Machine Learning- Exercise 2
Theoretical Part

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Multiclass Logistic Regression

(a) $P(Y = y|X = \boldsymbol{x}) = softmax(\boldsymbol{Wx} + \boldsymbol{b})_{[y]} = \frac{e^{\boldsymbol{w}_{[y]}\boldsymbol{x}+b_{[y]}}}{\sum_i e^{\boldsymbol{w}_{[i]}\boldsymbol{x}+b_{[i]}}}$, where $[i]$ indicates the i-th index of the vector / matrix, **W** the weights matrix and **b** the bias vector.

(b) $\Theta^* = \underset{\Theta}{argmin}\frac{1}{m}\sum_{t=1}^{m} -\log\left(P(Y_t = y|X_t = \boldsymbol{x})\right) = \underset{\Theta}{argmin}\sum_t -\log\left(softmax(\boldsymbol{Wx}+\boldsymbol{b})_{[y]}\right) \overset{\boldsymbol{w} := \boldsymbol{W}_{[y]}, b:=\boldsymbol{b}_{[y]}}{\triangleq} \underset{\Theta}{argmin}\sum_t -\log\left(\frac{e^{\boldsymbol{wx}+b}}{\sum_i e^{\boldsymbol{W}_{[i]}\boldsymbol{x}+\boldsymbol{b}_{[i]}}}\right) = \underset{\Theta}{argmin}\sum_t -\boldsymbol{wx} - b + \log(\sum_i \boldsymbol{W}_{[i]}\boldsymbol{x} + \boldsymbol{b}_{[i]})$, where Θ is **W** and **b**.

(c) I'll calculate the gradients of the average loss for all the training examples w.r.t each weight ($w_1, \dots, w_n - \ n\ is\ the\ number\ of\ classes$) and the bias ($b$):

Weights: $\nabla_{w_i} loss(\boldsymbol{W};\boldsymbol{b}) = \nabla_{w_i}\frac{1}{m}\sum_{t=1}^{m} -\log\left(P(Y_t = y|X_t = \boldsymbol{x})\right) = \frac{1}{m}\sum_{t=1}^{m}\nabla_{w_i} -\log\left(P(Y_t = y|X_t = \boldsymbol{x})\right) = \frac{1}{m}\sum_{t=1}^{m}\nabla_{w_i} -\log\left(\frac{e^{\boldsymbol{w_y x}+b_y}}{\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\right) = \frac{1}{m}\sum_{t=1}^{m} -\nabla_{w_i}\log\left(e^{\boldsymbol{w_y x}+b_y}\right) + \nabla_{w_i}\log\left(\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right) = \frac{1}{m}\sum_{t=1}^{m} -\nabla_{w_i}(\boldsymbol{w_y x} + b_y) + \frac{1}{\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\nabla_{w_i}\left(\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right)$

We'll call the derivative of the loss of example t as $\nabla_{w_i} loss_t(\boldsymbol{W};\boldsymbol{b}) = -\nabla_{w_i}(\boldsymbol{w_y x} + b_y) + \frac{1}{\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\nabla_{w_i}\left(\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right)$, so in total $\nabla_{w_i} loss(\boldsymbol{W};\boldsymbol{b}) = \frac{1}{m}\sum_{t=1}^{m} loss_t(\boldsymbol{W};\boldsymbol{b})$. For $i = y$ (where y is the correct tag), $loss_t(\boldsymbol{W};\boldsymbol{b}) = -\nabla_{w_y}(\boldsymbol{w_y x} + b_y) + \frac{1}{\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\nabla_{w_y}\left(\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right) = -\boldsymbol{x} + \frac{1}{\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\left(\sum_{j=1}^{n}\nabla_{w_y} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right) = -\boldsymbol{x} + \frac{1}{\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\left(\nabla_{w_y} e^{\boldsymbol{W}_0\boldsymbol{x}+\boldsymbol{b}_0} + \cdots \nabla_{w_y} e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y} + \cdots \nabla_{w_y} e^{\boldsymbol{W}_n\boldsymbol{x}+\boldsymbol{b}_n}\right) = -\boldsymbol{x} + \frac{1}{\sum_{j=1}^{n} e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\left(e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}\boldsymbol{x}\right) =$

$\boldsymbol{x}\left(\frac{e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}-1\right)=\boldsymbol{x}\left(softmax_{[y]}(\boldsymbol{Wx}+\boldsymbol{b})-1\right)$. For $i\neq y$: $loss_t(\boldsymbol{W};\boldsymbol{b})=-\nabla_{w_i}(\boldsymbol{w_y}\boldsymbol{x}+b_y)+\frac{1}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\nabla_{w_i}\left(\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right)=-0+\frac{1}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\left(\sum_{j=1}^{n}\nabla_{w_i}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right)=\frac{e^{\boldsymbol{W}_i\boldsymbol{x}+\boldsymbol{b}_i}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\boldsymbol{x}=softmax(\boldsymbol{Wx}+\boldsymbol{b})_{[i]}*\boldsymbol{x}$.

In conclusion, $\nabla_{w_i}loss(\boldsymbol{W};\boldsymbol{b})=\frac{1}{m}\sum_{t=1}^{m}\nabla_{w_i}loss_t(\boldsymbol{W};\boldsymbol{b})$,

where $\nabla_{w_i}loss_t(\boldsymbol{W};\boldsymbol{b})=\begin{cases}-\boldsymbol{x}+\frac{e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\boldsymbol{x}, & i=y\\ \frac{e^{\boldsymbol{W}_i\boldsymbol{x}+\boldsymbol{b}_i}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\boldsymbol{x} & ,i\neq y\end{cases}$.

Bias: $\nabla_{b_i}loss(\boldsymbol{W};\boldsymbol{b})=\nabla_{b_i}\frac{1}{m}\sum_{t=1}^{m}-\log\left(P(Y_t=y|X_t=\boldsymbol{x})\right)=\frac{1}{m}\sum_{t=1}^{m}\nabla_{b_i}-\log\left(P(Y_t=y|X_t=\boldsymbol{x})\right)=\frac{1}{m}\sum_{t=1}^{m}\nabla_{b_i}-\log\left(\frac{e^{\boldsymbol{w}_y\boldsymbol{x}+\boldsymbol{b}_y}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\right)=\frac{1}{m}\sum_{t=1}^{m}-\nabla_{b_i}\log\left(e^{\boldsymbol{w}_y\boldsymbol{x}+\boldsymbol{b}_y}\right)+\nabla_{b_i}\log\left(\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right)=\frac{1}{m}\sum_{t=1}^{m}-\nabla_{b_i}(\boldsymbol{w_y}\boldsymbol{x}+b_y)+\frac{1}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\nabla_{b_i}\left(\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right)$, so like before we'll look at the case $i=y$ for a single example t:

$-\nabla_{b_y}(\boldsymbol{w_y}\boldsymbol{x}+b_y)+\frac{1}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\nabla_{b_y}\left(\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}\right)=-1+\frac{1}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\left(\nabla_{b_y}e^{\boldsymbol{W}_0\boldsymbol{x}+\boldsymbol{b}_0}+\cdots\nabla_{b_y}e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}+\cdots\ \nabla_{b_y}e^{\boldsymbol{W}_n\boldsymbol{x}+\boldsymbol{b}_n}\right)=-1+\frac{e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}*1}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}=softmax(\boldsymbol{Wx}+\boldsymbol{b})_{[y]}-1$, and for $i\neq y$ it's the same without the -1.

For conclusion, $\nabla_{b_i}loss(\boldsymbol{W};\boldsymbol{b})=\frac{1}{m}\sum_{t=1}^{m}\nabla_{b_i}loss_t(\boldsymbol{W};\boldsymbol{b})$,

where $\nabla_{b_i}loss_t(\boldsymbol{W};\boldsymbol{b})=\begin{cases}\frac{e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}-1, & i=y\\ \frac{e^{\boldsymbol{W}_i\boldsymbol{x}+\boldsymbol{b}_i}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}} & ,i\neq y\end{cases}$.

Now, for the update rules: the general SGD update rule is $\boldsymbol{w_i}=\eta\nabla_{\boldsymbol{w}_i}loss(\boldsymbol{W};\boldsymbol{b})$ for each row $\boldsymbol{w_i}$ in the weight matrix $\boldsymbol{W}$, and $b_i=\eta\nabla_{b_i}loss(\boldsymbol{W};\boldsymbol{b})$ for each element b_i in the bias vector $\boldsymbol{b}$. So the update rules are:

$$\boldsymbol{w_i}=\begin{cases}-\eta\boldsymbol{x}+\eta\frac{e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\boldsymbol{x}, & i=y\\ \eta\frac{e^{\boldsymbol{W}_i\boldsymbol{x}+\boldsymbol{b}_i}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}\boldsymbol{x} & ,i\neq y\end{cases}$$

$$b_i=\begin{cases}\eta\frac{e^{\boldsymbol{W}_y\boldsymbol{x}+\boldsymbol{b}_y}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}}-\eta, & i=y\\ \eta\frac{e^{\boldsymbol{W}_i\boldsymbol{x}+\boldsymbol{b}_i}}{\sum_{j=1}^{n}e^{\boldsymbol{W}_j\boldsymbol{x}+\boldsymbol{b}_j}} & ,i\neq y\end{cases}$$

Practical Part – Graph