Module 4.5: Backpropagation: Computing Gradients w.r.t. the Output Units

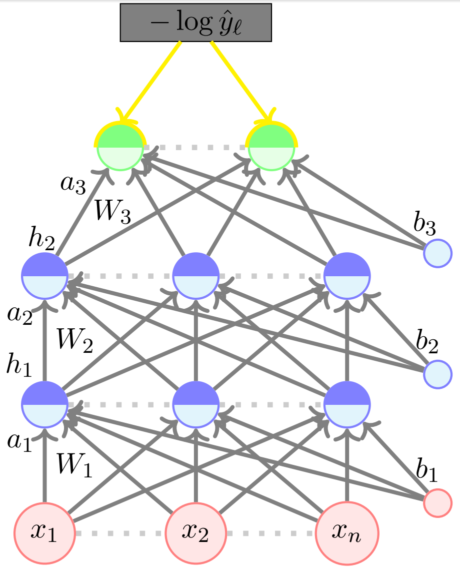
Quantities of interest (roadmap for the remaining part):

- Gradient w.r.t. output units
- Gradient w.r.t. hidden units
- Gradient w.r.t. weights

$$\underbrace{\frac{\partial \mathscr{L}(\theta)}{\partial W_{111}}}_{\text{Talk to the weight directly}} = \underbrace{\frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_3}}_{\text{Talk to the output layer}} \underbrace{\frac{\partial a_3}{\partial h_2} \frac{\partial h_2}{\partial a_2}}_{\text{Talk to the previous hidden layer}} \underbrace{\frac{\partial a_2}{\partial h_1} \frac{\partial h_1}{\partial a_1}}_{\text{Talk to the previous hidden layer}} \underbrace{\frac{\partial a_1}{\partial W_{111}}}_{\text{and now talk to the weights}}$$

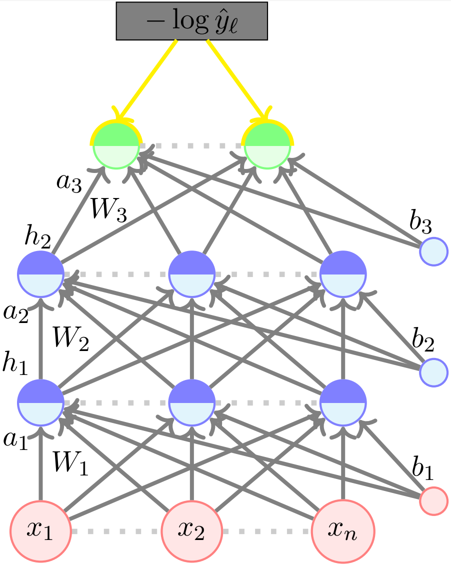
- Our focus is on *Cross entropy loss* and *Softmax* output.

Let us first consider the partial derivative w.r.t. i-th output



Let us first consider the partial derivative w.r.t. i-th output

$$\mathscr{L}(\theta) = -\log \hat{y}_\ell \quad (\ell = \text{true class label})$$



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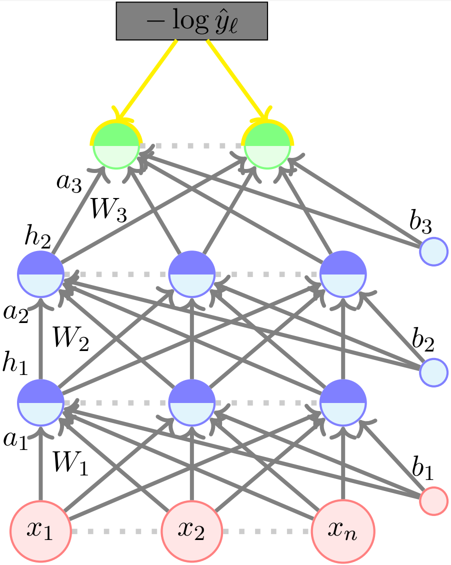
$$\frac{\partial}{\partial \hat{y}_i}(\mathscr{L}(\theta)) =$$



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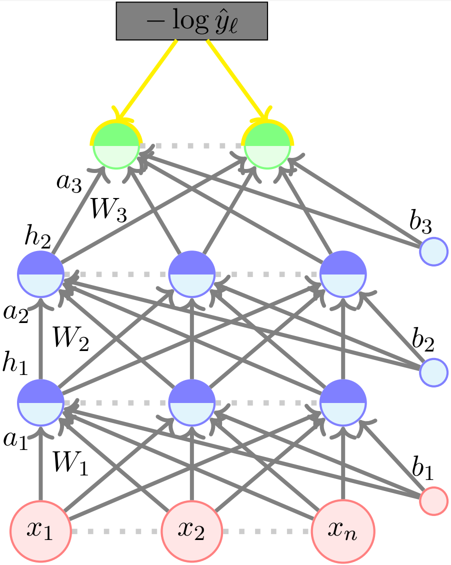

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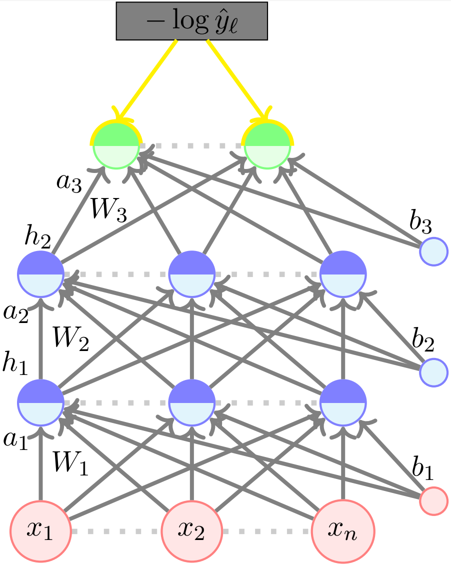
$$= -\frac{1}{\hat{y}_\ell} \quad \text{if } i = \ell$$



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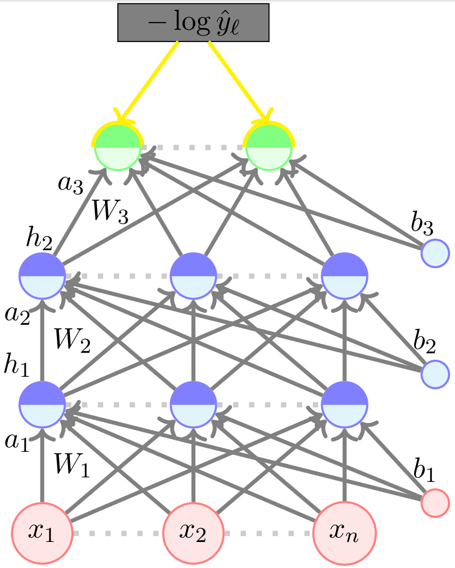
$$= 0 \qquad \textit{otherwise}$$



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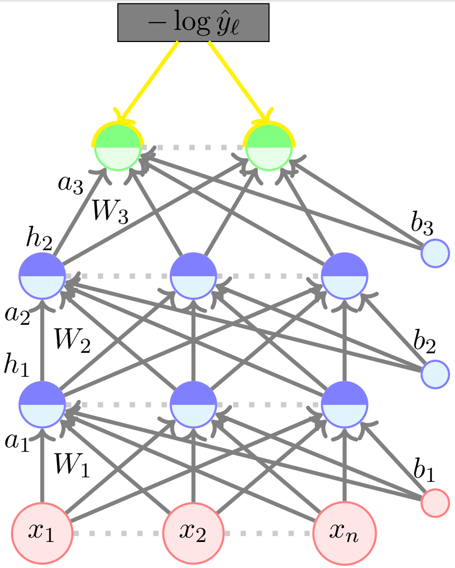
More compactly,



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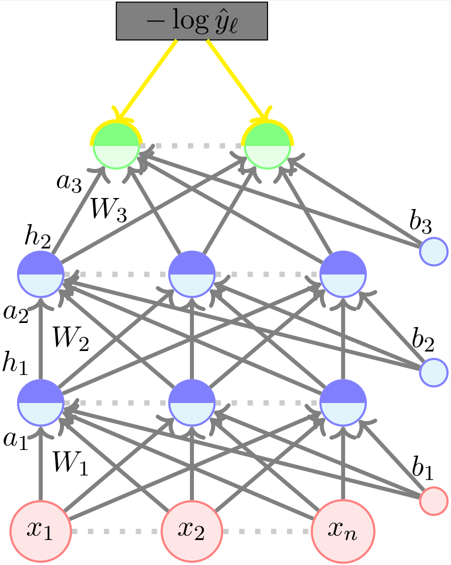
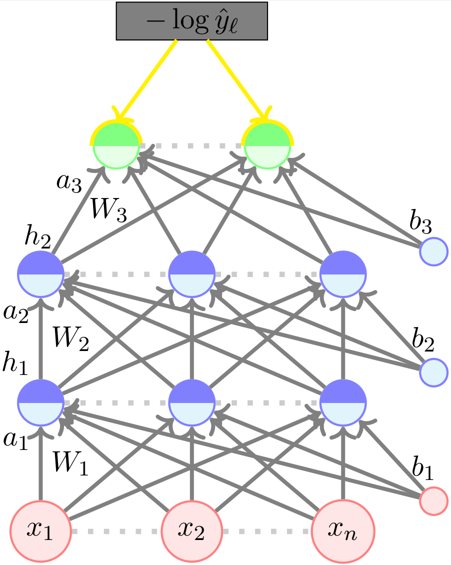
More compactly,

$$\frac{\partial}{\partial \hat{y}_i}(\mathscr{L}(\theta)) = -\frac{\mathbb{1}_{(i=\ell)}}{\hat{y}_\ell}$$

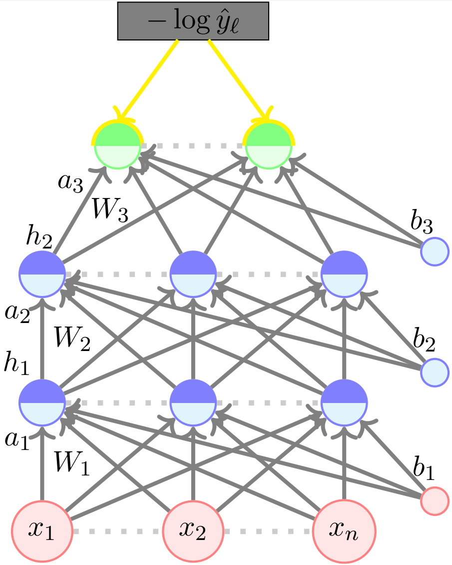


$$\frac{\partial}{\partial \hat{y}_i}\left(\mathscr{L}(\theta)\right) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$



$$\frac{\partial}{\partial \hat{y}_i}(\mathscr{L}(\theta)) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$

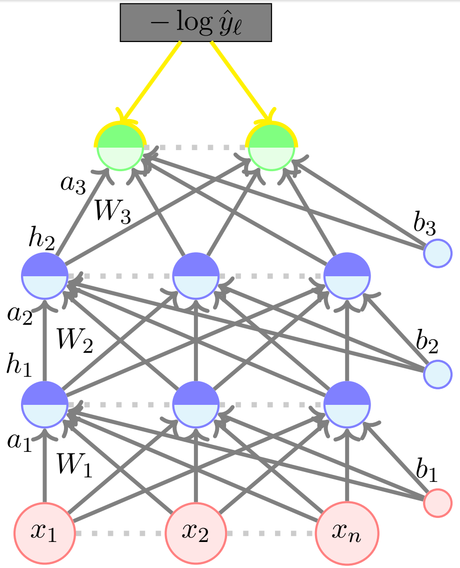
We can now talk about the gradient w.r.t. the vector $\hat{y}$



$$\frac{\partial}{\partial \hat{y}_i}(\mathscr{L}(\theta)) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$

We can now talk about the gradient w.r.t. the vector $\hat{y}$

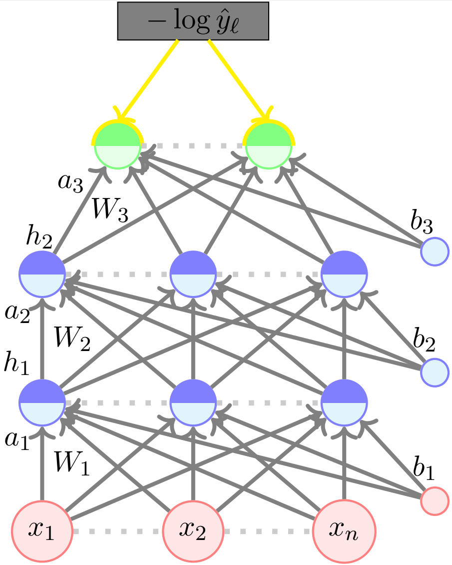
$$\nabla_{\hat{\mathbf{y}}}\mathscr{L}(\theta) = \begin{bmatrix} \\ \\ \\ \end{bmatrix}$$



$$\frac{\partial}{\partial \hat{y}_i}(\mathscr{L}(\theta)) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$

We can now talk about the gradient w.r.t. the vector $\hat{y}$

$$\nabla_{\hat{\mathbf{y}}}\mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}_1} \\ \\ \\ \end{bmatrix}$$



$$\frac{\partial}{\partial \hat{y}_i}(\mathscr{L}(\theta)) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$

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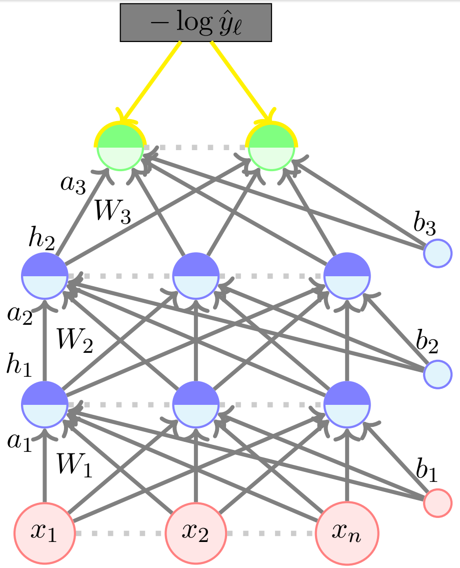
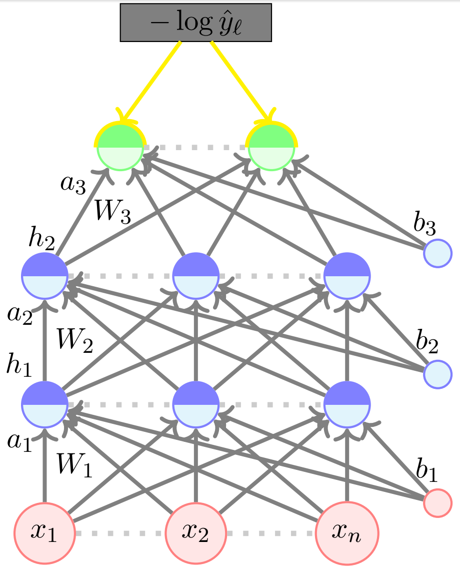
$$\nabla_{\hat{\mathbf{y}}}\mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}_1} \\ \vdots \\ \\ \end{bmatrix}$$



$$\frac{\partial}{\partial \hat{y}_i}\left(\mathscr{L}(\theta)\right) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$

We can now talk about the gradient w.r.t. the vector $\hat{y}$

$$\nabla_{\hat{\mathbf{y}}}\mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}_1} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}_k} \end{bmatrix}$$



$$\frac{\partial}{\partial \hat{y}_i}(\mathscr{L}(\theta)) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$

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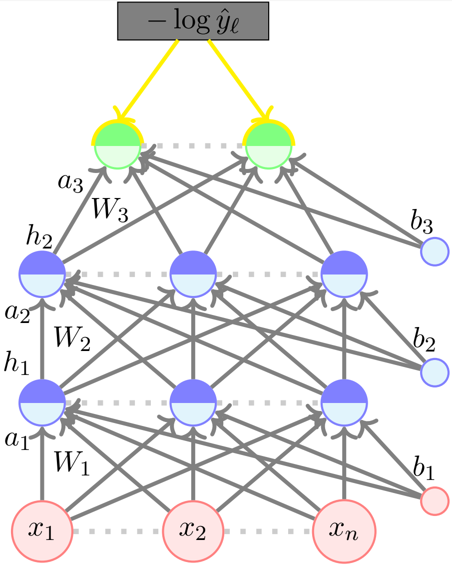
$$\nabla_{\hat{\mathbf{y}}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}_1} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}_k} \end{bmatrix} = -\frac{1}{\hat{y}_\ell}$$



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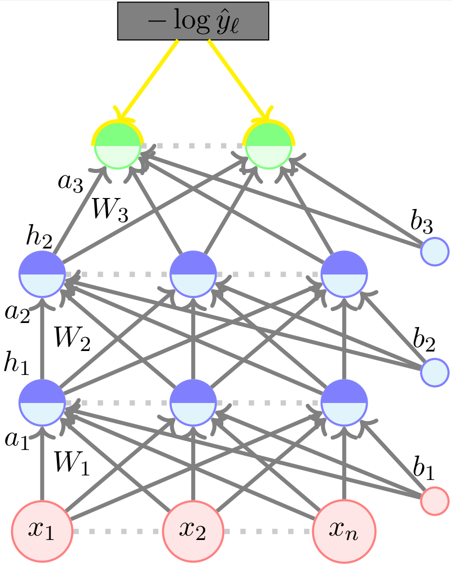

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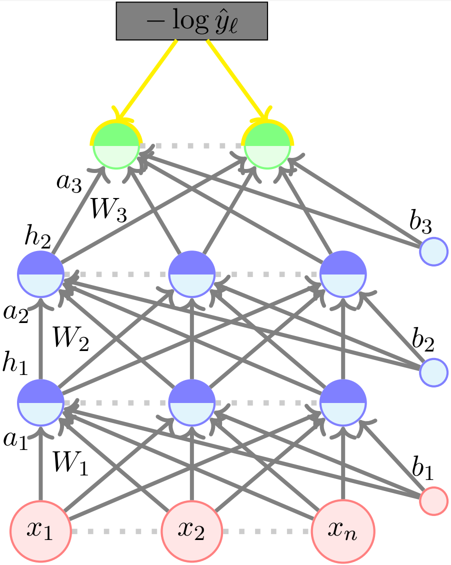

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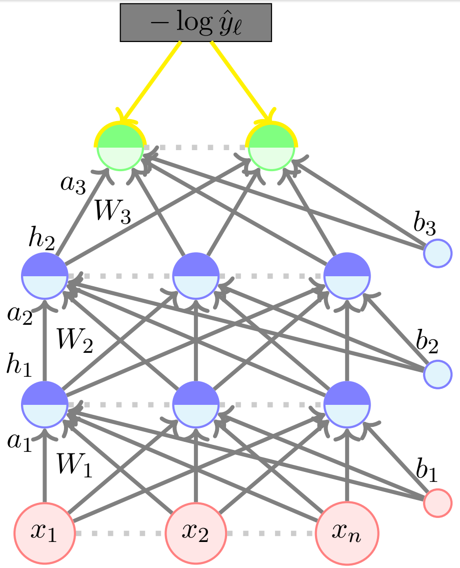

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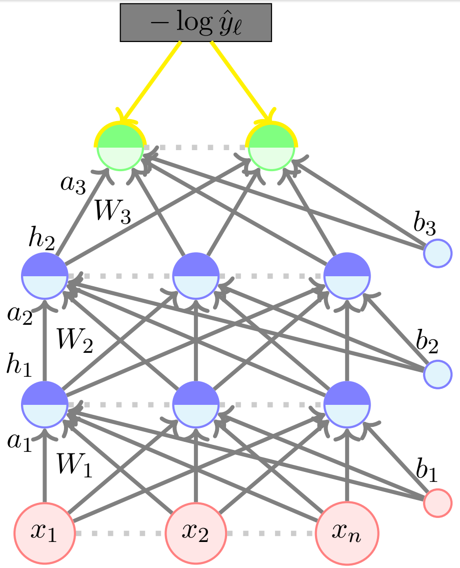

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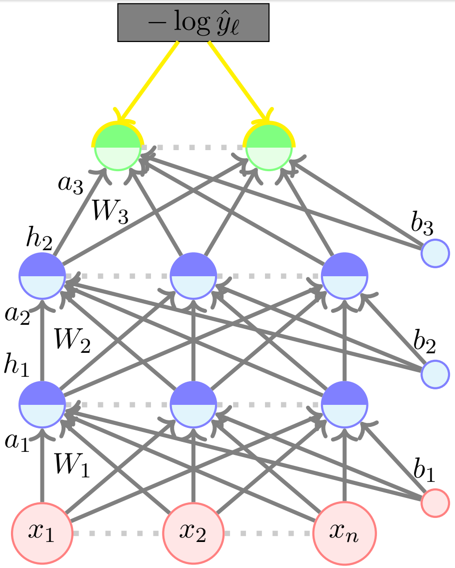

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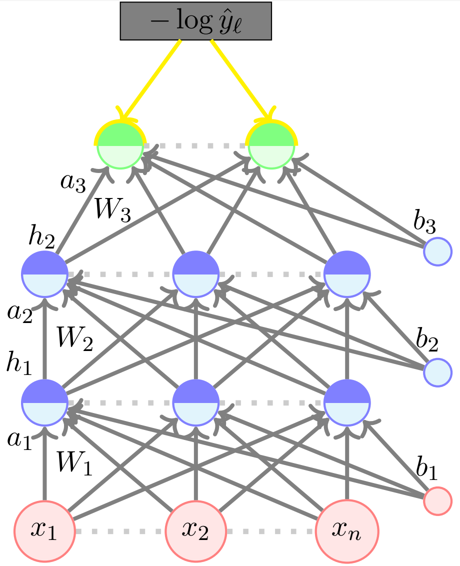
$$= -\frac{1}{\hat{y}_\ell} e_\ell$$



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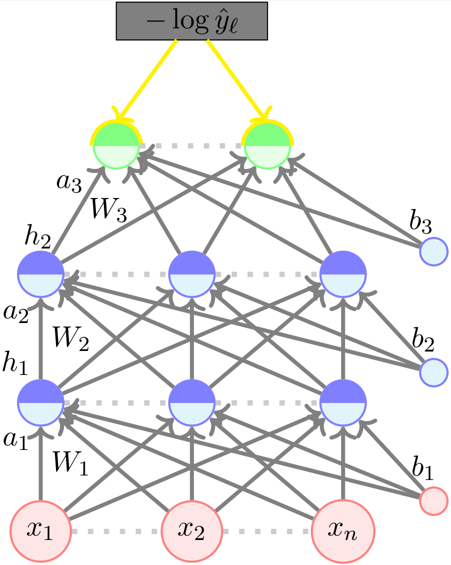
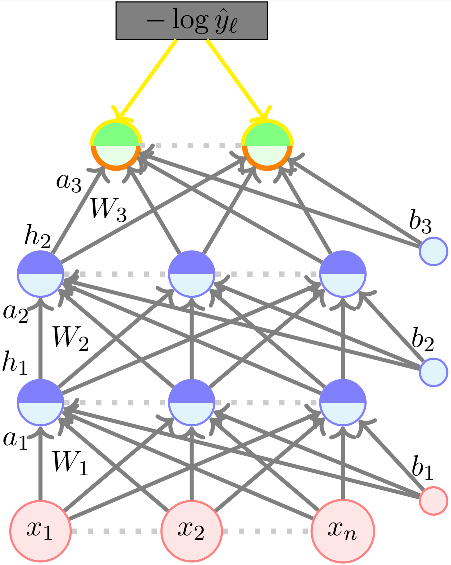
$$= -\frac{1}{\hat{y}_\ell} e_\ell$$

where $e(\ell)$ is a k-dimensional vector whose ℓ-th element is 1 and all other elements are 0.



What we are actually interested in is

$$\frac{\partial \mathscr{L}(\theta)}{\partial a_{Li}} = \frac{\partial(-\log \hat{y}_\ell)}{\partial a_{Li}}$$



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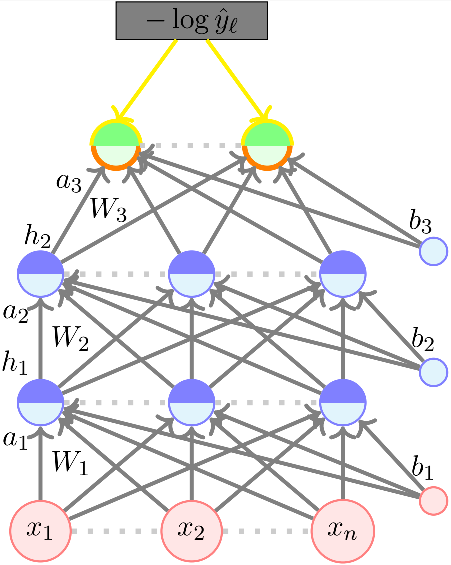

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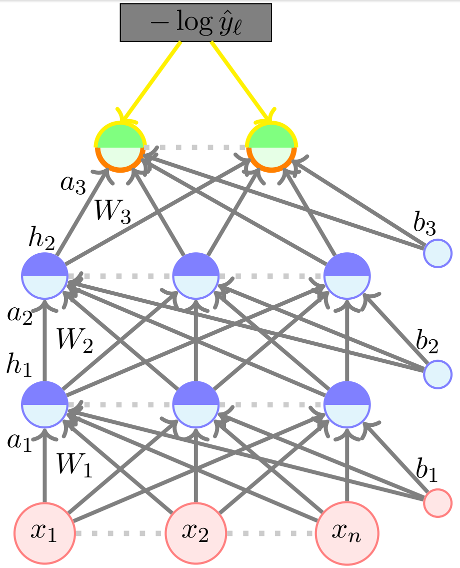
Does $\hat{y}_\ell$ depend on a_{Li} ?



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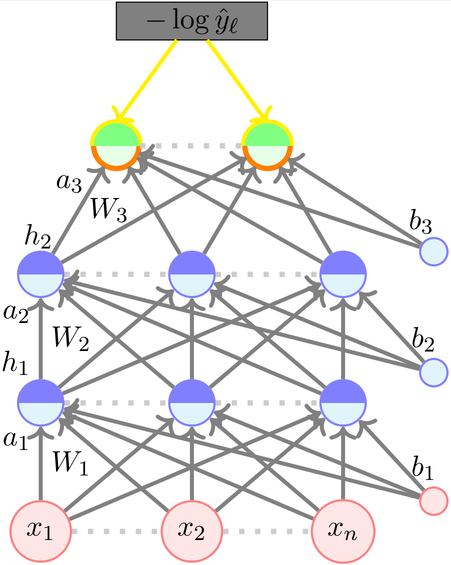
Does $\hat{y}_\ell$ depend on a_{Li} ? Indeed, it does.



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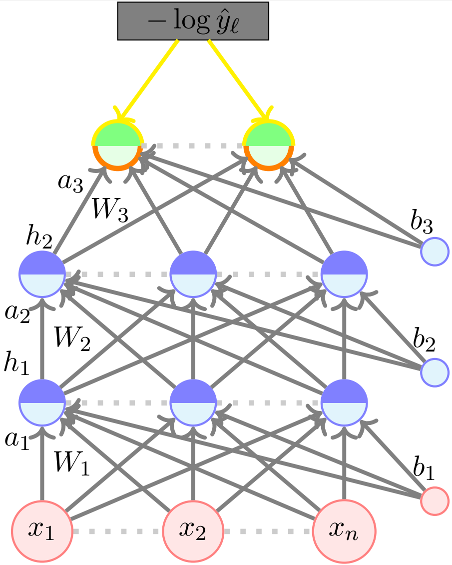
Does $\hat{y}_\ell$ depend on a_{Li} ? Indeed, it does.

$$\hat{y}_\ell = \frac{exp(a_{L\ell})}{\sum_i exp(a_{Li})}$$



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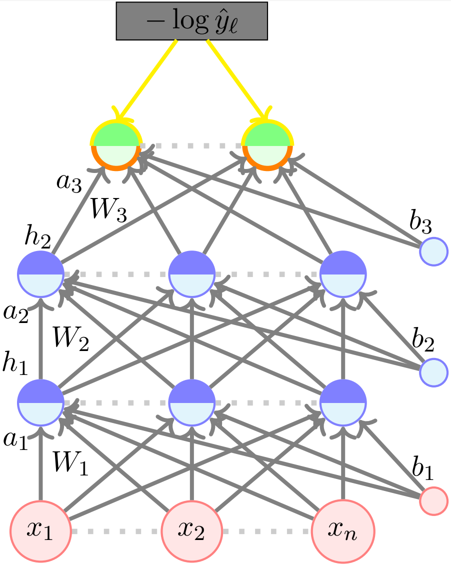
Does $\hat{y}_\ell$ depend on a_{Li} ? Indeed, it does.

$$\hat{y}_\ell = \frac{exp(a_{L\ell})}{\sum_i exp(a_{Li})}$$

Having established this, we will now derive the full expression on the next slide



$$\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell =$$

$$\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell = \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \hat{y}_\ell$$

$$\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell = \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \hat{y}_\ell$$

$$= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} softmax(\mathbf{a}_L)_\ell$$

$$
\begin{aligned}
\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell &= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \hat{y}_\ell \\
&= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} softmax(\mathbf{a}_L)_\ell \\
&= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_\ell}
\end{aligned}
$$

$$\begin{aligned}\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell &= \frac{-1}{\hat{y}_\ell}\frac{\partial}{\partial a_{Li}}\hat{y}_\ell \\ &= \frac{-1}{\hat{y}_\ell}\frac{\partial}{\partial a_{Li}} softmax(\mathbf{a}_L)_\ell \\ &= \frac{-1}{\hat{y}_\ell}\frac{\partial}{\partial a_{Li}} \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'}\exp(\mathbf{a}_L)_\ell}\end{aligned}$$

$$\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x}\frac{1}{h(x)} - \frac{g(x)}{h(x)^2}\frac{\partial h(x)}{\partial x}$$

$$
\begin{aligned}
\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell &= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \hat{y}_\ell \\
&= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} softmax(\mathbf{a}_L)_\ell \\
&= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_\ell} \\
&= \frac{-1}{\hat{y}_\ell} \left(\frac{\frac{\partial}{\partial a_{Li}} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell \left(\frac{\partial}{\partial a_{Li}} \sum_{i'} \exp(\mathbf{a}_L)_{i'} \right)}{(\sum_{i'} (\exp(\mathbf{a}_L)_{i'})^2} \right)
\end{aligned}
$$

$$
\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x} \frac{1}{h(x)} - \frac{g(x)}{h(x)^2} \frac{\partial h(x)}{\partial x}
$$

$$
\begin{aligned}
\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell &= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \hat{y}_\ell \\
&= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} softmax(\mathbf{a}_L)_\ell \\
&= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_\ell} \\
&= \frac{-1}{\hat{y}_\ell} \left(\frac{\frac{\partial}{\partial a_{Li}} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell \left(\frac{\partial}{\partial a_{Li}} \sum_{i'} \exp(\mathbf{a}_L)_{i'} \right)}{(\sum_{i'} (\exp(\mathbf{a}_L)_{i'})^2} \right) \\
&= \frac{-1}{\hat{y}_\ell} \left(\frac{\mathbb{1}_{(\ell=i)} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} \frac{\exp(\mathbf{a}_L)_i}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} \right)
\end{aligned}
$$

$$
\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x} \frac{1}{h(x)} - \frac{g(x)}{h(x)^2} \frac{\partial h(x)}{\partial x}
$$

$$\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell = \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \hat{y}_\ell$$

$$= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} softmax(\mathbf{a}_L)_\ell$$

$$= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_\ell}$$

$$= \frac{-1}{\hat{y}_\ell} \left(\frac{\frac{\partial}{\partial a_{Li}} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell \left(\frac{\partial}{\partial a_{Li}} \sum_{i'} \exp(\mathbf{a}_L)_{i'} \right)}{(\sum_{i'} (\exp(\mathbf{a}_L)_{i'})^2} \right)$$

$$= \frac{-1}{\hat{y}_\ell} \left(\frac{\mathbb{1}_{(\ell=i)} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} \frac{\exp(\mathbf{a}_L)_i}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} \right)$$

$$= \frac{-1}{\hat{y}_\ell} \left(\mathbb{1}_{(\ell=i)} softmax(\mathbf{a}_L)_\ell - softmax(\mathbf{a}_L)_\ell softmax(\mathbf{a}_L)_i \right)$$

$$\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x} \frac{1}{h(x)} - \frac{g(x)}{h(x)^2} \frac{\partial h(x)}{\partial x}$$

$$\frac{\partial}{\partial a_{Li}} - \log \hat{y}_\ell = \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \hat{y}_\ell$$

$$\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x} \frac{1}{h(x)} - \frac{g(x)}{h(x)^2} \frac{\partial h(x)}{\partial x}$$

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$$= \frac{-1}{\hat{y}_\ell} \frac{\partial}{\partial a_{Li}} \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_\ell}$$

$$= \frac{-1}{\hat{y}_\ell} \left(\frac{\frac{\partial}{\partial a_{Li}} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell \left(\frac{\partial}{\partial a_{Li}} \sum_{i'} \exp(\mathbf{a}_L)_{i'} \right)}{(\sum_{i'} (\exp(\mathbf{a}_L)_{i'})^2} \right)$$

$$= \frac{-1}{\hat{y}_\ell} \left(\frac{\mathbb{1}_{(\ell=i)} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} \frac{\exp(\mathbf{a}_L)_i}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} \right)$$

$$= \frac{-1}{\hat{y}_\ell} \left(\mathbb{1}_{(\ell=i)} softmax(\mathbf{a}_L)_\ell - softmax(\mathbf{a}_L)_\ell softmax(\mathbf{a}_L)_i \right)$$

$$= \frac{-1}{\hat{y}_\ell} \left(\mathbb{1}_{(\ell=i)} \hat{y}_\ell - \hat{y}_\ell \hat{y}_i \right)$$

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$$= \frac{-1}{\hat{y}_\ell} \left(\frac{\frac{\partial}{\partial a_{Li}} \exp(\mathbf{a}_L)_\ell}{\sum_{i'} \exp(\mathbf{a}_L)_{i'}} - \frac{\exp(\mathbf{a}_L)_\ell \left(\frac{\partial}{\partial a_{Li}} \sum_{i'} \exp(\mathbf{a}_L)_{i'} \right)}{(\sum_{i'} (\exp(\mathbf{a}_L)_{i'})^2} \right)$$

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$$= \frac{-1}{\hat{y}_\ell} \left(\mathbb{1}_{(\ell=i)} softmax(\mathbf{a}_L)_\ell - softmax(\mathbf{a}_L)_\ell softmax(\mathbf{a}_L)_i \right)$$

$$= \frac{-1}{\hat{y}_\ell} \left(\mathbb{1}_{(\ell=i)} \hat{y}_\ell - \hat{y}_\ell \hat{y}_i \right)$$

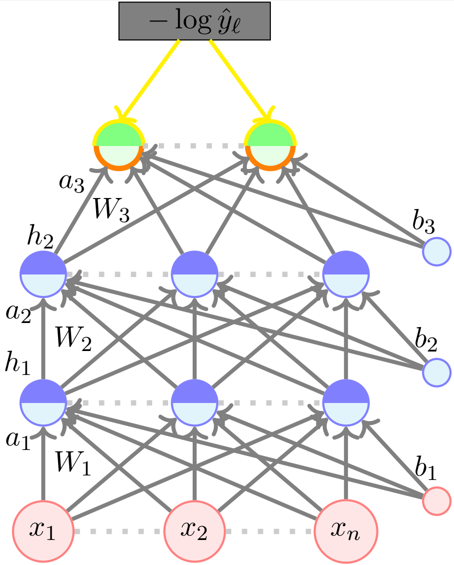
$$= -\left(\mathbb{1}_{(\ell=i)} - \hat{y}_i \right)$$

$$\frac{\partial \frac{g(x)}{h(x)}}{\partial x} = \frac{\partial g(x)}{\partial x} \frac{1}{h(x)} - \frac{g(x)}{h(x)^2} \frac{\partial h(x)}{\partial x}$$

So far we have derived the partial derivative w.r.t. the i-th element of $\mathbf{a}_L$

$$\frac{\partial \mathscr{L}(\theta)}{\partial a_{L,i}} = -(\mathbb{1}_{\ell=i} - \hat{y}_i)$$

We can now write the gradient w.r.t. the vector $\mathbf{a}_L$



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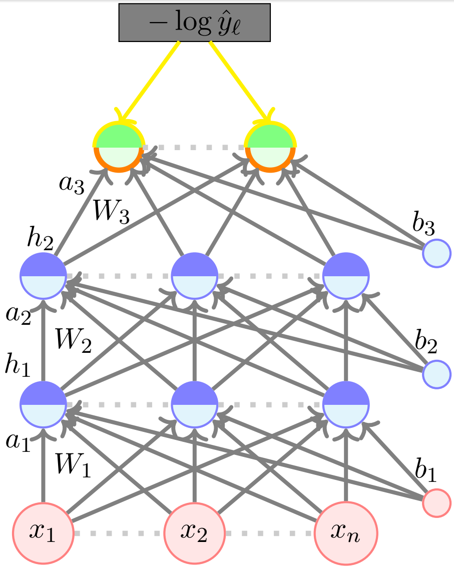
We can now write the gradient w.r.t. the vector $\mathbf{a}_L$

$$\nabla_{\mathbf{a_L}} \mathscr{L}(\theta)$$



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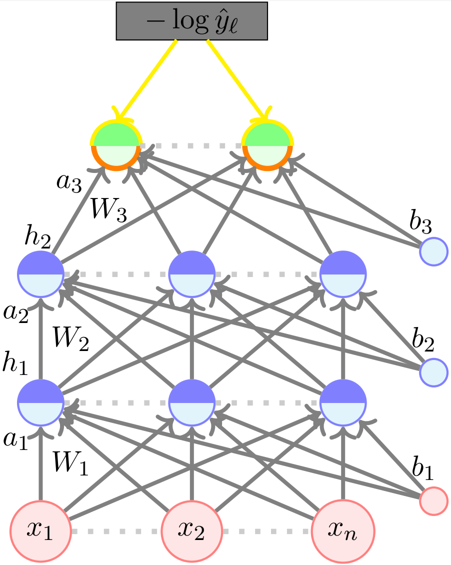
$$\frac{\partial \mathscr{L}(\theta)}{\partial a_{L,i}} = -(\mathbb{1}_{\ell=i} - \hat{y}_i)$$

We can now write the gradient w.r.t. the vector $\mathbf{a}_L$

$$\nabla_{\mathbf{a_L}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{L1}} \\ \\ \\ \end{bmatrix}$$



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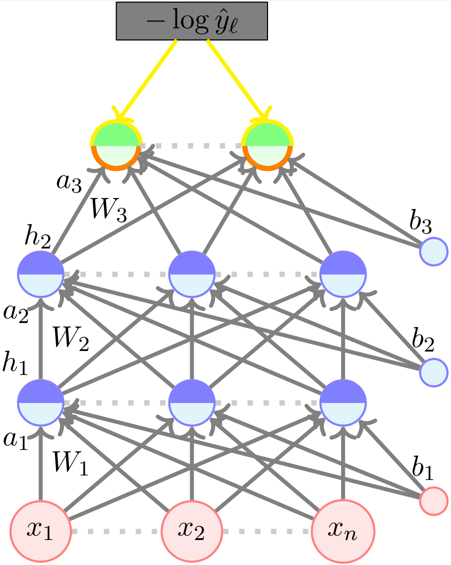
$$\nabla_{\mathbf{a_L}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{L1}} \\ \vdots \\ \\ \end{bmatrix}$$



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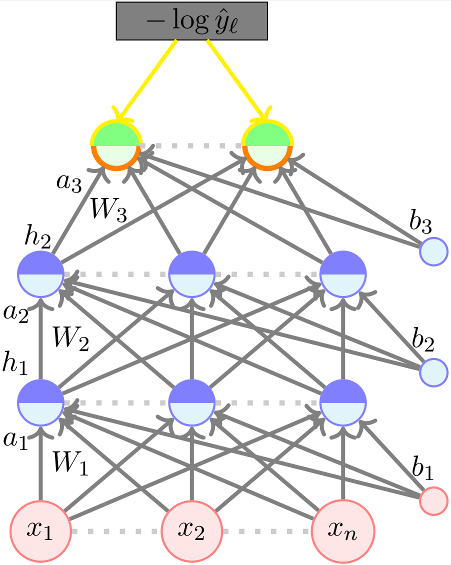
We can now write the gradient w.r.t. the vector $\mathbf{a}_L$

$$\nabla_{\mathbf{a_L}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{L1}} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial a_{Lk}} \end{bmatrix}$$



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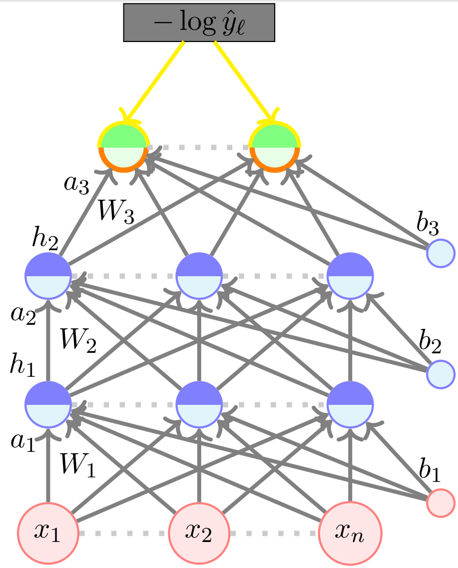

So far we have derived the partial derivative w.r.t. the i-th element of $\mathbf{a}_L$

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We can now write the gradient w.r.t. the vector $\mathbf{a}_L$

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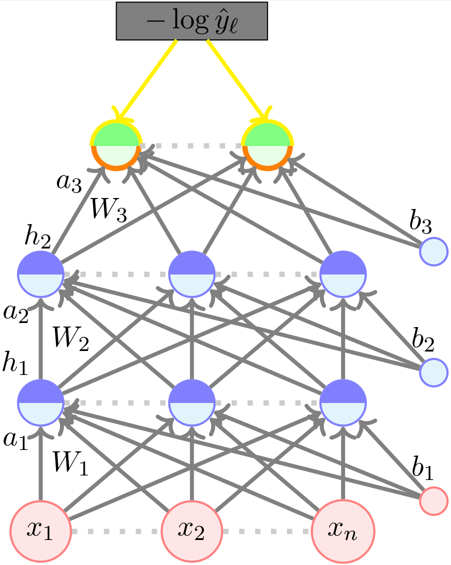

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We can now write the gradient w.r.t. the vector $\mathbf{a}_L$

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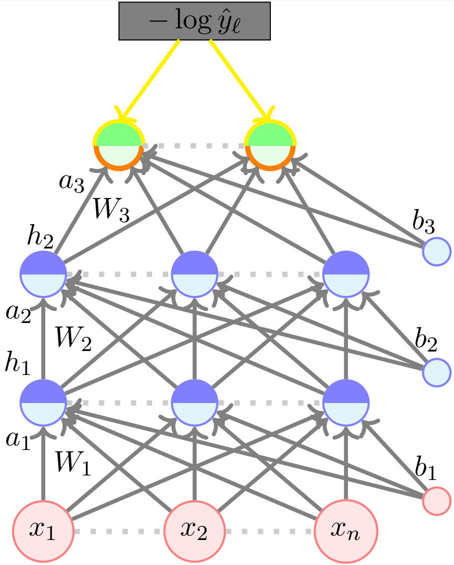

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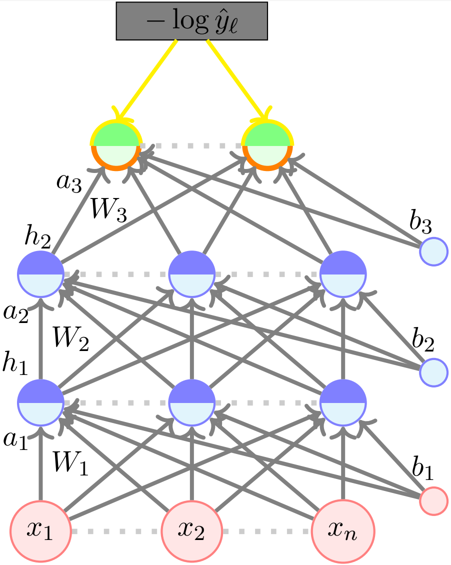

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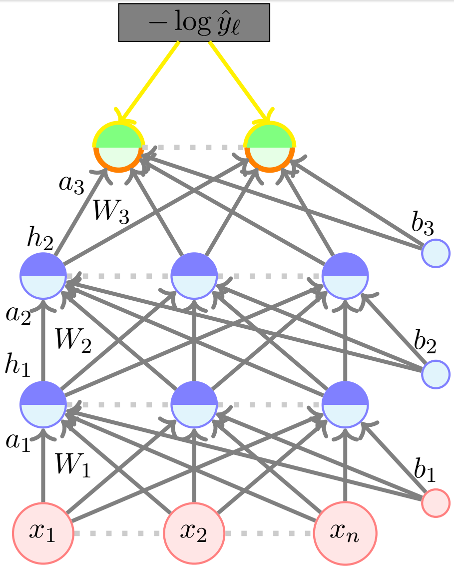
$$\frac{\partial \mathscr{L}(\theta)}{\partial a_{L,i}} = -(\mathbb{1}_{\ell=i} - \hat{y}_i)$$

We can now write the gradient w.r.t. the vector $\mathbf{a}_L$

$$\nabla_{\mathbf{a_L}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{L1}} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial a_{Lk}} \end{bmatrix} = \begin{bmatrix} -(\mathbb{1}_{\ell=1} - \hat{y}_1) \\ -(\mathbb{1}_{\ell=2} - \hat{y}_2) \\ \vdots \\ -(\mathbb{1}_{\ell=k} - \hat{y}_k) \end{bmatrix}$$



So far we have derived the partial derivative w.r.t. the i-th element of $\mathbf{a}_L$

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We can now write the gradient w.r.t. the vector $\mathbf{a}_L$

$$\nabla_{\mathbf{a_L}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{L1}} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial a_{Lk}} \end{bmatrix} = \begin{bmatrix} -(\mathbb{1}_{\ell=1} - \hat{y}_1) \\ -(\mathbb{1}_{\ell=2} - \hat{y}_2) \\ \vdots \\ -(\mathbb{1}_{\ell=k} - \hat{y}_k) \end{bmatrix}$$

$$= -(\mathbf{e}(\ell) - \hat{y})$$