

Proofs for Neural Network Library

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1 Math prem

Trace is cyclic.

$$\text{trace}(AB) = \text{trace}(BA)$$

Dot product is related with trace in this fashion.

$$\langle A, B \rangle = \text{trace}(A^T B)$$

$$\text{trace}(ABC) = \text{trace}(BCA) = \text{trace}(CAB)$$

$$\langle AB, C \rangle = \text{trace}((AB)^T C)$$

$\text{trace}(s) = s$, if s is scalar.

Common notion of gradient form in multi-dimension input and output.

$$\Delta y = \langle \frac{dy}{dx}, \Delta x \rangle = \frac{dy^T}{dx} \Delta x = \text{trace}(\frac{dy^T}{dx} \Delta x)$$

2 Neural Network

y_0 be input, y^* be label (desired output). N_1, N_2, \dots, N_m be m layers.

$$y_i = N_i(y_{i-1})$$

So, y_m is the output of NN (Neural Network). Let L be the loss function,

$$l = L(y_m, y^*)$$

3 mse

Let $x \in \mathbf{R}^n$ be input, $y^* \in \mathbf{R}^m$ be the label, $y \in \mathbf{R}^m$ be the output of mse layer.

Let $L \in \mathbf{R}$ be mean squared loss.

3.0.1 Forward pass

$$y = L(x, y^*) = 1/2 \|x - y^*\|^2$$

3.1 Backward pass

$$dy := \frac{dL}{dy} = \frac{dL}{dL} = 1$$

$$y = 1/2(x - y^*)^T(y_m - y^*)$$

$$\begin{aligned}\Delta y &= 1/2(x + \Delta x - y^*)^T(x + \Delta x - y^*) - 1/2(x - y^*)^T(x - y^*) \\ &= 1/2((\Delta x)^T(x - y^*) + (x - y^*)^T \Delta x + (\Delta x)^T \Delta x) \\ &= \Delta x^T(x - y^*) \\ &= \langle (x - y^*), \Delta x \rangle\end{aligned}$$

We got,

$$\begin{aligned}\Delta y &= \langle (x - y^*), \Delta x \rangle \\ \Rightarrow \frac{dy}{dx} &= (x - y^*)\end{aligned}$$

By chain rule,

$$\frac{dL}{dx} = \frac{dL}{dy} \frac{dy}{dx}$$

Putting the values,

$$\begin{aligned}\frac{dL}{dx} &= (dy)(x - y^*) = (x - y^*) \\ dx &:= \frac{dL}{dx} = dy(x - y^*)\end{aligned}$$

3.2 Weight gradient

Since, there is no weights in mse layer, so nothing is required.

4 Linear

Let $x \in \mathbf{R}^n$ be input, $y \in \mathbf{R}^m$ be the output of linear layer. $w \in \mathbf{R}^{m \times n}$ be the weight matrix and $L \in \mathbf{R}$ be loss. $dy := \frac{dL}{dy} \in \mathbf{R}^m$ be output loss gradient.

4.1 forward pass

$$y = wx$$

4.2 backward pass

$$\begin{aligned}y &= wx \\ \Delta y &= w(x + \Delta x) - wx = w\Delta x \\ \Delta L &= \left\langle \frac{dL}{dy}, \Delta y \right\rangle \\ &= \left\langle \frac{dL}{dy}, w\Delta x \right\rangle \\ &= \frac{dL}{dy}^T w \Delta x \\ &= \left(\frac{dL}{dy}^T w \right) \Delta x \\ &= \left\langle \left(\frac{dL}{dy}^T w \right)^T, \Delta x \right\rangle \\ &= \left\langle w^T \frac{dL}{dy}, \Delta x \right\rangle\end{aligned}$$

So we got the terms in required form,

$$\begin{aligned}\Delta L &= \left\langle w^T \frac{dL}{dy}, \Delta x \right\rangle \\ \frac{dL}{dx} &= w^T \frac{dL}{dy} \\ dx &:= \frac{dL}{dx} = w^T \frac{dL}{dy}\end{aligned}$$

4.3 Gradient pass

$$\begin{aligned}y &= wx \\ \Delta y &= (w + \Delta w)x - wx = \Delta wx \\ \Delta L &= \left\langle \frac{dL}{dy}, \Delta y \right\rangle \\ &= \left\langle \frac{dL}{dy}, \Delta wx \right\rangle \\ &= \frac{dL}{dy}^T \Delta wx \\ &= \text{trace}\left(\frac{dL}{dy}^T \Delta wx\right) \\ &= \text{trace}\left(x \frac{dL}{dy}^T \Delta w\right)\end{aligned}$$

$$\begin{aligned}
&= \langle x \frac{dL}{dy}^T, \Delta w \rangle \\
&= \langle \frac{dL}{dy} x^T, \Delta w \rangle
\end{aligned}$$

we got,

$$\begin{aligned}
\Delta L &= \langle \frac{dL}{dy} x^T, \Delta w \rangle \\
\Rightarrow \frac{dL}{dw} &= \frac{dL}{dy} x^T
\end{aligned}$$

5 Add

Let $x \in \mathbf{R}^n$ be input, $y \in \mathbf{R}^n$ be the output of linear layer. $w \in \mathbf{R}^n$ be the weight matrix and $L \in \mathbf{R}$ be loss. $dy := \frac{dL}{dy} \in \mathbf{R}^n$ be output loss gradient.

5.1 Forward pass

$$y = x + w$$

5.2 Backward pass

$$\begin{aligned}
y &= x + w \\
\Delta y &= x + \Delta x + w - (x + w) = \Delta x \\
\Delta L &= \langle \frac{dL}{dy}, \Delta y \rangle \\
\Delta L &= \langle \frac{dL}{dy}, \Delta x \rangle \\
\Rightarrow \frac{dL}{dx} &= \frac{dL}{dy}
\end{aligned}$$

5.3 Gradient pass

$$\begin{aligned}
y &= x + w \\
\Delta y &= x + \Delta w + w - (x + w) = \Delta w \\
\Delta L &= \langle \frac{dL}{dy}, \Delta y \rangle \\
\Delta L &= \langle \frac{dL}{dy}, \Delta w \rangle \\
\Rightarrow \frac{dL}{dw} &= \frac{dL}{dy}
\end{aligned}$$

6 Convolution with infinite dimension input

Let $x \in \mathbf{R}^\infty$ be input, $y \in \mathbf{R}^\infty$ be the output of convolution layer. $w \in \mathbf{R}^\infty$ be the weight matrix (filter) and $L \in \mathbf{R}$ be loss. $dy := \frac{dL}{dy} \in \mathbf{R}^\infty$ be output loss gradient.

We take $x \in \mathbf{R}^\infty$ to ignore the mode of padding (like 'full', 'valid', 'same', 'custom') in convolution, as in infinite dimensional input padding of input is meaningless. It makes proof little simple and yet conveys basic idea. Proof follows even if $w \in \mathbf{R}^k$ but breaks down with finite dimensional input. Reader is encouraged to find out in below proof where it would break down in case of finite-dimensional input.

Note - All summation index below runs from $-\infty$ to ∞

6.1 Definition

- Correlation

$$y = x \odot w$$

$$y_i := \sum_j x_{i+j} w_j$$

- Convolution

$$y = x \otimes w$$

$$y_i := \sum_j x_{i-j} w_j$$

6.2 Properties

Linearity of Convolution and Correlation

$$(A + B) \odot C = A \odot C + B \odot C$$

$$A \odot (B + C) = A \odot B + A \odot C$$

$$(A + B) \otimes C = A \otimes C + B \otimes C$$

$$A \otimes (B + C) = A \otimes B + A \otimes C$$

It is very easy to verify from the definition above.

Dot product with correlation and convolution

$$1) \quad \langle A, B \odot C \rangle = \langle C, B \odot A \rangle$$

$$2) \quad \langle A, B \otimes C \rangle = \langle A, B \otimes A \rangle$$

$$3) \quad \langle A, B \odot C \rangle = \langle B, A \otimes C \rangle$$

$$4) \quad \langle A, B \otimes C \rangle = \langle B, A \odot C \rangle$$

Proof,

$$1) \quad \langle A, B \odot C \rangle = \sum_i A_i (B \odot C)_i \quad \text{—def of dot product}$$

$$= \sum_i A_i (\sum_j B_{i+j} C_j) \quad \text{— def of correlation}$$

$$= \sum_i \sum_j A_i B_{i+j} C_j$$

$$= \sum_j \sum_i C_j B_{i+j} A_i \quad - \text{switching summation}$$

$$= \sum_j C_j \sum_i B_{i+j} A_i$$

$$= \sum_j C_j (\sum_i B_{i+j} A_i)$$

$$= \sum_j C_j (B \odot A)_j \quad - \text{def of correlation}$$

$$< C, B \odot A > \quad - \text{def dot product}$$

2). Similary,

$$< A, B \otimes C > = < A, B \otimes A > \quad \text{just interchanging correlation and convolution.}$$

$$3). < A, B \odot C > = \sum_i A_i (B \odot C)_i \quad - \text{def of dot product}$$

$$= \sum_i A_i (\sum_p B_{i+j} C_j) \quad - \text{def of correlation.}$$

$$= \sum_i \sum_p A_i B_{i+j} C_j \quad -$$

Change of variable, putting $p = i + j$ and $j = j$, $\Rightarrow i = p - j$

$$= \sum_p \sum_p A_{p-j} B_p C_j$$

$$= \sum_p B_p (\sum_p A_{p-j} C_j)$$

$$= \sum_p B_p (A \otimes C)_p$$

$$< B, A \otimes C >$$

$$4) \text{ Similary, } < A, B \otimes C > = < B, A \odot C >$$

7 Correlation1D

$x \in \mathbf{R}^n$ is input, $y \in \mathbf{R}^m$ is output, $w \in \mathbf{R}^{k \times l}$ is filter, $L \in \mathbf{R}$ is scalar valued Loss/cost.

7.1 Forward Pass

$$y = x \odot w$$

7.2 Backward Pass

$$y = x \odot w$$

$$\Delta y = (x + \Delta x) \odot w - x \odot w$$

$$= \Delta x \odot w$$

$$\Delta L = \langle \frac{dL}{dy}, \Delta y \rangle$$

$$= \langle \frac{dL}{dy}, \Delta x \odot w \rangle$$

$$= \langle \Delta x, \frac{dL}{dy} \otimes w \rangle$$

$$= \langle \frac{dL}{dy} \odot w, \Delta x \rangle$$

So, we got things in desired form,

$$\Delta L = \langle \frac{dL}{dy} \otimes w, \Delta x \rangle$$

$$\Rightarrow \frac{dL}{dx} = \frac{dL}{dy} \otimes w$$

7.3 Gradient Pass

$$y = x \odot w$$

$$\Delta y = x \odot (w + \Delta w) - x \odot w$$

$$= x \odot \Delta w$$

$$\Delta L = \langle \frac{dL}{dy}, \Delta y \rangle \quad - \text{ def of } \Delta$$

$$= \langle \frac{dL}{dy}, x \odot \Delta w \rangle \quad - \text{ putting value of } \Delta y$$

$$= \langle \Delta w, x \odot \frac{dL}{dy} \rangle \quad - \text{ switching variable, see property 6.2.1}$$

$$= \langle x \odot \frac{dL}{dy}, \Delta w \rangle$$

So, we got things in desired form,

$$\Delta L = \langle x \odot \frac{dL}{dy}, \Delta w \rangle$$

$$\Rightarrow \frac{dL}{dw} = x \odot \frac{dL}{dy}$$