Assignment 1

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1 Q1

 $\operatorname{softmax}(\mathbf{x}) = \operatorname{softmax}(\mathbf{x} + c)$ (Note, remember softmax is defined as a function taking in a vector)

Considering element i

$$\frac{e^{x_i}}{\sum_j e^{x_j}} = \frac{e^{x_i + c}}{\sum_j e^{x_j + c}} \tag{1}$$

since,

$$\frac{e^{x_i}e^c}{\sum_j e^{x_j}e^c} = \frac{e^{x_i}e^c}{\sum_j e^{x_j}e^c} \tag{2}$$

QED

This is useful for the trick where $c = -\max_{i=1}^{n} \mathbf{x}_{i}$, since the largest number in the exponential possible is now 0. That is it prevents overflow.

2 Q2 a)

The sigmoid function is

$$y = \frac{1}{1 + e^{-x}} = \sigma(x) = (1 + e^{-x})^{-1} = (z)^{-1}$$
(3)

Where $z = 1 + e^{-x} = 1 + e^{r}$, and r = -x

Then by simple chain rule

$$\frac{dy}{dx} = \frac{dy}{dz} * \frac{dz}{dr} * \frac{dr}{dx} \tag{4}$$

$$\frac{dy}{dx} = -(1 + e^{-x})^{-2} * e^{-x} * (-1) = e^{-x} * \left(\frac{1}{1 + e^{-x}}\right)^2 = e^{-x}\sigma(x)\sigma(x)$$
 (5)

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

$$\frac{1 - \frac{1}{1 + e^{-x}}}{\frac{1}{1 + e^{-x}}} = (1 + e^{-x}) - \frac{1 + e^{-x}}{1 + e^{-x}} = (1 + e^{-x}) - 1 = e^{-x}$$
(6)

Then

$$e^{-x}\sigma(x)\sigma(x) = \frac{1 - \sigma(x)}{\sigma(x)}\sigma(x) = (1 - \sigma(x))(\sigma(x))$$
 (7)

QED

3 Q2 b)

Asume K classes, $\hat{y} = \text{softmax}(\theta) = [\hat{y}_1, ..., \hat{y}_K] = [\text{softmax}(\theta_1), ..., \text{softmax}(\theta_K)] = g(\theta_i) = \frac{e^{\theta_i}}{\sum_{c} e^{\theta_c}}$

$$J = CE(y, \hat{y}) = -\sum_{i}^{K} y_i \log(\hat{y}_i)$$
(8)

Note that the sum is over all the classes and that y is 1-hot so that the sum only picks out one value

$$\nabla_{\theta} J = -\sum_{i}^{K} \frac{\partial}{\partial \theta} y_{i} \log(\hat{y}_{i}) = -\sum_{i}^{K} y_{i} \frac{\partial}{\partial \theta} \log(g(\theta_{i})) = -\sum_{i}^{K} y_{i} \frac{1}{g(\theta_{i})} \frac{\partial}{\partial \theta} g(\theta_{i})$$
(9)

Considering $\frac{\partial}{\partial \theta}g(\theta_i)$, for an element j of θ, θ_j there are two cases. Case 1) j=i then note

$$\frac{\partial}{\partial \theta_j} g(\theta_i) = \frac{\partial}{\partial \theta_j} g(\theta_j) = \frac{\partial}{\partial \theta_i} g(\theta_i)$$
(10)

$$\frac{dg(\theta_i)}{d\theta_i} = \frac{d}{d\theta_i} \frac{e^{\theta_i}}{\sum_{c} e^{\theta_c}} = \frac{\left(\frac{d}{d\theta_j} e^{\theta_i}\right) \left(\sum_{c} e^{\theta_c}\right) - \left(\frac{d}{d\theta_j} \sum_{c} e^{\theta_c}\right) (e^{\theta_i})}{\left(\sum_{c} e^{\theta_c}\right)^2} \tag{11}$$

Where $(\frac{d}{d\theta_j}\sum_c e^{\theta_c})(e^{\theta_i}) = \frac{d}{d\theta_j}e^{\theta_1} + \ldots + e^{\theta_j} + \ldots + e^{\theta_K} = e^{\theta_j} = e^{\theta_i}$ So

$$=\frac{(e^{\theta_i})(\sum_c e^{\theta_c}) - (e^{\theta_i})(e^{\theta_i})}{(\sum_c e^{\theta_c})(\sum_c e^{\theta_c})} = \frac{(e^{\theta_i})}{(\sum_c e^{\theta_c})} \frac{(\sum_c e^{\theta_c} - e^{\theta_i})}{(\sum_c e^{\theta_c})} = g(\theta_i) \left(\frac{\sum_c e^{\theta_c}}{\sum_c e^{\theta_c}} - \frac{e^{\theta_i}}{\sum_c e^{\theta_c}}\right)$$
(12)

$$= g(\theta_i)(1 - g(\theta_i)) = g(\theta_i)(1 - g(\theta_i)) \tag{13}$$

Now in the case there $j \neq i$

$$\frac{dg(\theta_i)}{d\theta_j} = \frac{d}{d\theta_j} \frac{e^{\theta_i}}{\sum_c e^{\theta_c}} = \frac{d}{d\theta_j} e^{\theta_i} \left(\sum_c e^{\theta_c}\right)^{-1} = -e^{\theta_i} \left(\sum_c e^{\theta_c}\right)^{-2} e^{\theta_j}$$
(14)

$$= \frac{-(e^{\theta_i})}{(\sum_c e^{\theta_c})} \frac{(e^{\theta_j})}{(\sum_c e^{\theta_c})} = -g(\theta_i)g(\theta_j)$$
(15)

Let $t_{ij} = 1$ if i = j and i = 0, if $i \neq j$, then we can combine both cases as

$$\frac{dg(\theta_i)}{d\theta_j} = g(\theta_i)(t_{ij} - g(\theta_i)) \tag{16}$$

Which can be confirmed with i = j, $g(\theta_i)(1 - g(\theta_i)) = g(\theta_i)(1 - g(\theta_j))$ and with $j \neq i$, $g(\theta_i)(0 - g(\theta_i)) = g(\theta_i)(-g(\theta_i)) = -g(\theta_i)(g(\theta_i))$

Now putting it all together we get

$$\nabla_{\theta} J = -\sum_{i}^{K} y_{i} \frac{1}{g(\theta_{i})} \overline{g(\theta_{i})} (t_{ij} - g(\theta_{i}))$$
(17)

Let t = y = yt, and since y is 1-hot, this gets vectorized as

$$= -y - g(\theta) = -y - \hat{y} = \hat{y} - y \tag{18}$$

Q2c4

Note I used 'Practical Guide to Matrix Calculus for Deep Learning' by Andrew Delong [HERE] for this question, which was very helpful in giving identities for matrix calculus. I am using the Hadamard (element-wise) product as ⊙

Remember

$$\frac{\partial x^T a}{x} = \frac{\partial a^T x}{x} = a \tag{19}$$

Some definitions:

 $\hat{y} = g(\theta) = g(hW_2 + b_2)$, which has dims \mathbb{R}^{1*K} (same as y)

 $\theta = hW_2 + b_2$, which has dims \mathbb{R}^{1*K}

 $h = \sigma(z) = \sigma(xW_1 + b_1)$, which has dims \mathbb{R}^{1*D_h} (same as the derivative $\sigma'(z)$)

 $z = xW_1 + b_1$, which has dims \mathbb{R}^{1*D_h}

and $W_2 \in \mathbb{R}^{D_h*K}$, $W_1 \in \mathbb{R}^{D_x*D_h}$, $x \in \mathbb{R}^{1*D_x}$ Let $\Delta_2 = \hat{y} - y \in \mathbb{R}^{1*K}$ be the last error message

$$\nabla_x J = (\hat{y} - y) \left(\frac{d\theta}{dx} \right) = \left(\triangle_2 \left(\frac{d\theta}{dh} \right) \right) \odot \left(\frac{dh}{dx} \right)$$
 (20)

$$= \left(\triangle_2 \left(\frac{d}{dh} h W_2 + b_2 \right) \right) \odot \left(\frac{dh}{dx} \right) = \left(\triangle_2 W_2^T \right) \odot \left(\frac{dh}{dx} \right) = \left(\left(\triangle_2 W_2^T \right) \odot \left(\frac{dh}{dz} \right) \right) \frac{dz}{dx} \quad (21)$$

$$= \left(\left(\triangle_2 W_2^T \right) \odot \left(\sigma'(xW_1 + b_1) \right) \right) W_1^T \tag{22}$$

Let $\triangle_1 = (\triangle_2 W_2^T) \odot (\sigma'(xW_1 + b_1)) = (\sigma'(xW_1 + b_1)) \odot (\triangle_2 W_2^T) \in \mathbb{R}^{1*D_h}$ be the hidden error message

Then $\triangle_1 W_1^T \in \mathbb{R}^{1*D_x}$ which is the size we were hoping for.

5 Q2d)

There are the same number of parameters as there are weights and biases which is the size of W_1, W_2, b_1 , and b_2 which is $(D_x * D_h) + (D_h * K) + (1 * D_h) + (1 * K)$

6 Q3a)

From Slide 22 of Lecture 2, the global objective is

$$J(\theta) = \frac{1}{T} \sum_{t=-c < j < c, j \neq 0}^{T} -\log(P(w_{t+j}|w_t))$$
 (23)

For a specific outer word w_i and an inner word \hat{r}

$$J_{i} = -\log(P(\text{word}_{i}|\hat{r}, W)) = -\log\left(\frac{e^{w_{i}^{T}\hat{r}}}{\sum_{j}^{|V|} e^{w_{j}^{T}\hat{r}}}\right) = -\left(w_{i}^{T}\hat{r} - \log\left(\sum_{j}^{|V|} e^{w_{j}^{T}\hat{r}}\right)\right)$$
(24)

$$= -w_i^T \hat{r} + \log\left(\sum_{i}^{|V|} e^{w_j^T \hat{r}}\right) \tag{25}$$

$$\nabla_{\hat{r}} J_i = \frac{\partial}{\partial \hat{r}} w_i^T \hat{r} + \frac{\partial}{\partial \hat{r}} log \left(\sum_{j=1}^{|V|} e^{w_j^T \hat{r}} \right) = -w_i + \frac{1}{\sum_{j=1}^{|V|} e^{w_j^T \hat{r}}} \left(\frac{\partial}{\partial \hat{r}} \sum_{k=1}^{|V|} e^{w_k^T \hat{r}} \right)$$
(26)

$$= -w_i + \frac{1}{\sum_{j}^{|V|} e^{w_j^T \hat{r}}} \left(\sum_{k}^{|V|} e^{w_k^T \hat{r}} \right) w_k^T = -w_i + \sum_{k}^{|V|} \frac{(e^{w_k^T \hat{r}}) w_k^T}{\sum_{j}^{|V|} e^{w_j^T \hat{r}}} = -w_i + \sum_{k}^{|V|} P(\operatorname{word}_k | \hat{r}, W) w_k^T$$
(27)

7 Q3b)

Just to write down the dimensions of all the variables:

 $\hat{r}, w_i, \frac{\partial J_i}{\hat{r}}, \frac{\partial J_i}{w_j} \in \mathbb{R}^{1*D}$ and $w_k^T \hat{r} \in \mathbb{R}, \ \sigma(w_k^T \hat{r}) w_k, \sigma(w_k^T \hat{r}) \hat{r} \in \mathbb{R}^{1*D}$

There are two cases

Case 1) j = i

$$\nabla_{w_j} J_i = -\hat{r} + \frac{1}{\sum_{k}^{|V|} e^{w_k^T \hat{r}}} \frac{\partial}{\partial w_j} \sum_{l}^{|V|} e^{w_l^T \hat{r}}$$

$$(28)$$

But the last partial is only not zero when l = j so

$$\nabla_{w_j} J_i = -\hat{r} + \frac{e^{w_j^T \hat{r}} \hat{r}}{\sum_k^{|V|} e^{w_k^T \hat{r}}}$$
 (29)

Case 2) $j \neq i$

$$\nabla_{w_j} J_i = -(0) + \frac{e^{w_j^T \hat{r}} \hat{r}}{\sum_k^{|V|} e^{w_k^T \hat{r}}} = \frac{e^{w_j^T \hat{r}} \hat{r}}{\sum_k^{|V|} e^{w_k^T \hat{r}}}$$
(30)

The two cases can be combined with t_{ij} , where t_{ij} is 1 when i = j and 0 otherwise

$$\nabla_{w_j} J_i = -\hat{r}(t_{ij}) + \frac{e^{w_j^T \hat{r}} \hat{r}}{\sum_k^{|V|} e^{w_k^T \hat{r}}}$$
(31)

8 Q3c)a)

$$J_i(\hat{r}, w_i, w_1, ..., w_K) = -\log(\sigma(w_i^T \hat{r})) - \sum_{k=1}^{K} \log(\sigma(-w_k^T \hat{r})) = z_1 + z_2$$
 (32)

$$\nabla_{\hat{r}} z_1 = \frac{-1}{\sigma(w_i^T \hat{r})} \sigma'(w_i^T \hat{r}) w_i = \frac{-\sigma(w_i^T \hat{r}) (1 - \sigma(w_i^T \hat{r})) w_i}{\sigma(w_i^T \hat{r})} = (\sigma(w_i^T \hat{r}) - 1) w_i$$
(33)

$$\nabla_{\hat{r}} z_2 = -\sum_{k}^{K} \frac{1}{\sigma(-w_k^T \hat{r})} \sigma'(-w_k^T \hat{r})(-w_k) = \sum_{k}^{K} \frac{\overline{\sigma(-w_k^T \hat{r})}(1 - \sigma(-w_k^T \hat{r}))w_k}{\overline{\sigma(-w_k^T \hat{r})}} = \sum_{k}^{K} (1 - \sigma(-w_k^T \hat{r}))w_k$$
(34)

$$\nabla_{\hat{r}} J_i = (\sigma(w_i^T \hat{r}) - 1) w_i + \sum_{k}^{K} (1 - \sigma(-w_k^T \hat{r})) w_k$$
 (35)

9 Q3c)b)

$$J_i(\hat{r}, w_i, w_1, ..., w_K) = -\log(\sigma(w_i^T \hat{r})) - \sum_{k=1}^{K} \log(\sigma(w_k^T \hat{r})) = z_1 + z_2$$
 (36)

Case 1) j = i

Since $i \notin K$, then $\nabla_{\hat{r}} z_2 = 0$

$$\nabla_{\hat{r}} z_1 = \nabla_{\hat{r}} J_i = \frac{-1}{\sigma(w_i^T \hat{r})} \sigma'(w_i^T \hat{r}) \hat{r} = \frac{-\overline{\sigma(w_i^T \hat{r})} (1 - \sigma(w_i^T \hat{r})) \hat{r}}{\overline{\sigma(w_i^T \hat{r})}} = (\sigma(w_i^T \hat{r}) - 1) \hat{r}$$
(37)

Case 2) $j \neq i$

 $\nabla_{w_i} z_1 = 0$

Then for $\nabla_{w_j} z_1$ there are two cases, if $j \neq k$, then $\nabla_{w_j} z_2 = 0$.

If j = k,

$$\nabla_{w_j} z_2 = \frac{-1}{\sigma(-w_k^T \hat{r})} \sigma'(-w_k^T \hat{r})(-\hat{r}) = \frac{\sigma(-w_k^T \hat{r})(1 - \sigma(-w_k^T \hat{r}))\hat{r}}{\sigma(-w_k^T \hat{r})} = (1 - \sigma(-w_k^T \hat{r}))\hat{r}$$
(38)

A side note that $1 - \sigma(-x) = \sigma(x)$. Proof:

$$1 - \frac{1}{1 + e^{-(-x)}} = \frac{1 + e^x}{1 + e^x} - \frac{1}{1 + e^x} = \frac{1 - 1 + e^x}{1 + e^x} = \frac{e^x}{1 + e^x}$$
(39)

$$=\frac{1(e^x)}{(1/e^x+1)(e^x)} = \frac{1}{(1/e^x+1)} = \frac{1}{(e^{-x}+1)} = \frac{1}{1+e^{-x}}$$
(40)

The two cases can then be combined with t_{ij} , where t_{ij} is 1 when i = j and 0 otherwise

$$\nabla_{w_i} J_i = \nabla_{w_i} z_1 + \nabla_{w_i} z_2 = (\sigma(w_k^T \hat{r}) - t_{ij})\hat{r}$$

$$\tag{41}$$

Which works for if j = k (i.e. only update the gradient for words which are in the negative samples and not all words cause that would be a lot unchanging updates)

10 Q3d)

$$J(\theta_{w_i}) = \sum_{-c \le j \le c, j \ne 0} -\log(P(v'_{w_{i+j}}|v_{w_i})) = \sum_{-c \le j \le c, j \ne 0} F(v'_{w_{i+j}}|v_{w_i})$$
(42)

Where F is either softmax-CE or negative sampling

$$\nabla J = \sum_{-c \le j \le c, j \ne 0} F'(v'_{w_{i+j}} | v_{w_i}) \tag{43}$$

Which is easily found given the above parts for both $\nabla_{v'_{w_{i+1}}} J$ and $\nabla_{v_{w_i}} J$