

Big Data Computing

Master's Degree in Computer Science

2021-2022

Gabriele Tolomei

Department of Computer Science

Sapienza Università di Roma

tolomei@di.uniroma1.it



SAPIENZA
UNIVERSITÀ DI ROMA

Recap from Last Lecture

- 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 training heuristic
- Regression Trees:
 - Use Residual Sum of Squares (RSS) as splitting criterion
 - At inference time, predictions are the mean of the leaf observations

Classification Trees

- Very similar to a regression tree

Classification Trees

- Very similar to a regression tree
- Used to predict a **categorical** response rather than a numerical one

Classification Trees

- Very similar to a regression tree
- Used to predict a **categorical** response rather than a numerical one
- Tree building is still based on **Recursive Binary Splitting** algorithm but RSS cannot be used as a criterion for splitting nodes

Classification Trees

- Very similar to a regression tree
- Used to predict a **categorical** response rather than a numerical one
- 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**"

Classification Trees

- Very similar to a regression tree
- Used to predict a **categorical** response rather than a numerical one
- 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

- A node containing instances all with the same label is **perfectly pure**

The "Impurity" of a Node

- A node containing instances all with the same label is **perfectly pure**
- We would like to grow a tree whose nodes are as purest as possible

The "Impurity" of a Node

- A node containing instances all with the same label is **perfectly pure**
- We would like to grow a tree whose nodes are as purest as possible
- Several different measures to represent this notion of node "impurity":
 - Classification Error Rate
 - Gini Index
 - Entropy

The "Impurity" of a Node

- A node containing instances all with the same label is **perfectly pure**
- We would like to grow a tree whose nodes are as purest as possible
- Several different measures to represent this notion of node "impurity":
 - Classification Error Rate
 - Gini Index
 - Entropy
- It is often convenient to refer to the **information gain** of a split

Classification Trees: Notation

Subset of training instances falling into **region** R

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

Classification Trees: Notation

Subset of training instances falling into **region** R

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

(f, s) -split

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

Classification Trees: Notation

Subset of training instances falling into **region** R

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

(f, s) -split

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

impurity of a region

$$I(\mathcal{D}_R)$$

Classification Trees: Notation

Subset of training instances falling into **region** R

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

(f, s)-split

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

impurity of a region

$$I(\mathcal{D}_R)$$

information gain obtained with an (f, s) -split

$$IG(\mathcal{D}_R, f, s)$$

Classification Trees: Notation

Subset of training instances falling into **region** R

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

(f, s) -split

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

impurity of a region

$$I(\mathcal{D}_R)$$

information gain obtained with an (f, s) -split

$$IG(\mathcal{D}_R, f, s)$$

Maximize Information Gain

At each step, the best (f, s) -split is found so as to minimize the children nodes' impurity

Maximize Information Gain

At each step, the best (f, s) -split is found so as to minimize the children nodes' impurity

This corresponds to select the (f, s) -split that maximizes the information gain

Maximize Information Gain

At each step, the best (f, s) -split is found so as to minimize the children nodes' impurity

This corresponds to select the (f, s) -split that maximizes the information gain

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

Node Impurity: Classification Error Rate

- Classification error rate is the fraction of the training observations in that region that are not labeled with the most common class

Node Impurity: Classification Error Rate

- Classification error rate is the fraction of the training observations in that region that are **not** labeled with the most common class

$$I_E(\mathcal{D}_{R_j}) = 1 - \max_k \{\hat{p}_{jk}\}$$

Node Impurity: Classification Error Rate

- Classification error rate is the fraction of the training observations in that region that are **not** labeled with the most common class

$$I_E(\mathcal{D}_{R_j}) = 1 - \max_k \{\hat{p}_{jk}\}$$

proportion of training observations in the j -th region that are from the k -th class

Node Impurity: Classification Error Rate

- Classification error rate is the fraction of the training observations in that region that are **not** labeled with the most common class

$$I_E(\mathcal{D}_{R_j}) = 1 - \max_k \{\hat{p}_{jk}\}$$

proportion of training observations in the j -th region that are from the k -th class

- Although this is the most intuitive notion of impurity we will see how this may not be a great choice

Node Impurity: Classification Error Rate

- Classification error rate is the fraction of the training observations in that region that are **not** labeled with the most common class

$$I_E(\mathcal{D}_{R_j}) = 1 - \max_k \{\hat{p}_{jk}\}$$

proportion of training observations in the j -th region that are from the k -th class

- Although this is the most intuitive notion of impurity we will see how this may not be a great choice
- Other 2 measures are preferable: **Gini Index** and **Entropy**

Node Impurity: Gini Index

- Measures the variance across the K classes

$$I_G(\mathcal{D}_{R_j}) = \sum_{k=1}^K \hat{p}_{jk}(1 - \hat{p}_{jk})$$

Node Impurity: Gini Index

- Measures the variance across the K classes

$$I_G(\mathcal{D}_{R_j}) = \sum_{k=1}^K \hat{p}_{jk}(1 - \hat{p}_{jk})$$

- A small value of Gini is obtained whenever all the proportions are either close to 1 or to 0

Node Impurity: Gini Index

- Measures the variance across the K classes

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

- A small value of Gini is obtained whenever all the proportions are either close to 1 or to 0
- A small value indicates that a node contains predominantly observations from a single class

Node Impurity: Entropy

- Alternative, yet similar to Gini

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

Node Impurity: Entropy

- Alternative, yet similar to Gini

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

- It ranges between $[0, +\infty]$

Node Impurity: Entropy

- Alternative, yet similar to Gini

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

- It ranges between $[0, +\infty]$
- Like Gini, a small value of entropy is obtained whenever all the proportions are either close to 1 or to 0

Node Impurity: Entropy

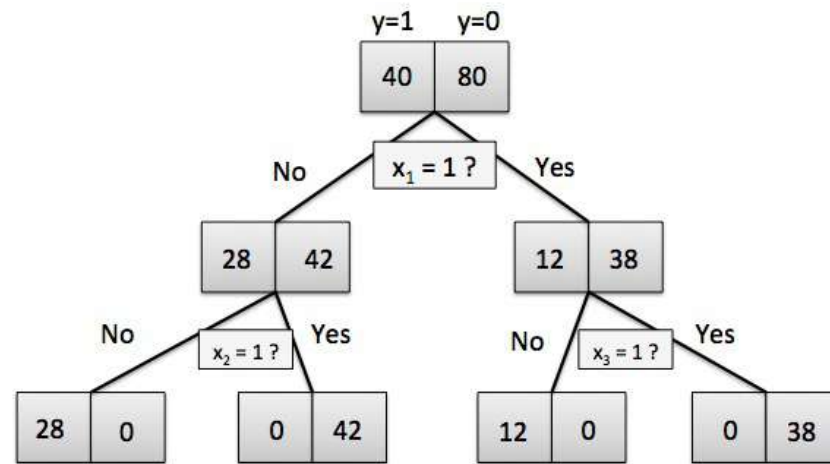
- Alternative, yet similar to Gini

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

- It ranges between $[0, +\infty]$
- 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

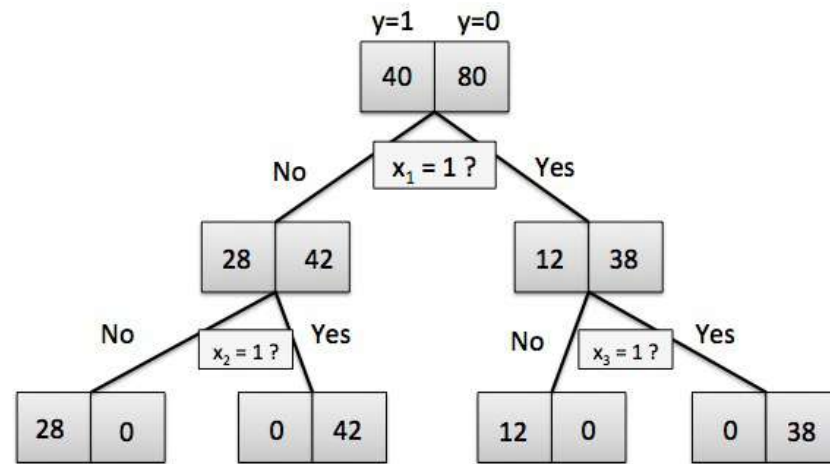
Classification Error Rate vs. Entropy (Gini)

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



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

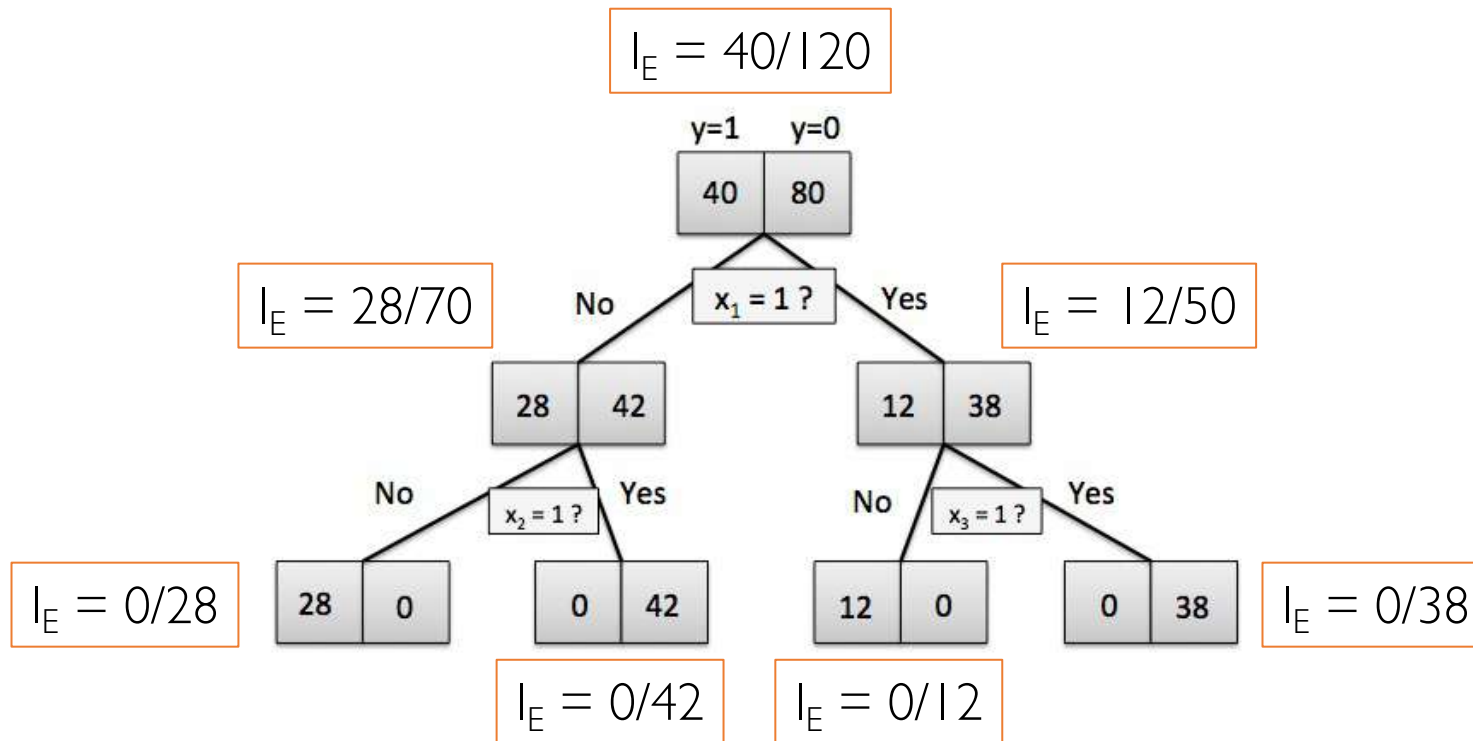


Question

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

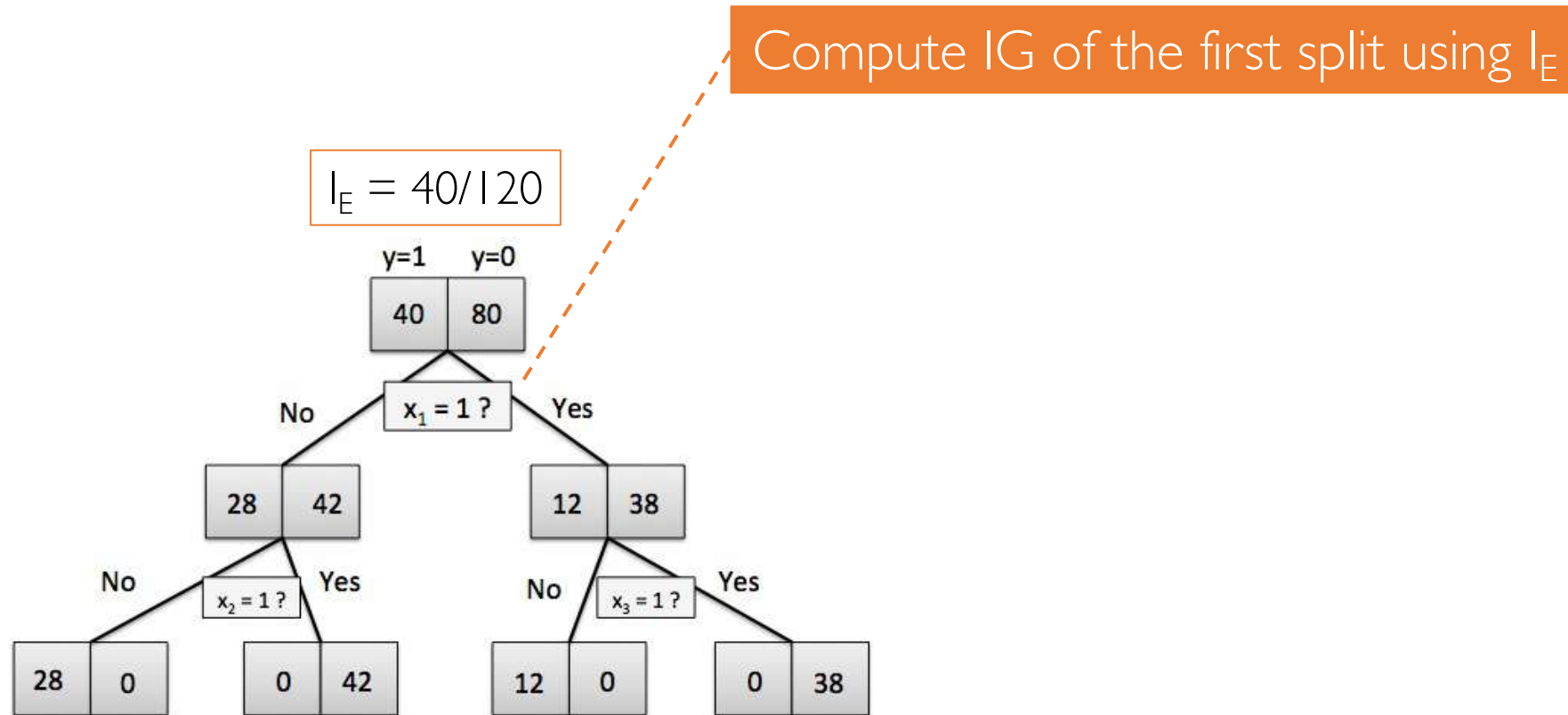
Classification Error Rate vs. Entropy (Gini)

Node impurity using I_E



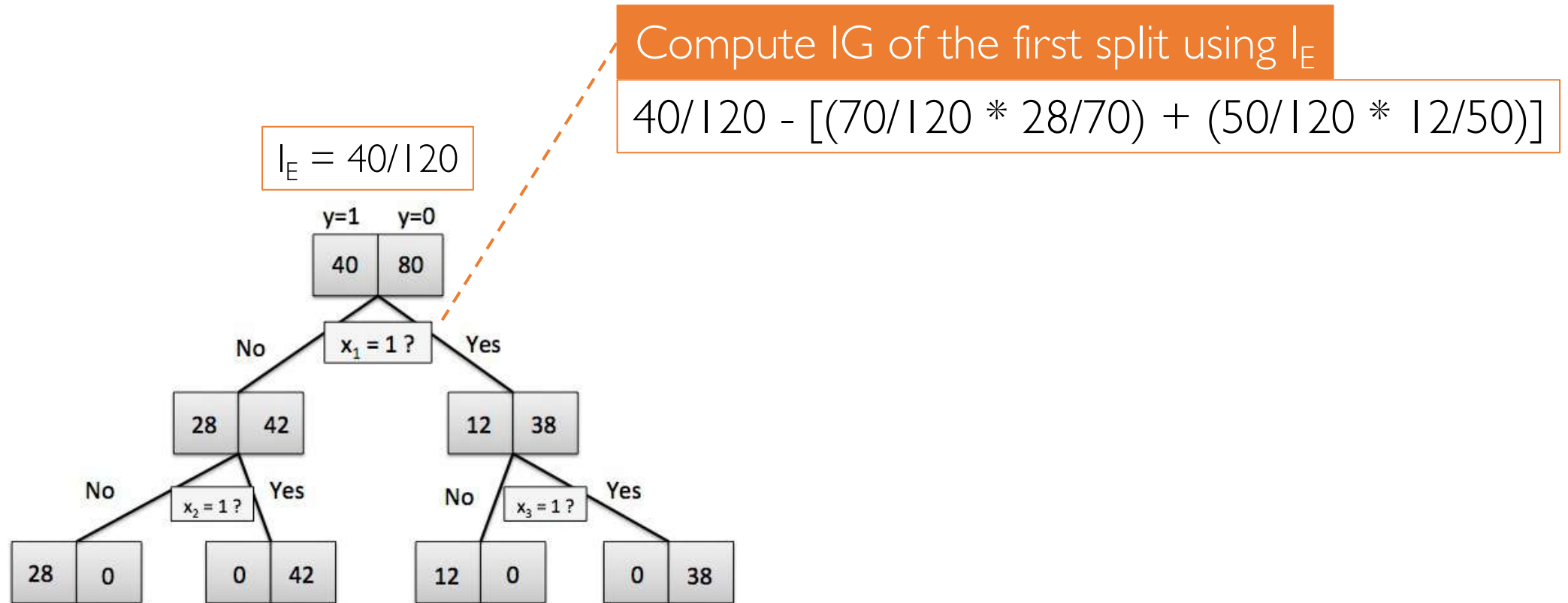
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



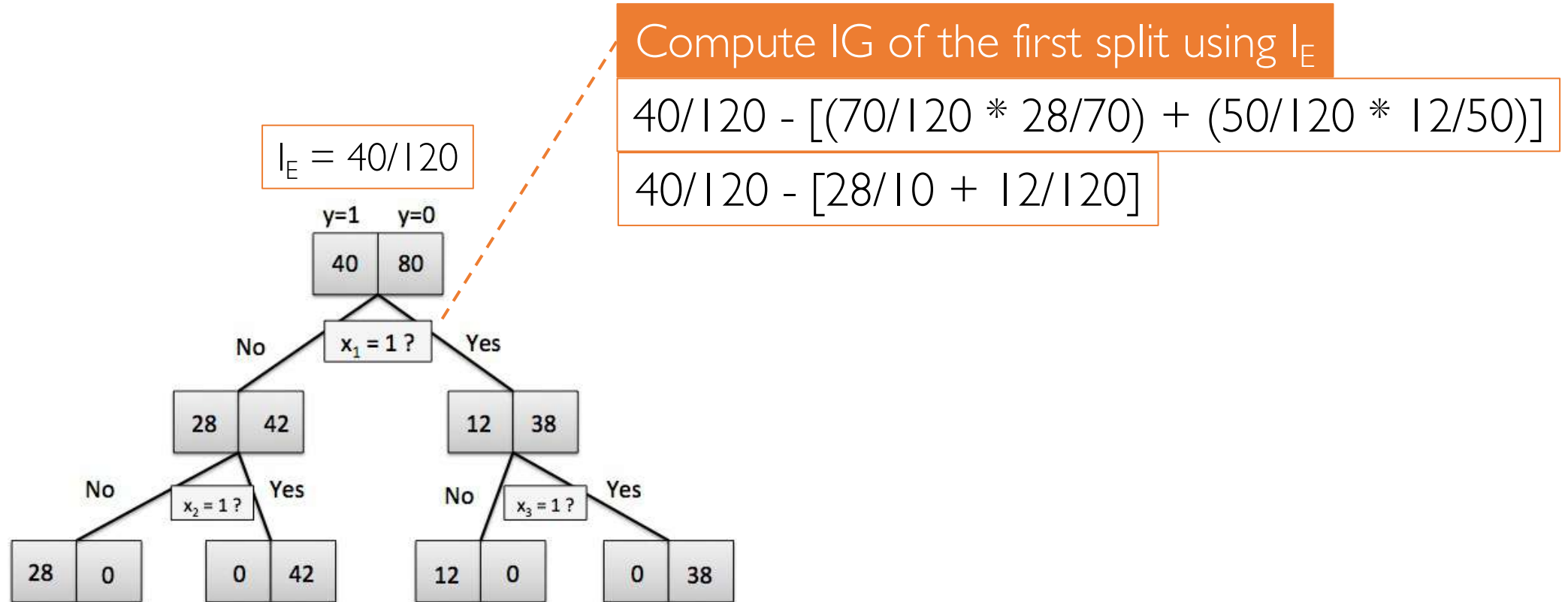
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



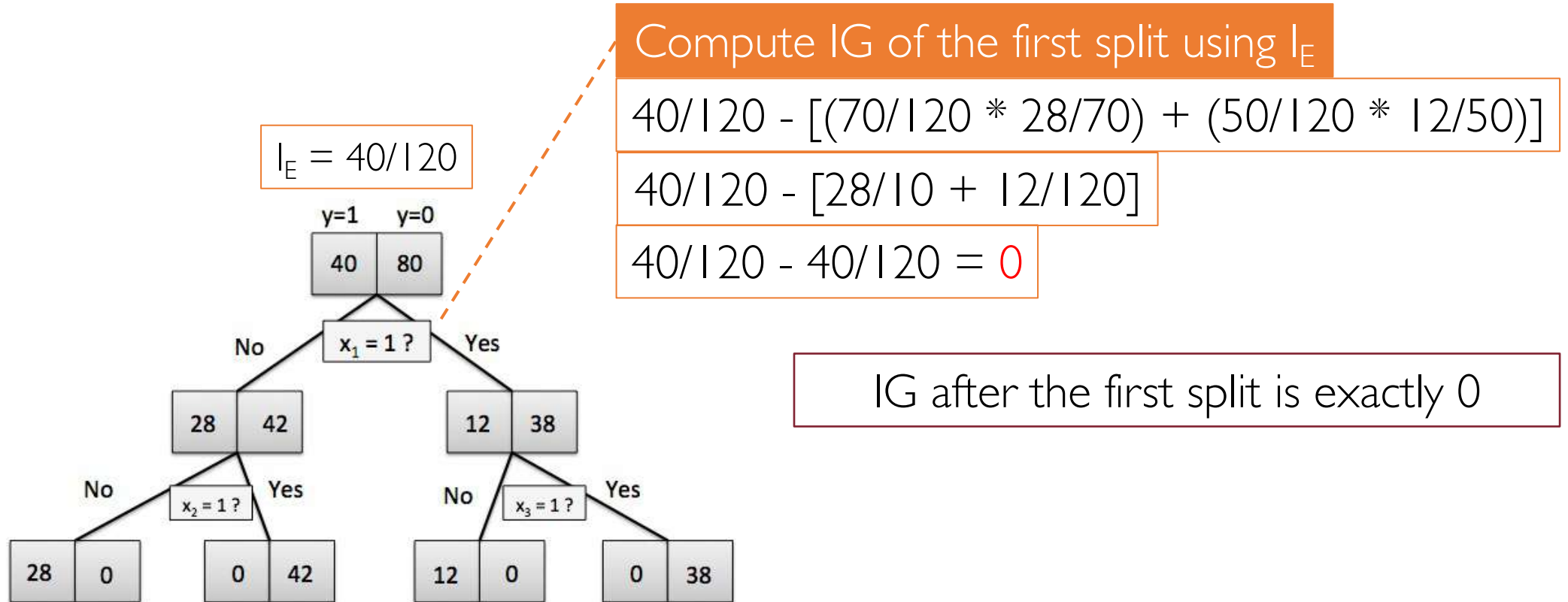
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



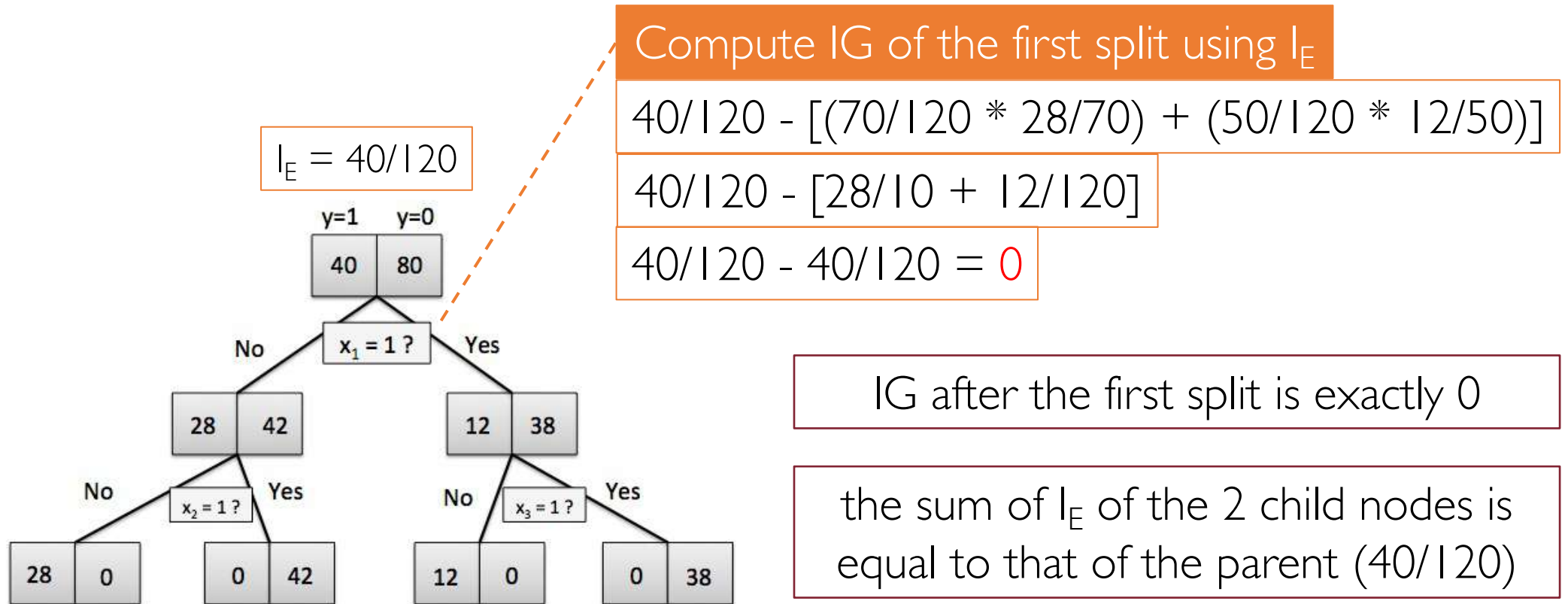
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



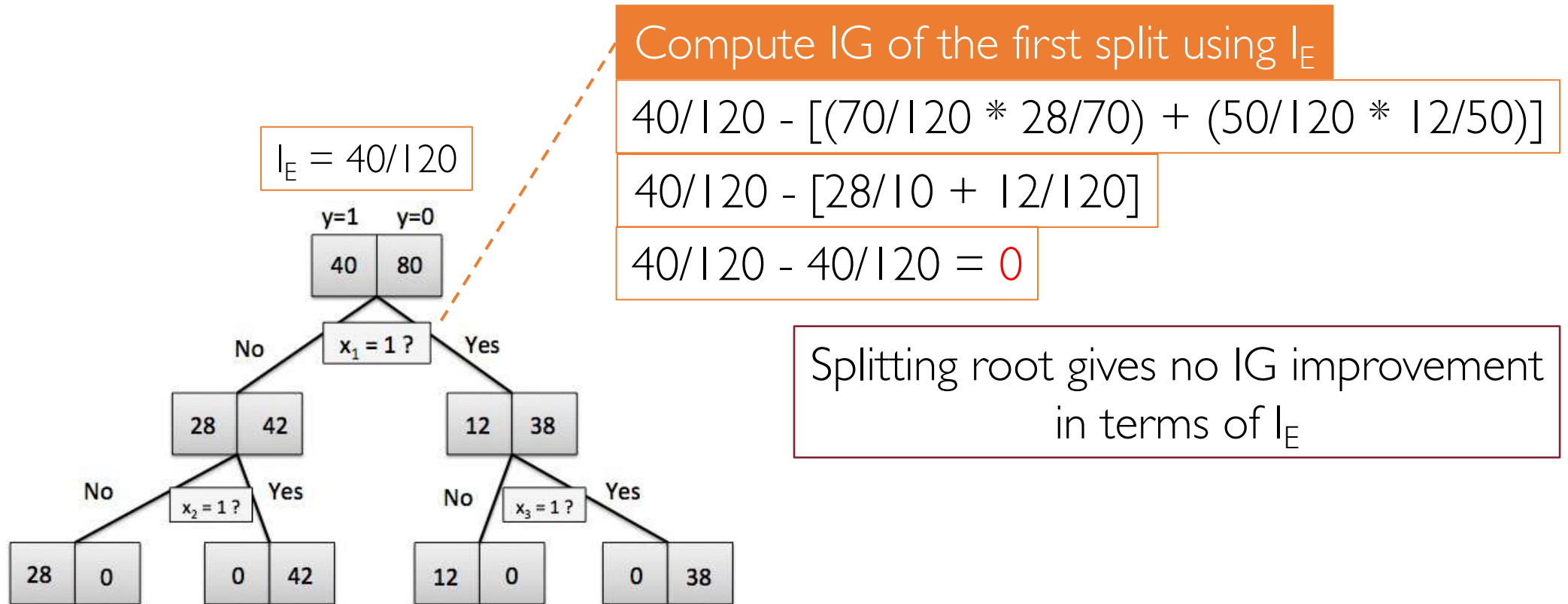
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



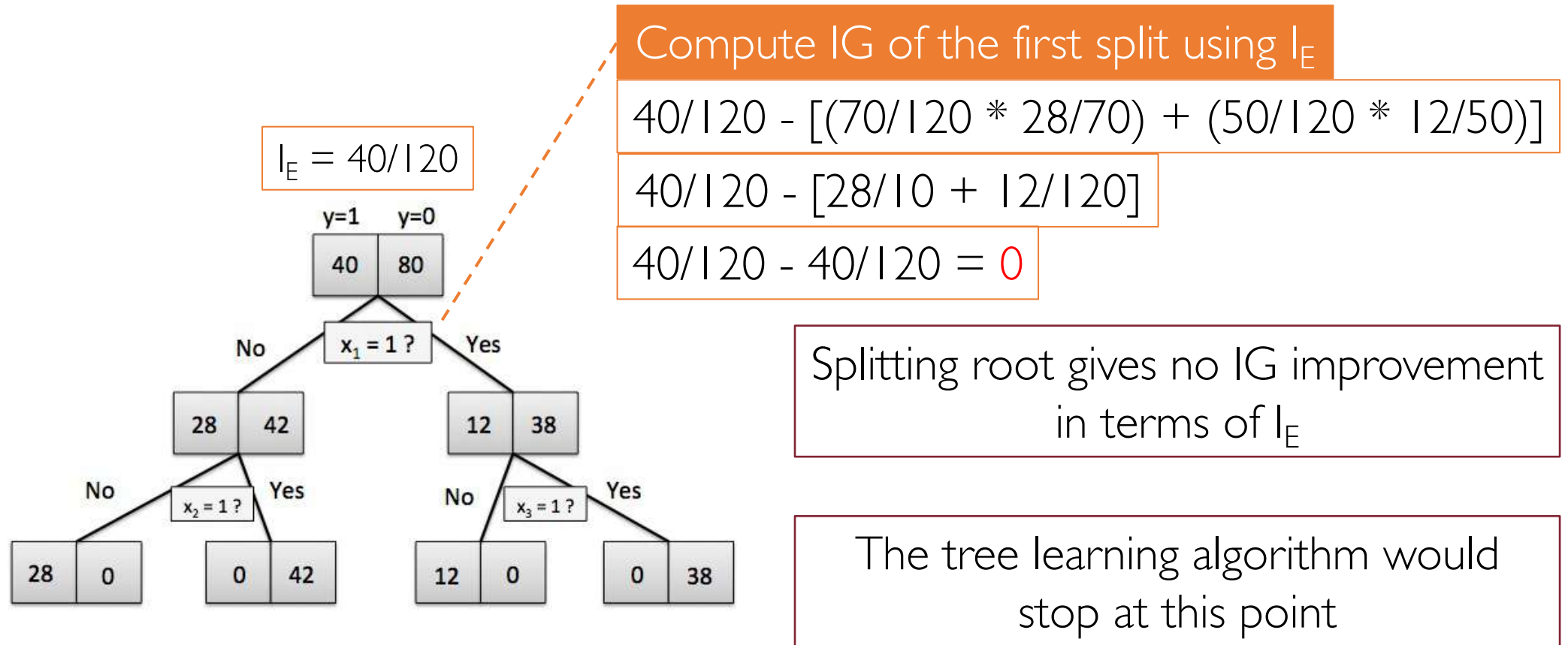
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



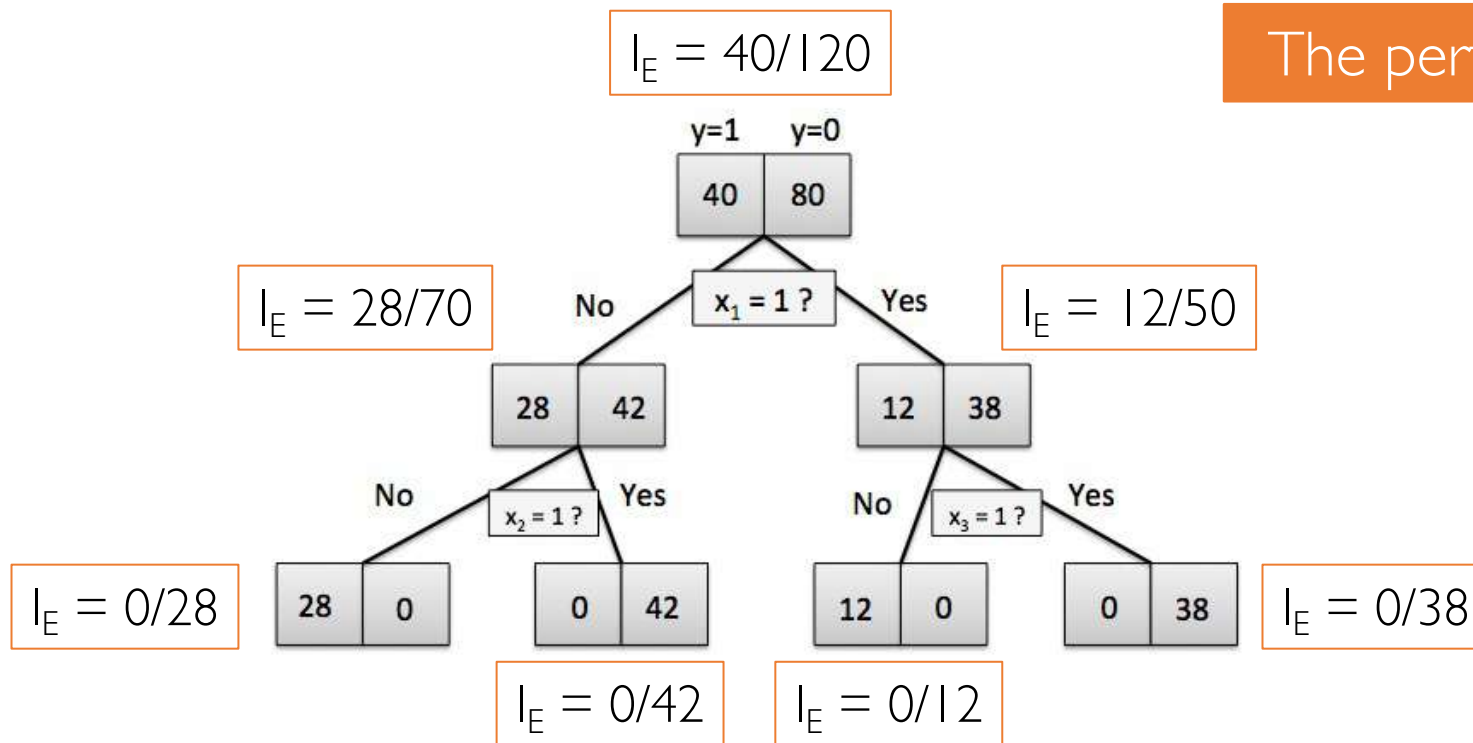
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



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

Classification Error Rate vs. Entropy (Gini)

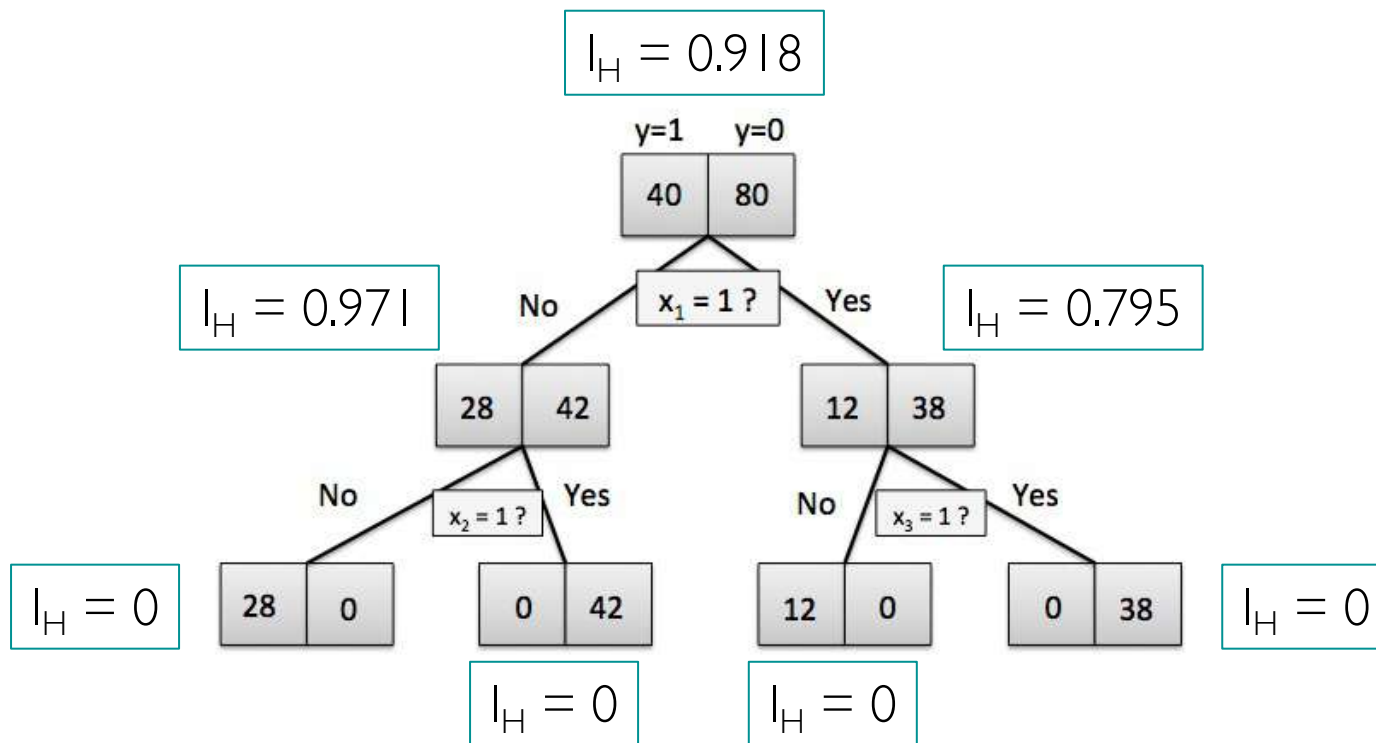


The perfect tree cannot be built using I_E

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

Classification Error Rate vs. Entropy (Gini)

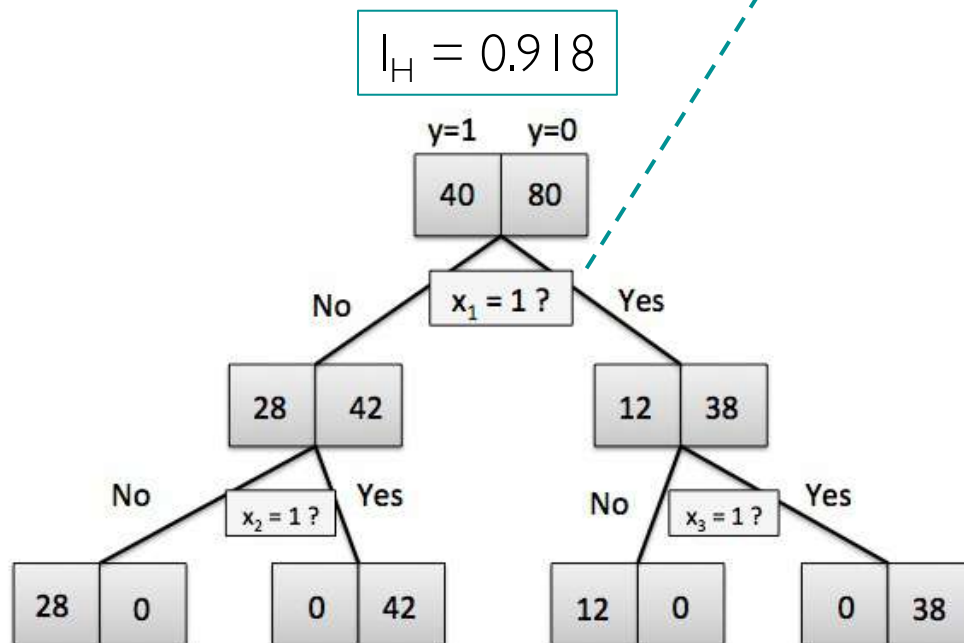
Node impurity using I_H



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

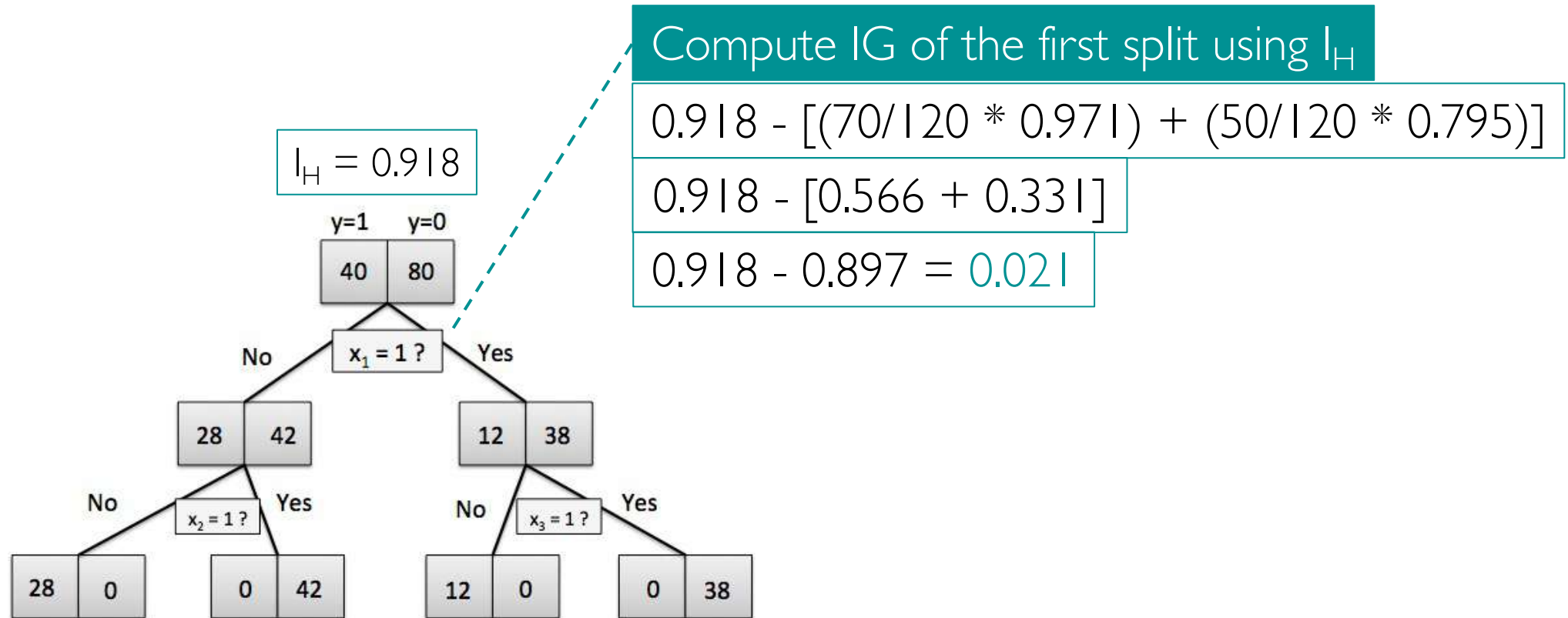
Classification Error Rate vs. Entropy (Gini)

Compute IG of the first split using I_H



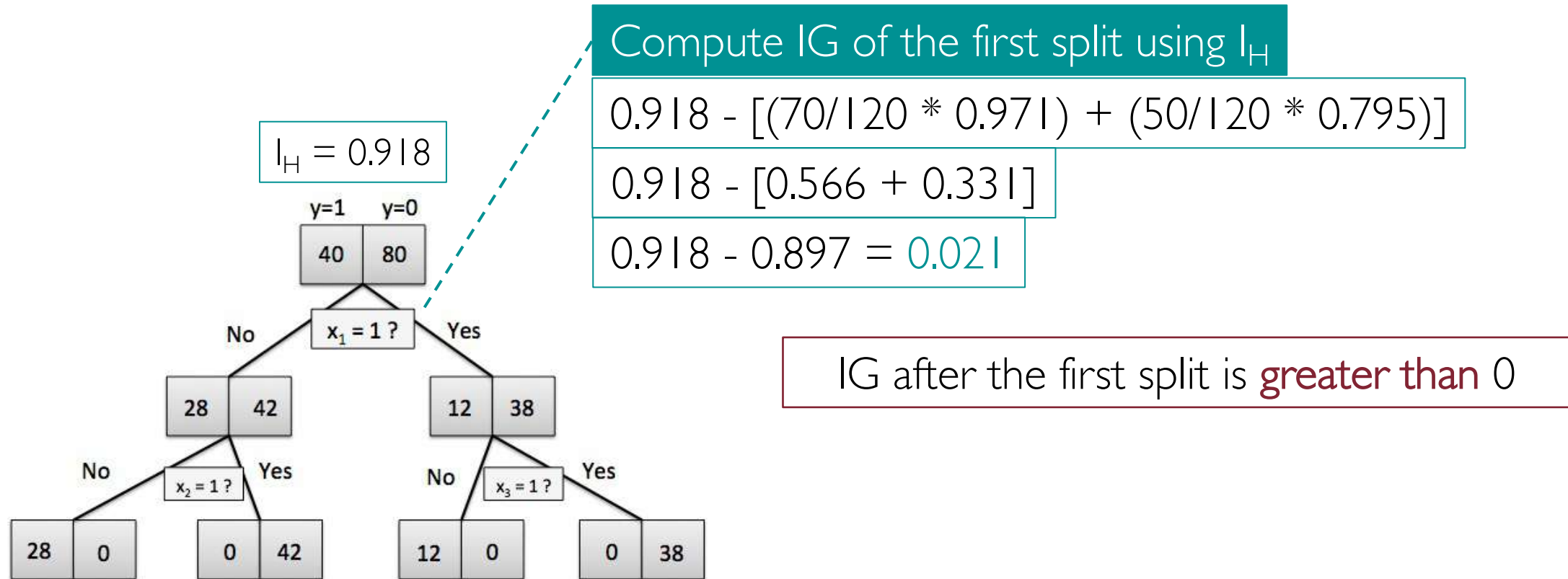
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



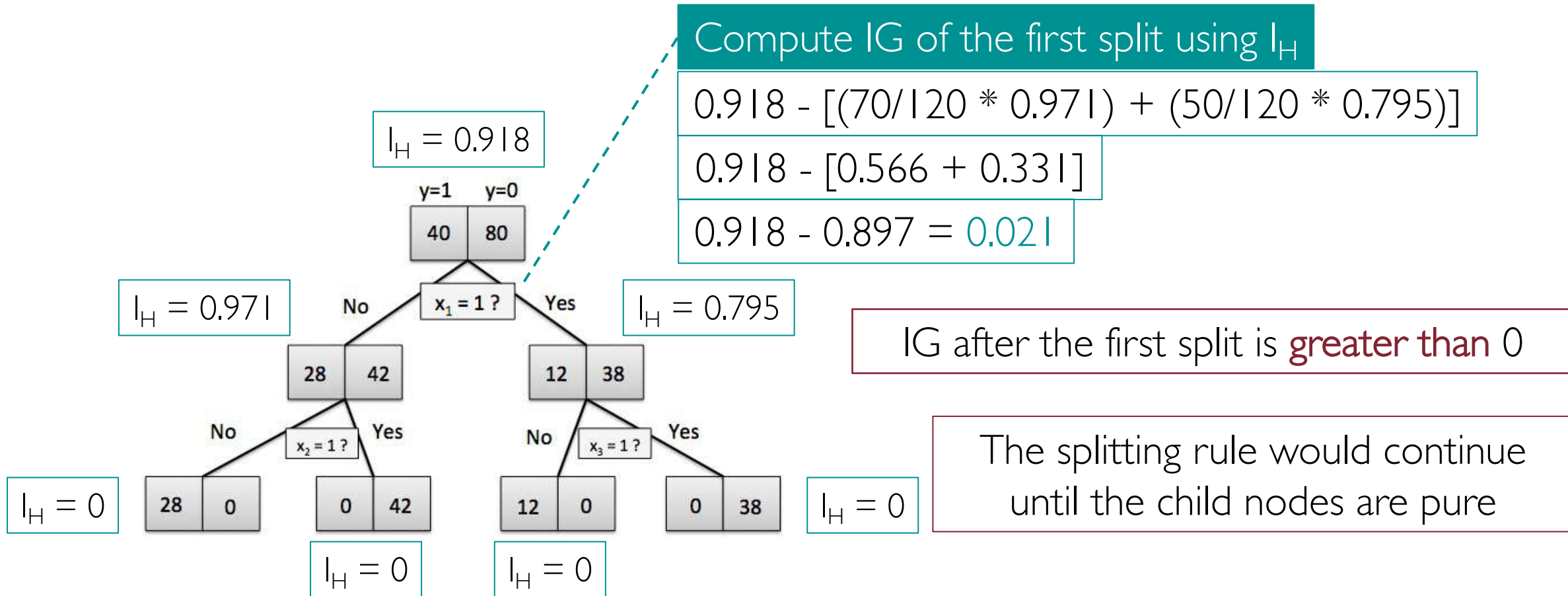
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)



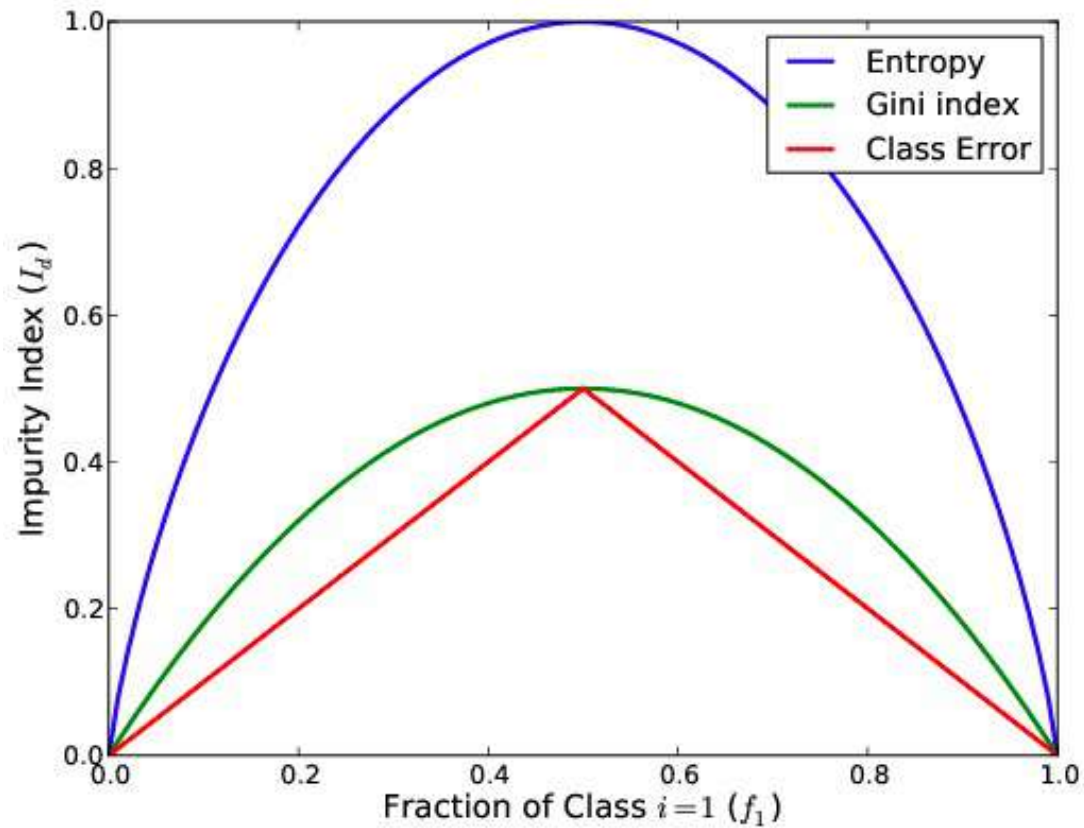
source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)

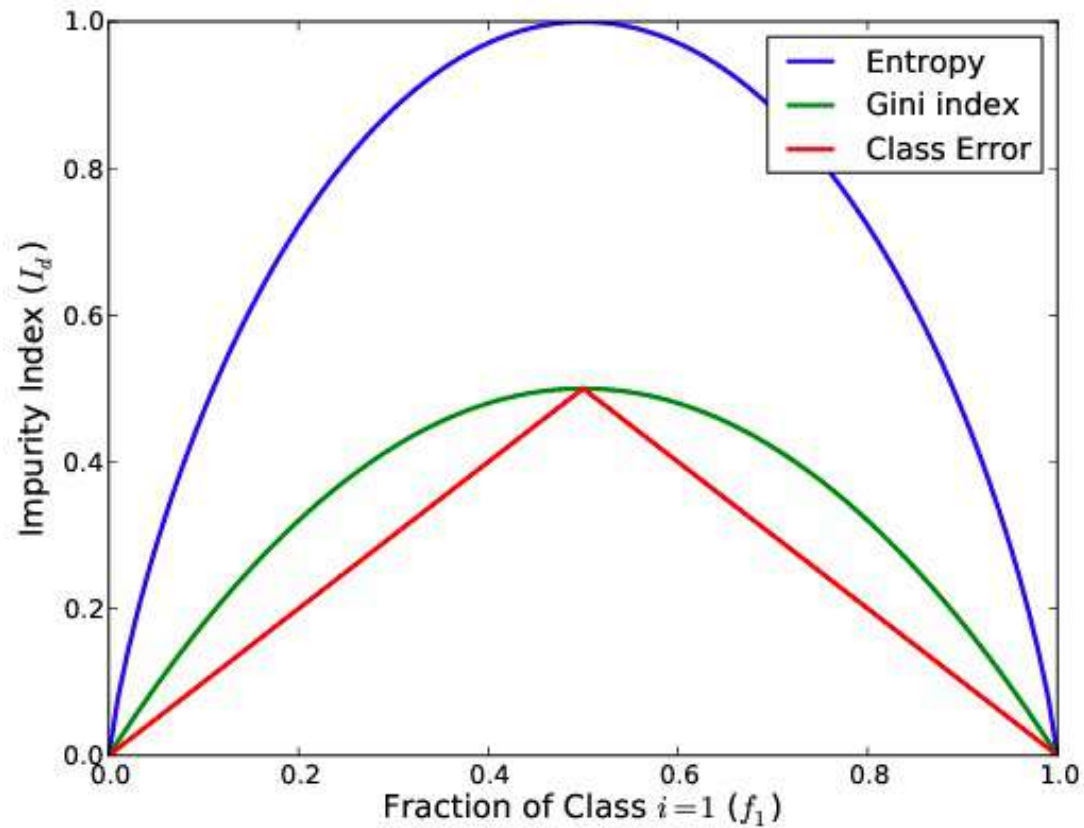


source: <https://sebastianraschka.com/faq/docs/decisiontree-error-vs-entropy.html>

Classification Error Rate vs. Entropy (Gini)

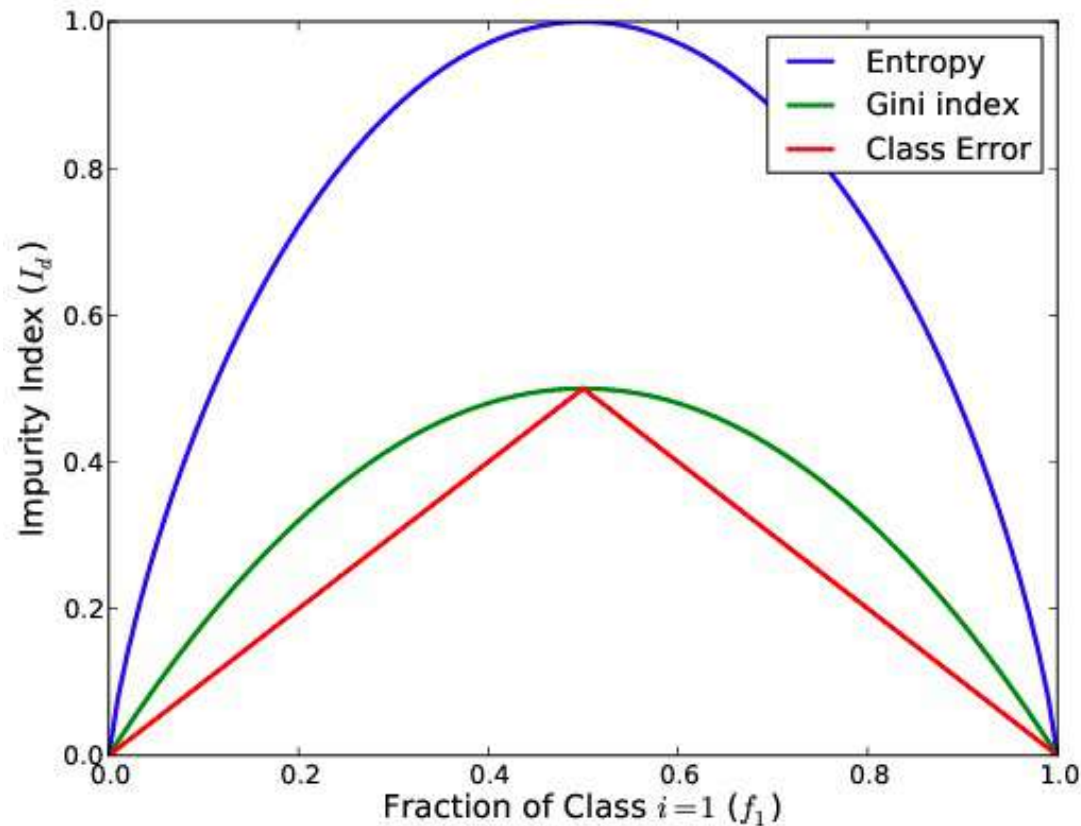


Classification Error Rate vs. Entropy (Gini)

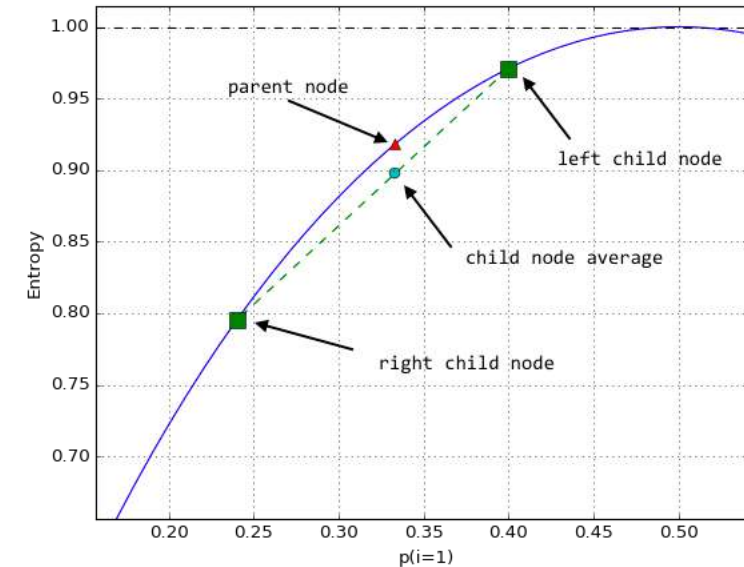


Gini and Entropy are "smoother" than classification error

Classification Error Rate vs. Entropy (Gini)



Gini and Entropy are "smoother" than classification error



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

Evolution of Entropy

- Suppose we have x_1, \dots, x_N N items

Evolution of Entropy

- Suppose we have x_1, \dots, x_N N items
- Each item is labelled either as positive ($y=1$) or negative ($y=0$)

Evolution of Entropy

- Suppose we have x_1, \dots, x_N N items
- Each item is labelled either as positive ($y=1$) or negative ($y=0$)
- Let N^+ (N^-) be the number of positive (negative) elements

Evolution of Entropy

- Suppose we have x_1, \dots, x_N N items
- Each item is labelled either as positive ($y=1$) or negative ($y=0$)
- Let N^+ (N^-) be the number of positive (negative) elements
- We define the ratio $p = N^+/N$ and $q = N^-/N$

Evolution of Entropy

- Suppose we have x_1, \dots, x_N N items
- Each item is labelled either as positive ($y=1$) or negative ($y=0$)
- 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:

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

Evolution of Entropy

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

Evolution of Entropy

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

- 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

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

- 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)
- H is **maximum** (i.e., $H=1$) when $N^+ = N^- = N/2$
 - worst case (half of the elements labelled positive, half negative)

Evolution of Entropy

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

- 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)
- H is **maximum** (i.e., $H=1$) when $N^+ = N^- = N/2$
 - worst case (half of the elements labelled positive, half negative)
- H ranges in $[0, 1]$ independently of the size of the set

Evolution of Entropy

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

- 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)
- H is **maximum** (i.e., $H=1$) when $N^+ = N^- = N/2$
 - worst case (half of the elements labelled positive, half negative)
- H ranges in $[0, 1]$ independently of the size of the set

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

Evolution of Entropy in Tree Splitting

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

Evolution of Entropy in Tree Splitting

- Suppose we start with a node whose entropy is 1 (half +/half -)
- The worst split will occur if the two resulting children nodes will both contain half +/half - examples
 - In such a case, each child node will still have entropy = 1

Evolution of Entropy in Tree Splitting

- Suppose we start with a node whose entropy is 1 (half +/half -)
- The worst split will occur if the two resulting children nodes will both contain half +/half - examples
 - In such a case, each child node will still have entropy = 1
- To account for the number of elements, the **weighted average** of children entropies are computed

$$H_{\text{split}} = \frac{N_{\text{left}}}{N} H_{\text{left}} + \frac{N_{\text{right}}}{N} H_{\text{right}}$$

Evolution of Entropy in Tree Splitting

- Suppose we start with a node whose entropy is 1 (half +/half -)
- The worst split will occur if the two resulting children nodes will both contain half +/half - examples
 - In such a case, each child node will still have entropy = 1
- To account for the number of elements, the **weighted average** of children entropies are computed

$$H_{\text{split}} = \frac{N_{\text{left}}}{N} H_{\text{left}} + \frac{N_{\text{right}}}{N} H_{\text{right}}$$

splitting can't do worst!

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

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

Which one is better?

Linear Models vs. Decision Trees

Linear Models

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

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

Which one is better?

If there is a strong linear relationship between input and output

Linear Models vs. Decision Trees

Linear Models

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

Decision Trees

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

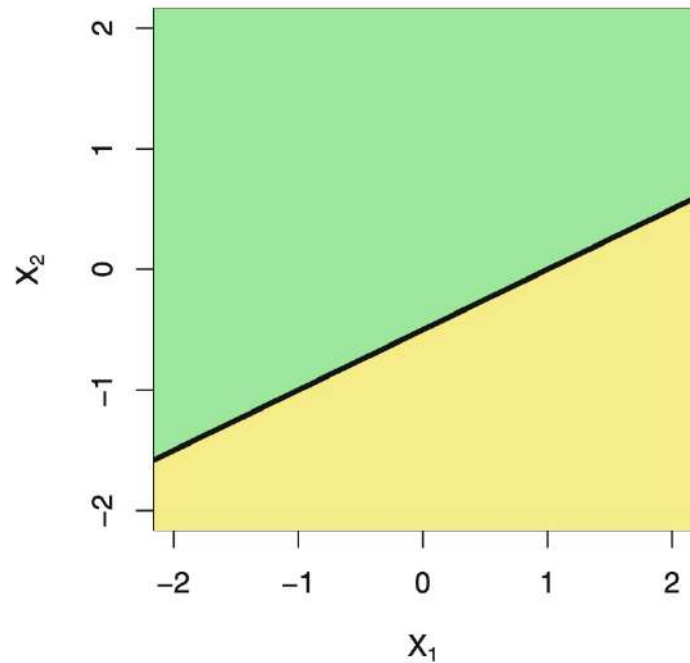
Learned hypothesis is constant within a region

Which one is better?

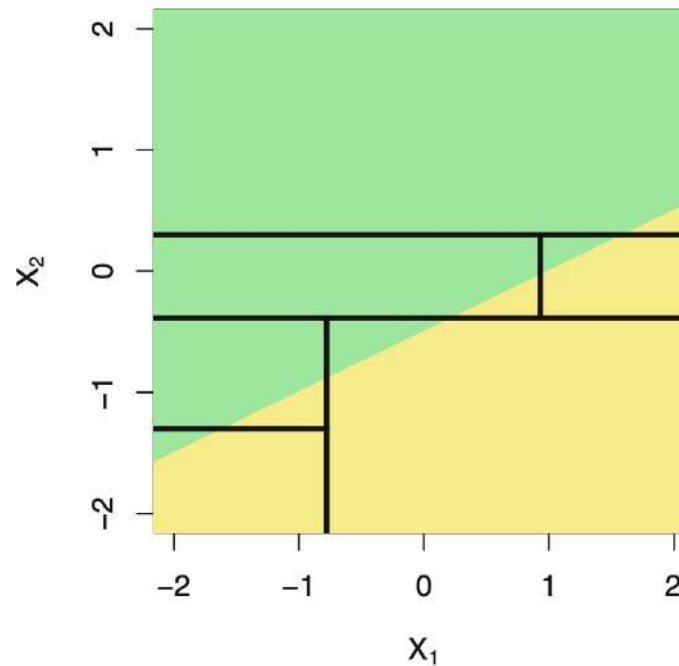
If there is a highly non-linear relationship between input and output

Linear Models vs. Decision Trees: Example

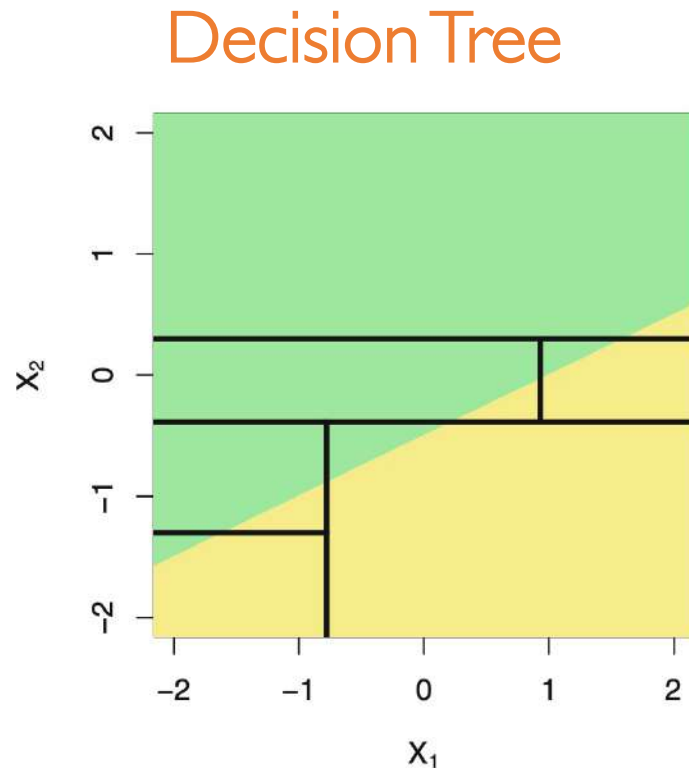
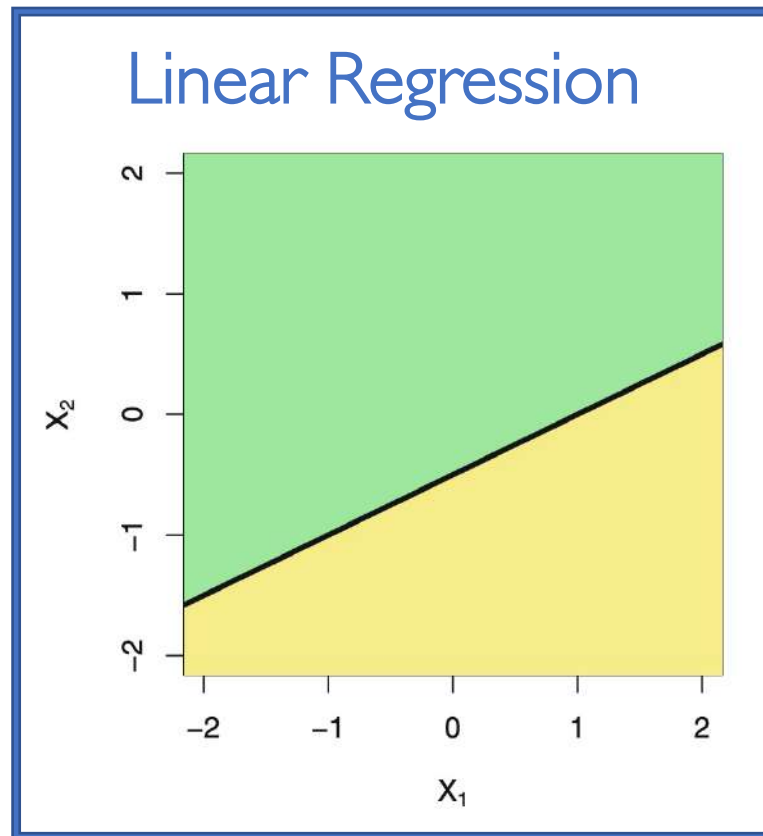
Linear Regression



Decision Tree



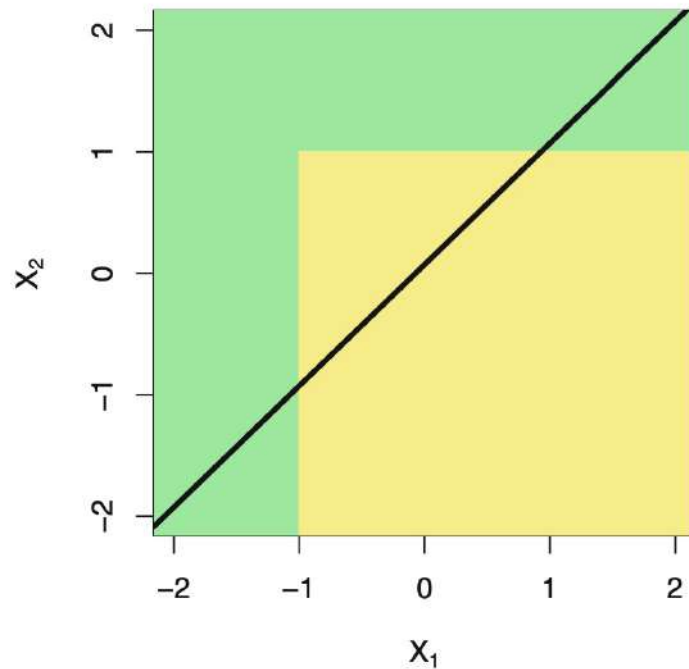
Linear Models vs. Decision Trees: Example



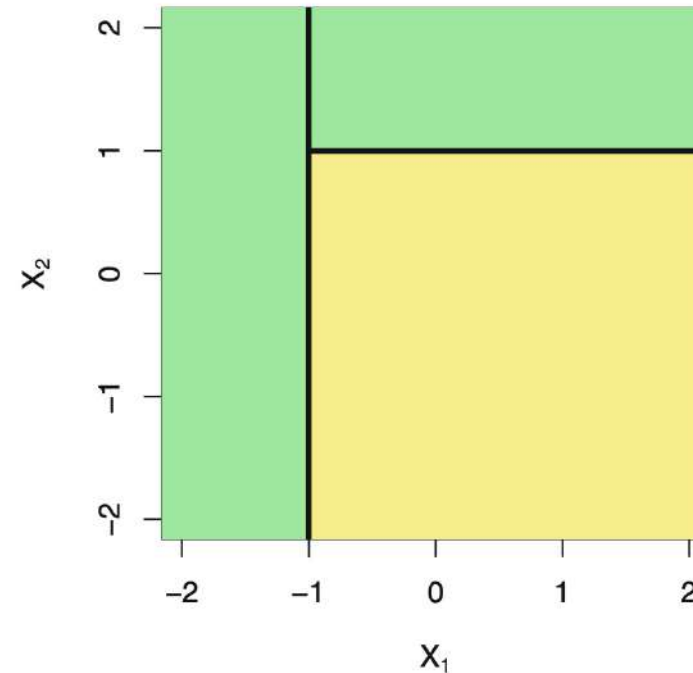
Nice linear decision boundary

Linear Models vs. Decision Trees: Example

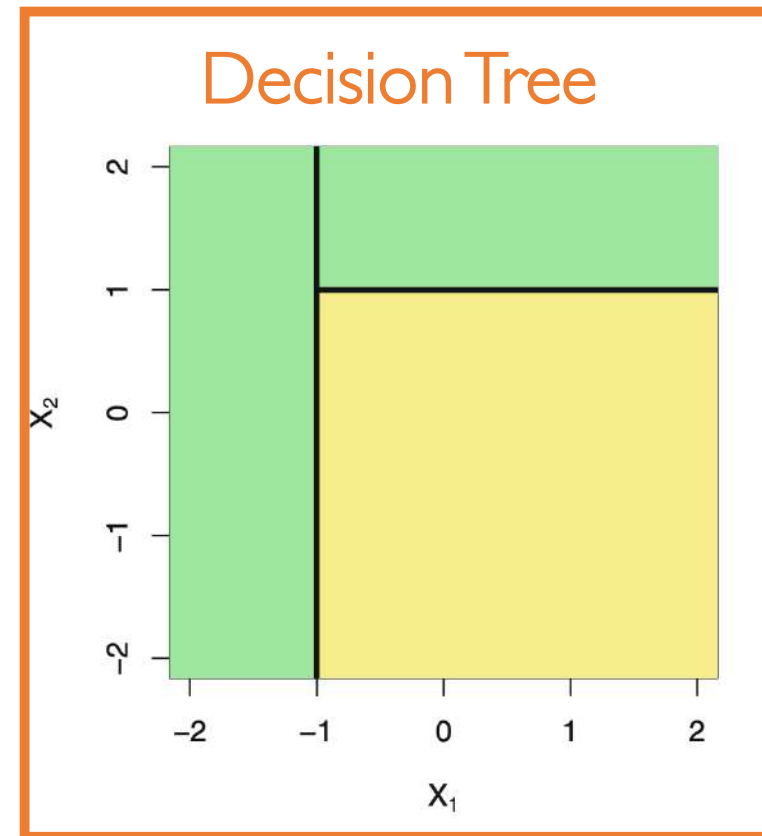
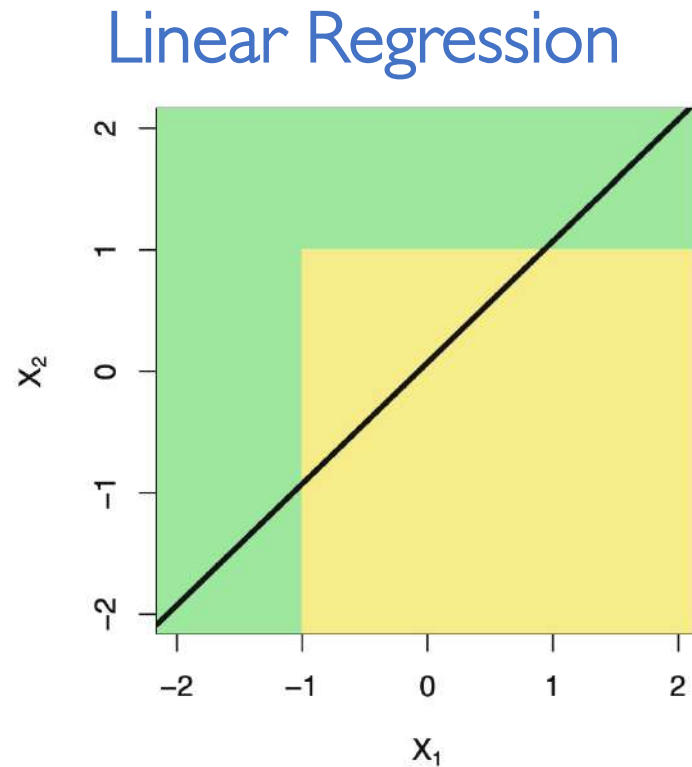
Linear Regression



Decision Tree



Linear Models vs. Decision Trees: Example



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

Decision Trees: Pruning

- Greedy tree growing strategy may lead to:
 - **Overfitting** → if we keep splitting as long as there is an information gain
 - **Underfitting** → if we early-stop the splitting process

Decision Trees: Pruning

- Greedy tree growing strategy may lead to:
 - **Overfitting** → if we keep splitting as long as there is an information gain
 - **Underfitting** → if we early-stop the splitting process
- A better strategy is to grow a very large tree T_0 , and then **prune** it back in order to obtain a subtree

Decision Trees: Pruning

- Greedy tree growing strategy may lead to:
 - **Overfitting** → if we keep splitting as long as there is an information gain
 - **Underfitting** → if we early-stop the splitting process
- A better strategy is to grow a very large tree T_0 , and then **prune** it back in order to obtain a subtree

How do we determine such a subtree?

Decision Trees: Pruning

- Greedy tree growing strategy may lead to:
 - **Overfitting** → if we keep splitting as long as there is an information gain
 - **Underfitting** → if we early-stop the splitting process
- A better strategy is to grow a very large tree T_0 , and then **prune** it back in order to obtain a subtree

How do we determine such a subtree?

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

Decision Trees: Pruning

- Given a subtree, we can estimate its test error using cross-validation or the validation set approach

Decision Trees: Pruning

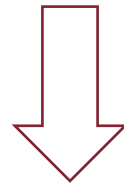
- Given a subtree, we can estimate its test error using cross-validation or the validation set approach
- Problem: too many subtrees to consider (unfeasible!)

Decision Trees: Pruning

- Given a subtree, we can estimate its test error using cross-validation or the validation set approach
- Problem: too many subtrees to consider (unfeasible!)
- We need a way to select a small set of subtrees for consideration

Decision Trees: Pruning

- Given a subtree, we can estimate its test error using cross-validation or the validation set approach
- Problem: too many subtrees to consider (unfeasible!)
- We need a way to select a small set of subtrees for consideration



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

Cost Complexity Pruning

- Rather than considering every possible subtree, we consider a sequence of trees indexed by a non-negative **tuning parameter** α

Cost Complexity Pruning

- Rather than considering every possible subtree, we consider a sequence of trees indexed by a non-negative **tuning parameter** α
- For each value of α there is a subtree $T \subset T_0$ so as to minimize:

$$\sum_{j=1}^{|T|} \sum_{i: \mathbf{x}_i \in R_j} (y_i - \hat{y}_{R_j})^2 + \alpha |T|$$

Cost Complexity Pruning

- Rather than considering every possible subtree, we consider a sequence of trees indexed by a non-negative **tuning parameter** α
- For each value of α there is a subtree $T \subset T_0$ so as to minimize:

$$\sum_{j=1}^{|T|} \sum_{i: \mathbf{x}_i \in R_j} (y_i - \hat{y}_{R_j})^2 + \alpha |T|$$

- $|T|$ indicates the number of terminal nodes of the tree T

Cost Complexity Pruning

- Rather than considering every possible subtree, we consider a sequence of trees indexed by a non-negative **tuning parameter** α
- For each value of α there is a subtree $T \subset T_0$ so as to minimize:

$$\sum_{j=1}^{|T|} \sum_{i: \mathbf{x}_i \in R_j} (y_i - \hat{y}_{R_j})^2 + \alpha |T|$$

- $|T|$ indicates the number of terminal nodes of the tree T
- R_j is the subset of feature space corresponding to the j -th leaf

Cost Complexity Pruning

- The tuning parameter α controls a **trade-off** between the subtree's **complexity** and its **fit** to the training data

Cost Complexity Pruning

- The tuning parameter α controls a **trade-off** between the subtree's **complexity** and its **fit** to the training data
 - When $\alpha = 0$ $T = T_0$ (just minimize the training error)

Cost Complexity Pruning

- The tuning parameter α controls a **trade-off** between the subtree's **complexity** and its **fit** to the training data
 - When $\alpha = 0$ $T = T_0$ (just minimize the training error)
 - As α increases there is a price to pay for the extra complexity of the tree

Cost Complexity Pruning

- The tuning parameter α controls a **trade-off** between the subtree's **complexity** and its **fit** to the training data
 - When $\alpha = 0$ $T = T_0$ (just minimize the training error)
 - As α increases there is a price to pay for the extra complexity of the tree
- The cost complexity pruning is similar to LASSO regularization of linear models

Cost Complexity Pruning

- The tuning parameter α controls a **trade-off** between the subtree's **complexity** and its **fit** to the training data
 - When $\alpha = 0$ $T = T_0$ (just minimize the training error)
 - As α increases there is a price to pay for the extra complexity of the tree
- The cost complexity pruning is similar to LASSO regularization of linear models
- We can select a value of α using a validation set or cross-validation

Decision Trees: PROs

- Trees are very **easy to explain** (even easier than linear regression!)

Decision Trees: PROs

- Trees are very **easy to explain** (even easier than linear regression!)
- Some people think decision trees mimic **human decision-making**

Decision Trees: PROs

- Trees are very **easy to explain** (even easier than linear regression!)
- Some people think decision trees mimic **human decision-making**
- Trees can be **displayed graphically**, and are easily interpreted even by a non-expert (especially if they are small)

Decision Trees: PROs

- Trees are very **easy to explain** (even easier than linear regression!)
- Some people think decision trees mimic **human decision-making**
- Trees can be **displayed graphically**, and are easily interpreted even by a non-expert (especially if they are small)
- Trees can easily **handle categorical features** without the need to create dummy variables (i.e., one-hot encoding)

Decision Trees: CONs

- Trees generally have **lower predictive accuracy** than regression and classification approaches

Decision Trees: CONs

- Trees generally have **lower predictive accuracy** than regression and classification approaches
- Trees may be **not very robust**: a small change in the data can cause a large change in the final estimated tree

Decision Trees: CONs

- Trees generally have **lower predictive accuracy** than regression and classification approaches
- Trees may be **not very robust**: a small change in the data can cause a large change in the final estimated tree

Improvement: **Ensembles** of Decision Trees

Decision Trees: CONs

- Trees generally have **lower predictive accuracy** than regression and classification approaches
- Trees may be **not very robust**: a small change in the data can cause a large change in the final estimated tree

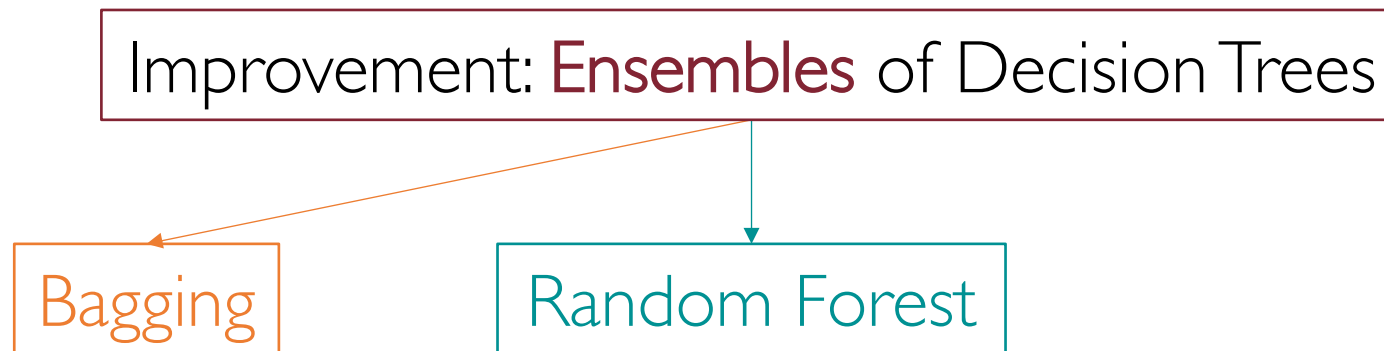
Improvement: **Ensembles** of Decision Trees

Bagging

A diagram consisting of a rectangular box with a dark red border containing the text 'Improvement: Ensembles of Decision Trees'. An orange arrow originates from the word 'Ensembles' and points diagonally down and to the left to a smaller rectangular box with an orange border containing the word 'Bagging'.

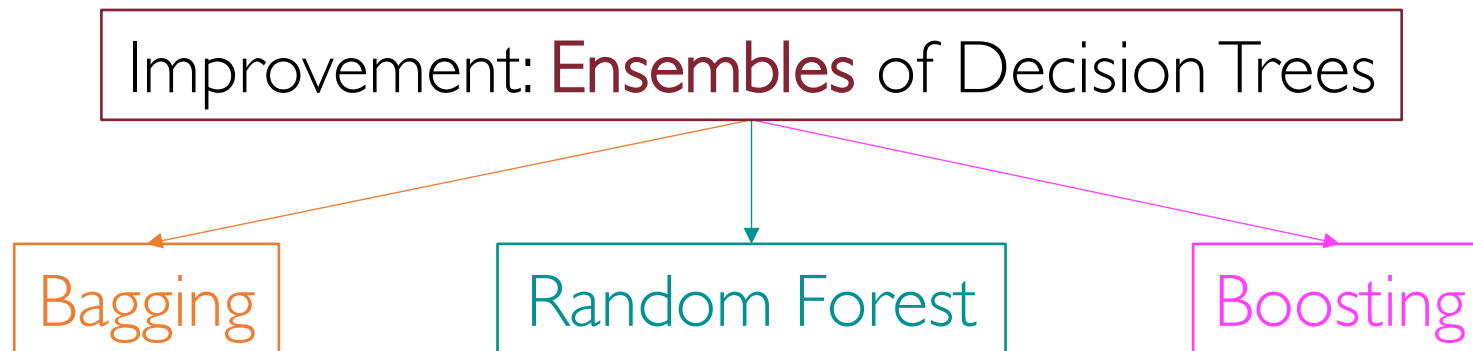
Decision Trees: CONs

- Trees generally have **lower predictive accuracy** than regression and classification approaches
- Trees may be **not very robust**: a small change in the data can cause a large change in the final estimated tree



Decision Trees: CONs

- Trees generally have **lower predictive accuracy** than regression and classification approaches
- Trees may be **not very robust**: a small change in the data can cause a large change in the final estimated tree



Tree Ensembles: Bagging

- Standard decision trees suffer from **high variance** (overfitting)

Tree Ensembles: Bagging

- Standard decision trees suffer from **high variance** (overfitting)
- If we randomly split a training set in two halves and fit a decision tree on each, chances are we end up with 2 very different trees

Tree Ensembles: Bagging

- Standard decision trees suffer from **high variance** (overfitting)
- If we randomly split a training set in two halves and fit a decision tree on each, chances are we end up with 2 very different trees
- Low-variance approaches, instead, are less sensitive to different training sets

Tree Ensembles: Bagging

- Standard decision trees suffer from **high variance** (overfitting)
- If we randomly split a training set in two halves and fit a decision tree on each, chances are we end up with 2 very different trees
- 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

Bagging: Intuition

- Given a set of n i.i.d. observations Z_1, \dots, Z_n , each with variance σ^2

Bagging: Intuition

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

Bagging: Intuition

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

$$\bar{Z} = \frac{1}{n} (Z_1 + \dots + Z_n)$$

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

$$\frac{1}{n^2} [\text{Var}(Z_1) + \dots + \text{Var}(Z_n)] =$$

$$\frac{1}{n^2} \left(\underbrace{\sigma^2 + \dots + \sigma^2}_n \right) = \frac{n\sigma^2}{n^2} = \frac{\sigma^2}{n}$$

Bagging: Intuition

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

$$\bar{Z} = \frac{1}{n} (Z_1 + \dots + Z_n)$$

$$\begin{aligned} \text{Var}(\bar{Z}) &= \text{Var} \left[\frac{1}{n} (Z_1 + \dots + Z_n) \right] = \\ &\frac{1}{n^2} [\text{Var}(Z_1) + \dots + \text{Var}(Z_n)] = \\ &\frac{1}{n^2} \left(\underbrace{\sigma^2 + \dots + \sigma^2}_n \right) = \frac{n\sigma^2}{n^2} = \frac{\sigma^2}{n} \end{aligned}$$

$$\begin{aligned} \text{Var}(\alpha X) &= \alpha^2 \text{Var}(X) \\ \text{Var} \left(\sum_{i=1}^n X_i \right) &= \sum_{i=1}^n \text{Var}(X_i) \quad \text{if } X_i \text{ are independent} \end{aligned}$$

Bagging: Intuition

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

$$\bar{Z} = \frac{1}{n} (Z_1 + \dots + Z_n)$$

$$\begin{aligned} \text{Var}(\bar{Z}) &= \text{Var} \left[\frac{1}{n} (Z_1 + \dots + Z_n) \right] = \\ &\frac{1}{n^2} [\text{Var}(Z_1) + \dots + \text{Var}(Z_n)] = \\ &\frac{1}{n^2} \left(\underbrace{\sigma^2 + \dots + \sigma^2}_n \right) = \frac{n\sigma^2}{n^2} = \frac{\sigma^2}{n} \end{aligned}$$

$$\begin{aligned} \text{Var}(\alpha X) &= E[(\alpha X - E[\alpha X])^2] = E[(\alpha X - \alpha E[X])^2] = \\ &E[\alpha^2 (X - E[X])^2] = \\ &\alpha^2 E[(X - E[X])^2] = \alpha^2 \text{Var}(X) \end{aligned}$$

$$\text{Var}(\alpha X) = \alpha^2 \text{Var}(X)$$

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

Bagging: Intuition

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

$$\bar{Z} = \frac{1}{n} (Z_1 + \dots + Z_n)$$

$$\begin{aligned} \text{Var}(\bar{Z}) &= \text{Var} \left[\frac{1}{n} (Z_1 + \dots + Z_n) \right] = \\ &\frac{1}{n^2} [\text{Var}(Z_1) + \dots + \text{Var}(Z_n)] = \\ &\frac{1}{n^2} \left(\underbrace{\sigma^2 + \dots + \sigma^2}_n \right) = \frac{n\sigma^2}{n^2} = \boxed{\frac{\sigma^2}{n}} \end{aligned}$$

$$\begin{aligned} \text{Var}(\alpha X) &= E[(\alpha X - E[\alpha X])^2] = E[(\alpha X - \alpha E[X])^2] = \\ &E[\alpha^2 (X - E[X])^2] = \\ &\alpha^2 E[(X - E[X])^2] = \alpha^2 \text{Var}(X) \end{aligned}$$

$$\text{Var}(\alpha X) = \alpha^2 \text{Var}(X)$$

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

Averaging a set of observations reduces variance!

Bagging: Intuition

Take many training sets, build a separate prediction model on each, and average the resulting predictions

Bagging: Intuition

Take many training sets, build a separate prediction model on each, and average the resulting predictions

$$h^1(\mathbf{x}), \dots, h^B(\mathbf{x})$$

B predictive models learned from B training sets

Bagging: Intuition

Take many training sets, build a separate prediction model on each, and average the resulting predictions

$$h^1(\mathbf{x}), \dots, h^B(\mathbf{x})$$

B predictive models learned from B training sets

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

Final model obtained averaging the B predictions

Bagging: Intuition

Take many training sets, build a separate prediction model on each, and average the resulting predictions

$$h^1(\mathbf{x}), \dots, h^B(\mathbf{x})$$

B predictive models learned from B training sets

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

Final model obtained averaging the B predictions

Unfortunately, we generally do not have access to multiple training sets

Bagging: Intuition

Take many training sets, build a separate prediction model on each, and average the resulting predictions

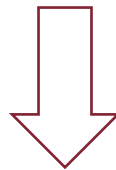
$$h^1(\mathbf{x}), \dots, h^B(\mathbf{x})$$

B predictive models learned from B training sets

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

Final model obtained averaging the B predictions

Unfortunately, we generally do not have access to multiple training sets



Bootstrap

Taking repeated samples from the same training set

Bagging: Intuition

Generate **B** different bootstrapped samples from the original training set

Bagging: Intuition

Generate **B** different bootstrapped samples from the original training set

Train a model on each bootstrapped sample

Bagging: Intuition

Generate **B** different bootstrapped samples from the original training set

Train a model on each bootstrapped sample

Average the **B** predictions

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

Bagging

- Note that bagging is a general-purpose framework

Bagging

- Note that bagging is a general-purpose framework
- It can be used in combination with *any* model

Bagging

- Note that bagging is a general-purpose framework
- 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

Bagging: Variable Importance

- The improved prediction accuracy of bagging trees comes at the expense of the interpretability of a single tree

Bagging: Variable Importance

- The improved prediction accuracy of bagging trees comes at the expense of the interpretability of a single tree
- Still, one can obtain an overall summary of the importance of each feature using RSS (**regression**) or Gini index/Entropy (**classification**)

Bagging: Variable Importance

- The improved prediction accuracy of bagging trees comes at the expense of the interpretability of a single tree
- 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

- Improve bagging trees through **decorrelating** individual trees

Tree Ensemble: Random Forests

- Improve bagging trees through **decorrelating** individual trees
- As in bagging, there will be **B** decision trees learned on bootstrapped samples of the original training set

Tree Ensemble: Random Forests

- Improve bagging trees through **decorrelating** individual trees
- As in bagging, there will be **B** decision trees learned on bootstrapped samples of the original training set
- But for each individual tree, every time it comes to splitting a node only a **random sample** of $k < n$ features is considered

Tree Ensemble: Random Forests

- Improve bagging trees through **decorrelating** individual trees
- As in bagging, there will be **B** decision trees learned on bootstrapped samples of the original training set
- But for each individual tree, every time it comes to splitting a node only a **random sample** of $k < n$ features is considered
- Each split is allowed to use only one of those k features

Random Forests: Sample Feature Split

- A fresh sample of k features is taken at each split

Random Forests: Sample Feature Split

- A fresh sample of k features is taken at each split
- A typical value of k is $\sim \sqrt{n}$

Random Forests: Sample Feature Split

- A fresh sample of k features is taken at each split
- A typical value of k is $\sim \sqrt{n}$
- At each split in the tree, the algorithm is not even allowed to consider a majority of the available features!

Random Forests: Sample Feature Split

- A fresh sample of k features is taken at each split
- A typical value of k is $\sim \sqrt{n}$
- At each split in the tree, the algorithm is not even allowed to consider a majority of the available features!
- This may sound crazy, but it has a clever rationale

Random Forests: Rationale

- Suppose a dataset contains a very strongly predictive feature along with a set of other moderately predictive variables

Random Forests: Rationale

- Suppose a dataset contains a very strongly predictive feature along with a set of other moderately predictive variables
- If we use "vanilla" bagging, most of the bagged trees will use that highly predictive feature as the top split

Random Forests: Rationale

- Suppose a dataset contains a very strongly predictive feature along with a set of other moderately predictive variables
- If we use "vanilla" bagging, most of the bagged trees will use that highly predictive feature as the top split
- As a result, most (if not all) the bagged trees will look **very similar**

Random Forests: Rationale

- Suppose a dataset contains a very strongly predictive feature along with a set of other moderately predictive variables
- If we use "vanilla" bagging, most of the bagged trees will use that highly predictive feature as the top split
- As a result, most (if not all) the bagged trees will look **very similar**
- Predictions from the individual bagged trees will be **highly correlated**

Random Forests: Rationale

- Suppose a dataset contains a very strongly predictive feature along with a set of other moderately predictive variables
- If we use "vanilla" bagging, most of the bagged trees will use that highly predictive feature as the top split
- As a result, most (if not all) the bagged trees will look **very similar**
- Predictions from the individual bagged trees will be **highly correlated**

Lower variance reduction

Random Forests: Rationale

- Enforce random sampling of k out of n features at each split

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
 - For $k = \sqrt{n}$ this means $1/\sqrt{n}$

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
 - For $k = \sqrt{n}$ this means $1/\sqrt{n}$
- We can think of this process as **decorrelating** the trees

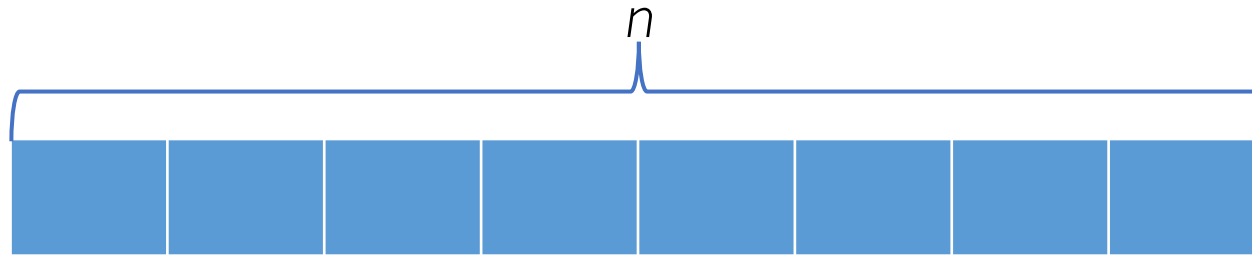
Random Forests: Rationale

- Enforce random sampling of k out of n features at each split
- The probability a split considers the strongest predictor is k/n
 - 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

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
 - 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

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?

Why k/n ? – Approach 1.a.

We want to compute the following:

$P(f \text{ is extracted as 1st})$

Why k/n ? – Approach 1.a.

We want to compute the following:

$P(f \text{ is extracted as 1st})$

OR $\left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right]$

Why k/n ? – Approach 1.a.

We want to compute the following:

$P(f \text{ is extracted as 1st})$

OR $\left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right]$

OR $\left[P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } f \text{ is extracted as 3rd}) \right]$

Why k/n ? – Approach 1.a.

We want to compute the following:

$P(f \text{ is extracted as 1st})$

OR $\left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right]$

OR $\left[P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } f \text{ is extracted as 3rd}) \right]$

...

OR $\left[P(f \text{ is NOT extracted as 1st AND } \dots \text{ AND } f \text{ is NOT extracted as } k - 1\text{-th AND } f \text{ is extracted as } k\text{-th}) \right]$

Why k/n ? – Approach 1.a.

We want to compute the following:

$$P(f \text{ is extracted as 1st}) \quad \frac{1}{n}$$

$$\text{OR } \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right]$$

$$\text{OR } \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } f \text{ is extracted as 3rd}) \right]$$

...

$$\text{OR } \left[P(f \text{ is NOT extracted as 1st AND } \dots \text{ AND } f \text{ is NOT extracted as } k-1\text{-th AND } f \text{ is extracted as } k\text{-th}) \right]$$

Why k/n ? – Approach 1.a.

We want to compute the following:

$$P(f \text{ is extracted as 1st}) \quad \frac{1}{n}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right] \quad \frac{n-1}{n} * \frac{1}{n-1}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } f \text{ is extracted as 3rd}) \right]$$

...

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } \dots \text{ AND } f \text{ is NOT extracted as } k-1\text{-th AND } f \text{ is extracted as } k\text{-th}) \right]$$

Why k/n ? – Approach 1.a.

We want to compute the following:

$$P(f \text{ is extracted as 1st}) \quad \frac{1}{n}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right] \quad \frac{n-1}{n} * \frac{1}{n-1}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } f \text{ is extracted as 3rd}) \right] \quad \frac{n-1}{n} * \frac{n-2}{n-1} * \frac{1}{n-2}$$

...

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } \dots \text{ AND } f \text{ is NOT extracted as } k-1\text{-th AND } f \text{ is extracted as } k\text{-th}) \right]$$

Why k/n ? – Approach 1.a.

We want to compute the following:

$$P(f \text{ is extracted as 1st}) \quad \frac{1}{n}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right] \quad \frac{n-1}{n} * \frac{1}{n-1}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } f \text{ is extracted as 3rd}) \right] \quad \frac{n-1}{n} * \frac{n-2}{n-1} * \frac{1}{n-2}$$

...

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } \dots \text{ AND } f \text{ is NOT extracted as } k-1\text{-th AND } f \text{ is extracted as } k\text{-th}) \right] \\ \frac{n-1}{n} * \frac{n-2}{n-1} * \dots * \frac{n-(k-1)}{n-k} * \frac{1}{n-(k-1)}$$

Why k/n ? – Approach 1.a.

We want to compute the following:

$$P(f \text{ is extracted as 1st}) \quad \frac{1}{n}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is extracted as 2nd}) \right] \quad \frac{n-1}{n} * \frac{1}{n-1}$$

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } f \text{ is extracted as 3rd}) \right] \quad \frac{n-1}{n} * \frac{n-2}{n-1} * \frac{1}{n-2}$$

...

$$\text{OR} \left[P(f \text{ is NOT extracted as 1st AND } \dots \text{ AND } f \text{ is NOT extracted as } k-1\text{-th AND } f \text{ is extracted as } k\text{-th}) \right]$$

$$\frac{n-1}{n} * \frac{n-2}{n-1} * \dots * \frac{n-(k-1)}{n-(k-2)} * \frac{1}{n-(k-1)}$$

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

Why k/n ? – Approach 1.b.

It might be easier to compute the following:

$1 - P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } \dots \text{ AND } f \text{ is NOT extracted as } k\text{-th})$

Why k/n ? – Approach 1.b.

It might be easier to compute the following:

$1 - P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } \dots \text{ AND } f \text{ is NOT extracted as } k\text{-th})$

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

Why k/n ? – Approach 1.b.

It might be easier to compute the following:

$1 - P(f \text{ is NOT extracted as 1st AND } f \text{ is NOT extracted as 2nd AND } \dots \text{ AND } f \text{ is NOT extracted as } k\text{-th})$

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

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

Why k/n ? – Approach 2

We can achieve the same result from the subsets of size k of n elements

Why k/n ? – Approach 2

We can achieve the same result from the subsets of size k of n elements

We want to compute how many subsets contain the feature f out of all the combinations of k elements taken from the initial set of n

Why k/n ? – Approach 2

We can achieve the same result from the subsets of size k of n elements

We want to compute how many subsets contain the feature f out of all the combinations of k elements taken from the initial set of n

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

Why k/n ? – Approach 2

We can achieve the same result from the subsets of size k of n elements

We want to compute how many subsets contain the feature f out of all the combinations of k elements taken from the initial set of n

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

f is already chosen: we need to count the subsets of size $k-1$ of $n-1$ elements

$$\binom{n}{k}$$

Why k/n ? – Approach 2

We can achieve the same result from the subsets of size k of n elements

We want to compute how many subsets contain the feature f out of all the combinations of k elements taken from the initial set of n

$\frac{\binom{n-1}{k-1}}{\binom{n}{k}}$ f is already chosen: we need to count the subsets of size $k-1$ of $n-1$ elements

$\binom{n}{k}$ Combinations of k out of n elements " n choose k "

Why k/n ? – Approach 2

We can achieve the same result from the subsets of size k of n elements

We want to compute how many subsets contain the feature f out of all the combinations of k elements taken from the initial set of n

$$\frac{\binom{n-1}{k-1}}{\binom{n}{k}} \quad \begin{array}{l} f \text{ is already chosen: we need to count the subsets of size } k-1 \text{ of } n-1 \text{ elements} \\ \text{Combinations of } k \text{ out of } n \text{ elements "n choose k"} \end{array}$$

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

Tree Ensemble: Boosting

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

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

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

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

Boosting

- Unlike fitting a single large decision tree to the data, potentially leading to overfitting, the boosting approach instead **learns slowly**

Boosting

- Unlike fitting a single large decision tree to the data, potentially leading to overfitting, the boosting approach instead **learns slowly**
- 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 $b = 1, 2, \dots, B$, 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 shrunk version of the new tree:

$$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x). \quad (8.10)$$

- (c) Update the residuals,

$$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i). \quad (8.11)$$

3. Output the boosted model,

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

Boosting: Hyperparameters

- Boosting has 3 tuning hyperparameters:
 - The number of trees B (boosting can overfit if B is too large)

Boosting: Hyperparameters

- Boosting has 3 tuning hyperparameters:
 - The number of trees B (boosting can overfit if B is too large)
 - The shrinkage parameter λ (a small positive number) controls the rate at which boosting learns $[0.01 \div 0.001]$

Boosting: Hyperparameters

- Boosting has 3 tuning hyperparameters:
 - The number of trees B (boosting can overfit if B is too large)
 - The shrinkage parameter λ (a small positive number) controls the rate at which boosting learns $[0.01 \div 0.001]$
 - The number d of splits in each tree, which controls the complexity of the boosted ensemble (often $d = 1$ works well, in which case each tree is a **stump**)

Boosting: Hyperparameters

- Boosting has 3 tuning hyperparameters:
 - The number of trees B (boosting can overfit if B is too large)
 - The shrinkage parameter λ (a small positive number) controls the rate at which boosting learns $[0.01 \div 0.001]$
 - The number d of splits in each tree, which controls the complexity of the boosted ensemble (often $d = 1$ works well, in which case each tree is a **stump**)
- Tuning done via validation or cross-validation

Take-Home Message of Today

- Decision Trees (DTs) highly **expressive** yet **interpretable** models both for regression and classification

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

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**

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