

Consider some data $\{(x_i, y_i)\}_{i=1}^n$ and a differentiable loss function $\mathcal{L}(y, F(x))$ and a multiclass classification problem which should be solved by a gradient boosting algorithm. Let therefore be the cross-entropy loss function defined by the class probabilities gained from the softmax function so that :

$$softmax = \frac{e^{y_i}}{\sum_{k=1}^N e^{y_k}} \quad (1)$$

$$\mathcal{L}(y_i, \hat{y}_i) = - \sum y_i \log \hat{y}_i \quad (2)$$

where y_i defines the the relative frequencies of each class in our target variable y .

In this case we end up with the partial derivatives for the softmax function

$$D_j softmax_i = \frac{\delta softmax_i}{\delta y_j} = \begin{bmatrix} D_1 softmax_1 & \times & D_N softmax_1 \\ & \ddots & \\ D_1 softmax_N & \times & D_N softmax_N \end{bmatrix} \quad (3)$$

$$D_j softmax_i = \begin{cases} softmax_i - softmax_j^2 & i = j \\ -softmax_j \times softmax_i & i \neq j \end{cases} \quad (4)$$

And the derivative of the cross-entropy loss function w.r.t. $F(x)$

$$\frac{\partial \mathcal{L}}{\partial \hat{y}} = \left(- \sum_i y_i \log \hat{y}_i \right) = - \frac{y_i}{\hat{y}_i} \quad (5)$$

Combining both gradients leads to the gradient of the loss function

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \hat{y}} &= - \frac{y_i}{\hat{y}_i} \hat{y}_i (1 - \hat{y}_i) + \sum_{t \neq i} - \frac{y_t}{\hat{y}_t} (-\hat{y}_t \hat{y}_i) \\ &= -y_i + y_i \hat{y}_i + \sum_{t \neq i} y_t \hat{y}_i \\ &= -y_i + \sum_t y_t \hat{y}_i \\ &= \hat{y}_i \underbrace{\sum_t y_t}_{=1} - y_i \\ &= \hat{y}_i - y_i \end{aligned} \quad (6)$$

In this sense our initial model $F_0(x)$ should be :

$$F_0(x) = \frac{e^{y_i}}{\sum_{k=1}^N e^{y_k}} \quad (7)$$

One obtains the intial residuals $r_{i0} = y_i - F_0(x)$ which are then used to fit a classification tree with R_{im} terminal nodes.

The pseudo residuals are obtained through

$$\begin{aligned}
r_{im} &= - \left[\frac{\partial \mathcal{L}(y_i, F(x_i))}{\partial F(x_i)} \right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1, \dots, n \\
&= - \sum_{i=1}^N (\hat{y}_i - y_i) \\
&= \sum_{i=1}^N (y_i - \hat{y}_i)
\end{aligned} \tag{8}$$

The output values for each terminal node can be derived using a second-order Taylor approximation so that,

$$\begin{aligned}
\gamma_{lm} &= \underset{\gamma}{\operatorname{argmin}} \sum_{x_i \in R_{lm}} L(y_i, F_{m-1}(x_i) + \gamma) \\
&\approx - \left[\mathcal{L}(y_i, F(x_i)) + \frac{\partial \mathcal{L}(y_i, F(x_i))}{\partial F(x_i)} + \frac{\partial^2 \mathcal{L}(y_i, F(x_i))}{\partial^2 F(x_i)} \right] \\
&= y_i \log(\hat{y}_i) + \sum_{i=1}^N (y_i - \hat{y}_i) - 1
\end{aligned} \tag{9}$$

In the end our new predictions should be :

$$F_m(x) = F_{m-1}(x) + \nu \sum_{j=1}^m \gamma_{jm} I(x \in R_{jm}) \tag{10}$$