NE 795 Scientific Machine Learning Fall 2023

Homework 2

Fundamental Techniques of Machine Learning

Problem 1. Logistic Regression. *Using the notations given in the lecture slides, derive the partial derivative of LL*(β) *w.r.t.* β_i :

$$\frac{\partial LL(\beta)}{\partial \beta_j} = \sum_{i=1}^m \left[y^{(i)} - \sigma(\beta^T x^{(i)}) \right] \cdot x_j^{(i)}.$$

The log-likelihood function is

$$LL(\beta) = \sum_{i=1}^{m} \left[y^{(i)} \cdot \ln \left(\sigma(\beta^T x^{(i)}) \right) + \left(1 - y^{(i)} \right) \cdot \ln \left(1 - \sigma(\beta^T x^{(i)}) \right) \right],$$
$$\beta = \left[\beta_0, \beta_1, \dots, \beta_d \right].$$

Sigmoid function is

$$\sigma(z) = \frac{1}{1 + e^{-z}}.$$

The log-likelihood function derives from:

$$\begin{split} \frac{\partial}{\partial \beta_{j}} \sum_{i=1}^{m} y^{(i)} \cdot \ln \left(\sigma(\beta^{T} x^{(i)}) \right) &= \sum_{i=1}^{m} y^{(i)} \cdot \frac{\partial \ln \left(\sigma(\beta^{T} x^{(i)}) \right)}{\partial \sigma(\beta^{T} x^{(i)})} \cdot \frac{\partial \sigma(\beta^{T} x^{(i)})}{\partial (\beta^{T} x^{(i)})} \cdot \frac{\partial \beta^{T} x^{(i)}}{\partial \beta_{j}} &= \\ &= \sum_{i=1}^{m} y^{(i)} \cdot \frac{1}{\sigma(\beta^{T} x^{(i)})} \cdot \frac{\partial \left(\frac{1}{1 + e^{-\beta^{T} x^{(i)}}} \right)}{\partial (\beta^{T} x^{(i)})} \cdot \frac{\partial \beta^{T} x^{(i)}}{\partial \beta_{j}} &= \\ &= \sum_{i=1}^{m} y^{(i)} \cdot \left(e^{-\beta^{T} x^{(i)}} + 1 \right) \cdot \frac{e^{-\beta^{T} x^{(i)}}}{\left(e^{-\beta^{T} x^{(i)}} + 1 \right)^{2}} \cdot x^{(i)} &= \sum_{i=1}^{m} y^{(i)} \cdot \frac{e^{-\beta^{T} x^{(i)}}}{\left(e^{-\beta^{T} x^{(i)}} + 1 \right)} \cdot x^{(i)}; \\ &= \frac{\partial}{\partial \beta_{j}} \sum_{i=1}^{m} \left[\left(1 - y^{(i)} \right) \cdot \ln \left(1 - \sigma(\beta^{T} x^{(i)}) \right) \right] &= \\ &= \frac{\partial}{\partial \beta_{j}} \sum_{i=1}^{m} \left[\ln \left(1 - \sigma(\beta^{T} x^{(i)}) \right) - y^{(i)} \cdot \ln \left(1 - \sigma(\beta^{T} x^{(i)}) \right) \right]; \end{split}$$

$$\begin{split} \frac{\partial}{\partial \beta_{j}} \sum_{i=1}^{m} \ln \left(1 - \sigma(\beta^{T} x^{(i)}) \right) &= \sum_{i=1}^{m} \frac{\partial \ln \left(1 - \sigma(\beta^{T} x^{(i)}) \right)}{\partial (1 - \sigma(\beta^{T} x^{(i)}))} \cdot \frac{\partial \left(1 - \sigma(\beta^{T} x^{(i)}) \right)}{\partial (\beta^{T} x^{(i)})} \cdot \frac{\partial \beta^{T} x^{(i)}}{\partial \beta_{j}} &= \\ &= \sum_{i=1}^{m} \frac{1}{1 - \sigma(\beta^{T} x^{(i)})} \cdot \frac{-e^{-\beta^{T} x^{(i)}}}{\left(e^{-\beta^{T} x^{(i)}} + 1 \right)^{2}} \cdot x^{(i)} &= \sum_{i=1}^{m} \frac{1 + e^{-\beta^{T} x^{(i)}}}{e^{-\beta^{T} x^{(i)}}} \cdot \frac{-e^{-\beta^{T} x^{(i)}}}{\left(e^{-\beta^{T} x^{(i)}} + 1 \right)^{2}} \cdot x^{(i)} &= \\ &= \sum_{i=1}^{m} -\frac{1}{e^{-\beta^{T} x^{(i)}}} \cdot x^{(i)}; \\ &\frac{\partial}{\partial \beta_{j}} \sum_{i=1}^{m} -y^{(i)} \cdot \ln \left(1 - \sigma(\beta^{T} x^{(i)}) \right) &= \sum_{i=1}^{m} \frac{y^{(i)}}{e^{-\beta^{T} x^{(i)}} + 1} \cdot x^{(i)}; \\ &\frac{\partial LL(\beta)}{\partial \beta_{j}} &= \frac{\partial}{\partial \beta_{j}} \sum_{i=1}^{m} \left[y^{(i)} \cdot \ln \left(\sigma(\beta^{T} x^{(i)}) \right) + \left(1 - y^{(i)} \right) \cdot \ln \left(1 - \sigma(\beta^{T} x^{(i)}) \right) \right] &= \\ &= \sum_{i=1}^{m} y^{(i)} \cdot \frac{e^{-\beta^{T} x^{(i)}}}{e^{-\beta^{T} x^{(i)}} + 1} \cdot x^{(i)} + \sum_{i=1}^{m} -\frac{1}{e^{-\beta^{T} x^{(i)}} + 1} \cdot x^{(i)} + \sum_{i=1}^{m} \frac{y^{(i)}}{e^{-\beta^{T} x^{(i)}} + 1} \cdot x^{(i)} &= \\ &= \sum_{i=1}^{m} \frac{y^{(i)} \cdot e^{-\beta^{T} x^{(i)}} - 1 + y^{(i)}}{e^{-\beta^{T} x^{(i)}} + 1} \cdot x^{(i)} &= \sum_{i=1}^{m} \frac{y^{(i)} \cdot \left(e^{-\beta^{T} x^{(i)}} + 1 \right) - 1}{e^{-\beta^{T} x^{(i)}} + 1} \cdot x^{(i)} &= \\ &= \sum_{i=1}^{m} y^{(i)} - \frac{1}{e^{-\beta^{T} x^{(i)}} + 1} \cdot x^{(i)} &= \sum_{i=1}^{m} \left[y^{(i)} - \sigma(\beta^{T} x^{(i)}) \right] \cdot x_{j}^{(i)}. \end{split}$$