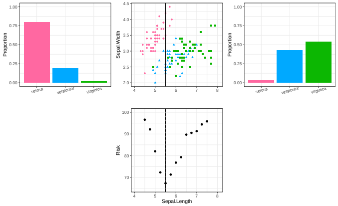
Introduction to Machine Learning

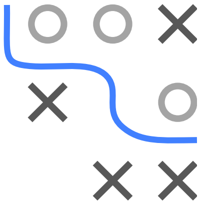
CART: Splitting Criteria for Classification



Learning goals

- Understand different splitting criteria for classification
- Know the connections between empirical risk minimization and impurity minimization

OPTIMAL CONSTANT MODELS



As losses in classification, we typically use:

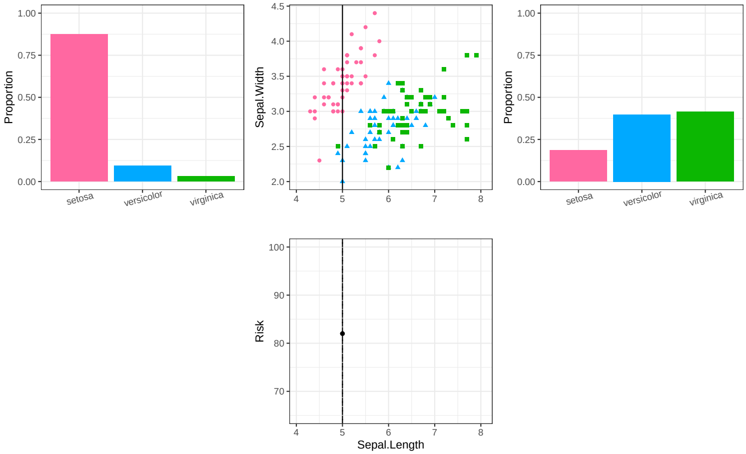
- (Multi-class) Brier score $L(y, \boldsymbol{\pi}) = \sum_{k=1}^{g} (\pi_k - o_k(y))^2$, a.k.a. L_2 loss on probabilities
- (Multi-class) Log loss $L(y, \boldsymbol{\pi}) = -\sum_{k=1}^{g} o_k(y) \log(\pi_k)$, as in logistic regression

Optimal constant predictions (in a node) for both losses are simply the proportions of the contained classes:

$$c_{\mathcal{N}} = (\hat{\pi}_1^{(\mathcal{N})}, \ldots, \hat{\pi}_g^{(\mathcal{N})}) \quad \text{with}$$
$$\hat{\pi}_k^{(\mathcal{N})} = \frac{1}{|\mathcal{N}|} \sum_{(\mathbf{x},y)\in\mathcal{N}} \mathbb{I}(y = k) \quad \forall k \in \{1, \ldots, g\}$$

FINDING THE BEST SPLIT

Let’s compute the Brier score for all splits, with optimal constant probability vectors in both children



FINDING THE BEST SPLIT

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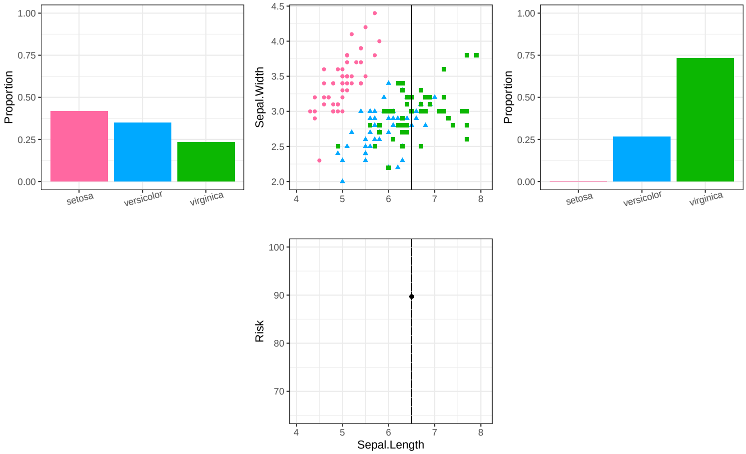
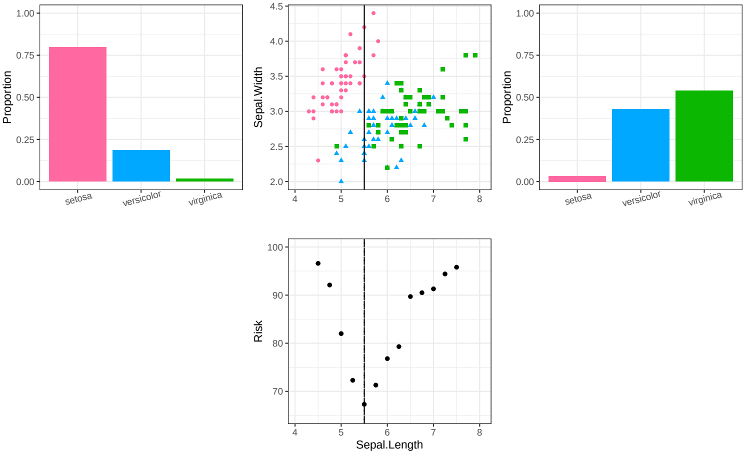
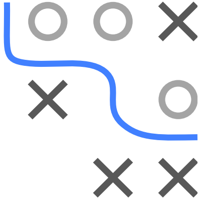


FINDING THE BEST SPLIT

The optimal split point typically creates greatest imbalance or purity of label distribution



RISK MINIMIZATION VS. IMPURITY



- Split crits are sometimes defined in terms of impurity reduction instead of ERM, where a measure of "impurity" is defined per node
- For regression trees, "impurity" is simply defined as variance of y, which is quite obviously L_2 loss
- Brier score is equivalent to Gini impurity

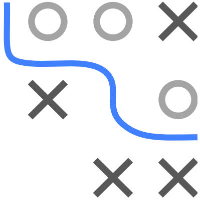
$$I(\mathcal{N}) = \sum_{k=1}^{g} \hat{\pi}_k^{(\mathcal{N})} \left(1 - \hat{\pi}_k^{(\mathcal{N})}\right)$$

- Log loss is equivalent to entropy

$$I(\mathcal{N}) = -\sum_{k=1}^{g} \hat{\pi}_k^{(\mathcal{N})} \log \hat{\pi}_k^{(\mathcal{N})}$$

- Trees can be understood completely through the lens of ERM, so this new terminology is unnecessary and perhaps confusing

SPLITTING WITH MISCLASSIFICATION LOSS



- Often, we want to minimize the MCE in classification
- Zero-One-Loss is not differentiable, but that is a non-issue in the tree-optimization based on loops
- Brier score and Log loss more sensitive to changes in the node probs, often produce purer nodes, and are still preferred

Split 1:

	class 0	class 1
$\mathcal{N}_1$	300	100
$\mathcal{N}_2$	100	300

Split 2:

	class 0	class 1
$\mathcal{N}_1$	400	200
$\mathcal{N}_2$	0	200

- Both splits are equivalent in MCE
- But: Split 2 results in purer nodes, both Brier score (Gini) and Log loss (Entropy) prefer 2nd split