CS 6301.503 Spring 2019 Scott C. Waggener (scw180000)
Homework 3 (Calculus) Problem 1

Honor statement:

Read:

Solution: Complete ■

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Homework 3 (Calculus) Problem 2

Read:

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Homework 3 (Calculus) Problem 3

Read:

Solution: Complete ■

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Homework 3 (Calculus) Problem 4

Let $\boldsymbol{x}$ be the $K \times 1$ vector output of the last layer of a xNN and $e = \text{crossEntropy}(\boldsymbol{p}^*, \text{softMax}(\boldsymbol{x}))$ be the error where $\boldsymbol{p}^*$ is a $K \times 1$ vector with a 1 in position k^* representing the correct class and 0s elsewhere. Derive $\partial e / \partial \boldsymbol{x}$

Solution:

$$\frac{\partial e}{\partial \boldsymbol{x}} = \begin{pmatrix} p(x_0) \\ \vdots \\ p(x_k) - 1 \\ \vdots \\ p(x_n) \end{pmatrix} \begin{matrix} \\ \\ \leftarrow k \\ \\ \\ \end{matrix} \tag{1}$$

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Proof: First, note that error function e is given by the cross entropy of a softmax, the typical error function chosen for **classification** networks. We can tell by the given error function that we will need to apply the chain rule. Specifically, we will need to compute the following for use in the chain rule.

$$\frac{d}{d\boldsymbol{x}}\text{softMax}(\boldsymbol{x}) \qquad\qquad \frac{\partial}{\partial \boldsymbol{p}}\text{crossEntropy}(\boldsymbol{p}^*, \boldsymbol{p}) \tag{2}$$

We will start with cross entropy. Recall that cross entropy is given by

$$\text{crossEntropy}(\boldsymbol{p}^*, \boldsymbol{p}) = c(\boldsymbol{p}^*, \boldsymbol{p}) \qquad = -\sum_{x_i \in \boldsymbol{x}} p^*(x_i) \log p(x_i) \tag{3}$$

Differentiating cross entropy for each of $x_i \in \boldsymbol{x}$ produces a gradient vector. We know that $\boldsymbol{p}^*$ is a one hot vector at position k meaning that our gradient will be nonzero only at position k upon differentiation. Applying the log derivative identity gives

$$\nabla_{\boldsymbol{x}} c(\boldsymbol{p}^*, \boldsymbol{p}) = \tag{4}$$

$$\nabla_{\boldsymbol{x}}\Big(-\sum_{x_i \in \boldsymbol{x}} p^*(x_i)\log p(x_i)\Big) = \begin{pmatrix} -\frac{\partial}{\partial x_1} p^*(x_1)\log p(x_1) \\ -\frac{\partial}{\partial x_2} p^*(x_2)\log p(x_2) \\ \vdots \\ -\frac{\partial}{\partial x_k} p^*(x_k)\log p(x_k) \\ \vdots \\ -\frac{\partial}{\partial x_N} p^*(x_N)\log p(x_N) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \underbrace{-\frac{\partial}{\partial x}\log p(x_k)}_{-1/p(x_k)} \\ \vdots \\ 0 \end{pmatrix} \tag{5}$$

$$= \begin{pmatrix} 0 \\ 0 \\ \vdots \\ -\frac{1}{p(x_k)} \\ \vdots \\ 0 \end{pmatrix} \leftarrow k \tag{6}$$

So our cross entropy gradient for a one hot vector $\boldsymbol{p}^*$ with nonzero position k is 0 everywhere except at position k.

Now we compute our next required derivative: softmax. The softmax function is given by

$$\text{softMax}(\boldsymbol{x}) = \frac{1}{\sum_{x_i \in \boldsymbol{x}} e^{x_i}} \begin{pmatrix} e^{x_0} \\ e^{x_1} \\ \vdots \\ e^{x_K} \end{pmatrix} \tag{7}$$

Calculating this derivative will yield a Jacobian

$$\frac{\partial s}{\partial \boldsymbol{x}} = \Big(\sum_{x_i \in \boldsymbol{x}} e^{x_i}\Big)^{-1} \frac{\partial}{\partial \boldsymbol{x}} \begin{pmatrix} e^{x_0} \\ e^{x_1} \\ \vdots \\ e^{x_K} \end{pmatrix} + \frac{\partial}{\partial \boldsymbol{x}}\Big(\sum_{x_i \in \boldsymbol{x}} e^{x_i}\Big)^{-1} \begin{pmatrix} e^{x_0} \\ e^{x_1} \\ \vdots \\ e^{x_K} \end{pmatrix} \tag{8}$$

$$= \underbrace{\Big(\sum_{x_i \in \boldsymbol{x}} e^{x_i}\Big)^{-1} \begin{pmatrix} e^{x_0} & 0 & \cdots & 0 \\ 0 & e^{x_1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{x_n} \end{pmatrix}}_{\substack{s(\boldsymbol{x})|i \quad \forall i = j \\ 0 \quad \forall i \neq j}} - \underbrace{\Big(\sum_{x_i \in \boldsymbol{x}} e^{x_i}\Big)^{-2} \begin{pmatrix} e^{2x_0} & e^{x_1+x_0} & \cdots & e^{x_n+x_0} \\ e^{x_0+x_1} & e^{2x_1} & \cdots & e^{x_n+x_1} \\ \vdots & \vdots & \ddots & \vdots \\ e^{x_0+x_n} & e^{x_1+x_n} & \cdots & e^{2x_n} \end{pmatrix}}_{\substack{s(\boldsymbol{x})^2|i \quad \forall i = j \\ s(\boldsymbol{x})|i \cdot s(\boldsymbol{x})|j \quad \forall i \neq j}} \tag{9}$$

$$\tag{10}$$

So we get this Jacobian matrix where the entries come from two possible cases that can be expressed in terms of the original function. To express this more cleanly let us denote the softmax at a given $x_i \in \boldsymbol{x}$ with the same $p(x_i)$ notation used for handling cross entropy. Then the entry of the ith row and jth column in the Jacobian matrix for softmax of vector $\boldsymbol{x}$ will be given by

$$J_s(\boldsymbol{x})_{ij} = \begin{cases} p(x_i) - p(x_i)^2 & \forall i = j \\ -p(x_i) \cdot p(x_j) & \forall i \neq j \end{cases} \tag{11}$$

Now we have found what we need to apply the chain rule

$$\frac{\partial e}{\partial \boldsymbol{x}} = \boldsymbol{J}_s(\boldsymbol{x}) \cdot \nabla_{\boldsymbol{x}} c(\boldsymbol{p}^*, \boldsymbol{p}) \tag{12}$$

$$= \begin{pmatrix} p(x_0) - p(x_0)^2 & -p(x_0) \cdot p(x_1) & \cdots & -p(x_0) \cdot p(x_n) \\ -p(x_1) \cdot p(x_0) & p(x_1) - p(x_1)^2 & \cdots & -p(x_1) \cdot p(x_n) \\ \vdots & \vdots & \ddots & \vdots \\ -p(x_n) \cdot p(x_0) & -p(x_n) \cdot p(x_1) & \cdots & p(x_n) - p(x_n)^2 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ \vdots \\ -\frac{1}{p(x_k)} \\ \vdots \\ 0 \end{pmatrix} \tag{13}$$

$$= \begin{pmatrix} \frac{p(x_0) \cdot p(x_k)}{p(x_k)} \\ \vdots \\ \frac{p(x_k)^2 - p(x_k)}{p(x_k)} \\ \vdots \\ \frac{p(x_n) \cdot p(x_k)}{p(x_k)} \end{pmatrix} \tag{14}$$

$$\frac{\partial e}{\partial \boldsymbol{x}} = \begin{pmatrix} p(x_0) \\ \vdots \\ p(x_k) - 1 \\ \vdots \\ p(x_n) \end{pmatrix} \leftarrow k \tag{15}$$

This result is very clean and intuitive. It shows that increasing the probabilities for incorrect labels increases error, and that decreasing probability for the correct label increases error. We were able to get this result by treating softmax and cross entropy derivatives together via the chain rule. This property can only be exploited in implementation by using procedures in the library that treat these layers together.

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Homework 2 (Linear Algebra) Problem 5

Solution:

$$\frac{\partial e}{\partial \boldsymbol{x}} = \left(\boldsymbol{H}^T \cdot \boldsymbol{I}_n \cdot \boldsymbol{I}_n\{0,1\} \cdot \boldsymbol{I}_n \cdot \frac{\partial e}{\partial \boldsymbol{y}} \right) + \boldsymbol{I}_n \tag{16}$$

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Proof: First we decompose the residual block representing the flow of information in backpropagation: resiudal input, pointwise nonlinearity, bias vector, and dense layer.

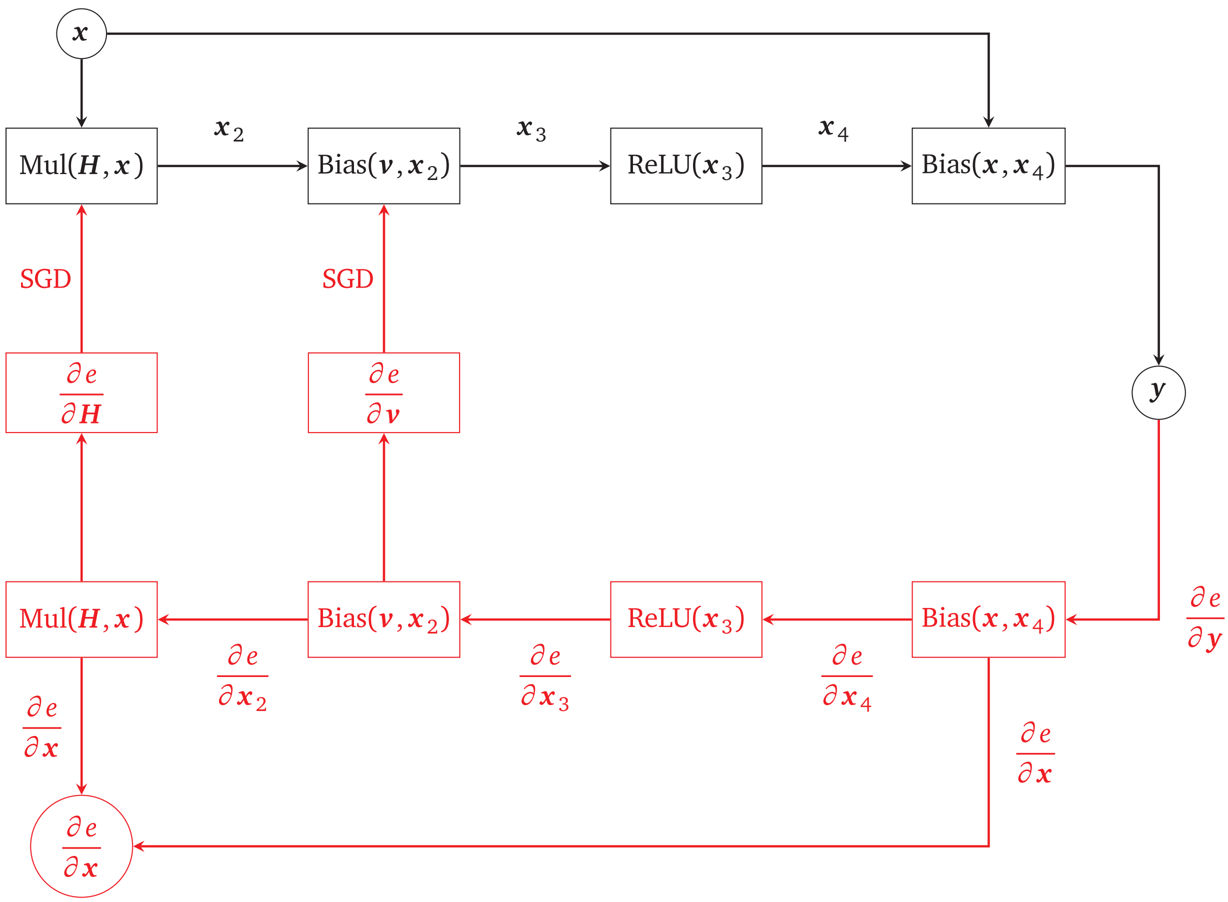
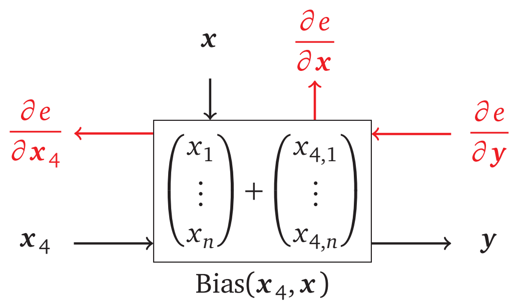


Figure 1. Decomposition of a residual layer

In order to obtain $\partial e / \partial \boldsymbol{x}$ we need to apply the chain rule to move along blocks in the backwards pass. Starting with residual bias block, we have



By definition the bias block is composed of a linear combination of independent vectors, meaning that our Jacobian reduces to an identity matrix before application of the chain rule.

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}_4} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 1 \end{pmatrix} = \boldsymbol{I}_n \tag{17}$$

And completing the chain rule we have

$$\frac{\partial e}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} \cdot \frac{\partial e}{\partial \boldsymbol{y}} \qquad \frac{\partial e}{\partial \boldsymbol{x}_4} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}_4} \cdot \frac{\partial e}{\partial \boldsymbol{y}} \tag{18}$$

$$= \boldsymbol{I}_n \cdot \frac{\partial e}{\partial \boldsymbol{y}} \qquad = \boldsymbol{I}_n \cdot \frac{\partial e}{\partial \boldsymbol{y}} \tag{19}$$

Next we have the ReLU block. This block has no weights to update, and we treat its Jacobian as an identity matrix

$$\frac{\partial e}{\partial \boldsymbol{x}_3} = \frac{\partial \boldsymbol{x}_4}{\partial \boldsymbol{x}_3} \cdot \frac{\partial e}{\partial \boldsymbol{x}_4} \tag{20}$$

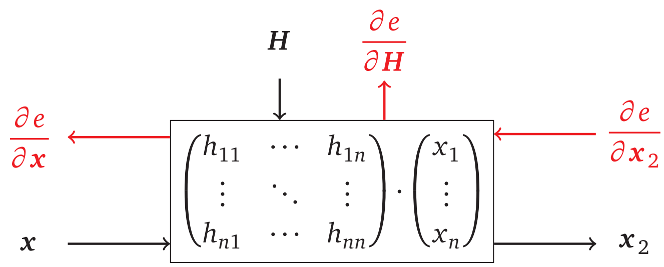
$$= \boldsymbol{I}_n\{0,1\} \cdot \left(\boldsymbol{I}_n \cdot \frac{\partial e}{\partial \boldsymbol{y}} \right) \tag{21}$$

We pass through another trivial bias block

$$\frac{\partial e}{\partial \boldsymbol{x}_2} = \frac{\partial \boldsymbol{x}_3}{\partial \boldsymbol{x}_2} \cdot \frac{\partial e}{\partial \boldsymbol{x}_3} \tag{22}$$

$$= \boldsymbol{I}_n \cdot \left(\boldsymbol{I}_n\{0,1\} \cdot \boldsymbol{I}_n \cdot \frac{\partial e}{\partial \boldsymbol{y}} \right) \tag{23}$$

Lastly we have a multiplication block



Mult($\boldsymbol{H}, \boldsymbol{x}$)

The Jacobian for a multiplication block is given in the notes as the transpose of the term that we are not differentiating with respect to. This can always be verified manually if needed.

$$\frac{\partial e}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{x}_2}{\partial \boldsymbol{x}} \cdot \frac{\partial e}{\partial \boldsymbol{x}_2} \tag{24}$$

$$= \boldsymbol{H}^T \cdot \left(\boldsymbol{I}_n \cdot \boldsymbol{I}_n\{0,1\} \cdot \boldsymbol{I}_n \cdot \frac{\partial e}{\partial \boldsymbol{y}} \right) \tag{25}$$

Finally, we must remember that as a residual layer the backwards pass graph has a two element merge into $\partial e / \partial \boldsymbol{x}$. One we finished computing through the dense layer, and the other comes from the residual block we computed first. This gives the final result

$$\frac{\partial e}{\partial \boldsymbol{x}} = \frac{\partial e}{\partial \boldsymbol{x}_2} \cdot \frac{\partial \boldsymbol{x}_2}{\partial \boldsymbol{x}} \tag{26}$$

$$= \left(\boldsymbol{H}^T \cdot \boldsymbol{I}_n \cdot \boldsymbol{I}_n\{0,1\} \cdot \boldsymbol{I}_n \cdot \frac{\partial e}{\partial \boldsymbol{y}} \right) + \boldsymbol{I}_n \tag{27}$$

Shown in the original figure, we have a flow of gradients that looks like

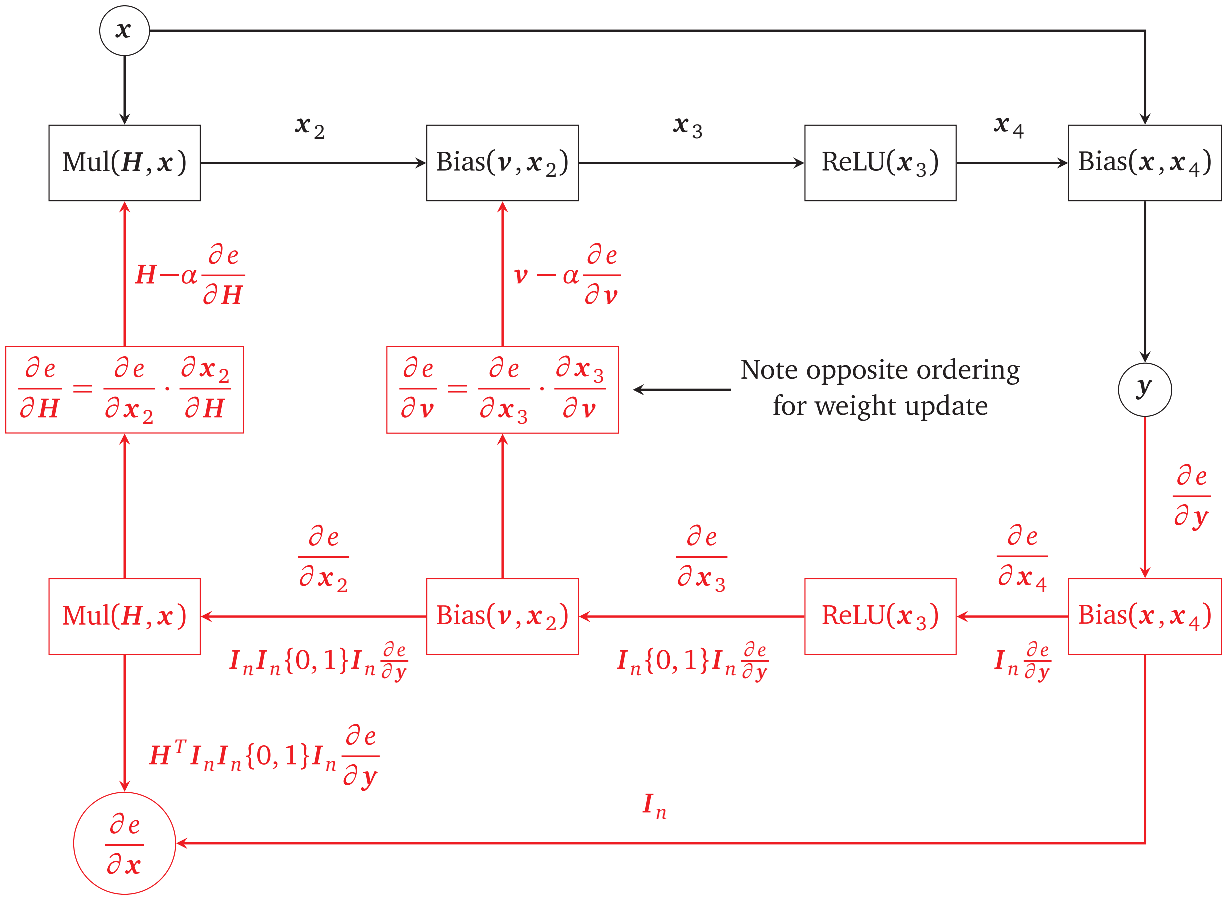


Figure 2. Chain rule applied over backwards pass

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Homework 3 (Calculus) Problem 6

Solution: At the end of the last problem we created a graph depicting the backward pass and how gradients flow across blocks. This graph also shows the generic form of the gradient descent updates. All we have to do is express these generic forms in terms of known variables

$$\boldsymbol{H} - \alpha \frac{\partial e}{\partial \boldsymbol{H}} = \boldsymbol{H} - \alpha \left(\frac{\partial e}{\partial \boldsymbol{x}_2} \cdot \frac{\partial \boldsymbol{x}_2}{\partial \boldsymbol{x}} \right) \tag{28}$$

$$= \boldsymbol{H} - \alpha \left(\left(\boldsymbol{I}_n \boldsymbol{I}_n \{0, 1\} \boldsymbol{I}_n \frac{\partial e}{\partial \boldsymbol{y}} \right) \cdot \left(\boldsymbol{x}^T \right) \right) \tag{29}$$

$$\boldsymbol{v} - \alpha \frac{\partial e}{\partial \boldsymbol{v}} = \boldsymbol{v} - \alpha \left(\frac{\partial e}{\partial \boldsymbol{x}_3} \cdot \frac{\partial \boldsymbol{x}_3}{\partial \boldsymbol{x}_2} \right) \tag{30}$$

$$= \boldsymbol{H} - \alpha \left(\left(\boldsymbol{I}_n \{0, 1\} \boldsymbol{I}_n \frac{\partial e}{\partial \boldsymbol{y}} \right) \cdot \left(\boldsymbol{I}_n \right) \right) \tag{31}$$

For the multiplication block we see that the weight update depends in part on $\boldsymbol{x}$. As such, we will need to store $\boldsymbol{x}$ from the forward pass in order to perform gradient descent during the backward pass.

Furthermore, the diagonal matrix produced as we differentiate ReLU will depend on what inputs were given to ReLU in the forward pass. Thus we must store input $\boldsymbol{x}_3$ where we map $x_i \in \boldsymbol{x}_3 < 0$ to 0 in $\boldsymbol{I}\{0, 1\}$.

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