Gated Recurrent Unit (GRU): back-propagation derivation

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Abstract

This document contains derivation of the gradients for a Gated Recurrent Unit (a type of RNN-block) using back-propagation (or reverse-mode differentiation). For the implementation of the neural-network see the accompanying notebooks.

1 Block Architecture

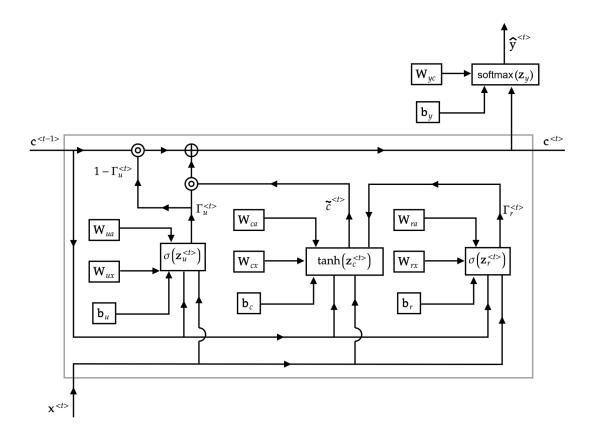


Figure 1: forward propagation diagram for a GRU-block at time-step t. The concentric circles represent a hadamard-product (i.e. $\mathbf{x} \circ \mathbf{y}$) of the input vectors.

2 Forward Propagation

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

$$\mathbf{z}_{u}^{\langle t \rangle} = \mathbf{W}_{uc}^{\dagger} \, \mathbf{c}^{\langle t-1 \rangle} + \mathbf{W}_{ux}^{\dagger} \, \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{u} \qquad \text{eq.} 1$$

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

$$\mathbf{z}_{r}^{\langle t \rangle} = \mathbf{W}_{rc}^{\dagger} \, \mathbf{c}^{\langle t-1 \rangle} + \mathbf{W}_{rx}^{\dagger} \, \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{r} \qquad \text{eq.} 3$$

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

$$\mathbf{z}_{c}^{\langle t \rangle} = \mathbf{W}_{cc}^{\dagger} \, \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle} \right) + \mathbf{W}_{cx}^{\dagger} \, \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{c} \qquad \text{eq.} 5$$

$$\tilde{\mathbf{c}}^{\langle t \rangle} = \tanh(\mathbf{z}_{c}^{\langle t \rangle}) \qquad \text{eq.} 6$$

$$\mathbf{c}^{\langle t \rangle} = \Gamma_{u}^{\langle t \rangle} \circ \tilde{\mathbf{c}}^{\langle t \rangle} + (1 - \Gamma_{u}^{\langle t \rangle}) \circ \mathbf{c}^{\langle t-1 \rangle} \qquad \text{eq.} 7$$

$$\mathbf{z}_{y}^{\langle t \rangle} = \mathbf{W}_{ya}^{\dagger} \, \mathbf{c}^{\langle t \rangle} + \mathbf{b}_{y} \qquad \text{eq.} 8$$

$$\hat{\mathbf{y}}^{\langle t \rangle} = \operatorname{softmax} \, \left(\mathbf{z}_{u}^{\langle t \rangle}\right) \qquad \text{eq.} 9$$

where,

$$\mathbf{x}^{\langle t \rangle} \text{ is a } (n_x,1)\text{-dimensional vector}$$

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

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

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

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

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

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

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

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

Also, the sub-scripts denote the following: $_r$ - relevance-gate, and $_u$ - update-gate.

3 Backward Propagation

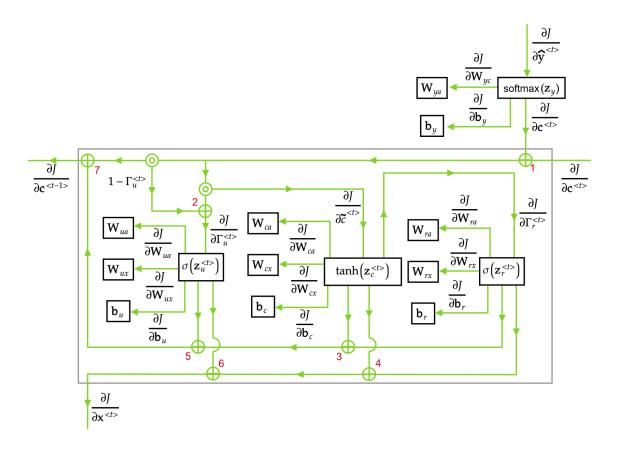


Figure 2: backward-propagation/gradient-flow diagram for a LSTM-block at time-step t. The concentric circles represent a hadamard-product (i.e. $\mathbf{x} \circ \mathbf{y}$) of the input vectors.

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

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,

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

3.2 Computing $\frac{\partial J}{\partial \mathbf{W}_{uc}}$ and $\frac{\partial J}{\partial \mathbf{b}_{y}}$

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

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

Note: for more on the derivation of the derivative of a **softmax()** function, see ..\notes\softmax-function.ipynb

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

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

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

$$\begin{aligned} \mathrm{d}\mathbf{z}_{y}^{\langle t \rangle} &= \mathrm{d}\left(\mathbf{W}_{yc}^{\intercal} \mathbf{c}^{\langle t \rangle} + \mathbf{b}_{y}\right) \\ &= \mathrm{d}\left(\mathbf{W}_{yc}^{\intercal}\right) \mathbf{c}^{\langle t \rangle} + \mathbf{W}_{yc}^{\intercal} \mathrm{d}\mathbf{c}^{\langle t \rangle} + \mathrm{d}\mathbf{b}_{y} \end{aligned} \quad \text{eq.9-1}$$

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

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

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

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

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

when differentiating w.r.t. \mathbf{b}_y , we have $d\mathbf{c}^{\langle t \rangle} = 0$, and $d\mathbf{W}_{yc} = 0$. 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 $\frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}}$

This derivative has two components

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

Comp-2 flows-in as the derivative from $\hat{\mathbf{y}}^{\langle t \rangle}$. This derivative is computed using eq.9-1 as follows,

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

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

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{c}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{z}_{y}^{\langle t \rangle}} \mathbf{W}_{yc}^{\mathsf{T}}$$

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

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

3.4 Computing $\frac{\partial J}{\partial \tilde{\mathbf{c}}^{(t)}}$ and $\frac{\partial J}{\partial \Gamma_{s}^{(t)}}$

From eq.7 (see section-2), we have

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

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

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

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

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

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

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

$$d\mathbf{z}_{c}^{\langle t \rangle} = d\left(\mathbf{W}_{cc}^{\mathsf{T}} \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right) + \mathbf{W}_{cx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{c}\right)$$

$$= d\mathbf{W}_{cc}^{\mathsf{T}} \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right) + \mathbf{W}_{cc}^{\mathsf{T}} d\left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right) + d\mathbf{W}_{cx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle}$$

$$+ \mathbf{W}_{cx}^{\mathsf{T}} d\mathbf{x}^{\langle t \rangle} + d\mathbf{b}_{c} \qquad \text{eq.9-2}$$

when differentiating w.r.t. \mathbf{W}_{cc} , we have $d\mathbf{W}_{cx} = 0$, $d\left(\Gamma_r^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right) = 0$, $d\mathbf{b}_c = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} d\mathbf{W}_{cc}^{\intercal} \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right)\right)$$

$$= \operatorname{tr}\left(\left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right)^{\intercal} d\mathbf{W}_{cc} \left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\intercal}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\intercal} \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right)^{\intercal} d\mathbf{W}_{cc}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{cc}} = \left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}}\right)^{\intercal} \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right)^{\intercal}$$

when differentiating w.r.t. \mathbf{W}_{cx} , we have $d\mathbf{W}_{cc} = 0$, $d\left(\Gamma_r^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right) = 0$, $d\mathbf{b}_c = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$= d\mathbf{W}_{uc}^{\mathsf{T}} \mathbf{c}^{\langle t-1 \rangle} + \mathbf{W}_{uc}^{\mathsf{T}} d\mathbf{c}^{\langle t-1 \rangle} + d\mathbf{W}_{ux}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{W}_{ux}^{\mathsf{T}} d\mathbf{x}^{\langle t \rangle} + d\mathbf{b}_{u} \qquad \text{eq.9-2}$$

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

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

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

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

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

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

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

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

3.7 Computing $\frac{\partial J}{\partial \Gamma_r^{(t)}}$

From the results in section-3.5 and, from eq.9-2, we have

$$\begin{split} \frac{\partial J}{\partial \Gamma_r^{\langle t \rangle}} &= \frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}} \frac{\partial \tilde{\mathbf{c}}^{\langle t \rangle}}{\partial \Gamma_r^{\langle t \rangle}} \\ &= \frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}} \frac{\partial \tilde{\mathbf{c}}^{\langle t \rangle}}{\partial \left(\Gamma_r^{\langle t \rangle} \circ \mathbf{c}^{\langle t - 1 \rangle} \right)} \frac{\partial \left(\Gamma_r^{\langle t \rangle} \circ \mathbf{c}^{\langle t - 1 \rangle} \right)}{\partial \Gamma_r^{\langle t \rangle}} \\ &= \frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}} \mathbf{W}_{cc}^\intercal \operatorname{diag} \left(\mathbf{c}^{\langle t - 1 \rangle} \right) \\ &= \left(\frac{\partial J}{\partial \tilde{\mathbf{c}}^{\langle t \rangle}} \mathbf{W}_{cc}^\intercal \right) \circ \left(\mathbf{c}^{\langle t - 1 \rangle} \right)^\intercal \end{split}$$

Note: for more information on the derivative of a Hadamard product, see the Appendix-A in .\backprop-lstm.pdf.

3.8 Computing $\frac{\partial J}{\partial \mathbf{W}_{rc}}$, $\frac{\partial J}{\partial \mathbf{W}_{rx}}$, and $\frac{\partial J}{\partial \mathbf{b}_r}$

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

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

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

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

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

$$d\mathbf{z}_{r}^{\langle t \rangle} = d\left(\mathbf{W}_{rc}^{\mathsf{T}} \mathbf{c}^{\langle t-1 \rangle} + \mathbf{W}_{rx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{b}_{r}\right)$$

$$= d\mathbf{W}_{rc}^{\mathsf{T}} \mathbf{c}^{\langle t-1 \rangle} + \mathbf{W}_{rc}^{\mathsf{T}} d\mathbf{c}^{\langle t-1 \rangle} + d\mathbf{W}_{rx}^{\mathsf{T}} \mathbf{x}^{\langle t \rangle} + \mathbf{W}_{rx}^{\mathsf{T}} d\mathbf{x}^{\langle t \rangle} + d\mathbf{b}_{r} \qquad \text{eq.9-3}$$

when differentiating w.r.t. \mathbf{W}_{rc} , we have $d\mathbf{W}_{rx} = 0$, $d\mathbf{c}^{\langle t-1 \rangle} = 0$, $d\mathbf{b}_r = 0$, and $d\mathbf{x}^{\langle t \rangle} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{\partial J}{\partial \mathbf{z}_{r}^{\langle t \rangle}} d\mathbf{W}_{rc}^{\intercal} \mathbf{c}^{\langle t-1 \rangle}\right)$$

$$= \operatorname{tr}\left(\left(\mathbf{c}^{\langle t-1 \rangle}\right)^{\intercal} d\mathbf{W}_{rc} \left(\frac{\partial J}{\partial \mathbf{z}_{r}^{\langle t \rangle}}\right)^{\intercal}\right)$$

$$= \operatorname{tr}\left(\left(\frac{\partial J}{\partial \mathbf{z}_{r}^{\langle t \rangle}}\right)^{\intercal} \left(\mathbf{c}^{\langle t-1 \rangle}\right)^{\intercal} d\mathbf{W}_{rc}\right)$$

$$\Longrightarrow \frac{\partial J}{\partial \mathbf{W}_{rc}} = \left(\frac{\partial J}{\partial \mathbf{z}_{r}^{\langle t \rangle}}\right)^{\intercal} \left(\mathbf{c}^{\langle t-1 \rangle}\right)^{\intercal}$$

when differentiating w.r.t. \mathbf{W}_{rx} , we have $d\mathbf{W}_{rc} = 0$, $d\mathbf{c}^{\langle t-1\rangle} = 0$, $d\mathbf{b}_r = 0$, and $d\mathbf{x}^{\langle t\rangle} = 0$. So,

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

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

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

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

when differentiating w.r.t. \mathbf{b}_r , we have $d\mathbf{W}_{rc} = 0$, $d\mathbf{c}^{\langle t-1\rangle} = 0$, $d\mathbf{W}_{rx} = 0$, and $d\mathbf{x}^{\langle t\rangle} = 0$. So,

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

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

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

The derivative $\frac{\partial J}{\partial \mathbf{c}^{(t-1)}}$ has four components, as follows

Comp-1 flows-in as part of the derivative $\frac{\partial J}{\partial \mathbf{c}^{(t)}}$. This derivative is computed as follows

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

Comp-2 flows-in as derivative from $\Gamma_r^{\langle t \rangle}$ (see eq.9-3), and is computed as follows

$$\frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} = \frac{\partial J}{\partial \mathbf{z}_r^{\langle t \rangle}} \frac{\partial \mathbf{z}_r^{\langle t \rangle}}{\partial \mathbf{c}^{\langle t-1 \rangle}}$$
$$= \frac{\partial J}{\partial \mathbf{z}_r^{\langle t \rangle}} \mathbf{W}_{rc}^{\mathsf{T}}$$

Comp-3 flows-in as derivative from $\Gamma_u^{\langle t \rangle}$ (see eq.9-2), and is computed as follows

$$\frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} = \frac{\partial J}{\partial \mathbf{z}_{u}^{\langle t \rangle}} \frac{\partial \mathbf{z}_{u}^{\langle t \rangle}}{\partial \mathbf{c}^{\langle t-1 \rangle}}$$
$$= \frac{\partial J}{\partial \mathbf{z}_{v}^{\langle t \rangle}} \mathbf{W}_{uc}^{\mathsf{T}}$$

Comp-4 flows-in as derivative from $\tilde{\mathbf{c}}^{\langle t \rangle}$ (see eq.9-2), and is computed as follows

$$\frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} = \frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} \frac{\partial \mathbf{z}_{c}^{\langle t \rangle}}{\partial \mathbf{c}^{\langle t-1 \rangle}}
= \frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} \frac{\partial \mathbf{z}_{c}^{\langle t \rangle}}{\partial \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right)} \frac{\partial \left(\Gamma_{r}^{\langle t \rangle} \circ \mathbf{c}^{\langle t-1 \rangle}\right)}{\partial \mathbf{c}^{\langle t-1 \rangle}}
= \frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} \mathbf{W}_{cc}^{\mathsf{T}} \operatorname{diag}\left(\Gamma_{r}^{\langle t \rangle}\right)
= \left(\frac{\partial J}{\partial \mathbf{z}_{c}^{\langle t \rangle}} \mathbf{W}_{cc}^{\mathsf{T}}\right) \circ \left(\Gamma_{r}^{\langle t \rangle}\right)^{\mathsf{T}}$$

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

$$\frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} = \frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} \bigg|_{\mathbf{Comp-1}} + \frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} \bigg|_{\mathbf{Comp-2}} + \frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} \bigg|_{\mathbf{Comp-3}} + \frac{\partial J}{\partial \mathbf{c}^{\langle t-1 \rangle}} \bigg|_{\mathbf{Comp-4}}$$
(see \oplus labeled as β , β , and β in figure-2)

The derivative $\frac{\partial J}{\partial \mathbf{c}^{(t-1)}}$ has three components, as follows

Comp-1 flows-in as derivative from $\Gamma_r^{\langle t \rangle}$ (see eq.9-3), and is computed as follows

$$\begin{split} \frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} &= \frac{\partial J}{\partial \mathbf{z}_r^{\langle t \rangle}} \frac{\partial \mathbf{z}_r^{\langle t \rangle}}{\partial \mathbf{x}^{\langle t \rangle}} \\ &= \frac{\partial J}{\partial \mathbf{z}_r^{\langle t \rangle}} \mathbf{W}_{rx}^{\intercal} \end{split}$$

Comp-2 flows-in as derivative from $\Gamma_u^{\langle t \rangle}$ (see eq. 9-2), and is computed as follows

$$\frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{z}_u^{\langle t \rangle}} \frac{\partial \mathbf{z}_u^{\langle t \rangle}}{\partial \mathbf{x}^{\langle t \rangle}}$$
$$= \frac{\partial J}{\partial \mathbf{z}_r^{\langle t \rangle}} \mathbf{W}_{ux}^{\mathsf{T}}$$

Comp-3 flows-in as derivative from $\tilde{\mathbf{c}}^{\langle t \rangle}$ (see eq.9-2), and is computed as follows

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

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

$$\frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} = \frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} \bigg|_{\mathbf{Comp-1}} + \frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} \bigg|_{\mathbf{Comp-2}} + \frac{\partial J}{\partial \mathbf{x}^{\langle t \rangle}} \bigg|_{\mathbf{Comp-3}}$$
(see \oplus labeled as 4, and 6 in figure-2)

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.