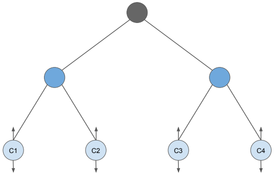
Introduction to Machine Learning

Gradient Boosting with Trees 2



Learning goals

- Loss optimal terminal coefficients
- GB with trees for multiclass problems

ADAPTING TERMINAL COEFFICIENTS

- Tree as additive model: $b(\mathbf{x}) = \sum_{t=1}^{T} c_t \mathbb{1}_{\{\mathbf{x} \in R_t\}}$,
- R_t are the terminal regions; c_t are terminal constants

The GB model is still additive in the regions:

$$\begin{aligned} f^{[m]}(\mathbf{x}) &= f^{[m-1]}(\mathbf{x}) + \alpha^{[m]} b^{[m]}(\mathbf{x}) \\ &= f^{[m-1]}(\mathbf{x}) + \alpha^{[m]} \sum_{t=1}^{T^{[m]}} c_t^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_t^{[m]}\}} \\ &= f^{[m-1]}(\mathbf{x}) + \sum_{t=1}^{T^{[m]}} \tilde{c}_t^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_t^{[m]}\}}. \end{aligned}$$

With $\tilde{c}_t^{[m]} = \alpha^{[m]} \cdot c_t^{[m]}$ in the case that $\alpha^{[m]}$ is a constant learning rate

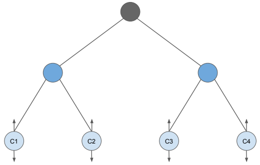
ADAPTING TERMINAL COEFFICIENTS

After the tree has been fitted against the PRs, we can adapt terminal constants in a second step to become more loss optimal.

$$f^{[m]}(\mathbf{x}) = f^{[m-1]}(\mathbf{x}) + \sum_{t=1}^{T^{[m]}} \tilde{c}_t^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_t^{[m]}\}}.$$

We can determine/change all $\tilde{c}_t^{[m]}$ individually and directly L-optimally:

$$\tilde{c}_t^{[m]} = \arg\min_c \sum_{\mathbf{x}^{(i)} \in R_t^{[m]}} L(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + c).$$



ADAPTING TERMINAL COEFFICIENTS

An alternative approach ist to directly fit a loss-optimal tree. Risk for data in a node:

$$\mathcal{R}(\mathcal{N}') = \sum_{i \in \mathcal{N}'} L(y^{(i)}, f^{[m-1]}(\mathbf{x}^{(i)}) + c)$$

with $\mathcal{N}'$ being the index set of a specific (left or right) node after splitting and c the constant of the node.

c can be found by line search or analytically for some losses.

GB MULTICLASS WITH TREES

- From Friedman, J. H. - Greedy Function Approximation: A Gradient Boosting Machine (1999)
- We again model one discriminant function per class.
- Determining the tree structure works just like before.
- In the estimation of the c values, i.e., the heights of the terminal regions, however, all models depend on each other because of the definition of L. Optimizing this is more difficult, so we will skip some details and present the main idea and results.

GB MULTICLASS WITH TREES

- There is no closed-form solution for finding the optimal $\hat{c}_{tk}^{[m]}$ values. Additionally, the regions corresponding to the different class trees overlap, so that the solution does not reduce to a separate calculation within each region of each tree.
- Hence, we approximate the solution with a single Newton-Raphson step, using a diagonal approximation to the Hessian (we leave out the details here).
- This decomposes the problem into a separate calculation for each terminal node of each tree.
- The result is

$$\hat{c}_{tk}^{[m]} = \frac{g-1}{g} \frac{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} \tilde{r}_k^{[m](i)}}{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} \left|\tilde{r}_k^{[m](i)}\right| \left(1 - \left|\tilde{r}_k^{[m](i)}\right|\right)}.$$

GB MULTICLASS WITH TREES

Algorithm 1 Gradient Boosting for g-class Classification.

1: Initialize $f_k^{[0]}(\mathbf{x}) = 0,\ k = 1, \ldots, g$
2: **for** $m = 1 \to M$ **do**
3: Set $\pi_k(\mathbf{x}) = \frac{\exp(f_k^{[m]}(\mathbf{x}))}{\sum_j \exp(f_j^{[m]}(\mathbf{x}))}, k = 1, \ldots, g$
4: **for** $k = 1 \to g$ **do**
5: For all i: Compute $\tilde{r}_k^{[m](i)} = \mathbb{1}_{\{y^{(i)}=k\}} - \pi_k(\mathbf{x}^{(i)})$
6: Fit regr. tree to the $\tilde{r}_k^{[m](i)}$ giving terminal regions $R_{tk}^{[m]}$
7: Compute
8: $$\hat{c}_{tk}^{[m]} = \frac{g-1}{g} \frac{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} \tilde{r}_k^{[m](i)}}{\sum_{\mathbf{x}^{(i)} \in R_{tk}^{[m]}} \left|\tilde{r}_k^{[m](i)}\right| \left(1 - \left|\tilde{r}_k^{[m](i)}\right|\right)}$$
9: Update $\hat{f}_k^{[m]}(\mathbf{x}) = \hat{f}_k^{[m-1]}(\mathbf{x}) + \sum_t \hat{c}_{tk}^{[m]} \mathbb{1}_{\{\mathbf{x} \in R_{tk}^{[m]}\}}$
10: **end for**
11: **end for**
12: Output $\hat{f}_1^{[M]}, \ldots, \hat{f}_g^{[M]}$