Convolutional Neural Network: back-propagation for 2D-convolution

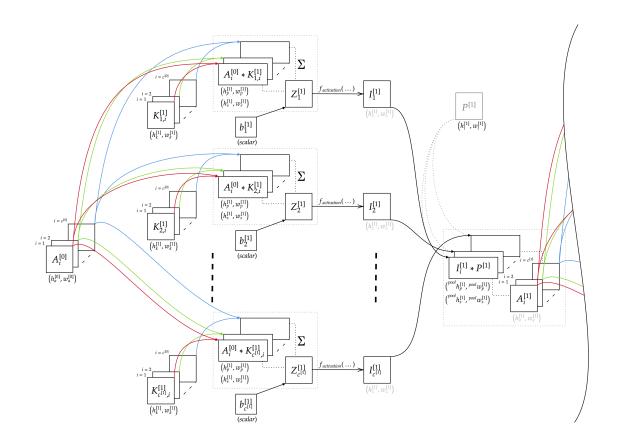
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Abstract

This document contains derivation of the gradients for a 3-layer convolutional neural-network (with 2D-convolution), using back-propagation (or reverse-mode differentiation). For the implementation of the neural-network see the accompanying notebooks.

1 Network Architecture



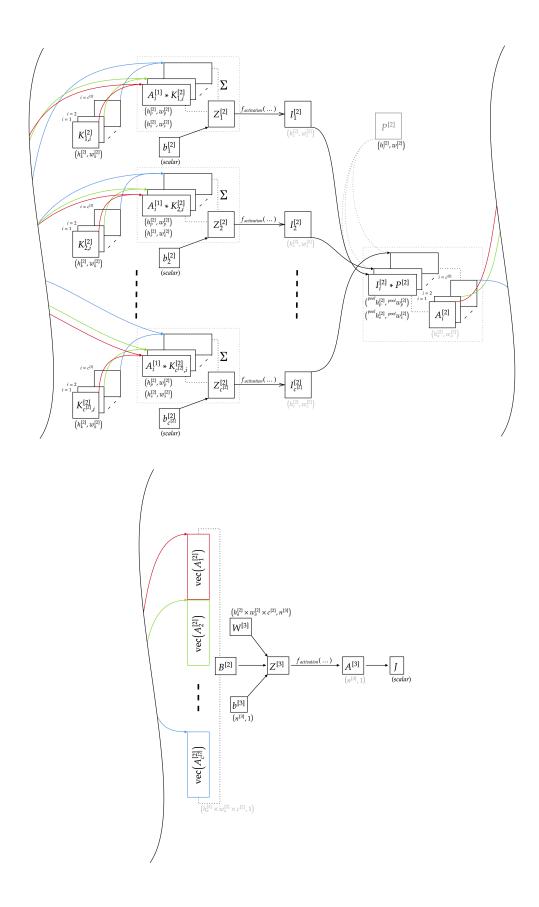


Figure 1: a three layer CNN with layers-1 & layer-2 being convolutional layers, and layer-3 a fully-connected layer

2 Forward Propagation

The equations for forward-propagation are as follows:

$$\begin{split} \mathbf{Z}_{j}^{[l]} &= \sum_{i=1}^{c^{[l-1]}} \mathbf{A}_{i}^{[l-1]} * \mathbf{K}_{j,i}^{[l]} + b_{j}^{[l]} \vec{\mathbf{I}}_{(h_{z}^{[l]}, w_{z}^{[l]})} \quad, \forall 1 \leq j \leq c^{[l]} \\ \mathbf{I}^{[l]} &= f_{activation}(\mathbf{Z}^{[l]}) \\ \mathbf{A}_{j}^{[l]} &= f_{pool}(\mathbf{I}_{j}^{[l]}) \quad, \forall 1 \leq j \leq c^{[l]} \end{split}$$

where,

$$\begin{aligned} \mathbf{K}_{j,i}^{[l]} &\in \mathbb{R}^{h_k^{[l]} \times w_k^{[l]}} & \text{is the } i^{th}\text{-channel of the } j^{th}\text{-kernel in } l^{th}\text{-layer, with } 1 \leq i \leq c^{[l-1]} \ \& \ 1 \leq j \leq c^{[l]} \\ b_j^{[l]} &\in \mathbb{R} & \text{is the } j^{th}\text{-component of the bias-vector } \mathbf{b}^{[l]}, \text{ with } 1 \leq j \leq c^{[l]} \\ \mathbf{A}_i^{[l-1]} &\in \mathbb{R}^{h_a^{[l-1]} \times w_a^{[l-1]}} & \text{is the } i^{th}\text{-channel of the output of } (l-1)^{th}\text{-layer, with } 1 \leq i \leq c^{[l-1]} \\ f_{activation}(\dots) & \text{is the activation function} \\ \mathbf{I}^{[l]} &\in \mathbb{R}^{h_z^{[l]} \times w_z^{[l]}} & \text{is an intermediate result of } l^{th}\text{-layer} \\ f_{pool}(\dots) & \text{is the pooling-function. And, in the above diagram this is average/mean-pooling} \\ P^{[l]} & \text{is an abstract representation of the pooling window. And, } \\ \binom{pool}{h_p^{[l]}, pool} w_p^{[l]}) &\& \binom{pool}{h_s^{[l]}, pool} w_s^{[l]}) \text{ are the padding and stride, respectively, for the pooling operation} \end{aligned}$$

Note: when an input of size (h_a, w_a) is convolved with a kernel of size (h_k, w_k) , using a stride of (h_s, w_s) & padding of (h_p, w_p) , the size of the resulting output (h_z, w_z) is given by

$$h_z = \left| \frac{h_a + 2h_p - h_k}{h_s} + 1 \right|; \qquad w_z = \left| \frac{w_a + 2w_p - w_k}{w_s} + 1 \right|$$

3 Optimization: gradient-descent

The optimization is performed according to the following equations:

$$\begin{aligned} \mathbf{K}_{j,i}^{[l]} &:= \mathbf{K}_{j,i}^{[l]} - \alpha \nabla_{K_{j,i}^{[l]}} J \\ \mathbf{b}^{[l]} &:= \mathbf{b}^{[l]} - \alpha \nabla_{b^{[l]}} J \end{aligned}$$

where, α is the learning-rate/step-size.

3.1 Back-propagation

The gradients in the above equations are derived using back-propagation, as follows:

• Since, J is a scalar, we can write $J = \operatorname{tr}(J) = J^{\mathsf{T}} = \operatorname{tr}(J^{\mathsf{T}})$. And the derivative can be computed as follows:

$$dJ = d(tr(J))$$
$$= tr(dJ)$$

The objective while computing the above derivative, is to massage the expression to the following form:

$$dy = tr(\mathbf{A}d\mathbf{X})$$

then,

$$\frac{\mathrm{d}y}{\mathrm{d}\mathbf{X}} = \mathbf{A}$$

• Let **A** and **B** be $m \times n$ and $p \times q$ matrices. Then the essence of the derivative $\frac{d\mathbf{A}}{d\mathbf{B}}$ is to compute the derivative of every entry of **A** w.r.t. every entry of **B**. Therefore, we can simplify this matrix derivative by vectorizing (using the vec operator) the matrices and perform a vector-by-vector derivative.

In the following computations, by $_{v}\mathbf{A}$ we denote $vec(\mathbf{A})$; where,

- if **A** is an $m \times n$ matrix, then ${}_{v}$ **A** is the $mn \times 1$ vector obtained by stacking columns of **A** one below the other.
- if **A** is an $m \times n \times c$ matrix, then ${}_{v}$ **A** is the $mn \times c$ dimensional matrix whose columns are the vectors ${}_{v}$ **A**_j, $\forall 1 \leq j \leq c$.

See [1] and [2] for more information.

3.1.1 Computing $\frac{dJ}{d\mathbf{W}^{[3]}}$, $\frac{dJ}{d\mathbf{b}^{[3]}}$, and $\frac{dJ}{d\mathbf{B}^{[2]}}$

We have,

$$\frac{\mathrm{d}J}{\mathrm{d}\mathbf{Z}^{[3]}} = \frac{\mathrm{d}J}{\mathrm{d}\mathbf{A}^{[3]}} \frac{\mathrm{d}\mathbf{A}^{[3]}}{\mathrm{d}\mathbf{Z}^{[3]}}$$

where,

$$\frac{\mathrm{d}J}{\mathrm{d}\mathbf{A}^{[3]}} = \begin{bmatrix} \frac{\partial}{\partial a_1^{[3]}} & \frac{\partial}{\partial a_2^{[3]}} & \cdots & \frac{\partial}{\partial a_{n}^{[3]}} \end{bmatrix} \otimes J$$
$$= \begin{bmatrix} \frac{\partial J}{\partial a_1^{[3]}} & \frac{\partial J}{\partial a_2^{[3]}} & \cdots & \frac{\partial J}{\partial a_{n}^{[3]}} \end{bmatrix}$$

and,

$$\frac{\mathrm{d}\mathbf{A}^{[3]}}{\mathrm{d}\mathbf{Z}^{[3]}} = \begin{bmatrix} \frac{\partial}{\partial z_{1}^{[3]}} & \frac{\partial}{\partial z_{2}^{[3]}} & \dots & \frac{\partial}{\partial z_{n}^{[3]}} \end{bmatrix} \otimes \begin{bmatrix} a_{1}^{[3]} \\ a_{2}^{[3]} \\ \vdots \\ a_{n}^{[3]} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{1}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{2}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{2}^{[3]}}{\partial z_{2}^{[3]}} & \dots & \frac{\partial a_{2}^{[3]}}{\partial z_{n}^{[3]}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial a_{n}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{n}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{2}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{n}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{2}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{n}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{2}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{n}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{2}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{n}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{1}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \dots & \frac{\partial a_{n}^{[3]}}{\partial z_{n}^{[3]}} \\ \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3]}} & \frac{\partial a_{1}^{[3]}}{\partial z_{1}^{[3$$

Note: for the derivatives in this section, we have $\mathbf{A}^{[3]} = {}_{v}\mathbf{A}^{[3]}$, $\mathbf{Z}^{[3]} = {}_{v}\mathbf{Z}^{[3]}$, and $\mathbf{B}^{[2]} = {}_{v}\mathbf{B}^{[2]}$; since, $\mathbf{Z}^{[3]}$, $\mathbf{A}^{[3]}$, and $\mathbf{B}^{[2]}$ are already vectors.

Then,

$$dJ = \operatorname{tr}\left(\frac{dJ}{d\mathbf{Z}^{[3]}}d\mathbf{Z}^{[3]}\right)$$

where, $d\mathbf{Z}^{[3]}$ can be expanded as,

$$\begin{split} \mathrm{d}\mathbf{Z}^{[3]} &= \mathrm{d}((\mathbf{W}^{[3]})^{\intercal}\mathbf{B}^{[2]} + \mathbf{b}^{[3]}) \\ &= \mathrm{d}(\mathbf{W}^{[3]})^{\intercal}\mathbf{B}^{[2]} + (\mathbf{W}^{[3]})^{\intercal}\mathrm{d}(\mathbf{B}^{[2]}) + \mathrm{d}\mathbf{b}^{[3]} \end{split}$$

when differentiating w.r.t. $\mathbf{W}^{[3]}$, we have $d\mathbf{b}^{[3]} = d\mathbf{B}^{[2]} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{dJ}{d\mathbf{Z}^{[3]}}d(\mathbf{W}^{[3]})^{\mathsf{T}}\mathbf{B}^{[2]}\right)$$

$$= \operatorname{tr}\left((\mathbf{B}^{[2]})^{\mathsf{T}}d\mathbf{W}^{[3]}\left(\frac{dJ}{d\mathbf{Z}^{[4]}}\right)^{\mathsf{T}}\right)$$

$$= \operatorname{tr}\left(\left(\frac{dJ}{d\mathbf{Z}^{[3]}}\right)^{\mathsf{T}}(\mathbf{B}^{[2]})^{\mathsf{T}}d\mathbf{W}^{[3]}\right)$$

$$\Longrightarrow \frac{dJ}{d\mathbf{W}^{[3]}} = \left(\frac{dJ}{d\mathbf{Z}^{[3]}}\right)^{\mathsf{T}}(\mathbf{B}^{[2]})^{\mathsf{T}}$$

when differentiating w.r.t. $\mathbf{b}^{[3]}$, we have $d(\mathbf{W}^{[3]})^{\mathsf{T}} = d\mathbf{B}^{[2]} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{dJ}{d\mathbf{Z}^{[3]}}d\mathbf{b}^{[3]}\right)$$

$$\Longrightarrow \frac{dJ}{d\mathbf{b}^{[3]}} = \frac{dJ}{d\mathbf{Z}^{[3]}}$$

when differentiating w.r.t. $\mathbf{B}^{[2]}$, we have $d(\mathbf{W}^{[3]})^{\intercal} = d\mathbf{b}^{[3]} = 0$. So,

$$dJ = \operatorname{tr}\left(\frac{dJ}{d\mathbf{Z}^{[3]}}(\mathbf{W}^{[3]})^{\mathsf{T}}d\mathbf{B}^{[2]}\right)$$
$$\Longrightarrow \frac{dJ}{d\mathbf{B}^{[2]}} = \frac{dJ}{d\mathbf{Z}^{[3]}}(\mathbf{W}^{[3]})^{\mathsf{T}}$$

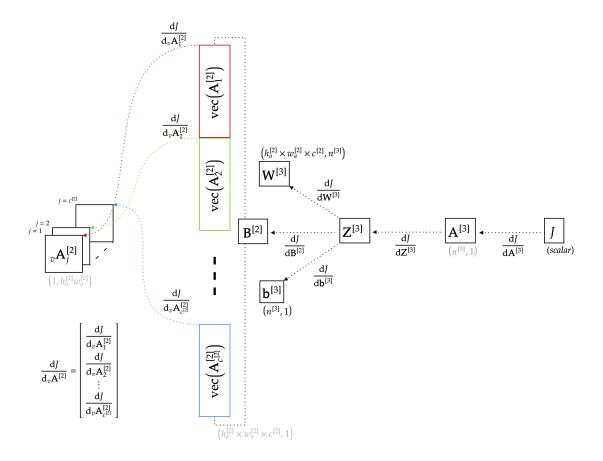


Figure 2: backward-propagation through the fully-connected layer, and the reshaping of the Jacobian $\frac{\mathrm{d}J}{\mathrm{d}\mathbf{B}^{[2]}}$ into the combined (in terms of channels) Jacobian $\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{A}^{[2]}}$.

3.1.2 Computing $\frac{dJ}{d_v \mathbf{A}^{[2]}}$

The vector $\mathbf{B}^{[2]}$, obtained by flattening the tensor $\mathbf{A}^{[2]}$, has the following structure:

$$B^{[2]} = \begin{bmatrix} \operatorname{vec}(\mathbf{A}_{1}^{[2]}) \\ \operatorname{vec}(\mathbf{A}_{2}^{[2]}) \\ \vdots \\ \operatorname{vec}(\mathbf{A}_{c^{[2]}}^{[2]}) \end{bmatrix} = \begin{bmatrix} a_{1,11}^{[2]} \\ a_{1,h_{a}^{[2]}w_{a}^{[2]}}^{[2]} \\ a_{2,11}^{[2]} \\ \vdots \\ a_{2,h_{a}^{[2]}w_{a}^{[2]}}^{[2]} \\ \vdots \\ \vdots \\ a_{c^{[2]},11}^{[2]} \\ \vdots \\ a_{c^{[2]},11}^{[2]} \end{bmatrix}$$

where,

Therefore, the derivative $\frac{dJ}{d\mathbf{B}^{[2]}}$ assumes the following structure:

$$\frac{\mathrm{d}J}{\mathrm{d}\mathbf{B}^{[2]}} = \begin{bmatrix} \frac{\partial}{\partial a_{1,11}^{[2]}} & \cdots & \frac{\partial}{\partial a_{1,h_a^{[2]}w_a^{[2]}}^{[2]}} & \frac{\partial}{\partial a_{2,11}^{[2]}} & \cdots \\ & \frac{\partial}{\partial a_{2,h_a^{[2]}w_a^{[2]}}^{[2]}} & \cdots & \cdots & \frac{\partial}{\partial a_{c^{[2]},11}^{[2]}} & \cdots & \frac{\partial}{\partial a_{c^{[2]},h_a^{[2]}w_a^{[2]}}^{[2]}} \end{bmatrix} \otimes J$$

$$= \begin{bmatrix} \frac{\partial J}{\partial a_{1,11}^{[2]}} & \cdots & \frac{\partial J}{\partial a_{1,h_a^{[2]}w_a^{[2]}}^{[2]}} & \frac{\partial J}{\partial a_{2,11}^{[2]}} & \cdots \\ & \frac{\partial J}{\partial a_{c^{[2]},h_a^{[2]}w_a^{[2]}}^{[2]}} & \cdots & \cdots & \frac{\partial J}{\partial a_{c^{[2]},11}^{[2]}} & \cdots & \frac{\partial J}{\partial a_{c^{[2]},h_a^{[2]}w_a^{[2]}}} \end{bmatrix}$$

We now reshape the vector $\frac{\mathrm{d}J}{\mathrm{d}\mathbf{B}^{[2]}}$ into a $c^{[2]} \times h_a^{[2]} w_a^{[2]}$ dimensional matrix such that each row corresponds to a channel of $\mathbf{A}^{[2]}$, (figure 2) i.e. each row is a derivative of J w.r.t. $\mathrm{vec}(\mathbf{A}_i^{[2]})$, as follows:

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{A}^{[2]}} = \begin{bmatrix}
\frac{\partial J}{\partial a_{1,11}^{[2]}} & \frac{\partial J}{\partial a_{1,21}^{[2]}} & \cdots & \frac{\partial J}{\partial a_{1,21}^{[2]}w_{a}^{[2]}} \\
\frac{\partial J}{\partial a_{2,11}^{[2]}} & \frac{\partial J}{\partial a_{2,21}^{[2]}} & \cdots & \frac{\partial J}{\partial a_{a}^{[2]}w_{a}^{[2]}} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial J}{\partial a_{c[2],11}^{[2]}} & \frac{\partial J}{\partial a_{a}^{[2]}} & \cdots & \frac{\partial J}{\partial a_{a}^{[2]}w_{a}^{[2]}}
\end{bmatrix}$$

3.1.3 Computing $\frac{dJ}{d_{n}\mathbf{I}^{[2]}}$

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{I}^{[2]}} = \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{A}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{A}^{[2]}}{\mathrm{d}_{v}\mathbf{I}^{[2]}}$$

Where, $\frac{d_v \mathbf{A}^{[2]}}{d_v \mathbf{I}^{[2]}}$ is computed based on the type of pooling, as follows:

Average Pooling: Let $P^{[2]}$ be a $h_l^{[2]} \times w_l^{[2]}$ dimensional matrix with all entries equal to $\frac{1}{h_l^{[2]}w_l^{[2]}}$. Then, the average pooled matrix $\mathbf{A}_j^{[2]}$ is obtained by convolving $P^{[2]}$ with $\mathbf{I}_j^{[2]}$, with a padding of $({}^lh_p^{[2]}, {}^lw_p^{[2]})$ and a stride of $({}^lh_s^{[2]}, {}^lw_s^{[2]})$, i.e.

$$\mathbf{A}_{j}^{[2]} = \mathbf{I}_{j}^{[2]} * P^{[2]}$$

Now, let $I_{j,pq}^{[2]}$ be the (p,q)-th entry of the matrix $\mathbf{I}_j^{[2]}$, for any $1 \leq j \leq c^{[2]}$. Then the derivative $\frac{\mathrm{d}_v A_j^{[2]}}{\mathrm{d}I_{j,pq}^{[2]}}$ is computed as follows:

$$\frac{\mathrm{d}\mathbf{A}_{j}^{[2]}}{\mathrm{d}I_{j,pq}} = \frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,pq}^{[2]}} * P^{[2]} \implies \frac{\mathrm{d}_{v}\mathbf{A}_{j}^{[2]}}{\mathrm{d}I_{j,pq}^{[2]}} = \mathrm{vec}\bigg(\frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,pq}^{[2]}} * P^{[2]}\bigg)$$

where, the convolution is performed with the same padding and stride as that used for computing $\mathbf{A}_{j}^{[2]}$ from $\mathbf{I}_{j}^{[2]}$, i.e. a padding of $({}^{l}h_{p}^{[2]}, {}^{l}w_{p}^{[2]})$ and a stride of $({}^{l}h_{s}^{[2]}, {}^{l}w_{s}^{[2]})$. Also, notice that the value of the derivative $\frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,pq}^{[2]}}$ is independent of the entries in

 $\mathbf{I}_{j}^{[2]}$, i.e. for any $1 \leq p \leq h_{z}^{[2]}$ & $1 \leq q \leq w_{z}^{[2]}$ the value of the derivative $\frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,pq}^{[2]}}$ is the same for all $1 \leq j \leq c^{[2]}$.

Extending the above derivative w.r.t. all the entries in $_v\mathbf{I}_j^{[2]}$ results in a $h_a^{[2]}w_a^{[2]}\times h_z^{[2]}w_z^{[2]}$ dimensional matrix, defined as follows

$$\begin{split} \frac{\mathrm{d}_{v}\mathbf{A}_{j}^{[2]}}{\mathrm{d}_{v}\mathbf{I}_{j}^{[2]}} &= \left[\frac{\partial}{\partial I_{j,11}^{[2]}} \quad \frac{\partial}{\partial I_{j,21}^{[2]}} \quad \cdots \quad \frac{\partial}{\partial I_{j,h_{z}^{[2]}w_{z}^{[2]}}^{[2]}}\right] \otimes {}_{v}\mathbf{A}_{j}^{[2]} \\ &= \left[\frac{\partial_{v}\mathbf{A}_{j}^{[2]}}{\partial I_{j,11}^{[2]}} \quad \frac{\partial_{v}\mathbf{A}_{j}^{[2]}}{\partial I_{j,21}^{[2]}} \quad \cdots \quad \frac{\partial_{v}\mathbf{A}_{j}^{[2]}}{\partial I_{j,h_{z}^{[2]}w_{z}^{[2]}}}\right] \\ &= \left[\operatorname{vec}\left(\frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,11}^{[2]}} * P^{[2]}\right) \quad \operatorname{vec}\left(\frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,21}^{[2]}} * P^{[2]}\right) \quad \cdots \quad \operatorname{vec}\left(\frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,h_{z}^{[2]}w_{z}^{[2]}}} * P^{[2]}\right)\right] \\ &= \operatorname{and, is equal for all channels } 1 \leq j \leq c^{[2]}. \text{ Hence, we have,} \\ &= \frac{\mathrm{d}_{v}\mathbf{A}^{[2]}}{\mathrm{d}_{v}\mathbf{I}^{[2]}} \end{split}$$

Max-pooling: the backward pass for a max-pooling operation is performed by routing the gradient to the input that had the highest value in the forward pass. Hence, during the forward pass of a pooling layer it is common to keep track of the index of the max activation (sometimes also called the switches) so that gradient routing is efficient during back-propagation. [3]

 L^2 -norm pooling: TODO

3.1.4 Computing $\frac{dJ}{d_{1}\mathbf{Z}^{[2]}}$

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}^{[2]}} = \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{I}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{I}^{[2]}}{\mathrm{d}_{v}\mathbf{Z}^{[2]}}$$

Here, the derivative $\frac{d_v \mathbf{I}^{[2]}}{d_v \mathbf{Z}^{[2]}}$ has to be computed channel-wise because the value of the derivative is dependent on the values of the entries of $\mathbf{I}_j^{[2]}$, i.e. for some channel $1 \leq j \leq c^{[2]}$, we have

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}_{i}^{[2]}} = \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{I}_{i}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{I}_{i}^{[2]}}{\mathrm{d}_{v}\mathbf{Z}_{i}^{[2]}}$$

and then stacked as follows

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}^{[2]}} = \begin{bmatrix} \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}_{1}^{[2]}} \\ \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}_{2}^{[2]}} \\ \vdots \\ \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}_{c}^{[2]}} \end{bmatrix} = \begin{bmatrix} \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{I}_{1}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{I}_{1}^{[2]}}{\mathrm{d}_{v}\mathbf{Z}_{2}^{[2]}} \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}_{2}^{[2]}} \\ \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{I}_{2}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{I}_{2}^{[2]}}{\mathrm{d}_{v}\mathbf{Z}_{2}^{[2]}} \\ \vdots \\ \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{I}_{c}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{I}_{2}^{[2]}}{\mathrm{d}_{v}\mathbf{Z}_{c}^{[2]}} \end{bmatrix}$$

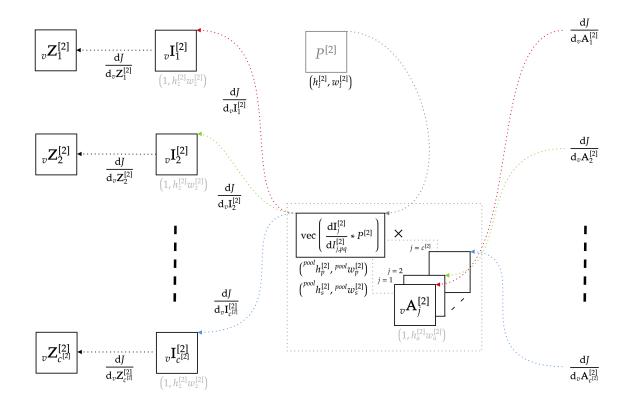


Figure 3: backward-propagation through a average-pooling layer. The derivative $\frac{\mathrm{d}\mathbf{I}_{j}^{[2]}}{\mathrm{d}I_{j,pq}^{[2]}}$ is computed $\forall 1 \leq p \leq h_{z}^{[2]}$ & $\forall 1 \leq q \leq w_{z}^{[2]}$. It is independent of the choice of the channel $1 \leq j \leq c^{[2]}$ for $\mathbf{I}_{j}^{[2]}$, and hence is equal for all the channels.

3.1.5 Computing $\frac{dJ}{d_n \mathbf{K}^{[2]}}$, $\frac{dJ}{d\mathbf{b}^{[2]}}$, and $\frac{dJ}{d_n \mathbf{A}^{[1]}}$

The matrix $\mathbf{Z}_{j}^{[2]}$ is computed as per the following equation

$$\mathbf{Z}_{j}^{[2]} = \sum_{i=1}^{c^{[1]}} \mathbf{A}_{i}^{[1]} * \mathbf{K}_{j,i}^{[2]} + b_{j}^{[2]} \ \vec{\mathbf{1}}_{(h_{z}^{[2]}, w_{z}^{[2]})} \quad , \forall 1 \leq j \leq c^{[2]}$$

where, the convolution is performed with a padding of $(h_p^{[2]}, w_p^{[2]})$ and a stride of $(h_s^{[2]}, w_s^{[2]})$.

Derivative w.r.t. $_{v}\mathbf{K}^{[2]}$: For computing the derivative of J w.r.t. $_{v}\mathbf{K}^{[2]}$, lets start by considering each channel of each kernel in layer-2 separately, as follows

$$\frac{\mathrm{d}J}{\mathrm{d}_v \mathbf{K}_{j,i}^{[2]}} = \frac{\mathrm{d}J}{\mathrm{d}_v \mathbf{Z}_j^{[2]}} \frac{\mathrm{d}_v \mathbf{Z}_j^{[2]}}{\mathrm{d}_v \mathbf{K}_{j,i}^{[2]}}$$

where,

 $_{v}\mathbf{K}_{j,i}^{[2]}$ is the i^{th} -channel of the j^{th} -kernel in layer-2, and $1 \leq j \leq c^{[2]}$ & $1 \leq i \leq c^{[1]}$

 $\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{Z}_j^{[2]}} \qquad \text{is the derivative of } J \text{ w.r.t. the } j^{th}\text{-channel of } \mathbf{Z}^{[2]}, \text{ i.e. the } j^{th}\text{-row of the matrix } \frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{Z}^{[2]}}$

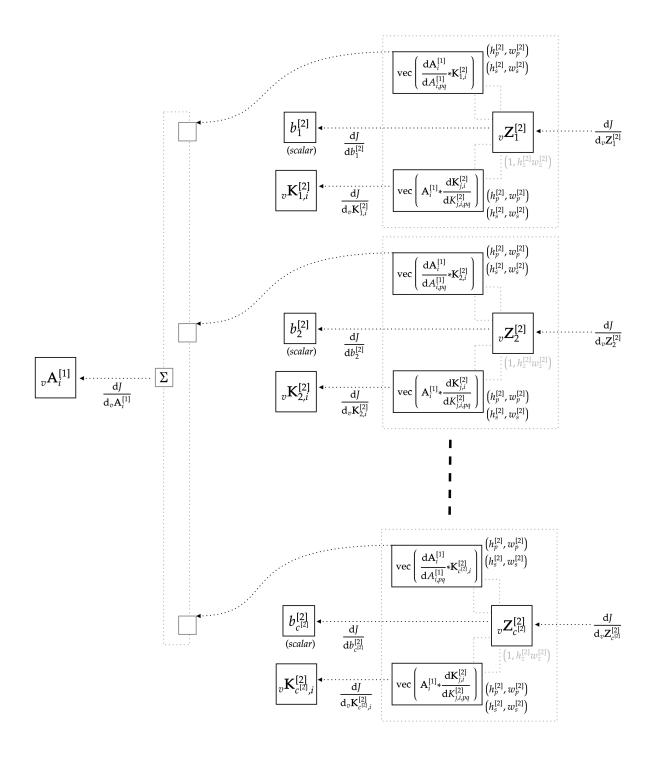


Figure 4: back-propagation through a convolutional for some channel-i, and must be performed for each $1 \leq i \leq c^{[1]}$. The derivative $\frac{\mathrm{d}\mathbf{K}_{j,i}^{[2]}}{\mathrm{d}K_{j,i,pq}^{[2]}}$ must be computed $\forall 1 \leq p \leq h_k^{[2]}$ & $\forall 1 \leq q \leq w_k^{[2]}$. Also, the value of this derivative is independent of the choice of the kernel, and hence is equal for all $1 \leq j \leq c^{[2]}$.

Then the derivative of $\mathbf{Z}_{j}^{[2]}$ w.r.t. $K_{j,i,pq}^{[2]}$, the $(p,q)^{th}$ -entry of $\mathbf{K}_{j,i}^{[2]}$, is computed as follows

$$\frac{\mathrm{d}\mathbf{Z}_{j}^{[2]}}{\mathrm{d}K_{j,i,pq}^{[2]}} = \mathbf{A}_{i}^{[1]} * \frac{\mathrm{d}\mathbf{K}_{j,i}^{[2]}}{\mathrm{d}K_{j,i,pq}^{[2]}} \implies \frac{\mathrm{d}_{v}\mathbf{Z}_{j}^{[2]}}{\mathrm{d}K_{j,i,pq}^{[2]}} = \mathrm{vec}\bigg(\mathbf{A}_{i}^{[1]} * \frac{\mathrm{d}\mathbf{K}_{j,i}^{[2]}}{\mathrm{d}K_{j,i,pq}^{[2]}}\bigg) \qquad \textit{See section-4}$$

Extending the above derivative w.r.t. all the entries of ${}_{v}\mathbf{K}_{j,i}^{[2]}$ results in a $h_{z}^{[2]}w_{z}^{[2]} \times h_{k}^{[2]}w_{k}^{[2]}$ dimensional matrix, defined as follows

$$\begin{split} \frac{\mathrm{d}_{v}\mathbf{Z}_{j}^{[2]}}{\mathrm{d}_{v}\mathbf{K}_{j,i}^{[2]}} &= \left[\frac{\partial}{\partial K_{j,i,11}^{[2]}} \quad \frac{\partial}{\partial K_{j,i,21}^{[2]}} \quad \cdots \quad \frac{\partial}{\partial K_{j,i,h_{k}^{[2]}w_{k}^{[2]}}^{[2]}}\right] \otimes_{v}\mathbf{Z}_{j}^{[2]} \\ &= \left[\frac{\partial_{v}\mathbf{Z}_{j}^{[2]}}{\partial K_{j,i,11}^{[2]}} \quad \frac{\partial_{v}\mathbf{Z}_{j}^{[2]}}{\partial K_{j,i,21}^{[2]}} \quad \cdots \quad \frac{\partial_{v}\mathbf{Z}_{j}^{[2]}}{\partial K_{k}^{[2]}}\right] \\ &= \left[\operatorname{vec}\left(\mathbf{A}_{i}^{[1]} * \frac{\mathrm{d}\mathbf{K}_{j,i}^{[2]}}{\mathrm{d}K_{j,i,11}^{[2]}}\right) \quad \operatorname{vec}\left(\mathbf{A}_{i}^{[1]} * \frac{\mathrm{d}\mathbf{K}_{j,i}^{[2]}}{\mathrm{d}K_{j,i,21}^{[2]}}\right) \quad \cdots \quad \operatorname{vec}\left(\mathbf{A}_{i}^{[1]} * \frac{\mathrm{d}\mathbf{K}_{j,i}^{[2]}}{\mathrm{d}K_{j,i,21}^{[2]}}\right)\right] \end{split}$$

The value of the above derivative, given a channel-i, is equal for all kernels $1 \le j \le c^{[2]}$, i.e. the derivative is independent of the values of the entries of $\mathbf{K}_{j,i}^{[2]}$ and depends only on the entries of i^{th} -channel of $\mathbf{A}^{[2]}$. Therefore,

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{K}_{:,i}^{[2]}} = \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{Z}^{[2]}}{\mathrm{d}_{v}\mathbf{K}_{j,i}^{[2]}} \quad \text{for any } 1 \le j \le c^{[2]}$$

gives the derivative of J w.r.t. the i^{th} -channel of all the kernels in layer-2. And, the above computation must be performed for each $1 \le i \le c^{[1]}$ to get the gradient of J w.r.t. all the layer-2 kernels' entries.

Derivative w.r.t. $\mathbf{b}^{[2]}$: Vectorizing the above equation and taking the derivative of $_{v}\mathbf{Z}_{j}^{[2]}$ w.r.t. $b_{j}^{[2]}$, we get

$$v\mathbf{Z}_{j}^{[2]} = \operatorname{vec}\left(\sum_{i=1}^{c^{[1]}} \mathbf{A}_{i}^{[1]} * \mathbf{K}_{j,i}^{[2]}\right) + b_{j}^{[2]} \operatorname{vec}\left(\mathbf{1}_{(h_{z}^{[2]}, w_{z}^{[2]})}\right) \\
 = \operatorname{vec}\left(\sum_{i=1}^{c^{[1]}} \mathbf{A}_{i}^{[1]} * \mathbf{K}_{j,i}^{[2]}\right) + b_{j}^{[2]} \mathbf{1}_{(h_{z}^{[2]} w_{z}^{[2]}, 1)} \\
 \Longrightarrow \frac{\operatorname{d}_{v} \mathbf{Z}_{j}^{[2]}}{\operatorname{d} b_{j}^{[2]}} = \mathbf{1}_{(h_{z}^{[2]} w_{z}^{[2]}, 1)} \quad \forall 1 \leq j \leq c^{[2]}$$

This derivative is independent of the value of $b_j^{[2]}$, and hence is equal for all the kernels in layer-2. Therefore, we have

$$\frac{\mathrm{d}J}{\mathrm{d}b_{j}^{[2]}} = \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}_{j}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{Z}_{j}^{[2]}}{\mathrm{d}b_{j}^{[2]}}$$
$$= \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}_{j}^{[2]}} \mathbf{1}_{(h_{z}^{[2]}w_{z}^{[2]},1)}$$

Now, expanding the above derivative w.r.t. all components of $\mathbf{b}^{[2]}$, we get

$$\frac{\mathrm{d}J}{\mathrm{d}\mathbf{b}^{[2]}} = \begin{bmatrix} \frac{\mathrm{d}J}{\mathrm{d}_v \mathbf{Z}_1^{[2]}} \mathbf{1}_{(h_z^{[2]} w_z^{[2]}, 1)} & \frac{\mathrm{d}J}{\mathrm{d}_v \mathbf{Z}_2^{[2]}} \mathbf{1}_{(h_z^{[2]} w_z^{[2]}, 1)} & \dots & \frac{\mathrm{d}J}{\mathrm{d}_v \mathbf{Z}_{c^{[2]}}^{[2]}} \mathbf{1}_{(h_z^{[2]} w_z^{[2]}, 1)} \end{bmatrix} \\
= \begin{pmatrix} \frac{\mathrm{d}J}{\mathrm{d}_v \mathbf{Z}^{[2]}} \mathbf{1}_{(h_z^{[2]} w_z^{[2]}, 1)} \end{pmatrix}^{\mathsf{T}}$$

Derivative w.r.t. $\mathbf{A}^{[1]}$: Each channel of $\mathbf{A}^{[1]}$ is convolved by the corresponding channels of all the kernels in layer-2. Therefore, the gradient w.r.t. $\mathbf{A}^{[2]}_i$, for any $1 \leq i \leq c^{[1]}$, is the sum of gradients flowing in from all the kernels, i.e.

$$\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{A}_i^{[1]}} = \sum_{j=1}^{c^{[2]}} \frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{Z}_j^{[2]}} \frac{\mathrm{d}_v\mathbf{Z}_j^{[2]}}{\mathrm{d}_v\mathbf{A}_i^{[1]}}$$

Let, $A_{i,pq}^{[1]}$ be the $(p,q)^{th}$ -entry of the i^{th} -channel of $\mathbf{A}^{[1]}$. Then, the derivative of $\mathbf{Z}_{j}^{[2]}$ w.r.t. $A_{i,pq}^{[1]}$ is computed as follows

$$\frac{\mathrm{d}\mathbf{Z}_{j}^{[2]}}{\mathrm{d}A_{i,pq}^{[1]}} = \frac{\mathrm{d}\mathbf{A}_{i}^{[1]}}{\mathrm{d}A_{i,pq}^{[1]}} * \mathbf{K}_{j,i}^{[2]} \implies \frac{\mathrm{d}_{v}\mathbf{Z}_{j}^{[2]}}{\mathrm{d}A_{i,pq}^{[1]}} = \mathrm{vec}\left(\frac{\mathrm{d}\mathbf{A}_{i}^{[1]}}{\mathrm{d}A_{i,pq}^{[1]}} * \mathbf{K}_{j,i}^{[2]}\right) \qquad See \ section-4$$

where, the above convolution is performed with the same padding and stride as that used to compute $\mathbf{Z}_j^{[2]}$, i.e. with a padding of $(h_p^{[2]}, w_p^{[2]})$ and a stride of $(h_s^{[2]}, w_s^{[2]})$.

Extending the above derivative w.r.t. all the entries of $\mathbf{A}_i^{[1]}$ results in a $h_z^{[2]}w_z^{[2]} \times h_a^{[2]}w_a^{[2]}$ dimensional matrix, defined as follows

$$\frac{d_{v} \mathbf{Z}_{j}^{[2]}}{d_{v} \mathbf{A}_{i}^{[2]}} = \begin{bmatrix} \frac{\partial}{\partial A_{i,11}^{[1]}} & \frac{\partial}{\partial A_{i,21}^{[1]}} & \cdots & \frac{\partial}{\partial A_{i,n}^{[1]} w_{a}^{[1]}} \end{bmatrix} \otimes_{v} \mathbf{Z}_{j}^{[2]} \\
= \begin{bmatrix} \frac{\partial_{v} \mathbf{Z}_{j}^{[2]}}{\partial A_{i,11}^{[1]}} & \frac{\partial_{v} \mathbf{Z}_{j}^{[2]}}{\partial A_{i,21}^{[1]}} & \cdots & \frac{\partial_{v} \mathbf{Z}_{j}^{[2]}}{\partial A_{i,n}^{[1]} w_{a}^{[1]}} \end{bmatrix} \\
= \begin{bmatrix} \operatorname{vec} \left(\frac{d \mathbf{A}_{i}^{[1]}}{d A_{i,11}^{[1]}} * \mathbf{K}_{j,i}^{[2]} \right) & \operatorname{vec} \left(\frac{d \mathbf{A}_{i}^{[1]}}{d A_{i,21}^{[1]}} * \mathbf{K}_{j,i}^{[2]} \right) & \cdots & \operatorname{vec} \left(\frac{d \mathbf{A}_{i}^{[1]}}{d A_{i,n}^{[1]} w_{a}^{[2]}} * \mathbf{K}_{j,i}^{[2]} \right) \end{bmatrix}$$

After computing $\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{A}_i^{[1]}}$ for all $1 \leq i \leq c^{[1]}$, the derivative $\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{A}^{[1]}}$, which is a $c^{[1]} \times h_a^{[1]}w_a^{[1]}$ dimensional matrix, is computed as follows

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{A}^{[1]}} = \begin{bmatrix} \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{A}_{1}^{[1]}} \\ \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{A}_{2}^{[1]}} \\ \vdots \\ \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{A}_{c}^{[1]}} \end{bmatrix}$$

3.1.6 Computing $\frac{dJ}{d_v \mathbf{Z}^{[1]}}$, $\frac{dJ}{d_v \mathbf{K}^{[1]}}$, and $\frac{dJ}{d\mathbf{b}^{[1]}}$

Given the derivative $\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{A}^{[1]}}$, we can compute the subsequent derivatives as follows

$$\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{I}^{[1]}} = \frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{A}^{[1]}} \frac{\mathrm{d}_v\mathbf{A}^{[1]}}{\mathrm{d}_v\mathbf{I}^{[1]}}$$

the derivative $\frac{d_v \mathbf{A}^{[1]}}{d_v \mathbf{I}^{[1]}}$ is computed based on the pooling strategy, as described in the above section-3.1.3

$$\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{Z}^{[1]}} = \frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{I}^{[1]}} \frac{\mathrm{d}_v\mathbf{I}^{[1]}}{\mathrm{d}_v\mathbf{Z}^{[1]}}$$

the derivative $\frac{d_v \mathbf{I}^{[1]}}{d_v \mathbf{Z}^{[1]}}$ is computed based on the activation function, as shown in *section-3.1.4*

$$\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{K}_{:,i}^{[2]}} = \frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{Z}^{[2]}} \frac{\mathrm{d}_{v}\mathbf{Z}^{[2]}}{\mathrm{d}_{v}\mathbf{K}_{j,i}^{[2]}}$$

the derivative $\frac{\mathrm{d}_{v}\mathbf{Z}^{[2]}}{\mathrm{d}_{v}\mathbf{K}^{[2]}_{j,i}}$ is computed as shown in section-3.1.5. And, the derivative $\frac{\mathrm{d}J}{\mathrm{d}_{v}\mathbf{K}^{[2]}_{:,i}}$ must be computed for each $1 \leq i \leq c^{[1]}$

 $\langle straightforward-to-compute \rangle$

$$\frac{\mathrm{d}J}{\mathrm{d}\mathbf{b}^{[1]}} = \left(\frac{\mathrm{d}J}{\mathrm{d}_v\mathbf{Z}^{[1]}}\mathbf{1}_{(h_z^{[1]}w_z^{[1]},1)}\right)^{\mathsf{T}}$$

3.2 Jacobian or Gradient?

In the above derivations, we have used the numerator layout while performing matrixderivatives. 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. So, based on our derivations the gradients would be the following:

$$\begin{aligned} \nabla_{K_{j,i}^{[l]}} J &= \left(\frac{\mathrm{d}J}{\mathrm{d}\mathbf{K}_{j,i}^{[l]}}\right)^{\mathsf{T}} \\ \nabla_{b^{[l]}} J &= \left(\frac{\mathrm{d}_v \mathbf{Z}^{[2]}}{\mathrm{d}_v \mathbf{b}^{[l]}}\right)^{\mathsf{T}} \end{aligned}$$

4 Appendix: derivative of a convolution

Here, we compute the derivative of a convolution w.r.t. its constituents. Let **A** be a (3,4) dimensional matrix, β be a (2,2) dimensional matrix, and **Z** be a (4,3) dimensional matrix obtained by convolving **A** by β with a padding of (1,1) and a stride of (1,2), i.e.

$$\mathbf{Z} = \mathbf{A} * \beta$$

$$= \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a_{11} & a_{12} & a_{13} & a_{14} & 0 \\ 0 & a_{21} & a_{22} & a_{23} & a_{24} & 0 \\ 0 & a_{31} & a_{32} & a_{33} & a_{34} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} * \begin{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & a_{11} \end{bmatrix} * \beta & \begin{bmatrix} 0 & 0 \\ a_{12} & a_{13} \end{bmatrix} * \beta & \begin{bmatrix} 0 & 0 \\ a_{12} & a_{13} \end{bmatrix} * \beta & \begin{bmatrix} a_{14} & 0 \\ a_{24} & 0 \end{bmatrix} * \beta \\ \begin{bmatrix} \begin{bmatrix} 0 & a_{21} \\ 0 & a_{21} \end{bmatrix} * \beta & \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} * \beta & \begin{bmatrix} a_{24} & 0 \\ a_{34} & 0 \end{bmatrix} * \beta \\ \begin{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & a_{31} \end{bmatrix} * \beta & \begin{bmatrix} a_{32} & a_{33} \\ a_{32} & a_{33} \end{bmatrix} * \beta & \begin{bmatrix} a_{34} & 0 \\ a_{34} & 0 \end{bmatrix} * \beta \\ \begin{bmatrix} \begin{bmatrix} 0 & 0 \\ 0 & a_{31} \end{bmatrix} * \beta & \begin{bmatrix} a_{32} & a_{33} \\ 0 & 0 \end{bmatrix} * \beta & \begin{bmatrix} a_{34} & 0 \\ 0 & 0 \end{bmatrix} * \beta \\ \end{bmatrix}$$

$$= \begin{bmatrix} a_{11}\beta_{22} & a_{12}\beta_{11} + a_{13}\beta_{12} + a_{22}\beta_{21} + a_{23}\beta_{22} & a_{14}\beta_{11} + a_{24}\beta_{21} \\ a_{21}\beta_{12} + a_{31}\beta_{22} & a_{22}\beta_{11} + a_{23}\beta_{12} + a_{32}\beta_{21} + a_{33}\beta_{22} & a_{24}\beta_{11} + a_{34}\beta_{21} \\ a_{31}\beta_{12} & a_{32}\beta_{11} + a_{33}\beta_{12} & a_{32}\beta_{11} + a_{33}\beta_{12} & a_{34}\beta_{11} \end{bmatrix}$$

$$= \begin{bmatrix} z_{11} & z_{12} & z_{13} \\ z_{11} & z_{12} & z_{13} \\ z_{21} & z_{22} & z_{23} \\ z_{31} & z_{32} & z_{33} \\ \end{bmatrix}$$
(rep.3)

Also, the vectorized forms of these matrices are as follows

$${}_{v}\mathbf{A} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{12} \\ a_{22} \\ a_{13} \\ a_{23} \\ a_{23} \\ a_{33} \\ a_{14} \\ a_{24} \\ a_{34} \end{bmatrix}; \qquad {}_{v}\beta = \begin{bmatrix} \beta_{11} \\ \beta_{21} \\ \beta_{12} \\ \beta_{22} \end{bmatrix}; \qquad {}_{v}\mathbf{Z} = \begin{bmatrix} z_{11} \\ z_{21} \\ z_{31} \\ z_{41} \\ z_{12} \\ z_{22} \\ z_{32} \\ z_{42} \\ z_{23} \\ z_{23} \\ z_{23} \\ z_{23} \\ z_{23} \end{bmatrix}$$

Essence of matrix/vector derivative: Let M and N be any two vectors/matrices. Then, the objective of the derivative $\frac{dM}{dN}$ is to compute the derivative of each entry of M w.r.t. each entry of N. And, the representation of a group of entries as matrices, vectors, or tensors is merely a matter of notation.

Now, consider the following derivatives:

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}\beta} = \mathrm{reshape}\left(\frac{\mathrm{d}_v\mathbf{Z}}{\mathrm{d}_v\beta}\right)$$
:

$$\frac{\mathbf{d}_{v}\mathbf{Z}}{\mathbf{d}_{v}\beta} = \begin{bmatrix} \frac{\partial}{\partial\beta_{11}} & \frac{\partial}{\partial\beta_{21}} & \frac{\partial}{\partial\beta_{12}} & \frac{\partial}{\partial\beta_{22}} \end{bmatrix} \otimes_{v}\mathbf{Z}$$

$$= \begin{bmatrix} \frac{\partial_{v}\mathbf{Z}}{\partial\beta_{11}} & \frac{\partial_{v}\mathbf{Z}}{\partial\beta_{21}} & \frac{\partial_{v}\mathbf{Z}}{\partial\beta_{12}} & \frac{\partial_{v}\mathbf{Z}}{\partial\beta_{22}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial_{z_{11}}}{\partial\beta_{11}} & \frac{\partial z_{11}}{\partial\beta_{21}} & \frac{\partial z_{11}}{\partial\beta_{12}} & \frac{\partial z_{11}}{\partial\beta_{22}} \\ \frac{\partial z_{21}}{\partial\beta_{11}} & \frac{\partial z_{21}}{\partial\beta_{21}} & \frac{\partial z_{21}}{\partial\beta_{12}} & \frac{\partial z_{21}}{\partial\beta_{22}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial z_{43}}{\partial\beta_{11}} & \frac{\partial z_{43}}{\partial\beta_{21}} & \frac{\partial z_{43}}{\partial\beta_{12}} & \frac{\partial z_{43}}{\partial\beta_{22}} \end{bmatrix}$$
eq.a1-1

Let's compute the value of an arbitrary element of this matrix, say derivative of z_{32} w.r.t. β_{21} (you should try out with some other combination of entries)

$$\frac{\partial z_{32}}{\partial \beta_{21}} = \frac{\partial (a_{22}\beta_{11} + a_{23}\beta_{12} + a_{32}\beta_{21} + a_{33}\beta_{22})}{\partial \beta_{21}} \quad \text{using rep.2}$$

$$= a_{32}$$

$$= \frac{\partial \left(\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} * \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} \right)}{\partial \beta_{21}} \quad \text{using rep.1}$$

$$= \frac{\partial \left(\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} \right)}{\partial \beta_{21}} * \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} + \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} * \frac{\partial \left(\begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} \right)}{\partial \beta_{21}}$$

$$= \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} * \frac{\partial \left(\begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} \right)}{\partial \beta_{21}} = \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} * \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \quad \text{eq.a1-2}$$

In the matrix in eq.a1-1 above, each column involves the derivative of $_v\mathbf{Z}$ w.r.t. a single entry of β , hence, the value of the derivative $\frac{\partial \beta}{\partial \beta_{21}}$ is equal for all entries in the column corresponding to β_{21} . Extending the derivative in eq.a1-2 to all the entries z_{pq} , $\forall 1 \leq p \leq 4 \& \forall 1 \leq q \leq 3$ and using rep.2, we get the following

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}\beta_{21}} = \mathbf{A} * \frac{\mathrm{d}\beta}{\mathrm{d}\beta_{21}} = \mathbf{A} * \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

where, the convolution is performed with the same padding and stride as that used for computing \mathbf{Z} . And, vectorizing the above derivative we get

$$\frac{\mathrm{d}_{v}\mathbf{Z}}{\mathrm{d}\beta_{21}} = \mathrm{vec}\left(\mathbf{A} * \frac{\mathrm{d}\beta}{\mathrm{d}\beta_{21}}\right) \qquad \text{eq.a1-3}$$

Extending the derivative in eq.a1-3 to all the entries β_{rs} , $\forall 1 \leq r \leq 2 \& \forall 1 \leq s \leq 2$, we get the following

$$\frac{\mathrm{d}_{v}\mathbf{Z}}{\mathrm{d}_{v}\beta} = \left[\operatorname{vec}\left(\mathbf{A} * \frac{\mathrm{d}\beta}{\mathrm{d}\beta_{1}1}\right) \quad \operatorname{vec}\left(\mathbf{A} * \frac{\mathrm{d}\beta}{\mathrm{d}\beta_{2}1}\right) \quad \operatorname{vec}\left(\mathbf{A} * \frac{\mathrm{d}\beta}{\mathrm{d}\beta_{1}2}\right) \quad \operatorname{vec}\left(\mathbf{A} * \frac{\mathrm{d}\beta}{\mathrm{d}\beta_{2}2}\right) \right]$$

$$\frac{d\mathbf{Z}}{d\mathbf{A}} = \text{reshape}(\frac{d_v\mathbf{Z}}{d_v\mathbf{A}})$$
:

$$\frac{\mathbf{d}_{v}\mathbf{Z}}{\mathbf{d}_{v}\mathbf{A}} = \begin{bmatrix} \frac{\partial}{\partial A_{11}} & \frac{\partial}{\partial A_{21}} & \dots & \frac{\partial}{\partial \beta_{34}} \end{bmatrix} \otimes_{v}\mathbf{Z}$$

$$= \begin{bmatrix} \frac{\partial_{v}\mathbf{Z}}{\partial A_{11}} & \frac{\partial_{v}\mathbf{Z}}{\partial A_{21}} & \dots & \frac{\partial_{v}\mathbf{Z}}{\partial A_{34}} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{\partial z_{11}}{\partial A_{11}} & \frac{\partial z_{11}}{\partial A_{21}} & \dots & \frac{\partial z_{11}}{\partial A_{34}} \\ \frac{\partial z_{21}}{\partial A_{11}} & \frac{\partial z_{21}}{\partial A_{21}} & \dots & \frac{\partial z_{21}}{\partial A_{34}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial z_{43}}{\partial A_{11}} & \frac{\partial z_{43}}{\partial A_{21}} & \dots & \frac{\partial z_{43}}{\partial A_{34}} \end{bmatrix}$$
eq.a2-1

Let's compute the value of an arbitrary element of this matrix, say derivative of z_{32} w.r.t. A_{23} (you should try out with some other combination of entries)

$$\begin{split} \frac{\partial z_{32}}{\partial A_{23}} &= \frac{\partial \left(a_{22}\beta_{11} + a_{23}A_{12} + a_{32}\beta_{21} + a_{33}\beta_{22}\right)}{\partial A_{23}} \quad \text{using rep.2} \\ &= \beta_{12} \\ &= \frac{\partial \left(\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} * \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix}\right)}{\partial A_{23}} \quad \text{using rep.1} \\ &= \frac{\partial \left(\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix}\right)}{\partial A_{23}} * \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} + \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} * \frac{\partial \left(\begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix}\right)}{\partial A_{23}} \\ &= \frac{\partial \left(\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix}\right)}{\partial A_{23}} * \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} * \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} \quad \text{eq.a2-2} \end{split}$$

In the matrix in eq.a2-1 above, each column involves the derivative of $_v\mathbf{Z}$ w.r.t. a single entry of \mathbf{A} , hence, the value of the derivative $\frac{\partial \mathbf{A}}{\partial A_{23}}$ is equal for all entries in the column corresponding to A_{23} . Extending the derivative in eq.a2-2 to all the entries z_{pq} , $\forall 1 \leq p \leq 4 \& \forall 1 \leq q \leq 3$ and using rep.2, we get the following

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}A_{23}} = \frac{\mathrm{d}\mathbf{A}}{\mathrm{d}A_{23}} * \beta = \begin{bmatrix} 0 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 0 \end{bmatrix} * \beta$$

where, the convolution is performed with the same padding and stride as that used for computing \mathbf{Z} . And, vectorizing the above derivative we get

$$\frac{\mathrm{d}_{v}\mathbf{Z}}{\mathrm{d}A_{23}} = \mathrm{vec}\left(\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}A_{23}} * \beta\right) \qquad \text{eq.a2-3}$$

Extending the derivative in eq.a2-3 to all the entries A_{rs} , $\forall 1 \leq r \leq 3 \& \forall 1 \leq s \leq 4$, we get the following

$$\frac{\mathrm{d}_{v}\mathbf{Z}}{\mathrm{d}_{v}\beta} = \left[\operatorname{vec} \left(\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}A_{11}} * \beta \right) \quad \operatorname{vec} \left(\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}A_{21}} * \beta \right) \quad \dots \quad \operatorname{vec} \left(\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}A_{34}} * \beta \right) \right]$$

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