Introduction to Machine Learning

CART Splitting Criteria for Regression

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Learning goals

- Understand how to define split criteria via ERM
- Understand how to find splits in regression with *L*₂ loss

SPLITTING CRITERIA



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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?



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RISK OF A SPLIT



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

The total risk is the sum of the individual losses:

23.4 + 72.4 = 95.8 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.



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SEARCHING THE BEST SPLIT

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



We have reduced the problem to a simple loop.

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FORMALIZATION

- $\bullet \ \mathcal{N} \subseteq \mathcal{D}$ 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_i at split point *t* divides a parent node N into

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

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

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

 $\bullet\,$ Finding the best way to split $\mathcal N$ into $\mathcal N_1,\mathcal N_2$ means solving

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

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

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

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