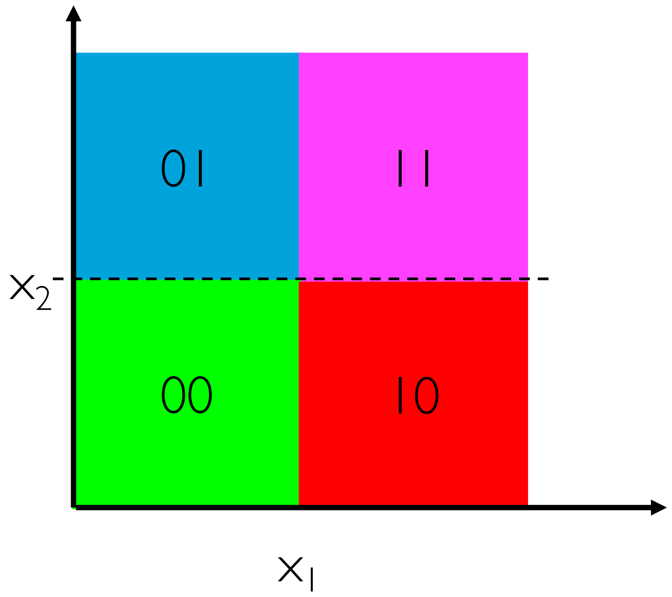

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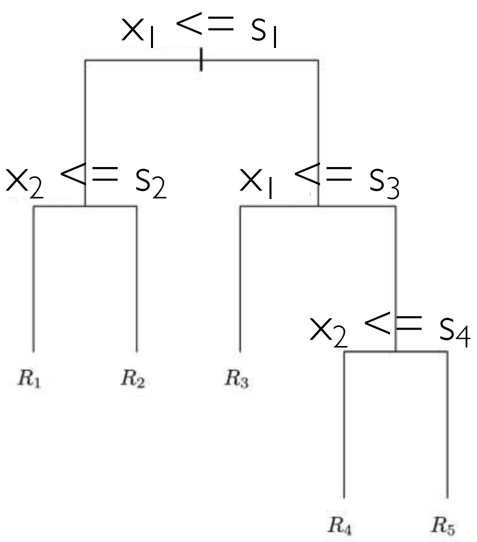
For each attribute, find a split point s

Test x_j <= s and create 2 branches

The same attribute may be further split in each subtree



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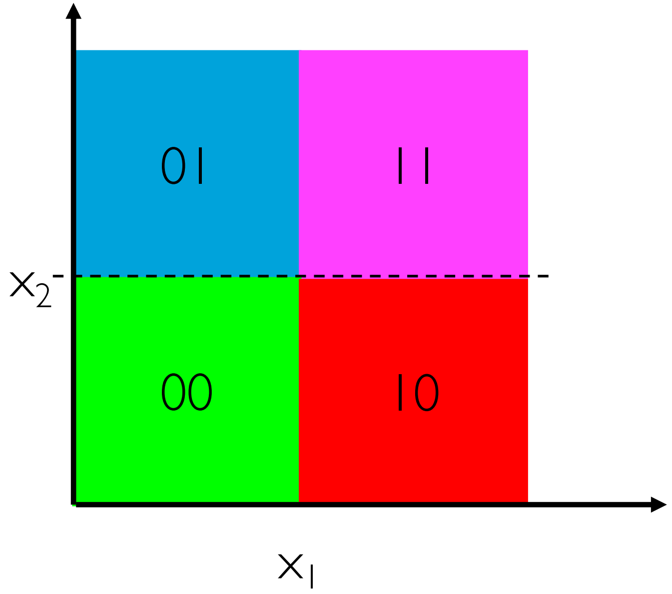

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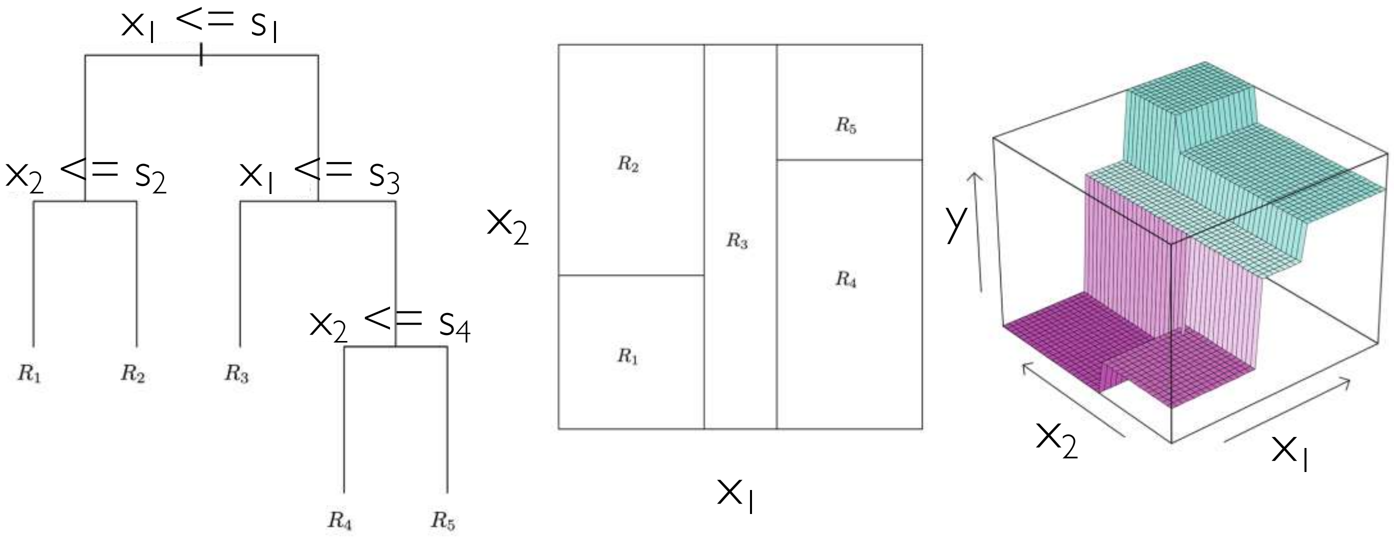

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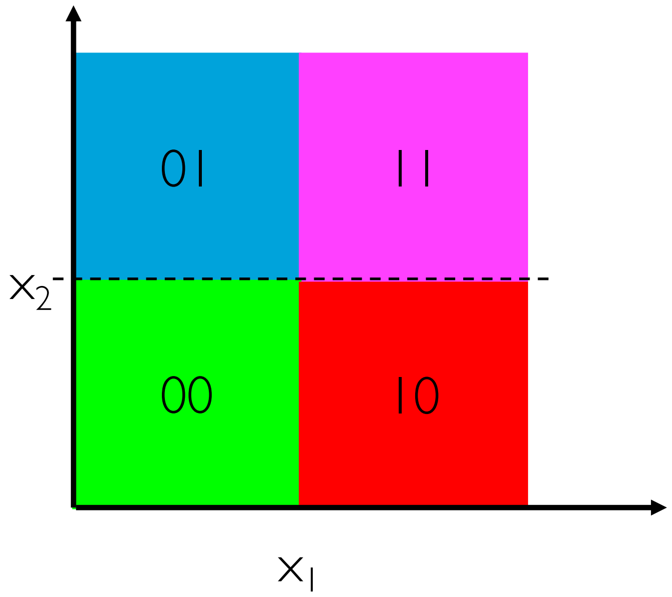

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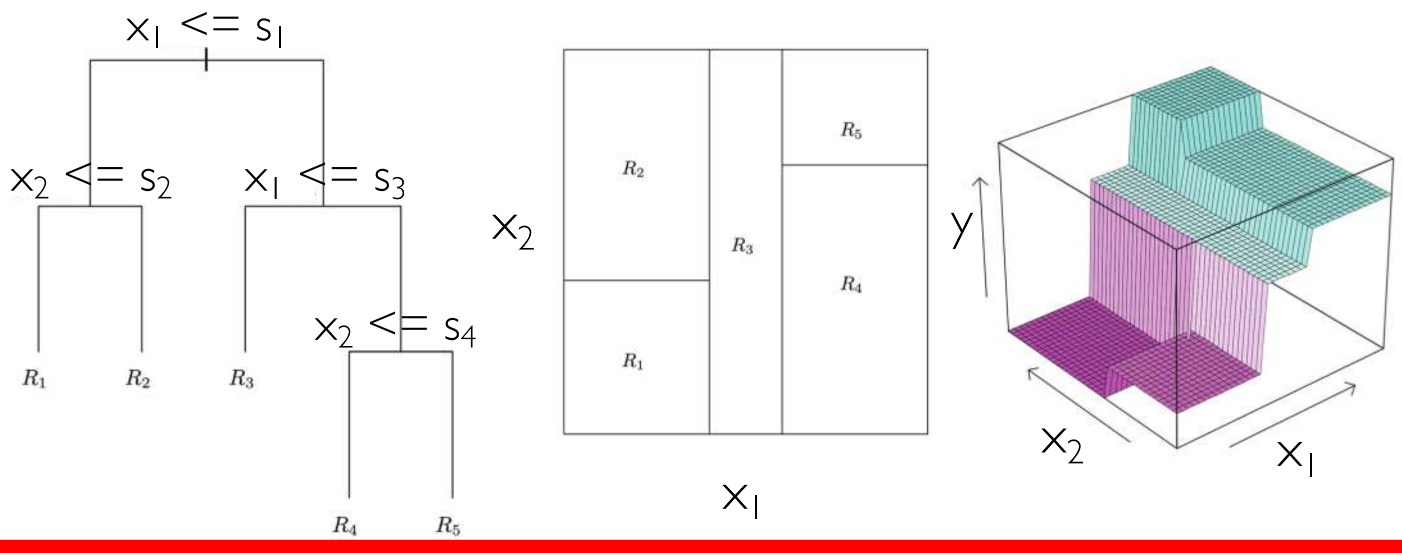

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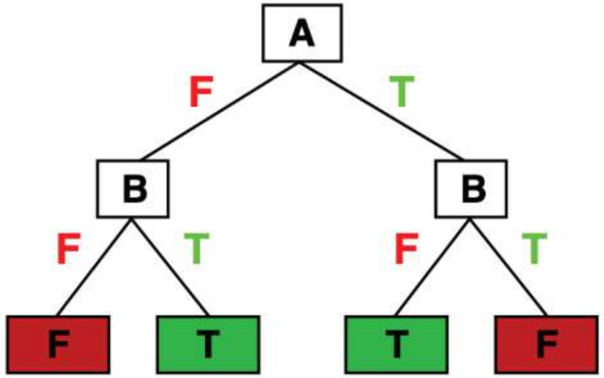
F	T	T
T	F	T
T	T	F



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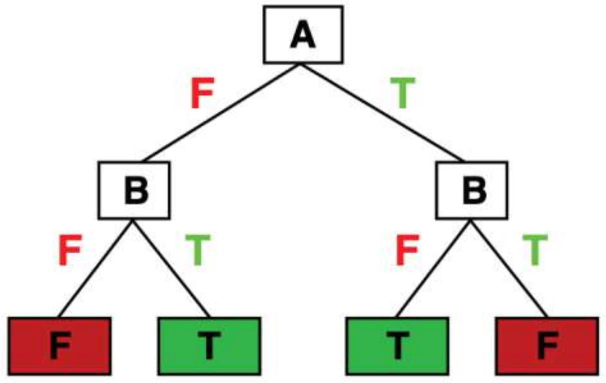

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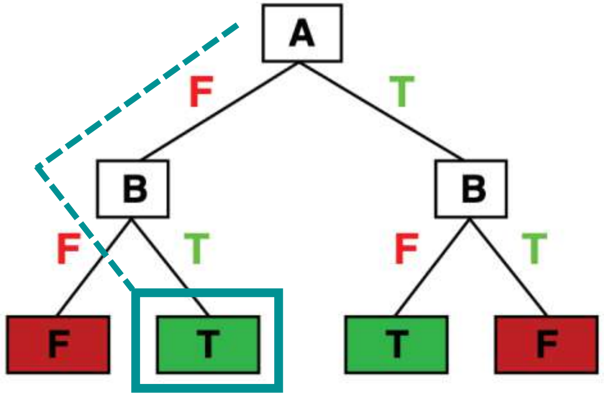

Each row of the truth table maps to a root-to-leaf path on the tree

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Such a tree will have one dedicated root-to-leaf path for each training instance

Of course, this tree clearly overfits the training data and it will not generalize to unseen examples (needs regularization)

Hypothesis Space

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Each boolean function of n boolean inputs is represented by a truth table

x_1	x_1	…	x_n	y
0	0	…	0	
1	0	…	0	
1	1	…	0	
…	…	…	…	
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2^n rows

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For each input y = 0 or 1

Hypothesis Space

A possible boolean function is the one which will output all 0s

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x_1	x_1	…	x_n	y
0	0	…	0	0
1	0	…	0	0
1	1	…	0	0
…	…	…	…	0
…	…	…	…	0
…	…	…	…	0
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Hypothesis Space

Another possible boolean function is the one which will output all 1s

2^n rows

x_1	x_1	…	x_n	y
0	0	…	0	1
1	0	…	0	1
1	1	…	0	1
…	…	…	…	1
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Larger hypothesis space means also it is generally harder for the learning algorithm to find the best hypothesis (larger space to explore)

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Solution

Top-Down greedy heuristic Recursive Binary Splitting

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top-down

- Greedy strategy:
  - At each step, the best "local" split is made
  - Looking ahead might result in a different split, which leads to a better tree

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$$\{x_{i,f} \le s\}$$

is the region of the feature space in which the *f*-th feature takes on values less than or equal to *s*

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Goal: find the pair (f, s) which minimizes the following

$$\sum_{i:\ \mathbf{x}_i \in R_{\text{left}}(f,s)} (y_i - \hat{y}_{R_{\text{left}}})^2 + \sum_{i:\ \mathbf{x}_i \in R_{\text{right}}(f,s)} (y_i - \hat{y}_{R_{\text{right}}})^2$$

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- Finding the pair (f, s) which minimizes the quantity below can be done "easily", especially when the number of features d is not too large

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- Possible stopping criteria (tree grows until):
  - no region contains more than N observations
  - max depth of the tree is D
  - RSS is reduced by at least a threshold value t

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- Tree building is still based on Recursive Binary Splitting algorithm but RSS cannot be used as a criterion for splitting nodes
- A natural alternative to RSS minimization is to minimize the "impurity"
- The predicted label of a test instance is the most frequent label (mode) of the instances belonging to the region where it falls

The "Impurity" of a Node

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- It is often convenient to refer to the information gain of a split

Classification Trees: Notation

Subset of training instances falling into region R

$$\mathcal{D}_R = \mathcal{D} \cap R = \{(\mathbf{x}_i, y_i) \in \mathcal{D} \mid \mathbf{x}_i \in R\}$$

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$$IG(\mathcal{D}_R, f, s) = \underbrace{I(\mathcal{D}_R)}_{\text{parent node's impurity}} - \underbrace{\left[\frac{|\mathcal{D}_{R_{\text{left}}(f,s)}|}{|\mathcal{D}_R|} I(\mathcal{D}_{R_{\text{left}}(f,s)}) + \frac{|\mathcal{D}_{R_{\text{right}}(f,s)}|}{|\mathcal{D}_R|} I(\mathcal{D}_{R_{\text{right}}(f,s)})\right]}_{\text{children nodes' impurity}}$$

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- Other 2 measures are preferable: Gini Index and Entropy

Node Impurity: Gini Index

- Measures the variance across the K classes

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- A small value indicates that a node contains predominantly observations from a single class

Node Impurity: Entropy

- Alternative, yet similar to Gini

$$I_H(\mathcal{D}_{Rj}) = -\sum_{k=1}^{K} \hat{p}_{jk} \log_2(\hat{p}_{jk})$$

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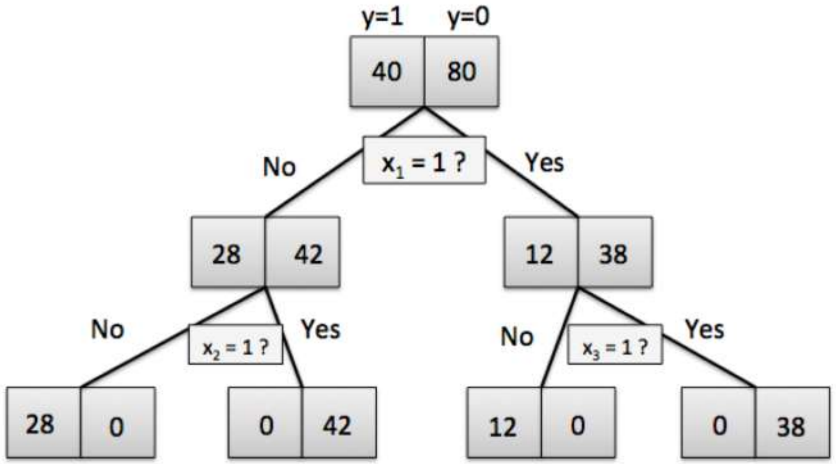
- Like Gini, a small value of entropy is obtained whenever all the proportions are either close to 1 or to 0
- In practice, both entropy and Gini can be used to grow a tree

Classification Error Rate vs. Entropy (Gini)

Consider this decision tree which perfectly separates positive (y=1) from negative (y=0) samples using 3 splits on 3 binary features x_1, x_2, x_3



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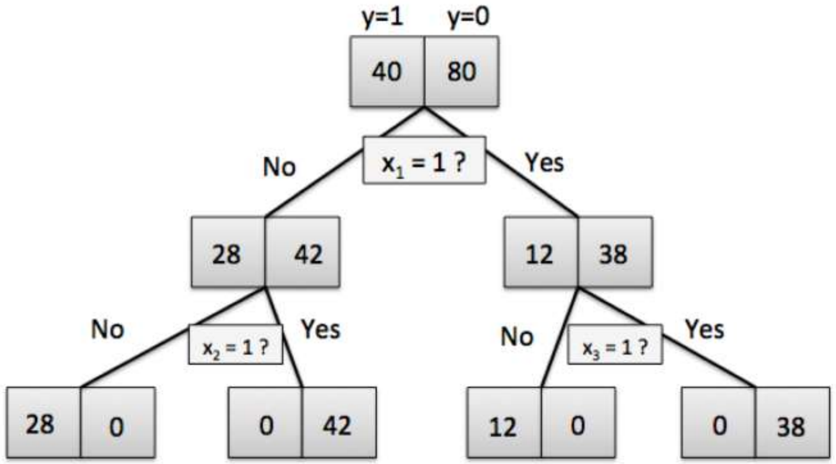
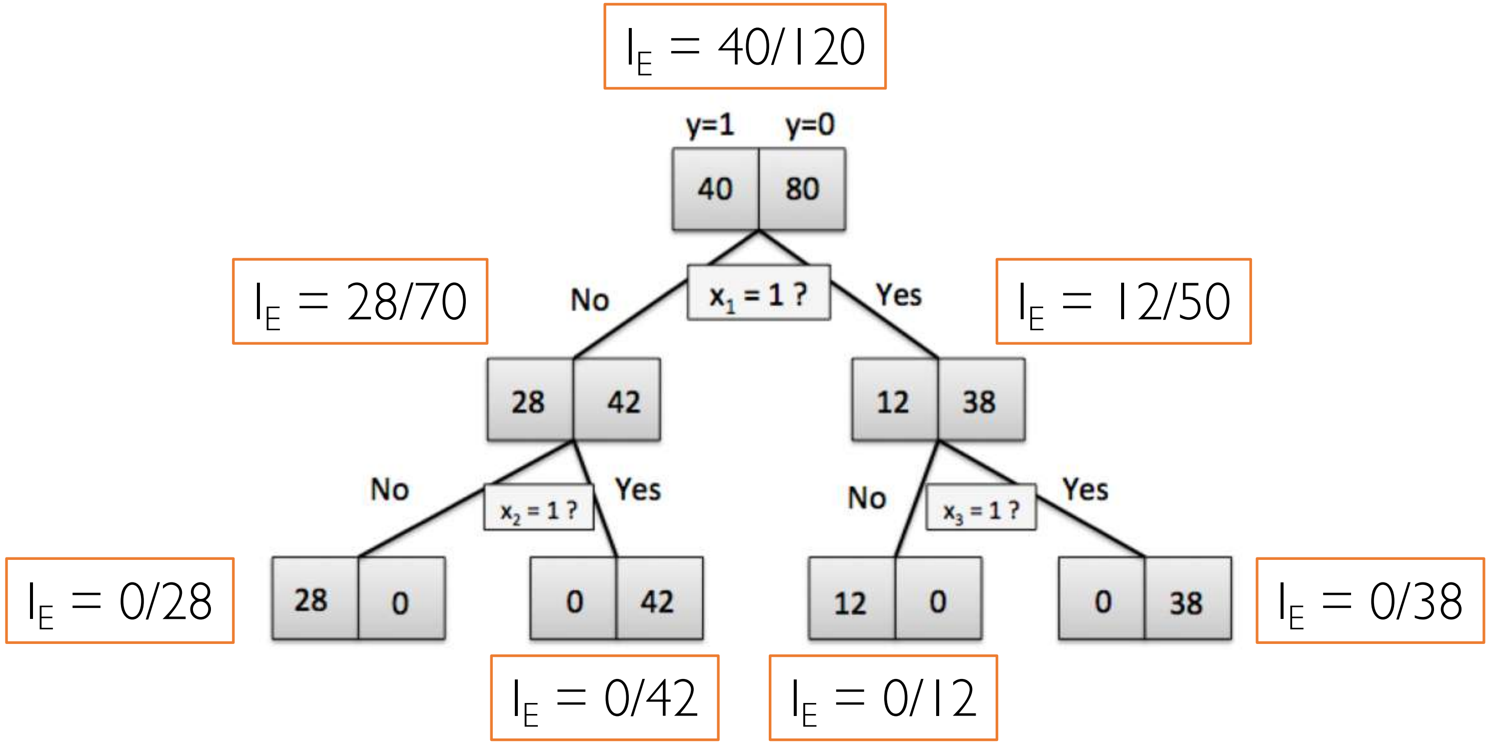


Question

Would we be able to learn the tree above using classification error rate as splitting criterion?

Classification Error Rate vs. Entropy (Gini)

Node impurity using I_E

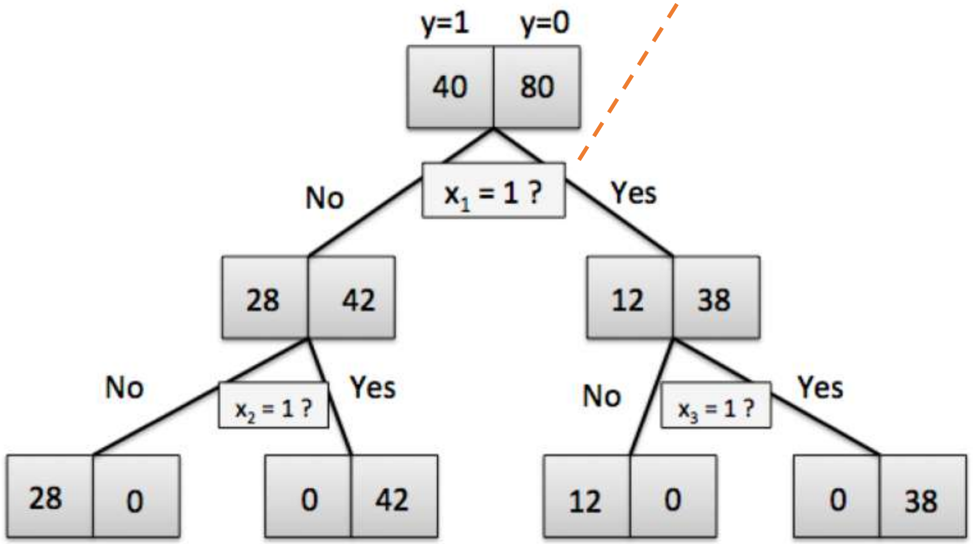


source: https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html

Classification Error Rate vs. Entropy (Gini)

Compute IG of the first split using I_E

$I_E = 40/120$



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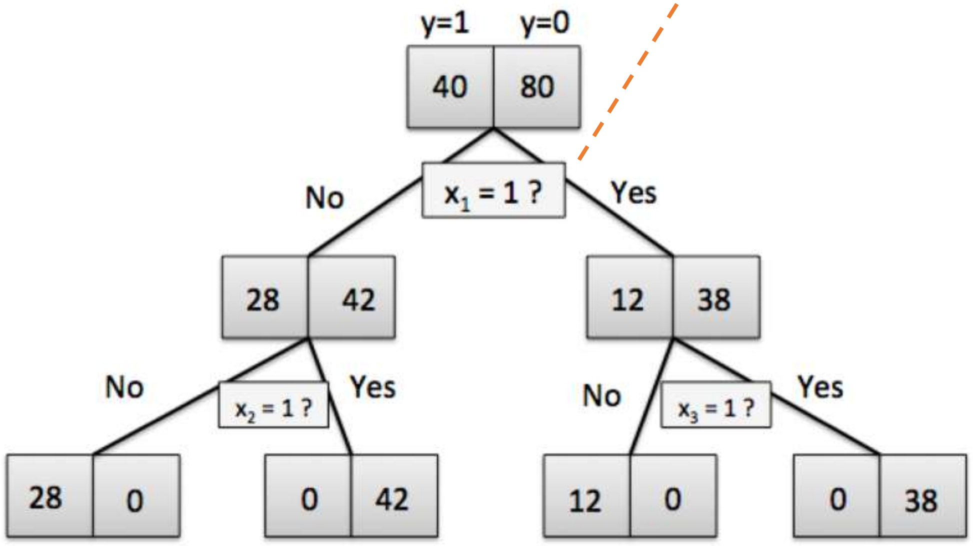

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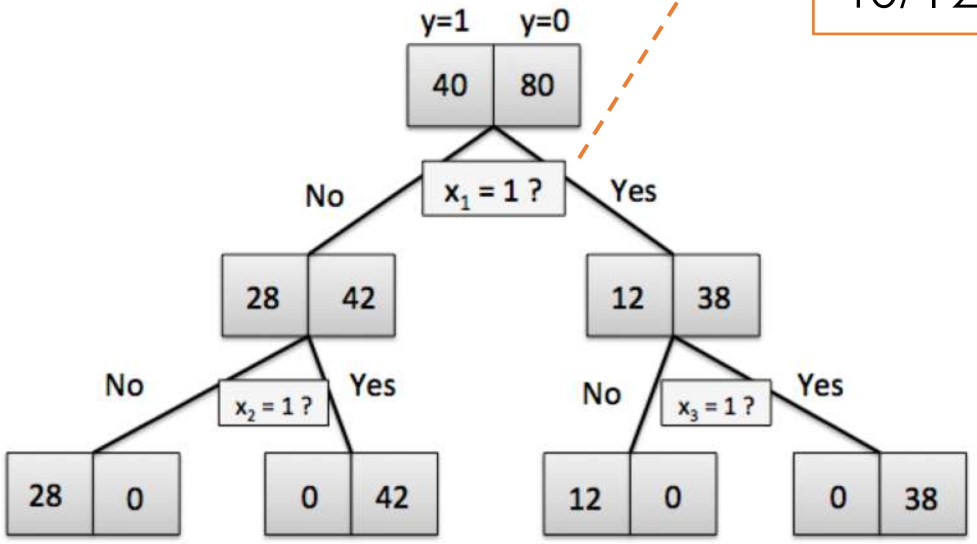

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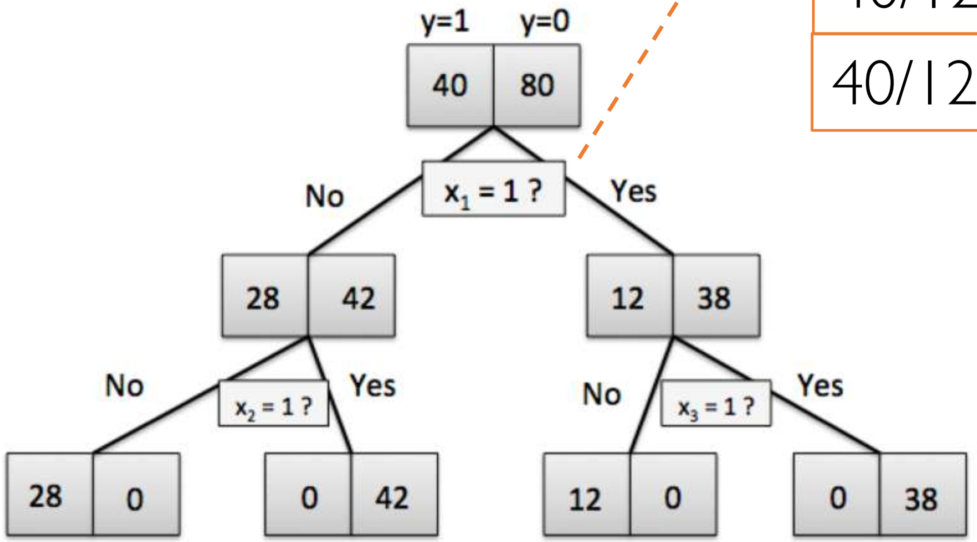

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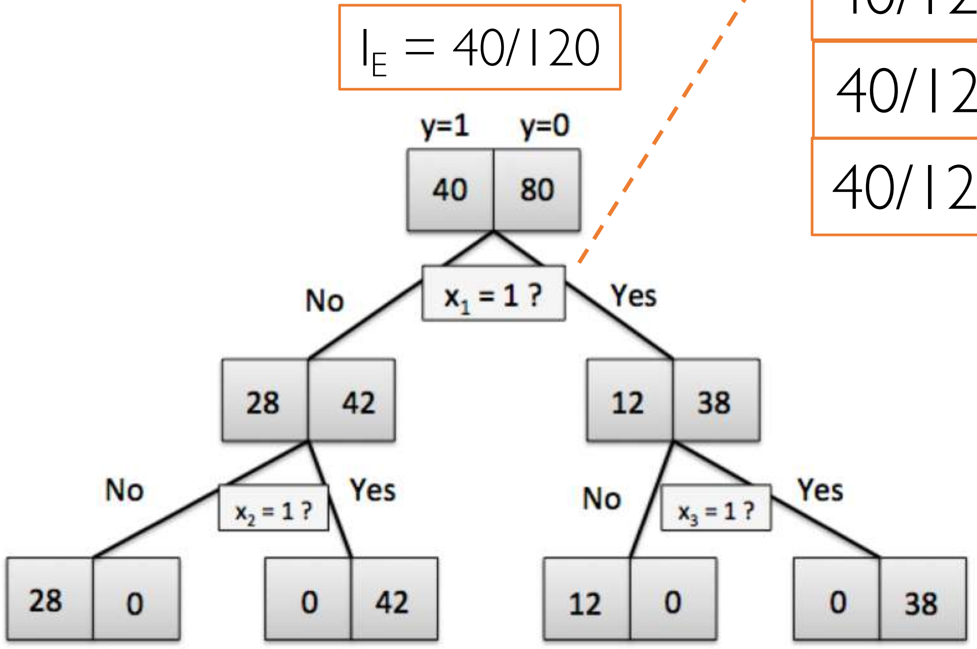

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the sum of I_E of the 2 child nodes is equal to that of the parent (40/120)

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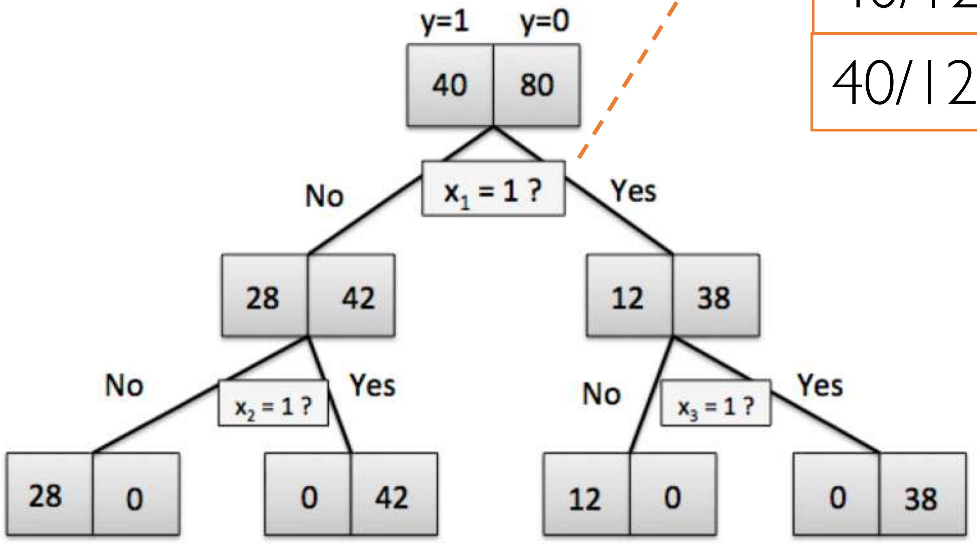

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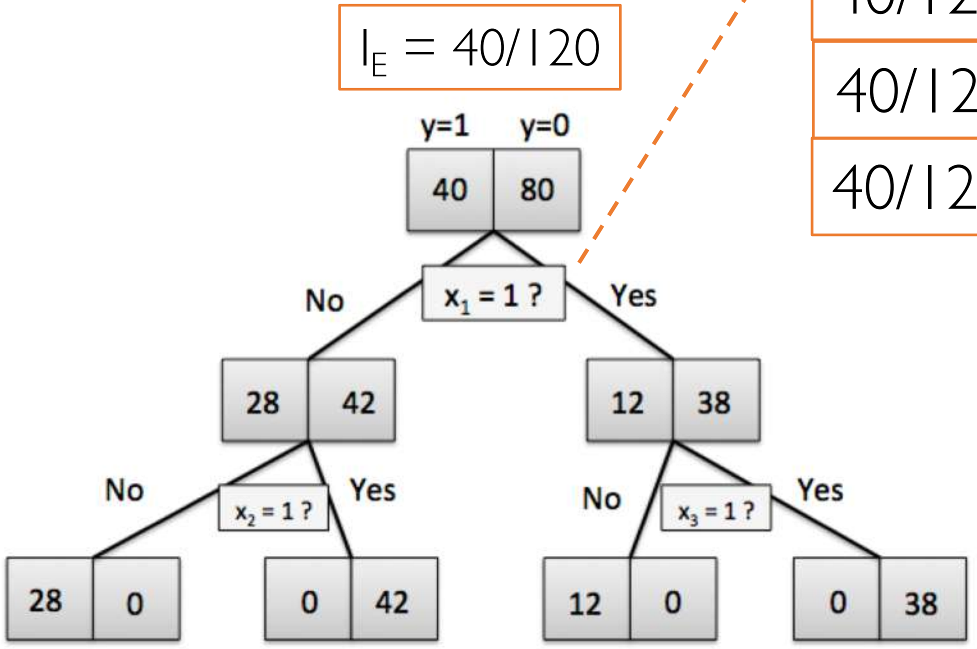

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The tree learning algorithm would stop at this point

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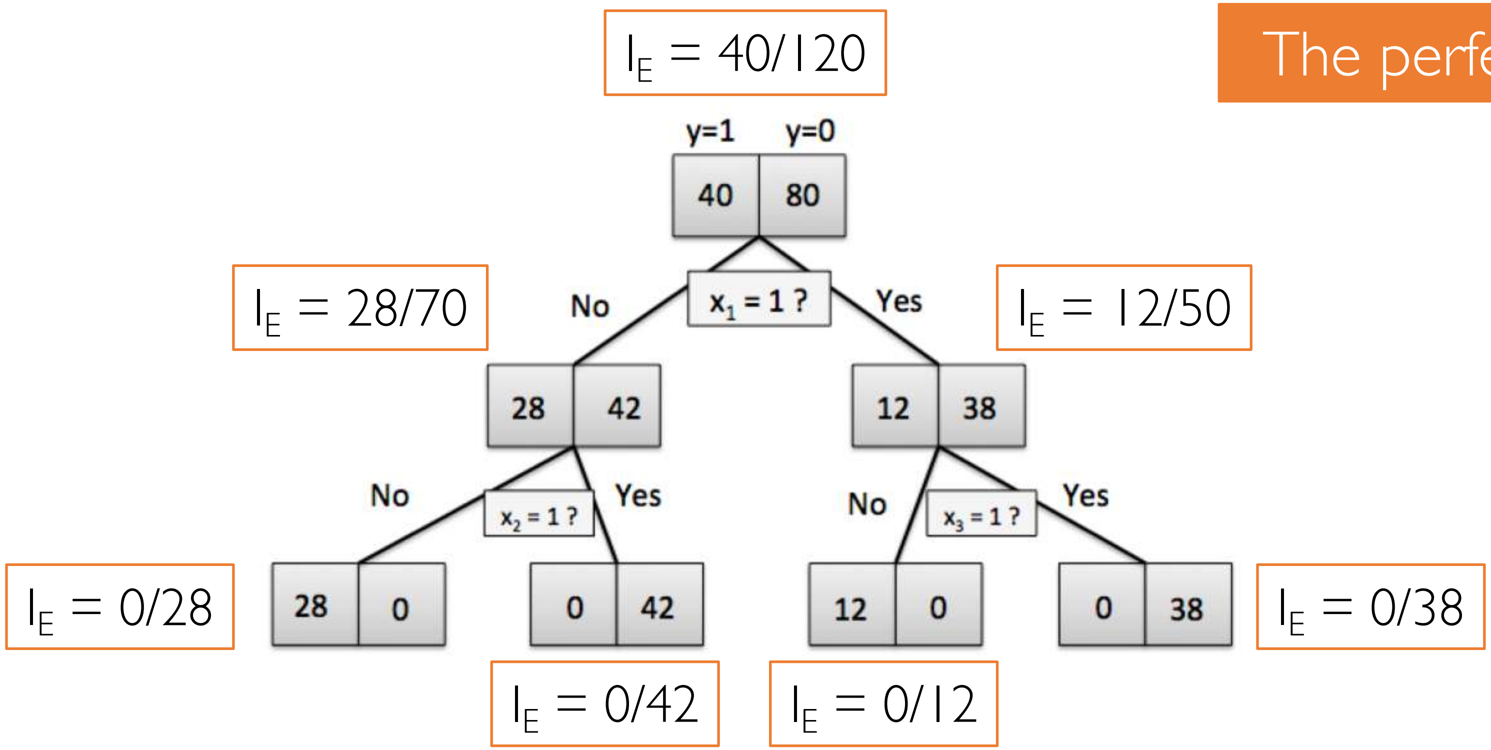
Classification Error Rate vs. Entropy (Gini)

The perfect tree cannot be built using I_E



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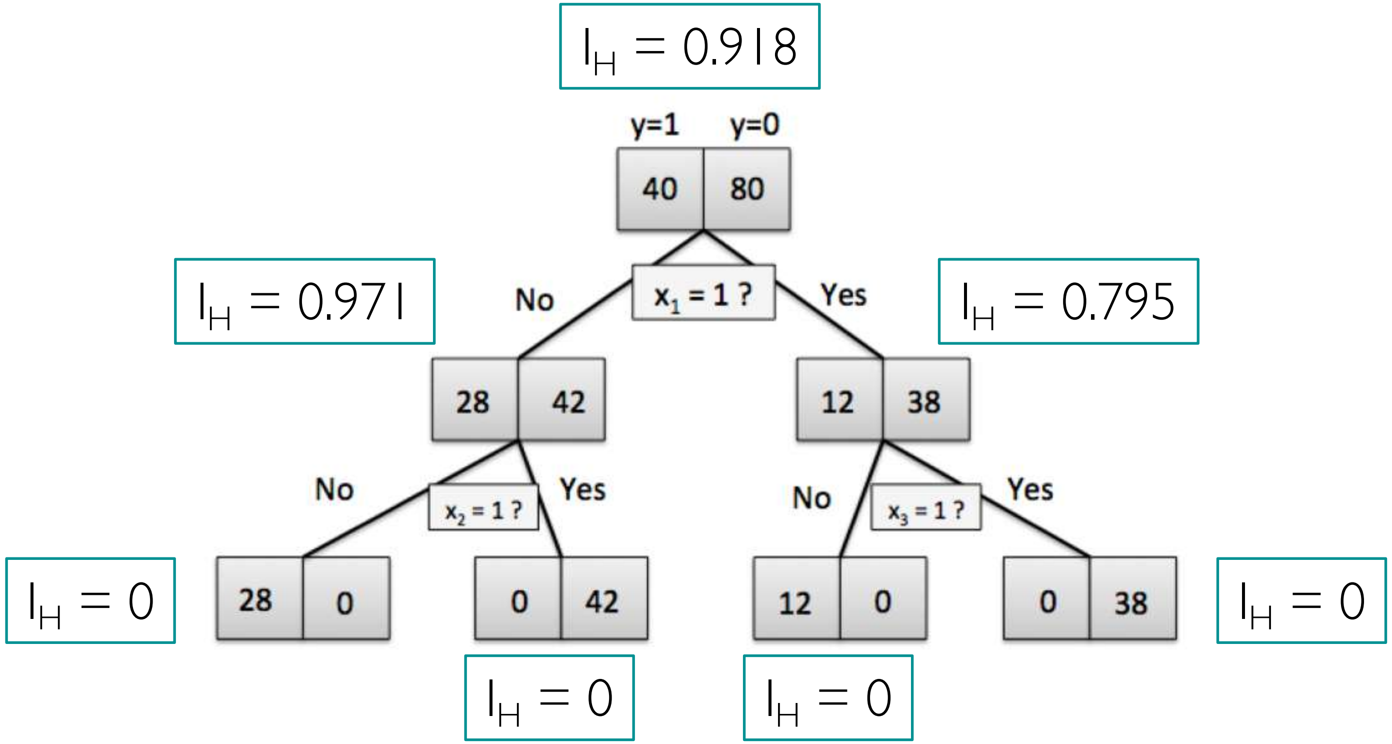
Classification Error Rate vs. Entropy (Gini)

Node impurity using I_H



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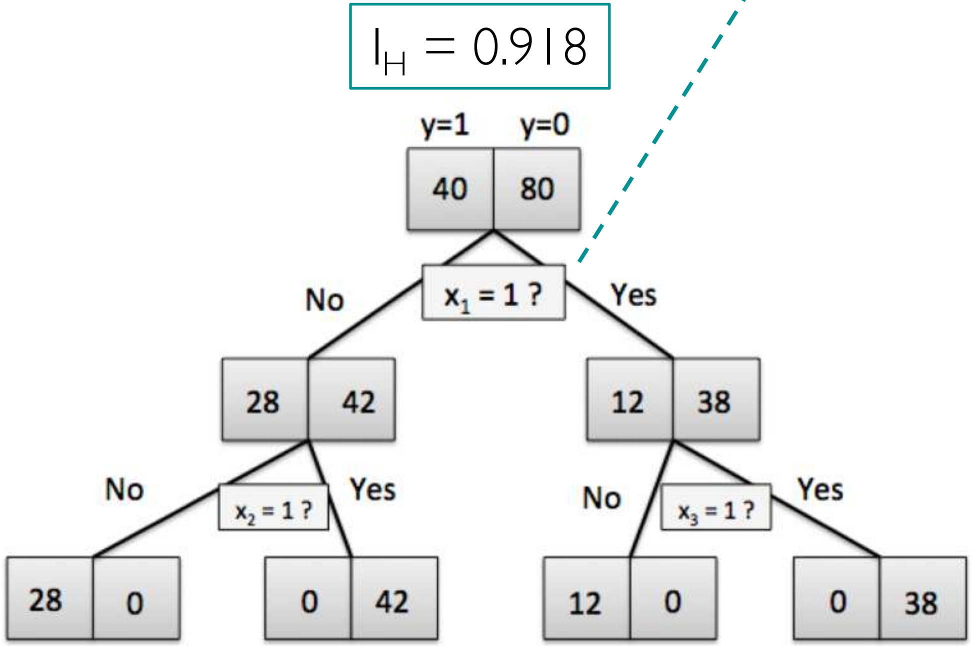

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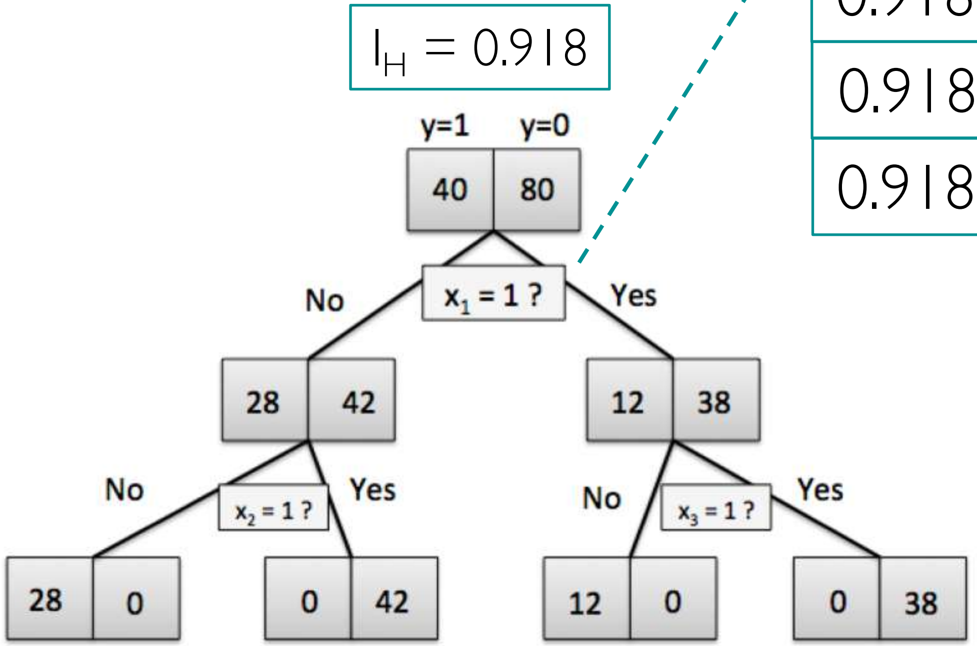

Compute IG of the first split using I_H

$0.918 - [(70/120 * 0.971) + (50/120 * 0.795)]$

$0.918 - [0.566 + 0.331]$

$0.918 - 0.897 = 0.021$

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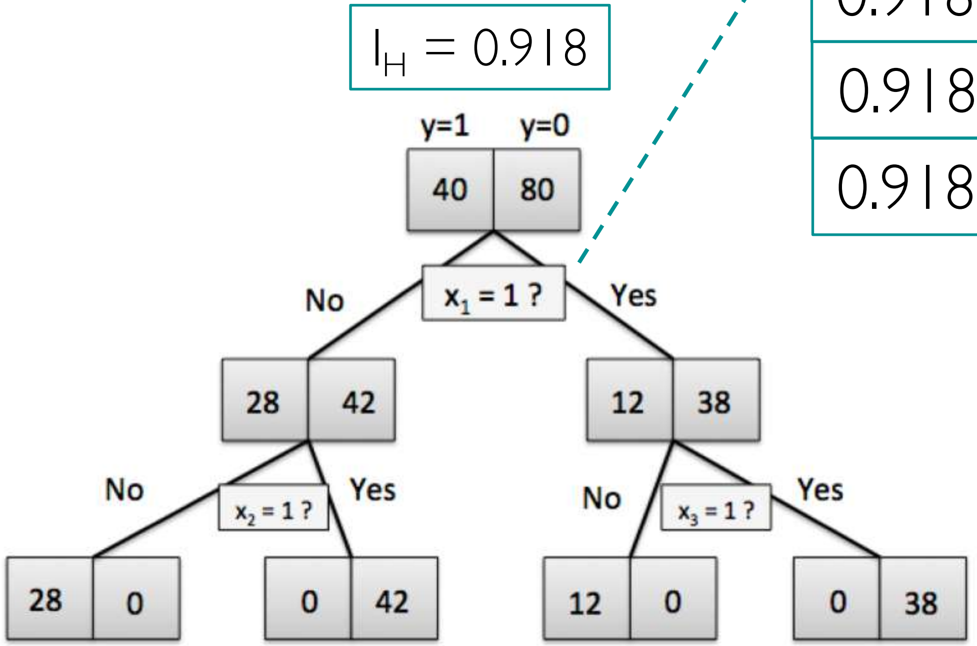

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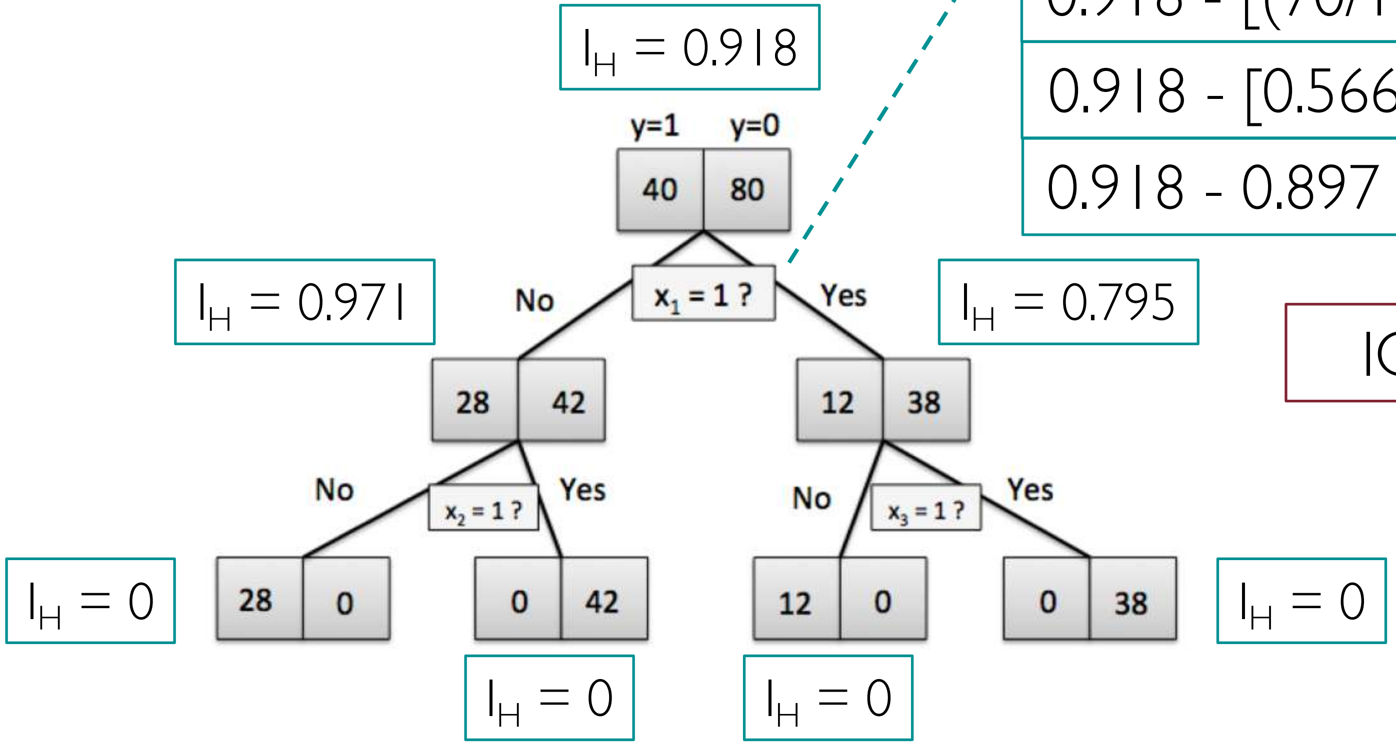

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The splitting rule would continue until the child nodes are pure

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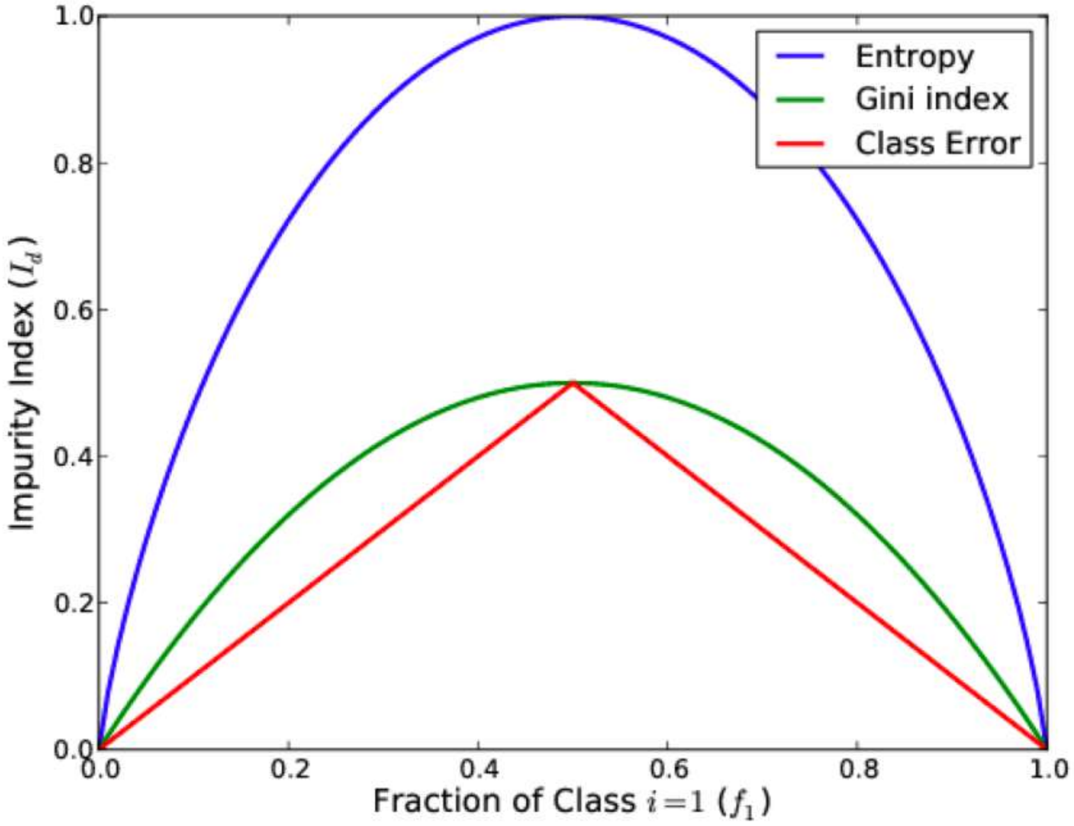

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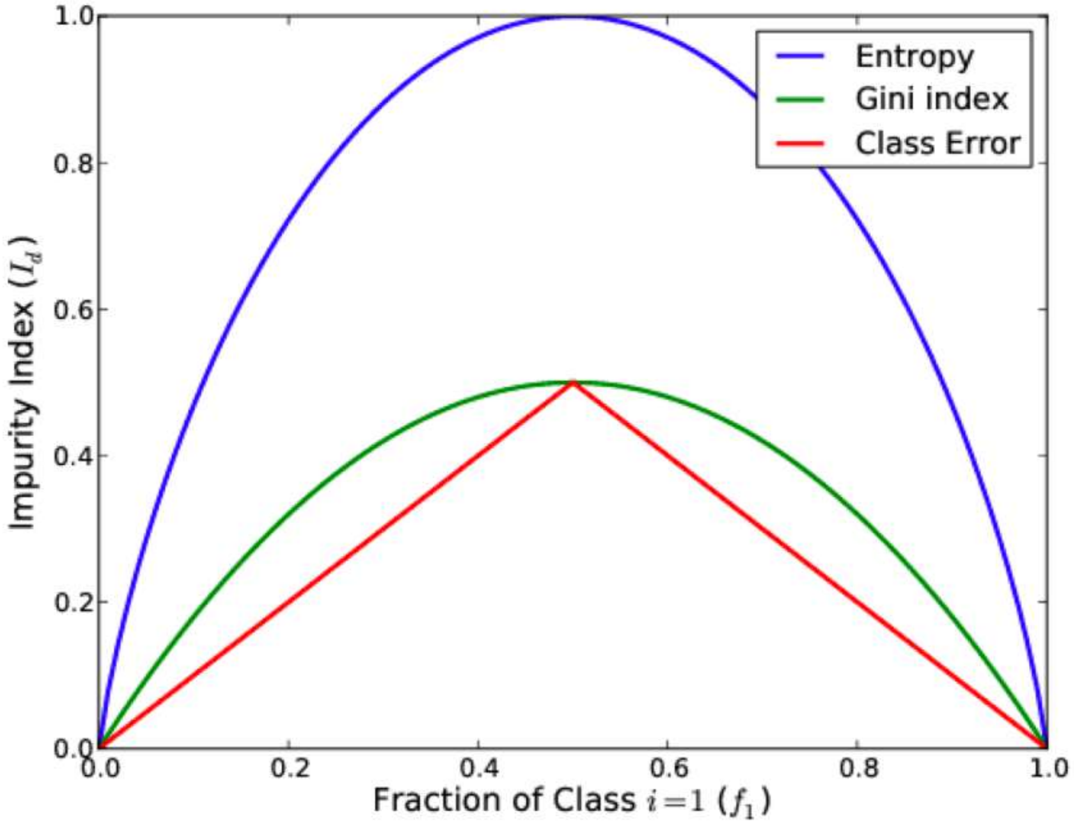

Gini and Entropy are "smoother" than classification error

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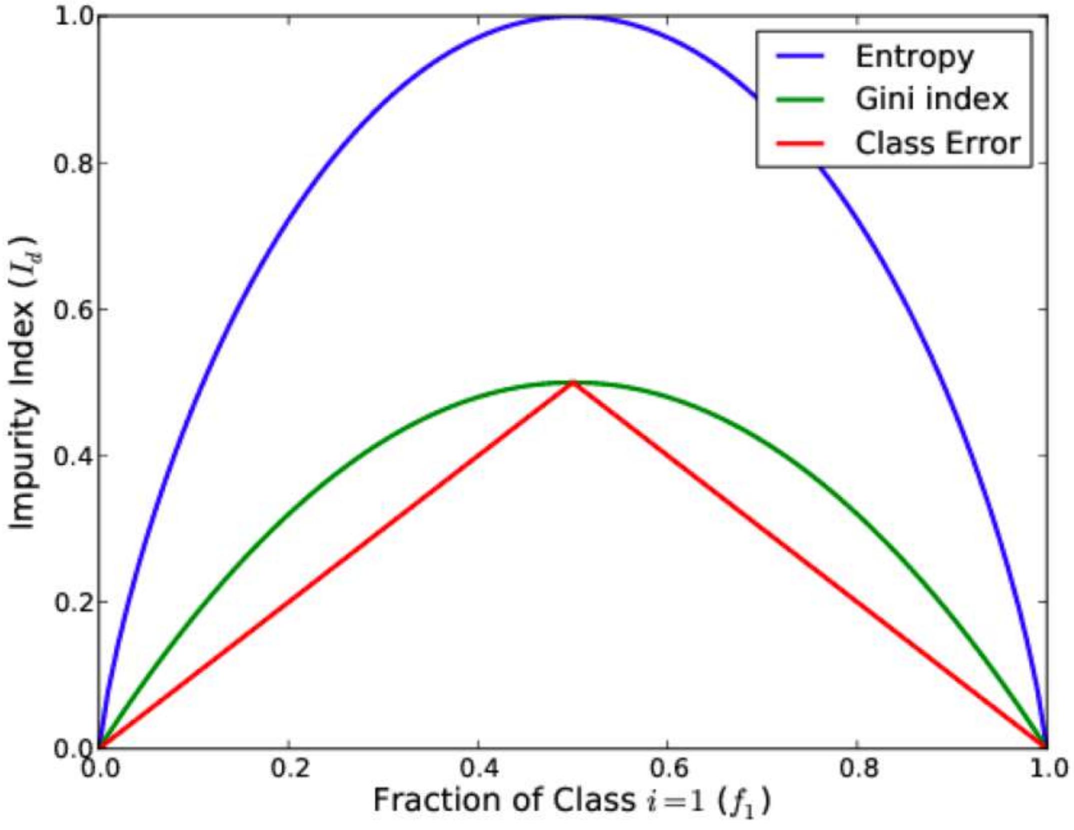

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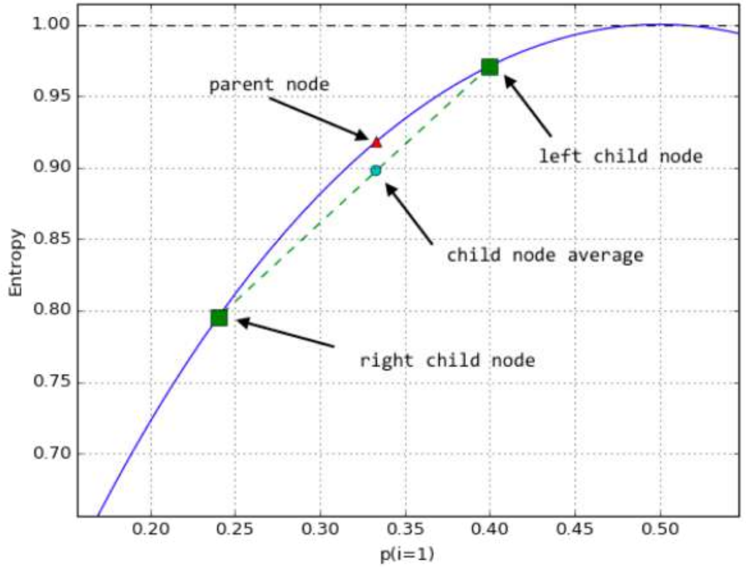

Entropy is always larger than the weighted averaged entropy due to its "bell shape"

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- Let N^+ (N^-) be the number of positive (negative) elements
- We define the ratio $p = N^+/N$ and $q = N^-/N$
- The entropy is defined as:

$$H = -\Big[p\log_2(p) + q\log_2(q)\Big] = -\frac{N^+}{N}\log_2\left(\frac{N^+}{N}\right) - \frac{N^-}{N}\log_2\left(\frac{N^-}{N}\right)$$

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- H is minimum (i.e., H=0) when either N^+ or N^- is equal to N
  - best case of a pure set (all the elements have the same label)

Evolution of Entropy

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Only because each x_i takes on a binary value, in general H ranges in [0, +infinity]

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splitting can't do worst!

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Linear Models vs. Decision Trees

Linear Models

$$h_{\boldsymbol{\theta}}(\mathbf{x}) = \theta_0 + \sum_{i=1}^{n} \theta_i x_i$$

Decision Trees

$$h(\mathbf{x}) = \sum_{j=1}^{J} c_j \cdot \mathbf{1}_{R_j}(\mathbf{x})$$

Learned hypothesis is constant within a region

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If there is a strong linear relationship between input and output

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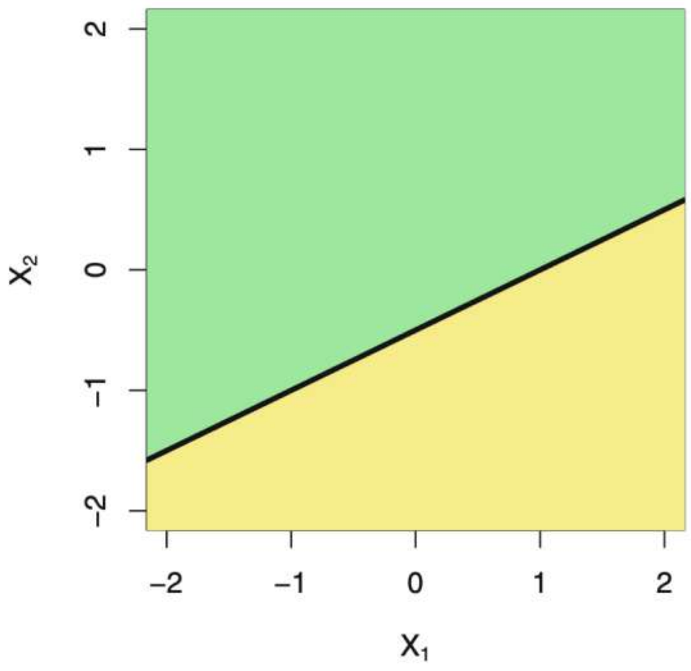
Which one is better?

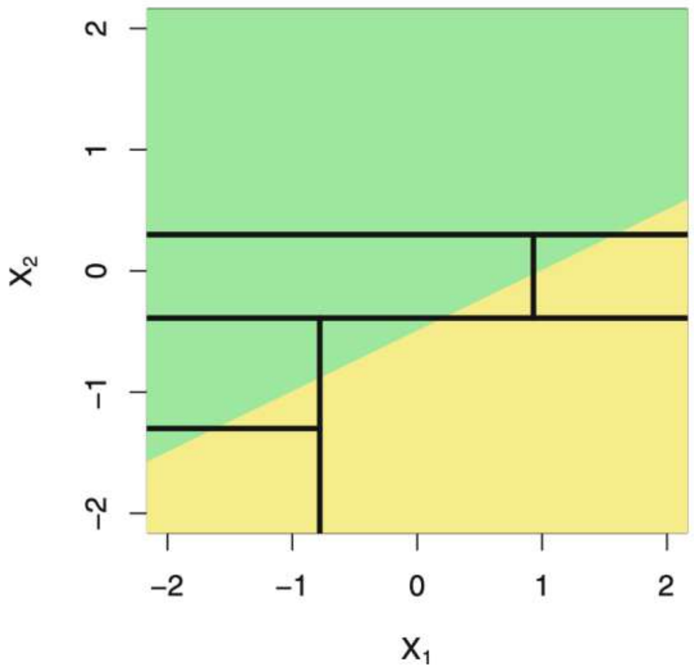
If there is a highly non-linear relationship between input and output

Linear Models vs. Decision Trees: Example

Linear Regression



Decision Tree



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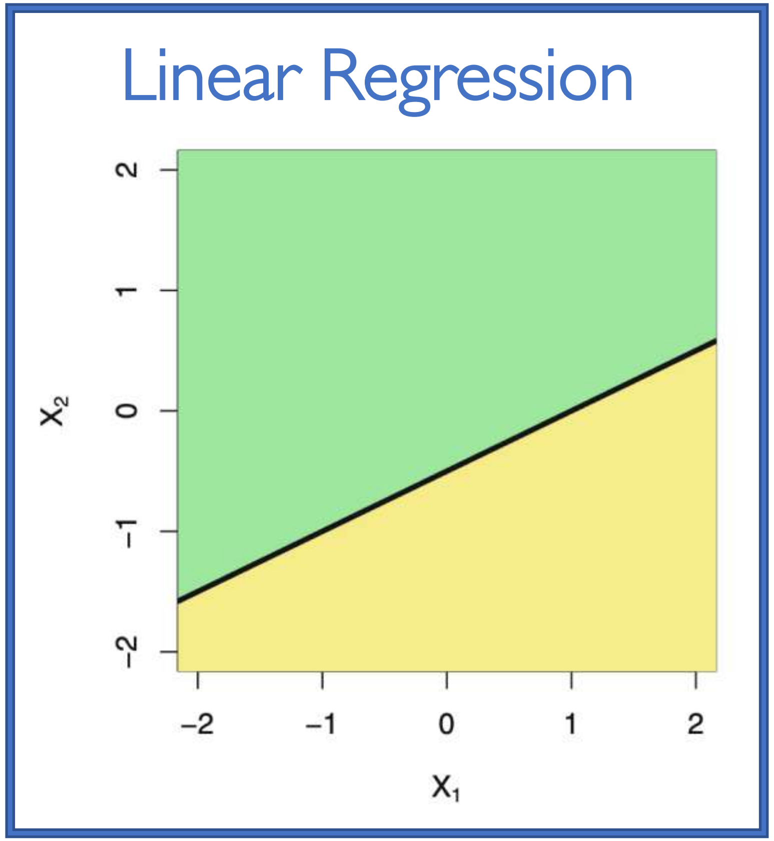

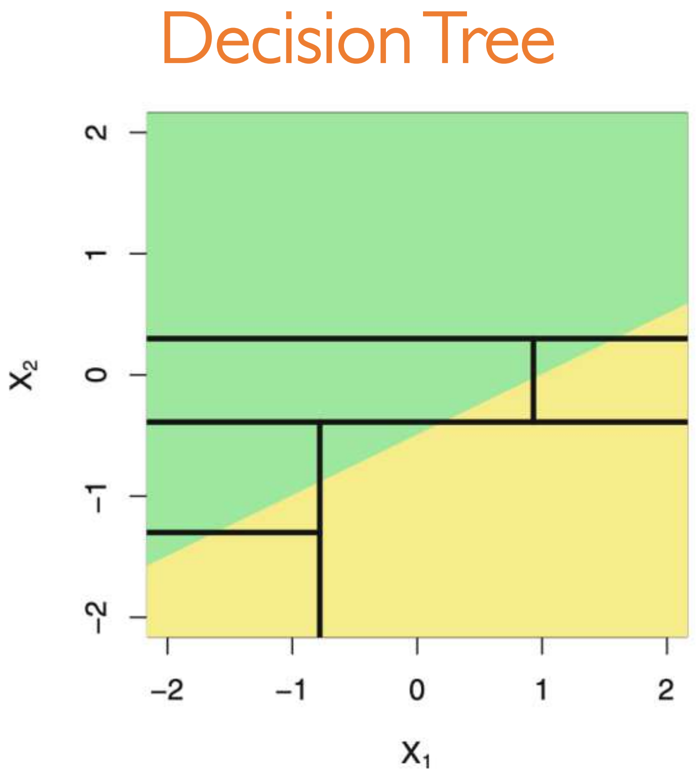

Nice linear decision boundary

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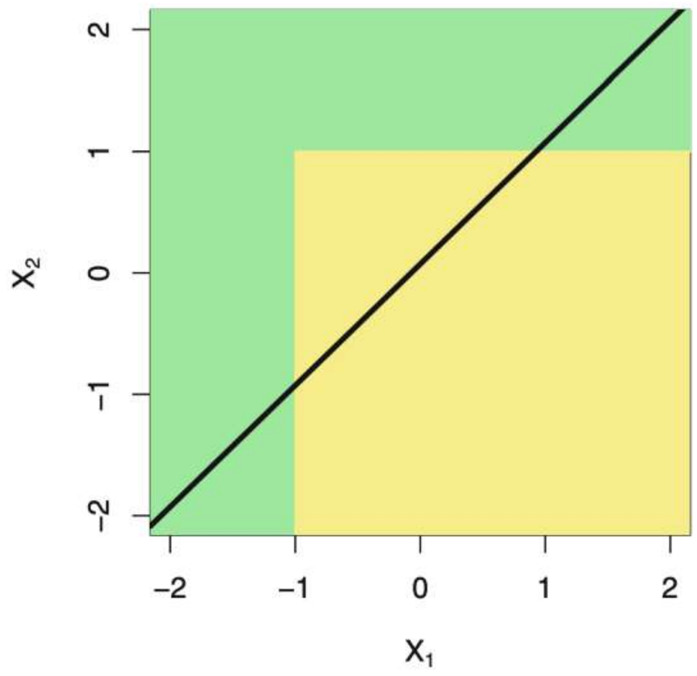

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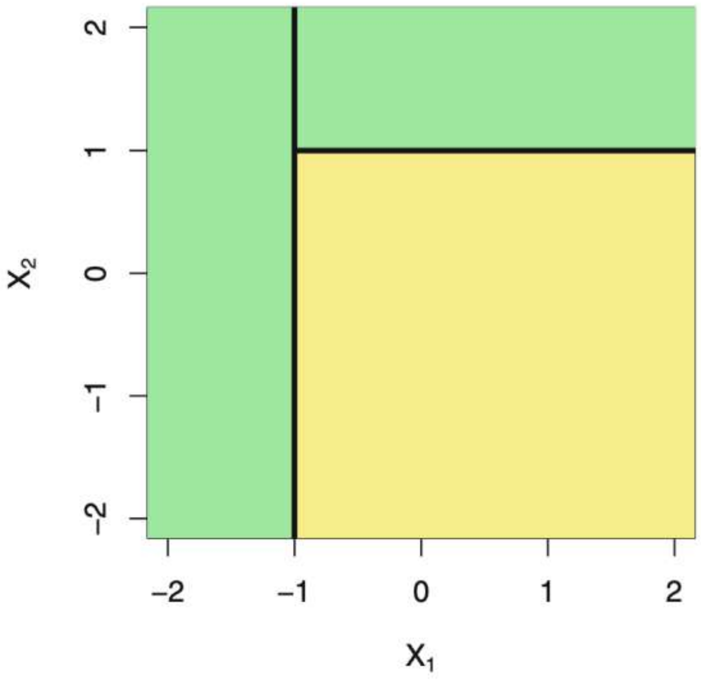

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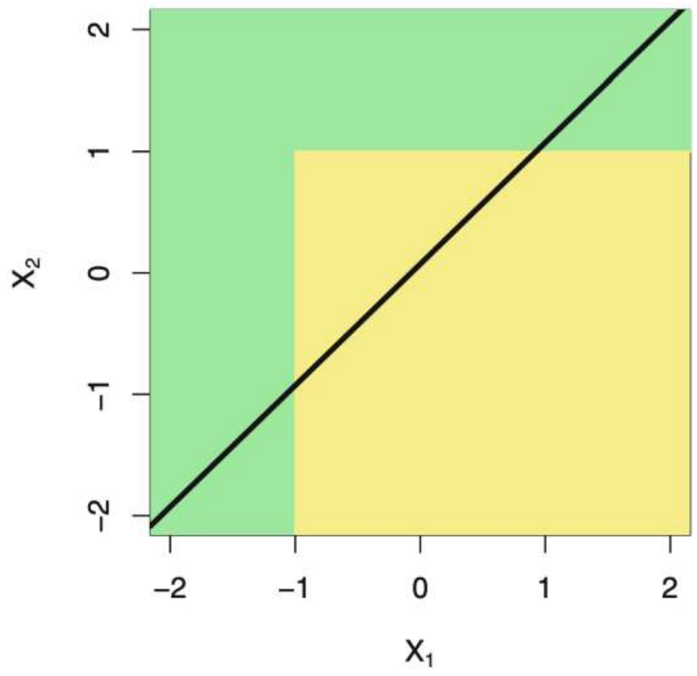

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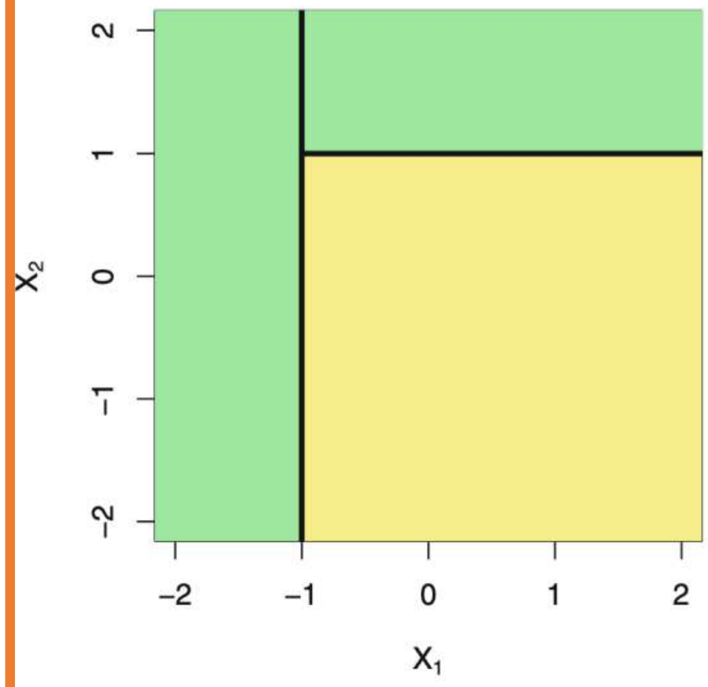

Non-linear decision boundary

Decision Trees: Pruning

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Intuitively, by selecting the subtree with the smalles test error!

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Cost Complexity Pruning (a.k.a. Weakest Link Pruning)

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- We can select a value of α using a validation set or cross-validation

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- Trees can easily handle categorical features without the need to create dummy variables (i.e., one-hot encoding)

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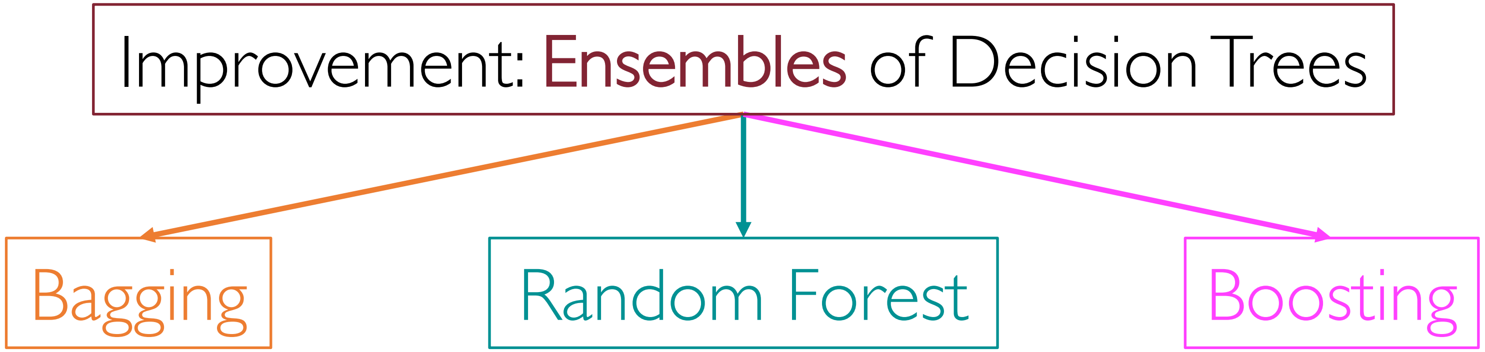

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- Low-variance approaches, instead, are less sensitive to different training sets
- Bootstrap aggregation (Bagging) is a general-purpose method to lower the variance of a statistical learning method

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Averaging a set of observations reduces variance!

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$\Downarrow$

Bootstrap

Taking repeated samples from the same training set

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Generate B different bootstrapped samples from the original training set

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- When used with classification trees the final prediction is typically obtained via majority voting
  - The overall prediction is just the most common across the B models

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- Still, one can obtain an overall summary of the importance of each feature using RSS (regression) or Gini index/Entropy (classification)
- Add up the total RSS/Gini index reduction obtained splitting on a certain feature and take the average over all the B trees

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- This may sound crazy, but it has a clever rationale

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Lower variance reduction

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Random Forests: Rationale

- Enforce random sampling of k out of n features at each split
- The probability a split considers the strongest predictor is k/n
  - Hypergeometric distribution (1 success, k draws with replacement, pop. size = n)
  - For k = sqrt(n) this means 1/sqrt(n)
- We can think of this process as **decorrelating** the trees
- Note that when $k = n$ this simply resembles to bagging
- As with bagging, random forests will not overfit if we increase B

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- In bagging, each tree is built on a bootstrap data set, independent of the other trees
- Boosting works in a similar way, except that the trees are grown sequentially using information from previously grown trees
- Boosting does not involve bootstrap sampling; instead each tree is fit on a modified version of the original data set

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- Consider boosting regression trees:
  1. Fit the tree to the current residuals rather than the actual response Y
  2. Add this new decision tree into the fitted function so as to update the residuals
  3. Each of these trees can be rather small, with just a few terminal nodes, determined by a model's hyperparameter (d)
  4. The shrinkage parameter λ slows the process down even further, allowing more and different shaped trees to attack the residuals

Boosting: Algorithm

Algorithm 8.2 *Boosting for Regression Trees*

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all i in the training set.
2. For $b = 1, 2, \ldots, B$, repeat:
   (a) Fit a tree $\hat{f}^b$ with d splits ($d+1$ terminal nodes) to the training data (X, r).
   (b) Update $\hat{f}$ by adding in a shrunken version of the new tree:
   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x). \tag{8.10}$$
   (c) Update the residuals,
   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i). \tag{8.11}$$
3. Output the boosted model,
$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x). \tag{8.12}$$

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- Tuning done via validation or cross-validation

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Take-Home Message of Today

- Decision Trees (DTs) highly expressive yet interpretable models both for regression and classification
- Learning the optimal DT is NP-Complete: Recursive Binary Splitting algorithm is an effective greedy heuristic
- DTs tend to overfit and have a low prediction accuracy
- Pruning and Ensembling techniques overcome both issues