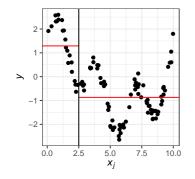
Introduction to Machine Learning

CART: Splitting Criteria for Regression



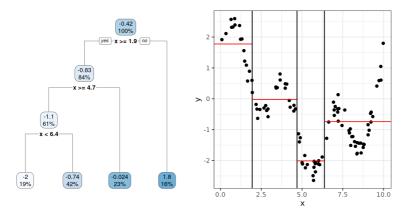


Learning goals

- Understand how to define split criteria via ERM
- Understand how to find splits in regression with L₂ loss



SPLITTING CRITERIA





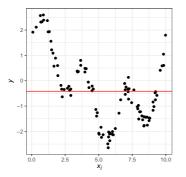
How to find good splitting rules? \implies Empirical Risk Minimization

OPTIMAL CONSTANTS IN LEAVES

Idea: A split is good if each child's point predictor reflects its data well.

For each child \mathcal{N} , predict with optimal constant, e.g., the mean $c_{\mathcal{N}} = \frac{1}{|\mathcal{N}|} \sum_{(\mathbf{x}, y) \in \mathcal{N}} y$ for the L_2 loss, i.e., $\mathcal{R}(\mathcal{N}) = \sum_{(\mathbf{x}, y) \in \mathcal{N}} (y - c_{\mathcal{N}})^2$.

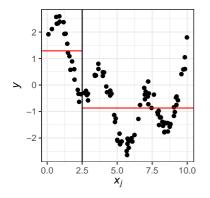
Root node:

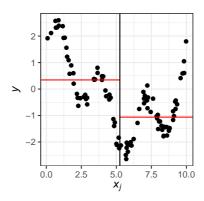




OPTIMAL CONSTANTS IN LEAVES

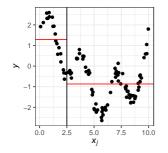
Which of these two splits is better?

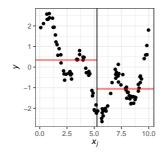






RISK OF A SPLIT







$$\mathcal{R}(\mathcal{N}_1) = 23.4, \, \mathcal{R}(\mathcal{N}_2) = 72.4$$
 $\mathcal{R}(\mathcal{N}_1) = 78.1, \, \mathcal{R}(\mathcal{N}_2) = 46.1$

$$\mathcal{R}(\mathcal{N}_1)=$$
 78.1, $\mathcal{R}(\mathcal{N}_2)=$ 46.1

The total risk is the sum of the individual losses:

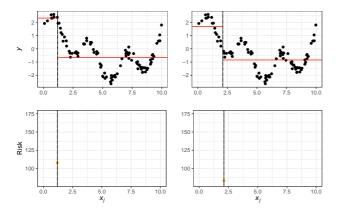
$$23.4 + 72.4 = 95.8$$

$$78.0 + 46.1 = 124.1$$

Based on the SSE, we prefer the first split.

SEARCHING THE BEST SPLIT

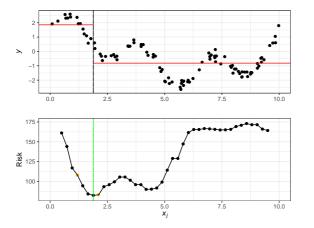
Let's find the best split for this feature by tabulating results.





SEARCHING THE BEST SPLIT

Let's iterate – quantile-wise or over all points.





We have reduced the problem to a simple loop.

FORMALIZATION

- $\mathcal{N} \subseteq \mathcal{D}$ is the data contained in this node
- Let $c_{\mathcal{N}}$ be the predicted constant for ${\mathcal{N}}$
- The risk $\mathcal{R}(\mathcal{N})$ for a node is:

$$\mathcal{R}(\mathcal{N}) = \sum_{(\mathbf{x}, y) \in \mathcal{N}} \mathcal{L}(y, c_{\mathcal{N}})$$

- ullet The optimal constant is $c_{\mathcal{N}} = rg \min_{c} \sum_{(\mathbf{x}, \mathbf{y}) \in \mathcal{N}} L(\mathbf{y}, c)$
- We often know what that is from theoretical considerations or we can perform a simple univariate optimization



FORMALIZATION / 2

• A split w.r.t. **feature** x_i **at split point** t divides a parent node \mathcal{N} into

$$\mathcal{N}_1 = \{(\mathbf{x}, y) \in \mathcal{N} : x_j < t\} \text{ and } \mathcal{N}_2 = \{(\mathbf{x}, y) \in \mathcal{N} : x_j \ge t\}.$$

To evaluate its quality, we compute the risk of our new, finer model

$$\mathcal{R}(\mathcal{N}, j, t) = \mathcal{R}(\mathcal{N}_1) + \mathcal{R}(\mathcal{N}_2)$$

$$= \left(\sum_{(\mathbf{x}, y) \in \mathcal{N}_1} L(y, c_{\mathcal{N}_1}) + \sum_{(\mathbf{x}, y) \in \mathcal{N}_2} L(y, c_{\mathcal{N}_2})\right)$$

• Finding the best way to split \mathcal{N} into $\mathcal{N}_1, \mathcal{N}_2$ means solving

$$arg min_{j,t} \mathcal{R}(\mathcal{N}, j, t)$$

FORMALIZATION / 3

- $\mathcal{R}(\mathcal{N}, j, t) = \mathcal{R}(\mathcal{N}_1) + \mathcal{R}(\mathcal{N}_2)$, makes sense if \mathcal{R} is a simple sum
- If we use averages, we have to reweight the terms to obtain a global average w.r.t. ${\cal N}$ as the children have different sizes

$$\bar{\mathcal{R}}(\mathcal{N},j,t) = \frac{|\mathcal{N}_1|}{|\mathcal{N}|} \bar{\mathcal{R}}(\mathcal{N}_1) + \frac{|\mathcal{N}_2|}{|\mathcal{N}|} \bar{\mathcal{R}}(\mathcal{N}_2)$$



 We mention this for clarity, as quite a few texts contain only the (more complicated) weighted formula without clear explanation