Big Data Computing

Master's Degree in Computer Science

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Gabriele Tolomei

Department of Computer Science

Sapienza Università di Roma

tolomei@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

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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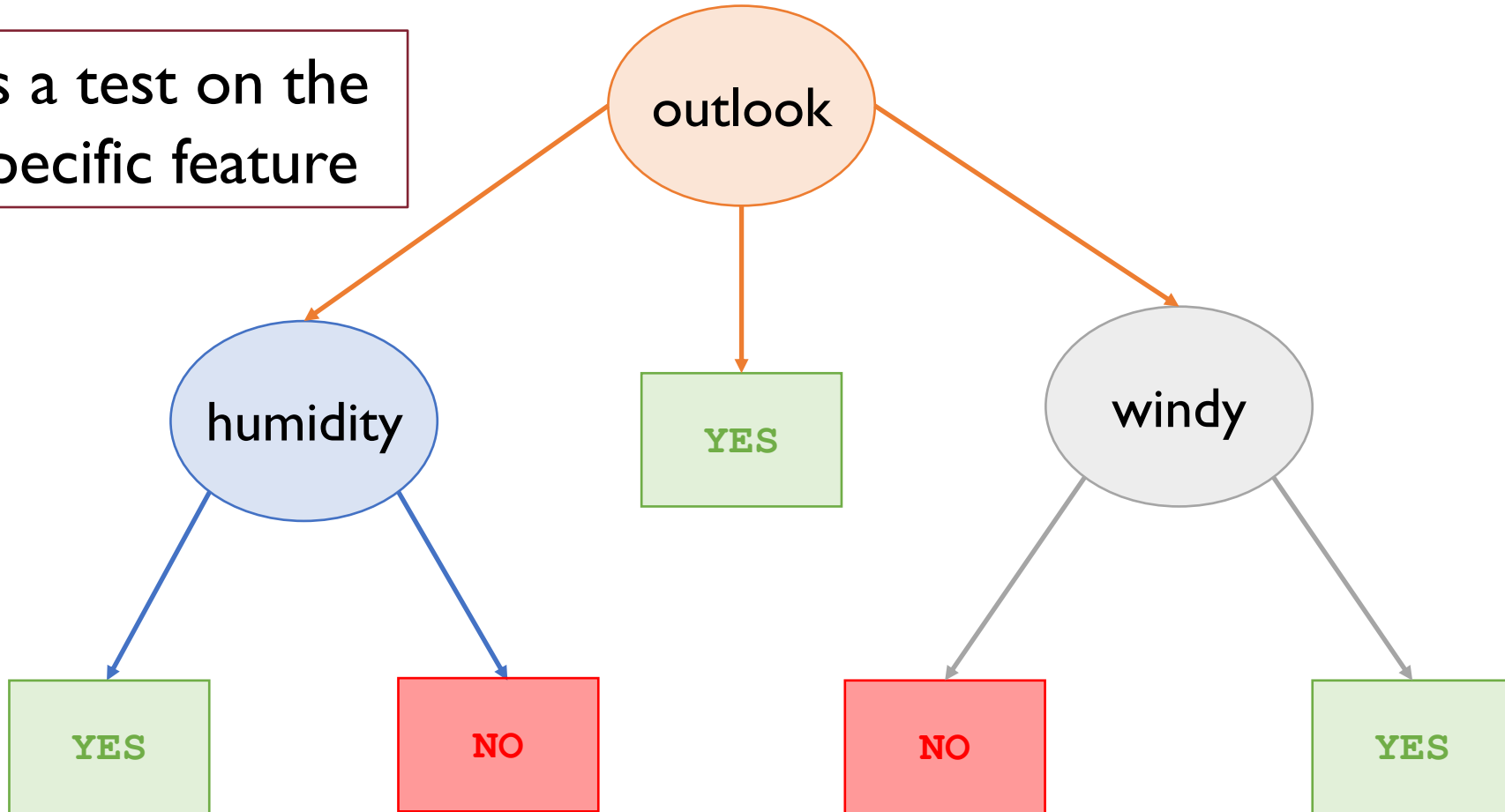
- Highly human-interpretable models
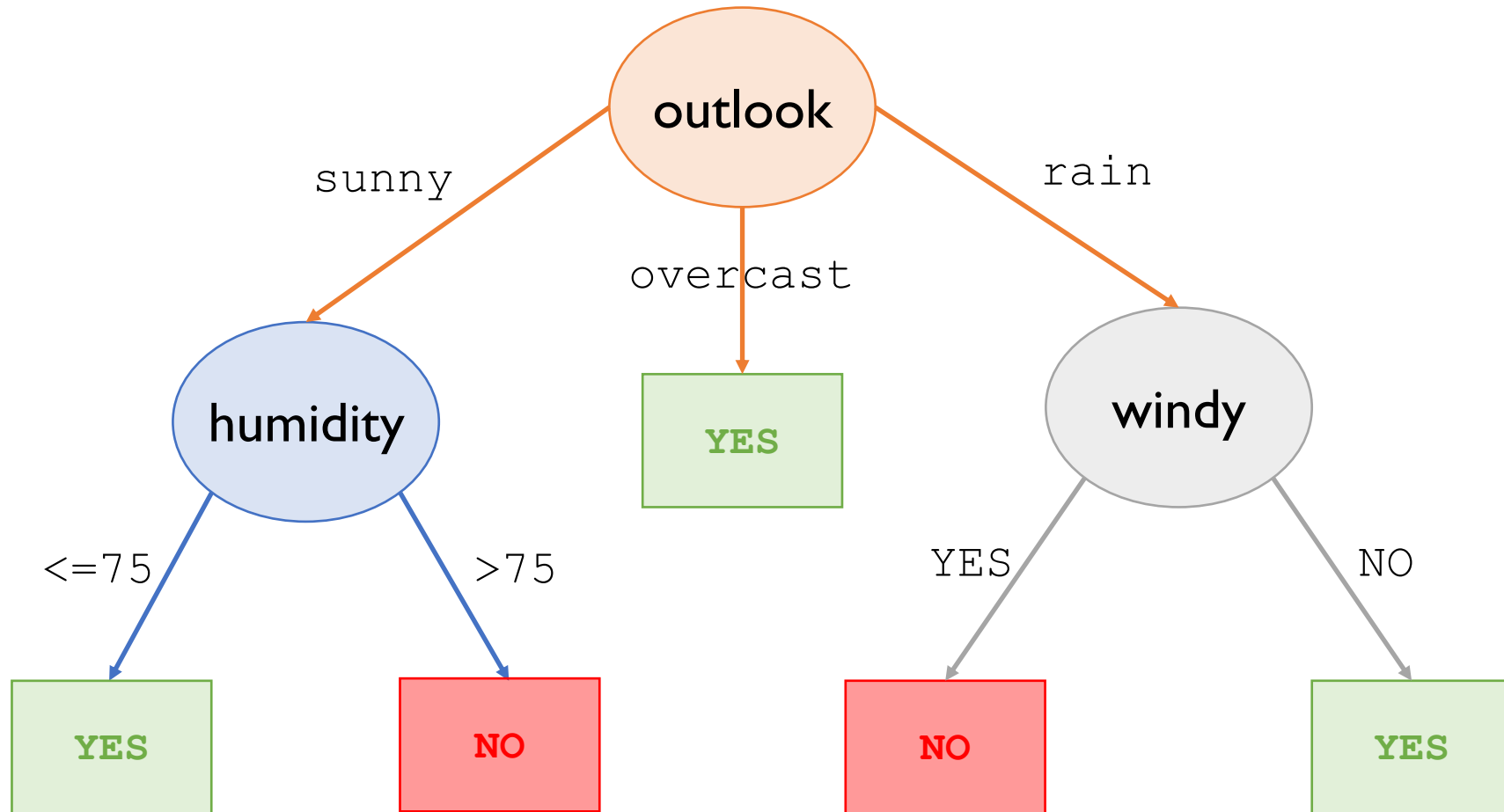
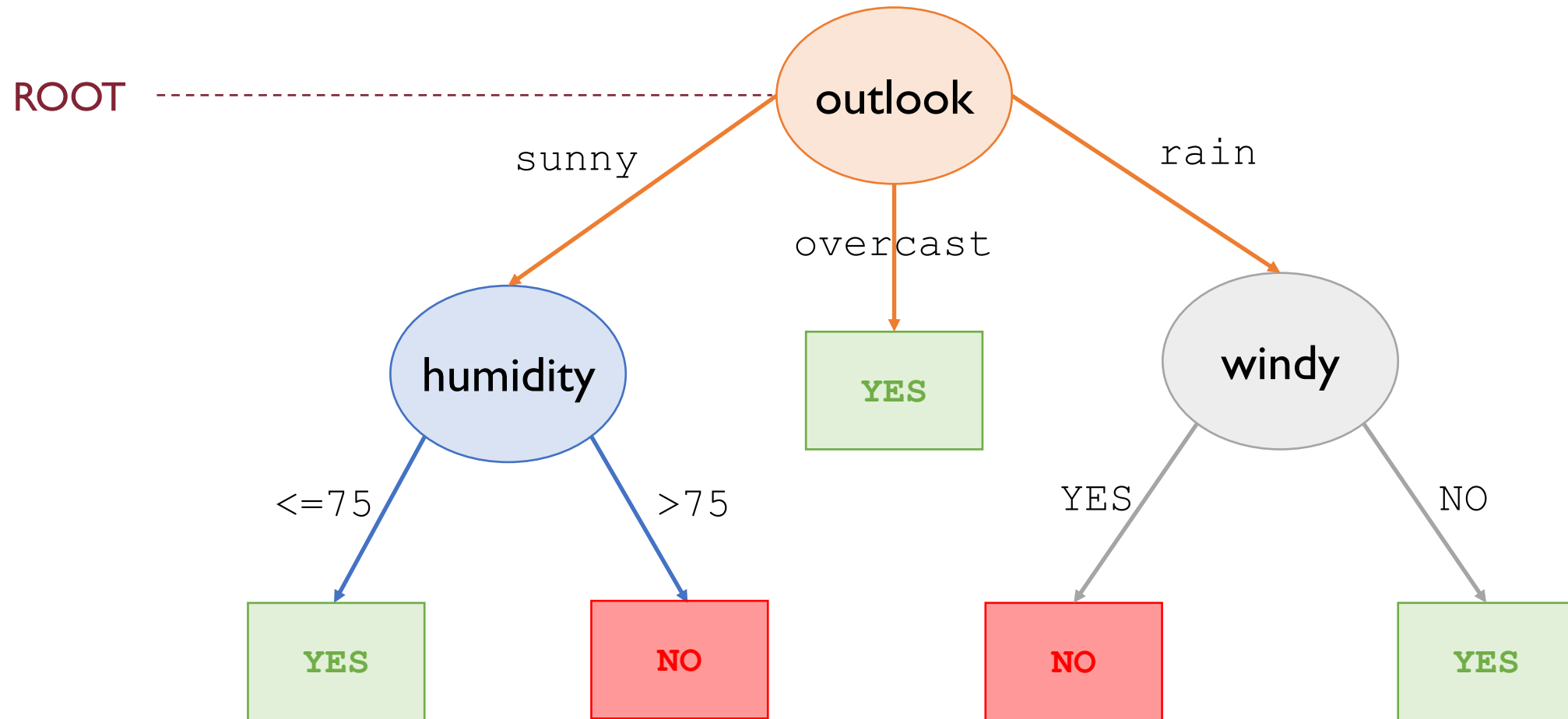# Decision Tree: An Example
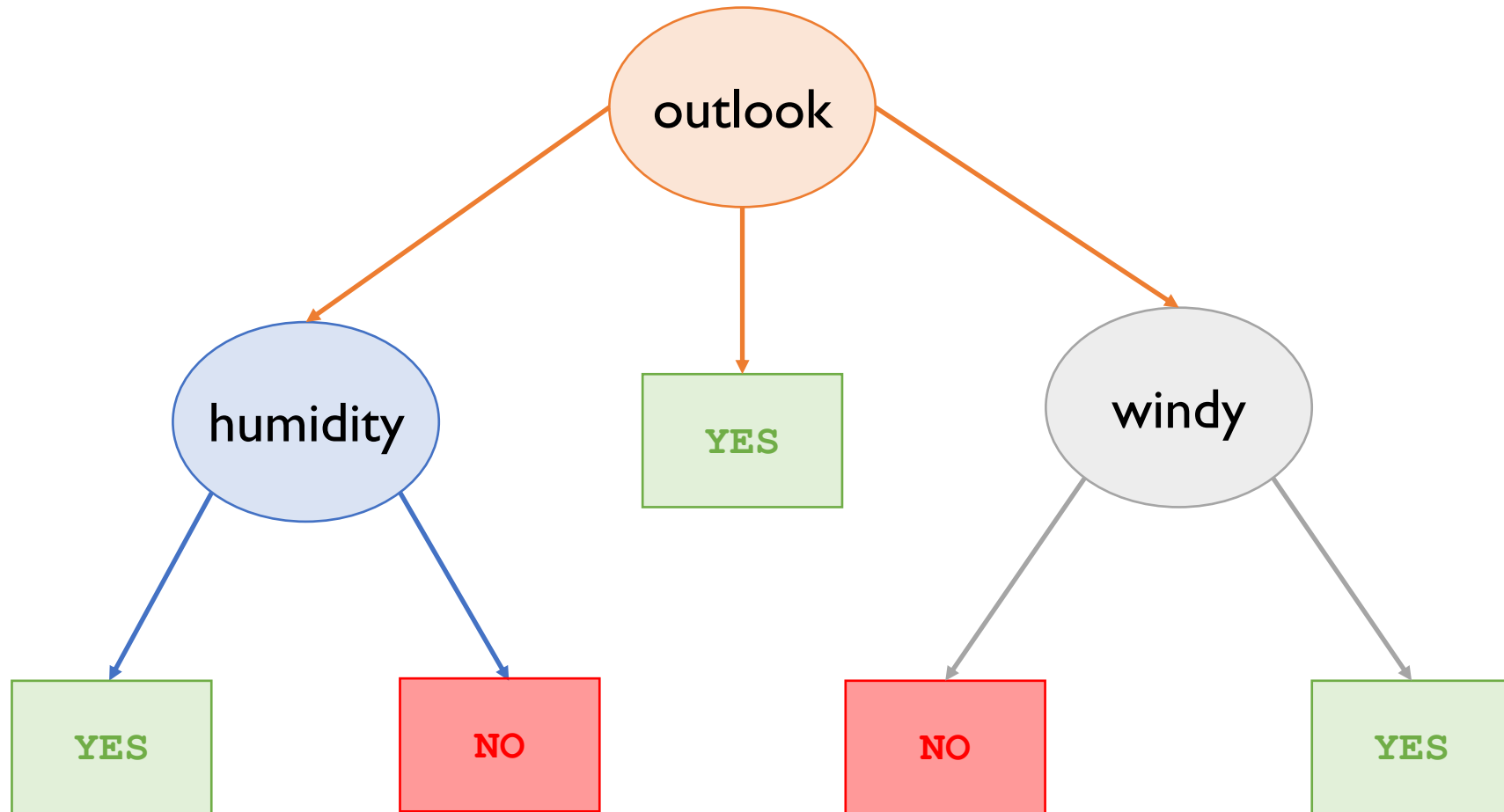
Decision Tree: An Example

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

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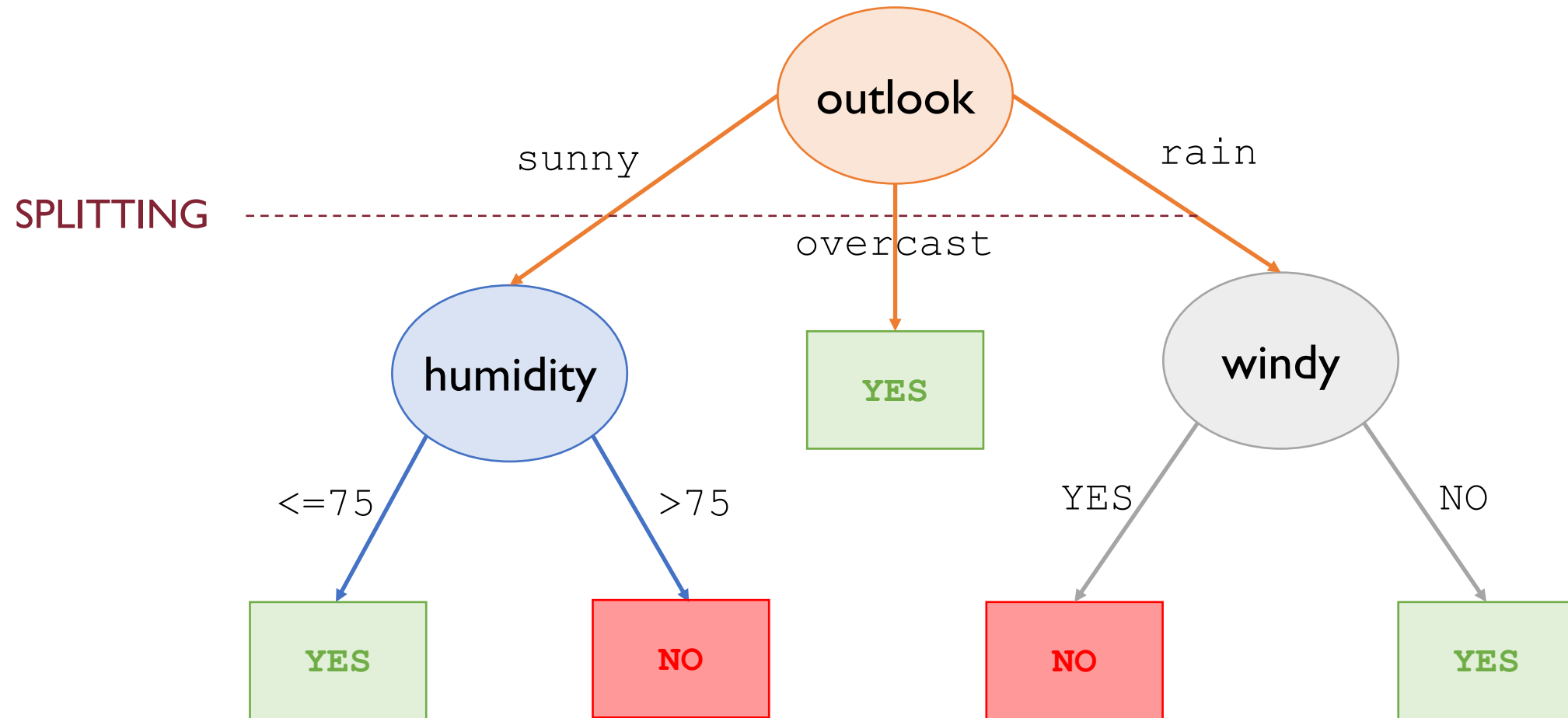
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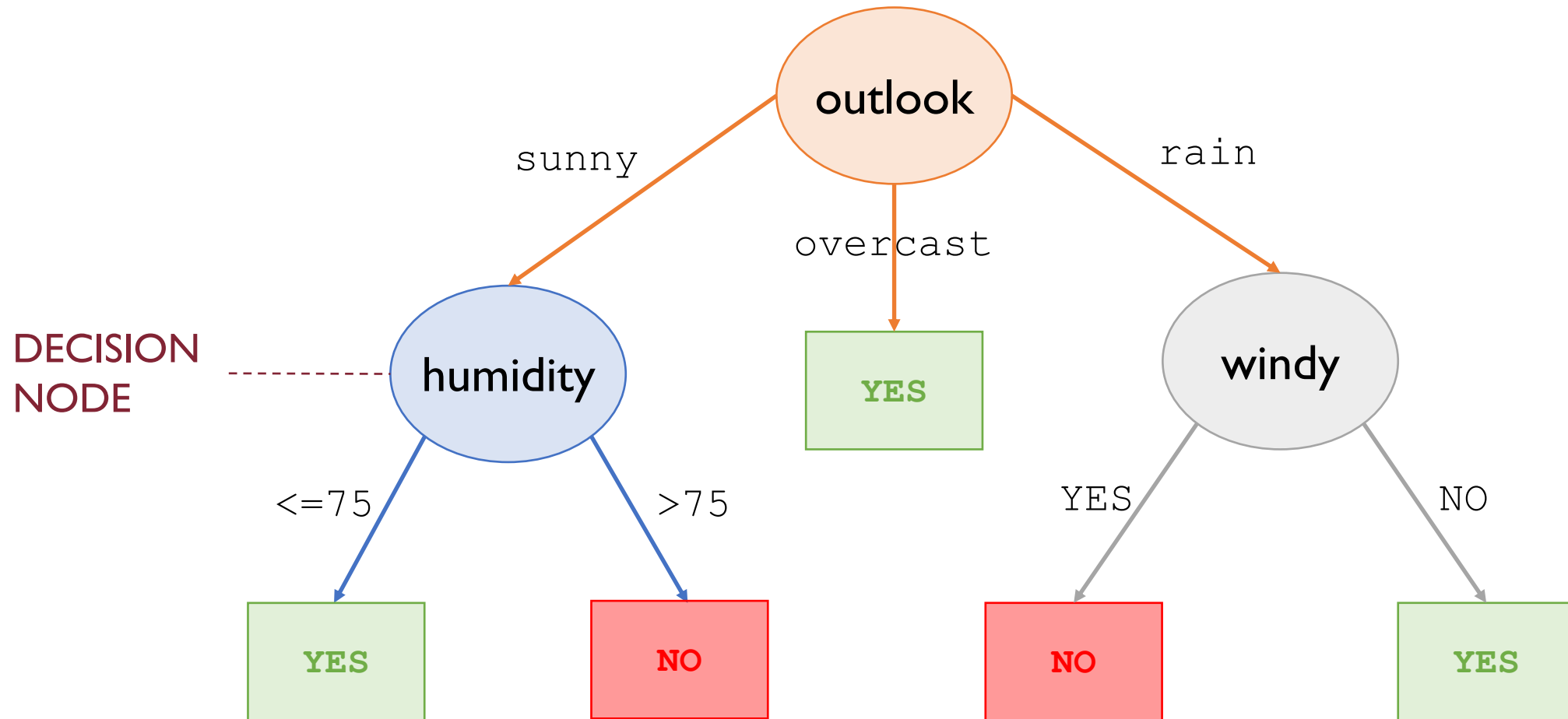
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ROOT ----------- outlook

SPLITTING -----------

DECISION NODE ----- humidity

sunny

overcast

rain

YES

windy

<=75

>75

YES

NO

LEAF ----- YES   NO

NO   YES

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

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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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The mean computed from observations in R_j

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Discrete Inputs
(e.g., boolean)

One branch for each value

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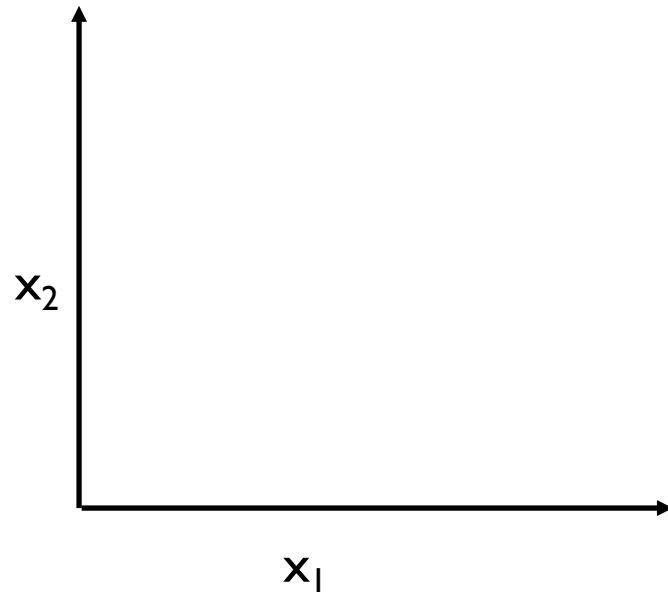
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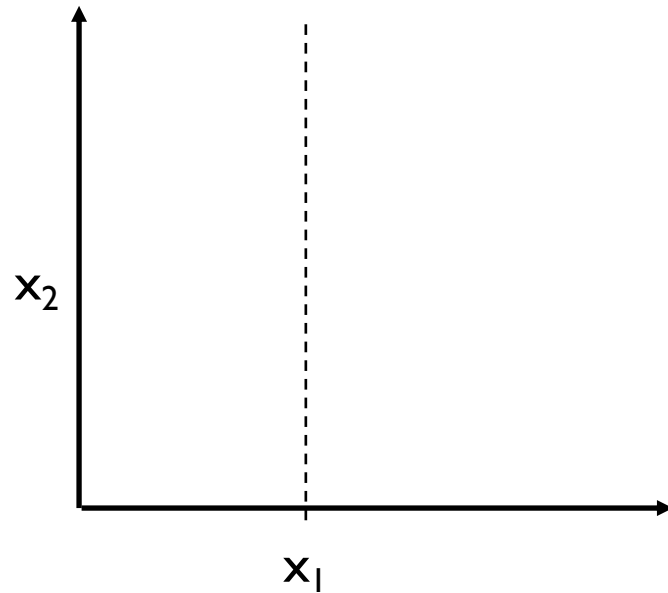(e.g., boolean)

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Test $x_j <= s$ and create 2 branches

The same attribute may be further split in each subtree

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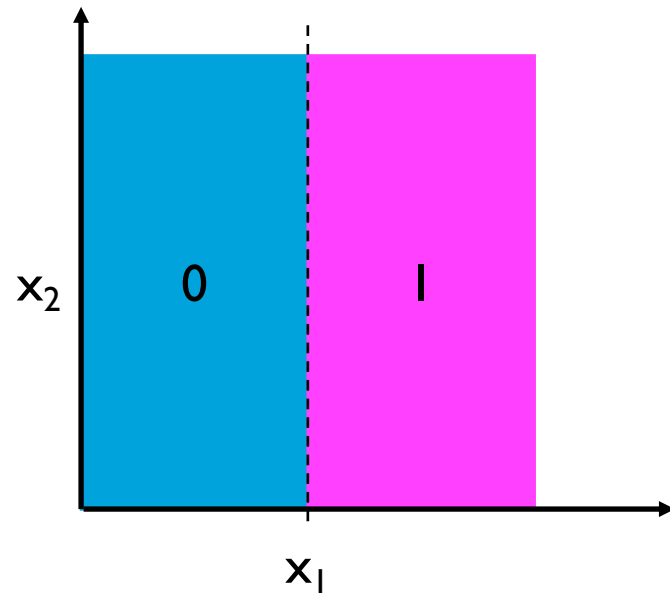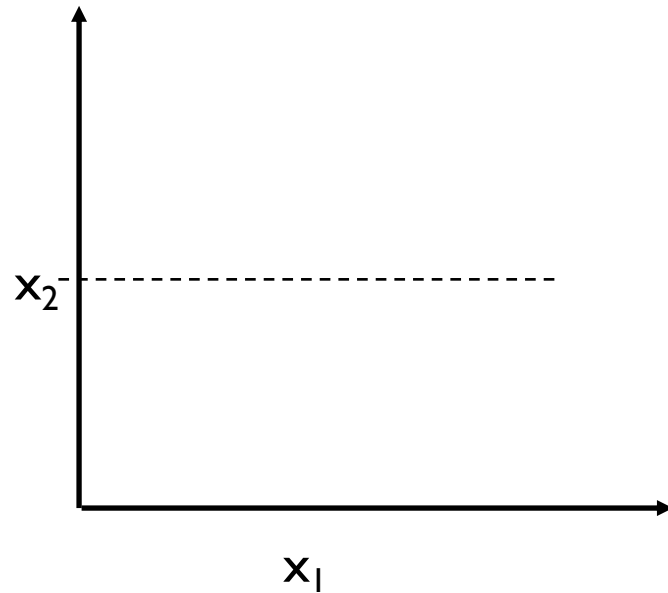Test $x_j <= s$ and create 2 branches

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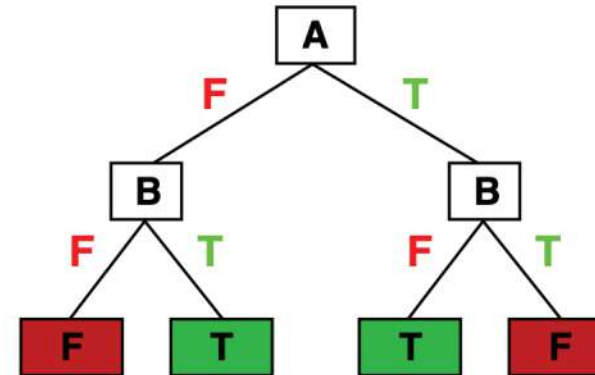
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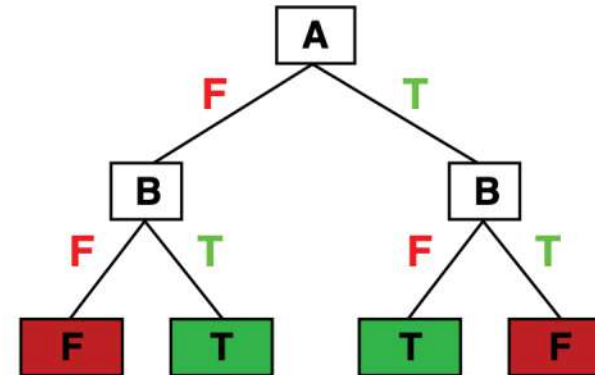
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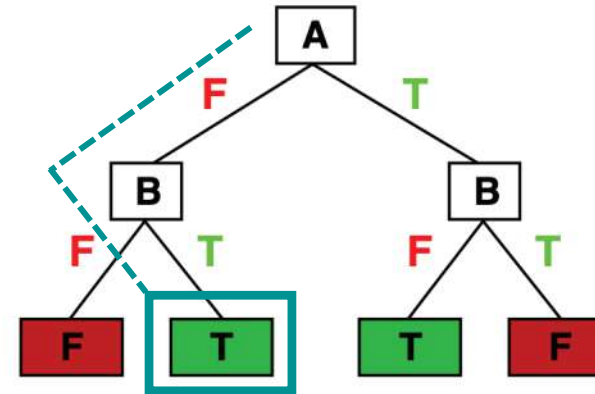
Each row of the truth table maps to a root-to-leaf path on the tree

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

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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For each input y = 0 or 1

Hypothesis Space

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

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

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Hypothesis Space

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

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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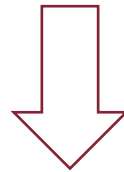
Solution
Top-Down greedy heuristic Recursive Binary Splitting

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- 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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- Such a splitting will lead to the partitioning of the feature space into the following regions:

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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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- 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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- The prediction for that test instance will be the **mean** of the region R_j

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- Tree building is still based on Recursive Binary Splitting 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

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- Several different measures to represent this notion of node "impurity":

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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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(*f*, *s*)-split

$$R_{\mathrm{left}}(f, s) = \{\mathbf{x}_i \mid x_{i,f} \leq s\} \quad R_{\mathrm{right}}(f, s) = \{\mathbf{x}_i \mid x_{i,f} > s\}$$

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$$
IG(\mathcal{D}_R, f, s) = \underbrace{I(\mathcal{D}_R)}_{\text{parent node's impurity}} - \underbrace{\left[\frac{\left|\mathcal{D}_{R_{\text{left}(f,s)}}\right|}{\left|\mathcal{D}_R\right|} I(\mathcal{D}_{R_{\text{left}(f,s)}}) + \frac{\left|\mathcal{D}_{R_{\text{right}(f,s)}}\right|}{\left|\mathcal{D}_R\right|} I(\mathcal{D}_{R_{\text{right}(f,s)}}) \right]}_{\text{children nodes' impurity}}
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- Classification error rate is the fraction of the training observations in that region that are not labeled with the most common class

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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
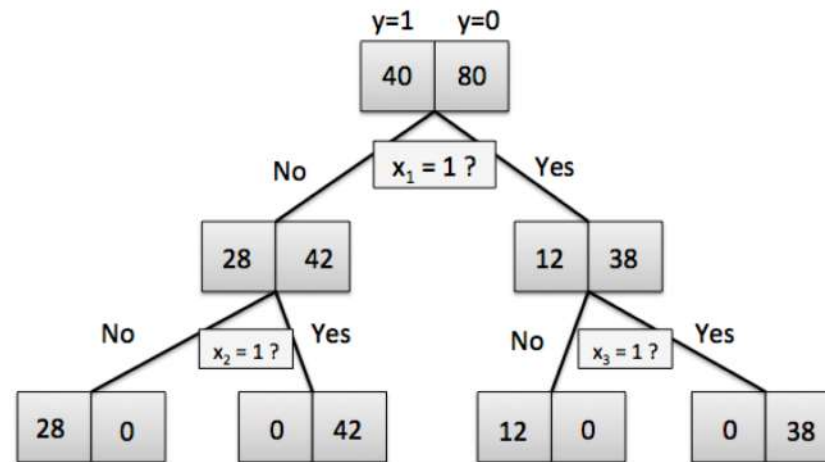
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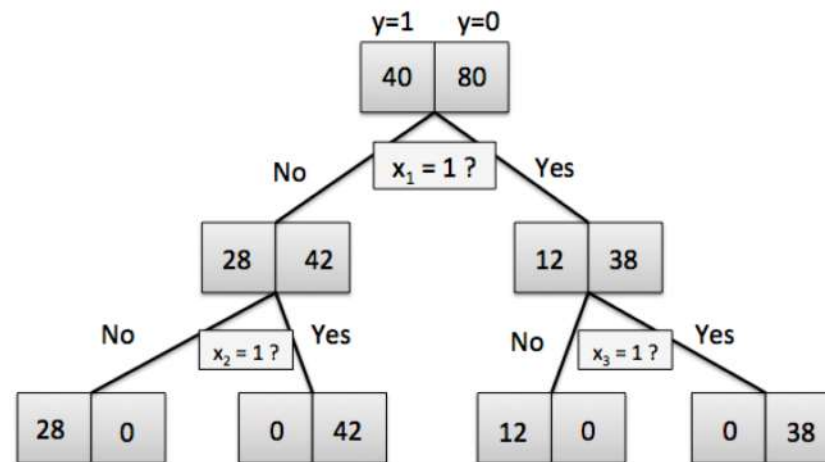
Question

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

$I_E = 40/120$

y=1   y=0

| 40 | 80 |

$I_E = 28/70$

No $x_1 = 1$?   Yes

$I_E = 12/50$

| 28 | 42 |

| 12 | 38 |

No $x_2 = 1$?   Yes

No $x_3 = 1$?   Yes

$I_E = 0/28$

| 28 | 0 |

| 0 | 42 |

| 12 | 0 |

| 0 | 38 |

$I_E = 0/38$

$I_E = 0/42$

$I_E = 0/12$

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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Compute IG of the first split using I_E

$$40/120 - [(70/120 * 28/70) + (50/120 * 12/50)]$$

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$40/120 - [28/10 + 12/120]$

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40/120 - 40/120 = 0

IG after the first split is exactly 0

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$40/120 - 40/120 = 0$

IG after the first split is exactly 0

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

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Classification Error Rate vs. Entropy (Gini)

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Splitting root gives no IG improvement in terms of IE

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Splitting root gives no IG improvement in terms of IE

The tree learning algorithm would stop at this point

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

Classification Error Rate vs. Entropy (Gini)

$I_E = 40/120$
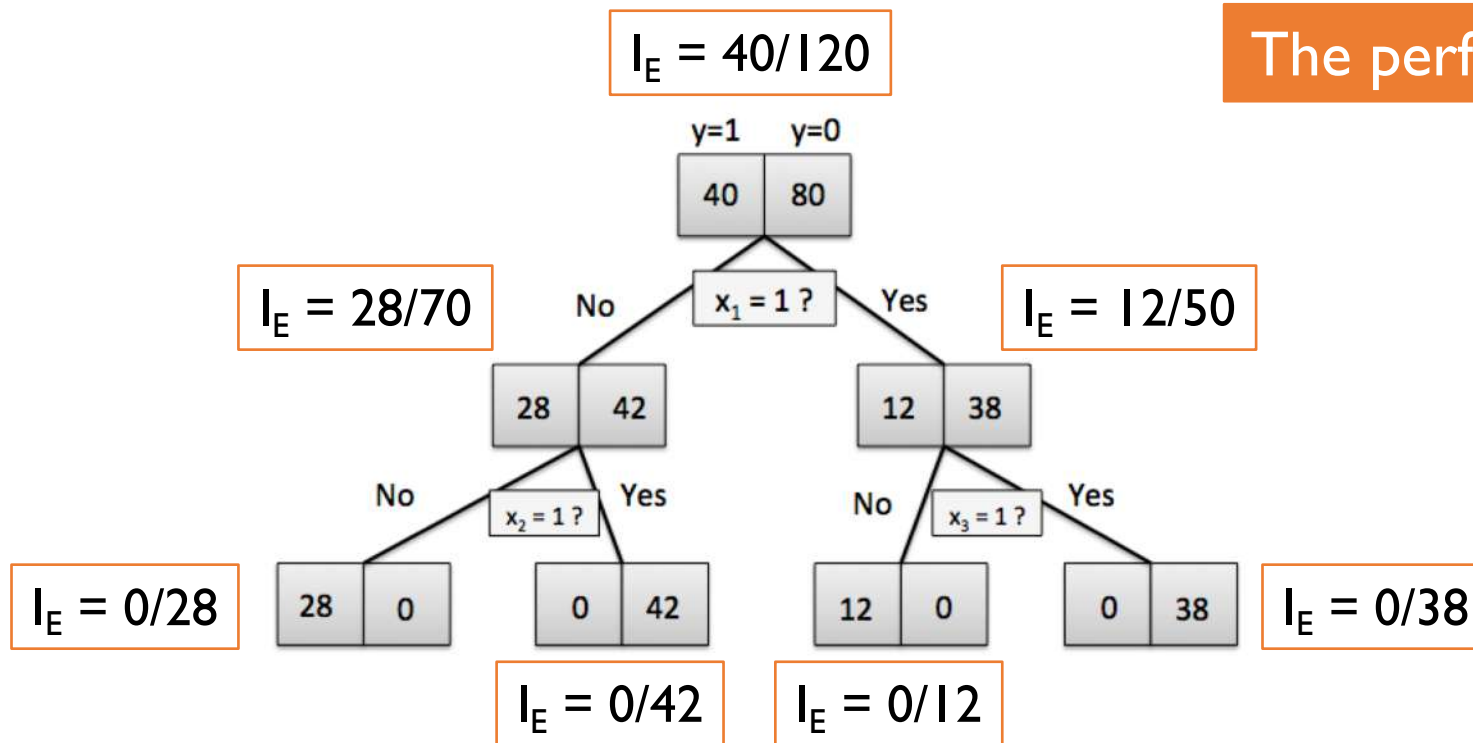
The perfect tree cannot be built using I_E

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Classification Error Rate vs. Entropy (Gini)

Node impurity using I_H

$I_H = 0.918$

y=1   y=0

| 40 | 80 |

No $x_1 = 1$?   Yes

$I_H = 0.971$

$I_H = 0.795$

| 28 | 42 | | 12 | 38 |

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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

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

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No $x_2 = 1?$ Yes   No $x_3 = 1?$ Yes

$I_H = 0$ | 28 | 0 | | 0 | 42 | | 12 | 0 | | 0 | 38 | $I_H = 0$

The splitting rule would continue until the child nodes are pure

$I_H = 0$ $I_H = 0$

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

Classification Error Rate vs. Entropy (Gini)
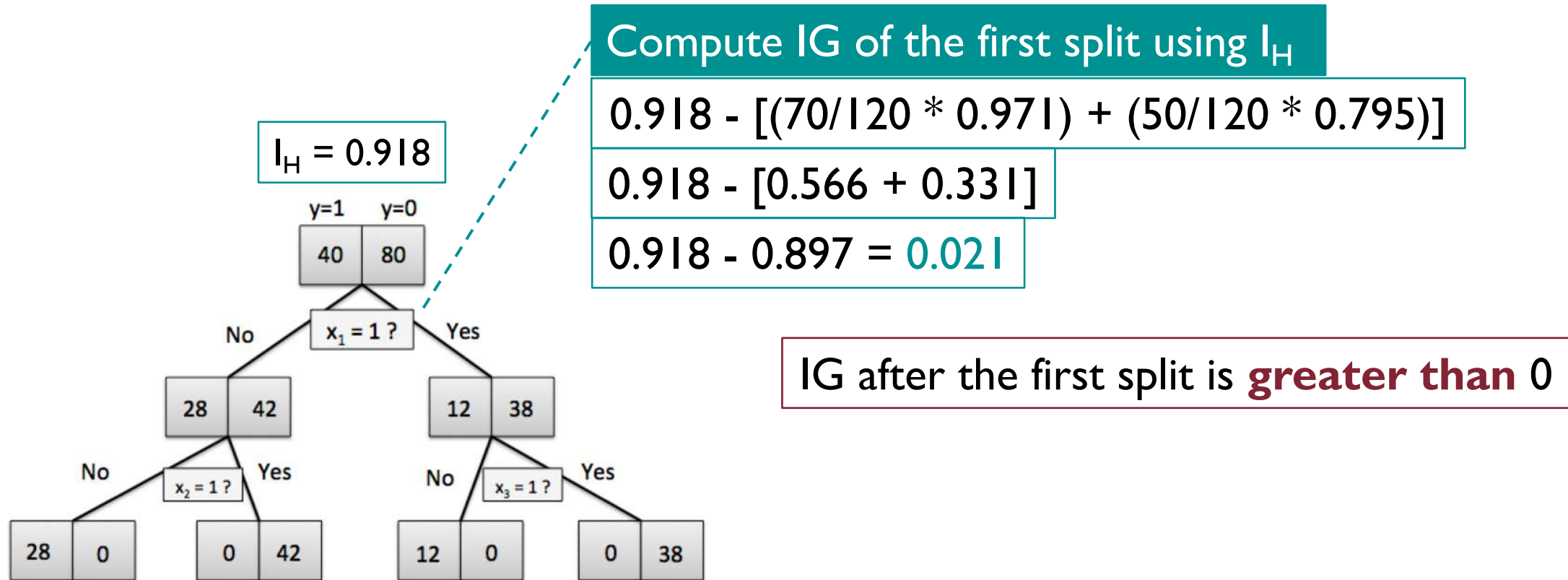
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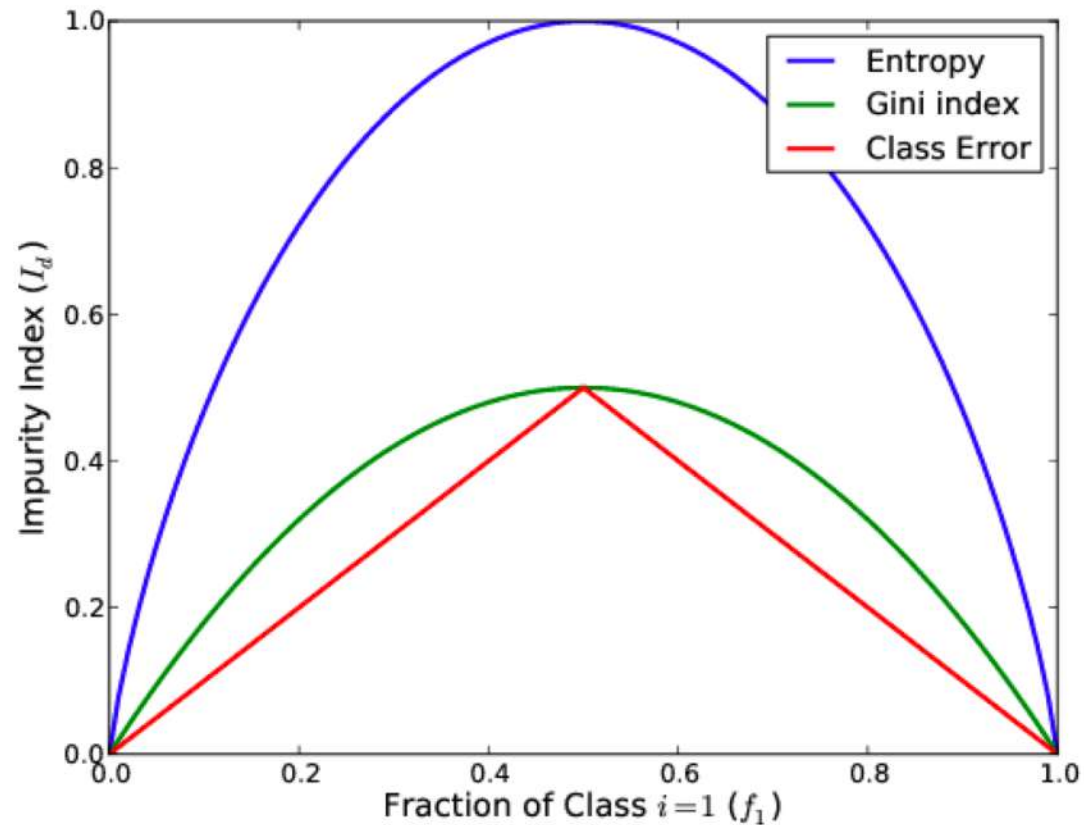
Gini and Entropy are "smoother" than classification error

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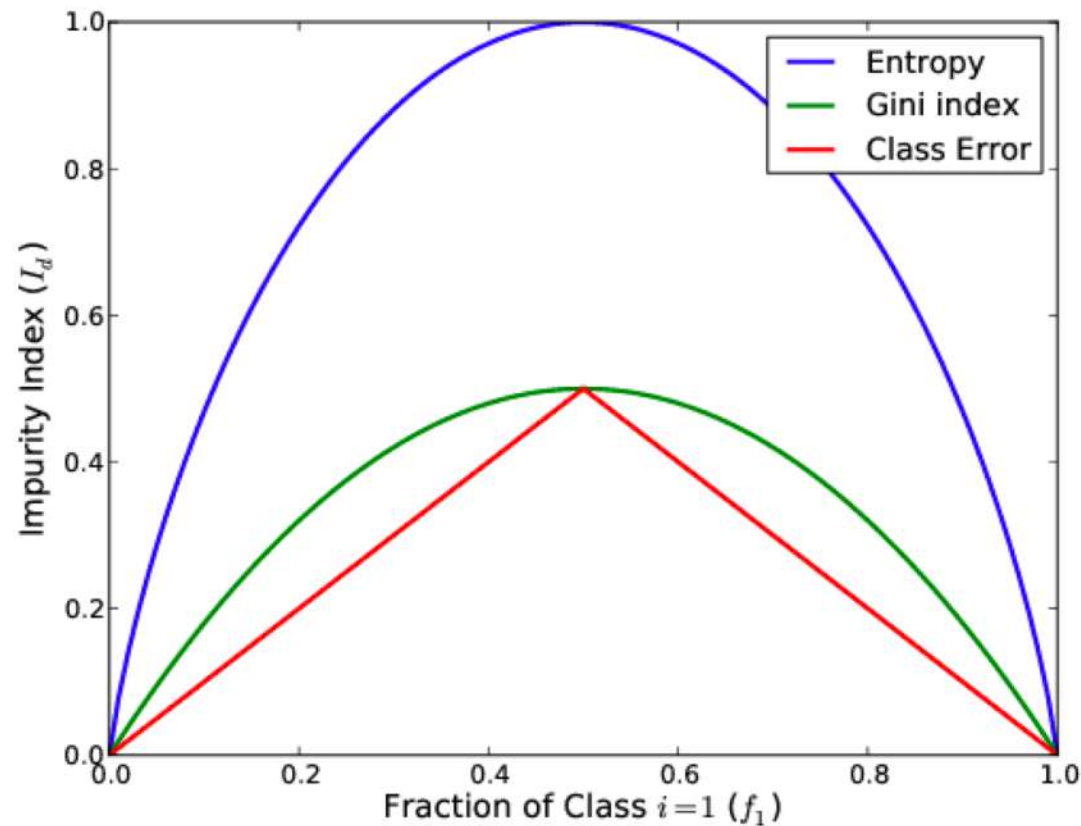
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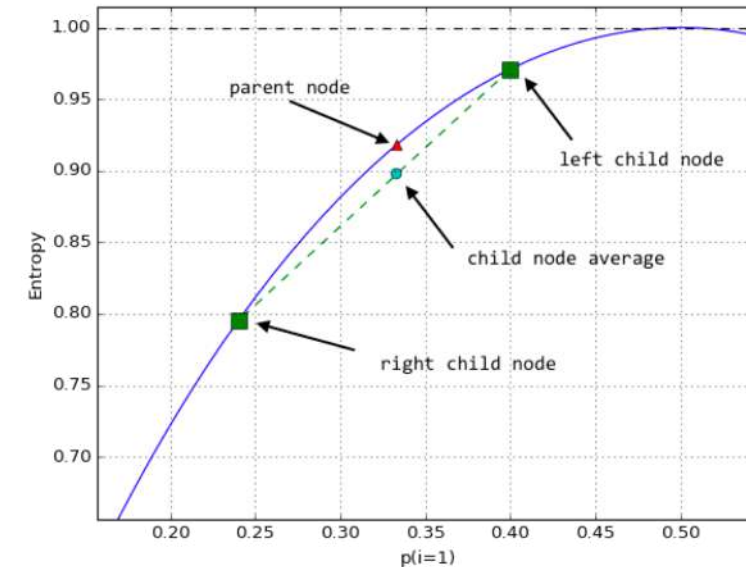
Entropy is always larger than the weighted averaged entropy due to its "bell shape"

Evolution of Entropy

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

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- We define the ratio $p = N^+/N$ and $q = N^-/N$

- The entropy is defined as:

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

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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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- Suppose we start with a node whose entropy is 1 (half +/half -)

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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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Which one is better?

If there is a strong linear relationship between input and output

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Learned hypothesis is constant within a region

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
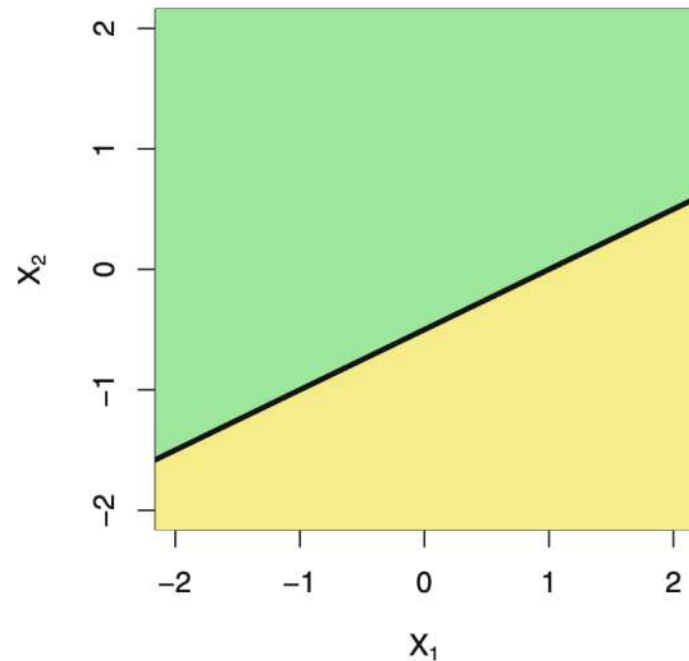
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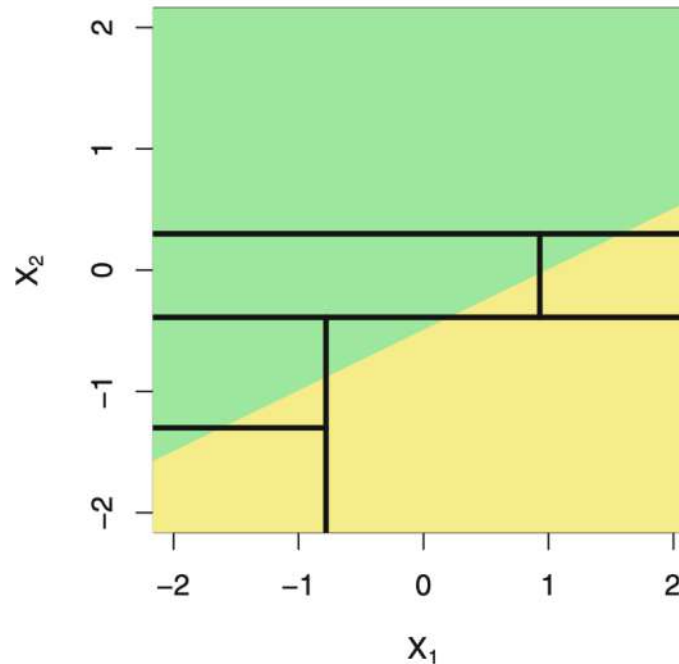
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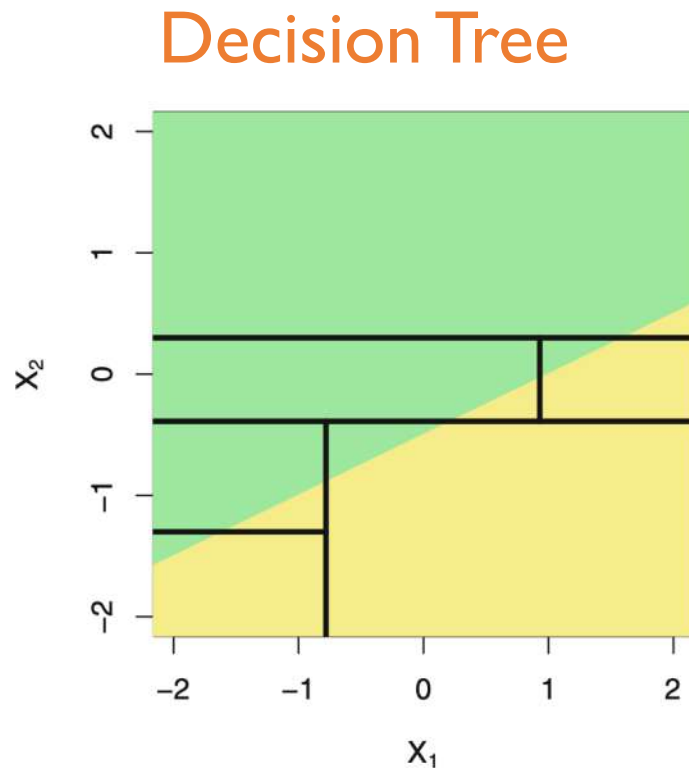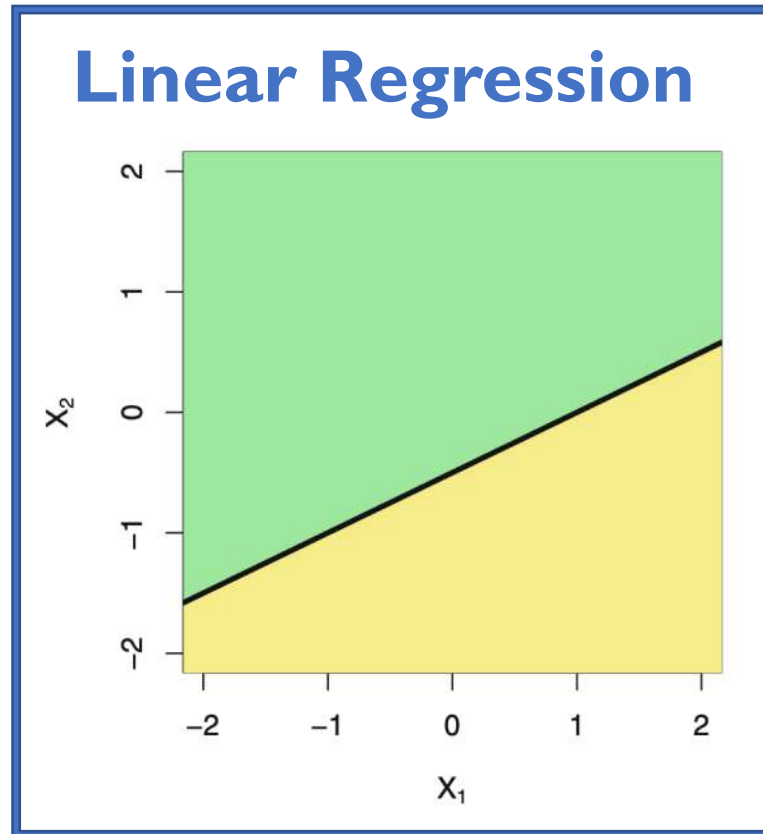
Decision Tree

Nice linear decision boundary

Linear Models vs. Decision Trees: Example

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Linear Models vs. Decision Trees: Example

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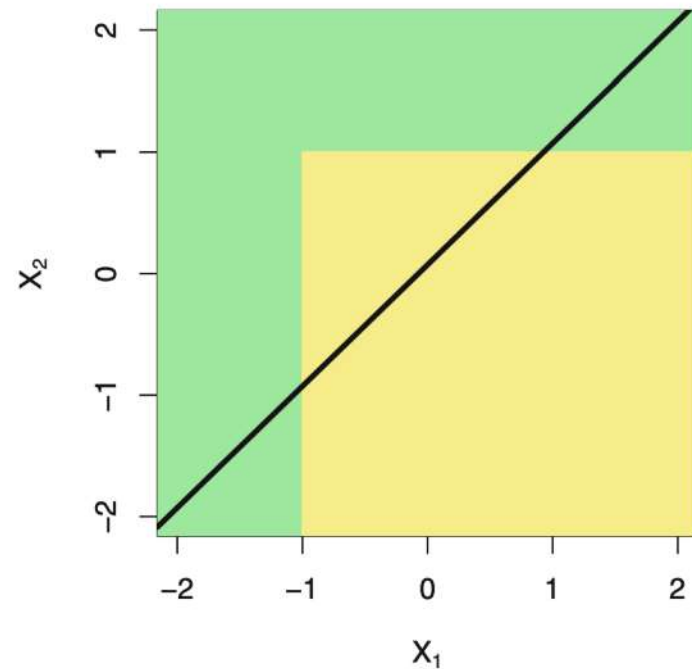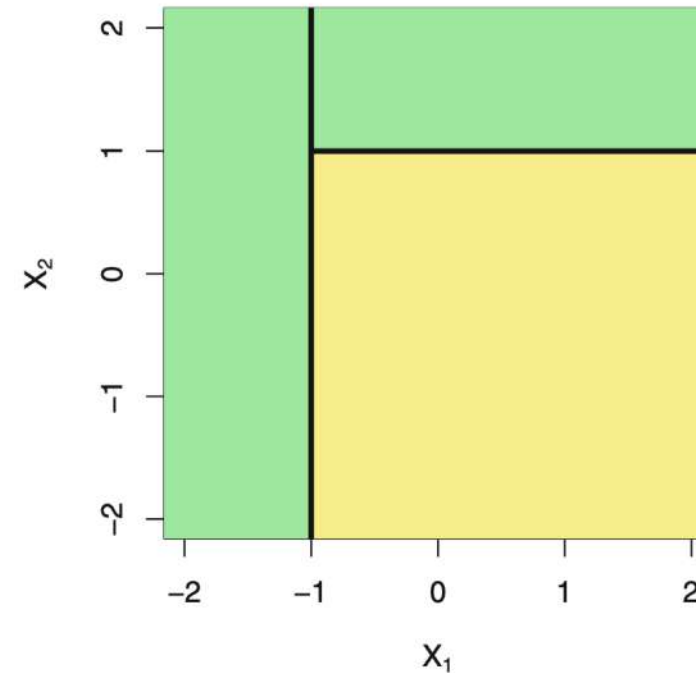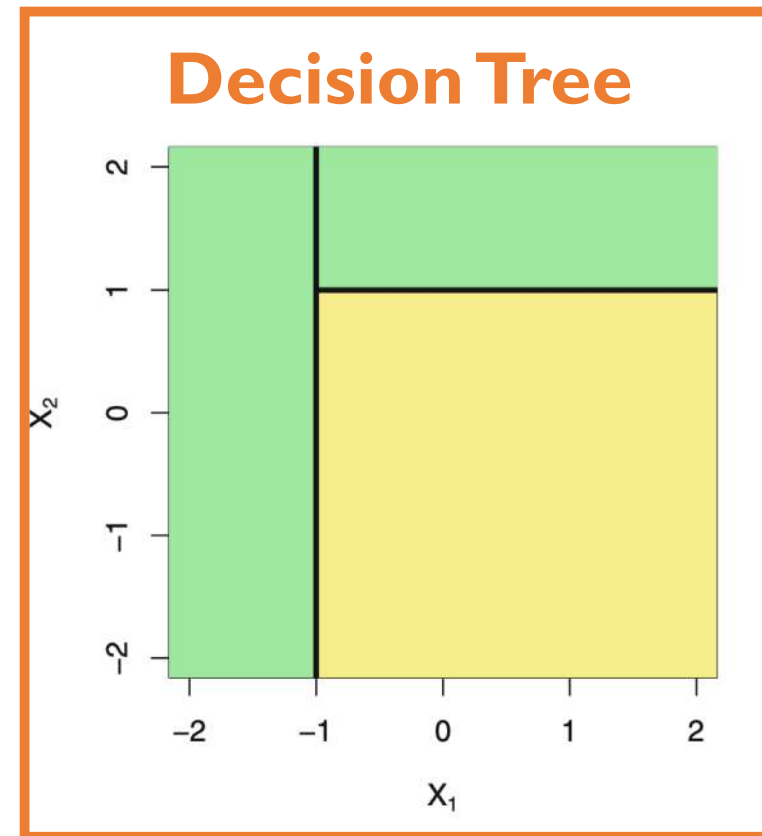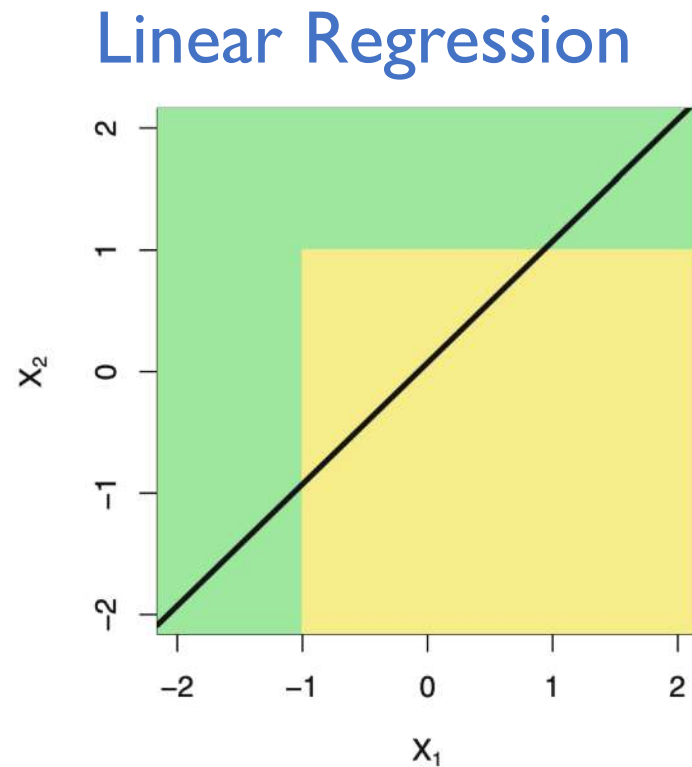
Decision Tree

Non-linear decision boundary

Decision Trees: Pruning

- Greedy tree growing strategy may lead to:

  - **Overfitting** → if we keep splitting as long as there is an information gain

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

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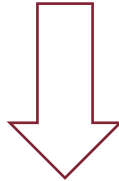
Cost Complexity Pruning (a.k.a. Weakest Link Pruning)

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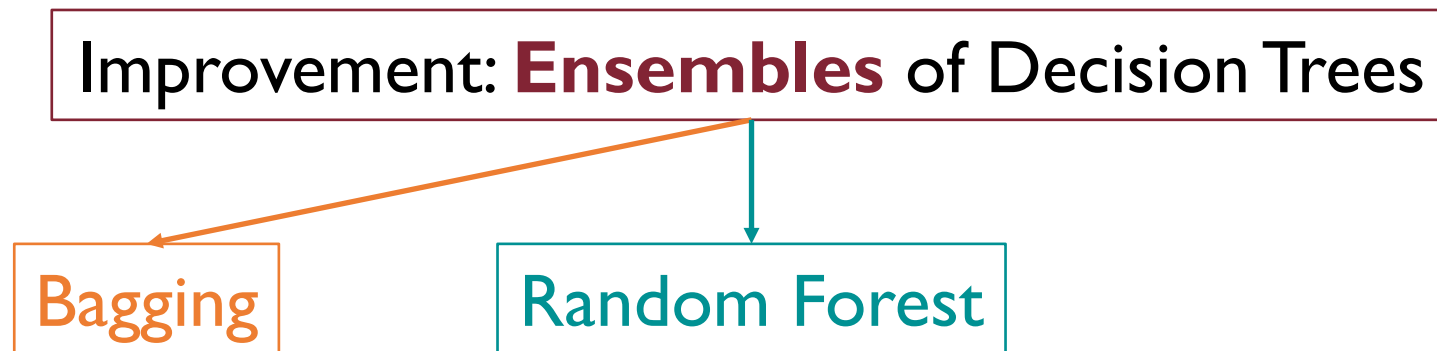
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- Bootstrap aggregation (**Bagging**) is a general-purpose method to lower the variance of a statistical learning method

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Averaging a set of observations reduces variance!

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Bootstrap

Taking repeated samples from the same 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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- As with bagging, random forests will not overfit if we increase B

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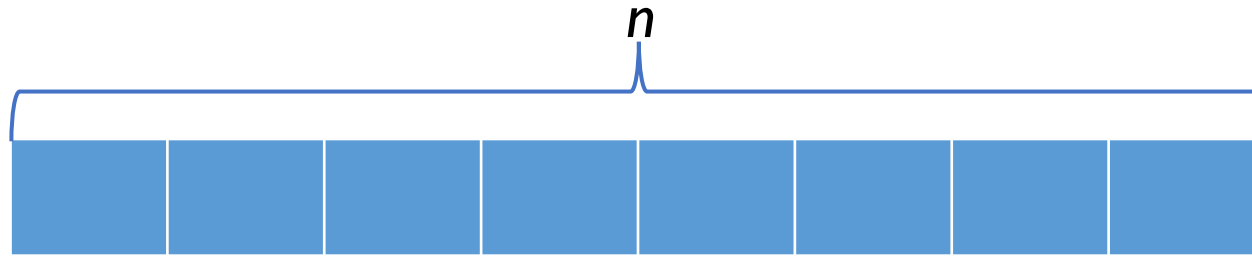
Randomly choose *k* features out of *n*, each with uniform probability $p = 1/n$

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

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$$\frac{1}{n} + \frac{n-1}{n} * \frac{1}{n-1} + \frac{n-1}{n} * \frac{n-2}{n-1} * \frac{1}{n-2} + \ldots + \frac{n-1}{n} * \frac{n-2}{n-1} * \ldots * \frac{n-(k-1)}{n-(k-2)} * \frac{1}{n-(k-1)} = \underbrace{\frac{1}{n} * \frac{1}{n} * \ldots * \frac{1}{n}}_{k} = \frac{k}{n}$$

Why *k/n?* – Approach 1.b.

It might be easier to compute the following:

$1 - P(f$ is **NOT** extracted as 1st **AND** f is **NOT** extracted as 2nd **AND** ... **AND** f is **NOT** extracted as k-th$)$

Why *k/n?* – Approach 1.b.

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$$1 - \underbrace{\left[\frac{n-1}{n} * \frac{n-2}{n-1} * \ldots * \frac{n-(k-1)}{n-(k-2)} * \frac{n-k}{n-(k-1)} \right]}_{k \text{ times}} =$$

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

Why *k/n*? – Approach 2

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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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- Again, general approach that can be applied to many statistical learning methods for regression or classification

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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

Boosting

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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,

   $$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x). \tag{8.12}$$

Boosting: Hyperparameters

- Boosting has **3** tuning **hyperparameters**:
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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