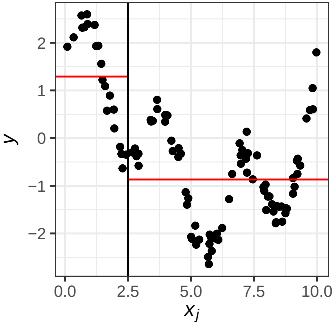
Introduction to Machine Learning

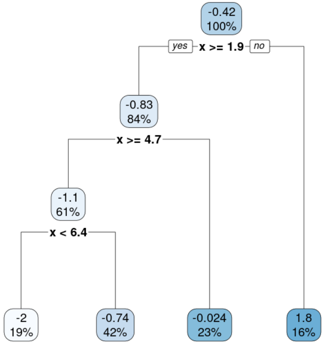
CART: Splitting Criteria for Regression

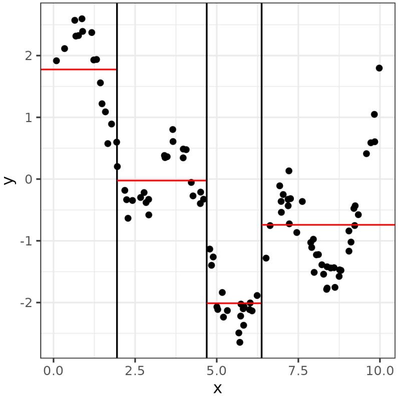


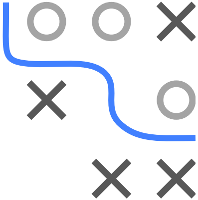
Learning goals

- Understand how to define split criteria via ERM
- Understand how to find splits in regression with L_2 loss

SPLITTING CRITERIA

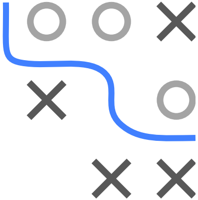






How to find good splitting rules? $\implies$ **Empirical Risk Minimization**

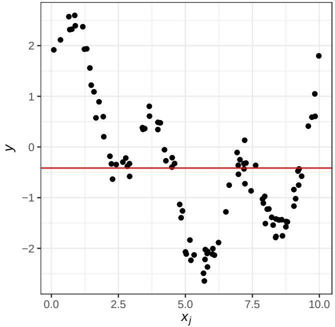
OPTIMAL CONSTANTS IN LEAVES



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

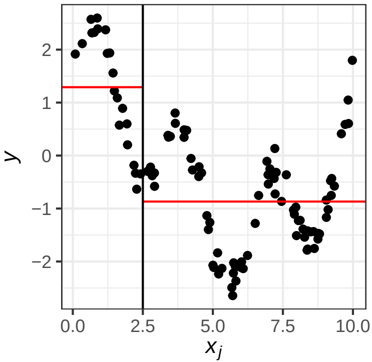
For each child $\mathcal{N}$, predict with optimal constant, e.g., the mean $c_{\mathcal{N}} = \frac{1}{|\mathcal{N}|} \sum\limits_{(\mathbf{x},y)\in\mathcal{N}} y$ for the L_2 loss, i.e., $\mathcal{R}(\mathcal{N}) = \sum\limits_{(\mathbf{x},y)\in\mathcal{N}} (y - c_{\mathcal{N}})^2$.

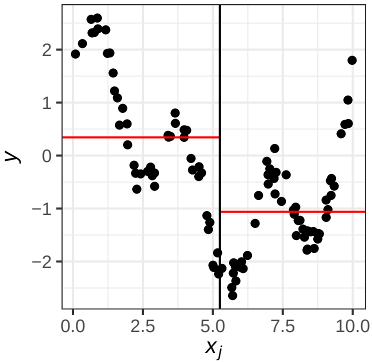
Root node:

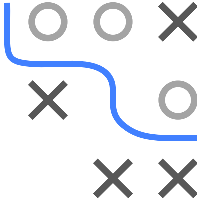


OPTIMAL CONSTANTS IN LEAVES

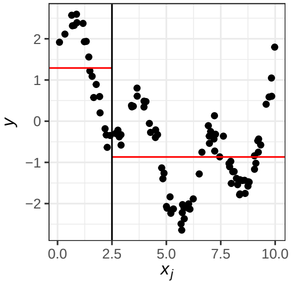
Which of these two splits is better?

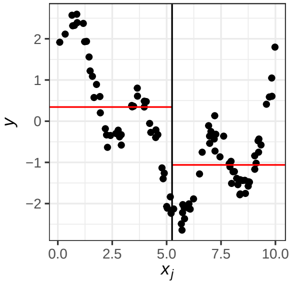


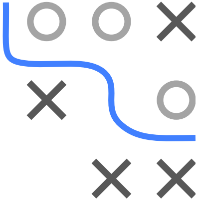




RISK OF A SPLIT







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

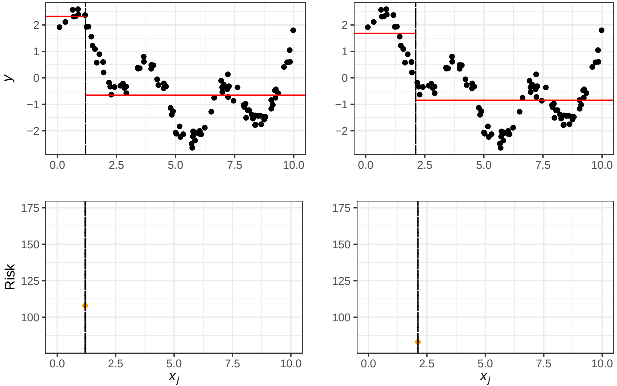
The total risk is the sum of the individual losses:

$23.4 + 72.4 = 95.8$ $\qquad$ $78.0 + 46.1 = 124.1$

Based on the SSE, we prefer the first split.

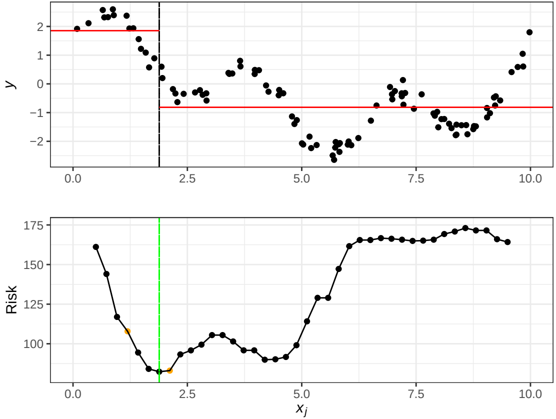
SEARCHING THE BEST SPLIT

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



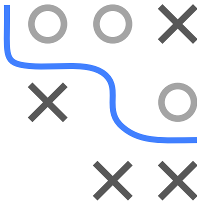
SEARCHING THE BEST SPLIT

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



We have reduced the problem to a simple loop.

FORMALIZATION

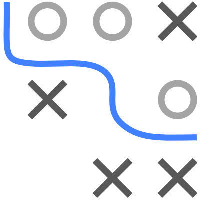


- $\mathcal{N} \subseteq \mathcal{D}$ is the data contained in this node
- Let $c_{\mathcal{N}}$ be the predicted constant for $\mathcal{N}$
- The risk $\mathcal{R}(\mathcal{N})$ for a node is:

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

- The optimal constant is $c_{\mathcal{N}} = \arg\min_{c} \sum_{(\mathbf{x},y)\in\mathcal{N}} L(y, c)$
- 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_j **at split point** t divides a parent node $\mathcal{N}$ into

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

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

$$\begin{aligned}\mathcal{R}(\mathcal{N}, j, t) &= \mathcal{R}(\mathcal{N}_1) + \mathcal{R}(\mathcal{N}_2) \\ &= \left(\sum_{(\mathbf{x},y)\in\mathcal{N}_1} L(y, c_{\mathcal{N}_1}) + \sum_{(\mathbf{x},y)\in\mathcal{N}_2} L(y, c_{\mathcal{N}_2}) \right)\end{aligned}$$

- 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. $\mathcal{N}$ 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