

**Solution 1:**

- Proceed as follows, when solving manually:

(a) Split  $x$  in two groups using the following split points.

- (1), (2, 7, 10, 20) (splitpoint 1.5)
- (1, 2), (7, 10, 20) (splitpoint 4.5)
- (1, 2, 7), (10, 20) (splitpoint 8.5)
- (1, 2, 7, 10), (20) (splitpoint 15)

(b) For each possible split point compute the sum of squares in both groups.

(c) Use as split point the point that splits both groups best w.r.t. minimizing the sum of squares in both groups.

Here, we have only one split variable  $x$ . A split point  $t$ , leads to the following half-spaces:

$$\mathcal{N}_1(t) = \{(x, y) \in \mathcal{N} : x \leq t\} \text{ and } \mathcal{N}_2(t) = \{(x, y) \in \mathcal{N} : x > t\}.$$

Remember the minimization Problem (here only for one split variable  $x$ ):

$$\min_t \left( \min_{c_1} \sum_{(x,y) \in \mathcal{N}_1} (y - c_1)^2 + \min_{c_2} \sum_{(x,y) \in \mathcal{N}_2} (y - c_2)^2 \right).$$

The inner minimization is solved through:  $\hat{c}_1 = \bar{y}_1$  and  $\hat{c}_2 = \bar{y}_2$

Which results in:

$$\min_t \left( \sum_{(x,y) \in \mathcal{N}_1} (y - \bar{y}_1)^2 + \sum_{(x,y) \in \mathcal{N}_2} (y - \bar{y}_2)^2 \right).$$

The sum of squares error of the parent is:

$$Impurity_{parent} = MSE_{parent} = \frac{1}{5} \sum_{i=1}^5 (y_i - 4.7)^2 = 22.56$$

Calculate the risk for each split point:

$$x \leq 1.5$$

$$\begin{aligned} \mathcal{R}(1, 1.5) &= \frac{1}{5} MSE_{left} + \frac{4}{5} MSE_{right} = \\ &= \frac{1}{5} \cdot \frac{1}{1} (1 - 1)^2 + \frac{4}{5} \cdot \frac{1}{4} ((1 - 5.625)^2 + (0.5 - 5.625)^2 + (10 - 5.625)^2 + (11 - 5.625)^2) \\ &= 19.1375 \end{aligned}$$

$$x \leq 4.5 \quad \mathcal{R}(1, 4.5) = 13.43$$

$$x \leq 8.5 \quad \mathcal{R}(1, 8.5) = 0.13$$

$$x \leq 15 \quad \mathcal{R}(1, 15) = 12.64$$

Minimal empirical risk is obtained by choosing the split point 8.5.

Doing the same for the log-transformation gives:

$$x \leq 0.3 \quad \mathcal{R}(1, 0.3) = 19.14$$

$$x \leq 1.3 \quad \mathcal{R}(1, 1.3) = 13.43$$

$$x \leq 2.1 \quad \mathcal{R}(1, 2.1) = 0.13$$

$$x \leq 2.6 \quad \mathcal{R}(1, 2.6) = 12.64$$

Minimal empirical risk is obtained by choosing the split point 2.1.

- Code example:

```
x = c(1,2,7,10,20)
y = c(1,1,0.5,10,11)

calculate_mse <- function(y) mean((y - mean(y))^2)
calculate_total_mse <- function(yleft, yright) {
  num_left <- length(yleft)
  num_right <- length(yright)

  w_mse_left <- num_left / (num_left + num_right) * calculate_mse(yleft)
  w_mse_right <- num_right / (num_left + num_right) * calculate_mse(yright)

  return(w_mse_left + w_mse_right)
}

split <- function(x, y) {
  # try out all unique points as potential split points and ...
  unique_sorted_x <- sort(unique(x))
  split_points <- unique_sorted_x[1:(length(unique_sorted_x) - 1)] +
    0.5 * diff(unique_sorted_x)
  node_mses <- lapply(split_points, function(i) {
    y_left <- y[x <= i]
    y_right <- y[x > i]

    # ... compute SS in both groups
    mse_split <- calculate_total_mse(y_left, y_right)
    print(sprintf("Split at %.1f: empirical Risk = %.2f", i, mse_split))

    return(mse_split)
  })
  # select the split point yielding the maximum impurity reduction
  best <- which.min(node_mses)
  split_points[best]
}

x

## [1] 1 2 7 10 20

split(x, y) # the 3rd observation is the best split point

## [1] "Split at 1.5: empirical Risk = 19.14"
## [1] "Split at 4.5: empirical Risk = 13.43"
## [1] "Split at 8.5: empirical Risk = 0.13"
## [1] "Split at 15.0: empirical Risk = 12.64"
## [1] 8.5
```

```
log(x)

## [1] 0.0000000 0.6931472 1.9459101 2.3025851 2.9957323

split(log(x), y) # also here, the 3rd observation is the best split point

## [1] "Split at 0.3: empirical Risk = 19.14"
## [1] "Split at 1.3: empirical Risk = 13.43"
## [1] "Split at 2.1: empirical Risk = 0.13"
## [1] "Split at 2.6: empirical Risk = 12.64"
## [1] 2.124248
```

## Solution 2:

According to the lecture for a target  $y$  with target space  $\mathcal{Y} = \{1, \dots, g\}$  the target class proportion  $\pi_k^{(\mathcal{N})}$  of class  $k \in \mathcal{Y}$  in a node can be computed, s.t.

$$\pi_k^{(\mathcal{N})} = \frac{1}{|\mathcal{N}|} \sum_{(x^{(i)}, y^{(i)}) \in \mathcal{N}} [y^{(i)} = k].$$

Now for any  $n \in \mathbb{N}$  let  $Y^{(1)}, \dots, Y^{(n)}, \hat{Y}^{(1)}, \dots, \hat{Y}^{(n)}$  be i.i.d. random variables, where  $Y^{(i)}$  and  $\hat{Y}^{(i)}$  are categorically distributed with

$$\mathbb{P}(Y^{(i)} = k | \mathcal{N}) = \mathbb{P}(\hat{Y}^{(i)} = k | \mathcal{N}) = \pi_k^{(\mathcal{N})} \quad \forall i \in \{1, \dots, n\}, \quad k \in \mathcal{Y}.$$

The random variables  $Y^{(1)}, \dots, Y^{(n)}$  represent data distributed like the training data<sup>1</sup> of size  $n$  and the random variables  $\hat{Y}^{(1)}, \dots, \hat{Y}^{(n)}$  the corresponding estimators using the randomizing rule. With these we can define the misclassification rate  $\text{err}_{\mathcal{N}}$  of node  $\mathcal{N}$  for data distributed like the training data, s.t

$$\text{err}_{\mathcal{N}} = \frac{1}{n} \sum_{i=1}^n [Y^{(i)} \neq \hat{Y}^{(i)}].$$

We're interested in the expected misclassification rate  $\text{err}_{\mathcal{N}}$  of node  $\mathcal{N}$  for data distributed like the training data, i.e.,

$$\begin{aligned} \mathbb{E}_{Y^{(1)}, \dots, Y^{(n)}, \hat{Y}^{(1)}, \dots, \hat{Y}^{(n)}} (\text{err}_{\mathcal{N}}) &= \mathbb{E}_{Y^{(1)}, \dots, Y^{(n)}, \hat{Y}^{(1)}, \dots, \hat{Y}^{(n)}} \left( \frac{1}{n} \sum_{i=1}^n [Y^{(i)} \neq \hat{Y}^{(i)}] \right) \\ &= \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{Y^{(i)}, \hat{Y}^{(i)}} ([Y^{(i)} \neq \hat{Y}^{(i)}]) \\ &= \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{Y^{(i)}} \left( \mathbb{E}_{\hat{Y}^{(i)}} ([Y^{(i)} \neq \hat{Y}^{(i)}]) \right) \\ &= \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{Y^{(i)}} \left( \sum_{k=1}^g [Y^{(i)} \neq k] \pi_k^{(\mathcal{N})} \right) \\ &= \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{Y^{(i)}} \left( \sum_{k \in \mathcal{Y} \setminus \{Y^{(i)}\}} \pi_k^{(\mathcal{N})} \right) \\ &= \frac{1}{n} \sum_{i=1}^n \mathbb{E}_{Y^{(i)}} (1 - \pi_{Y^{(i)}}^{(\mathcal{N})}) \\ &= \frac{1}{n} \sum_{i=1}^n \sum_{k=1}^g (1 - \pi_k^{(\mathcal{N})}) \pi_k^{(\mathcal{N})} \\ &= \frac{n}{n} \sum_{k=1}^g (1 - \pi_k^{(\mathcal{N})}) \pi_k^{(\mathcal{N})} \\ &= 1 - \sum_{k=1}^g \left( \pi_k^{(\mathcal{N})} \right)^2. \end{aligned}$$

This is exactly the Gini-Index which CART uses for splitting the tree.

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<sup>1</sup>under the independence assumption