

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 model. $F(x)$ is a model to predict \hat{y} . A loss function is an evaluation metric of a model $F(x)$ and our target variable y . The softmax transfer function is typically used to compute the estimated probability distribution in classification tasks involving multiple classes. Let therefore be the cross-entropy loss function defined by the estimated probability distributions gained from the softmax function so that :

$$\hat{y}_{i,softmax} = \frac{e^{\hat{y}_i}}{\sum_{k=1}^N e^{\hat{y}_k}} \quad (1)$$

$$\mathcal{L}(y_i, F(x)) = - \sum y_i \log \hat{y}_{i,softmax} \quad (2)$$

where y_i defines the the relative frequencies of each class in our target variable y and \hat{y}_i defines the predictions of y_i .

We need to initialize our gradient boosting model with an constant value. Let the initial model $F_0(x)$ be defined as :

$$F_0(x) = \frac{1}{N} \sum_{i=1}^{T_j} y_{i,j} \quad (3)$$

where T defines the number of observations in class j and N defines the number of observations of y . So the initial model is the class probability for each class j . Given that $F(x)$ is a model to predict \hat{y} the values of the model $F(x)$ can be used to define \hat{y}_i . So that we can calculate $\hat{y}_{i,softmax}$ with 1

Now we show that the loss function is differentiable.

$$D_j \hat{y}_{i,softmax} = \frac{\partial \hat{y}_{i,softmax}}{\partial \hat{y}_j} = \begin{bmatrix} D_1 \hat{y}_{1,softmax} & \times & D_N \hat{y}_{1,softmax} \\ & \vdots & \ddots & \vdots \\ D_1 \hat{y}_{N,softmax} & \times & D_N \hat{y}_{N,softmax} \end{bmatrix} \quad (4)$$

$$D_j \hat{y}_{i,softmax} = \frac{\partial \hat{y}_{i,softmax}}{\partial \hat{y}_j} \begin{cases} \hat{y}_{i,softmax} - \hat{y}_{j,softmax}^2 & i = j \\ -\hat{y}_{j,softmax} \times \hat{y}_{i,softmax} & i \neq j \end{cases} \quad (5)$$

And the derivative of the cross-entropy loss function w.r.t. \hat{y}_i

$$\frac{\partial \mathcal{L}}{\partial \hat{y}_{i,softmax}} = \left(- \sum y_i \log \hat{y}_{i,softmax} \right) = - \sum \frac{y_i}{\hat{y}_{i,softmax}} \quad (6)$$

Combining both gradients leads to the gradient of the loss function

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \hat{y}_{i,softmax}} &= -\frac{y_i}{\hat{y}_{i,softmax}} \hat{y}_{i,softmax} (1 - \hat{y}_{i,softmax}) + \sum_{j \neq i} -\frac{y_j}{\hat{y}_j} (-\hat{y}_{j,softmax} \hat{y}_{i,softmax}) \\
&= -y_i + y_i \hat{y}_{i,softmax} + \sum_{j \neq i} y_j \hat{y}_{i,softmax} \\
&= -y_i + \sum_j y_j \hat{y}_{i,softmax} \\
&= \hat{y}_{i,softmax} \underbrace{\sum_j y_j}_{=1} - y_i \\
&= \hat{y}_{i,softmax} - y_i
\end{aligned} \tag{7}$$

where y_j is the probability of class j

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

The pseudo residuals are obtained through

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

The output values for each terminal node l of each tree m γ_{lm} can be derived using a second-order Taylor approximation so that,

$$\begin{aligned}
\gamma_{lm} &= \underset{\gamma}{\operatorname{argmin}} \sum_{x_i \in R_{lm}} L(y_i, F_{m-1}(x_i) + \gamma) \\
&\approx \frac{\frac{\partial \mathcal{L}(y_i, F(x_i))}{\partial \hat{y}_{i,softmax}} + \frac{\partial \mathcal{L}(y_i, F(x_i))}{\partial \hat{y}_{i,softmax}} \gamma + \frac{1}{2} \frac{\partial^2 \mathcal{L}(y_i, F(x_i))}{\partial^2 \hat{y}_{i,softmax}} \gamma^2}{\partial \gamma} \\
&= \hat{y}_{i,softmax} - y_i + \gamma \stackrel{!}{=} 0 \\
\gamma &= y_i - \hat{y}_{i,softmax}
\end{aligned} \tag{9}$$

In the end our updated model should be :

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

where ν is a learning rate to weight the output values of the tree m .