2. Neural Network Basics (1)

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1. $\sigma(x) = \dfrac{1}{1+e^{-x}}$

$$\sigma'(x) = -(1+e^{-x})^{-2} \cdot e^{-x} \cdot (-1)$$
$$= \frac{e^{-x}}{(1+e^{-x})} \cdot \frac{1}{(1+e^{-x})}$$
$$= \frac{1}{e^{-(-x)}+1} \cdot \frac{1}{1+e^{-x}}$$
$$= \sigma(-x)\cdot\sigma(x)$$
lemma (a)
$$= \sigma(x)(1-\sigma(x))$$

$$\therefore \sigma'(x) = \sigma(x)(1-\sigma(x))$$

[Lemma (a)]

$\sigma(-x) = 1-\sigma(x)$

(pf) $\sigma(-x) = \dfrac{1}{1+e^{x}}$

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

$\therefore \sigma(-x) = 1-\sigma(x)$

2. $CE(y,\hat{y}) = -\sum_i y_i \log(\hat{y}_i)$

$$= -\sum_i y_i \log(\mathrm{softmax}(\theta)_i)$$

$$\Rightarrow \frac{\partial CE(y,\hat{y})}{\partial \theta_i} = \frac{\partial -\sum_j y_j \log(\hat{y}_j)}{\partial \theta_i}$$
$$= \frac{\partial -\sum_j y_j \log(S(\theta)_j)}{\partial \theta_i}$$
$$= \frac{\partial -y_k \log(S(\theta)_k)}{\partial \theta_i} \quad \left(\because y = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \rightarrow k\text{th element}\right)$$
$$= \frac{\partial -\log(S(\theta)_k)}{\partial \theta_i}$$
$$= -\frac{1}{S(\theta)_k} \cdot \frac{\partial S(\theta)_k}{\partial \theta_i}$$

$\boxed{\text{(i) } i=k \text{ case}}$

$$= -\frac{1}{\cancel{S(\theta)_k}} \cdot \cancel{S(\theta)_k}(1-S(\theta)_k) \quad (\because \text{lemma (b)})$$
$$= -(1-S(\theta)_i)$$
$$= \hat{y}_i - 1$$

$\boxed{\text{(ii) } i\neq k \text{ case}}$

$$= -\frac{1}{\cancel{S(\theta)_k}} \cdot -S(\theta)_i \cancel{S(\theta)_k} \quad (\because \text{lemma (b)})$$
$$= S(\theta)_i$$
$$= \hat{y}_i$$

$$\therefore \frac{\partial CE(y,\hat{y})}{\partial \theta_i} = \begin{cases} \hat{y}_i - 1 & \text{if } i=k \\ \hat{y}_i & \text{o.w} \end{cases}$$

$$\rightarrow \frac{\partial CE(y,\hat{y})}{\partial \theta} = \hat{y} - y$$

[Lemma (b)]

$\dfrac{\partial\, \mathrm{softmax}(\theta)_j}{\partial \theta_i}$? let's say $\mathrm{softmax}(\theta)_i = S(\theta)_i$

(i) $i=j$ case

$$\frac{\partial}{\partial \theta_i}\frac{e^{\theta_j}}{\sum_k e^{\theta_k}} = \frac{\partial}{\partial \theta_i}\frac{e^{\theta_i}}{\sum_k e^{\theta_k}}$$
$$= \frac{e^{\theta_i}\cdot\sum_k e^{\theta_k} - e^{\theta_i}\cdot e^{\theta_i}}{(\sum_k e^{\theta_k})^2}$$
$$= \frac{e^{\theta_i}}{\sum_k e^{\theta_k}} \cdot \frac{\sum_k e^{\theta_k} - e^{\theta_i}}{\sum_k e^{\theta_k}}$$
$$= S(\theta)_i(1-S(\theta)_i)$$

(ii) $i\neq j$ case

$$\frac{\partial}{\partial \theta_i}\frac{e^{\theta_j}}{\sum_k e^{\theta_k}} = \frac{-e^{\theta_j}e^{\theta_i}}{(\sum_k e^{\theta_k})^2}$$
$$= \frac{-e^{\theta_j}}{\sum_k e^{\theta_k}} \cdot \frac{e^{\theta_i}}{\sum_k e^{\theta_k}}$$
$$= -S(\theta)_i \cdot S(\theta)_j$$

$$\therefore \frac{\partial S(\theta)_j}{\partial \theta_i} = \begin{cases} S(\theta)_i(1-S(\theta)_j) & \text{if } i=j \\ -S(\theta)_i S(\theta)_j & \text{o.w} \end{cases}$$