Big Data Computing

Master's Degree in Computer Science

2019-2020

SAPIENZA
UNIVERSITÀ DI ROMA

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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)

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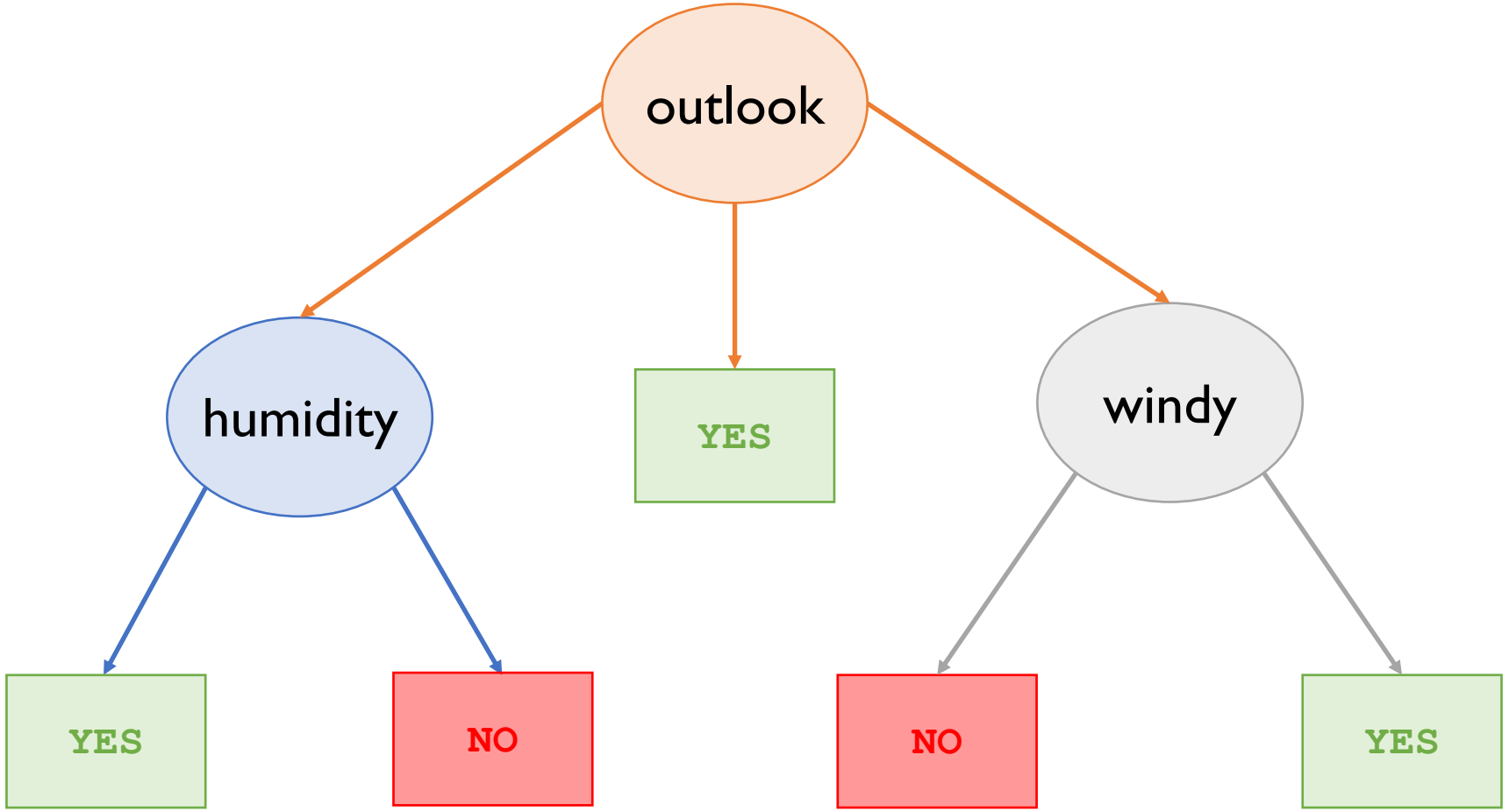
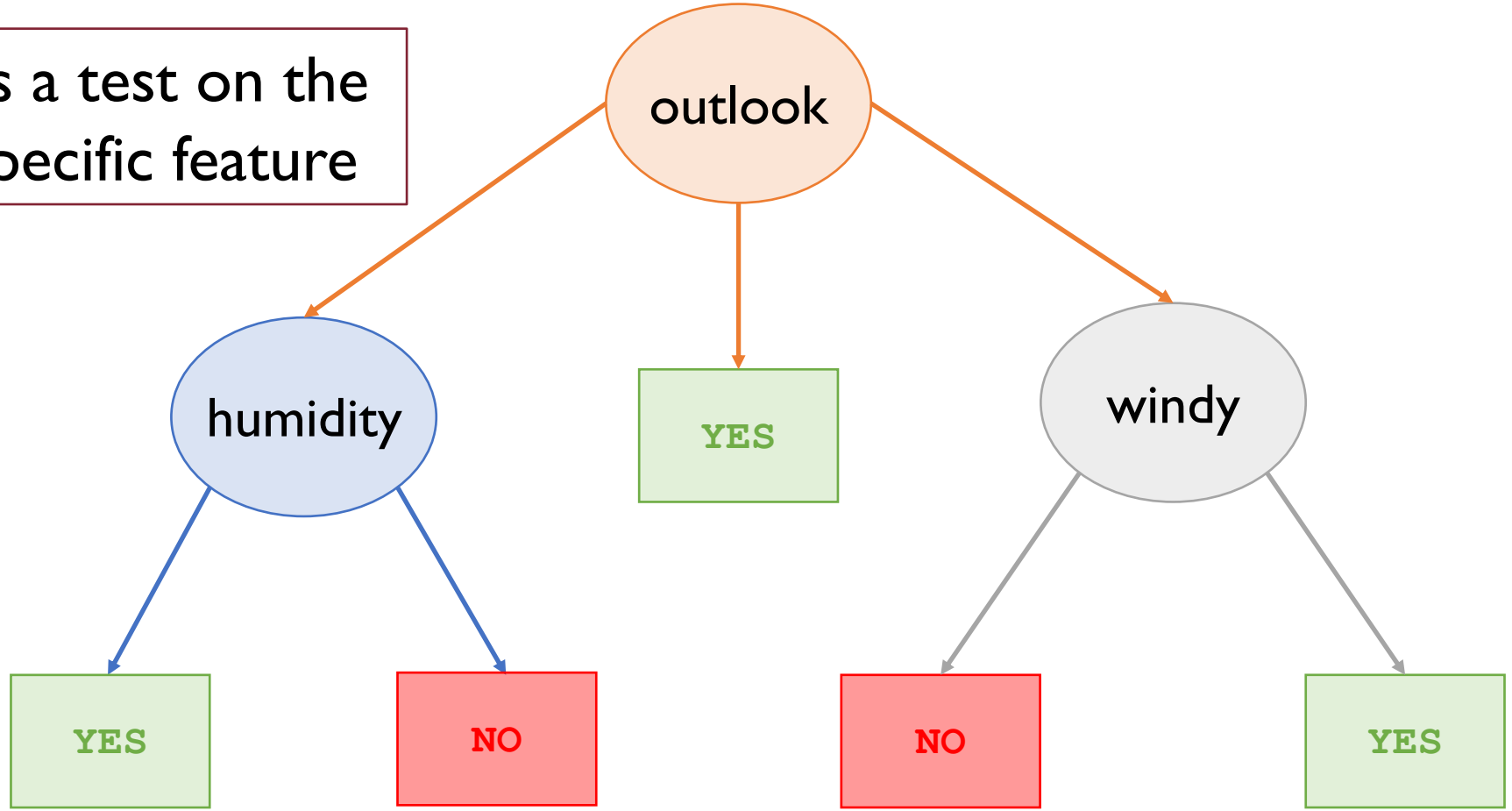
- The set of splitting rules can be represented as a tree (**decision tree**)
- Highly human-interpretable models

Decision Tree: An Example



Decision Tree: An Example

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



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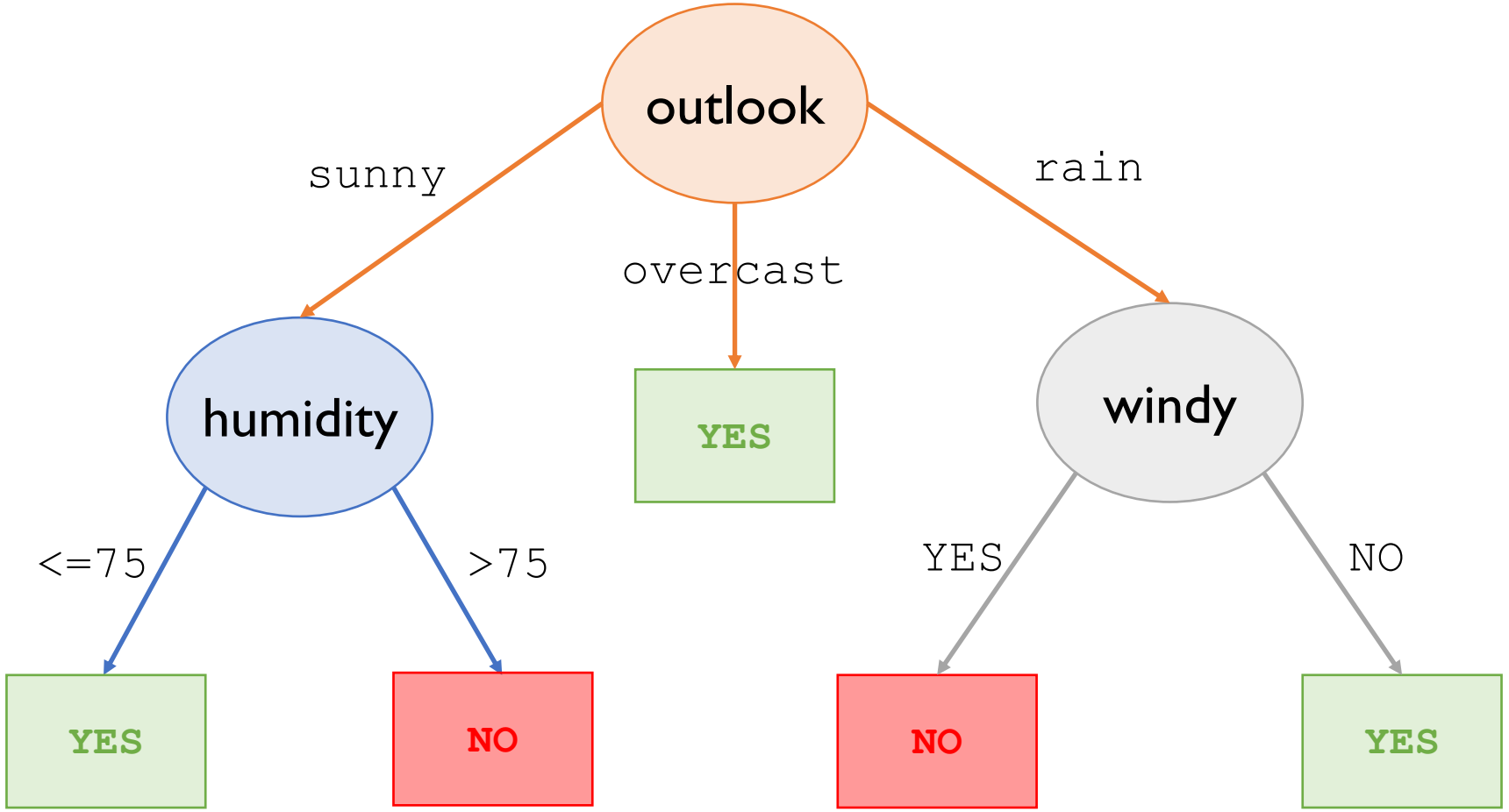

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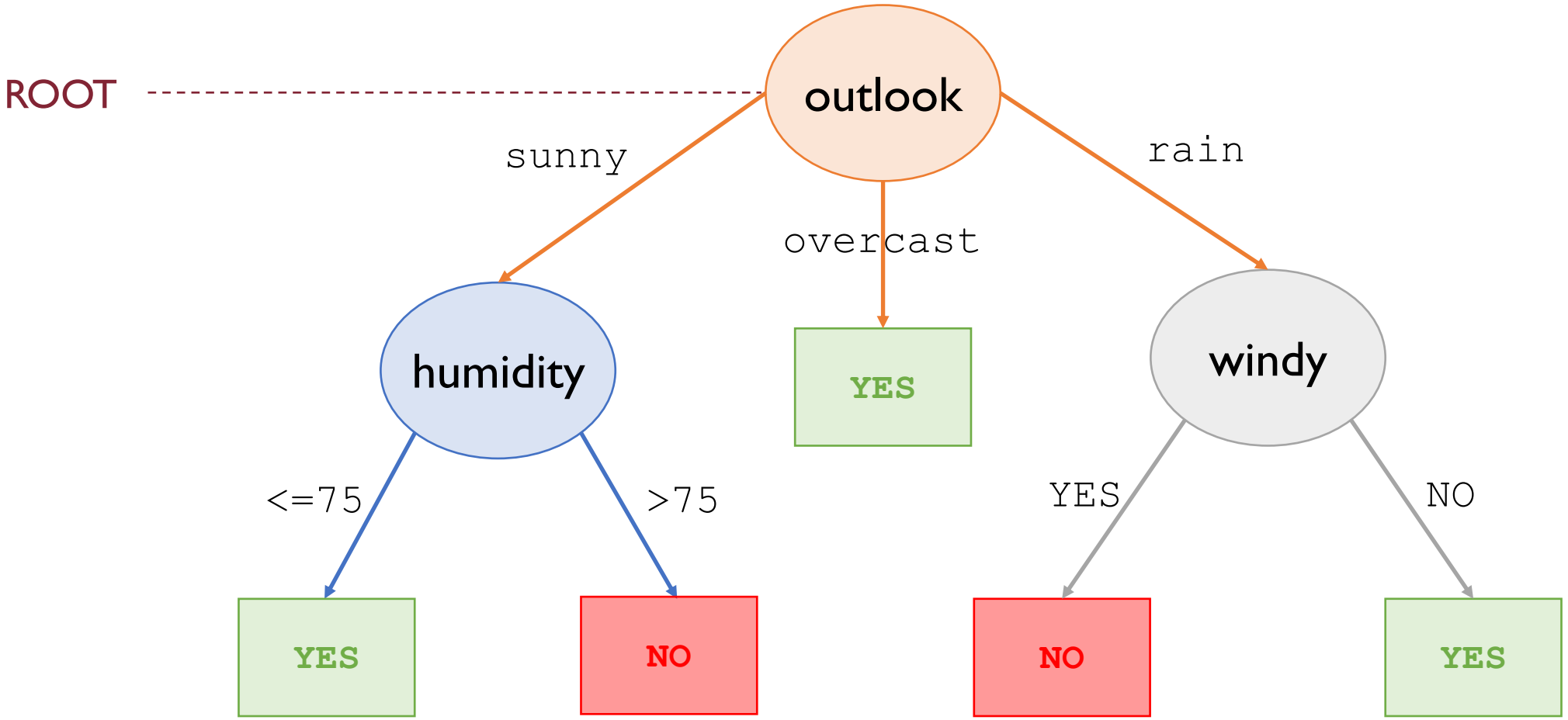

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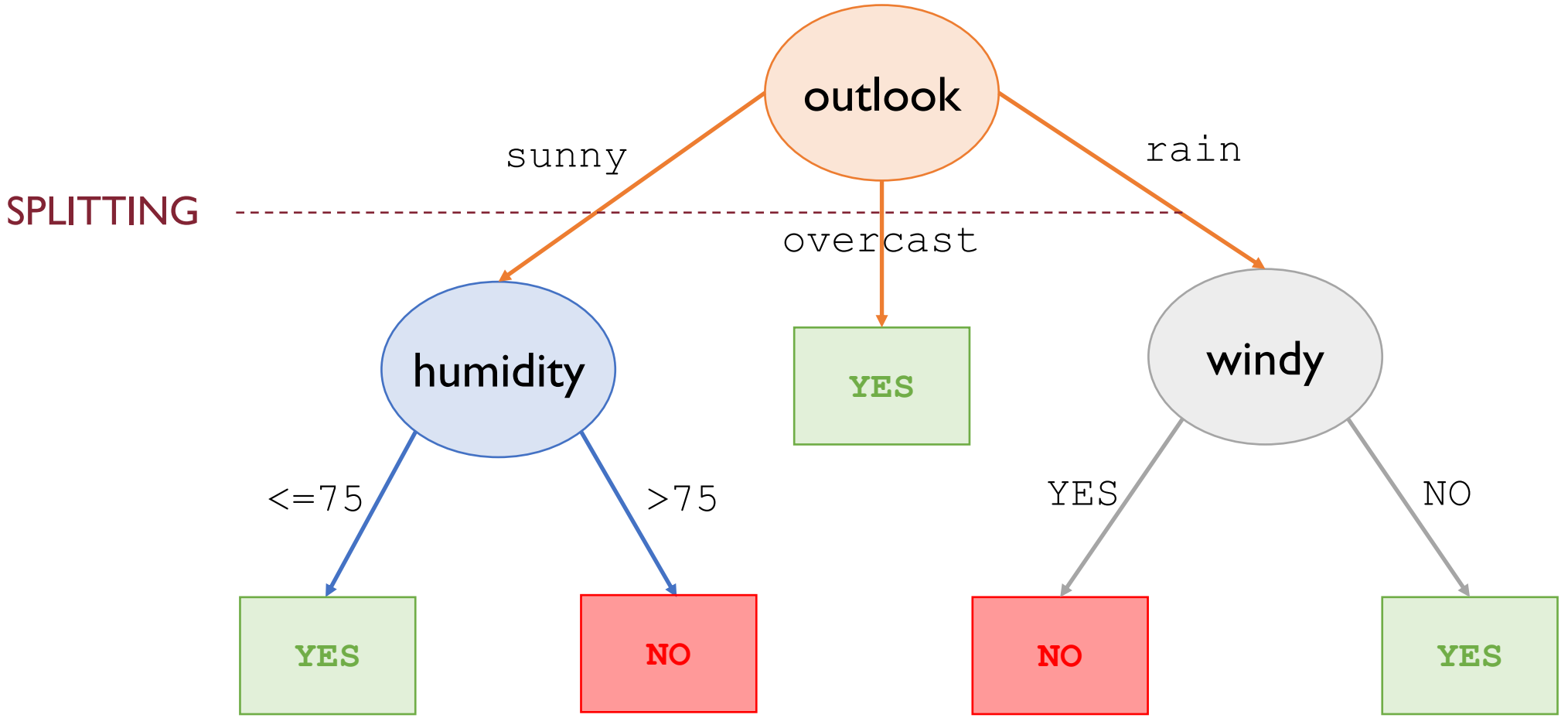

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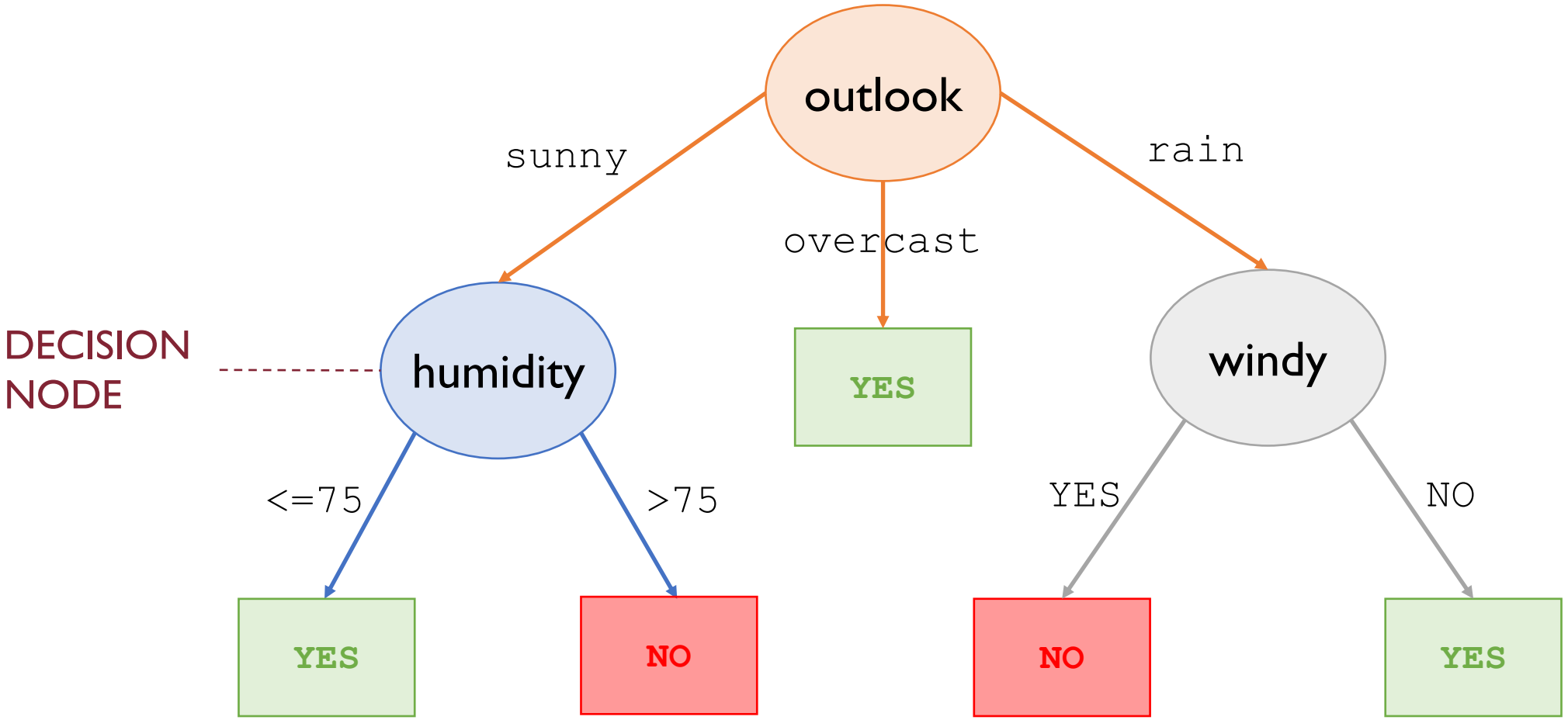

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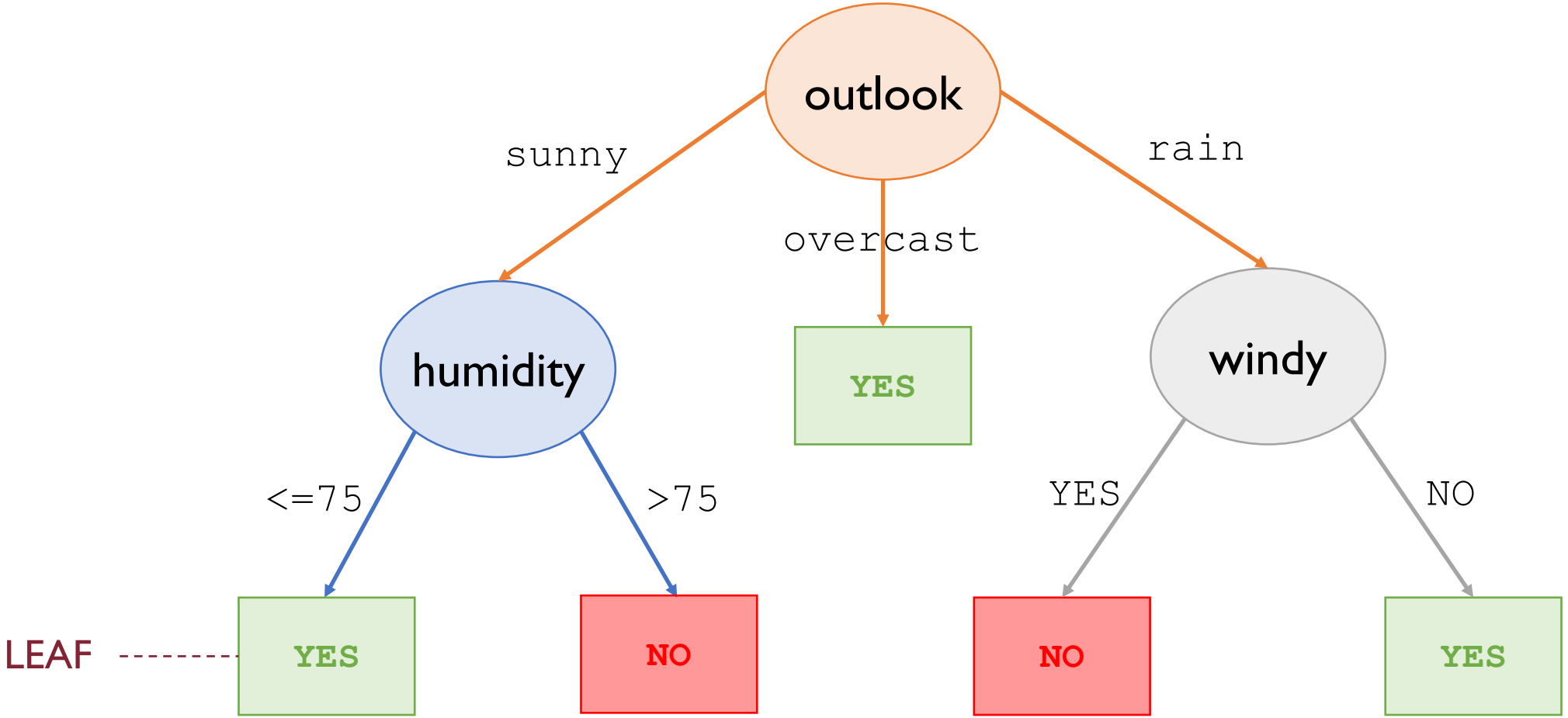

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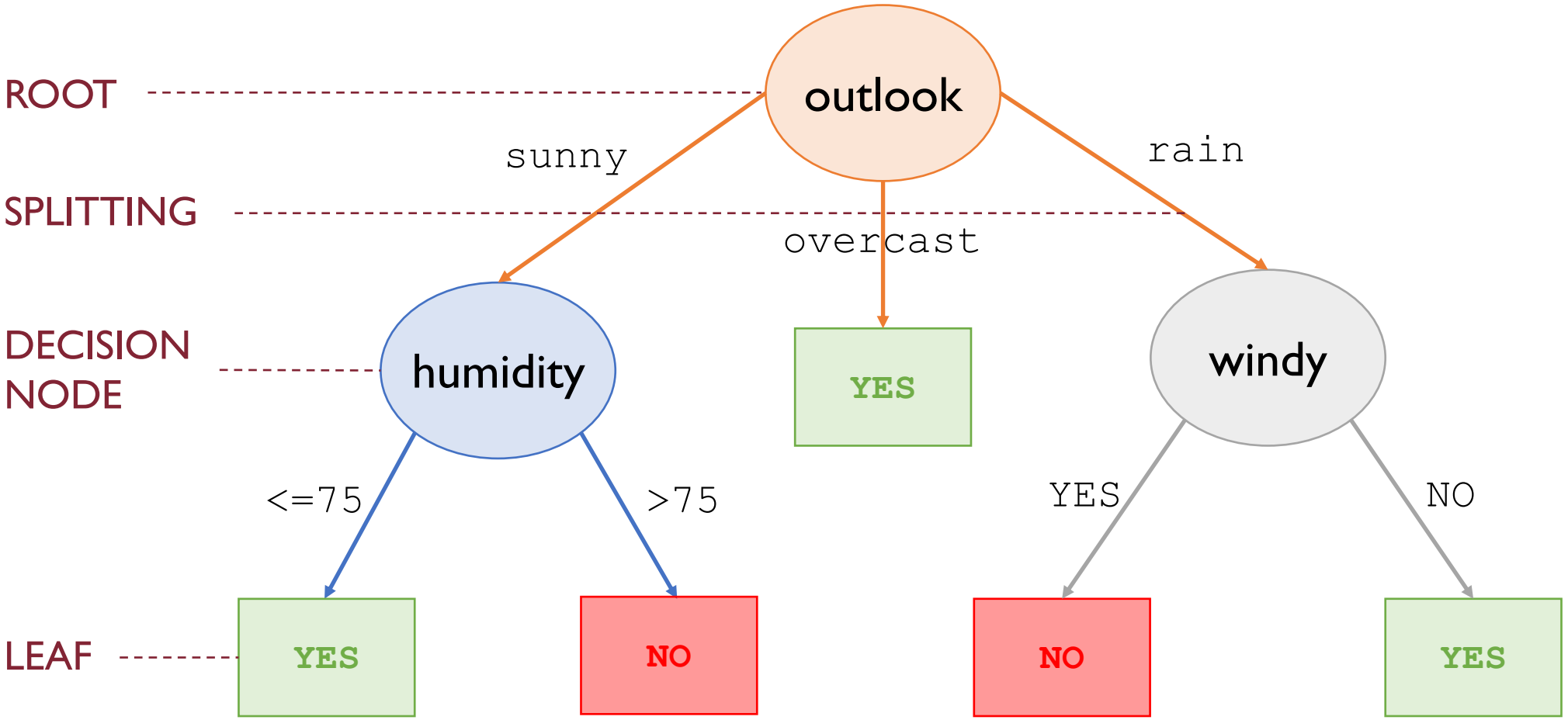
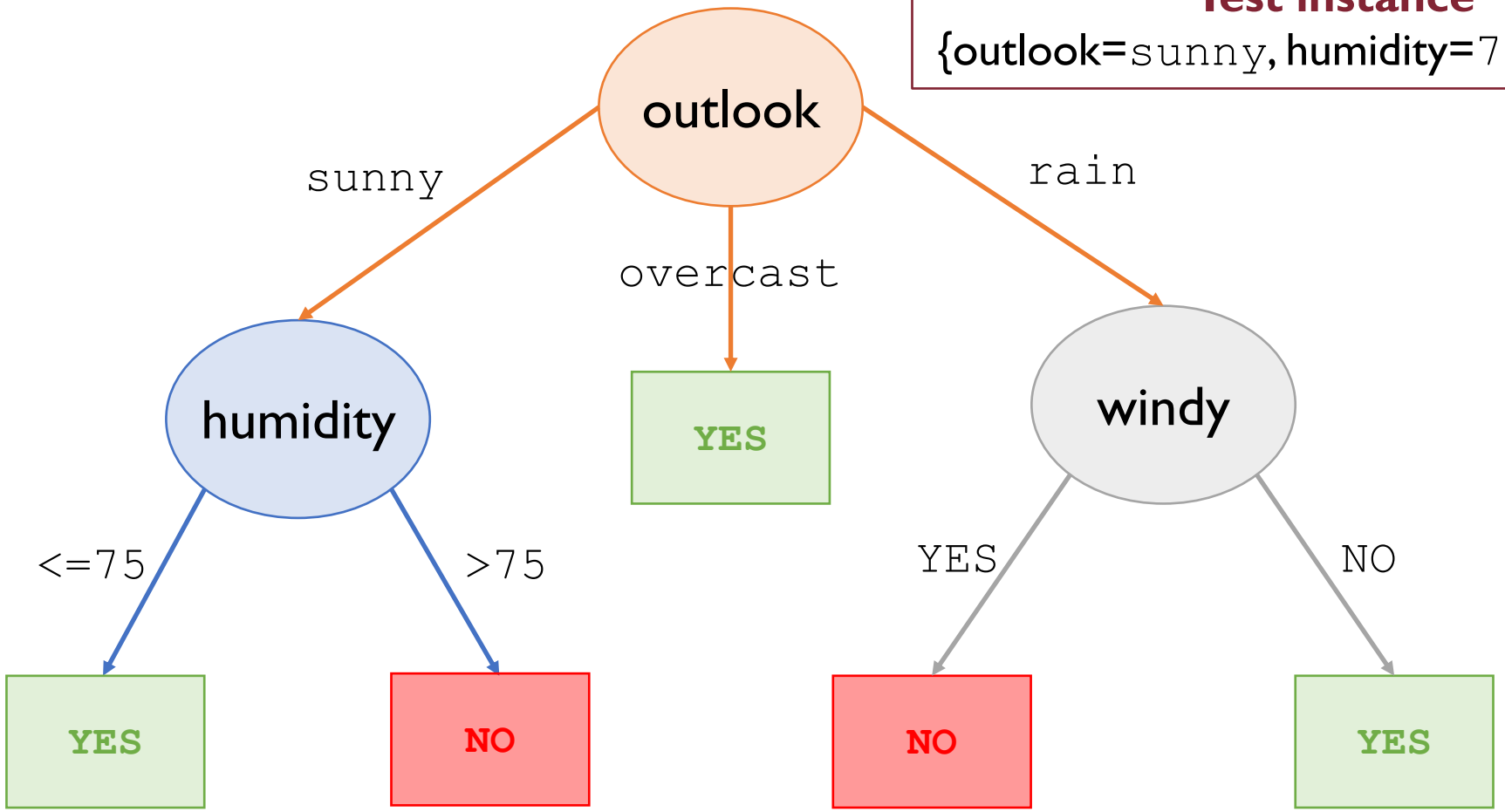


Decision Tree: An Example

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



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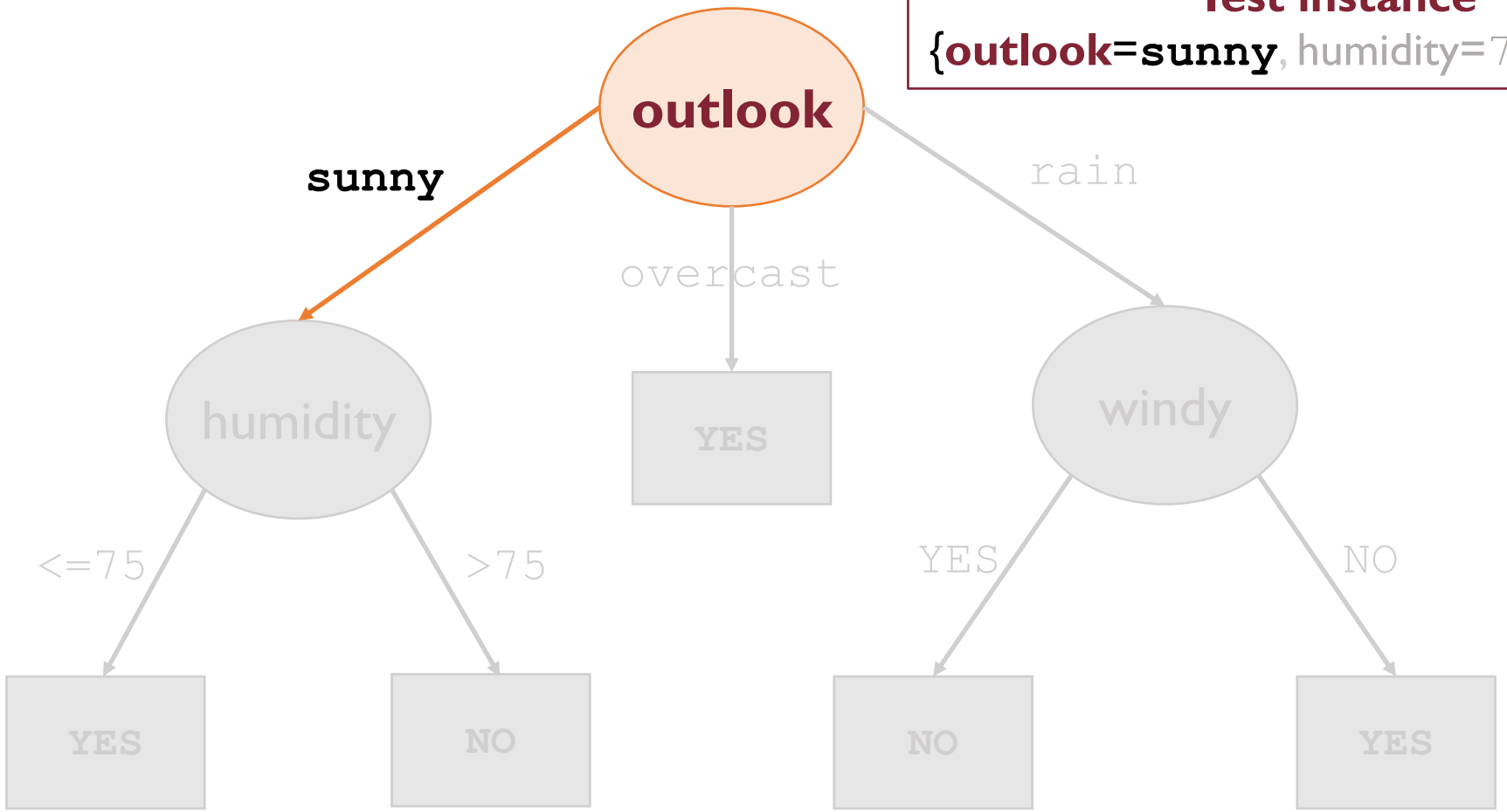

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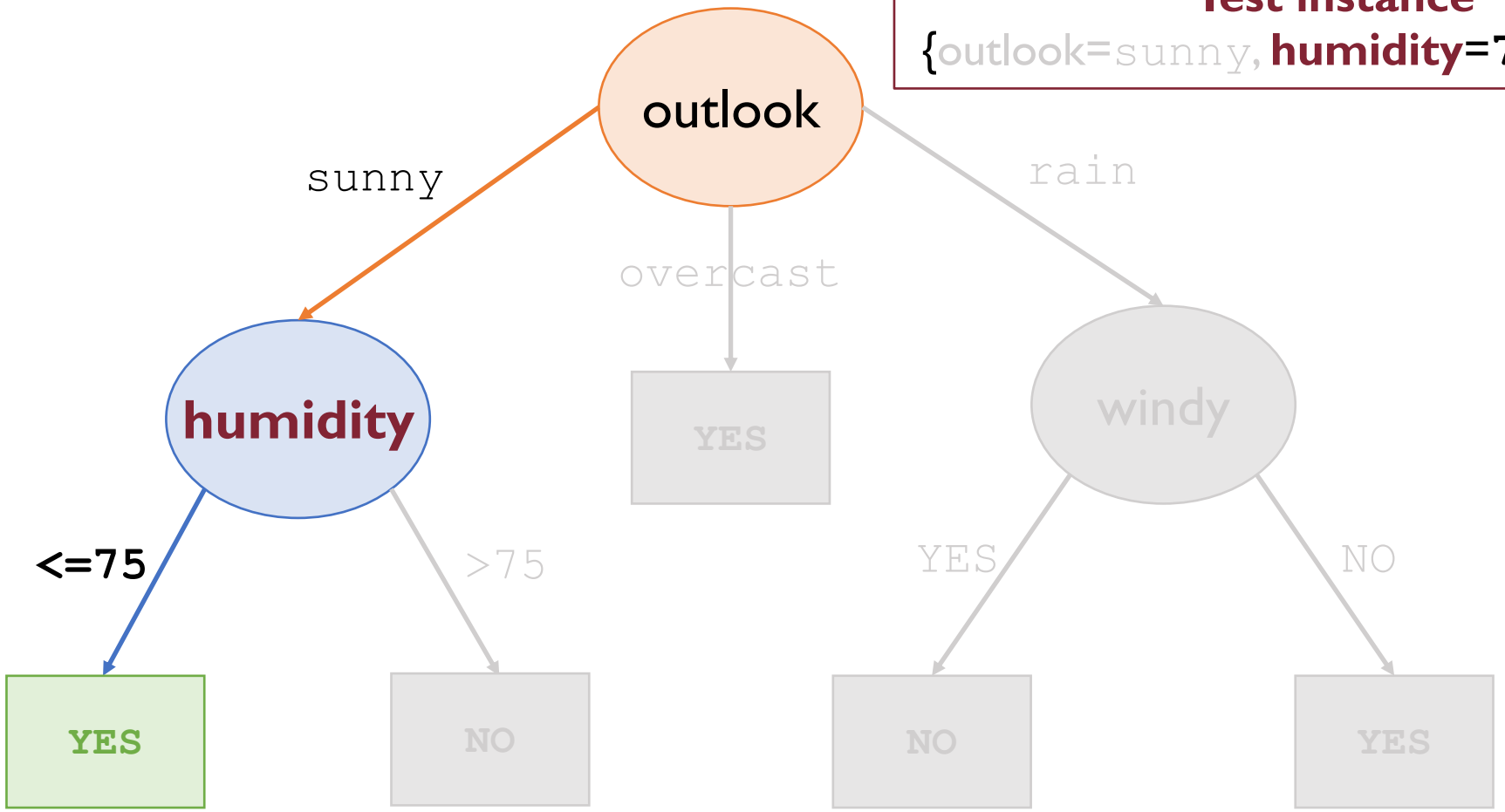

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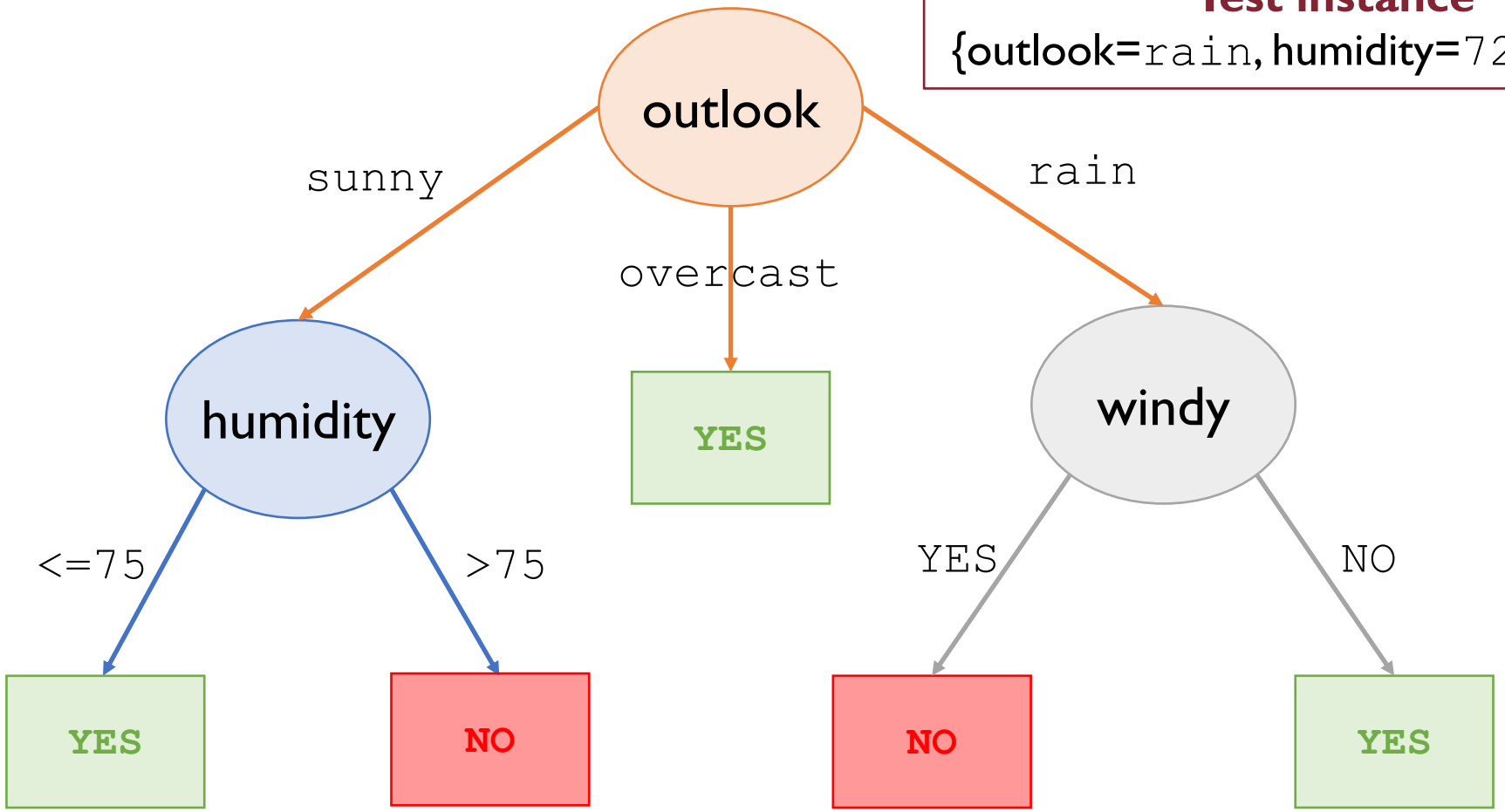

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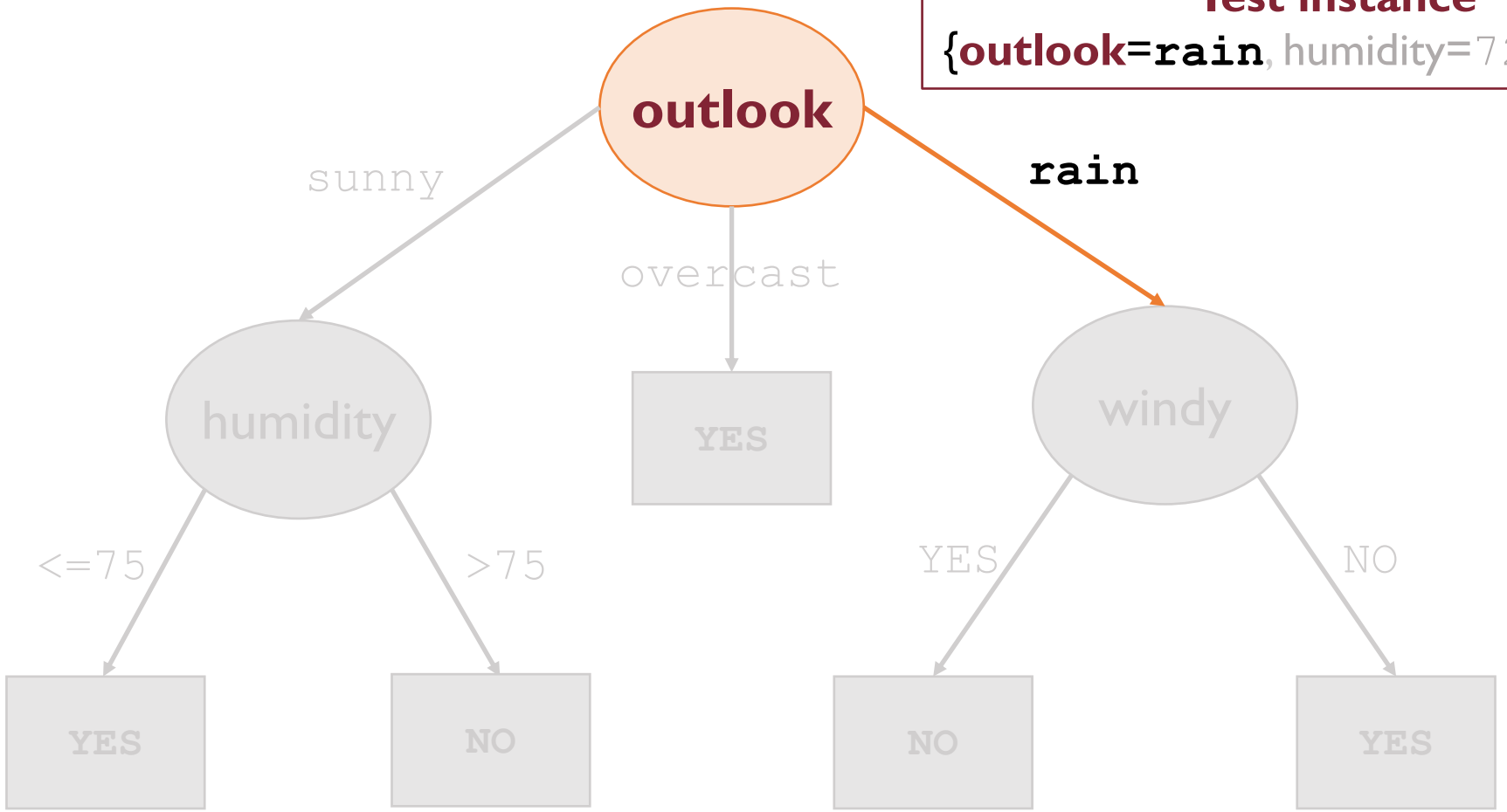

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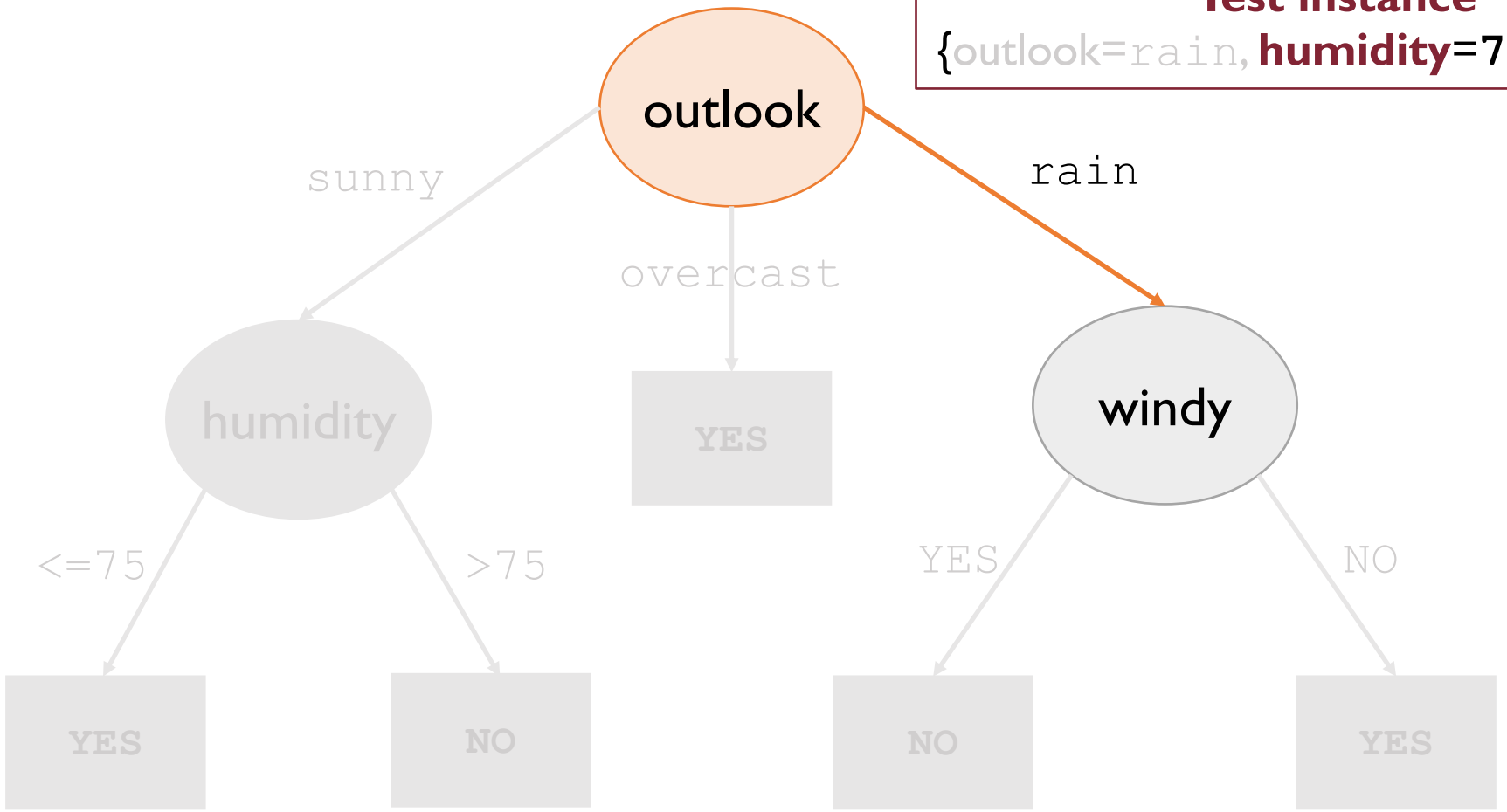

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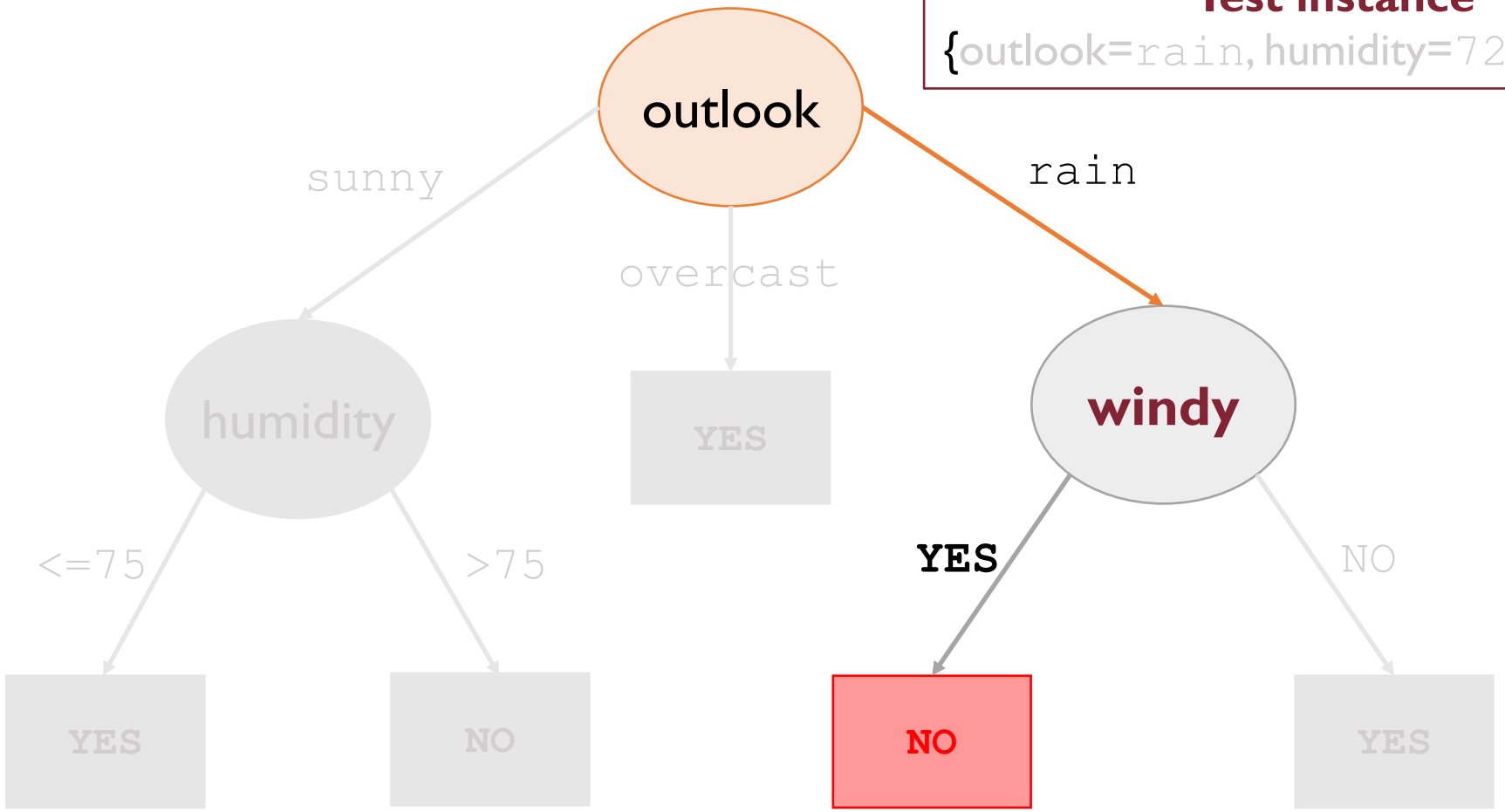

A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$ — input feature space

$\mathcal{Y}$ — output space

$\mathcal{Y} \in \mathbb{R}$ — real-value label of the *i*-th instance (regression)

$\mathcal{Y} \in \{1, \ldots, k\}$ — discrete-value label of the *i*-th instance (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

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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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Minimize the Residual Sum of Squares

$$\mathrm{RSS} = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \bar{y}_{R_j})^2$$

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The mean computed from observations in R_j

Discrete vs. Continuous Inputs

Discrete Inputs

(e.g., boolean)

One branch for each value

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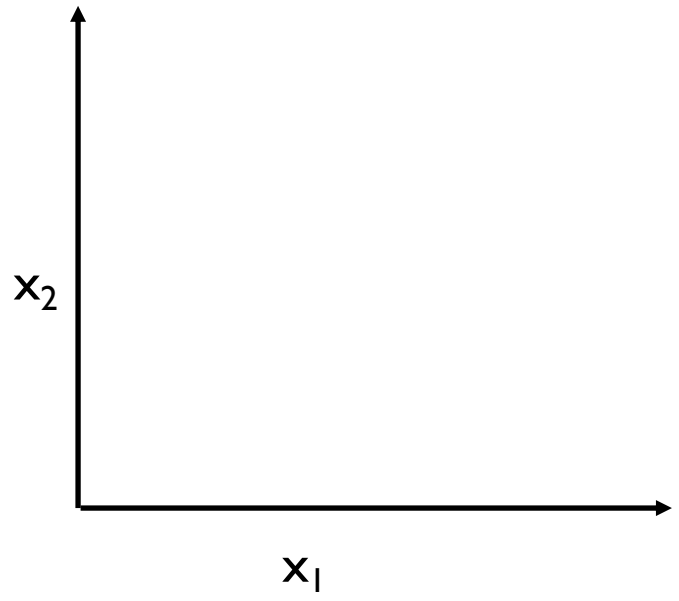

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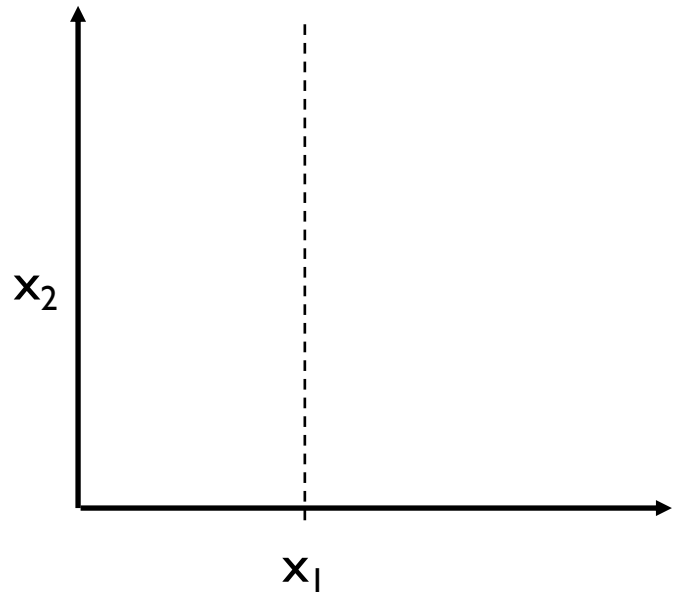

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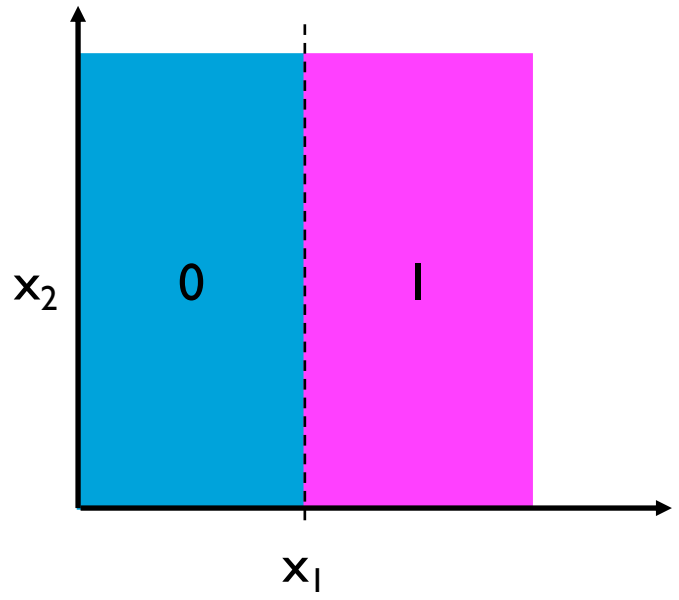

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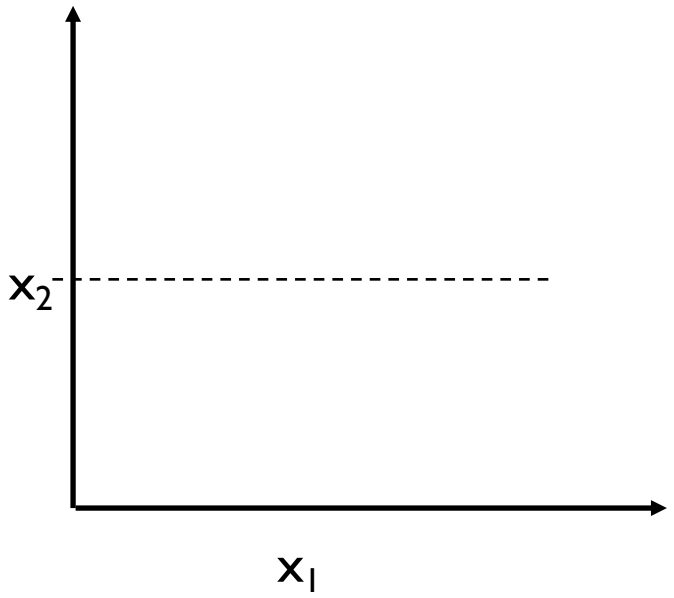

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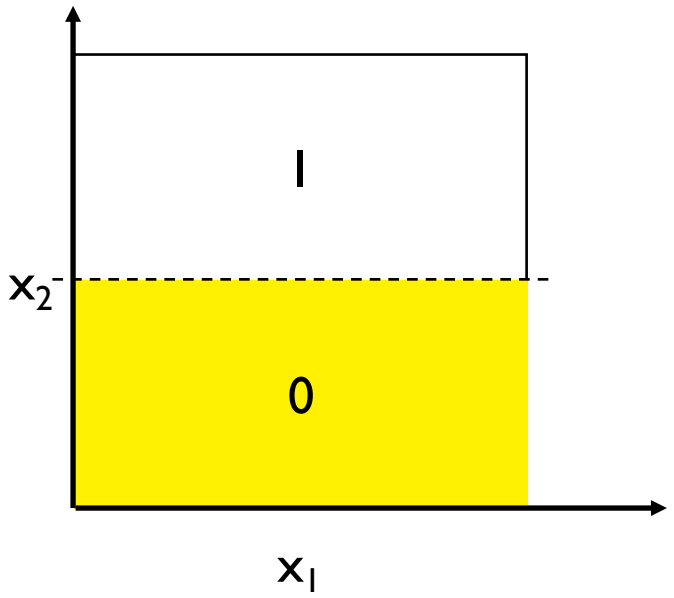

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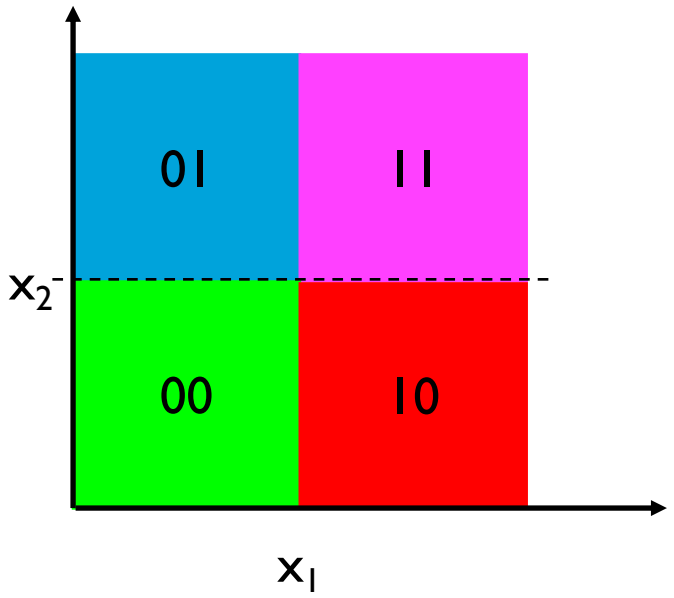

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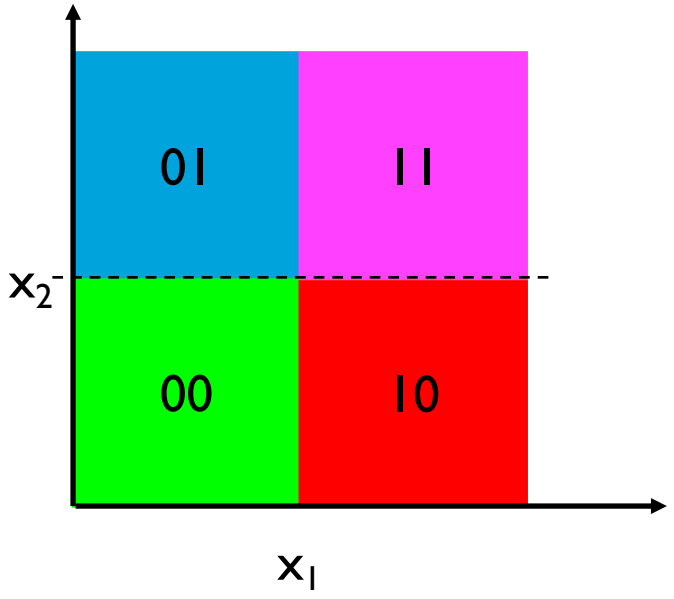

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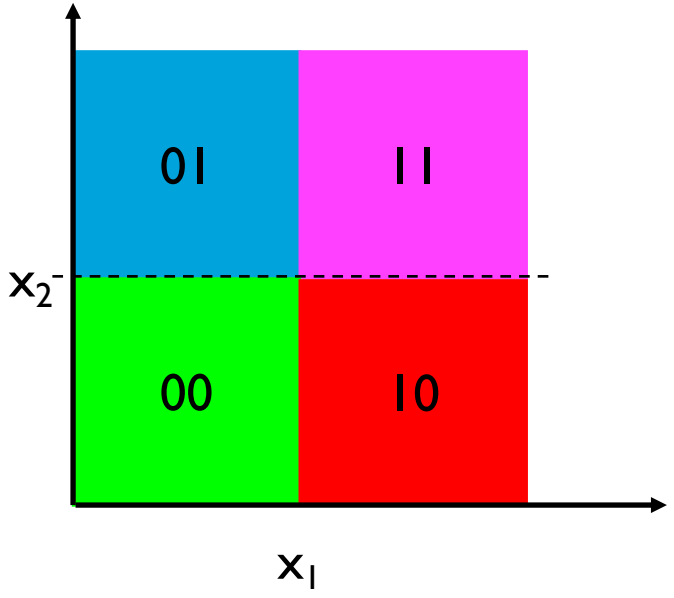

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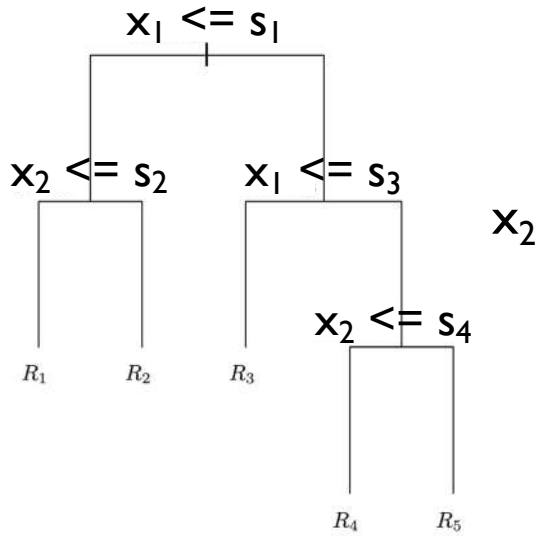

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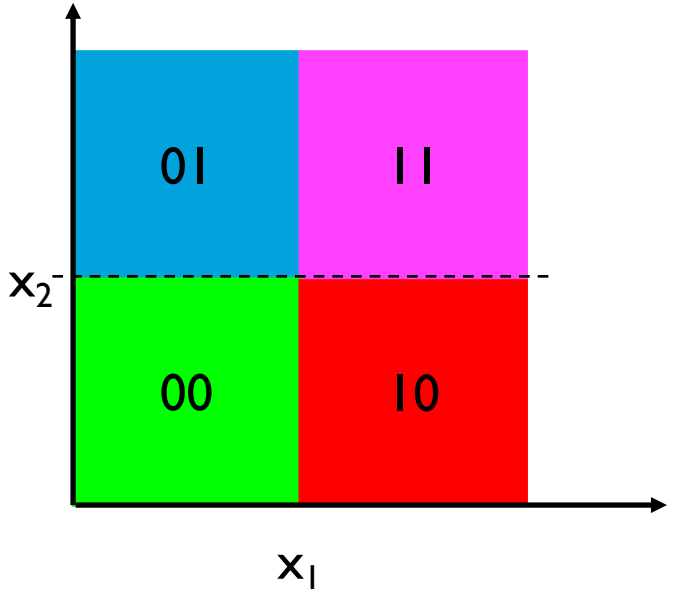

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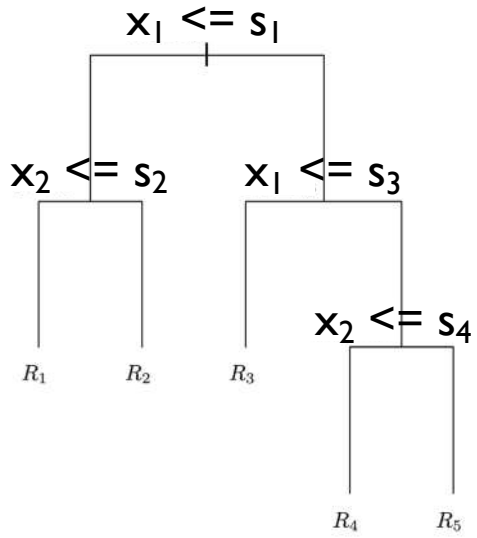

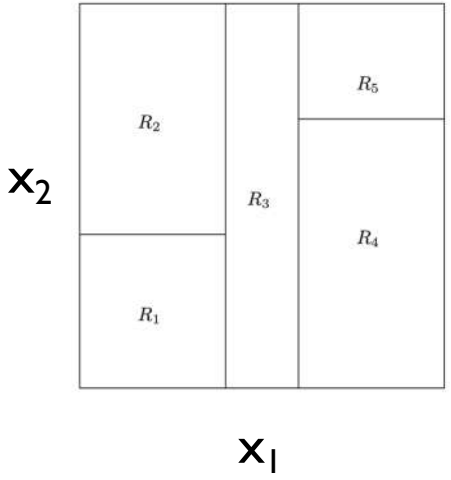

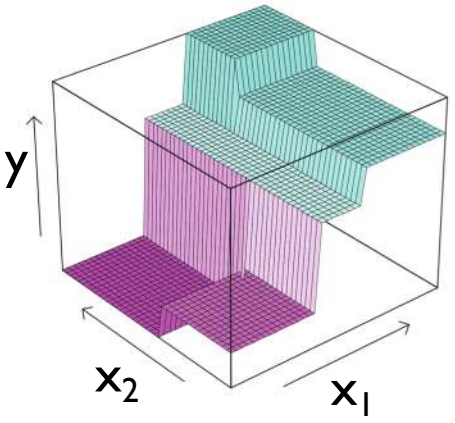

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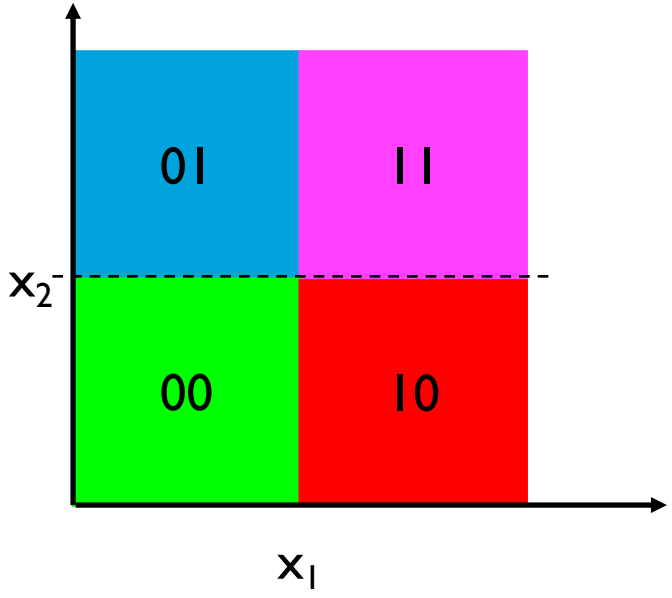

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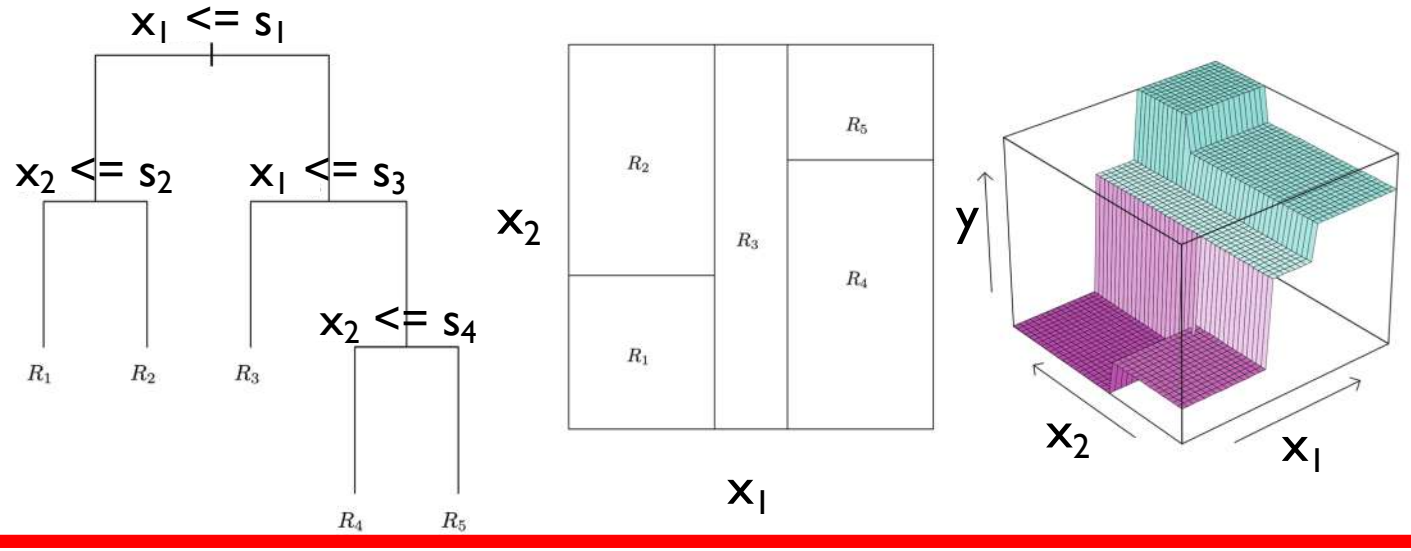

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F	T	T
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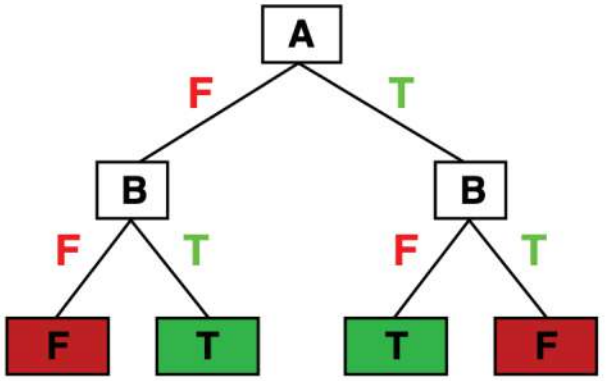
T	T	F



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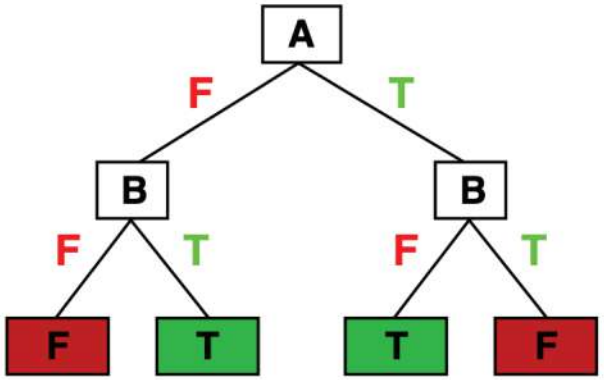

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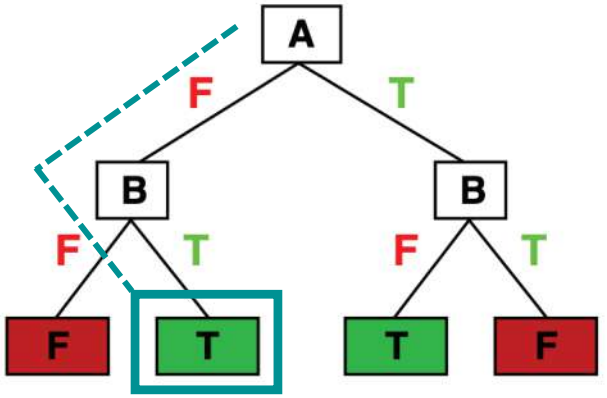

Each row of the truth table maps to a root-to-leaf path on the tree

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

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How many distinct decision trees can be built out of *n* boolean attributes?

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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	
…	…	…	…	
…	…	…	…	
…	…	…	…	
1	1	1	1	

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2^n rows

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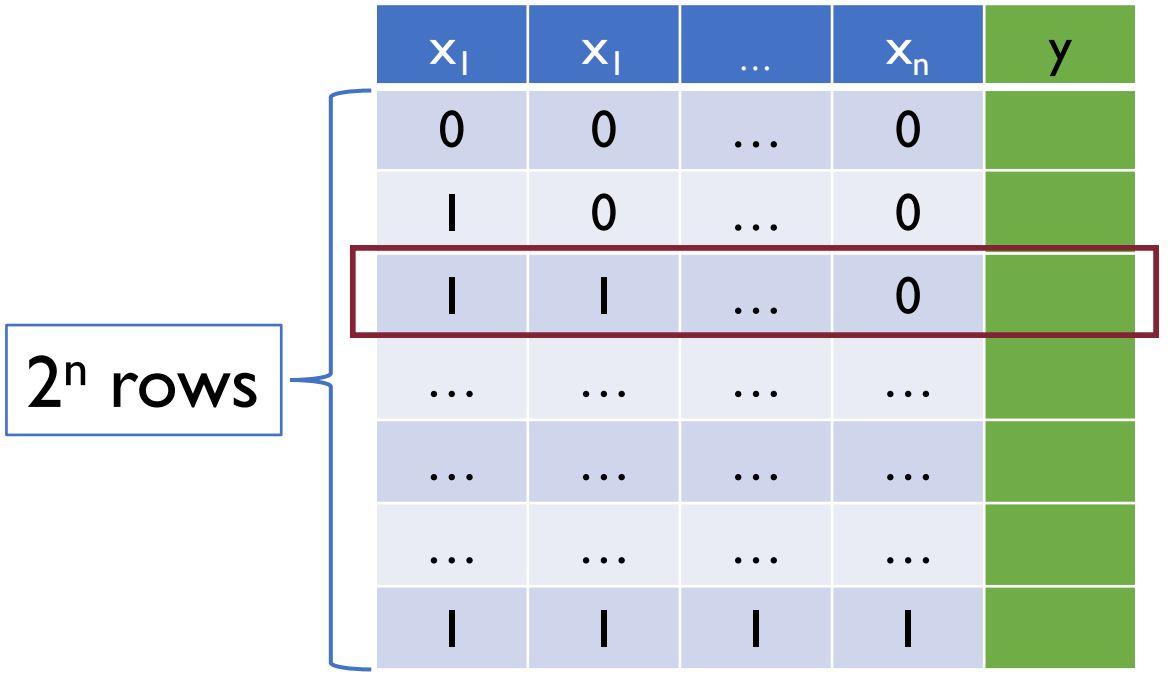


For each input y = 0 or 1

Hypothesis Space

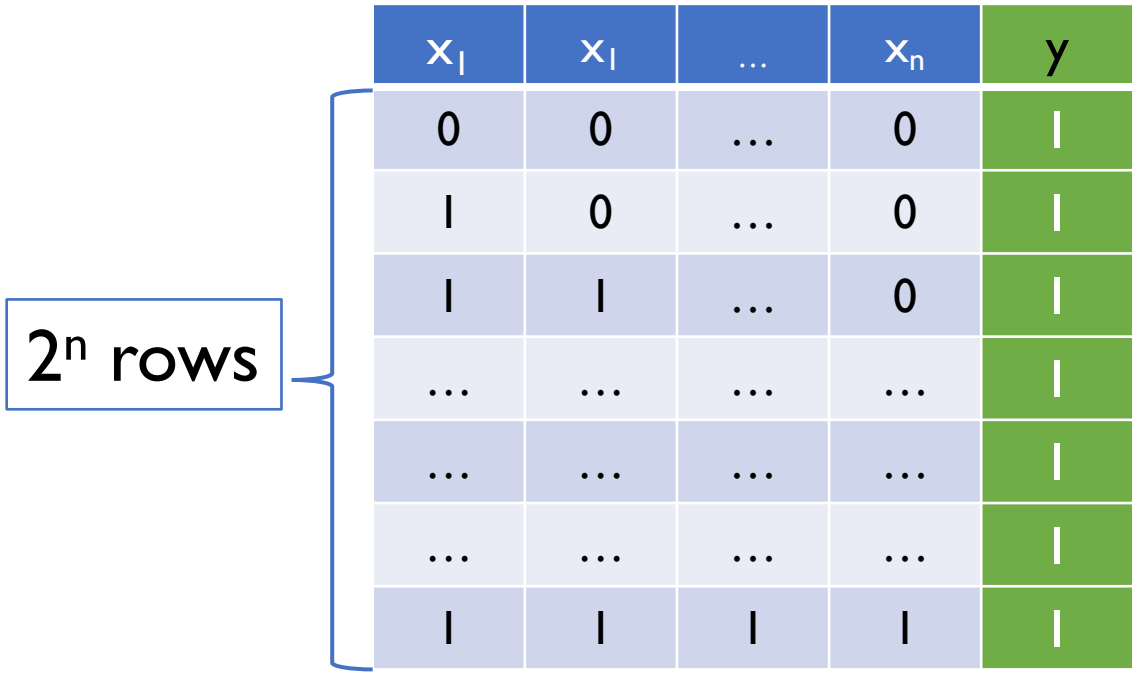
A possible boolean function is the one which will output all **0**s

2^n rows

x_1	x_1	…	x_n	y
0	0	…	0	0
1	0	…	0	0
1	1	…	0	0
…	…	…	…	0
…	…	…	…	0
…	…	…	…	0
1	1	1	1	0

Hypothesis Space

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



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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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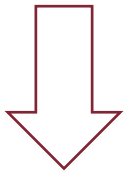

Solution

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

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

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

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- Each time, we reduce the RSS

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  - That would correspond to an overfitted tree
- 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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- 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

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  - Classification Error Rate
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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

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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**

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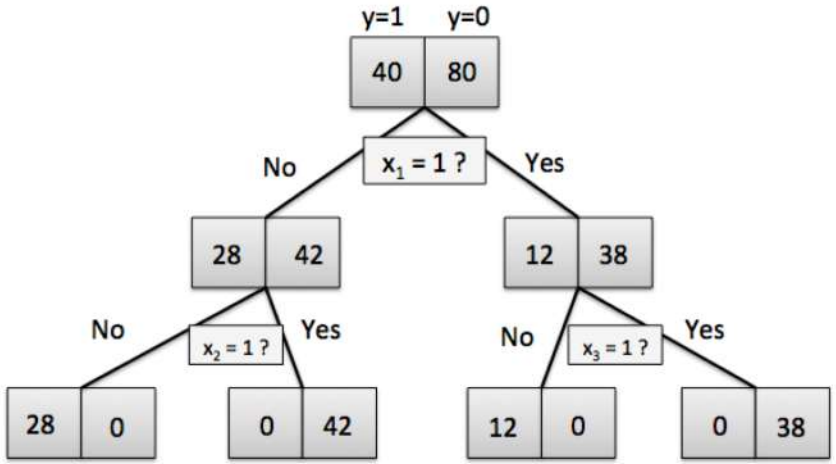
- In practice, both entropy and Gini can be used to grow a tree

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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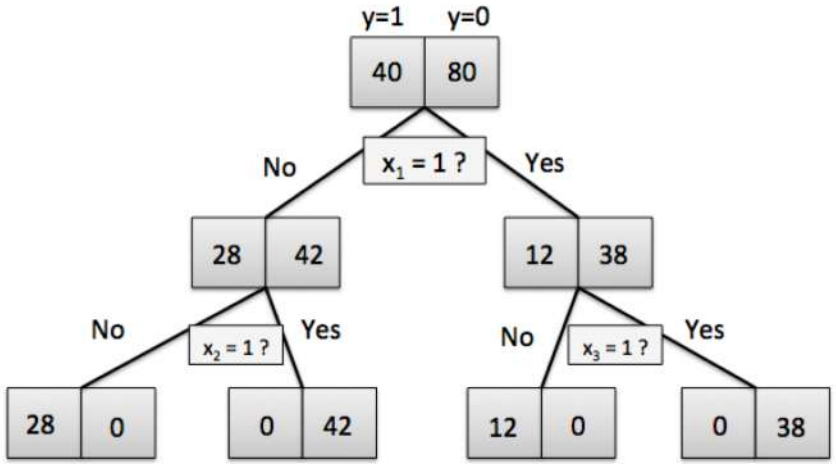
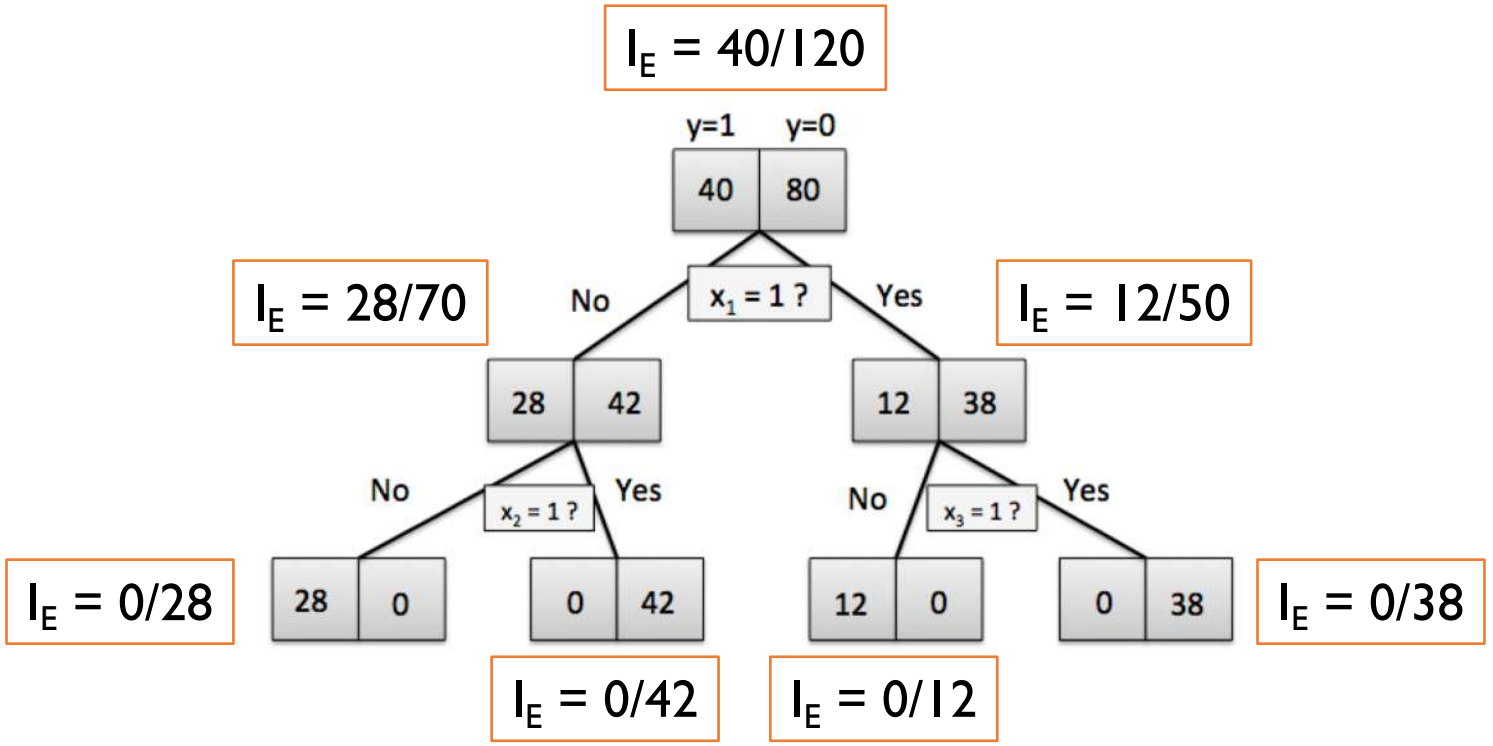


Question

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



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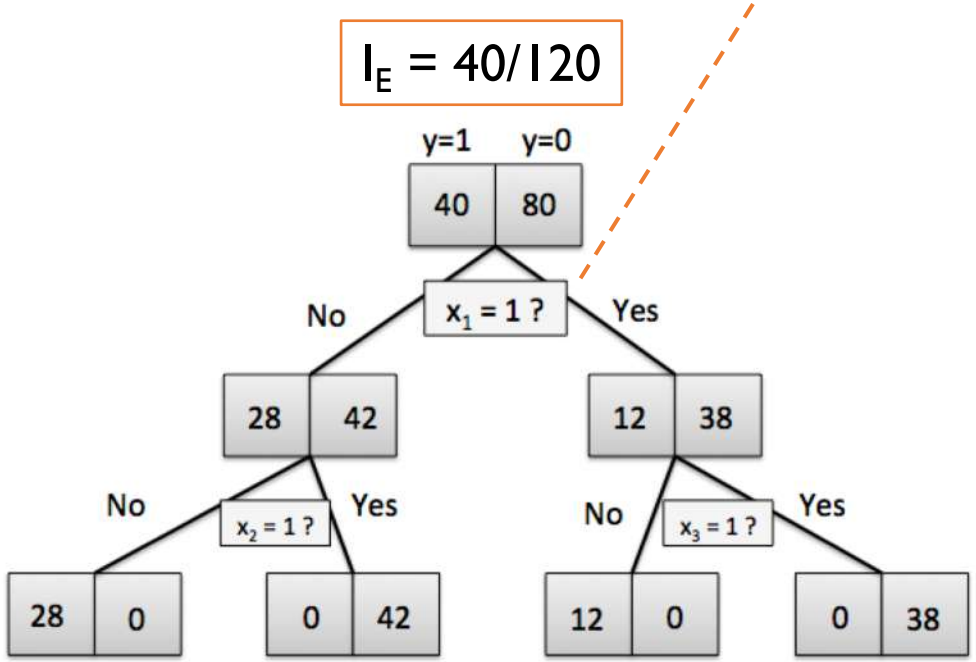
Compute IG of the first split using I_E



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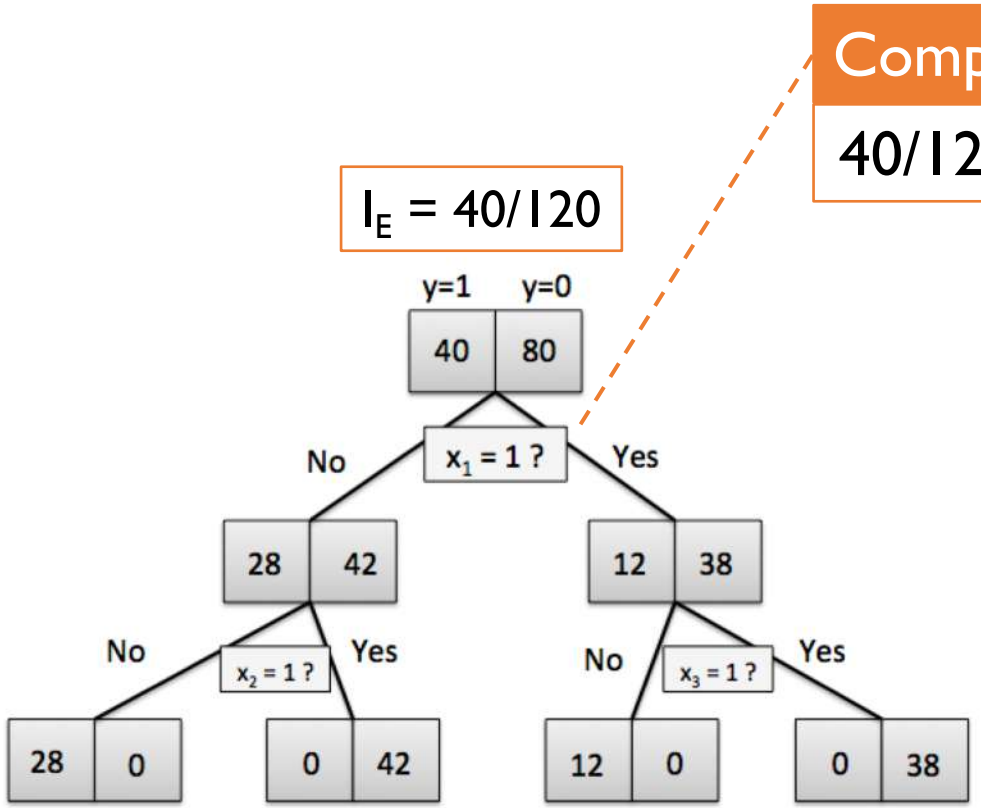

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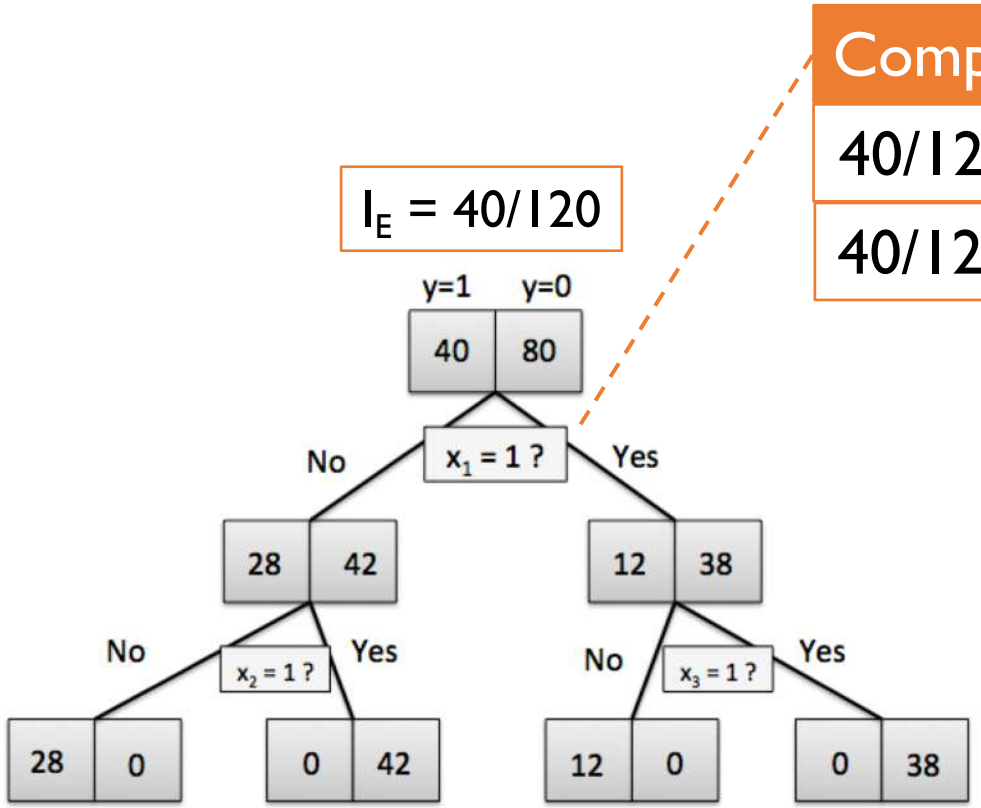

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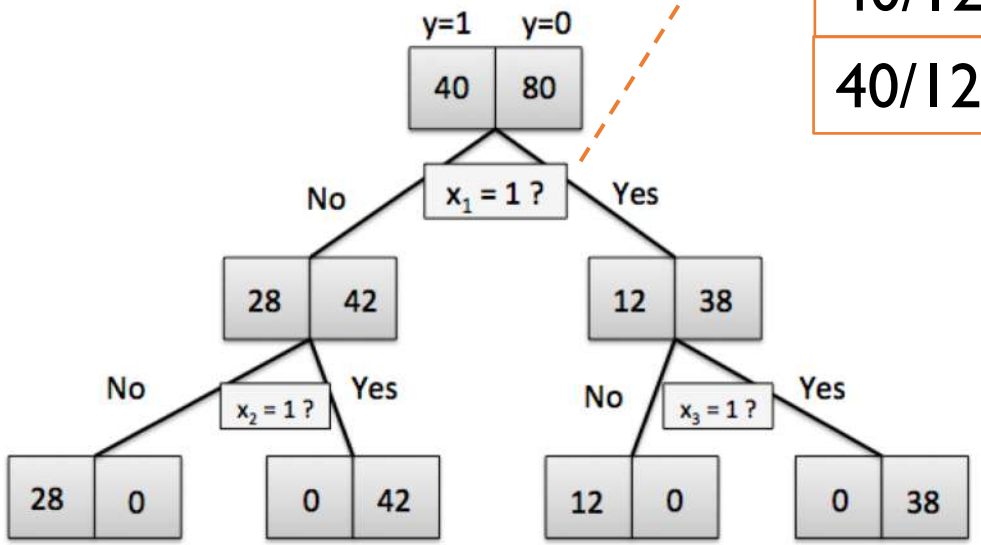

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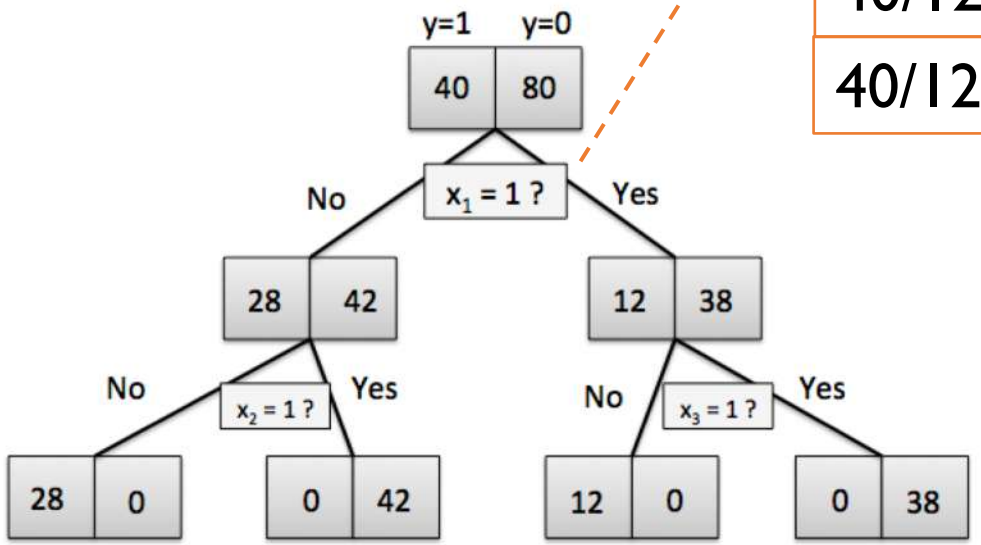

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the sum of I_E of the 2 child nodes is equal to that of the parent (40/120)

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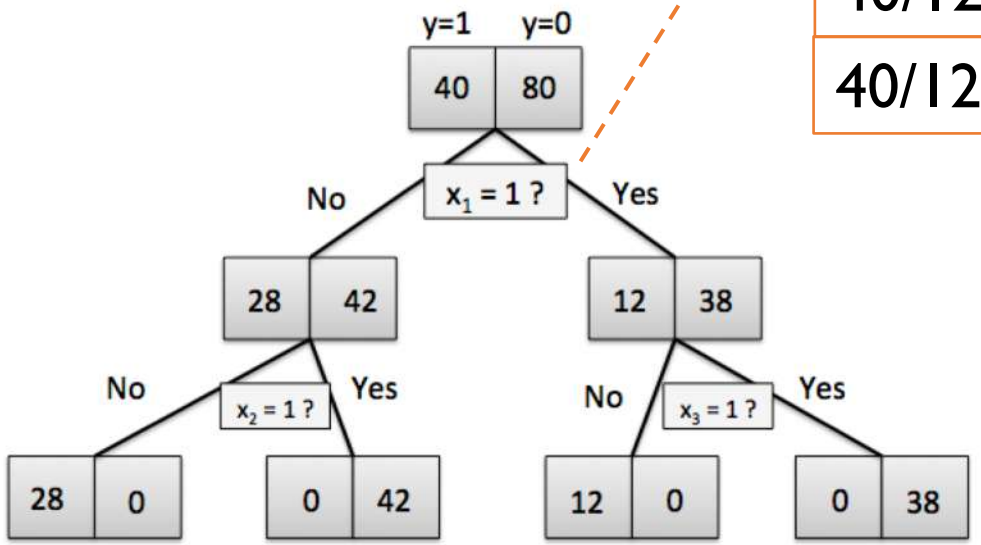

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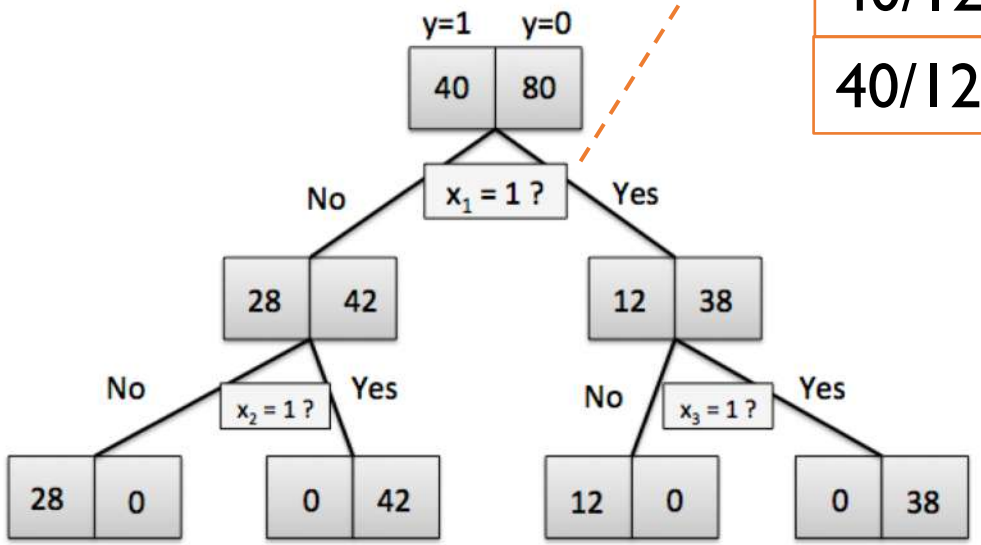

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The tree learning algorithm would stop at this point

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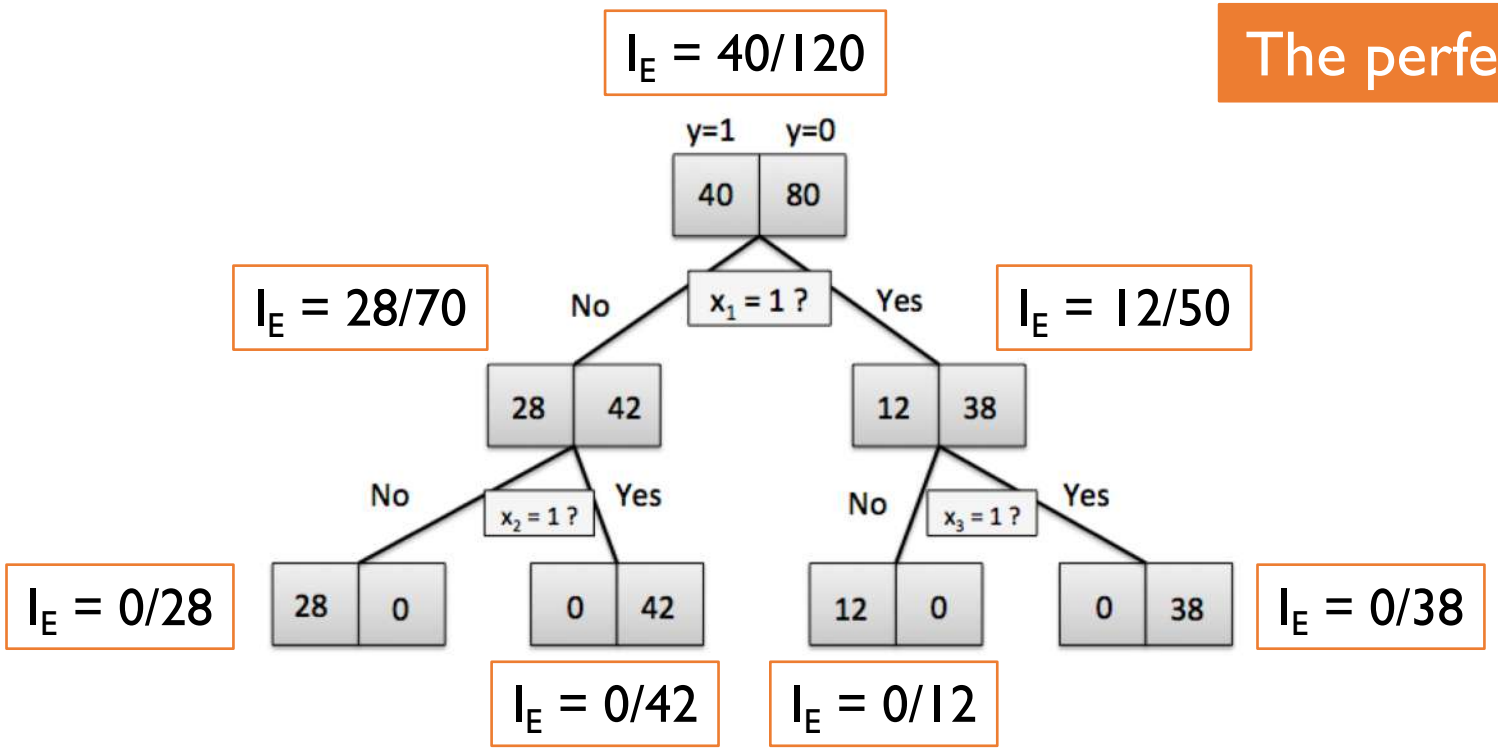

The perfect tree cannot be built using I_E

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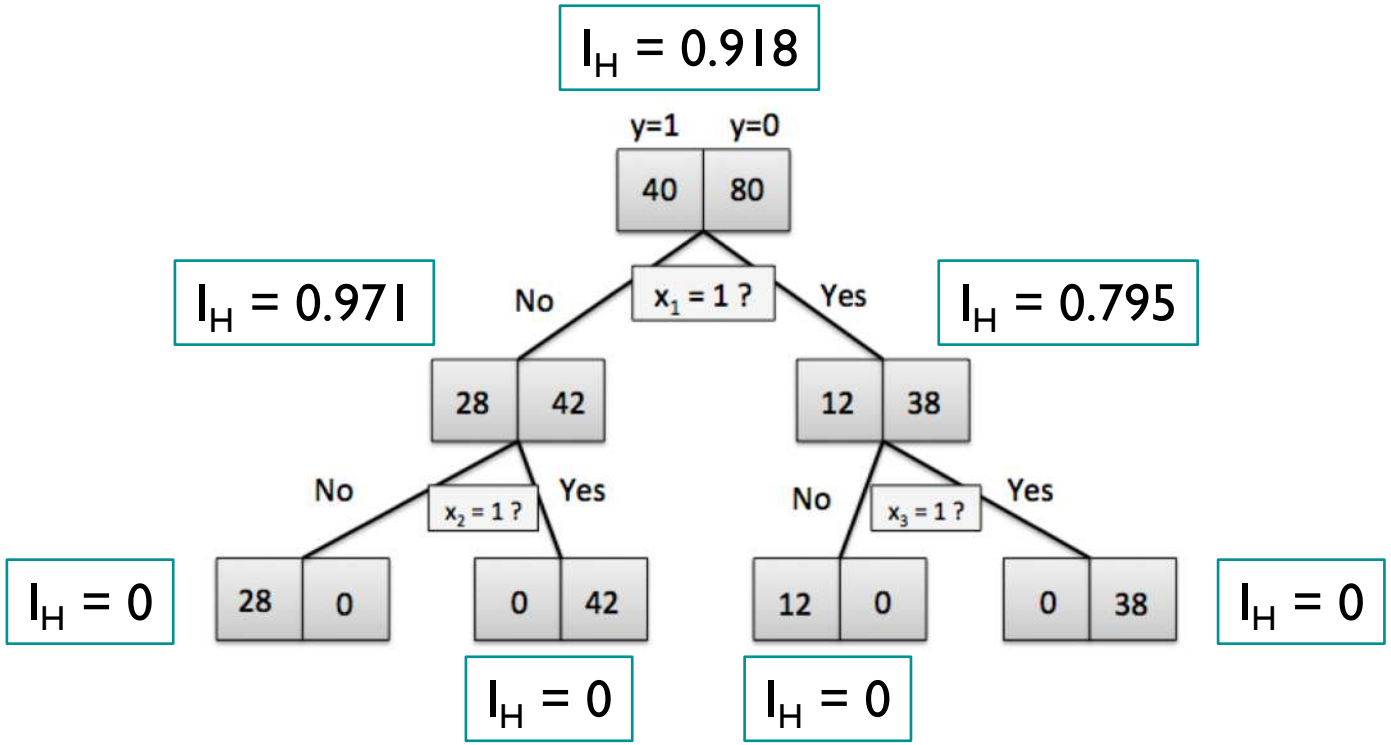
Classification Error Rate vs. Entropy (Gini)

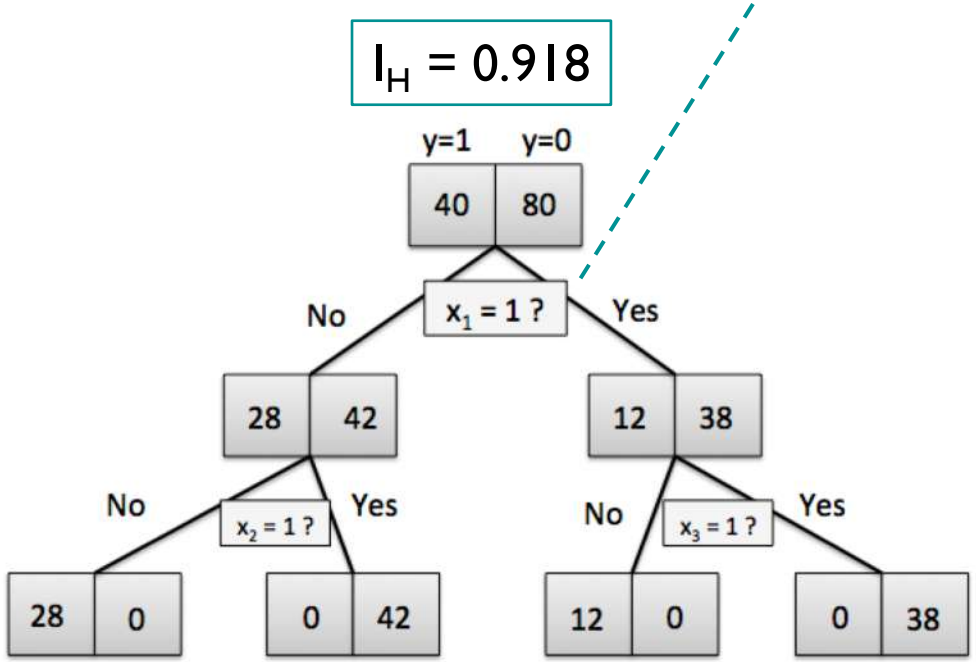
Node impurity using I_H



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_H



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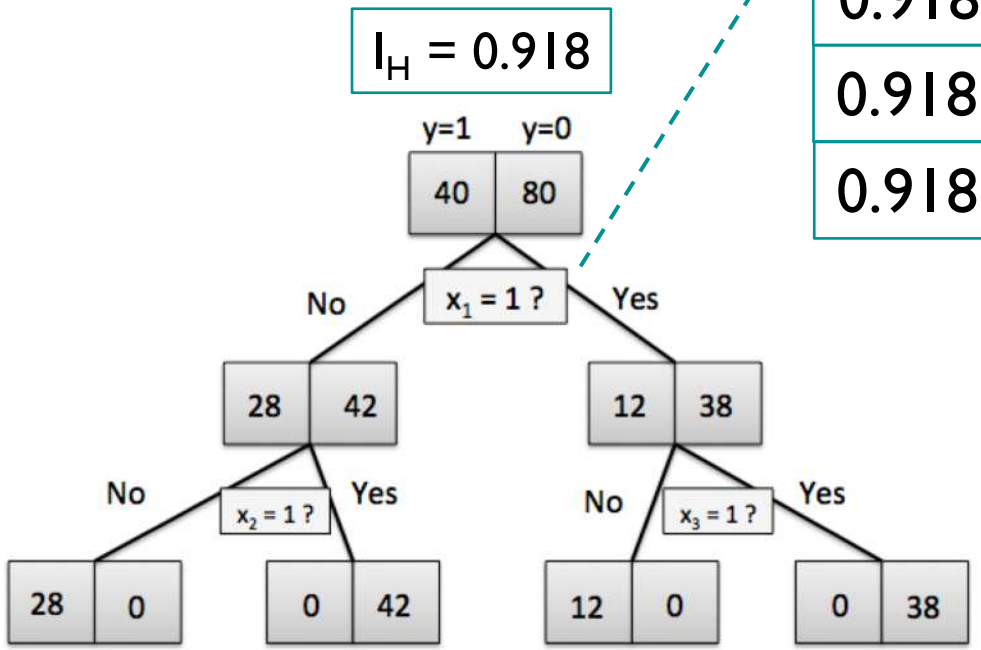

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0.918 - [(70/120 * 0.971) + (50/120 * 0.795)]

0.918 - [0.566 + 0.331]

0.918 - 0.897 = 0.021

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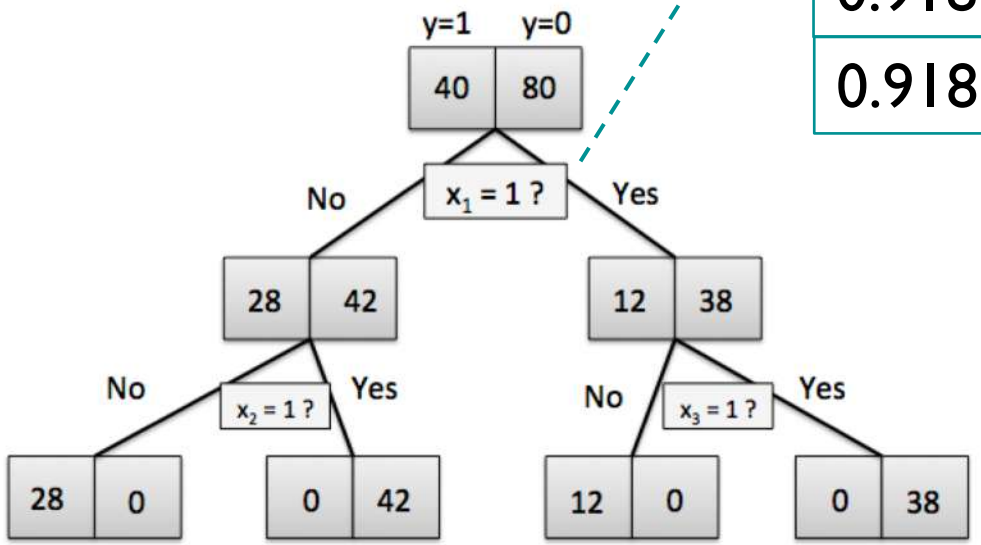

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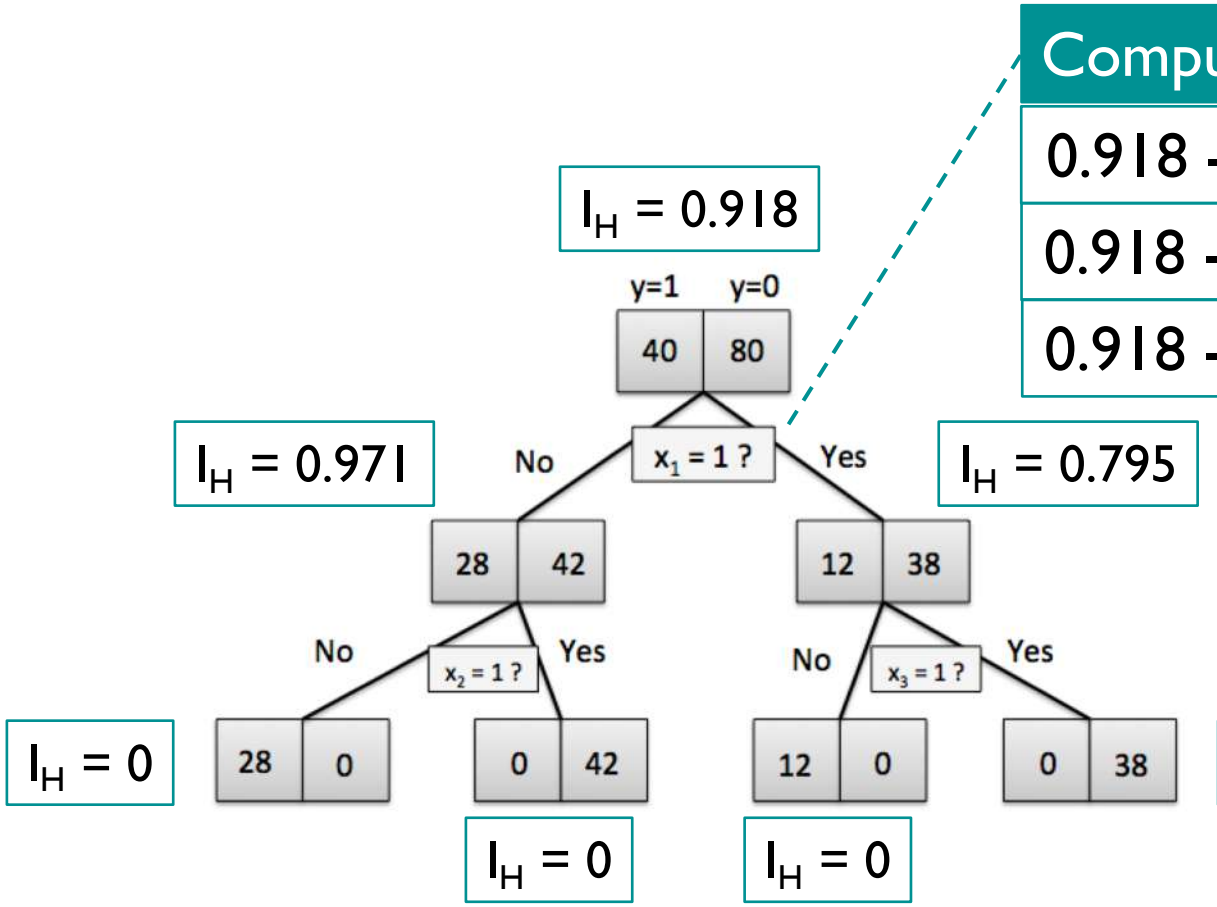

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The splitting rule would continue until the child nodes are pure

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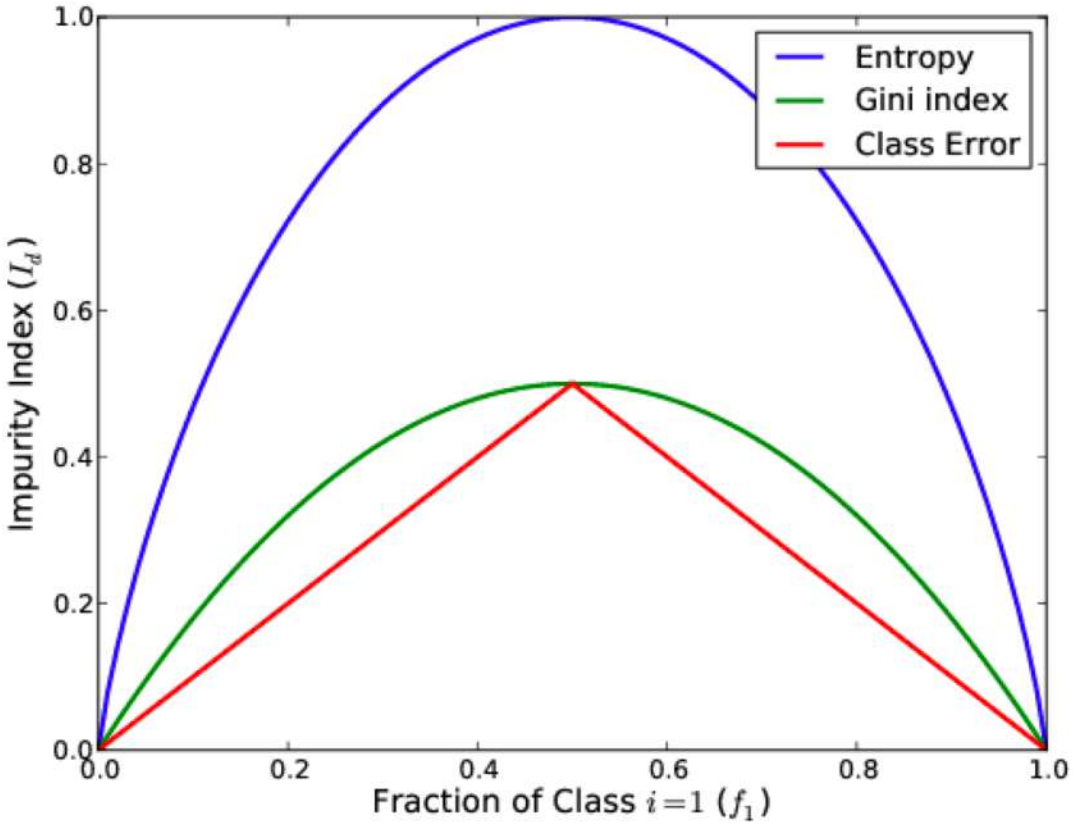

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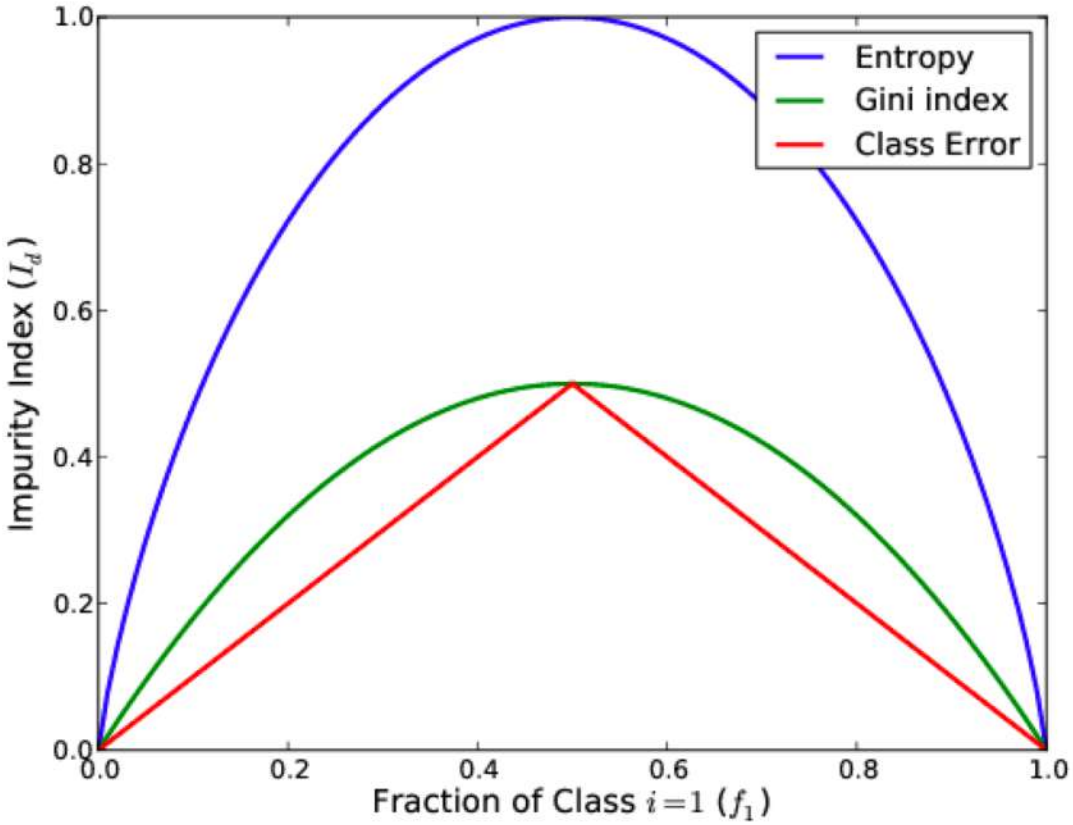

Gini and Entropy are "smoother" than classification error

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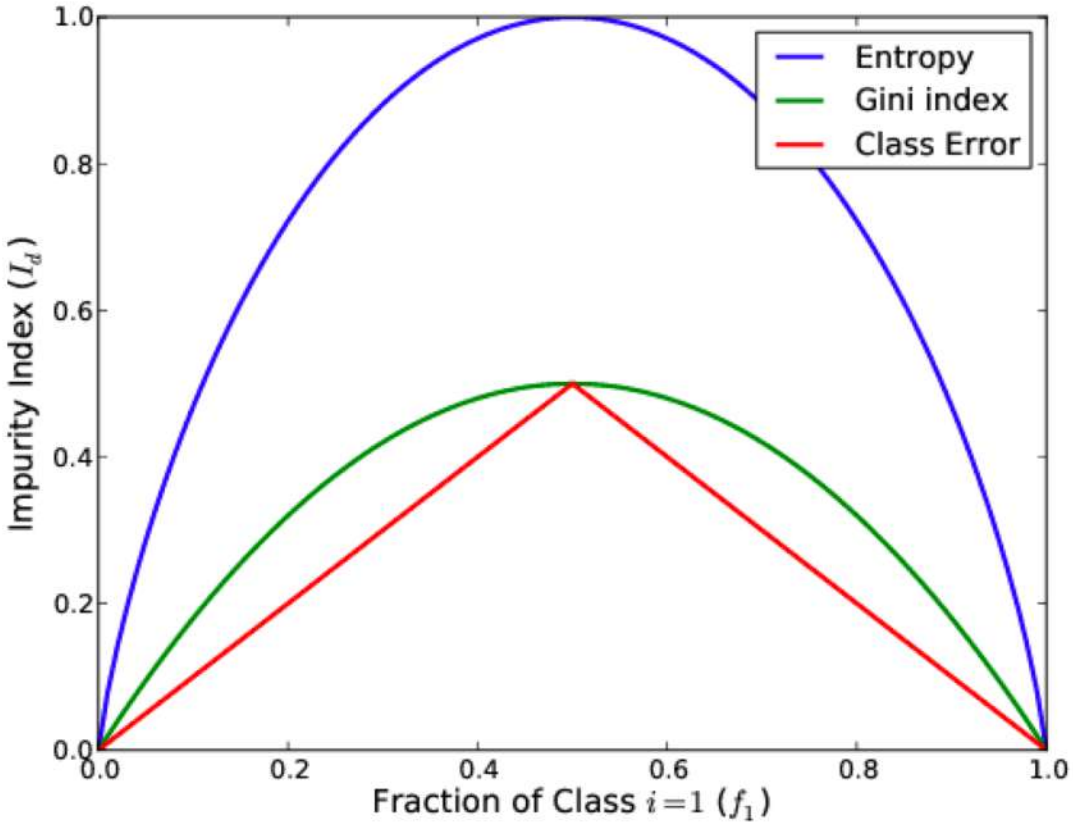

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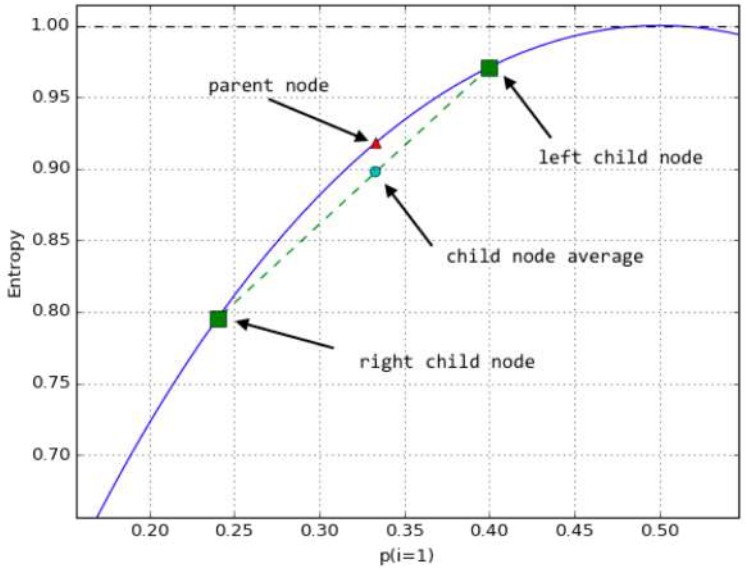

Entropy is always larger than the weighted averaged entropy due to its "bell shape"

Evolution of Entropy

- Suppose we have $x_1, \ldots, x_N$ N items

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- H always ranges in [0, 1] independently of the size of the set

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splitting can't do worst!

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Linear Models vs. Decision Trees

Linear Models

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

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

Learned hypothesis is constant within a region

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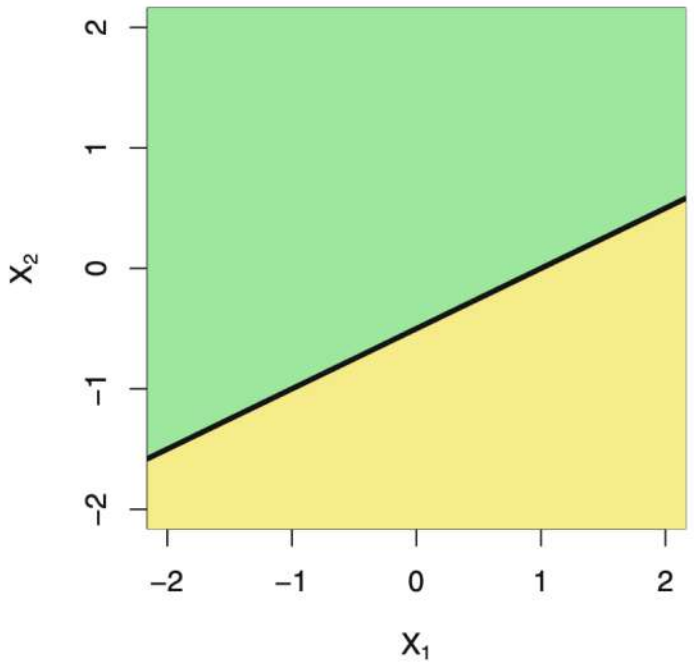
Linear Models vs. Decision Trees: Example

Linear Regression



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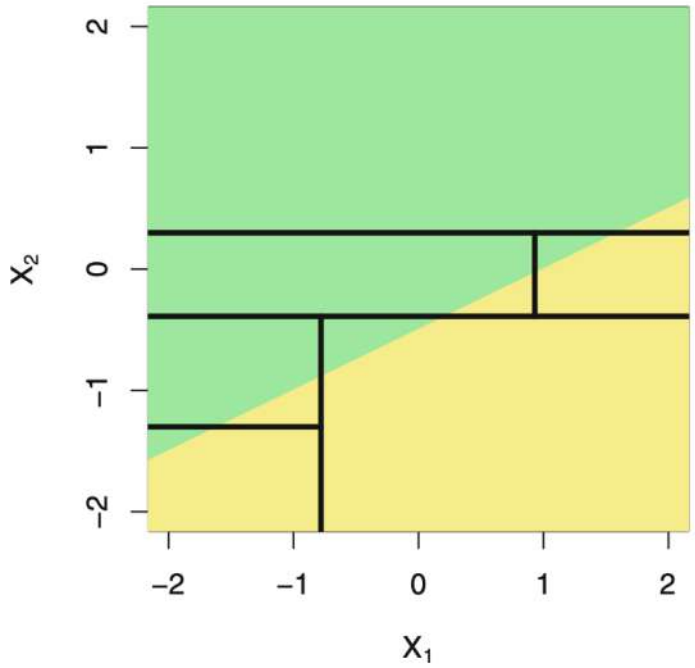

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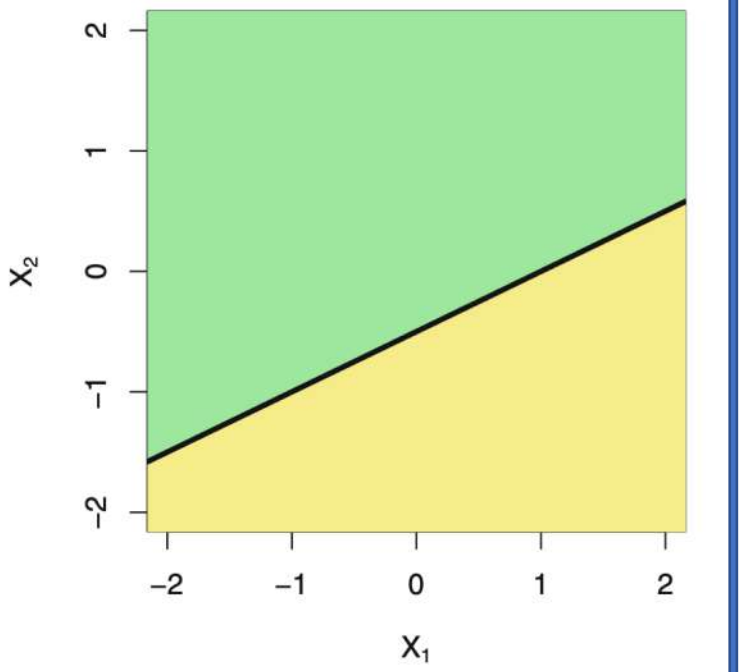

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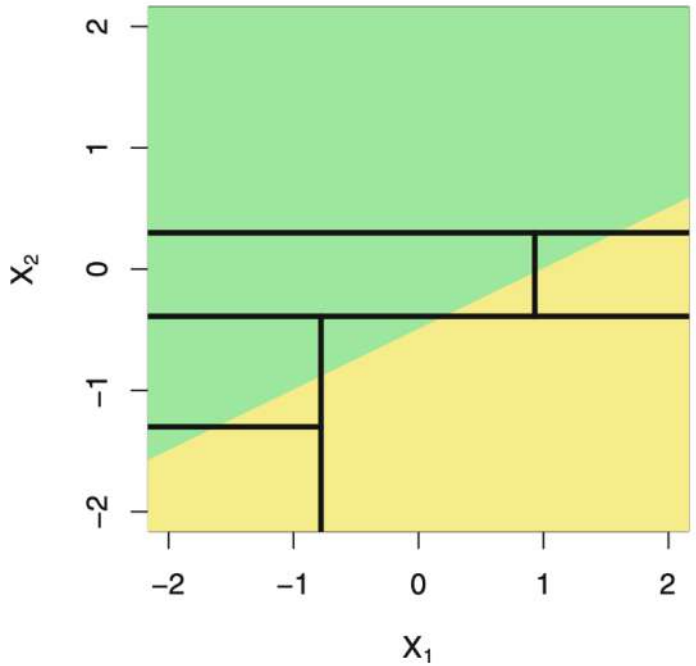

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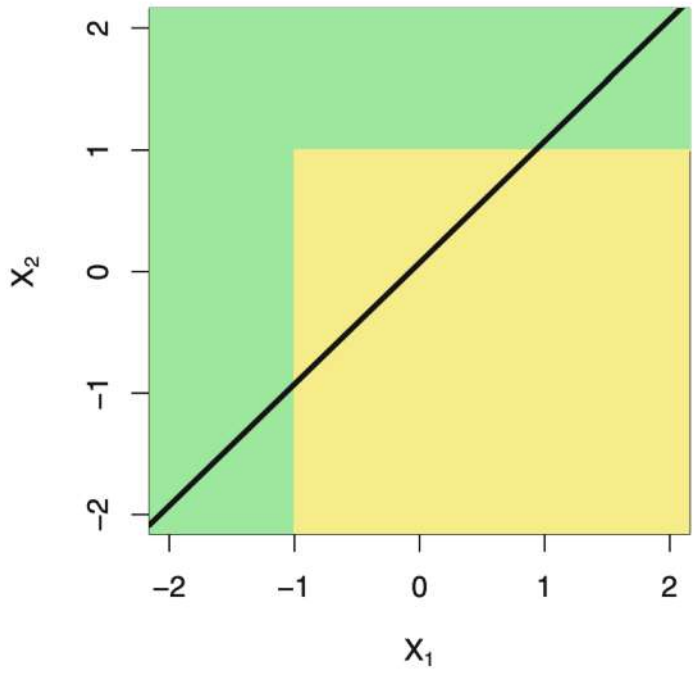

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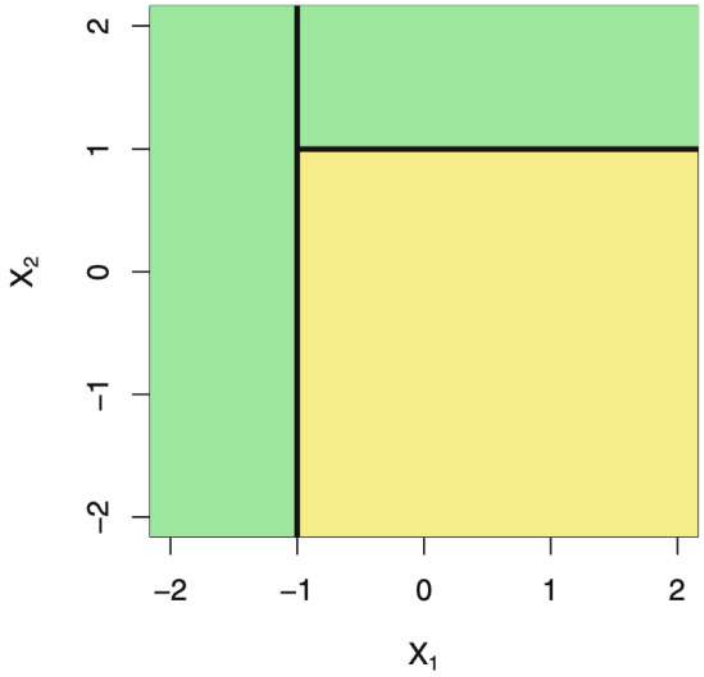

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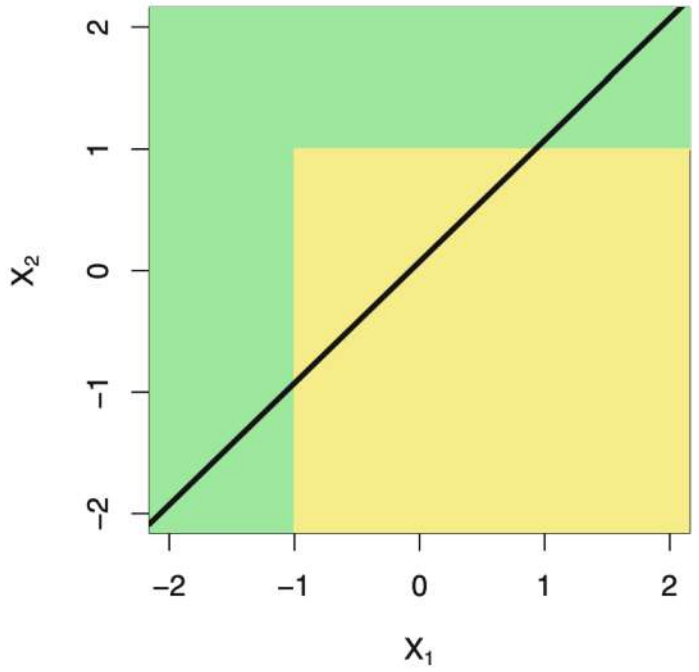

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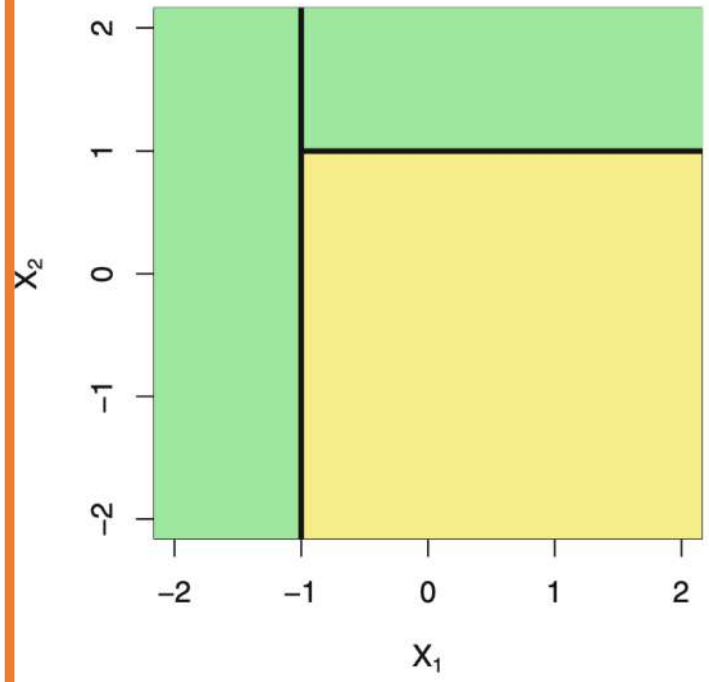

Non-linear decision boundary

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

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Improvement: **Ensembles** of Decision Trees

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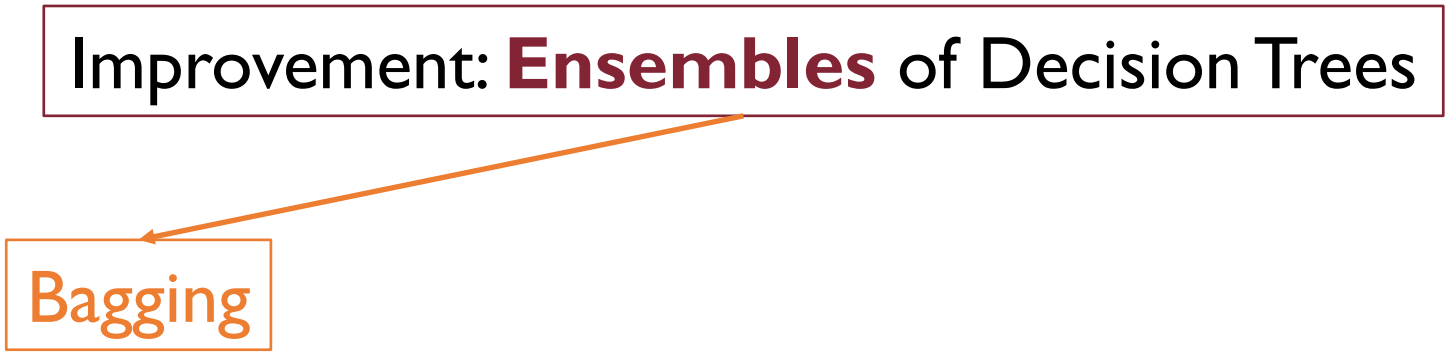

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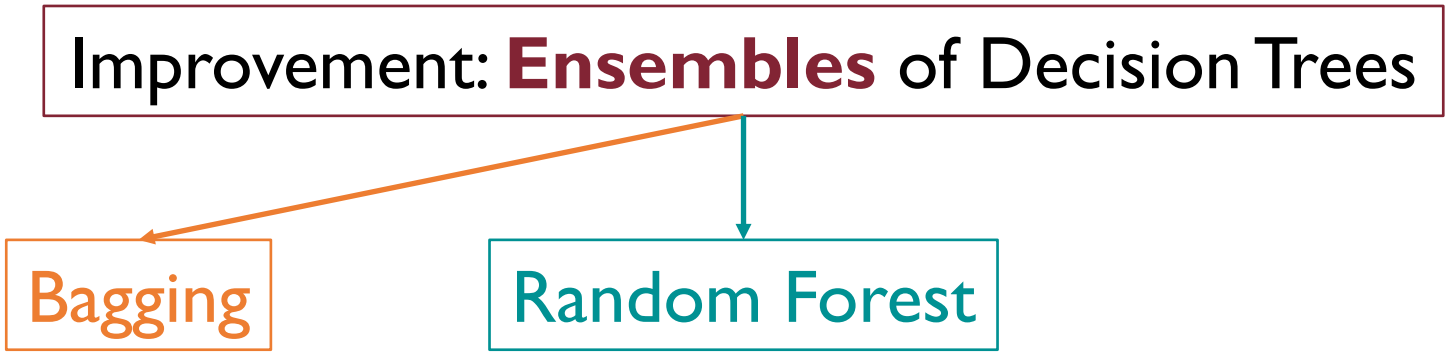

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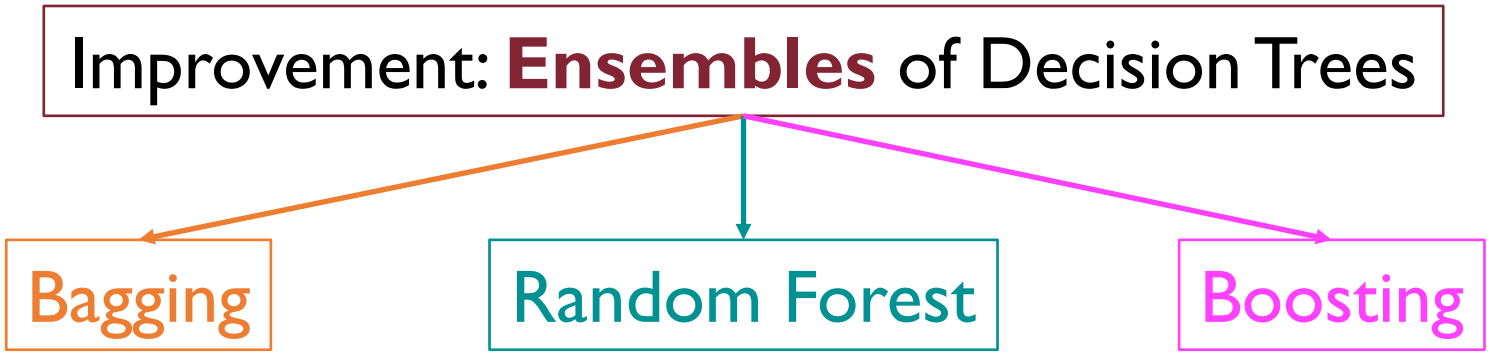

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- Low-variance approach, instead, are less sensitive to different training set
- Bootstrap aggregation (**Bagging**) is a general-purpose method to lower the variance of a statistical learning method

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$$\mathrm{Var}\left(\sum_{i=1}^{n} X_i\right) = \sum_{i=1}^{n} \mathrm{Var}(X_i) \quad \text{if } X_i \text{ are independent}$$

Bagging: Intuition

- Given a set of n i.i.d. observations $Z_1, \ldots, Z_n$, each with variance σ^2
- The variance of the empirical mean is σ^2/n

$$\bar{Z} = \frac{1}{n}\left(Z_1 + \ldots + Z_n\right)$$

$$\mathrm{Var}(\bar{Z}) = \mathrm{Var}\left[\frac{1}{n}\left(Z_1 + \ldots + Z_n\right)\right] =$$

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Averaging a set of observations reduces variance!

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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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$$h_{\text{bagging}}(\mathbf{x}) = \frac{1}{B}\sum_{b=1}^{B} h^{b*}(\mathbf{x})$$

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- It can be used in combination with *any* model
- 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

Tree Ensemble: Random Forests

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

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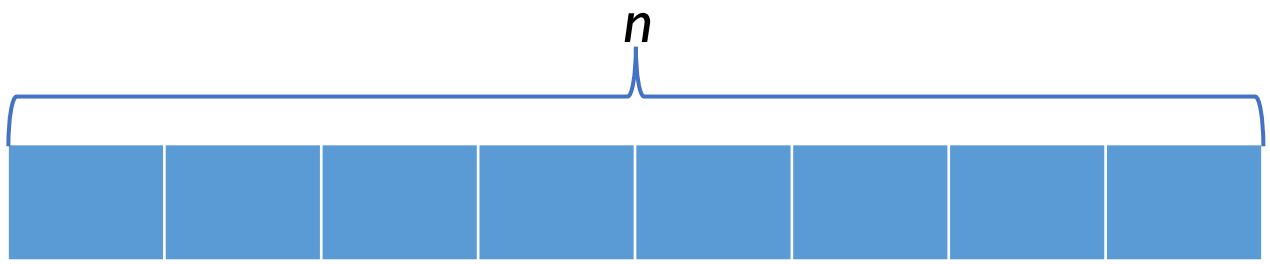
- We can think of this process as **decorrelating** the trees
- Note that when $k = n$ this simply resembles to bagging
- As with bagging, random forests will not overfit if we increase B

Why *k*/*n*?



Randomly choose *k* features out of *n*, each with uniform probability $p = 1/n$

What is the probability that the highly predictive feature *f* is contained in the *k*-sized random sample?

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We want to compute the following:

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It might be easier to compute the following:

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$$1 - \frac{n-k}{n} = \frac{k}{n}$$

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$$= \frac{\frac{(n-1)!}{(k-1)!(n-1-(k-1))!}}{\frac{n!}{k!(n-k)!}} = \frac{(n-1)!}{(k-1)!(n-k)!} * \frac{k!(n-k)!}{n!} = \boxed{\frac{k}{n}}$$

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Tree Ensemble: Boosting

- Again, general approach that can be applied to many statistical learning methods for regression or classification
- 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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- Decision Trees (DTs) highly **expressive** yet **interpretable** models both for regression and classification

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