Notes on analytic gradient derivation for iris neural network

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Having the iris dataset as input, we let Sx be a set of 4-dimensional input vectors,

$$Sx = \left\{ ..., \quad \begin{bmatrix} x_1 \\ \vdots \\ x_4 \end{bmatrix}, \quad ... \right\}.$$

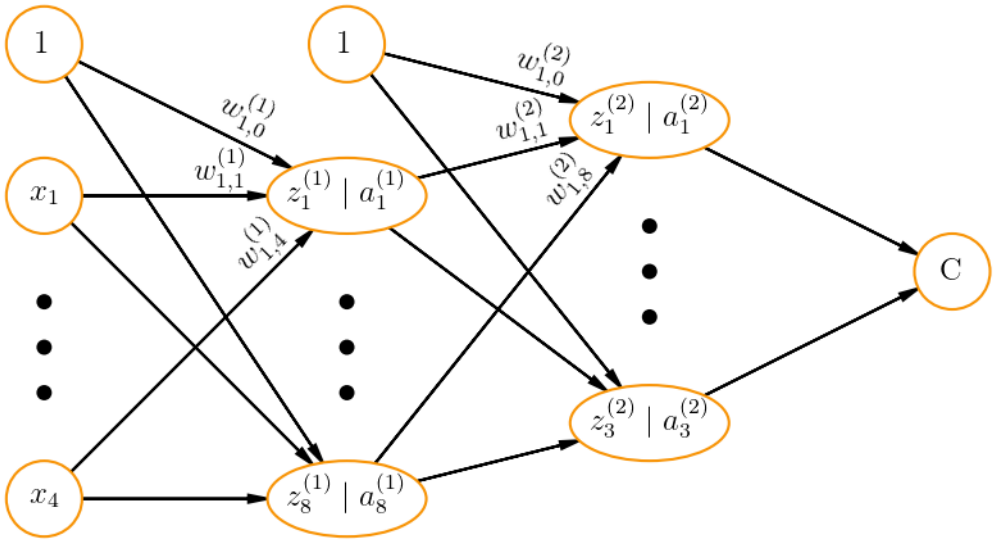
We denote $|Sx|$ to be the total number of such vectors in the set Sx.

We also have a set Sy of *one-hot* vectors transformed from the iris dataset's result variable with three classes,

$$Sy = \left\{ ..., \quad \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}, \quad ... \right\}.$$

Please note that although $|Sy|$ is never used in the derivation that follows, yet for the sake of clarity $|Sx| = |Sy|$.

And finally we define a neural network as depicted in the figure below



In addition we define neural network's functions as below. Note that these functions are pretty standard for neural networks and given here only as a reminder.

A sum of weighted inputs from the zero (input) layer that enters an arbitrary neuron

$$z_i^{(1)} = w_{i,0}^{(1)} + w_{i,1}^{(1)} x_1 + ... + w_{i,4}^{(1)} x_4, i \in [1, 8].$$

Using dot product, in matrix notation for the entire layer it transforms into

$$\begin{aligned} \mathbf{z^{(1)}} &= \begin{bmatrix} w_{1,0}^{(1)} & w_{1,1}^{(1)} & \cdots & w_{1,4}^{(1)} \\ \cdots & \cdots & \cdots & \cdots \\ w_{8,0}^{(1)} & w_{8,1}^{(1)} & \cdots & w_{8,4}^{(1)} \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_4 \end{bmatrix} \\ &= \mathbf{w^{(1)^T}} \cdot \mathbf{x}. \end{aligned}$$

A sigmoid function of an arbitrary neuron of the first layer

$$a_i^{(1)} = \frac{1}{1 + e^{-z_i^{(1)}}}, i \in [1, 8].$$

A sum of weighted inputs from the first (hidden) layer that enters an arbitrary neuron

$$z_i^{(2)} = w_{i,0}^{(2)} + w_{i,1}^{(2)} a_1^{(1)} + ... + w_{i,8}^{(2)} a_8^{(1)}, i \in [1, 3].$$

Using dot product, in matrix notation for the entire layer it transforms into

$$\begin{aligned} \mathbf{z^{(2)}} &= \begin{bmatrix} w_{1,0}^{(2)} & w_{1,1}^{(2)} & \cdots & w_{1,8}^{(2)} \\ \cdots & \cdots & \cdots & \cdots \\ w_{3,0}^{(2)} & w_{3,1}^{(2)} & \cdots & w_{3,8}^{(2)} \end{bmatrix} \begin{bmatrix} 1 \\ a_1^{(1)} \\ \vdots \\ a_8^{(1)} \end{bmatrix} \\ &= \mathbf{w^{(2)^T}} \cdot \mathbf{a^{(1)}}. \end{aligned}$$

A sigmoid function of an arbitrary neuron of the second layer

$$a_i^{(2)} = \frac{1}{1 + e^{-z_i^{(2)}}}, i \in [1, 3].$$

And a cross entropy loss function

$$C = -\frac{1}{|Sx|}\sum_{Sx}\sum_{j=1}^{3} y_j \ln a_j^{(2)} + (1-y_j)\ln(1-a_j^{(2)}). \tag{1}$$

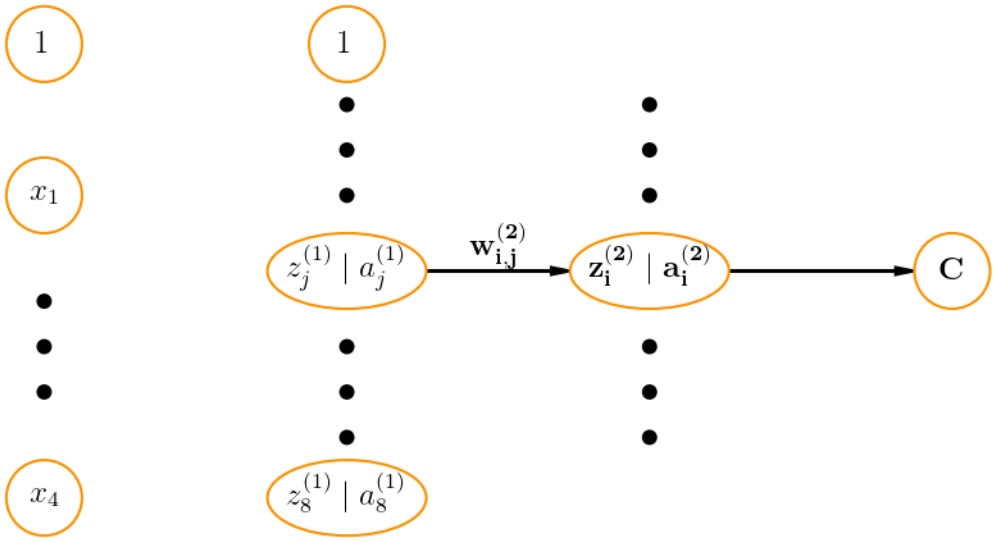
Finally, we are interested in obtainig a gradient of (1) w.r.t. the weights. In particular we will be deriving

$$\nabla_{w^{(2)}} C = \begin{bmatrix} \frac{\partial C}{\partial w^{(2)}_{1,0}} & \frac{\partial C}{\partial w^{(2)}_{1,1}} & \cdots & \frac{\partial C}{\partial w^{(2)}_{1,8}} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial C}{\partial w^{(2)}_{3,0}} & \frac{\partial C}{\partial w^{(2)}_{3,1}} & \cdots & \frac{\partial C}{\partial w^{(2)}_{3,8}} \end{bmatrix} \tag{2}$$

$$\nabla_{w^{(1)}} C = \begin{bmatrix} \frac{\partial C}{\partial w^{(1)}_{1,0}} & \frac{\partial C}{\partial w^{(1)}_{1,1}} & \cdots & \frac{\partial C}{\partial w^{(1)}_{1,4}} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial C}{\partial w^{(1)}_{8,0}} & \frac{\partial C}{\partial w^{(1)}_{8,1}} & \cdots & \frac{\partial C}{\partial w^{(1)}_{8,4}} \end{bmatrix}. \tag{3}$$

We will start from (2). Yet instead of calculating the gradient matrix in its entirety we are going to derive a partial derivative in general form first, namely $\frac{\partial C}{\partial w_{i,j}^{(2)}}$.

In order to spot all parts of (1) that depend on some arbitrary $w_{i,j}^{(2)}$ we will use a diagram that purposefully depicts only those dependencies



Thus applying the chain rule we arrive at the formula

$$\frac{\partial C}{\partial w_{i,j}^{(2)}} = \frac{\partial C}{\partial a_i^{(2)}} \frac{\partial a_i^{(2)}}{\partial z_i^{(2)}} \frac{\partial z_i^{(2)}}{\partial w_{i,j}^{(2)}}. \tag{4}$$

Now taking those partial derivatives independently we get

$$\begin{aligned}
\frac{\partial C}{\partial a_i^{(2)}} &= \frac{\partial}{\partial a_i^{(2)}}(-\frac{1}{|Sx|}\sum_{Sx}\sum_{j=1}^{3} y_j \ln a_j^{(2)} + (1-y_j)\ln(1-a_j^{(2)})) \\
&= -\frac{1}{|Sx|}\sum_{Sx} y_i \frac{1}{a_i^{(2)}} + (1-y_i)\frac{1}{1-a_i^{(2)}}(-1) \\
&= \frac{1}{|Sx|}\sum_{Sx} \frac{a_i^{(2)} - y_i}{a_i^{(2)}(1-a_i^{(2)})}. \qquad (5a) \\
\frac{\partial a_i^{(2)}}{\partial z_i^{(2)}} &= \frac{\partial}{\partial z_i^{(2)}} \frac{1}{1+e^{-z_i^{(2)}}} \\
&= \frac{\partial}{\partial z_i^{(2)}}(1+e^{-z_i^{(2)}})^{-1} \\
&= -(1+e^{-z_i^{(2)}})^{-2}(-1)e^{-z_i^{(2)}} \\
&= \frac{e^{-z_i^{(2)}}}{(1+e^{-z_i^{(2)}})^2} \\
&= \frac{1+e^{-z_i^{(2)}}-1}{(1+e^{-z_i^{(2)}})^2} \\
&= \frac{\cancel{1+e^{-z_i^{(2)}}}}{(1+e^{-z_i^{(2)}})\cancel{^2}} - \frac{1}{(1+e^{-z_i^{(2)}})^2} \\
&= \frac{1}{1+e^{-z_i^{(2)}}} - \frac{1}{(1+e^{-z_i^{(2)}})^2} \\
&= a_i^{(2)} - (a_i^{(2)})^2 \\
&= a_i^{(2)}(1-a_i^{(2)}). \qquad (5b) \\
\frac{\partial z_i^{(2)}}{\partial w_{i,j}^{(2)}} &= \frac{\partial}{\partial w_{i,j}^{(2)}}(w_{i,0}^{(2)} + w_{i,1}^{(2)}a_1^{(1)} + ... + w_{i,j}^{(2)}a_j^{(1)} + ... + w_{i,8}^{(2)}a_8^{(1)}) \\
&= \begin{cases} 1 & , j = 0 \\ a_j^{(1)} & , j \neq 0. \end{cases} \qquad (5c)
\end{aligned}$$

And finally combining (5a), (5b) and (5c) together we obtain

$$\begin{aligned}
\frac{\partial C}{\partial w_{i,j}^{(2)}} &= \frac{\partial C}{\partial a_i^{(2)}} \frac{\partial a_i^{(2)}}{\partial z_i^{(2)}} \frac{\partial z_i^{(2)}}{\partial w_{i,j}^{(2)}} \\
&= \frac{1}{|Sx|} \sum_{Sx} \frac{a_i^{(2)} - y_i}{\cancel{a_i^{(2)}(1 - a_i^{(2)})}} \cancel{a_i^{(2)}(1 - a_i^{(2)})} \frac{\partial z_i^{(2)}}{\partial w_{i,j}^{(2)}} \\
&= \frac{1}{|Sx|} \sum_{Sx} (a_i^{(2)} - y_i) \begin{cases} 1 & , j = 0 \\ a_j^{(1)} & , j \neq 0 \end{cases} \\
&= \begin{cases} \frac{1}{|Sx|} \sum_{Sx} (a_i^{(2)} - y_i) & , j = 0 \\ \frac{1}{|Sx|} \sum_{Sx} (a_i^{(2)} - y_i) a_j^{(1)} & , j \neq 0. \end{cases}
\end{aligned} \tag{6}$$

Using (6) our matrix gradient (2) now takes the form

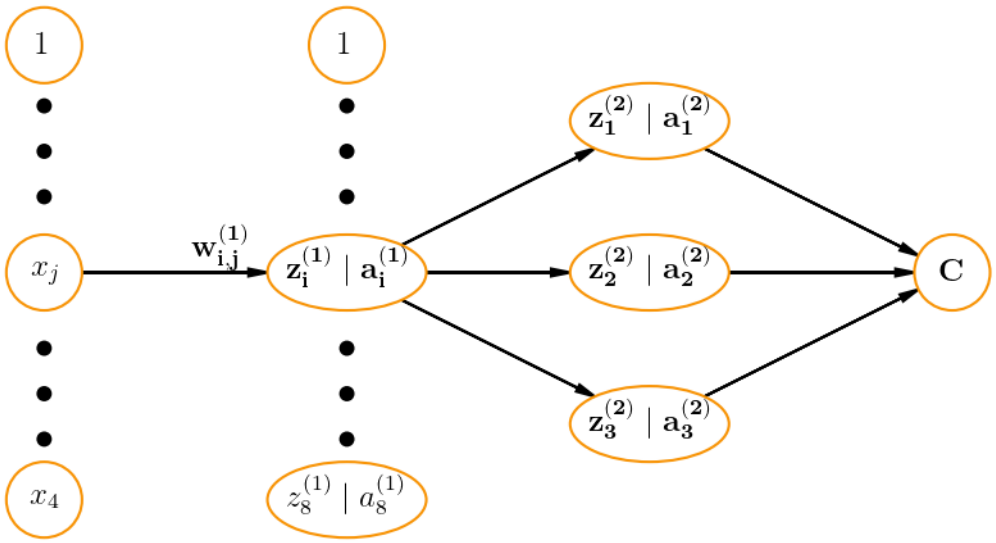
$$\begin{aligned}
\nabla_{w^{(2)}} C &= \begin{bmatrix} \frac{\partial C}{\partial w_{1,0}^{(2)}} & \frac{\partial C}{\partial w_{1,1}^{(2)}} & \cdots & \frac{\partial C}{\partial w_{1,8}^{(2)}} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial C}{\partial w_{3,0}^{(2)}} & \frac{\partial C}{\partial w_{3,1}^{(2)}} & \cdots & \frac{\partial C}{\partial w_{3,8}^{(2)}} \end{bmatrix} \\
&= \frac{1}{|Sx|} \begin{bmatrix} \sum_{Sx} (a_1^{(2)} - y_1) & \sum_{Sx} (a_1^{(2)} - y_1) a_1^{(1)} & ... & \sum_{Sx} (a_1^{(2)} - y_1) a_8^{(1)} \\ ... & ... & ... & ... \\ \sum_{Sx} (a_3^{(2)} - y_3) & \sum_{Sx} (a_3^{(2)} - y_3) a_1^{(1)} & ... & \sum_{Sx} (a_3^{(2)} - y_3) a_8^{(1)} \end{bmatrix}.
\end{aligned} \tag{7}$$

In addition, (7) can also take a nice vectorized form using dot product

$$\begin{aligned}
\nabla_{w^{(2)}} C &= \frac{1}{|Sx|} \begin{bmatrix} a_{1,1}^{(2)} - y_{1,1} & \cdots & a_{1,|Sx|}^{(2)} - y_{1,|Sx|} \\ \cdots & \cdots & \cdots \\ a_{3,1}^{(2)} - y_{3,1} & \cdots & a_{3,|Sx|}^{(2)} - y_{1,|Sx|} \end{bmatrix} \begin{bmatrix} 1 & a_{1,1}^{(1)} & \cdots & a_{1,8}^{(1)} \\ \vdots & \vdots & \cdots & \vdots \\ 1 & a_{|Sx|,1}^{(1)} & \cdots & a_{|Sx|,8}^{(1)} \end{bmatrix} \\
&= \frac{1}{|Sx|} (\mathbf{a^{(2)}} - \mathbf{y}) \cdot \mathbf{a^{(1)^T}}.
\end{aligned} \tag{8}$$

Please note that $\mathbf{a^{(1)^T}}$ includes a bias first column.

In order to obtain (3) we will use the same approach, i.e. we will derive a general formula of partial derivative, namely $\frac{\partial C}{\partial w_{i,j}^{(1)}}$.
Once again we are going to employ graphical approach to spot all parts of (1) that would get changed if some arbitrary $w_{i,j}^{(1)}$ was wiggled.



Thus according to the chain rule we have

$$\begin{aligned}\frac{\partial C}{\partial w_{i,j}^{(1)}} &= \frac{\partial C}{\partial a_1^{(2)}}\frac{\partial a_1^{(2)}}{\partial z_1^{(2)}}\frac{\partial z_1^{(2)}}{\partial a_i^{(1)}}\frac{\partial a_i^{(1)}}{\partial z_i^{(1)}}\frac{\partial z_i^{(1)}}{\partial w_{i,j}^{(1)}} + \frac{\partial C}{\partial a_2^{(2)}}\frac{\partial a_2^{(2)}}{\partial z_2^{(2)}}\frac{\partial z_2^{(2)}}{\partial a_i^{(1)}}\frac{\partial a_i^{(1)}}{\partial z_i^{(1)}}\frac{\partial z_i^{(1)}}{\partial w_{i,j}^{(1)}} \\ &+ \frac{\partial C}{\partial a_3^{(2)}}\frac{\partial a_3^{(2)}}{\partial z_3^{(2)}}\frac{\partial z_3^{(2)}}{\partial a_i^{(1)}}\frac{\partial a_i^{(1)}}{\partial z_i^{(1)}}\frac{\partial z_i^{(1)}}{\partial w_{i,j}^{(1)}} \\ &= \left(\sum_{k=1}^{3}\frac{\partial C}{\partial a_k^{(2)}}\frac{\partial a_k^{(2)}}{\partial z_k^{(2)}}\frac{\partial z_k^{(2)}}{\partial a_i^{(1)}}\right)\frac{\partial a_i^{(1)}}{\partial z_i^{(1)}}\frac{\partial z_i^{(1)}}{\partial w_{i,j}^{(1)}}.\end{aligned} \tag{9}$$

Let us recall that we have already carried out derivations for some of these partial derivatives. Specifically, $\frac{\partial C}{\partial a_k^{(2)}}$ is (5a) and $\frac{\partial a_k^{(2)}}{\partial z_k^{(2)}}$ is (5b). Hence only 3 partial derivatives left, and one of them, $\frac{\partial a_i^{(1)}}{\partial z_i^{(1)}}$, is in fact (5b) with a different upper index.

$$\frac{\partial z_k^{(2)}}{\partial a_i^{(1)}} = \frac{\partial}{\partial a_i^{(1)}}\left(w_{k,0}^{(2)} + w_{k,1}^{(2)}a_1^{(1)} + ... + w_{k,i}^{(2)}a_i^{(1)} + ... + w_{k,8}^{(2)}a_8^{(1)}\right)$$
$$= w_{k,i}^{(2)}. \tag{10a}$$
$$\frac{\partial z_i^{(1)}}{\partial w_{i,j}^{(1)}} = \frac{\partial}{\partial w_{i,j}^{(1)}}\left(w_{i,0}^{(1)} + w_{i,1}^{(1)}x_1 + ... + w_{i,j}^{(1)}x_j + ... + w_{i,4}^{(1)}x_4\right)$$
$$= \begin{cases} 1 & ,j = 0 \\ x_j & ,j \neq 0 \end{cases}. \tag{10b}$$
$$\frac{\partial a_i^{(1)}}{\partial z_i^{(1)}} = a_i^{(1)}(1 - a_i^{(1)}). \tag{10c}$$

Now combining (5a), (5b), (10a), (10b) and (10c) we have

$$\frac{\partial C}{\partial w_{i,j}^{(1)}} = \left(\sum_{k=1}^{3}\frac{\partial C}{\partial a_k^{(2)}}\frac{\partial a_k^{(2)}}{\partial z_k^{(2)}}\frac{\partial z_k^{(2)}}{\partial a_i^{(1)}}\right)\frac{\partial a_i^{(1)}}{\partial z_i^{(1)}}\frac{\partial z_i^{(1)}}{\partial w_{i,j}^{(1)}}$$
$$= \left(\sum_{k=1}^{3}\frac{1}{|Sx|}\sum_{Sx}\frac{a_k^{(2)} - y_k}{\cancel{a_k^{(2)}(1 - a_k^{(2)})}}\cancel{a_k^{(2)}(1 - a_k^{(2)})}w_{k,i}^{(2)}\right)a_i^{(1)}(1 - a_i^{(1)})\begin{cases} 1 & ,j = 0 \\ x_j & ,j \neq 0 \end{cases}$$
$$= \frac{1}{|Sx|}\sum_{Sx}\left(\sum_{k=1}^{3}(a_k^{(2)} - y_k)w_{k,i}^{(2)}\right)a_i^{(1)}(1 - a_i^{(1)})\begin{cases} 1 & ,j = 0 \\ x_j & ,j \neq 0 \end{cases}$$
$$= \begin{cases} \frac{1}{|Sx|}\sum_{Sx}\left(\sum_{k=1}^{3}(a_k^{(2)} - y_k)w_{k,i}^{(2)}\right)a_i^{(1)}(1 - a_i^{(1)}) & ,j = 0 \\ \frac{1}{|Sx|}\sum_{Sx}\left(\sum_{k=1}^{3}(a_k^{(2)} - y_k)w_{k,i}^{(2)}\right)a_i^{(1)}(1 - a_i^{(1)})x_j & ,j \neq 0 \end{cases}. \tag{11}$$

Before proceeding to the matrix gradient (3) we are going to introduce some additional notation for the sake of simplicity. We will denote

$$f_i^{(2)} = \left(\sum_{k=1}^{3}(a_k^{(2)} - y_k)w_{k,i}^{(2)}\right), i \in [1, 8] \tag{12a}$$
$$g_i^{(1)} = a_i^{(1)}(1 - a_i^{(1)}), i \in [1, 8]. \tag{12b}$$

Using (12a) and (12b) the matrix gradient (3) now takes the form

$$\begin{aligned}\nabla_{w^{(1)}} C &= \begin{bmatrix} \frac{\partial C}{\partial w^{(1)}_{1,0}} & \frac{\partial C}{\partial w^{(1)}_{1,1}} & \cdots & \frac{\partial C}{\partial w^{(1)}_{1,4}} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial C}{\partial w^{(1)}_{8,0}} & \frac{\partial C}{\partial w^{(1)}_{8,1}} & \cdots & \frac{\partial C}{\partial w^{(1)}_{8,4}} \end{bmatrix} \\ &= \frac{1}{|Sx|} \begin{bmatrix} \sum_{Sx} g^{(1)}_1 f^{(2)}_1 & \sum_{Sx} g^{(1)}_1 f^{(2)}_1 x_1 & \cdots & \sum_{Sx} g^{(1)}_1 f^{(2)}_1 x_4 \\ \cdots & \cdots & \cdots & \cdots \\ \sum_{Sx} g^{(1)}_8 f^{(2)}_8 & \sum_{Sx} g^{(1)}_8 f^{(2)}_8 x_1 & \cdots & \sum_{Sx} g^{(1)}_8 f^{(2)}_8 x_4. \end{bmatrix} \end{aligned} \tag{13}$$

In addition, (13) can also take a nice vectorized form using dot product

$$\begin{aligned}\nabla_{w^{(1)}} C &= \frac{1}{|Sx|} \begin{bmatrix} g^{(1)}_{1,1} f^{(2)}_{1,1} & \cdots & g^{(1)}_{1,|Sx|} f^{(2)}_{1,|Sx|} \\ \cdots & \cdots & \cdots \\ g^{(1)}_{8,1} f^{(2)}_{8,1} & \cdots & g^{(1)}_{8,|Sx|} f^{(2)}_{8,|Sx|} \end{bmatrix} \cdot \begin{bmatrix} 1 & x_{1,1} & \cdots & x_{1,4} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{|Sx|,1} & \cdots & x_{|Sx|,4} \end{bmatrix} \\ &= \frac{1}{|Sx|} \left(\mathbf{g^{(1)}} \odot \mathbf{f^{(2)}} \right) \cdot \mathbf{x^T}, \end{aligned} \tag{14}$$

where $\odot$ is Hadamard (element-wise) product.

Please note that $\mathbf{x^T}$ includes a bias first column. Heed that (12a) can aslo be vectorized if needed

$$\begin{aligned}\mathbf{f^{(2)}} &= \begin{bmatrix} a^{(2)}_{1,1} - y_{1,1} & \cdots & a^{(2)}_{1,3} - y_{1,3} \\ \cdots & \cdots & \cdots \\ a^{(2)}_{|Sx|,1} - y_{|Sx|,1} & \cdots & a^{(2)}_{|Sx|,3} - y_{|Sx|,3} \end{bmatrix} \begin{bmatrix} w^{(2)}_{1,1} & \cdots & w^{(2)}_{1,8} \\ \vdots & \vdots & \vdots \\ w^{(2)}_{3,1} & \cdots & w^{(2)}_{3,8} \end{bmatrix} \\ &= (\mathbf{a^{(2)}} - \mathbf{y})^{\mathrm{T}} \cdot \mathbf{w^{(2)}}. \end{aligned} \tag{15}$$