Introduction to Machine Learning

CART Splitting Criteria for Regression

Х \times \times

Learning goals

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

SPLITTING CRITERIA

X $\times\overline{\times}$

How to find good splitting rules? =⇒ **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 N , predict with optimal constant, e.g., the mean $c_{\cal N} = \frac{1}{|{\cal N}|}$ $\sum_{\cal A}$ (**x**,*y*)∈N *y* for the L_2 loss, i.e., $\mathcal{R}(\mathcal{N}) = \sum$ (**x**,*y*)∈N $(y - c_{\mathcal{N}})^2$. Root node:

 $\times\overline{\times}$

OPTIMAL CONSTANTS IN LEAVES

Which of these two splits is better?

X $\times\overline{\times}$

RISK OF A SPLIT

X $\times\overline{\times}$

 $\mathcal{R}(\mathcal{N}_1)=$ 23.4, $\mathcal{R}(\mathcal{N}_2)=$ 72.4 $\qquad\quad\mathcal{R}(\mathcal{N}_1)=$ 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 $\mathcal{N} \subset \mathcal{D}$ is the data contained in this node
- \bullet Let c_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 $c_{\mathcal{N}} = \argmin \quad \sum \quad \mathcal{L}(y, c)$ *c* $(x,y) \in \mathcal{N}$
- We often know what that is from theoretical considerations or we can perform a simple univariate optimization

FORMALIZATION / 2

 \bullet A split w.r.t. **feature** x_i at split point *t* divides a parent node 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

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

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

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

FORMALIZATION / 3

- $R(N, j, t) = R(N_1) + R(N_2)$, makes sense if 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

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

 $\overline{\mathbf{X}}$

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