Exercise Sheet 4

Exercise 1 - Hessian of logistic regression

$$L(w,X,y) = -\sum_{i=1}^{N}\left[y_i \log p(y_i=1|x_i,w) + (1-y_i)\log\left(1-p(y_i=1|x_i,w)\right)\right]$$

$$L_w = -\sum_{i=1}^{N}\left[y_i \log p_i + (1-y_i)\log(1-p_i)\right]$$

Gradient:

$$\nabla_w L_i = -\left(y_i \frac{\nabla_w p_i}{p_i} + (1-y_i)\frac{-\nabla_w p_i}{1-p_i}\right) = -\nabla_w p_i\left(\frac{y_i}{p_i} - \frac{1-y_i}{1-p_i}\right)$$

$$= -\nabla_w p_i\left(\frac{p_i - y_i}{p_i(1-p_i)}\right) \quad *$$

$\to \sigma(w^T x_i)(1-\sigma(w^T x_i))$

$$\nabla_w p_i = \nabla_w \sigma(w^T x_i) = \sigma'(w^T x_i)\cdot x_i = p_i(1-p_i)x_i \quad **$$

* and ** $\Rightarrow \boxed{\nabla_w L_i = (p_i - y_i)x_i} \Rightarrow$ first gradient

$$\begin{bmatrix} x_{i1} \\ \vdots \\ x_{im}\end{bmatrix} \quad (x_1 \cdots x_N)\begin{pmatrix} p_1 - y_1 \\ \vdots \\ p_n - y_n\end{pmatrix} = \begin{bmatrix} \ \end{bmatrix}_{m\times 1}$$

Sum for all samples $\Rightarrow \nabla_w L = \sum_{i=1}^{N}(p_i - y_i)x_i = X^T\cdot(P - Y)$

Hessian: for entry in (j,k)th position in Hessian: ?

$$\left[\nabla_w^2 L\right]_{jk} = \frac{\partial}{\partial w_j}\left(\sum_{i=1}^{N}(p_i - y_i)x_{i,k}\right) = \sum_{i=1}^{N}\frac{\partial p_i}{\partial w_j} * x_{ik}$$

$$\frac{\partial p_i}{\partial w_j} = \frac{\partial}{\partial w_j}\left(\sigma(w^T x_i)\right) = \sigma'(w^T x_i) * x_{ij} = p_i(1-p_i)x_{ij} \quad \Rightarrow$$

$$\Rightarrow \left[\nabla_w^2 L\right]_{jk} = \sum_{i=1}^{N} p_i(1-p_i)x_{ij} * x_{ik} \Rightarrow \text{element-wise results}$$

Diagonal matrix $S := \mathrm{diag}\left(p_1(1-p_1), p_2(1-p_2), \dots, p_N(1-p_N)\right) \in \mathbb{R}^{N\times N}$

$$\Rightarrow \sum_{i=1}^{N} x_{ij}\underbrace{p_i(1-p_i)}_{S_i}x_{ik} \xrightarrow{\text{for all entries}} = X^T S X$$

$$\Rightarrow \boxed{\nabla_w^2 L(w) = X^T . S . X}$$

Exercise 2 - Kullback-Leibler Divergence:

$$D_{KL}(P\|q) := \sum_{x\in\mathcal{X}} p(x) * \log \frac{p(x)}{q(x)}$$

① $D_{KL}(P\|q) \geq 0$ and $D_{KL}(P\|q) = 0 \iff P = q$

$$D_{KL}(P\|q) = \sum_x p(x) * \log\left(\frac{q(x)}{p(x)}\right)^{-1} = -\sum_x p(x)\log\frac{q(x)}{p(x)}$$

property of log => for $\forall x > 0$ => $\log x \leq x-1$ => $-\log x \geq 1-x$

$p(x)$ & $q(x) \geq 0$

$$\Rightarrow -\log\frac{q(x)}{p(x)} \geq 1 - \frac{q(x)}{p(x)}$$

$$\xrightarrow[\text{by } p(x)\geq 0]{\text{multiply both sides}} -p(x)\log\frac{q(x)}{p(x)} \geq p(x) - q(x) \xrightarrow{\text{Sum over all } x\in\mathcal{X}}$$

(sum of elements for any probability distribution)

$$-\sum_x p(x)\log\frac{q(x)}{p(x)} \geq \underbrace{\sum_{x\in\mathcal{X}} p(x)}_{=1} - \underbrace{\sum_{x\in\mathcal{X}} q(x)}_{=1} = 1 - 1 = 0$$

$$\Rightarrow \sum_{x\in\mathcal{X}} p(x)\log\frac{p(x)}{q(x)} \geq 0$$

$D_{KL}(P\|q) = 0 \iff P = q$

"$\Rightarrow$": $D_{KL}(P\|q) = 0 \Rightarrow \sum_{x\in\mathcal{X}} p(x) * \log\frac{p(x)}{q(x)} = 0 \Rightarrow \log\frac{p(x)}{q(x)} = 0 \Rightarrow \frac{p(x)}{q(x)} = 1$

for each term: $p(x)\log\frac{p(x)}{q(x)} = 0 \xrightarrow[\text{by } p(x)]{\text{divide}} \log\frac{p(x)}{q(x)} = 0 \Rightarrow p(x) = q(x)$ => $\boxed{p(x) = q(x)}$

"$\Leftarrow$": $P = q \Rightarrow \log\frac{p(x)}{q(x)} = \log 1 = 0 \Rightarrow D_{KL}(P\|q) = \sum_x p(x) * \log\frac{p(x)}{q(x)} = 0$

Exercise 2 - Kullback-Leibler Divergence

2 - Show that $D_{KL}(P\|Q) \neq D_{KL}(Q\|P)$ with an explicit example

Let $X = (a, b, c)$

dist $P \Rightarrow P = \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right)$

dist $Q \Rightarrow Q = \left(\frac{1}{8}, \frac{1}{8}, \frac{3}{4}\right)$

$$D_{KL}(P\|Q) = \sum_{x \in X} P(x) \log \frac{P(x)}{Q(x)} = \frac{1}{2} \log \frac{1/2}{1/8} + \frac{1}{4} \log \frac{1/4}{1/8} + \frac{1}{4} \log \frac{1/4}{3/4}$$

$$= \underbrace{\frac{1}{2} \underbrace{\log 4}_{0.602}}_{0.301} + \underbrace{\frac{1}{4} \underbrace{\log 2}_{0.301}}_{0.075} + \underbrace{\frac{1}{4} \underbrace{\log \frac{1}{3}}_{-0.477}}_{-0.119} \simeq 0.257 \; *$$

$$D_{KL}(Q\|P) = \sum_{x \in X} Q(x) \log \frac{Q(x)}{P(x)} = \frac{1}{8} \log \frac{1/8}{1/2} + \frac{1}{8} \log \frac{1/8}{1/4} + \frac{3}{4} \log \frac{3/4}{1/4}$$

$$= \frac{1}{8} \log \frac{1}{4} + \frac{1}{8} \log \frac{1}{2} + \frac{3}{4} \log 3 \simeq 0.245 \; **$$

$$0.257 \neq 0.245 \Rightarrow D_{KL}(P\|Q) \neq D_{KL}(Q\|P)$$