Notation Glossary:

z_j^l	Pre-Activation of j^{th} neuron in the l^{th} layer
a_j^l	(Post)-Activation of j^{th} neuron in the l^{th} layer
x_k	Input (0^{th}) layer activations
$A()$	General element-wise activation function
w_{jk}^l	Weight matrix of l^{th} layer
b_j^l	Bias vector of l^{th} layer
g_{jk}^l	Jacobian between layer l and $l-1$
J_{jk}^l	Jacobian between input (0^{th}) layer and layer l
H_{jk}^l	Diagonal Hessian between input (0^{th}) layer and layer l
$\odot$	Direct product over repeated index rather than summation

Network Jacobian:

In following derivations assume the standard feed forward relationships:

$$a_j^l = A(z_j^l) \tag{1}$$

$$z_j^l = \sum_k w_{jk}^l a_k^{l-1} + b_j^l \tag{2}$$

Note that the network's output corresponds to the L^{th} layer activations a_j^L. Begin by considering the layer to layer Jacobian:

$$\frac{\partial a_j^l}{\partial a_k^{l-1}} = \sum_q \frac{\partial a_j^l}{\partial z_q^l} \frac{\partial z_q^l}{\partial a_k^{l-1}} \tag{3}$$

$$= \sum_q \frac{\partial a_j^l}{\partial z_q^l} w_{qk}^l \tag{4}$$

$$g_{jk}^l = A'(z_j^l) \odot w_{jk}^l \tag{5}$$

Going 1 more layer back:

$$\frac{\partial a_j^l}{\partial a_k^{l-2}} = \sum_q \left[(A'(z_j^l) \odot w_{jq}^l)(A'(z_q^{l-1}) \odot w_{qk}^{l-1}) \right] \tag{6}$$

$$= \sum_q g_{jq}^l g_{qk}^{l-1} \tag{7}$$

This relationship can be recurred to obtain:

$$J_{jk}^l \equiv \frac{\partial a_j^l}{\partial x_k} = \sum_{\alpha,\beta...} g_{j\alpha}^l g_{\alpha\beta}^{l-1} ... g_{\mu k}^1 \tag{8}$$

Network Hessian:

The general l^{th} layer Hessian can be expressed as:

$$H_{jkm}^l \equiv \frac{\partial^2 a_j^l}{\partial x_m \partial x_k} = \frac{\partial J_{jk}^l}{\partial x_m} \tag{9}$$

For constructing Physics Loss functions, often only the diagonal Hessian is needed. Let:

$$\sum_k \delta_{mk} H^l_{jkm} \equiv H^l_{jk} \tag{10}$$

A further useful property of the full Hessian is its symmetry in the 2^{nd} and 3^{rd} indices (by property of partial derivatives):

$$H_{jkm} = H_{jmk} \tag{11}$$

We can also note the useful base cases:

$$J^0_{jk} = \delta_{jk} \tag{12}$$

$$H^0_{jkm} = 0 \tag{13}$$

To derive the full Hessian we consider a recursive method and start from:

$$J^l_{jk} \equiv \sum_q g^l_{jq} J^{l-1}_{qk} = \sum_q \left[A'(z^l_j) \odot w^l_{jq} J^{l-1}_{qk} \right] \tag{14}$$

Considering the Hessian as the derivative of the Jacobian:

$$H^l_{jkm} = \frac{\partial}{\partial x_m} \sum_q \left[A'(z^l_j) \odot w^l_{jq} J^{l-1}_{qk} \right] \tag{15}$$

$$= \sum_q \left[A''(z^l_j) \odot \frac{\partial z^l_j}{\partial x_m} \odot w^l_{jq} J^{l-1}_{qk} + A'(z^l_j) \odot w^l_{jq} \frac{\partial J^{l-1}_{qk}}{\partial x_m} \right] \tag{16}$$

We can recover several familiar terms from this expression, starting with

$$\frac{\partial J^{l-1}_{qk}}{\partial x_m} \equiv H^{l-1}_{qkm}, \tag{17}$$

and likewise, simplifying the first term:

$$\frac{\partial z^l_j}{\partial x_m} = \frac{\partial}{\partial x_m} \sum_q \left[w^l_{jq} a^{l-1}_q + b^l_j \right] = \sum_q w^l_{jq} \frac{\partial a^{l-1}_q}{\partial x_m} = \sum_q w^l_{jq} J^{l-1}_{qm}. \tag{18}$$

Putting these expressions together we yield a recursion relation for the full Hessian:

$$H^l_{jkm} = \sum_q \left[A''(z^l_j) \odot (w^l_{jq})^2 J^{l-1}_{qm} J^{l-1}_{qk} + A'(z^l_j) \odot w^l_{jq} H^{l-1}_{qkm} \right] \tag{19}$$

Finally, we can contract over $m \,\&\, k$ to obtain the diagonal Hessian of the l^{th} layer activations (with respect to the inputs x_k:

$$H^l_{jk} = \sum_q \left[A''(z^l_j) \odot (w^l_{jq} J^{l-1}_{qk})^2 + A'(z^l_j) \odot w^l_{jq} H^{l-1}_{qk} \right] \tag{20}$$

Jacobian and Hessian Loss Derivatives:

If we construct a Physics Loss using Jacobian and/or diagonal Hessian terms, we will need to propagate the according loss derivative through the network (standard backpropagation). This will require: $\frac{\partial J^L_{jk}}{\partial a^L_m}$

and $\frac{\partial H^L_{jk}}{\partial a^L_m}$. We begin with the simpler Jacobian using the form $J^l_{jk} = \sum_m A'(z^l_j) \odot w^l_{jm} J^{l-1}_{mk}$. First, a useful yet somewhat counterintuitive result is derived for $\frac{\partial J^{l-1}_{jk}}{\partial a^l_m}$ which is *not* in fact zero.

$$\frac{\partial a^l_m}{\partial J^{l-1}_{jk}} = \sum_p \frac{\partial a^l_m}{\partial x_p} \frac{\partial x_p}{\partial J^{l-1}_{jk}} \tag{21}$$

$$= \sum_p \frac{J^l_{mp}}{H^{l-1}_{jkp}} \tag{22}$$

$$\frac{\partial J^{l-1}_{jk}}{\partial a^l_m} = \sum_p \frac{H^{l-1}_{jkp}}{J^l_{mp}} \tag{23}$$

For the Jacobian derivative, a recursion relation is not needed and we can evaluate it directly for the L^{th} (output) layer:

$$\frac{\partial J^L_{jk}}{\partial a^L_m} = \frac{\partial}{\partial a^L_m} \sum_q \left[A'(z^L_j) \odot w^L_{jq} J^{L-1}_{qk} \right] \tag{24}$$

$$= \sum_q \left[A''(z^L_j) \odot \frac{\partial z^L_j}{\partial a^L_m} w^L_{jq} J^{L-1}_{qk} \right] + \sum_q \left[A'(z^L_j) \odot w^L_{jq} \frac{\partial J^{L-1}_{qk}}{\partial a^L_m} \right] \tag{25}$$

$$= \sum_q \left[\delta_{jm} \frac{A''(z^L_j)}{A'(z^L_m)} \odot w^L_{jq} J^{L-1}_{qk} \right] + \sum_{q,r} \left[A'(z^L_j) \odot w^L_{jq} \frac{H^{L-1}_{qkr}}{J^L_{mr}} \right] \tag{26}$$

$$= \delta_{jm} \frac{A''(z^L_j)}{[A'(z^L_m)]^2} \odot J^L_{jk} + \sum_{q,r} \left[A'(z^L_j) \odot w^L_{jq} \frac{H^{L-1}_{qkr}}{J^L_{mr}} \right] \tag{27}$$

The derivation for the Hessian derivative follows much of the same logic but is recursive (thus we consider it for a general l^{th} layer):

$$\frac{\partial H^l_{jk}}{\partial a^l_m} = \frac{\partial}{\partial a^l_m} \sum_q \left[A''(z^l_j) \odot \left(w^l_{jq} J^{l-1}_{qk} \right)^2 + A'(z^l_j) \odot w^l_{jq} H^{l-1}_{qk} \right] \tag{28}$$

$$\begin{aligned} &= \sum_q \Bigg[\delta_{jm} \frac{A'''(z^l_j)}{A'(z^l_m)} \odot \left(w^l_{jq} J^{l-1}_{qk} \right)^2 + 2A''(z^l_j) \odot w^l_{jq} \sum_p \left(\frac{H^{l-1}_{qkp}}{J^l_{mp}} \right) \\ &\quad + \delta_{jm} \frac{A''(z^l_j)}{A'(z^l_m)} \odot w^l_{jq} H^{l-1}_{qk} + A'(z^l_j) \odot w^l_{jq} \frac{\partial H^{l-1}_{qk}}{\partial a^l_m} \Bigg] \end{aligned} \tag{29}$$

The only problematic term here is $\frac{\partial H^{l-1}_{qk}}{\partial a^l_m}$ as it does not immediately lend itself to an obvious recursion relation. However, we can consider:

$$\frac{\partial H^{l-1}_{qk}}{\partial a^l_m} = \sum_p \frac{\partial H^{l-1}_{qk}}{\partial a^{l-1}_p} \frac{\partial a^{l-1}_p}{\partial a^l_m} \tag{30}$$

$$= \sum_p \frac{\partial H^{l-1}_{qk}}{\partial a^{l-1}_p} \frac{1}{A'(z^l_m) \odot w^l_{mp}} \tag{31}$$

This *does* seem recursive and we can also spot the base case for $l = 1$:

$$\frac{\partial H^0_{qk}}{\partial a^1_m} = \sum_p \frac{\partial H^0_{qk}}{\partial a^0_m} \frac{1}{A'(z^1_m) \odot w^1_{mp}} \tag{32}$$

$$= 0 \tag{33}$$

Where we have used the fact that $a_p^0 \equiv x_k$ (the input layer activations are identical to the model inputs) and from earlier we noted that $H_{jk}^0 = 0$. Performing the first recursion iteration to demonstrate:

$$\frac{\partial H_{jk}^1}{\partial a_m^1} = \sum_q \delta_{jm} \frac{A'''(z_j^1)}{A'(z_m^1)} \odot \left(w_{jq}^1 J_{qk}^0\right)^2 \tag{34}$$

All the terms proportional to H_{jkm}^0, H_{jk}^0 or $\frac{\partial H_{jk}^0}{\partial a_m^1}$ are zero. For completeness, this is substituted into the earlier equation to give:

$$\frac{\partial H_{jk}^l}{\partial a_m^l} = \frac{\partial}{\partial a_m^l} \sum_q \left[A''(z_j^l) \odot \left(w_{jq}^l J_{qk}^{l-1}\right)^2 + A'(z_j^l) \odot w_{jq}^l H_{qk}^{l-1}\right] \tag{35}$$

$$\begin{aligned} &= \sum_q \Bigg[\delta_{jm} \frac{A'''(z_j^l)}{A'(z_m^l)} \odot \left(w_{jq}^l J_{qk}^{l-1}\right)^2 + 2A''(z_j^l) \odot w_{jq}^l \sum_p \left(\frac{H_{qkp}^{l-1}}{J_{mp}^l}\right) \\ &\quad + \delta_{jm} \frac{A''(z_j^l)}{A'(z_m^l)} \odot w_{jq}^l H_{qk}^{l-1} + A'(z_j^l) \odot w_{jq}^l \sum_p \left(\frac{\partial H_{qk}^{l-1}}{\partial a_p^{l-1}} \frac{1}{A'(z_m^l) \odot w_{mp}^l}\right)\Bigg] \end{aligned} \tag{36}$$