

Let \mathbf{X} , \mathbf{y} represent the feature matrix and target vector. Suppose there are k classes and p features. Let \mathbf{Z}_i be the $(k \times p)$ -by- k matrix where

$$\mathbf{Z}_i = \begin{pmatrix} x_{i1} & 0 & \cdots & 0 \\ x_{i2} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ x_{ip} & 0 & \cdots & 0 \\ 0 & x_{i1} & \cdots & 0 \\ 0 & x_{i2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & x_{ip} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_{i1} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_{ip} \end{pmatrix}$$

Let $\hat{\beta}$ denote logistic regression optimum, put $\mathbf{u}_i = \mathbf{Z}_i^\top \hat{\beta}$, and let \mathbf{H} denote the hessian for logistic regression at $\hat{\beta}$.

1 ALO

We have

$$\begin{aligned} \mathbf{H}_{/i} &= \mathbf{H} - \mathbf{Z}_i \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{Z}_i^\top \\ \mathbf{g}_{/i} &= \mathbf{Z}_i \nabla \ell_i(\mathbf{u}_i) \end{aligned}$$

For ALO, we have

$$\tilde{\beta}_{/i} = \hat{\beta} - \mathbf{H}_{/i}^{-1} \mathbf{g}_{/i}$$

Put $\mathbf{K}_i = \mathbf{Z}_i^\top \mathbf{H}^{-1} \mathbf{Z}_i$. Then

$$\begin{aligned}
\mathbf{Z}_i^\top \tilde{\boldsymbol{\beta}}_{/i} &= \mathbf{Z}_i^\top \left[\hat{\boldsymbol{\beta}} - \mathbf{H}_{/i}^{-1} \mathbf{g}_{/i} \right] \\
&= \mathbf{u}_i - \mathbf{Z}_i^\top \left[\mathbf{H} - \mathbf{Z}_i \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{Z}_i^\top \right]^{-1} (-\mathbf{Z}_i \nabla \ell_i(\mathbf{u}_i)) \\
&= \mathbf{u}_i + \mathbf{Z}_i^\top \left[\mathbf{H} - \mathbf{Z}_i \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{Z}_i^\top \right]^{-1} (\mathbf{Z}_i \nabla \ell_i(\mathbf{u}_i)) \\
&= \mathbf{u}_i + \mathbf{Z}_i^\top \left[\mathbf{H}^{-1} - \mathbf{H}^{-1} \mathbf{Z}_i \left(\mathbf{K}_i - \nabla^2 \ell_i(\mathbf{u}_i)^{-1} \right)^{-1} \mathbf{Z}_i^\top \mathbf{H}^{-1} \right] (\mathbf{Z}_i \nabla \ell_i(\mathbf{u}_i)) \\
&= \mathbf{u}_i + \mathbf{K}_i \left[\mathbf{I} - \left(\mathbf{K}_i - \nabla^2 \ell_i(\mathbf{u}_i)^{-1} \right)^{-1} \mathbf{K}_i \right] \nabla \ell_i(\mathbf{u}_i) \\
&= \mathbf{u}_i + \mathbf{K}_i \left[\mathbf{I} - \left(\nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i - \mathbf{I} \right)^{-1} \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i \right] \nabla \ell_i(\mathbf{u}_i) \\
&= \mathbf{u}_i + \mathbf{K}_i \left[\mathbf{I} + \left(\mathbf{I} - \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i \right)^{-1} \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i \right] \nabla \ell_i(\mathbf{u}_i) \\
&= \mathbf{u}_i + \mathbf{K}_i \left(\mathbf{I} - \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i \right)^{-1} \left[\left(\mathbf{I} - \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i \right) + \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i \right] \nabla \ell_i(\mathbf{u}_i) \\
&= \mathbf{u}_i + \mathbf{K}_i \left[\mathbf{I} - \nabla^2 \ell_i(\mathbf{u}_i) \mathbf{K}_i \right]^{-1} \nabla \ell_i(\mathbf{u}_i)
\end{aligned}$$

Put

$$\begin{aligned}
\mathbf{A}_i &= \nabla^2 \ell_i(\mathbf{u}_i) \\
\mathbf{G}_i &= \mathbf{I} - \mathbf{A}_i \mathbf{K}_i \\
\tilde{\mathbf{u}}_i &= \mathbf{u}_i + \mathbf{K}_i \mathbf{G}_i^{-1} \nabla \ell_i(\mathbf{u}_i)
\end{aligned}$$

Then we can define ALO as

$$\text{ALO} = \frac{1}{n} \sum_i \ell_i(\tilde{\mathbf{u}}_i)$$