Long-short Term Memory (LSTM): back-propagation derivation

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Abstract

This document contains derivation of the gradients for a Long-short Term Memory Unit, using back-propagation (or reverse-mode differentiation). For the implementation of the neural-network see the accompanying notebooks.

1 Block Architecture

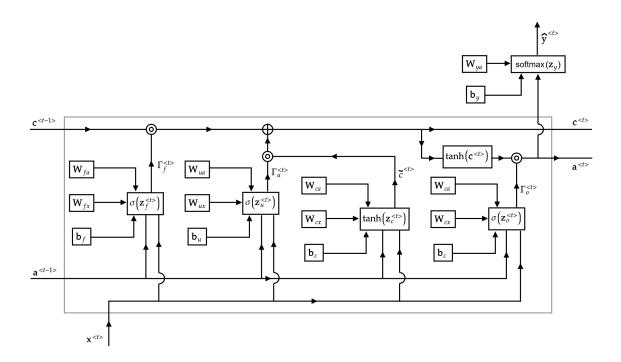


Figure 1: forward propagation diagram for a LSTM-block at time-step t. The concentric circles represent a hadamard-product (i.e. $\mathbf{x} \circ \mathbf{y}$) of the input vectors.

2 Forward Propagation

Given, $\mathbf{c}^{\langle t-1 \rangle}$ and $\mathbf{a}^{\langle t-1 \rangle}$ from the $(t-1)^{th}$ time-step, the equations for forward propagation through the t^{th} time-step, are as follows: (see figure-1)

$$\mathbf{z}_{f}^{\langle t \rangle} = \mathbf{W}_{fa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{fx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{f} \quad \text{eq.1}$$

$$\Gamma_{f}^{\langle t \rangle} = \sigma(\mathbf{z}_{f}^{\langle t \rangle}) \qquad \text{eq.2}$$

$$\mathbf{z}_{u}^{\langle t \rangle} = \mathbf{W}_{ua}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{ux}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{u} \quad \text{eq.3}$$

$$\Gamma_{u}^{\langle t \rangle} = \sigma(\mathbf{z}_{u}^{\langle t \rangle}) \qquad \text{eq.4}$$

$$\mathbf{z}_{o}^{\langle t \rangle} = \mathbf{W}_{oa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{ox}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{o} \quad \text{eq.5}$$

$$\Gamma_{o}^{\langle t \rangle} = \sigma(\mathbf{z}_{o}^{\langle t \rangle}) \qquad \text{eq.6}$$

$$\mathbf{z}_{c}^{\langle t \rangle} = \mathbf{W}_{ca}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{cx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{c} \quad \text{eq.7}$$

$$\tilde{\mathbf{c}}^{\langle t \rangle} = \mathbf{tanh}(\mathbf{z}_{c}^{\langle t \rangle}) \qquad \text{eq.8}$$

$$\mathbf{c}^{\langle t \rangle} = \Gamma_{u} \circ \tilde{\mathbf{c}}^{\langle t \rangle} + \Gamma_{f} \circ \mathbf{c}^{\langle t-1 \rangle} \qquad \text{eq.9}$$

$$\mathbf{a}^{\langle t \rangle} = \tanh(\mathbf{c}^{\langle t \rangle}) \circ \Gamma_{o} \qquad \text{eq.10}$$

$$\mathbf{z}_{y}^{\langle t \rangle} = \mathbf{W}_{ya}^{\mathsf{T}} \mathbf{a}^{\langle t \rangle} + \mathbf{b}_{y} \qquad \text{eq.11}$$

$$\hat{\mathbf{y}}^{\langle t \rangle} = \operatorname{softmax}(\mathbf{z}_{v}^{\langle t \rangle}) \qquad \text{eq.12}$$

where,

$$\mathbf{c}^{\langle t \rangle} \& \mathbf{c}^{\langle t-1 \rangle} \& \tilde{\mathbf{c}}^{\langle t \rangle} \text{ are } (n_a,1)\text{-dimensional vectors}$$

$$\mathbf{a}^{\langle t \rangle} \& \mathbf{a}^{\langle t-1 \rangle} \text{ are } (n_a,1)\text{-dimensional vectors}$$

$$\mathbf{W}_{*a}, * \in \{f, u, o, c\} \text{ are } (n_a, n_a)\text{-dimensional parameter matrices}$$

$$\mathbf{W}_{*x}, * \in \{f, u, o, c\} \text{ are } (n_x, n_a)\text{-dimensional parameter matrices}$$

$$\mathbf{b}_*, * \in \{f, u, o, c\} \text{ are } (n_a, 1)\text{-dimensional bias-vectors}$$

$$\Gamma_*^{\langle t \rangle}, * \in \{f, u, o\} \text{ are } (n_a, 1)\text{-dimensional vector, which represents a gate}$$

$$\mathbf{z}_*^{\langle t \rangle}, * \in \{f, u, o, c\} \text{ are } (n_a, 1)\text{-dimensional vector, is input to a gates' activation}$$

$$\mathbf{z}_y^{\langle t \rangle} \text{ is a } (n_y, 1)\text{-dimensional vector}$$

$$\mathbf{W}_{ya} \text{ is a } (n_a, n_y)\text{-dimensional parameter-matrix}$$

$$\mathbf{b}_y \text{ is a } (n_y, 1)\text{-dimensional bias vector}$$

Also, the sub-scripts denote the following: $_o$ - output-gate, $_u$ - update-gate, and $_f$ - forget-gate.

3 Backward Propagation

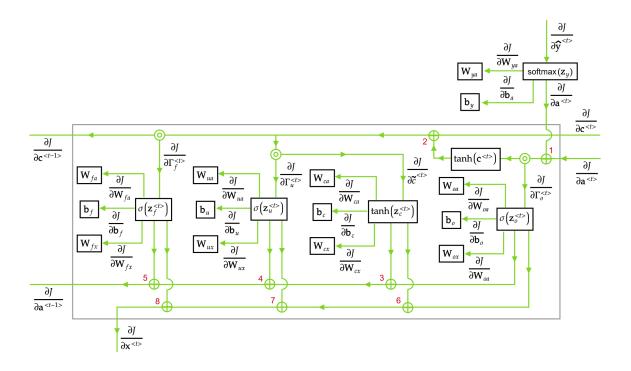


Figure 2: backward-propagation/gradient-flow diagram for a LSTM-block at time-step t. The concentric circles represent a hadamard-product (i.e. $\mathbf{x} \circ \mathbf{y}$) of the input vectors.

3.1 Computing $\frac{\partial J}{\partial \hat{\mathbf{y}}^{\langle t \rangle}}$

Since, $\hat{\mathbf{y}}^{\langle t \rangle}$ is computed using the softmax() activation-function, the loss J is computed using the cross-entropy loss. Also, let $\mathbf{y}^{\langle t \rangle}$ be the output-label corresponding to the t^{th} time-step. Then,

$$\frac{\partial J}{\partial \hat{\mathbf{y}}^{\langle t \rangle}} = \begin{bmatrix} \frac{\partial J}{\partial \hat{y}_{1}^{\langle t \rangle}} & \frac{\partial J}{\partial \hat{y}_{2}^{\langle t \rangle}} & \cdots & \frac{\partial J}{\partial \hat{y}_{ny}^{\langle t \rangle}} \end{bmatrix} \\
= \begin{bmatrix} y_{1}^{\langle t \rangle} & y_{2}^{\langle t \rangle} & y_{2}^{\langle t \rangle} & \cdots & y_{ny}^{\langle t \rangle} \\ \hat{y}_{1}^{\langle t \rangle} & \hat{y}_{2}^{\langle t \rangle} & \cdots & \hat{y}_{ny}^{\langle t \rangle} \end{bmatrix}$$

3.2 Computing $\frac{\partial J}{\partial \mathbf{W}_{ya}}$ and $\frac{\partial J}{\partial \mathbf{b}_y}$

From eq.12 (see section-2), we have

$$\begin{split} \frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}} &= \frac{\partial J}{\partial \hat{\mathbf{y}}^{\langle t \rangle}} \frac{\partial \hat{\mathbf{y}}^{\langle t \rangle}}{\partial \mathbf{z}_{y}^{\langle t \rangle}} \\ &= \frac{\partial J}{\partial \hat{\mathbf{y}}^{\langle t \rangle}} \left(\operatorname{diag}(\hat{\mathbf{y}}^{\langle t \rangle}) - \hat{\mathbf{y}}^{\langle t \rangle}(\hat{\mathbf{y}}^{\langle t \rangle})^{\intercal} \right) \end{split}$$

From eq.11 (see section-2), we have

$$\operatorname{tr}(J) = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle r \rangle}} d\mathbf{z}_{y}^{\langle t \rangle}\right)$$

where, $d\mathbf{z}_{y}^{\langle t \rangle}$ can be expanded as follows:

$$d\mathbf{z}_{y}^{\langle t \rangle} = d\left(\mathbf{W}_{ya}^{\mathsf{T}} \mathbf{a}^{\langle t \rangle} + \mathbf{b}_{y}\right)$$

$$= d\left(\mathbf{W}_{ya}^{\mathsf{T}}\right) \mathbf{a}^{\langle t \rangle} + \mathbf{W}_{ya}^{\mathsf{T}} d\left(\mathbf{a}^{\langle t \rangle}\right) + d\mathbf{b}_{y} \qquad \text{eq.13-1}$$

when differentiating w.r.t. \mathbf{W}_{ya} , we have $d\mathbf{a}^{\langle t \rangle} = 0$, and $d\mathbf{b}_y = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}} d\mathbf{W}_{ya}^{\mathsf{T}} \mathbf{a}^{\langle t \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{a}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ya} \left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ya}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{ya}} = \left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{b}_y , we have $d\mathbf{a}^{\langle t \rangle} = 0$, and $d\mathbf{W}_{ya} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}} d\mathbf{b}_{y}^{\mathsf{T}}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{b}_{y}} = \frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}}$$

3.3 Computing $\frac{\partial J}{\partial \mathbf{a}^{(t)}}$

This derivative has two components

Comp-1 one flows-in from the $(t+1)^{th}$ time-step, and

Comp-2 one flows-in as the derivative from $\hat{\mathbf{y}}^{\langle t \rangle}$. This derivative is computed from eq.13-1 as follows,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}} d\mathbf{z}_{y}^{\langle t \rangle}\right)$$

$$= \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}} \mathbf{W}_{ya}^{\intercal} d\mathbf{a}^{\langle t \rangle}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}} \mathbf{W}_{ya}^{\intercal}$$

Then, these two components are added to compute the true derivative (see the \oplus labeled as 1 in the figure-2), i.e.

$$\left. \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} = \left. \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} \right|_{\mathbf{Comp-1}} + \left. \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} \right|_{\mathbf{Comp-2}}$$

3.4 Computing $\frac{\partial J}{\partial \mathbf{c}^{(t)}}$, and $\frac{\partial J}{\partial \Gamma_o^{(t)}}$

From eq.10 (see section-2), we have

$$\frac{\partial J}{\partial \Gamma_o^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} \frac{\partial \mathbf{a}^{\langle t \rangle}}{\partial \Gamma_o^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} \operatorname{diag} \left(\tanh(\mathbf{c}^{\langle t \rangle}) \right)
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \circ \left(\tanh(\mathbf{c}^{\langle t \rangle}) \right)^{\mathsf{T}}$$

Note: For more information about computing the derivative of a Hadamard-product, see section-5.

The derivative $\frac{\partial J}{\partial \mathbf{c}^{(t)}}$ is made of two components, described as follows

Comp-1 one flows-in from the $(t+1)^{th}$ time-step, and

Comp-2 one flows-in as the derivative from the $\mathbf{a}^{\langle t \rangle}$. This derivative is computed as follows,

$$\frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} \frac{\partial \mathbf{a}^{\langle t \rangle}}{\partial \mathbf{c}^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} \frac{\partial \mathbf{a}^{\langle t \rangle}}{\partial \tanh(\mathbf{c}^{\langle t \rangle})} \frac{\partial \tanh(\mathbf{c}^{\langle t \rangle})}{\partial \mathbf{c}^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} (\mathbf{I}_{n_a \times n_a} \circ \Gamma_o^{\langle t \rangle}) (\mathbf{I}_{n_a \times n_a} - \mathbf{I}_{n_a \times n_a} \circ \tanh^2(\mathbf{c}^{\langle t \rangle}))
= \frac{\partial J}{\partial \mathbf{a}^{\langle t \rangle}} \circ \left[\Gamma_o^{\langle t \rangle} \circ (\mathbf{1}_{(n_a, 1)} - \tanh^2(\mathbf{c}^{\langle t \rangle})) \right]^{\mathsf{T}}$$

These two components are then added to compute the true derivative (see \oplus labeled as 2 in figure-2), i.e.

$$\frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} = \left. \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \right|_{\mathbf{Comp-1}} + \left. \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \right|_{\mathbf{Comp-2}}$$

3.5 Computing $\frac{\partial J}{\partial \mathbf{W}_{oa}}$, $\frac{\partial J}{\partial \mathbf{W}_{ox}}$, and $\frac{\partial J}{\partial \mathbf{b}_{o}}$

From eq.6 (see section-2), we have

$$\frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}} = \frac{\partial J}{\partial \Gamma_o^{\langle t \rangle}} \frac{\partial \Gamma_o^{\langle t \rangle}}{\partial \mathbf{z}_o^{\langle t \rangle}}
= \frac{\partial J}{\partial \Gamma_o^{\langle t \rangle}} \circ \left(\Gamma_o^{\langle t \rangle} \circ (\mathbf{1}_{(n_a,1)} - \Gamma_o^{\langle t \rangle}) \right)^{\mathsf{T}}$$

From eq.5 (see section-2), using the trace-method, we have

$$\operatorname{tr}(J) = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}} \, \mathrm{d}\mathbf{z}_o^{\langle t \rangle}\right)$$

where, $d\mathbf{z}_{o}^{\langle t \rangle}$ can be expanded as follows:

$$d\mathbf{z}_{o}^{\langle t \rangle} = d\left(\mathbf{W}_{oa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{ox}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{o}\right)$$

$$= d\mathbf{W}_{oa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{oa}^{\mathsf{T}} d\mathbf{a}^{\langle t-1 \rangle} + d\mathbf{W}_{ox}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{W}_{ox}^{\mathsf{T}} d\mathbf{x}^{\langle t \rangle} + d\mathbf{b}_{o} \qquad \text{eq. 13-2}$$

when differentiating w.r.t. \mathbf{W}_{oa} , we have $d\mathbf{W}_{ox} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_o = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}} d\mathbf{W}_{oa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{oa} \left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{oa}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{oa}} = \left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{W}_{ox} , we have $d\mathbf{W}_{oa} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_o = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}} d\mathbf{W}_{ox}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ox} \left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ox}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{ox}} = \left(\frac{\partial J}{\partial \mathbf{z}_{o}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{b}_o , we have $d\mathbf{W}_{oa} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{W}_{ox} = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}} d\mathbf{b}_o\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{b}_o} = \frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}}$$

3.6 Computing $\frac{\partial J}{\partial \Gamma_u^{\langle t \rangle}}$, $\frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}}$, $\frac{\partial J}{\partial \Gamma_f^{\langle t \rangle}}$, and $\frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}}$

From eq.9 (see section-2), we have

$$\frac{\partial J}{\partial \Gamma_u^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \frac{\partial \mathbf{c}^{\langle t \rangle}}{\partial \Gamma_u^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \operatorname{diag} \left(\tilde{\mathbf{c}}^{\langle t \rangle} \right)^{\mathsf{T}}
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \circ \left(\tilde{\mathbf{c}}^{\langle t \rangle} \right)^{\mathsf{T}}$$

$$\frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \frac{\partial \mathbf{c}^{\langle t \rangle}}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \operatorname{diag} \left(\Gamma_u^{\langle t \rangle} \right)
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \circ \left(\Gamma_u^{\langle t \rangle} \right)^{\mathsf{T}}
\frac{\partial J}{\partial \Gamma_f^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \frac{\partial \mathbf{c}^{\langle t \rangle}}{\partial \Gamma_f^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \operatorname{diag} \left(\mathbf{c}^{\langle t-1 \rangle} \right)^{\mathsf{T}}
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \circ \left(\mathbf{c}^{\langle t-1 \rangle} \right)^{\mathsf{T}}
\frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \frac{\partial \mathbf{c}^{\langle t \rangle}}{\partial \mathbf{c}^{\langle t-1 \rangle}}
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \operatorname{diag} \left(\Gamma_f^{\langle t \rangle} \right)^{\mathsf{T}}
= \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} \circ \left(\Gamma_f^{\langle t \rangle} \right)^{\mathsf{T}}$$

3.7 Computing $\frac{\partial J}{\partial \mathbf{W}_{ua}}$, $\frac{\partial J}{\partial \mathbf{W}_{ux}}$, and $\frac{\partial J}{\partial \mathbf{b}_u}$

From eq.4 (see section-2), we have

$$\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} = \frac{\partial J}{\partial \Gamma_{u}^{\langle t \rangle}} \frac{\partial \Gamma_{u}^{\langle t \rangle}}{\partial \mathbf{z}_{u}^{\langle t \rangle}}
= \frac{\partial J}{\partial \Gamma_{u}^{\langle t \rangle}} \circ \left(\Gamma_{u}^{\langle t \rangle} \circ (\mathbf{1}_{(n_{a},1)} - \Gamma_{u}^{\langle t \rangle}) \right)^{\mathsf{T}}$$

From eq.3 (see section-2), using the trace-method, we have

$$\operatorname{tr}(J) = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} \, \mathrm{d}\mathbf{z}_{u}^{\langle t \rangle}\right)$$

where, $\mathrm{d}\mathbf{z}_u^{\langle t\rangle}$ can be expanded as follows:

$$d\mathbf{z}_{u}^{\langle t \rangle} = d\left(\mathbf{W}_{ua}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{ux}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{u}\right)$$

$$= d\mathbf{W}_{ua}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{ua}^{\mathsf{T}} d\mathbf{a}^{\langle t-1 \rangle} + d\mathbf{W}_{ux}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{W}_{ux}^{\mathsf{T}} d\mathbf{x}^{\langle t \rangle} + d\mathbf{b}_{u} \qquad \text{eq.13-3}$$

when differentiating w.r.t. \mathbf{W}_{ua} , we have $d\mathbf{W}_{ux} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_u = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} d\mathbf{W}_{ua}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ua} \left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ua}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{ua}} = \left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{W}_{ux} , we have $d\mathbf{W}_{ua} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_u = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} d\mathbf{W}_{ux}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ux} \left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ux}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{ux}} = \left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{b}_u , we have $d\mathbf{W}_{ua} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{W}_{ux} = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} d\mathbf{b}_{u}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{b}_{u}} = \frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}}$$

3.8 Computing $\frac{\partial J}{\partial \mathbf{W}_{fa}}$, $\frac{\partial J}{\partial \mathbf{W}_{fx}}$, and $\frac{\partial J}{\partial \mathbf{b}_f}$

From eq.2 (see section-2), we have

$$\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}} = \frac{\partial J}{\partial \Gamma_{f}^{\langle t \rangle}} \frac{\partial \Gamma_{f}^{\langle t \rangle}}{\partial \mathbf{z}_{f}^{\langle t \rangle}}
= \frac{\partial J}{\partial \Gamma_{f}^{\langle t \rangle}} \circ \left(\Gamma_{f}^{\langle t \rangle} \circ (\mathbf{1}_{(n_{a},1)} - \Gamma_{f}^{\langle t \rangle}) \right)^{\mathsf{T}}$$

From eq.1 (see section-2), using the trace-method, we have

$$\operatorname{tr}(J) = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_f^{\langle t \rangle}} d\mathbf{z}_f^{\langle t \rangle}\right)$$

where, $\mathrm{d}\mathbf{z}_f^{\langle t\rangle}$ can be expanded as follows:

$$d\mathbf{z}_{f}^{\langle t \rangle} = d\left(\mathbf{W}_{fa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{fx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{f}\right)$$

$$= d\mathbf{W}_{fa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{fa}^{\mathsf{T}} d\mathbf{a}^{\langle t-1 \rangle} + d\mathbf{W}_{fx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{W}_{fx}^{\mathsf{T}} d\mathbf{x}^{\langle t \rangle} + d\mathbf{b}_{f} \qquad \text{eq. 13-4}$$

when differentiating w.r.t. \mathbf{W}_{fa} , we have $d\mathbf{W}_{fx} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_f = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}} d\mathbf{W}_{fa}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{fa} \left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{fa}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{fa}} = \left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{W}_{fx} , we have $d\mathbf{W}_{fa} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_f = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}} d\mathbf{W}_{fx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{fx} \left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{fx}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{fx}} = \left(\frac{\partial J}{\partial \mathbf{z}_{f}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{x}^{\langle t \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{b}_f , we have $d\mathbf{W}_{fa} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{W}_{fx} = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_f^{\langle t \rangle}} d\mathbf{b}_f\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{b}_f} = \frac{\partial J}{\partial \mathbf{z}_f^{\langle t \rangle}}$$

3.9 Computing $\frac{\partial J}{\partial \mathbf{W}_{ca}}$, $\frac{\partial J}{\partial \mathbf{W}_{cx}}$, and $\frac{\partial J}{\partial \mathbf{b}_c}$

From eq.8 (see section-2), we have

$$\begin{split} \frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} &= \frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}} \frac{\partial \tilde{\mathbf{c}}^{\langle t \rangle}}{\partial \mathbf{z}_{c}^{\langle t \rangle}} \\ &= \frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}} \circ \left[\mathbf{1}_{(n_{a},1)} - \tanh^{2}(\mathbf{z}_{c}^{\langle t \rangle}) \right]^{\mathsf{T}} \end{split}$$

From eq.7 (see section-2), using the trace-method, we have

$$\operatorname{tr}(J) = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} \, \mathrm{d}\mathbf{z}_{c}^{\langle t \rangle}\right)$$

where, $\mathrm{d}\mathbf{z}_{c}^{\langle t\rangle}$ can be expanded as follows:

$$d\mathbf{z}_{c}^{\langle t \rangle} = d\left(\mathbf{W}_{ca}^{\dagger} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{cx}^{\dagger} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{c}\right)$$

$$= d\mathbf{W}_{ca}^{\dagger} \mathbf{a}^{\langle t-1 \rangle} + \mathbf{W}_{ca}^{\dagger} d\mathbf{a}^{\langle t-1 \rangle} + d\mathbf{W}_{cx}^{\dagger} \mathbf{x}^{\langle t \rangle} + \mathbf{W}_{cx}^{\dagger} d\mathbf{x}^{\langle t \rangle} + d\mathbf{b}_{c} \qquad \text{eq.13-5}$$

when differentiating w.r.t. \mathbf{W}_{ca} , we have $d\mathbf{W}_{cx} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_c = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} d\mathbf{W}_{ca}^{\mathsf{T}} \mathbf{a}^{\langle t-1 \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ca} \left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}} d\mathbf{W}_{ca}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{ca}} = \left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\mathsf{T}} \left(\mathbf{a}^{\langle t-1 \rangle}\right)^{\mathsf{T}}$$

when differentiating w.r.t. \mathbf{W}_{cx} , we have $d\mathbf{W}_{ca} = 0$, $d\mathbf{a}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_c = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} d\mathbf{W}_{cx}^{\intercal} \mathbf{x}^{\langle t \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{x}^{\langle t \rangle}\right)^{\intercal} d\mathbf{W}_{cx} \left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\intercal}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\intercal} \left(\mathbf{x}^{\langle t \rangle}\right)^{\intercal} d\mathbf{W}_{cx}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{cx}} = \left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\intercal} \left(\mathbf{x}^{\langle t \rangle}\right)^{\intercal}$$

when differentiating w.r.t. \mathbf{b}_c , we have $d\mathbf{W}_{ca} = 0$, $d\mathbf{a}^{\langle t-1\rangle} = 0$, $d\mathbf{W}_{cx} = 0$, and $d\mathbf{x}^{\langle t\rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} d\mathbf{b}_{c}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{b}_{c}} = \frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}$$

3.10 Computing $\frac{\partial J}{\partial \mathbf{x}^{(t)}}$, and $\frac{\partial J}{\partial \mathbf{a}^{(t-1)}}$

Each of these derivatives has four components, described as follows

Comp-1 flows-in as derivative from $\Gamma_o^{\langle t \rangle}$

$$\frac{\partial J}{\partial \mathbf{a}^{\langle t-1 \rangle}} = \frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}} \frac{\partial \mathbf{z}_o^{\langle t \rangle}}{\partial \mathbf{a}^{\langle t-1 \rangle}}
= \frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}} \mathbf{W}_{oa}^{\mathsf{T}}
\frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}} \frac{\partial \mathbf{z}_o^{\langle t \rangle}}{\partial \mathbf{x}^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{z}_o^{\langle t \rangle}} \mathbf{W}_{ox}^{\mathsf{T}}$$

Comp-2 flows in as derivative from $\tilde{\mathbf{c}}^{\langle t \rangle}$

$$\frac{\partial J}{\partial \mathbf{a}^{\langle t-1 \rangle}} = \frac{\partial J}{\partial \mathbf{z}_c^{\langle t \rangle}} \frac{\partial \mathbf{z}_c^{\langle t \rangle}}{\partial \mathbf{a}^{\langle t-1 \rangle}}
= \frac{\partial J}{\partial \mathbf{z}_c^{\langle t \rangle}} \mathbf{W}_{ca}^{\mathsf{T}}
\frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{z}_c^{\langle t \rangle}} \frac{\partial \mathbf{z}_c^{\langle t \rangle}}{\partial \mathbf{x}^{\langle t \rangle}}
= \frac{\partial J}{\partial \mathbf{z}_c^{\langle t \rangle}} \mathbf{W}_{cx}^{\mathsf{T}}$$

Comp-3 flows-in as derivative from $\Gamma_u^{\langle t \rangle}$

$$\begin{split} \frac{\partial J}{\partial \mathbf{a}^{\langle t-1 \rangle}} &= \frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} \frac{\partial \mathbf{z}_{u}^{\langle t \rangle}}{\partial \mathbf{a}^{\langle t-1 \rangle}} \\ &= \frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} \mathbf{W}_{ua}^{\mathsf{T}} \\ \frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} &= \frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} \frac{\partial \mathbf{z}_{u}^{\langle t \rangle}}{\partial \mathbf{x}^{\langle t \rangle}} \\ &= \frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} \mathbf{W}_{ux}^{\mathsf{T}} \end{split}$$

Comp-4 flows-in as derivative from $\Gamma_f^{\langle t \rangle}$

$$\frac{\partial J}{\partial \mathbf{a}^{\langle t-1 \rangle}} = \frac{\partial J}{\partial \mathbf{z}_f^{\langle t \rangle}} \frac{\partial \mathbf{z}_f^{\langle t \rangle}}{\partial \mathbf{a}^{\langle t-1 \rangle}}$$

$$= \frac{\partial J}{\partial \mathbf{z}_f^{\langle t \rangle}} \mathbf{W}_{fa}^{\mathsf{T}}$$

$$\frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{z}_f^{\langle t \rangle}} \frac{\partial \mathbf{z}_f^{\langle t \rangle}}{\partial \mathbf{x}^{\langle t \rangle}}$$

$$= \frac{\partial J}{\partial \mathbf{z}_f^{\langle t \rangle}} \mathbf{W}_{fx}^{\mathsf{T}}$$

These four components are then added to compute the true derivative, i.e.

$$\begin{split} \frac{\partial J}{\partial \mathbf{a}^{\langle t-1\rangle}} &= \frac{\partial J}{\partial \mathbf{a}^{\langle t-1\rangle}} \bigg|_{\mathbf{Comp-1}} + \frac{\partial J}{\partial \mathbf{a}^{\langle t-1\rangle}} \bigg|_{\mathbf{Comp-2}} + \frac{\partial J}{\partial \mathbf{a}^{\langle t-1\rangle}} \bigg|_{\mathbf{Comp-3}} + \frac{\partial J}{\partial \mathbf{a}^{\langle t-1\rangle}} \bigg|_{\mathbf{Comp-4}} \\ & \text{(see } \oplus \text{ labeled as } 3, \ 4, \text{ and } 5 \text{ in figure-2}) \\ \frac{\partial J}{\partial \mathbf{x}^{\langle t\rangle}} &= \frac{\partial J}{\partial \mathbf{x}^{\langle t\rangle}} \bigg|_{\mathbf{Comp-1}} + \frac{\partial J}{\partial \mathbf{x}^{\langle t\rangle}} \bigg|_{\mathbf{Comp-2}} + \frac{\partial J}{\partial \mathbf{x}^{\langle t\rangle}} \bigg|_{\mathbf{Comp-3}} + \frac{\partial J}{\partial \mathbf{x}^{\langle t\rangle}} \bigg|_{\mathbf{Comp-4}} \\ & \text{(see } \oplus \text{ labeled as } 6, \ 7, \text{ and } 8 \text{ in figure-2}) \end{split}$$

4 Gradient or Jacobian?

In the above derivations, we have used the numerator layout while performing matrix-derivatives. One of the consequences of this decision is that the derivatives that we have computed are in-fact jacobians and not gradients. Fortunately, gradients are just transpose of jacobians.

5 Appendix-A:

In this section we will derive an expression for the derivative of a Hadamard product of two vectors. Let \mathbf{x} and \mathbf{y} be two vectors, and let $\mathbf{w} = \mathbf{x} \circ \mathbf{y}$ such that

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}; \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}; \qquad \mathbf{w} = \mathbf{x} \circ \mathbf{y} = \begin{bmatrix} x_1 y_1 \\ x_2 y_2 \\ \vdots \\ x_n y_n \end{bmatrix}$$

then, we have

$$\frac{\partial \mathbf{w}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \dots & \frac{\partial}{\partial x_n} \end{bmatrix} \otimes \begin{bmatrix} x_1 y_1 \\ x_2 y_2 \\ \vdots \\ x_n y_n \end{bmatrix} \\
= \begin{bmatrix} \frac{\partial(x_1 y_1)}{\partial x_1} & \frac{\partial(x_1 y_1)}{\partial x_2} & \dots & \frac{\partial(x_1 y_1)}{\partial x_n} \\ \frac{\partial(x_2 y_2)}{\partial x_1} & \frac{\partial(x_2 y_2)}{\partial x_2} & \dots & \frac{\partial(x_2 y_2)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial(x_n y_n)}{\partial x_1} & \frac{\partial(x_n y_n)}{\partial x_2} & \dots & \frac{\partial(x_n y_n)}{\partial x_n} \end{bmatrix} \\
= \begin{bmatrix} y_1 & 0 & \dots & 0 \\ 0 & y_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & y_n \end{bmatrix} \\
= \operatorname{diag}(\mathbf{y})$$
(1)