Q2 — Sigmoid 和交叉熵一起的求导推导.

因为 logistic regression 解决的是分类问题，在二元分类问题中，常使用 sigmoid 作为模型的假设函数：

$$\boxed{h_\theta(x^i) = \frac{1}{1+e^{-\theta^T x^i}}} \quad (**)$$

同样，对于二元分类，有 $p(\hat{y}^i=1|x^i;\theta) = h_\theta(x^i)$ ①

$$p(\hat{y}_i=0|x^i;\theta) = 1-h_\theta(x^i) \quad ②$$

合并①,②，则有：$\boxed{P(\hat{y}|x;\theta) = h_\theta(x)^y(1-h_\theta(x))^{1-y},\ y=0,1}$

↑ LR分布函数.

为了求出一个唯一最优模型，需使用MLE估计θ

(极大化已出现样本的联合概率求解θ).

$$\prod_i^n P(y^i|x^i;\theta) = \prod_{i=1}^n h_\theta(x^i)^{y^i}(1-h_\theta(x^i))^{1-y^i} \quad ③$$

对③两边取对数：

$$L(\theta) = \sum_{i=1}^n y^i\log h_\theta(x^i) + (1-y^i)\log(1-h_\theta(x^i)) \quad ④$$

④计算的是表征正确的概率

∴ 希望④越大越好.

∴ 定义损失函数为④的相反数：

$$\boxed{J(\theta) = -\frac{1}{n}\sum_{i=1}^n y^i\log h_\theta(x^i)+(1-y^i)\log(1-h_\theta(x^i))} \quad (*)$$

↑ loss.

对(*)求导.

有 $\log h_\theta(x^i) = \log\left(\frac{1}{1+e^{-\theta^T x^i}}\right) = -\log(1+e^{-\theta^T x^i})$

$$\log(1-h_\theta(x^i)) = \log\left(1-\frac{1}{1+e^{-\theta^T x^i}}\right)$$

$$= \log\left(\frac{1+e^{-\theta^T x^i}}{1+e^{-\theta^T x^i}} - \frac{1}{1+e^{-\theta^T x^i}}\right)$$

$$= \log\left(\frac{e^{-\theta^T x^i}}{1+e^{-\theta^T x^i}}\right)$$

$$= \log(e^{-\theta^T x^i}) - \log(1+e^{-\theta^T x^i})$$

$$= -\theta^T x^i - \log(1+e^{-\theta^T x^i})$$

$$\therefore J(\theta) = -\frac{1}{n}\sum_{i=1}^n\left[-y^i\log(1+e^{-\theta^T x^i}) + (1-y^i)(-\theta^T x^i-\log(1+e^{-\theta^T x^i}))\right]$$

$$= -\frac{1}{n}\sum_{i=1}^n\left[-\theta^T x^i - \log(1+e^{-\theta^T x^i}) + y^i\theta^T x^i\right]$$

$$= -\frac{1}{n}\sum_{i=1}^n\left[y^i\theta^T x^i - \log e^{\theta^T x^i} - \log(1+e^{-\theta^T x^i})\right]$$

$$= -\frac{1}{n}\sum_{i=1}^n\left[y^i\theta^T x^i - (\log e^{\theta^T x^i} + \log(1+e^{-\theta^T x^i}))\right]$$

$$= -\frac{1}{n}\sum_{i=1}^n\left[y^i\theta^T x^i - \log(e^{\theta^T x^i} + e^{\theta^T x^i-\theta^T x^i})\right]$$

$$= -\frac{1}{n}\sum_{i=1}^n\left[y^i\theta^T x^i - \log(1+e^{\theta^T x^i})\right].$$

$$\therefore \partial J(\theta)/\partial\theta_j = \partial/\partial\theta_j\left(\frac{-1}{n}\sum_{i=1}^n\left[y^i\theta^T x^i - \log(1+e^{\theta^T x^i})\right]\right)$$

$$= \frac{1}{n}\sum_{i=0}^n\left(\partial/\partial\theta_j\log(1+e^{\theta^T x^i}) - \partial/\partial\theta_j(y^i\theta^T x^i)\right)$$

$$= 1/n\sum_{i=0}^n\left(\frac{x^i_j e^{\theta^T x^i}}{1+e^{\theta^T x^i}} - y^i x^i_j\right)$$

$$\boxed{= 1/n\sum_{i=0}^n(h_\theta(x^i)-y^i)x^i_j}$$

对(*)求导(向量)：

(*)写成向量形式为 $\boxed{J(\theta)=-\left[y^T\log h_\theta(x)+(1-y^T)\log(1-h_\theta(x))\right]}$ (***)

将(**)代入(***)得：

$$J(\theta)=-\left[y^T\cdot\log\left(\frac{1}{1+e^{-\theta^T x}}\right)+(1-y^T)\log\left(\frac{e^{-\theta^T x}}{1+e^{-\theta^T x}}\right)\right]$$

$$=-\left[-y^T\log(1+e^{-\theta^T x})+(1-y^T)\log(e^{-\theta^T x})-(1-y^T)\log(1+e^{-\theta^T x})\right]$$

$$=-\left[(1-y^T)\log(e^{-\theta^T x})-\log(1+e^{-\theta^T x})\right]$$

$$=-\left[(1-y^T)(-\theta^T x)-\log(1+e^{-\theta^T x})\right]$$

$$\therefore \partial J(\theta)/\partial\theta_j=-\partial/\partial\theta_j\left((1-y^T)(-\theta^T x)-\log(1+e^{-\theta^T x})\right)$$

$$=(1-y^T)x-\frac{x\cdot e^{-\theta^T x}}{1+e^{-\theta^T x}}$$

$$=x\left(1-y^T-\frac{e^{-\theta^T x}}{1+e^{-\theta^T x}}\right)$$

$$=x\left(\frac{1}{1+e^{-\theta^T x}}-y^T\right)$$

$$=\boxed{x\left(h_\theta(x)-y^T\right)}$$