CS224N: NATURAL LANGUAGE PROCESSING WITH DEEP LEARNING ASSIGNMENT #1

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1. (a) For any input vector $\boldsymbol{x}$ and any constant c,

$$\begin{aligned}
\mathrm{softmax}(\boldsymbol{x}+c)_i &= \frac{e^{x_i+c}}{\sum_j e^{x_j+c}} \\
&= \frac{e^c e^{x_i}}{\sum_j e^c e^{x_j}} \\
&= \frac{e^c e^{x_i}}{e^c \sum_j e^{x_j}} \\
&= \frac{e^{x_i}}{\sum_j e^{x_j}} \\
&= \mathrm{softmax}(\boldsymbol{x})_i \qquad (1)
\end{aligned}$$

Since (1) is true for any arbitrary element i, we can conclude that:

$$\mathrm{softmax}(\boldsymbol{x}) = \mathrm{softmax}(\boldsymbol{x}+c)$$

(b) Please see the coding portion of the assignment.

2. (a) First, we can rearrange the definition of the sigmoid function to obtain:

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

Now we can derive the gradient of the sigmoid function w.r.t. x, assuming x is a scalar.

$$\begin{aligned}
\frac{\partial \sigma(x)}{\partial x} &= \frac{\partial}{\partial x}\frac{1}{1+e^{-x}} \\
&= \frac{-1}{(1+e^{-x})^2}\left(-e^{-x}\right) \\
&= \frac{1}{(1+e^{-x})^2}\left(e^{-x}\right) \\
&= (\sigma(x))^2\left(\frac{1}{\sigma(x)} - 1\right) \\
&= \sigma(x)\left(1-\sigma(x)\right)
\end{aligned}$$

(b) First, let's consider the fact that $\boldsymbol{y}$ is the one-hot label vector, i.e.

$$y_i = \begin{cases} 1, & \text{if } i = k \\ 0, & \text{otherwise} \end{cases}$$

where k is the index of the true label.
Therefore, we can simplify the cross entropy function as:

$$\mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_i y_i \log(\hat{y}_i) = -\log(\hat{y}_k)$$

To derive the gradient w.r.t the inputs of a softmax function when cross entropy loss is used for evaluation, let's consider its individual elements:

$$\begin{aligned}
\frac{\partial}{\partial \theta_i}\mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}}) &= \frac{\partial}{\partial \theta_i}\left[-\log(\hat{y}_k)\right] \\
&= \frac{\partial}{\partial \theta_i}\left[-\log(\frac{e^{\theta_k}}{\sum_j e^{\theta_j}})\right] \\
&= \frac{\partial}{\partial \theta_i}\left[-\theta_k + \log\sum_j e^{\theta_j}\right] \\
&= -\frac{\partial \theta_k}{\partial \theta_i} + \frac{\sum_j e^{\theta_j}\frac{\partial \theta_j}{\partial \theta_i}}{\sum_j e^{\theta_j}} \qquad (2)
\end{aligned}$$

By noting that:

$$\frac{\partial \theta_j}{\partial \theta_i} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}$$

We can simpify (2) as:

$$\frac{\partial}{\partial \theta_i}\mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -y_i + \frac{e^{\theta_i}}{\sum_j e^{\theta_j}} = -y_i + \hat{y}_i$$

Thus, the gradient w.r.t the inputs of a softmax function when cross entropy loss is used for evaluation is:

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

(c) Let's denote:

$$\begin{aligned}
\boldsymbol{\theta_1} &= \boldsymbol{x}\boldsymbol{W_1} + \boldsymbol{b_1} \\
\boldsymbol{\theta_2} &= \boldsymbol{h}\boldsymbol{W_2} + \boldsymbol{b_2}
\end{aligned}$$

By applying chain rule, we can rewrite the gradient as:

$$\frac{\partial J}{\partial \boldsymbol{x}} = \frac{\partial \mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{x}} = \frac{\partial \mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{\theta_2}}\frac{\partial \boldsymbol{\theta_2}}{\partial \boldsymbol{h}}\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{\theta_1}}\frac{\partial \boldsymbol{\theta_1}}{\partial \boldsymbol{x}}$$

The first component is simply the result of part (b):

$$\frac{\partial \mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{\theta_2}} = \hat{\boldsymbol{y}} - \boldsymbol{y}$$

The second component is:

$$\frac{\partial \boldsymbol{\theta_2}}{\partial \boldsymbol{h}} = \frac{\partial}{\partial \boldsymbol{h}}\left(\boldsymbol{h}\boldsymbol{W_2} + \boldsymbol{b_2}\right) = \boldsymbol{W_2}^\top$$

The third component is a $H \times H$ matrix and can be computed by examining its individual elements:

$$\left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{\theta_1}}\right)_{ij} = \left(\frac{\partial \sigma(\boldsymbol{\theta_1})}{\partial \boldsymbol{\theta_1}}\right)_{ij} = \frac{\partial \sigma(\theta_{1i})}{\partial \theta_{1j}} = \begin{cases} \sigma'(\theta_{1i}), & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}$$

where $\sigma'(\theta_{1i}) = \sigma(\theta_{1i})\left(1 - \sigma(\theta_{1i})\right)$ is the sigmoid gradient as shown in part (a).
Thus, we can define:

$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{\theta_1}} = \boldsymbol{S}(\boldsymbol{\theta_1})$$

where $\boldsymbol{S}$ denotes a $H \times H$ diagonal matrix where the diagonal elements are $\sigma'(\theta_i)$ for $i = 1, \cdots, H$.
The fourth component is similar to the second component:

$$\frac{\partial \boldsymbol{\theta_1}}{\partial \boldsymbol{x}} = \frac{\partial}{\partial \boldsymbol{x}}\left(\boldsymbol{x}\boldsymbol{W_1} + \boldsymbol{b_1}\right) = \boldsymbol{W_1}^\top$$

Therefore, the the gradient with respect to the inputs $\boldsymbol{x}$ to an one-hidden-layer neural network is:

$$\begin{aligned}\frac{\partial J}{\partial \boldsymbol{x}} &= \frac{\partial \mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{\theta_2}} \frac{\partial \boldsymbol{\theta_2}}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{\theta_1}} \frac{\partial \boldsymbol{\theta_1}}{\partial \boldsymbol{x}} \\ &= (\hat{\boldsymbol{y}} - \boldsymbol{y})\, \boldsymbol{W_2}^\top \boldsymbol{S}(\boldsymbol{\theta_1}) \boldsymbol{W_1}^\top \\ &= (\hat{\boldsymbol{y}} - \boldsymbol{y})\, \boldsymbol{W_2}^\top \boldsymbol{S}(\boldsymbol{x}\boldsymbol{W_1} + \boldsymbol{b_1}) \boldsymbol{W_1}^\top\end{aligned}$$

(d) The dimensions of the weights and biases are as follows:

Parameter	Dimension
W_1	$D_x \times H$
b_1	$1 \times H$
W_2	$H \times D_y$
b_2	$1 \times D_y$

Therefore, the number of parameters in this neural network is:

$$\#\text{ parameters} = D_x H + H + H D_y + D_y = (D_x + 1)H + D_y(H + 1)$$

(e) Please see the coding portion of the assignment.
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3. (a) Let's denote:

$$\begin{aligned}\theta_w &= \boldsymbol{u}_w^\top \boldsymbol{v}_c \\ \boldsymbol{\theta} &= \boldsymbol{U}^\top \boldsymbol{v}_c\end{aligned}$$

where θ_w is a scalar, $\boldsymbol{u}_w$ and $\boldsymbol{v}_c$ are column vectors of dimensions $N \times 1$, $\boldsymbol{\theta}$ is a column vector of dimension $V \times 1$, and $\boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \cdots, \boldsymbol{u}_V]$ is a matrix of dimension $N \times V$.
The softmax predictions for every word can then be written as:

$$\hat{\boldsymbol{y}} = \frac{\exp(\boldsymbol{U}^\top \boldsymbol{v}_c)}{\sum_{w=1}^{V} \exp(\boldsymbol{u}_w^\top \boldsymbol{v}_c)} = \frac{\exp(\boldsymbol{\theta})}{\sum_{w=1}^{V} \exp(\theta_w)}$$

where $\hat{\boldsymbol{y}}$ is a column vector of softmax predictions for every word of dimension $V \times 1$.
By using chain rule and the result of 2(b), the gradient of the cross entropy cost w.r.t. $\boldsymbol{v}_c$ can be derived as:

$$\begin{aligned}\frac{\partial}{\partial \boldsymbol{v}_c} J_{\text{softmax–CE}} &= \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{v}_c} \frac{\partial J}{\partial \boldsymbol{\theta}} \\ &= \frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{v}_c} \frac{\partial \mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{\theta}} \\ &= \boldsymbol{U}\,(\hat{\boldsymbol{y}} - \boldsymbol{y})\end{aligned}$$

where $\boldsymbol{y}$ is a column vector of expected word of dimension $V \times 1$.

(b) As in the previous part, we can apply chain rule and the result of 2(b):

$$\begin{aligned}\frac{\partial}{\partial \boldsymbol{u}_k} J_{\text{softmax–CE}} &= \frac{\partial \boldsymbol{\theta}}{\partial \boldsymbol{u}_k} \frac{\partial J}{\partial \boldsymbol{\theta}} \\ &= \frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k} \frac{\partial \mathrm{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}})}{\partial \boldsymbol{\theta}} \\ &= \frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k} (\hat{\boldsymbol{y}} - \boldsymbol{y}) \qquad (3)\end{aligned}$$

Rewriting matrix multiplication in (3) explicitly:

$$\begin{aligned}\frac{\partial}{\partial \boldsymbol{u}_k} J_{\text{softmax–CE}} &= \sum_{j}^{V} (\hat{\boldsymbol{y}} - \boldsymbol{y})_j \left(\frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k}\right)_{\cdot j} \\ &= \sum_{j}^{V} (\hat{y}_j - y_j) \left(\frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k}\right)_{\cdot j}\end{aligned}$$

where $\left(\frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k}\right)_{\cdot j}$ is the j-th column of $\frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k}$ which is a $N \times V$ matrix. It can be simplified to:

$$\left(\frac{\partial \boldsymbol{U}^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k}\right)_{\cdot j} = \begin{cases} \boldsymbol{v}_c, & \text{if } j = k \\ 0, & \text{otherwise} \end{cases}$$

Therefore,the gradient can be simplified to:

$$\frac{\partial}{\partial \boldsymbol{u}_k} J_{\text{softmax–CE}} = (\hat{y}_k - y_k)\, \boldsymbol{v}_c$$

Specifically,

$$\frac{\partial}{\partial \boldsymbol{u}_k} J_{\text{softmax–CE}} = \begin{cases} (\hat{y}_k - 1)\, \boldsymbol{v}_c, & \text{if } k = o \\ \hat{y}_k \boldsymbol{v}_c, & \text{otherwise} \end{cases}$$

(c) Let's denote:

$$\theta_o = \boldsymbol{u}_o^\top \boldsymbol{v}_c$$
$$\theta_k = -\boldsymbol{u}_k^\top \boldsymbol{v}_c$$

The gradient of the negative sampling loss w.r.t. $\boldsymbol{v}_c$ is:

$$\begin{aligned}
\frac{\partial}{\partial \boldsymbol{v}_c} J_{\text{neg-sample}} &= \frac{\partial}{\partial \boldsymbol{v}_c}\left[-\log(\sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c)) - \sum_{k=1}^{K} \log(\sigma(-\boldsymbol{u}_k^\top \boldsymbol{v}_c))\right] \\
&= \frac{\partial}{\partial \boldsymbol{v}_c}\left[-\log(\sigma(\theta_o)) - \sum_{k=1}^{K} \log(\sigma(\theta_k))\right] \\
&= -\frac{1}{\sigma(\theta_o)} \frac{\partial \sigma(\theta_o)}{\partial \theta_o} \frac{\partial \theta_o}{\partial \boldsymbol{v}_c} - \sum_{k=1}^{K} \frac{1}{\sigma(\theta_k)} \frac{\partial \sigma(\theta_k)}{\partial \theta_k} \frac{\partial \theta_k}{\partial \boldsymbol{v}_c} \\
&= -\frac{1}{\sigma(\theta_o)} \sigma(\theta_o)(1-\sigma(\theta_o)) \frac{\partial \theta_o}{\partial \boldsymbol{v}_c} - \sum_{k=1}^{K} \frac{1}{\sigma(\theta_k)} \sigma(\theta_k)(1-\sigma(\theta_k)) \frac{\partial \theta_k}{\partial \boldsymbol{v}_c} \\
&= (\sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c) - 1) \frac{\partial \boldsymbol{u}_o^\top \boldsymbol{v}_c}{\partial \boldsymbol{v}_c} + \sum_{k=1}^{K} (\sigma(-\boldsymbol{u}_k^\top \boldsymbol{v}_c) - 1) \frac{\partial (-\boldsymbol{u}_k^\top \boldsymbol{v}_c)}{\partial \boldsymbol{v}_c} \\
&= (\sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c) - 1)\boldsymbol{u}_o - \sum_{k=1}^{K} (\sigma(-\boldsymbol{u}_k^\top \boldsymbol{v}_c) - 1)\boldsymbol{u}_k
\end{aligned}$$

Similarly, the gradient of the negative sampling loss w.r.t. $\boldsymbol{u}_o$ is:

$$\begin{aligned}
\frac{\partial}{\partial \boldsymbol{u}_o} J_{\text{neg-sample}} &= (\sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c) - 1) \frac{\partial \boldsymbol{u}_o^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_o} + \sum_{k=1}^{K} (\sigma(-\boldsymbol{u}_k^\top \boldsymbol{v}_c) - 1) \frac{\partial (-\boldsymbol{u}_k^\top \boldsymbol{v}_c)}{\partial \boldsymbol{u}_o} \\
&= (\sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c) - 1)\boldsymbol{v}_c
\end{aligned}$$

And the gradient of the negative sampling loss w.r.t. $\boldsymbol{u}_k$ is (changing summation indices from k to j to avoid confusion):

$$\begin{aligned}
\frac{\partial}{\partial \boldsymbol{u}_k} J_{\text{neg-sample}} &= (\sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c) - 1) \frac{\partial \boldsymbol{u}_o^\top \boldsymbol{v}_c}{\partial \boldsymbol{u}_k} + \sum_{j=1}^{K} (\sigma(-\boldsymbol{u}_j^\top \boldsymbol{v}_c) - 1) \frac{\partial (-\boldsymbol{u}_j^\top \boldsymbol{v}_c)}{\partial \boldsymbol{u}_k} \\
&= (1 - \sigma(-\boldsymbol{u}_k^\top \boldsymbol{v}_c))\boldsymbol{v}_c
\end{aligned}$$

This cost function is much more efficient to compute than the softmax-CE loss because the computation of $\frac{\partial J}{\partial \boldsymbol{v}_c}$ for softmax-CE loss scales as V while the computation of $\frac{\partial J}{\partial \boldsymbol{v}_c}$ for negative sampling loss scales as K, resulting in a speed-up ratio of K/V, which could make a huge difference if one has a big vocabulary.

(d) For skip-gram, the cost for a context centered around c is:

$$J_{\text{skip-gram}}(w_{t-m}, \cdots, w_{t+m}) = \sum_{-m \le j \le m, j \ne 0} F(w_{t+j}, \boldsymbol{v}_c)$$

where

$$F(o, \boldsymbol{v}_c) = \begin{cases} J_{\text{softmax–CE}}(o, \boldsymbol{v}_c, \cdots) = \text{CE}(\boldsymbol{y}, \hat{\boldsymbol{y}}) = -\sum_i^V y_i \log(\hat{y}_i), & \text{for softmax–CE loss} \\ J_{\text{neg-sample}}(o, \boldsymbol{v}_c, \cdots) = -\log(\sigma(\boldsymbol{u}_o^\top \boldsymbol{v}_c)) - \sum_{k=1}^K \log(\sigma(-\boldsymbol{u}_k^\top \boldsymbol{v}_c)), & \text{for negative sampling loss} \end{cases}$$

Therefore, the gradients w.r.t. the word vectors for the skip-gram model are:

$$\frac{\partial}{\partial \boldsymbol{v}_k} J_{\text{skip-gram}}(w_{t-m}, \cdots, w_{t+m}) = \begin{cases} \sum_{-m \le j \le m, j \ne 0} \dfrac{\partial F(w_{t+j}, \boldsymbol{v}_c)}{\partial \boldsymbol{v}_c}, & \text{if } k = c \\ 0, & \text{otherwise} \end{cases}$$

$$\frac{\partial}{\partial \boldsymbol{u}_k} J_{\text{skip-gram}}(w_{t-m}, \cdots, w_{t+m}) = \sum_{-m \le j \le m, j \ne 0} \frac{\partial F(w_{t+j}, \boldsymbol{v}_c)}{\partial \boldsymbol{u}_k}$$

For CBOW, the cost is:

$$J_{\text{CBOW}}(w_{t-m}, \cdots, w_{t+m}) = F(w_t, \hat{\boldsymbol{v}})$$

where

$$\hat{\boldsymbol{v}} = \sum_{-m \le j \le m, j \ne 0} \boldsymbol{v}_{w_{t+j}}$$

Therefore, the gradients w.r.t. the word vectors for the CBOW model are:

$$\frac{\partial}{\partial \boldsymbol{v}_k} J_{\text{CBOW}}(w_{t-m}, \cdots, w_{t+m}) = \begin{cases} \dfrac{\partial F(w_t, \hat{\boldsymbol{v}})}{\partial \hat{\boldsymbol{v}}} \dfrac{\partial \hat{\boldsymbol{v}}}{\partial \boldsymbol{v}_k} = \dfrac{\partial F(w_t, \hat{\boldsymbol{v}})}{\partial \hat{\boldsymbol{v}}}, & \text{if } t - m \le k \le t + m \text{ and } k \ne t \\ 0, & \text{otherwise} \end{cases}$$

$$\frac{\partial}{\partial \boldsymbol{u}_k} J_{\text{CBOW}}(w_{t-m}, \cdots, w_{t+m}) = \frac{\partial F(w_t, \hat{\boldsymbol{v}})}{\partial \boldsymbol{u}_k}$$

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4. (a)
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