第四讲：前馈神经网络和反向传播

张盛平

s.zhang@hit.edu.cn

计算学部
哈尔滨工业大学

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致谢

- 讲稿中很多资料或素材来源于网络，包括国外一些大学的相关课程、一些博客、维基百科等。后面不一一列举来源，在此一并表示感谢
- 引用网络资源时，由于本人的理解能力，可能存在一些偏差
- 本讲稿会经常更新

References/Acknowledgments

See the excellent videos by Hugo Larochelle on Backpropagation

前馈神经网络 (又称多层神经网络)

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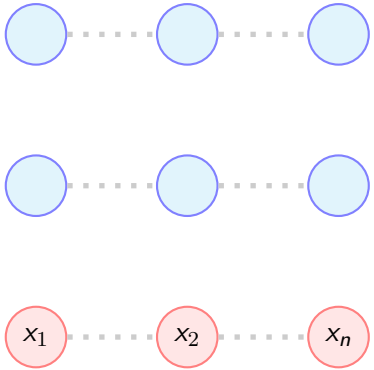

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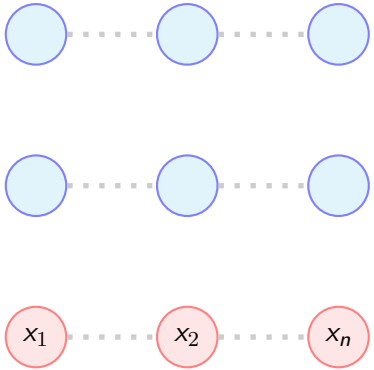

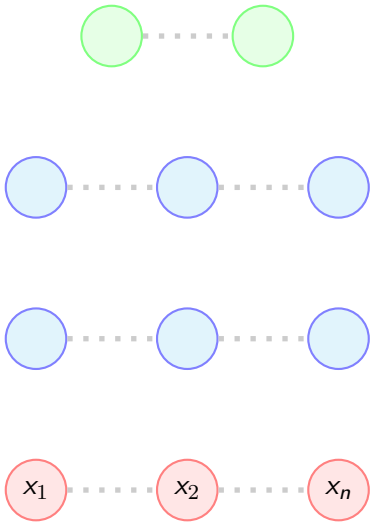

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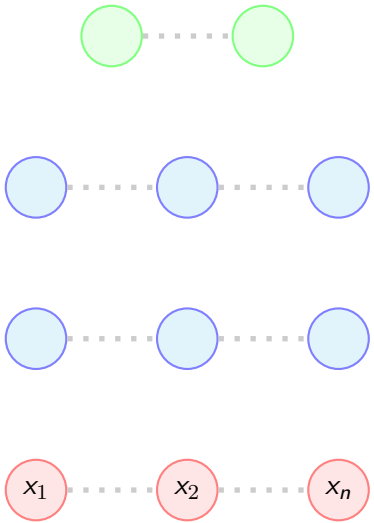

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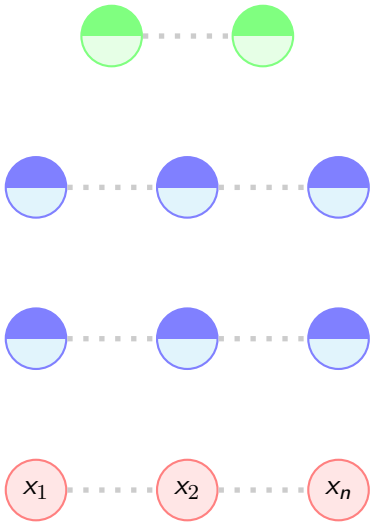

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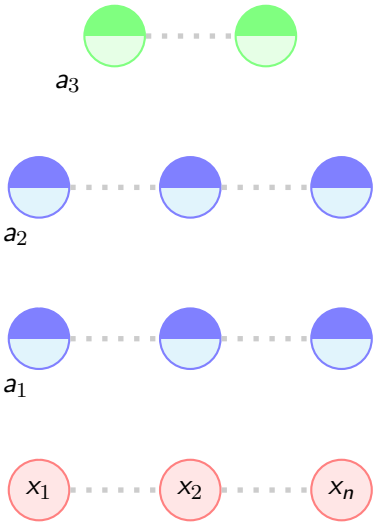

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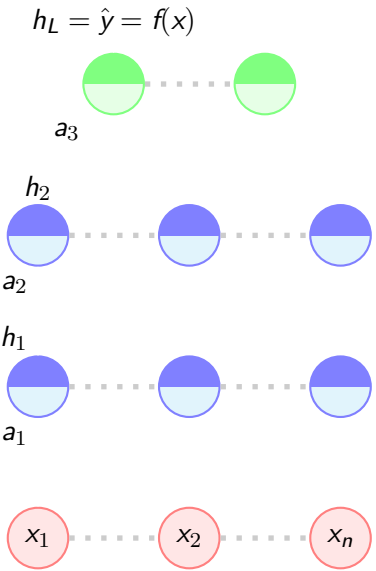

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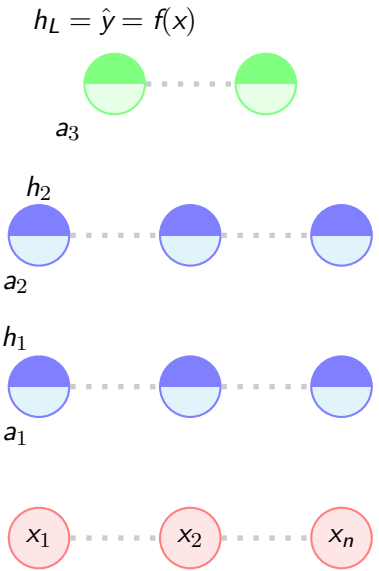

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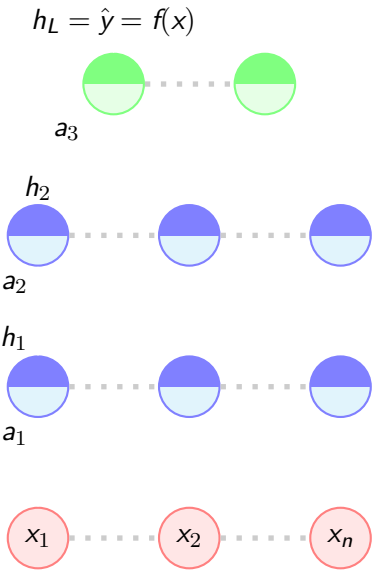

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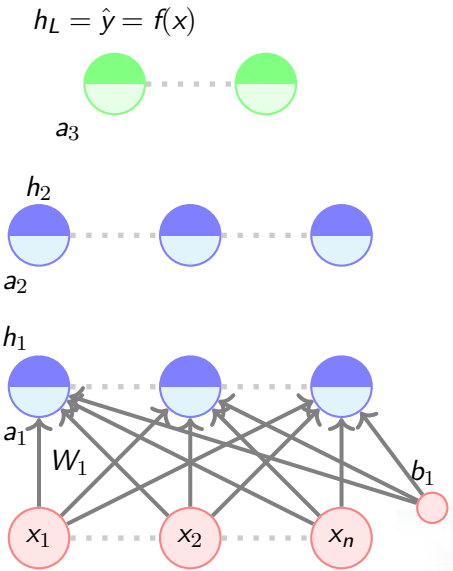

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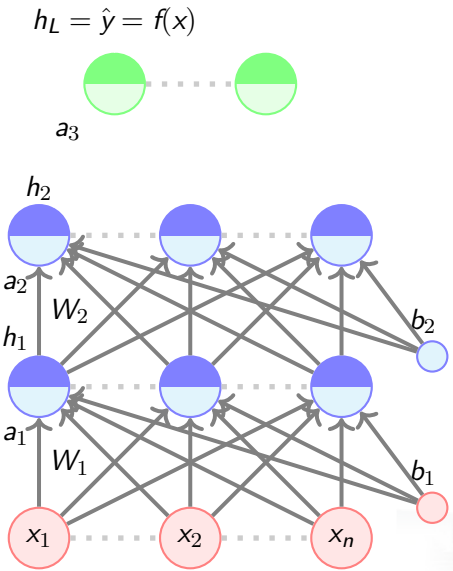

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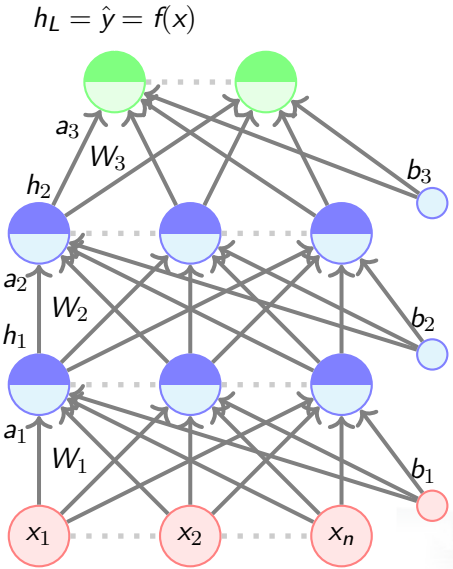

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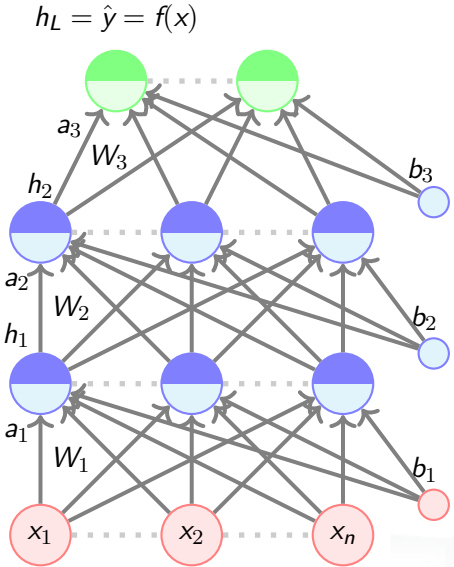
- $W_L \in \mathbb{R}^{n \times k}$ 和 $b_L \in \mathbb{R}^k$ 分别是最后一个隐含层到输出层的权重和偏置向量 ($L = 3$ in this case)



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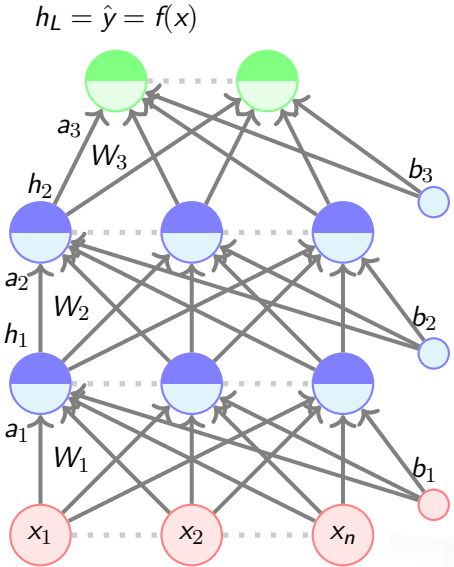

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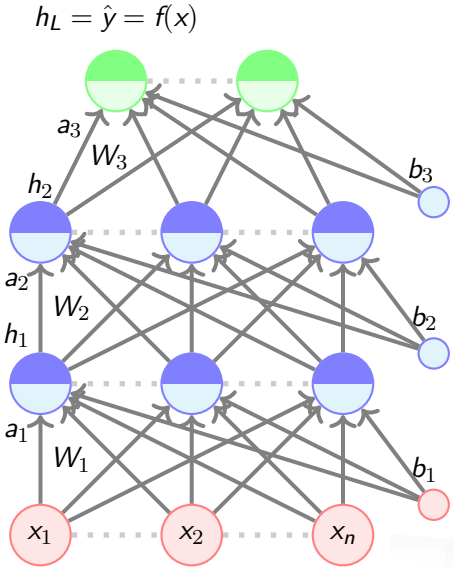

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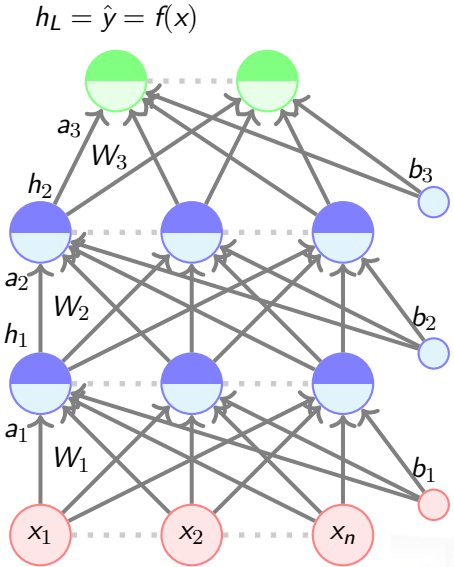

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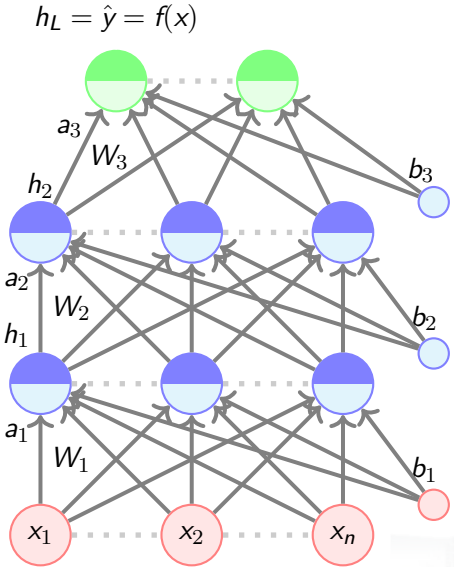

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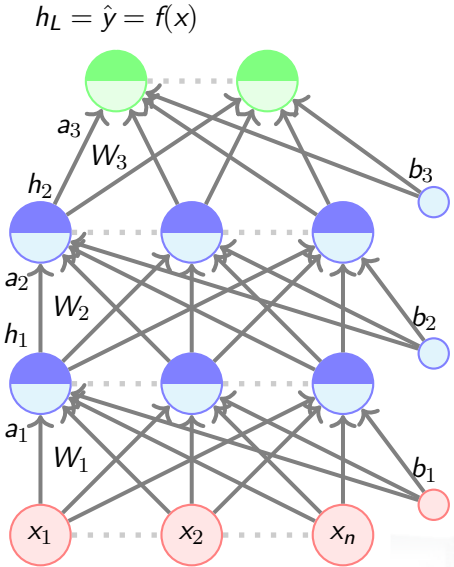

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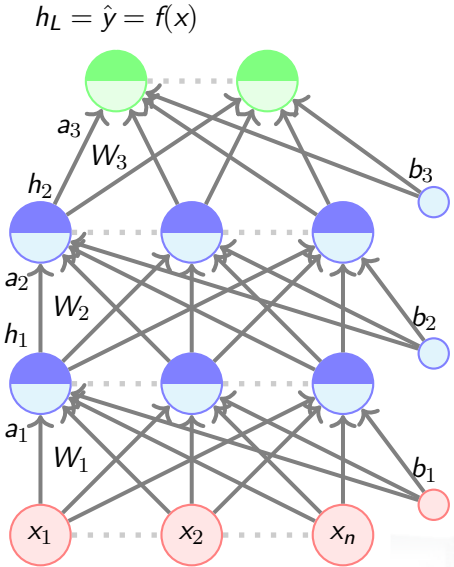
- 为了描述简单, 将 $a_i(x)$ 简化为 a_i, 将 $h_i(x)$ 简



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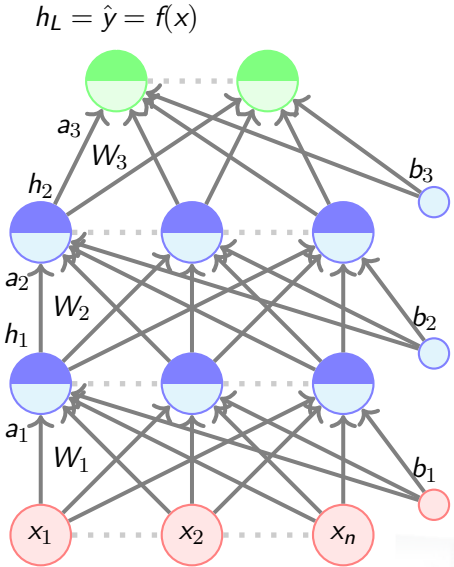
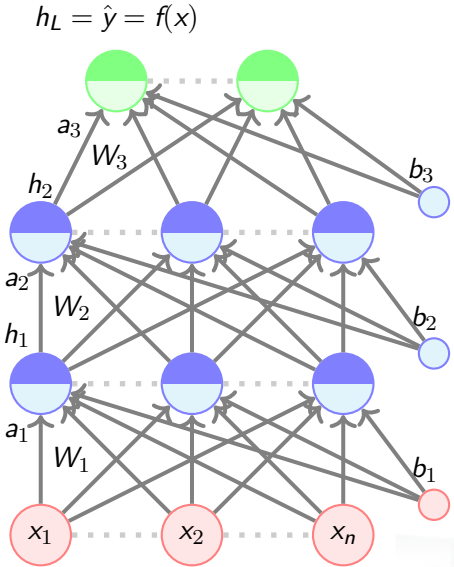


- **数据:** $\{x_i, y_i\}_{i=1}^{N}$



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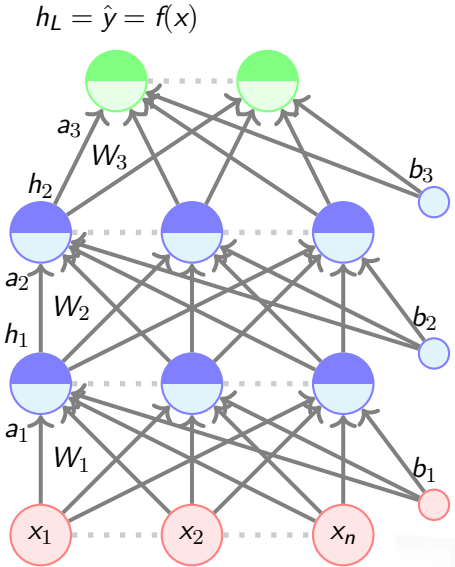

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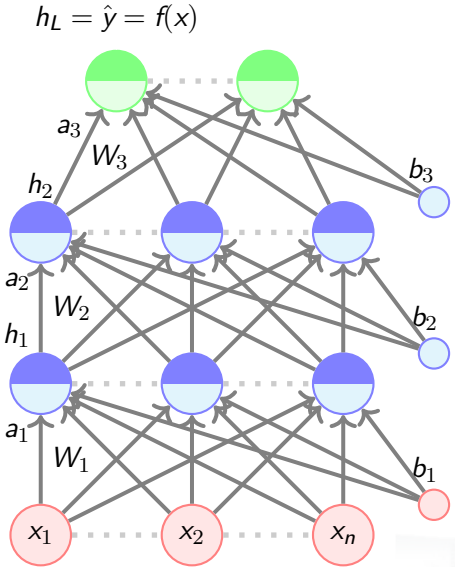

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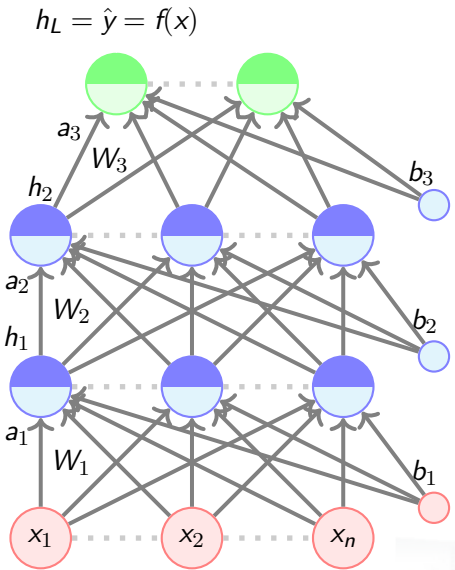
$$\theta = W_1, .., W_L, b_1, b_2, ..., b_L \quad (L = 3)$$



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- **目标/损失/误差函数:**

$$min \ \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{k} (\hat{y}_{ij} - y_{ij})^2$$

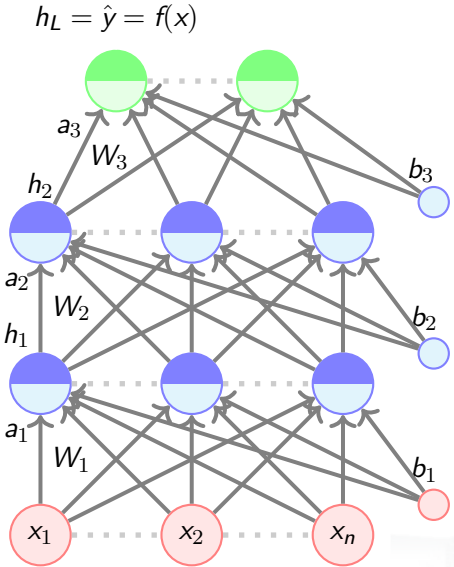
一般地, $min \ \mathscr{L}(\theta)$

其中 $\mathscr{L}(\theta)$ 是损失函数

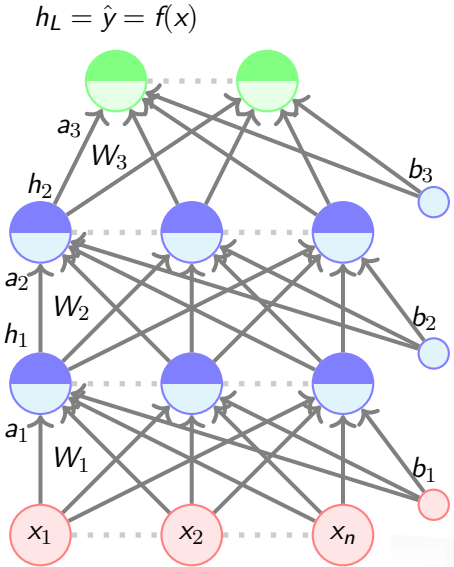
前馈神经网络参数学习 (Intuition)

The story so far...

- 已经介绍了前馈神经网络
- 希望找到一个算法来学习这个网络的参数



- 回忆一下梯度下降算法



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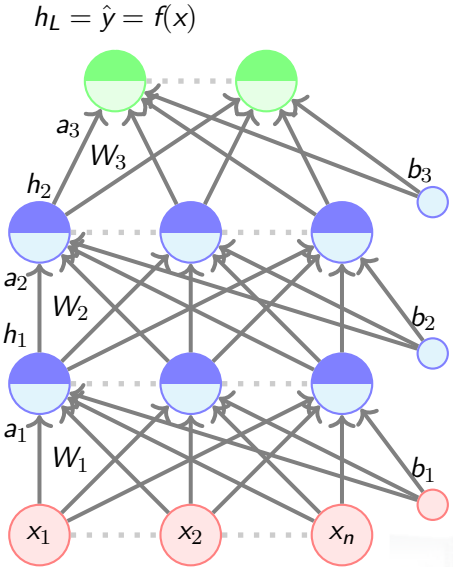
Algorithm: gradient_descent()

$t \leftarrow 0$;
$max\_iterations \leftarrow 1000$;
Initialize w_0, b_0;
while $t{+}{+} < max\_iterations$ **do**
  $w_{t+1} \leftarrow w_t - \eta \nabla w_t$;
  $b_{t+1} \leftarrow b_t - \eta \nabla b_t$;
end



- 回忆一下梯度下降算法
- 更紧凑的可以写为

Algorithm: gradient_descent()

$t \leftarrow 0$;
max_iterations $\leftarrow 1000$;
Initialize w_0, b_0;
while *t++* $<$ *max_iterations* **do**
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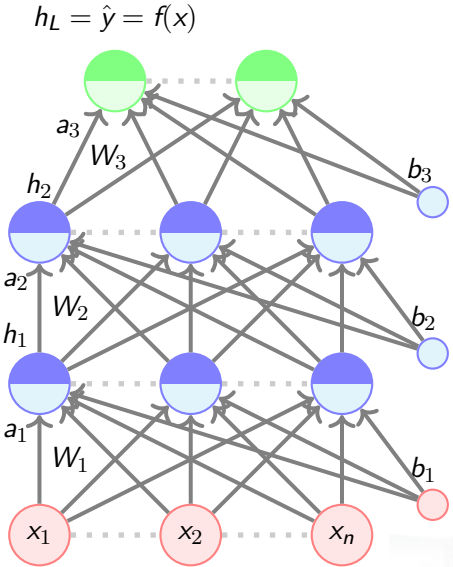
end



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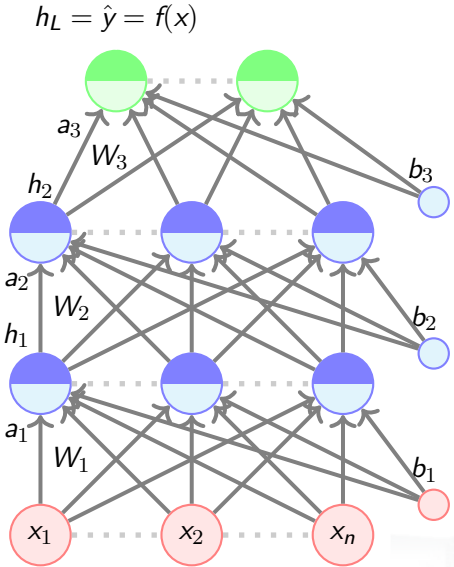

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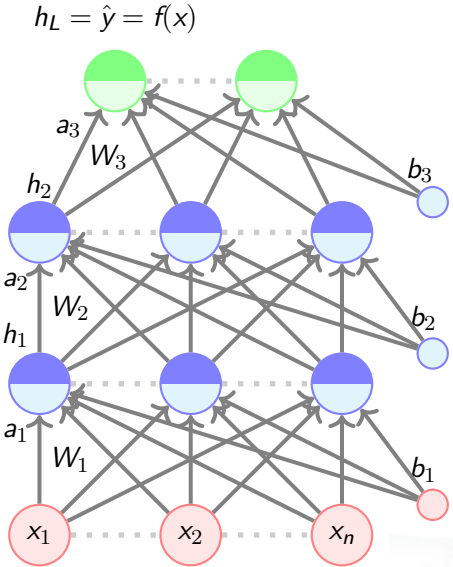

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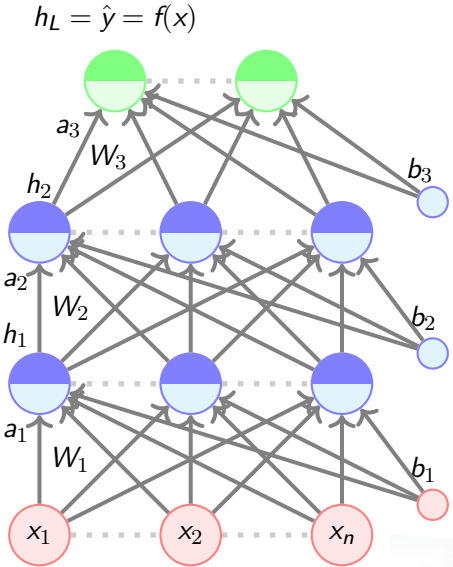

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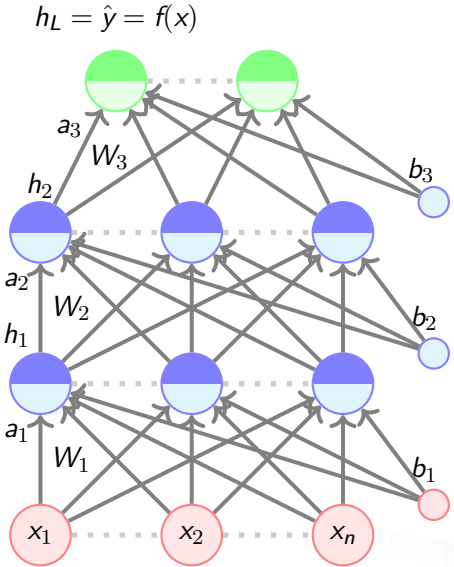

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Algorithm: gradient_descent()

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$max\_iterations \leftarrow 1000$;
Initialize $\theta_0 = [W_1^0, ..., W_L^0, b_1^0, ..., b_L^0]$;
while $t{+}{+} < max\_iterations$ **do**
  $\theta_{t+1} \leftarrow \theta_t - \eta \nabla \theta_t$;
end

- 其中 $\nabla \theta_t = \left[\frac{\partial \mathscr{L}(\theta)}{\partial W_{1,t}}, .., \frac{\partial \mathscr{L}(\theta)}{\partial W_{L,t}}, \frac{\partial \mathscr{L}(\theta)}{\partial b_{1,t}}, .., \frac{\partial \mathscr{L}(\theta)}{\partial b_{L,t}}\right]^T$
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$$\begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial W_{111}} & \cdots & \frac{\partial \mathscr{L}(\theta)}{\partial W_{11n}} \\ & & \\ & & \\ & & \\ & & \end{bmatrix}$$

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$$\begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial W_{111}} & \cdots & \frac{\partial \mathscr{L}(\theta)}{\partial W_{11n}} \\ \\ \frac{\partial \mathscr{L}(\theta)}{\partial W_{121}} & \cdots & \frac{\partial \mathscr{L}(\theta)}{\partial W_{12n}} \\ \vdots & \vdots & \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial W_{1n1}} & \cdots & \frac{\partial \mathscr{L}(\theta)}{\partial W_{1nn}} \end{bmatrix}$$

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- $\nabla\theta$ 由
  $\nabla W_1, \nabla W_2, ...\nabla W_{L-1} \in \mathbb{R}^{n\times n}, \nabla W_L \in \mathbb{R}^{n\times k}$,
  $\nabla b_1, \nabla b_2, ..., \nabla b_{L-1} \in \mathbb{R}^n$ and $\nabla b_L \in \mathbb{R}^k$ 组成

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输出函数和损失函数

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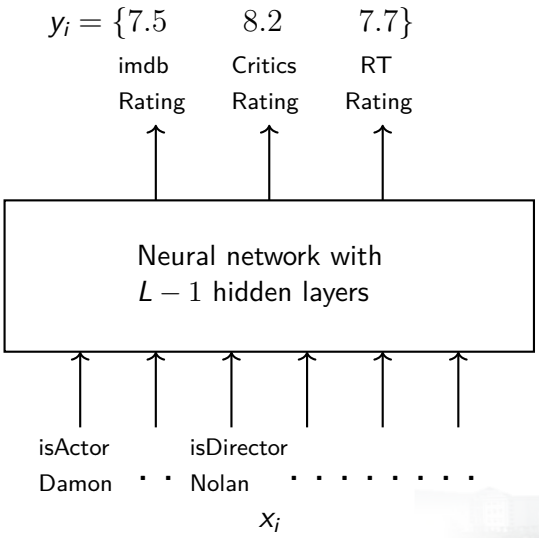

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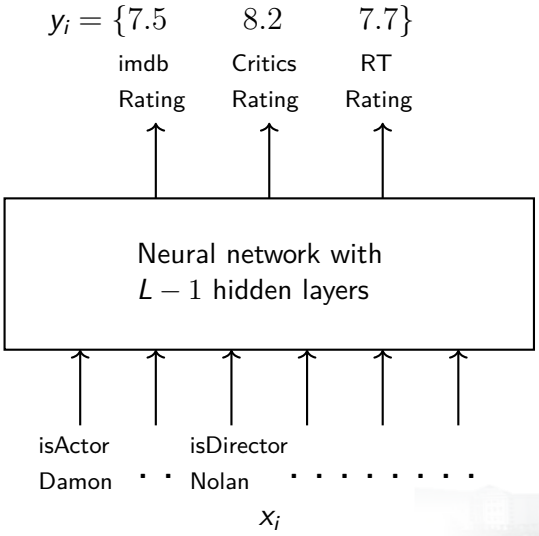

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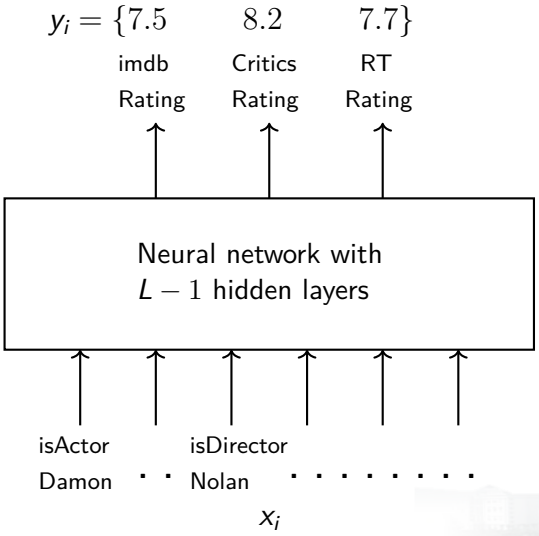

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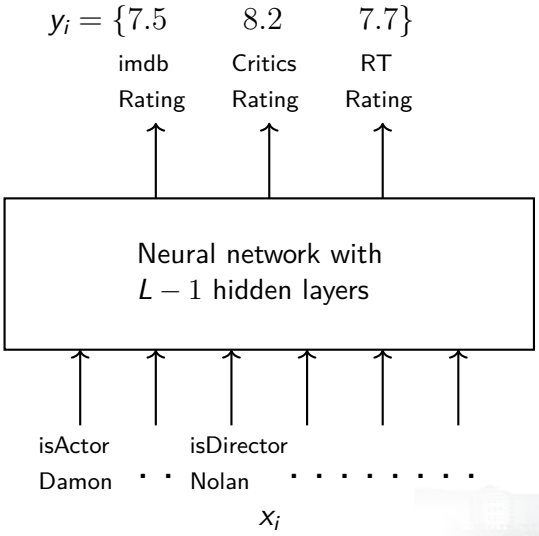

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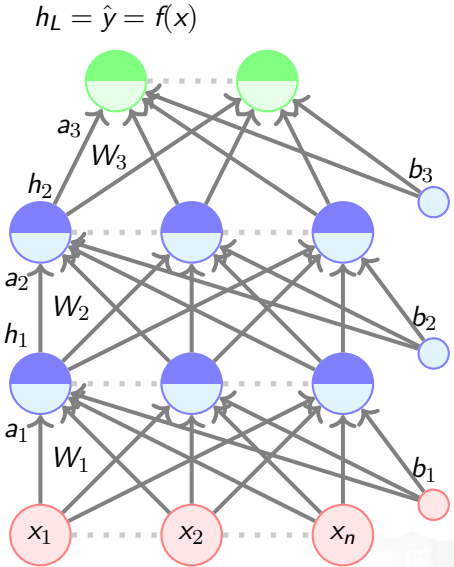
$$\mathscr{L}(\theta) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{3} (\hat{y}_{ij} - y_{ij})^2$$



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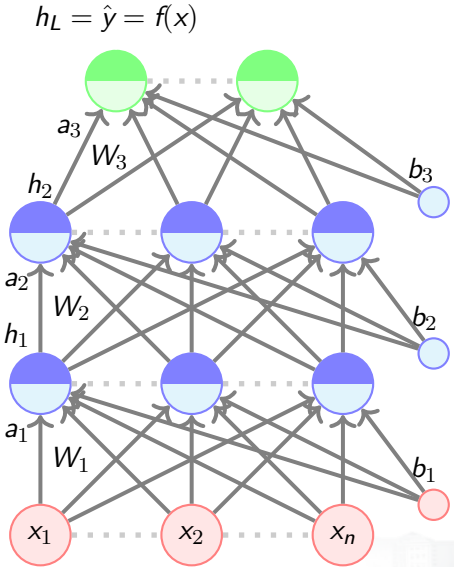

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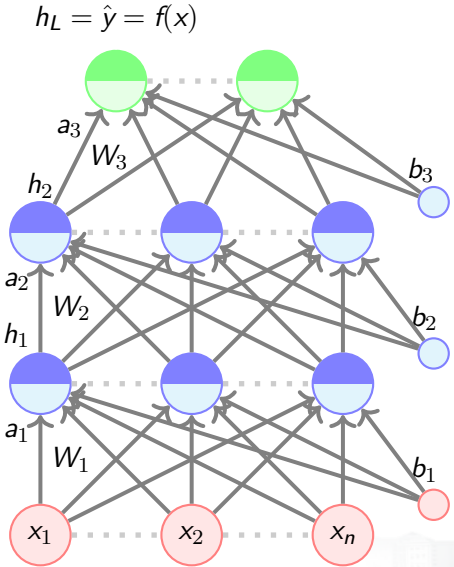

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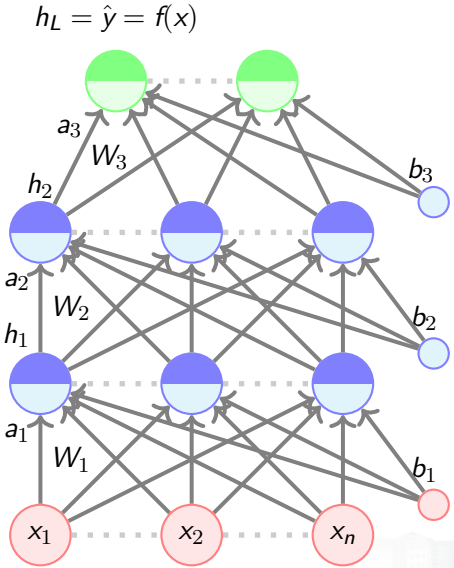

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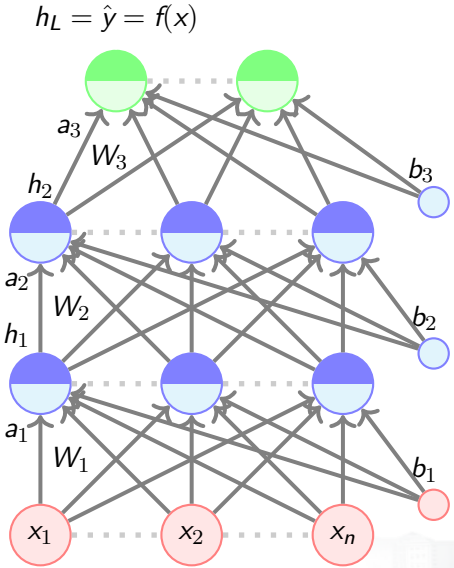
$$\begin{aligned} f(x) &= h_L = O(a_L) \\ &= W_O a_L + b_O \end{aligned}$$



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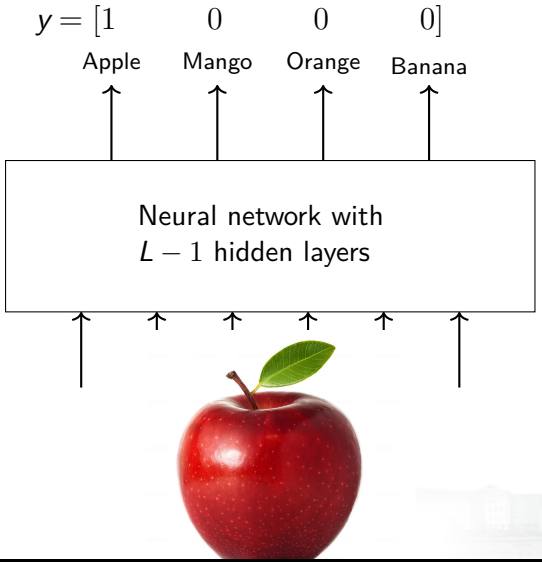
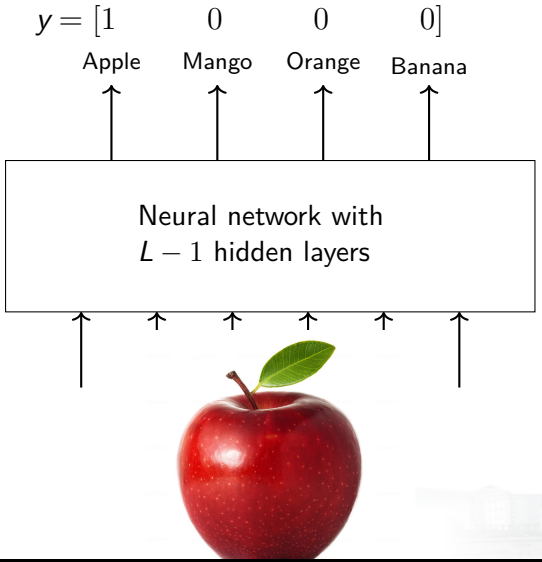
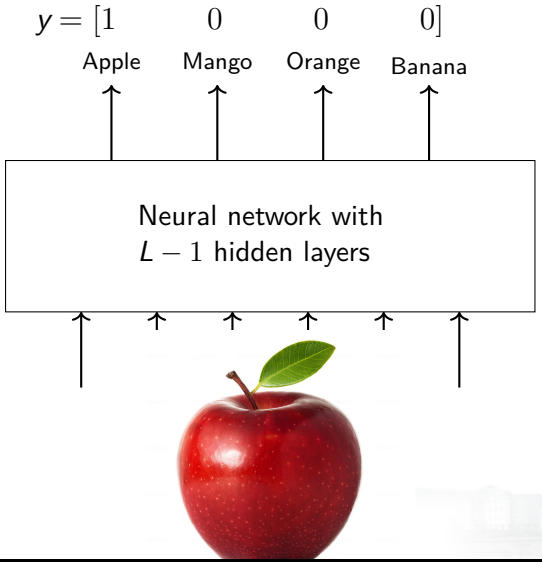
- $\hat{y}_i = f(x_i)$ 不再受限于 0 和 1 之间了


$y = [1 \quad 0 \quad 0 \quad 0]$
Apple
Mango
Orange
Banana
Neural network with
$L-1$ hidden layers

- 考虑另一个问题



- 考虑另一个问题
- 假定我们希望将一张图像分类成 k 个类中的一个



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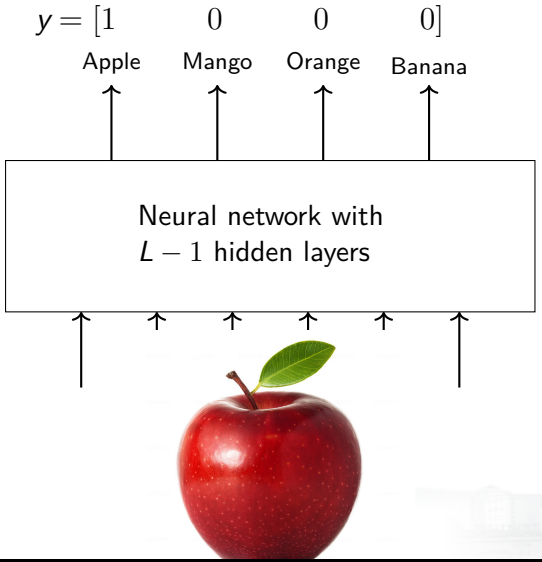

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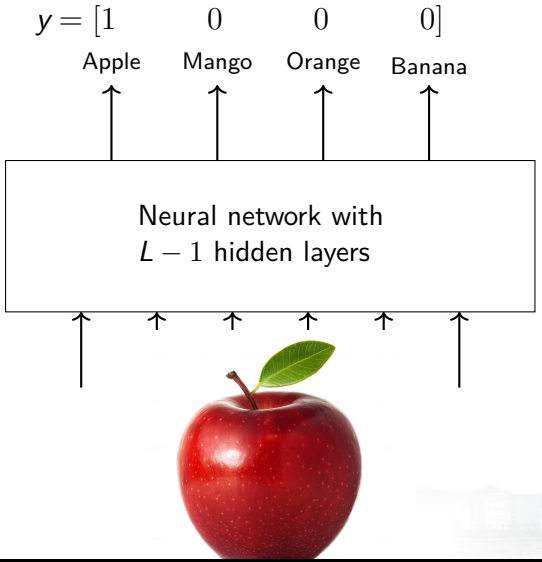
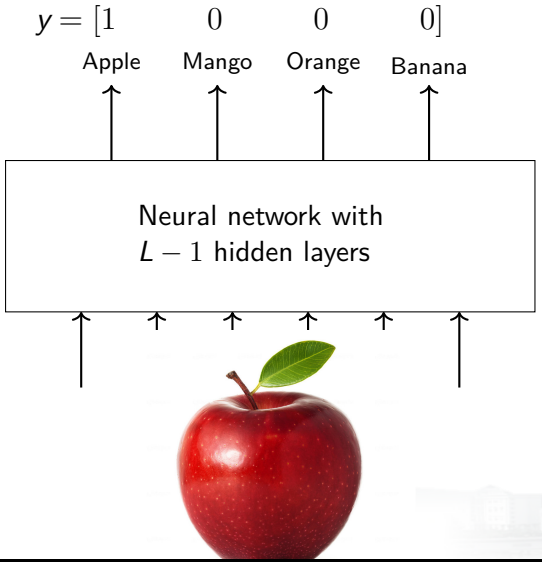
- 还有更好的损失函数吗?


$y = [1 \quad 0 \quad 0 \quad 0]$
Apple
Mango
Orange
Banana
Neural network with
$L-1$ hidden layers

- 注意：y 是一个概率分布



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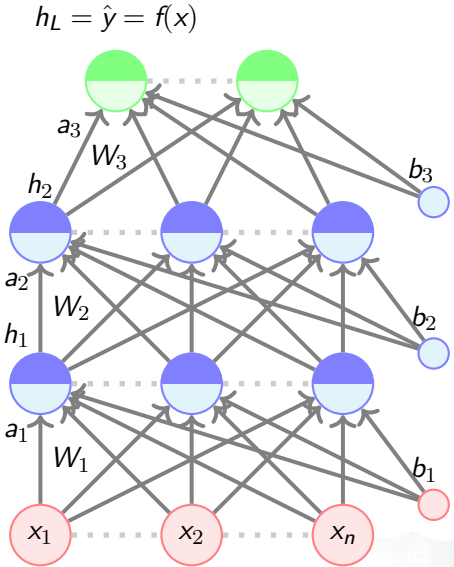

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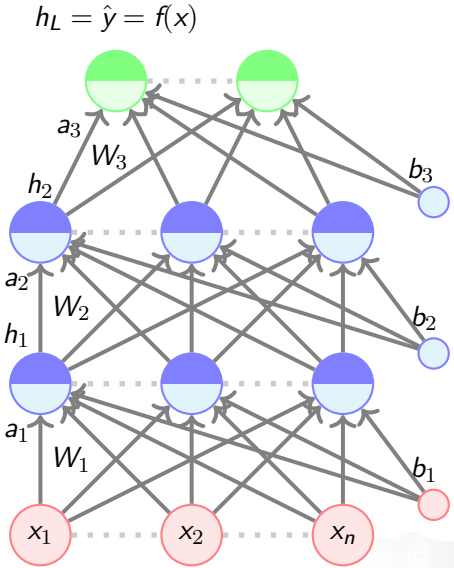
- 选择什么样的输出激活函数 'O' 才能确保输出是一个概率分布?

$$a_L = W_L h_{L-1} + b_L$$



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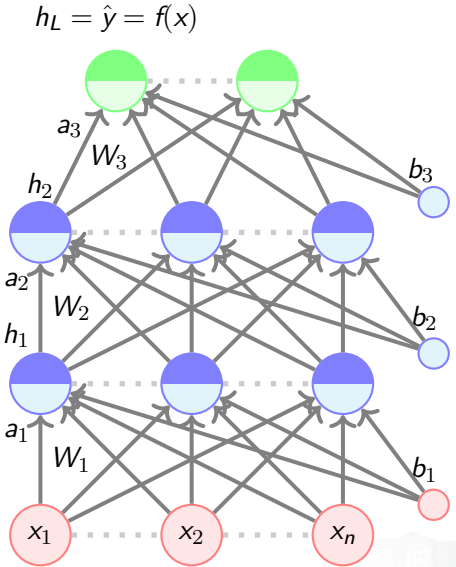
$O(a_L)_j$ 是 $\hat{y}$ 的第 j^{th} 个元素，$a_{L,j}$ 是向量 a_L 的第 j^{th} 个元素.



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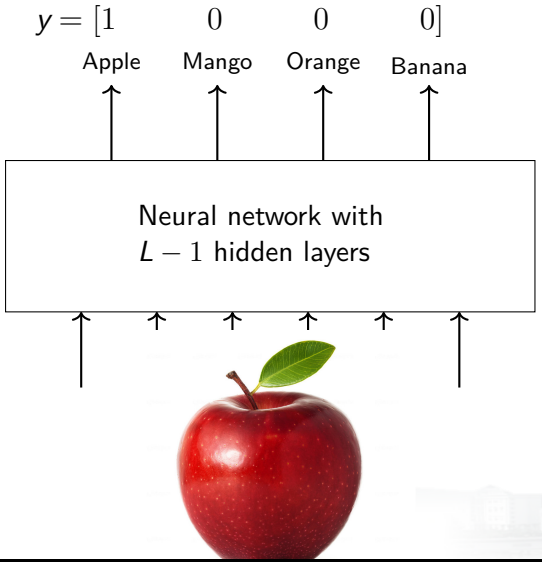
- 这个输出函数称作为 *softmax* 函数



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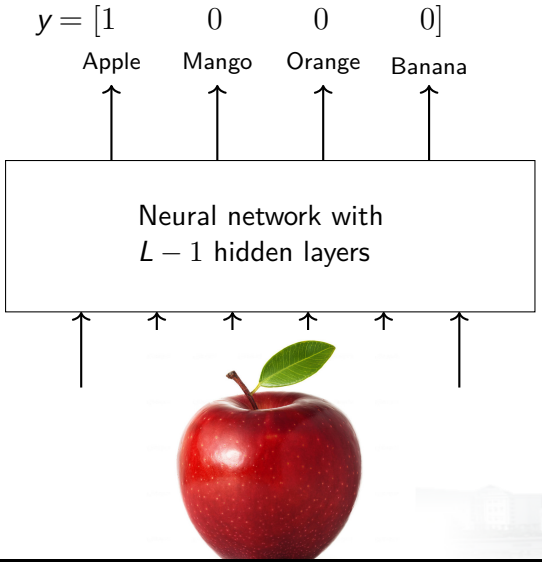

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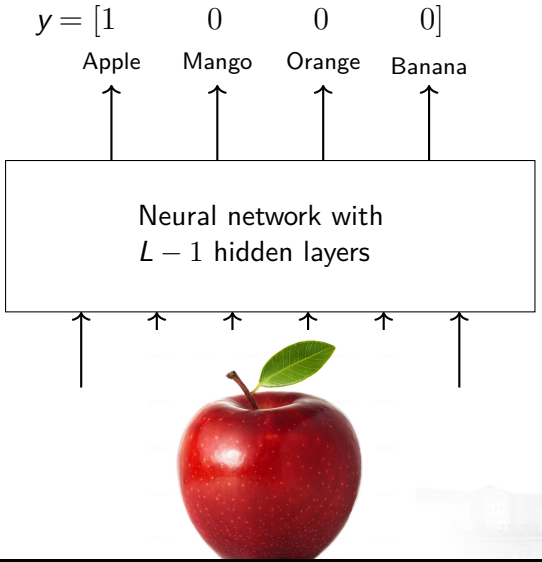
$$\mathscr{L}(\theta) = -\sum_{c=1}^{k} y_c \log \hat{y}_c$$



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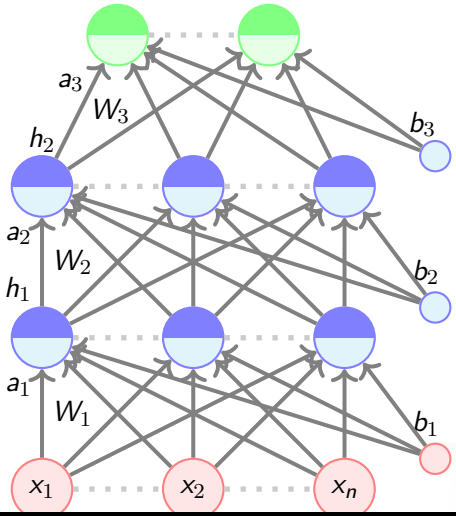
- 注意：

$$y_c = 1 \quad \text{if } c = \ell \text{ (the true class label)}$$
$$= 0 \quad \text{otherwise}$$
$$\therefore \ \mathscr{L}(\theta) = -\log \hat{y}_\ell$$

$h_L = \hat{y} = f(x)$



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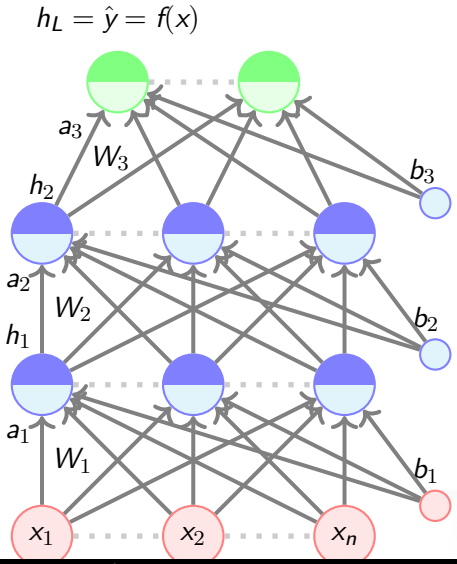

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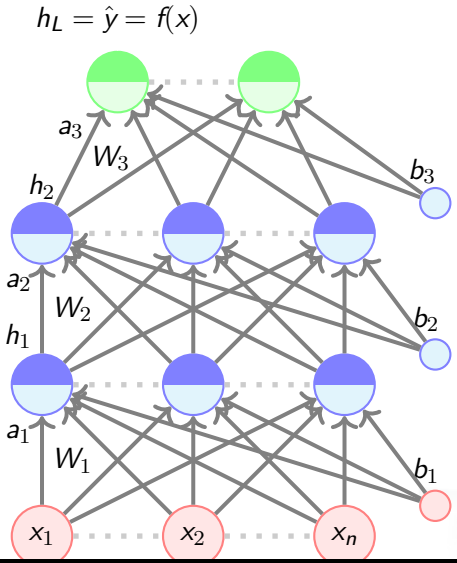

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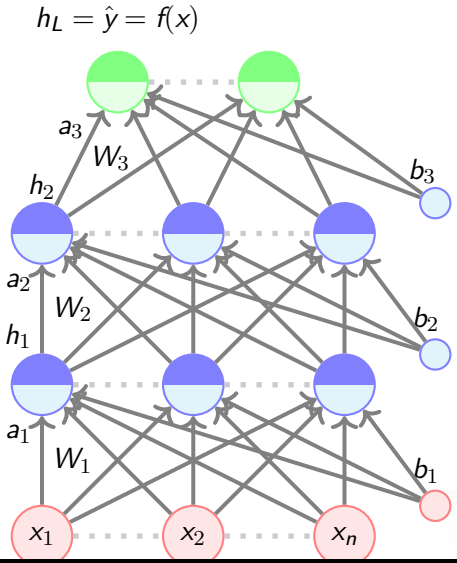

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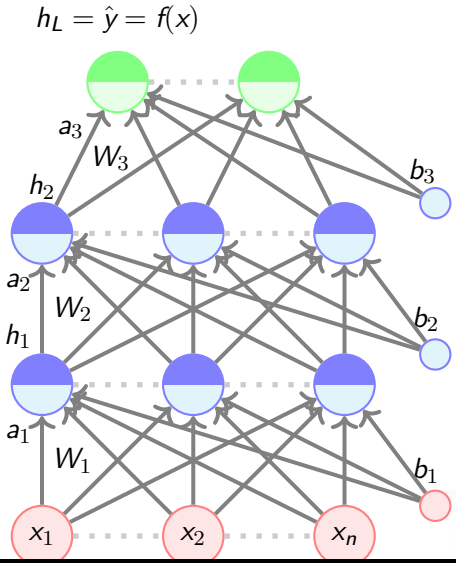

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- $\log \hat{y}_\ell$ 被称为数据的 *log-likelihood*

	Outputs	
	Real Values	Probabilities
Output Activation		
Loss Function		

	Outputs	
	Real Values	Probabilities
Output Activation	Linear	
Loss Function		

	Outputs	
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Output Activation	Linear	Softmax
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- 在本讲的后面内容中，将考虑激活函数是 softmax 函数，损失函数是交叉熵的情况

反向传播 (Intuition)

需要回答两个问题

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- 如何计算 $\nabla\theta$?

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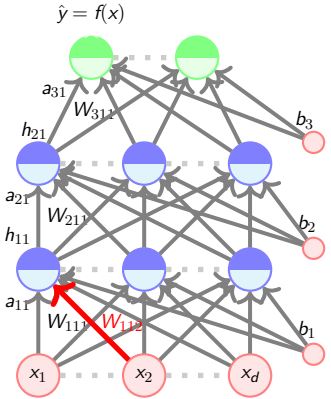
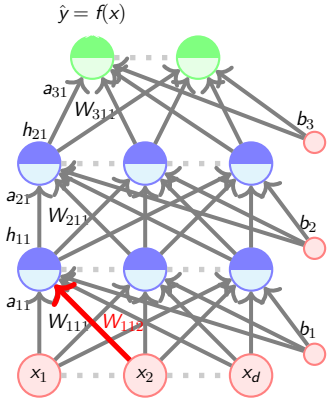
- 考虑这一个权重(W_{112}).



Algorithm 9: gradient descent()

$t \leftarrow 0$;
$max\_iterations \leftarrow 1000$;
Initialize θ_0;
while $t{+}{+} < max\_iterations$ **do**
  $\theta_{t+1} \leftarrow \theta_t - \eta \nabla \theta_t$;
end

- 考虑这一个权重(W_{112}).
- 使用 SGD 来学习这个权重，需要计算 $\frac{\partial \mathcal{L}(\theta)}{\partial W_{112}}$.



Algorithm 10: gradient descent()

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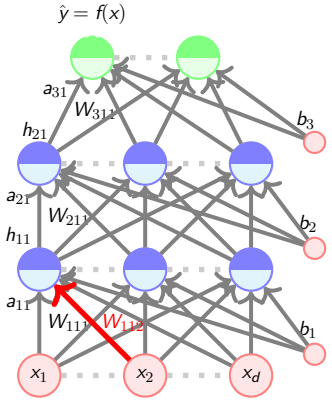

Algorithm 11: gradient descent()

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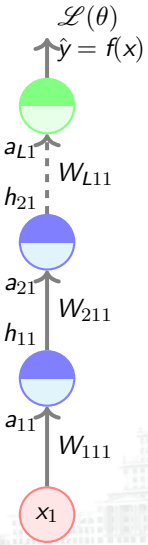

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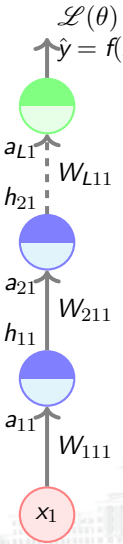
- 这种情况，很容易通过链式法则，求得



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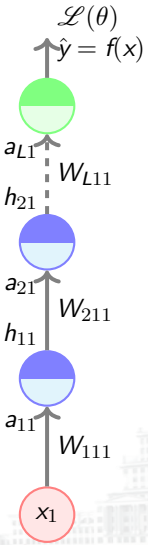

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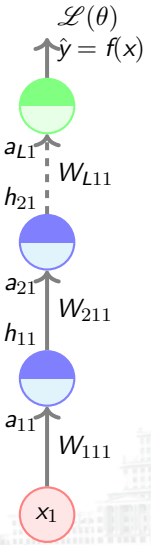
$$\frac{\partial \mathscr{L}(\theta)}{\partial W_{111}} = \frac{\partial \mathscr{L}(\theta)}{\partial h_{11}} \frac{\partial h_{11}}{\partial W_{111}}$$ (just compressing the chain rule)



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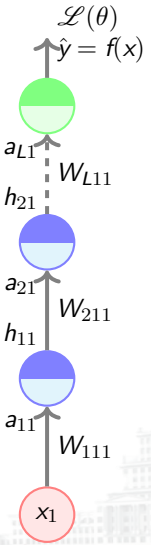
(just compressing the chain rule)



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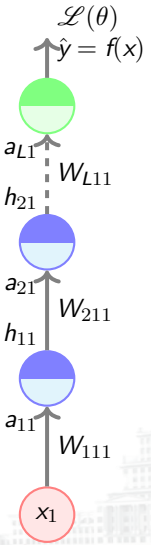

在进入具体的数学推导之前，先看看反向传播的直观解释

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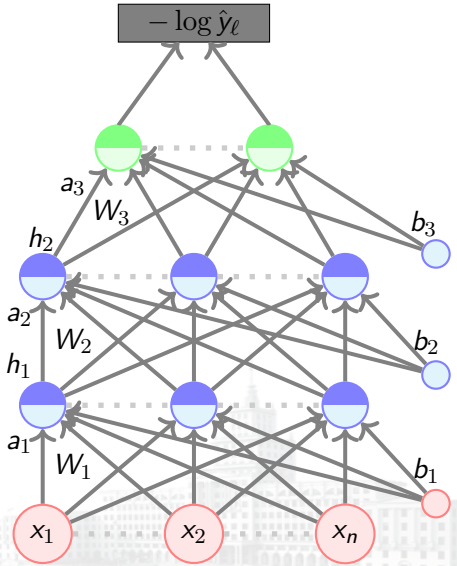

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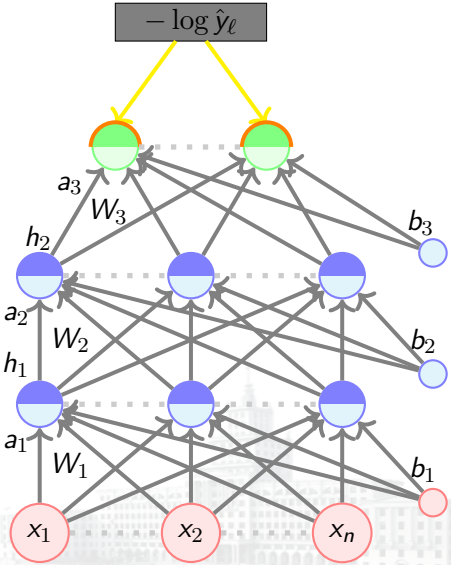

- 我们在输出层得到一个损失，我们希望找出谁应该对这个损失负责？
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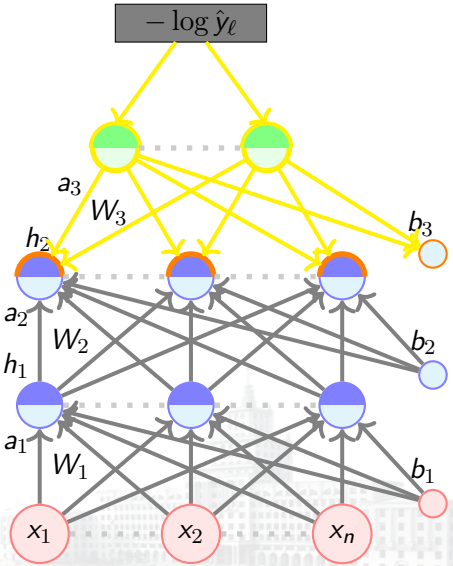
- 最后一层说“我已经尽了我能尽的责任了，请你理解，我只能做得想隐含层和我下面的权重好样好,”. After all ...

$$f(x) = \hat{y} = O(W_L h_{L-1} + b_L)$$



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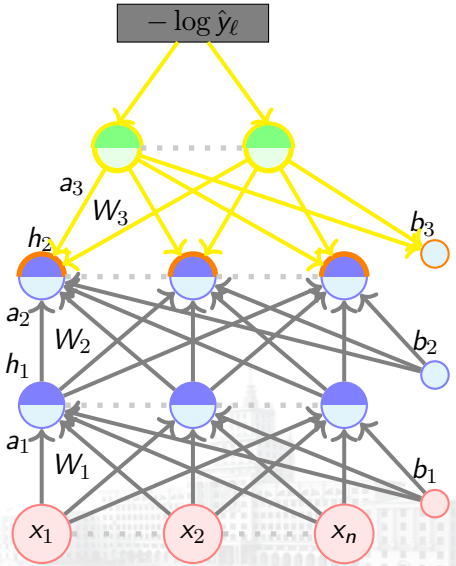

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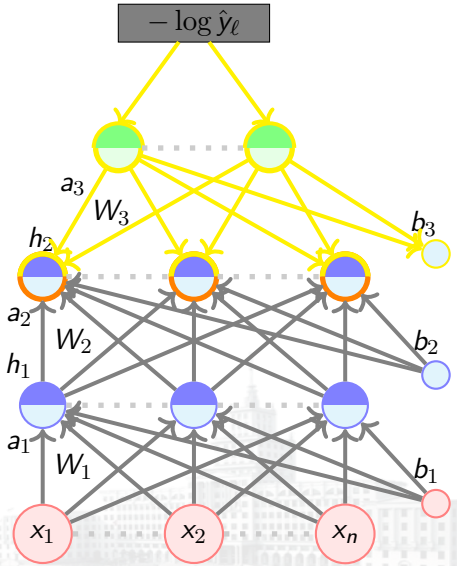

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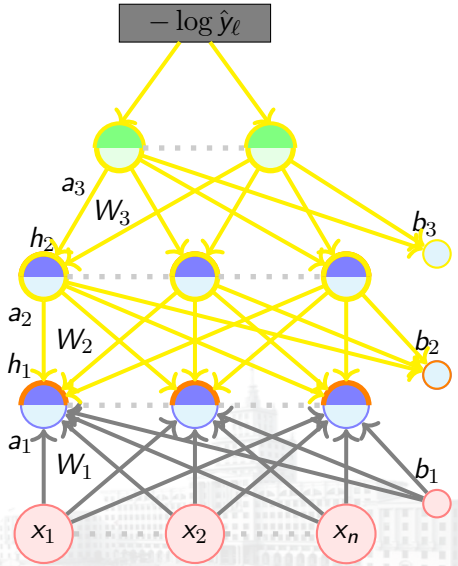

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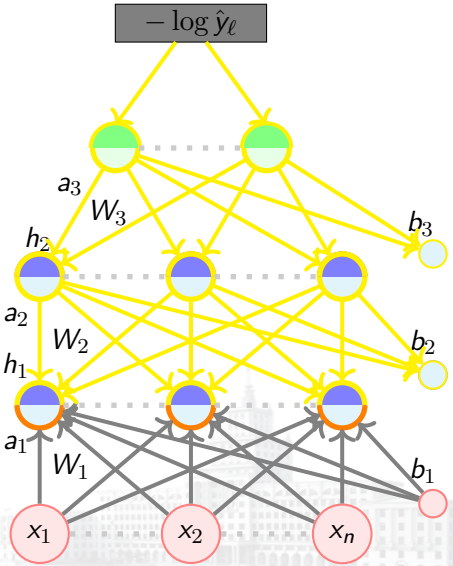

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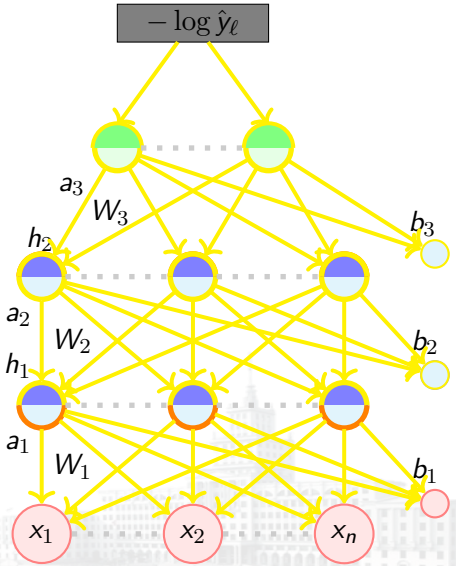
- 不同于直接和它们对话，通过隐含层和输出层来和它们对话会更容易（链式法则也允许我们这样做）



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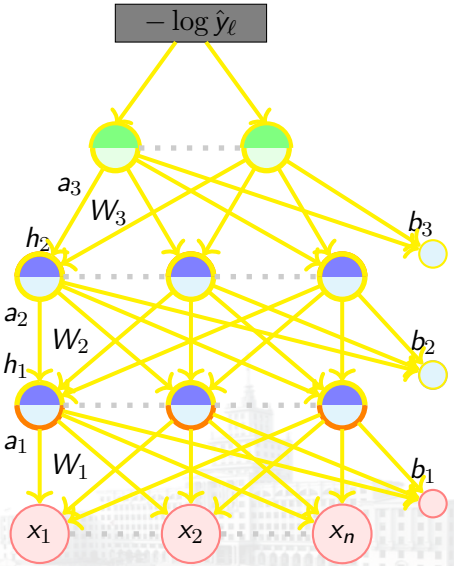
$$\underbrace{\frac{\partial \mathscr{L}(\theta)}{\partial W_{111}}}_{\text{Talk to the weight directly}} = \underbrace{\frac{\partial \mathscr{L}(\theta)}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial a_3}}_{\text{Talk to the output layer}} \underbrace{\frac{\partial a_3}{\partial h_2} \frac{\partial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



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需要计算的梯度:

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- Gradient w.r.t. output units

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需要计算的梯度:

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

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需要计算的梯度:

- Gradient w.r.t. output units
- Gradient w.r.t. hidden units
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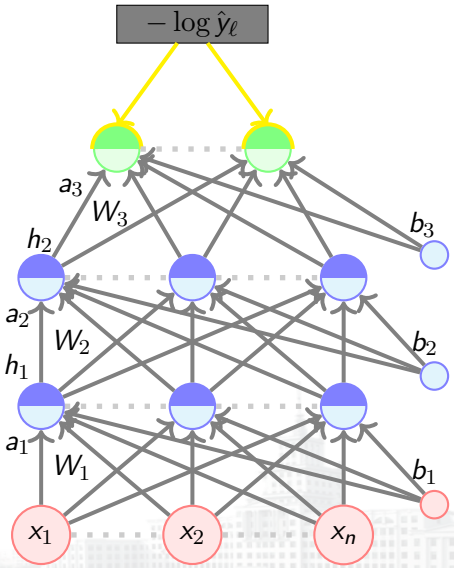
- 我们关注 交叉熵损失函数和 *Softmax* 输出函数

反向传播: 计算损失函数对输出单元的梯度（Gradients w.r.t. the Output Units)

首先，考虑对 i-th 输出的偏导数



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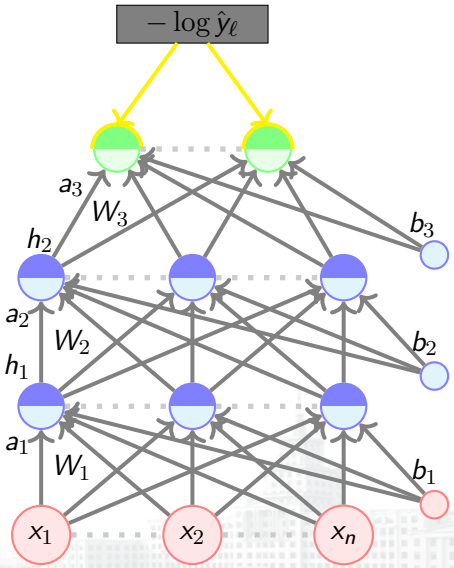
$$\mathscr{L}(\theta) = -\log \hat{y}_\ell \quad (\ell = \text{true class label})$$



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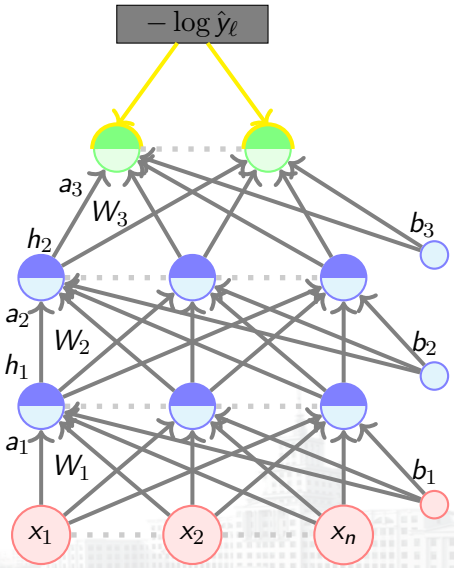

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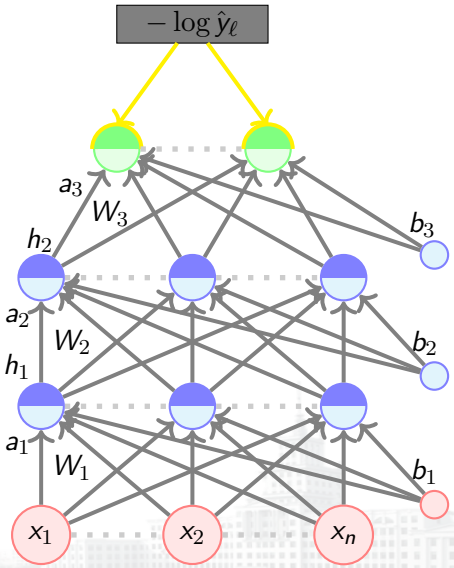

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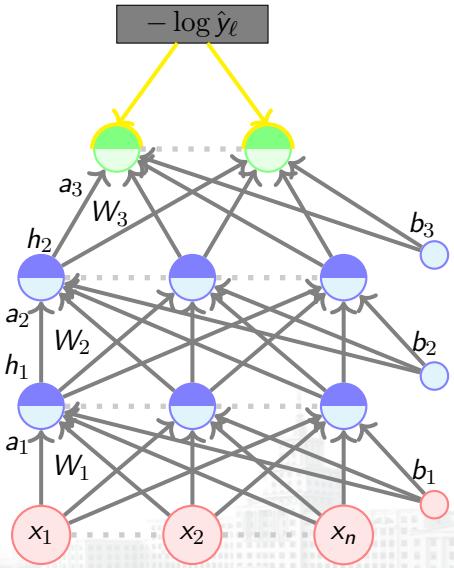

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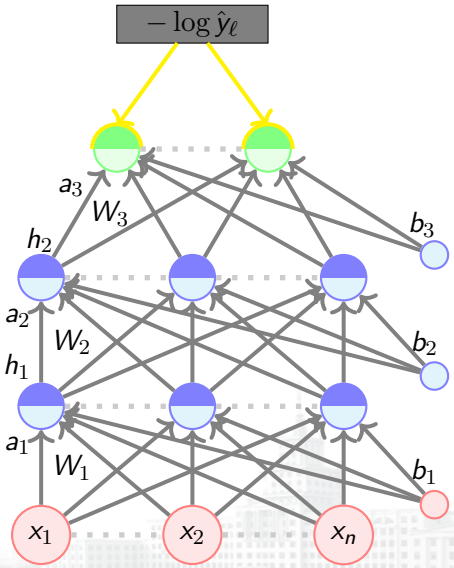

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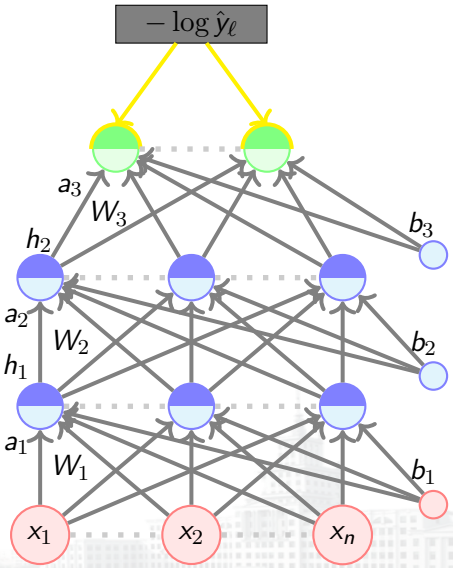

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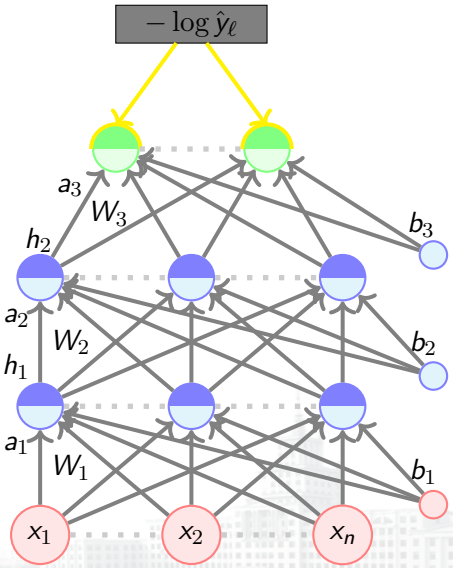
$$\frac{\partial}{\partial \hat{y}_i}\left(\mathscr{L}(\theta)\right) = -\frac{\mathbb{1}_{(i=\ell)}}{\hat{y}_\ell}$$



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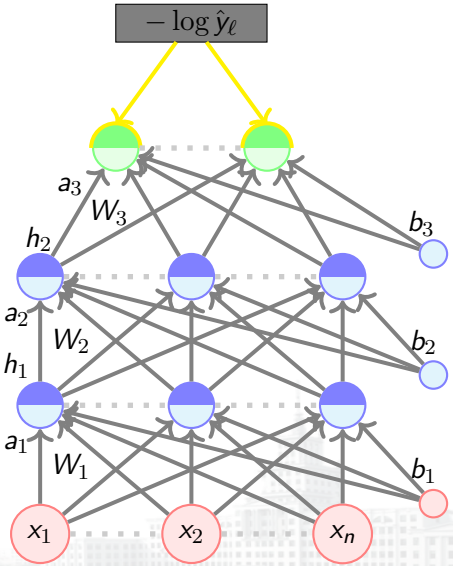

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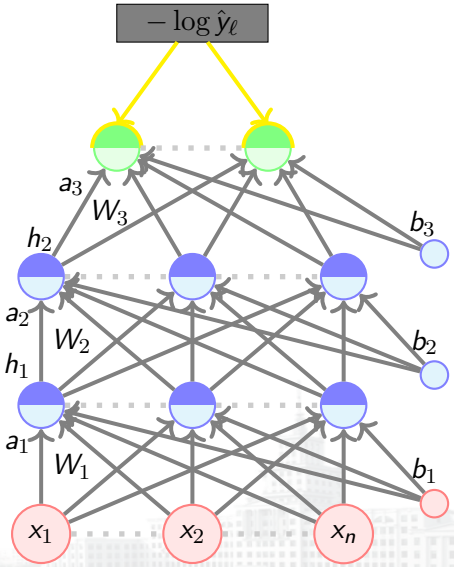

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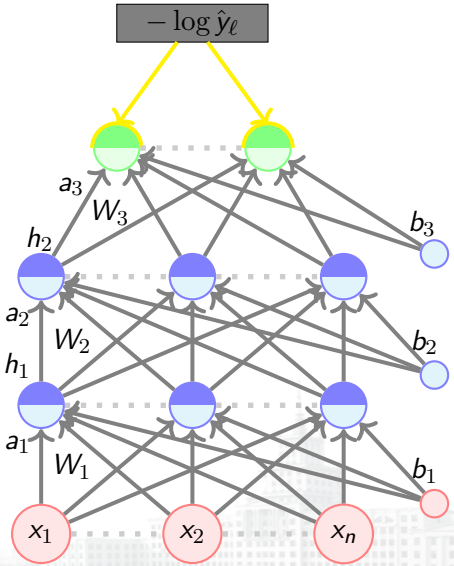

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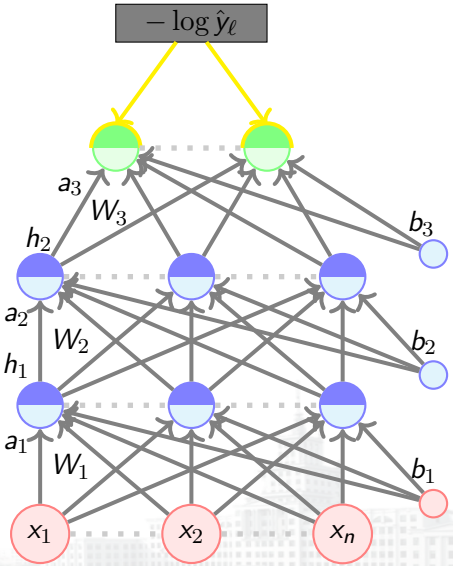

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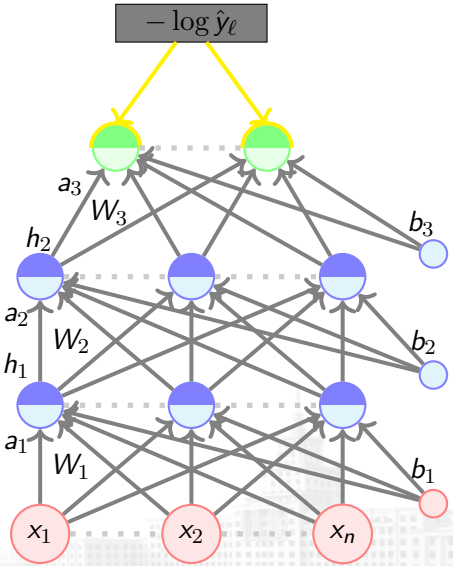

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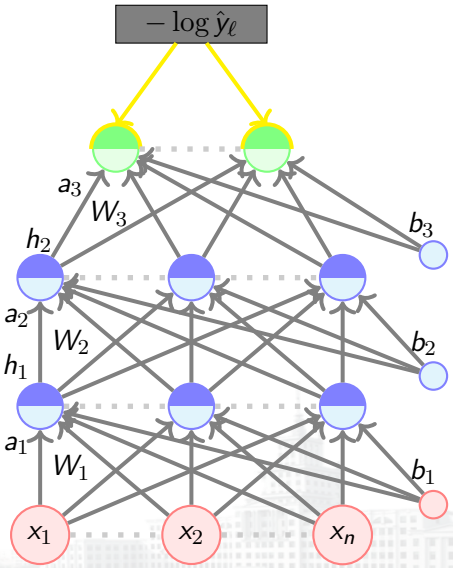

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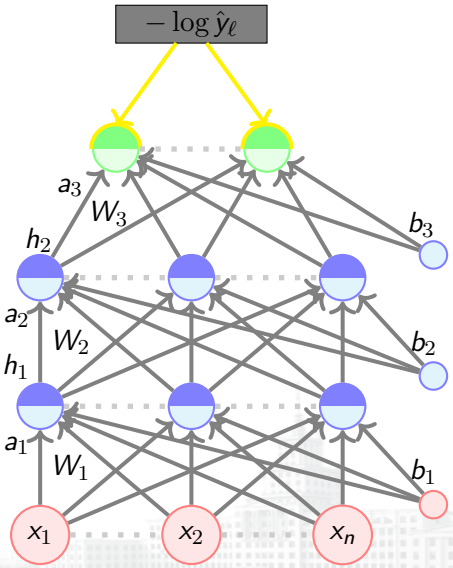

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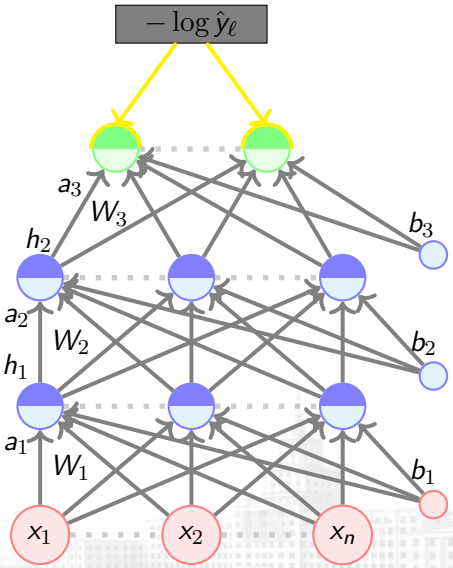

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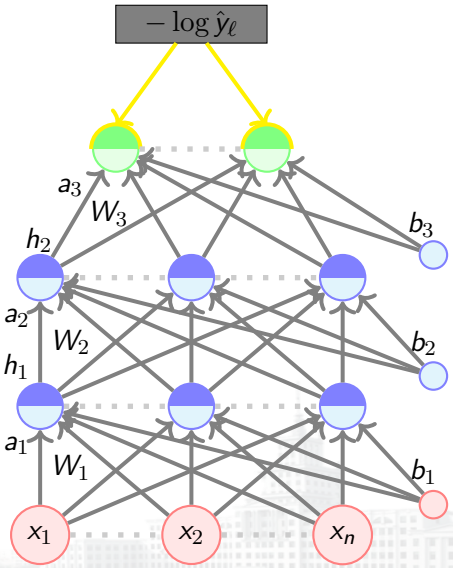

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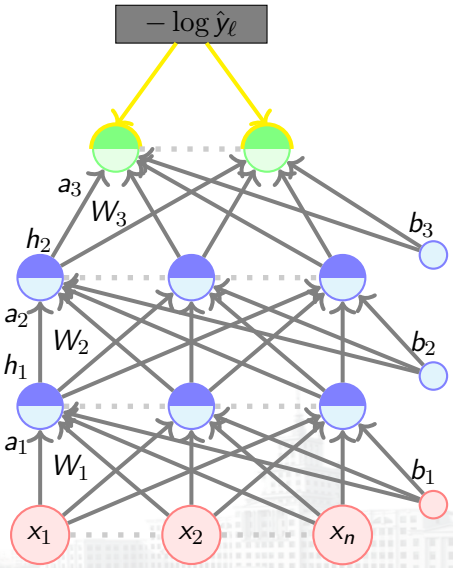

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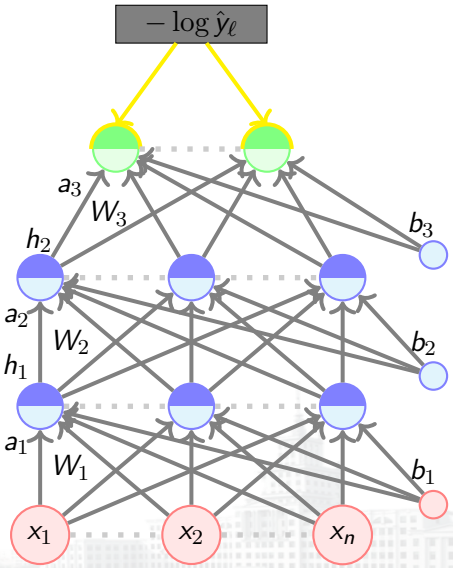

$$\frac{\partial}{\partial \hat{y}_i}\left(\mathscr{L}(\theta)\right) = -\frac{\mathbb{1}_{(\ell=i)}}{\hat{y}_\ell}$$

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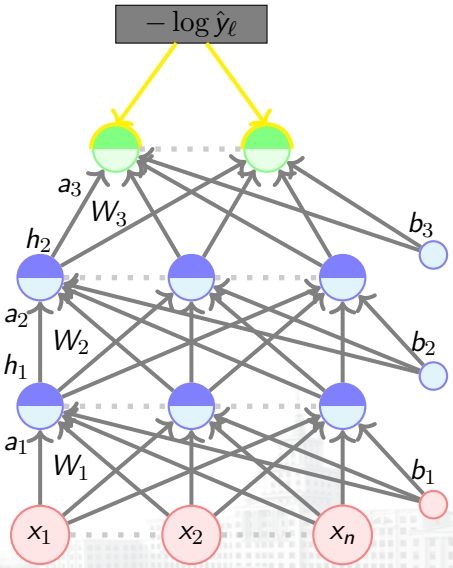

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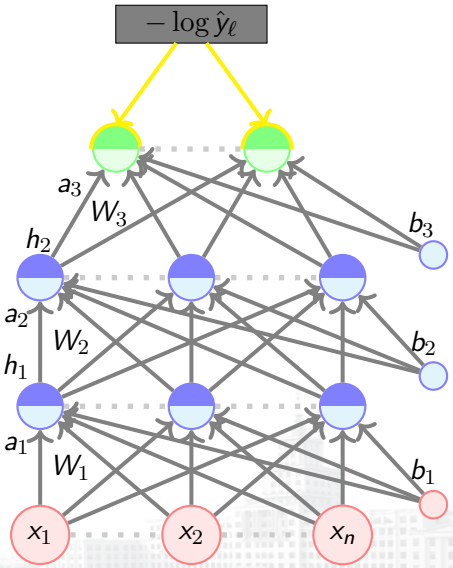
$$= -\frac{1}{\hat{y}_\ell}\mathbf{e}_\ell$$



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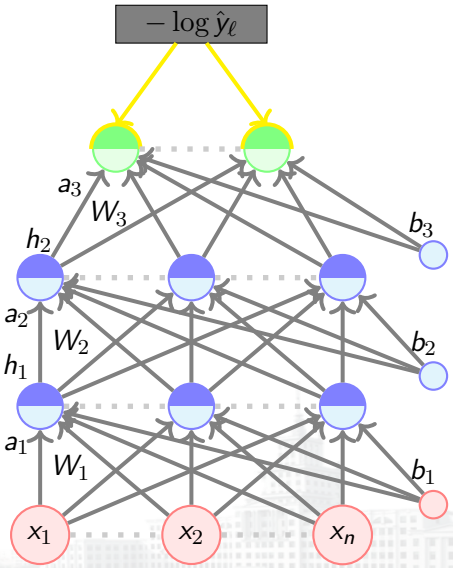
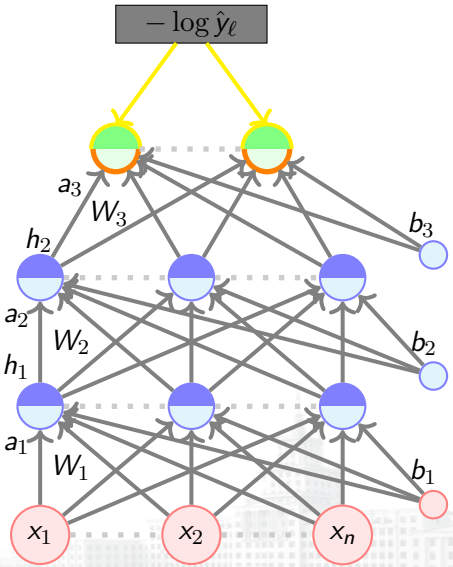
其中 $\mathbf{e}_\ell$ 是一个 k 维向量，它的第 ℓ 个元素是 1 其他元素是 0.



实际上，我们想要计算的是

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



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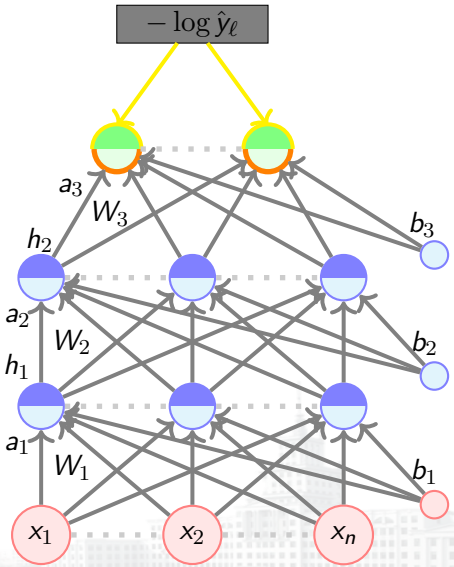

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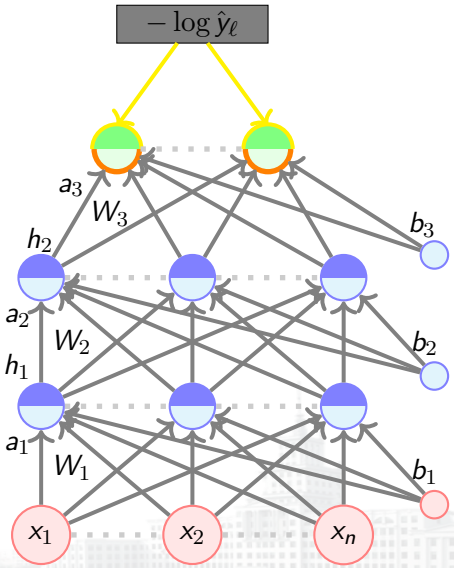
$\hat{y}_\ell$ 依赖于 a_{Li} 吗？



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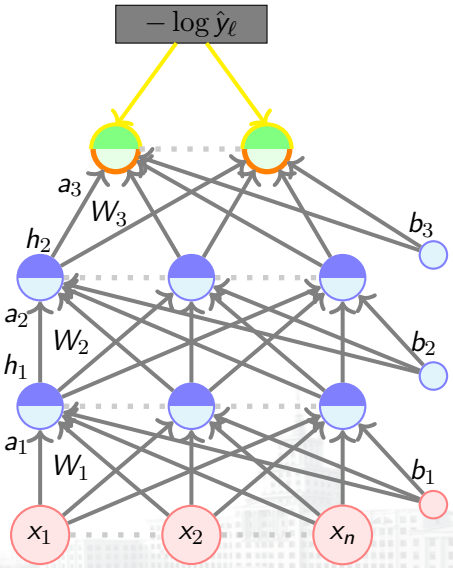

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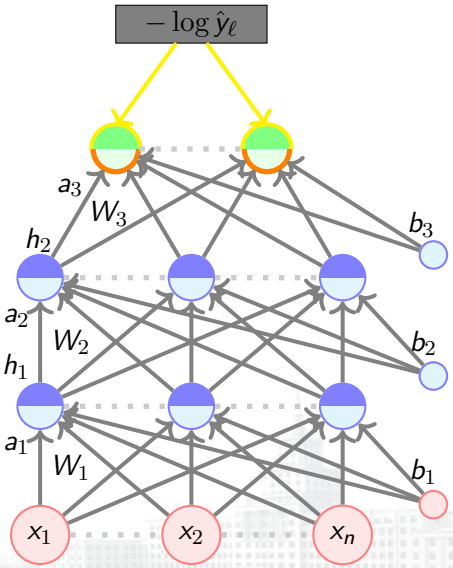
$$\hat{y}_\ell = \frac{exp(a_{L\ell})}{\sum_i exp(a_{Li})}$$



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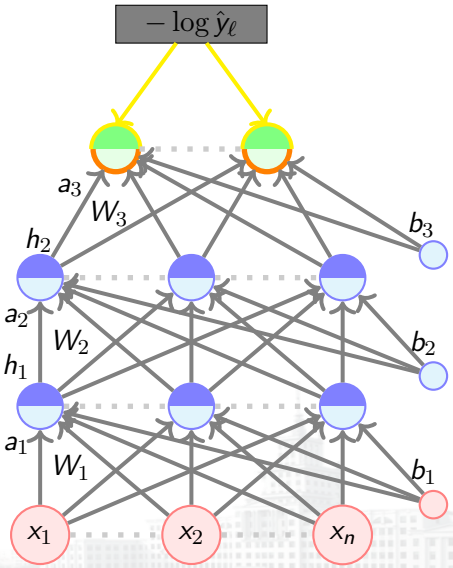
$$\hat{y}_\ell = \frac{exp(a_{L\ell})}{\sum_i exp(a_{Li})}$$

建立 $\hat{y}_\ell$ 和 a_{Li} 的依赖关系后，下面可以计算出对 a_{Li} 的偏导数



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

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

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

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

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

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

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

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现在，已经得到对 $\mathbf{a}_L$ 的 i 个元素的偏导

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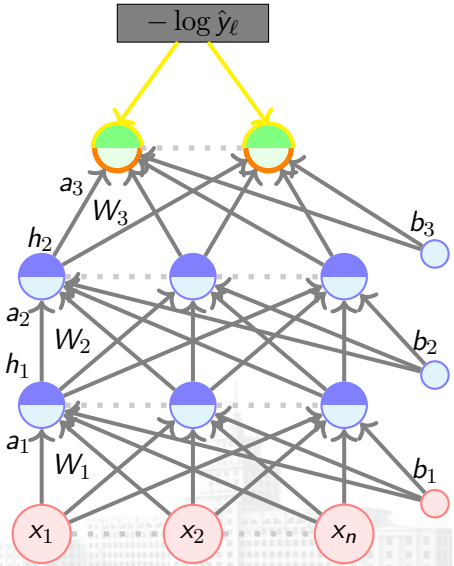
对向量 $\mathbf{a}_L$ 的导数可以计算为



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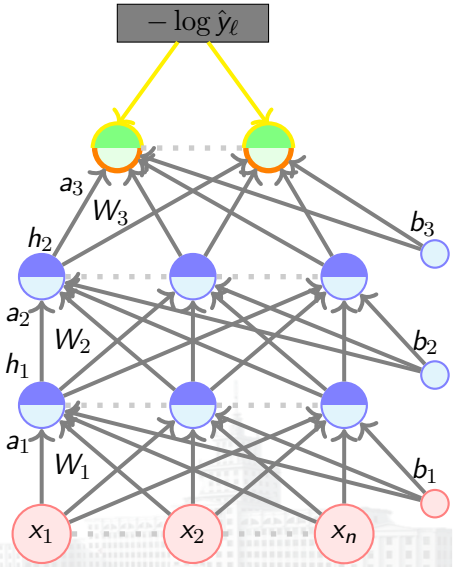

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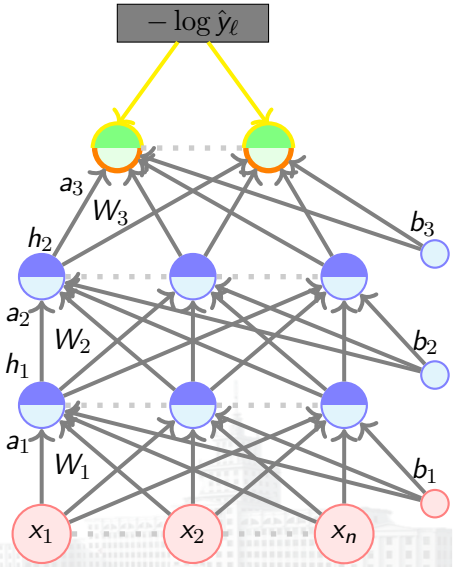

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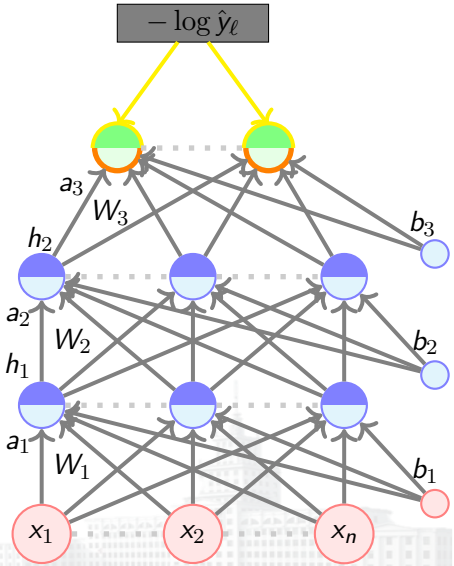

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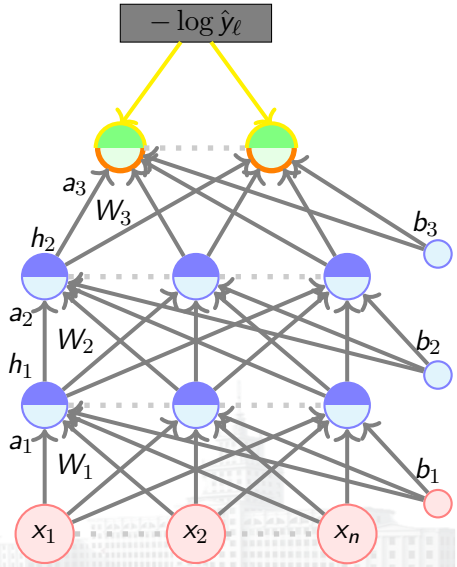

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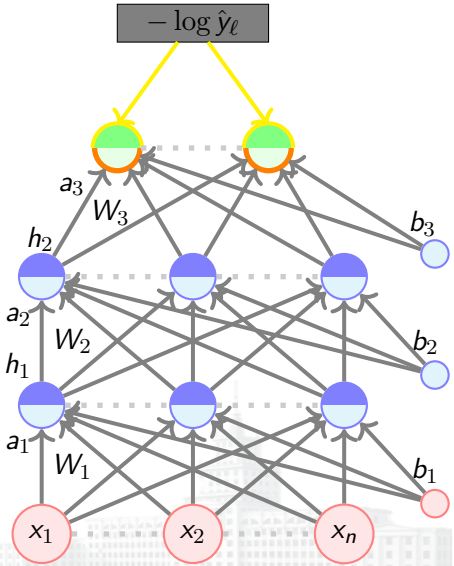

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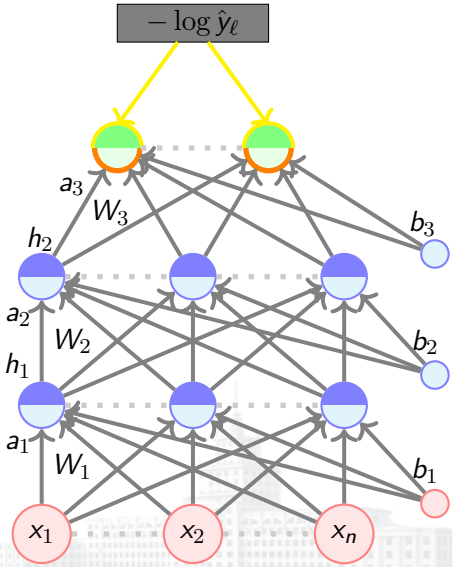

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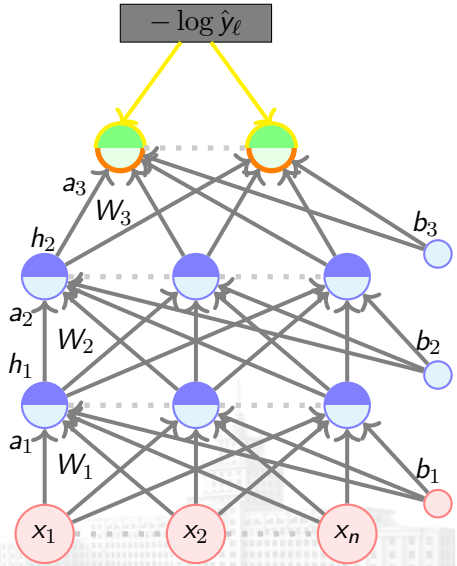

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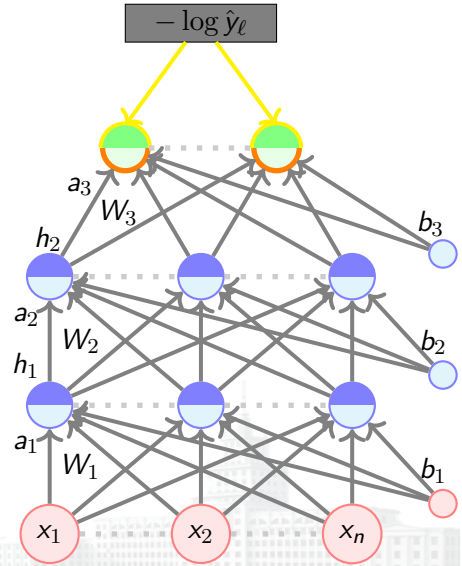
$$\frac{\partial \mathscr{L}(\theta)}{\partial a_{L,i}} = -(\mathbb{1}_{\ell=i} - \hat{y}_i)$$

对向量 $\mathbf{a}_L$ 的导数可以计算为

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



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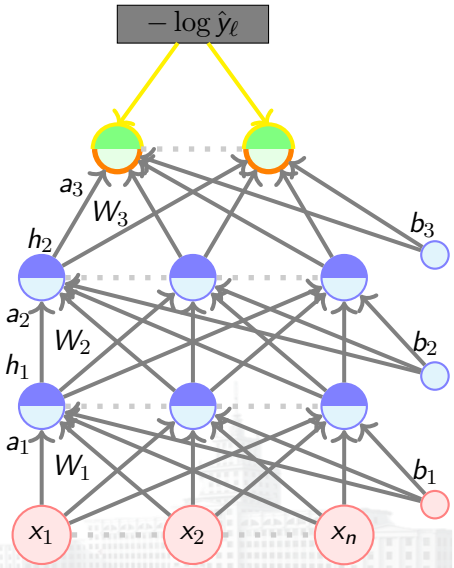

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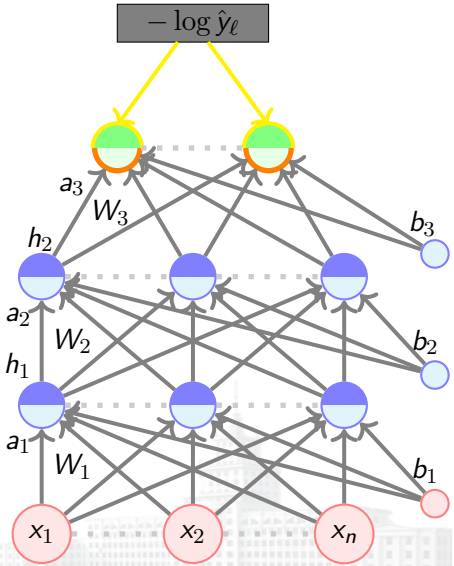


反向传播: 计算损失函数对隐含单元的梯度（Gradients w.r.t. Hidden Units)

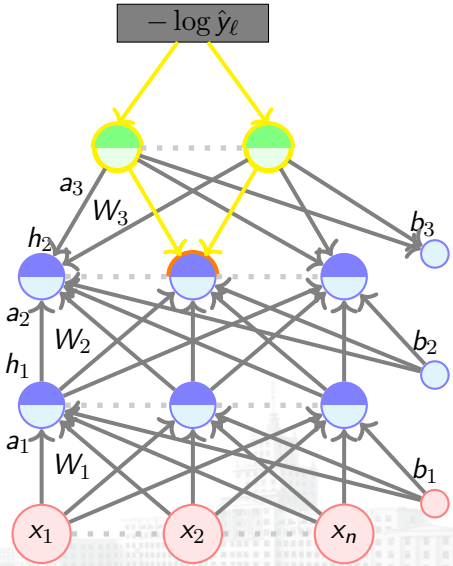
需要计算的梯度:

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

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

- 我们关注 交叉熵损失函数和 *Softmax* 输出函数

Chain rule along multiple paths: 如果一个函数 $p(z)$ 是中间结果 $q_i(z)$ 的函数:



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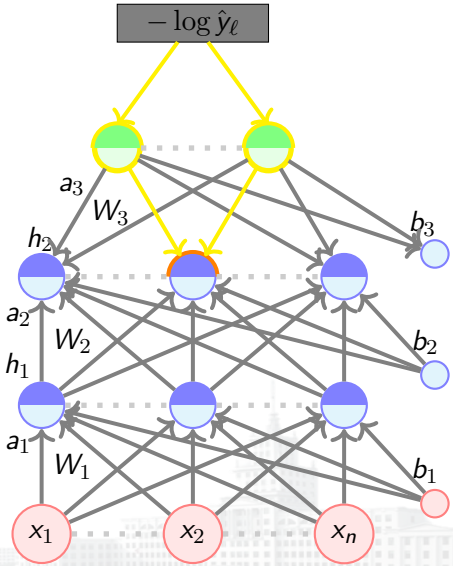

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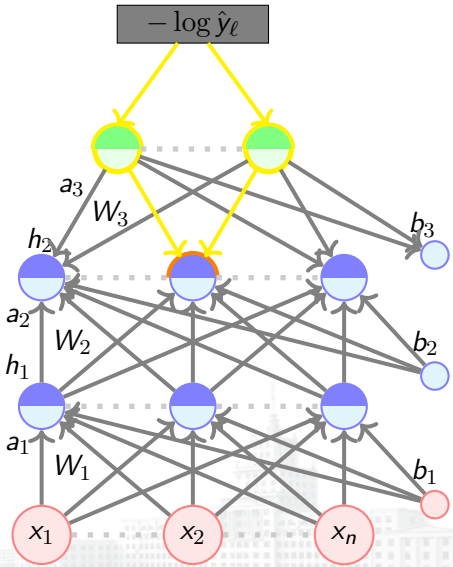
- $p(z)$ 就是损失函数 $\mathscr{L}(\theta)$



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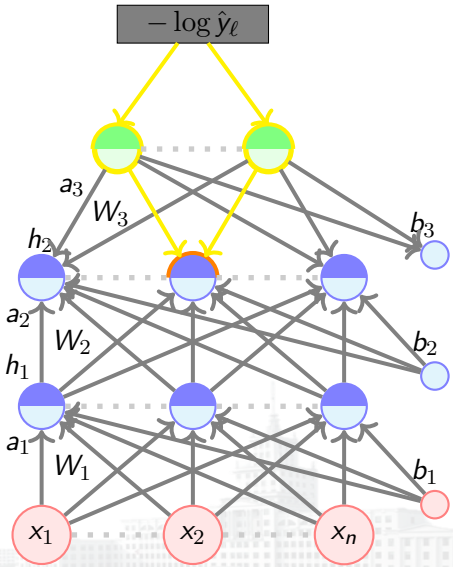

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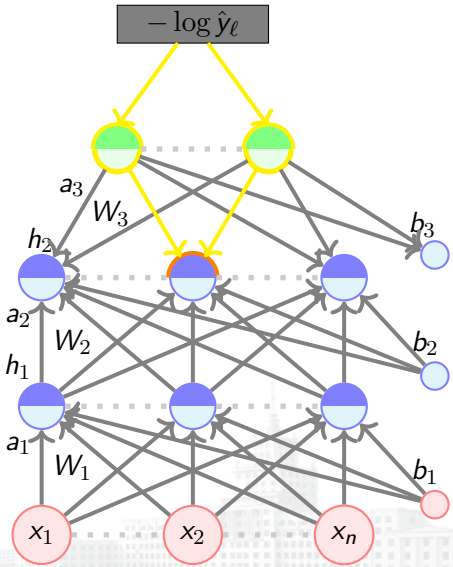
- $q_m(z) = a_{Lm}$



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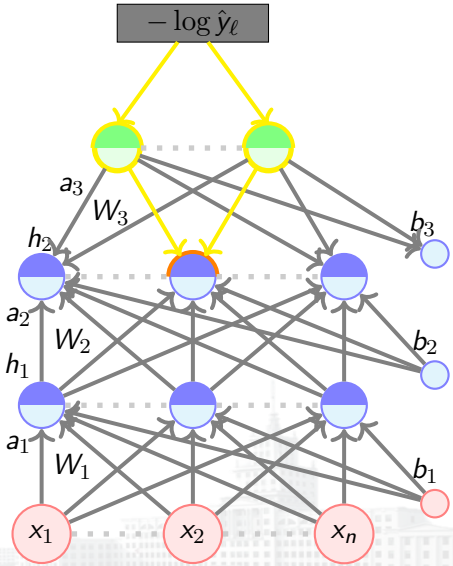
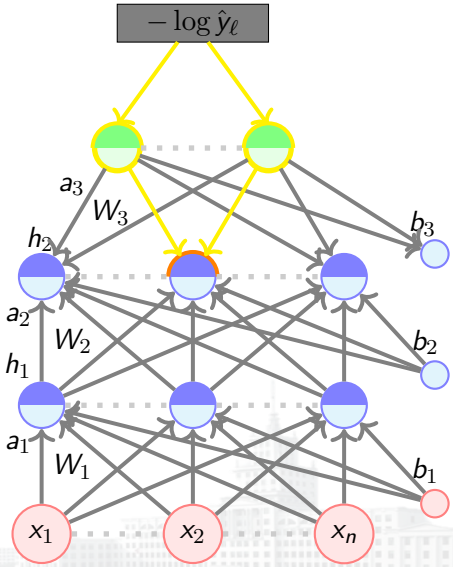
$$\frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}}$$



$$\frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} = \sum_{m=1}^{k} \frac{\partial \mathscr{L}(\theta)}{\partial a_{i+1,m}} \frac{\partial a_{i+1,m}}{\partial h_{ij}}$$



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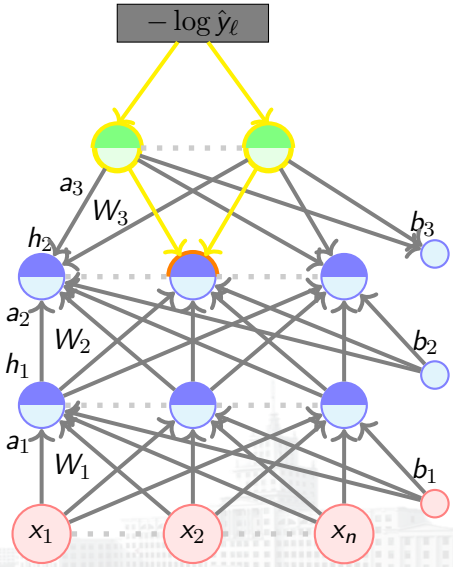

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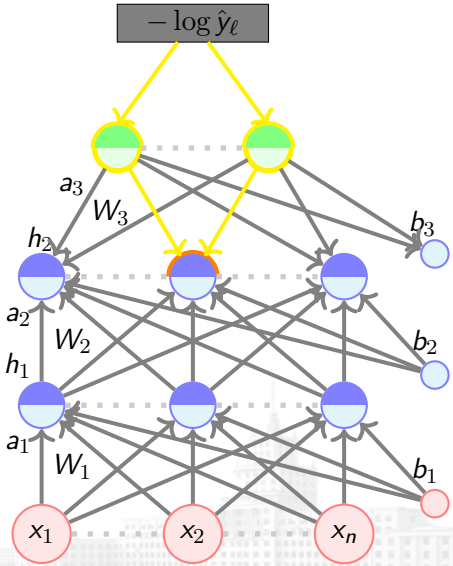

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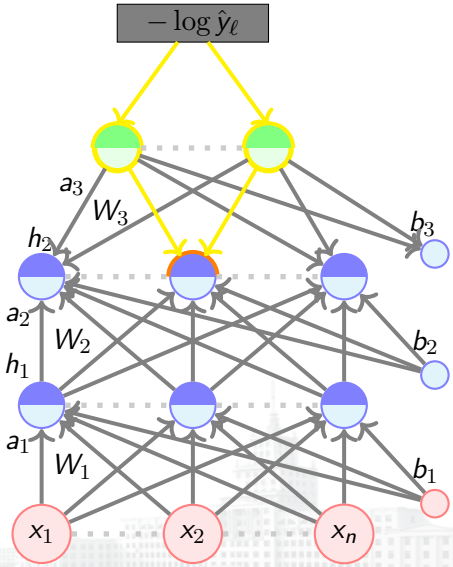

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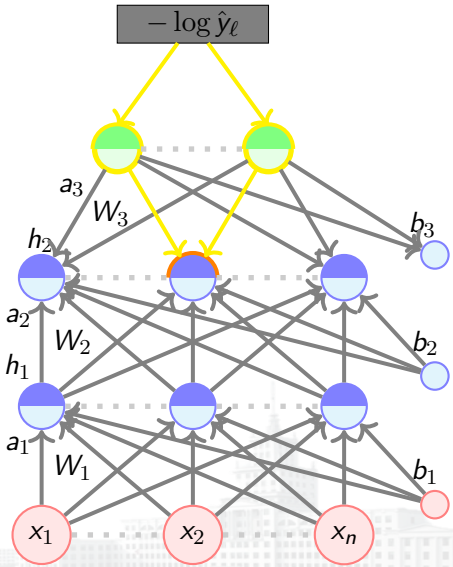

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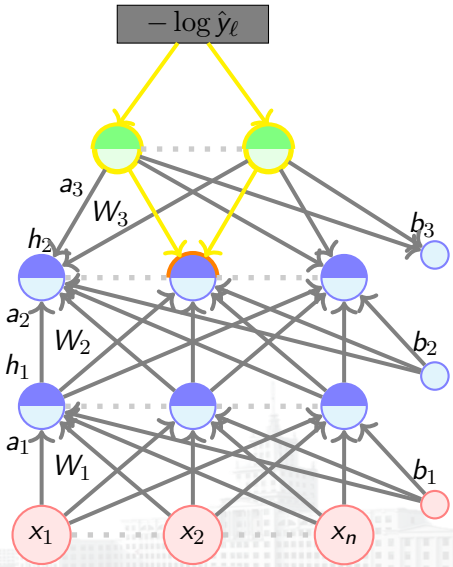

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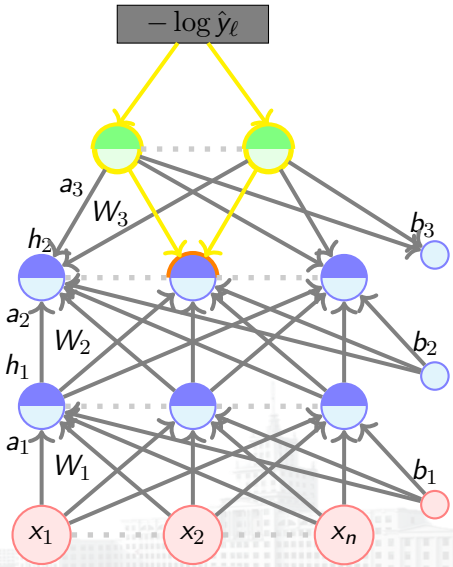

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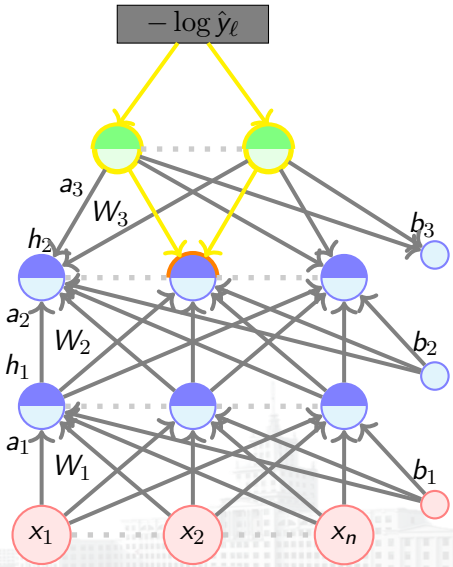

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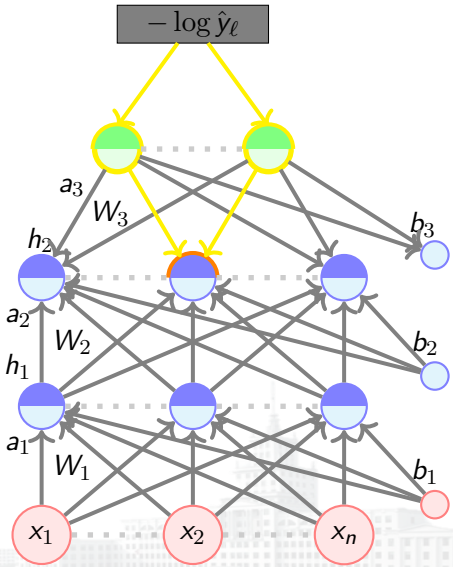

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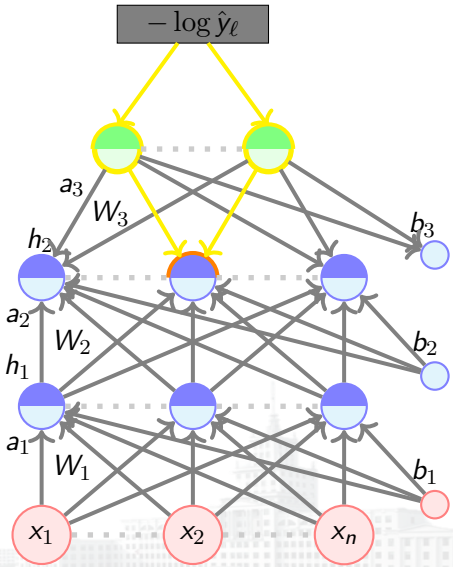

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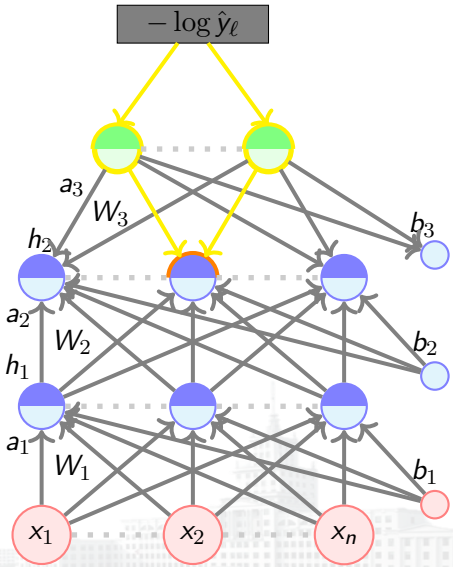

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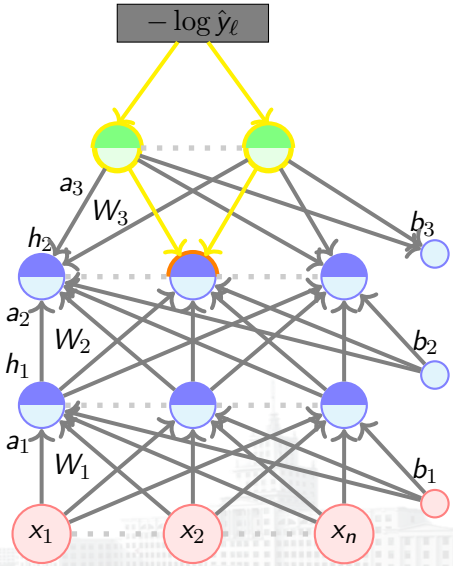

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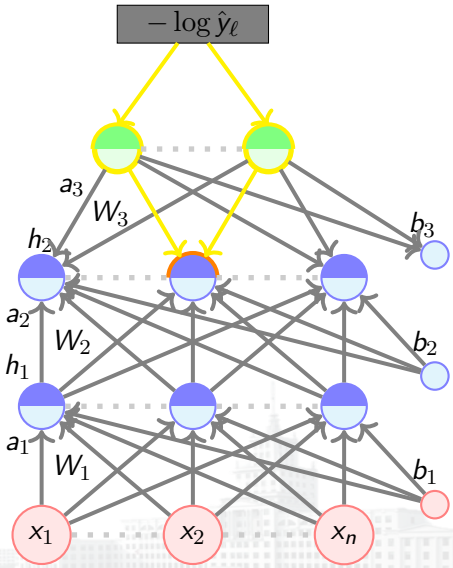
$$(W_{i+1,\cdot,j})^T \nabla_{a_{i+1}} \mathscr{L}(\theta) =$$



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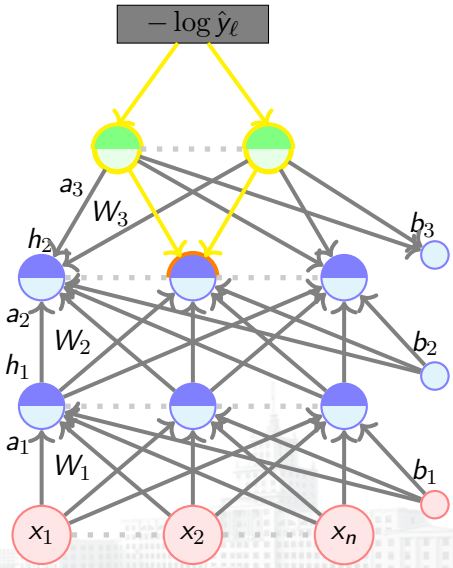
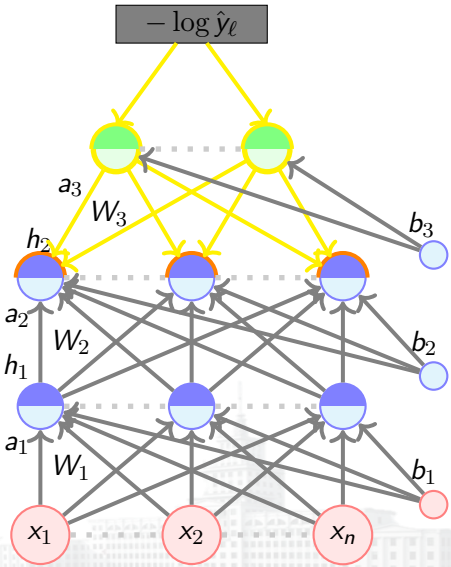


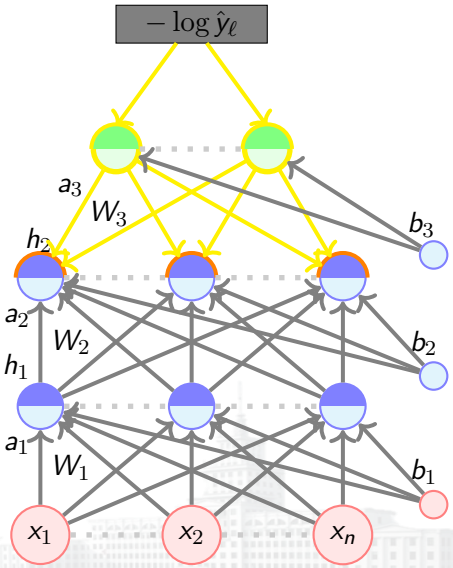
有, $\frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} = (W_{i+1,.,j})^T \nabla_{a_{i+1}} \mathscr{L}(\theta)$



有, $\frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} = (W_{i+1,.,j})^T \nabla_{a_{i+1}} \mathscr{L}(\theta)$

可以重写 gradient w.r.t. h_i

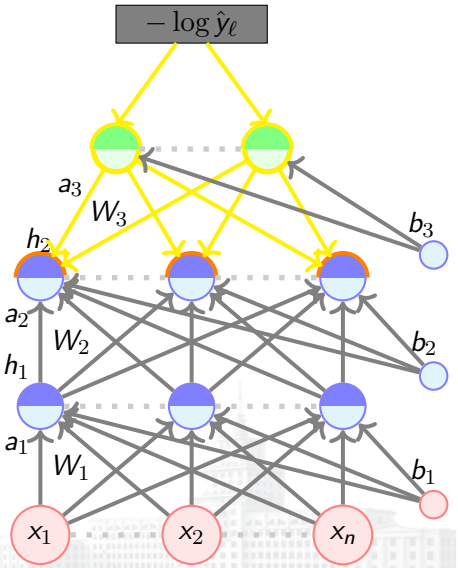
$\nabla_{\mathbf{h_i}} \mathscr{L}(\theta)$



有, $\frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} = (W_{i+1,.,j})^T \nabla_{a_{i+1}} \mathscr{L}(\theta)$

可以重写 gradient w.r.t. h_i

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



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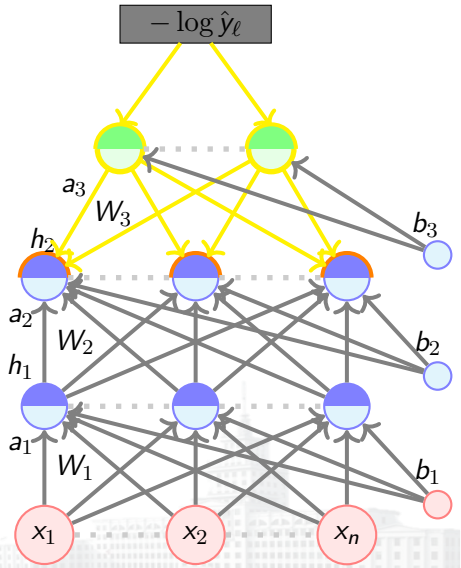
可以重写 gradient w.r.t. h_i

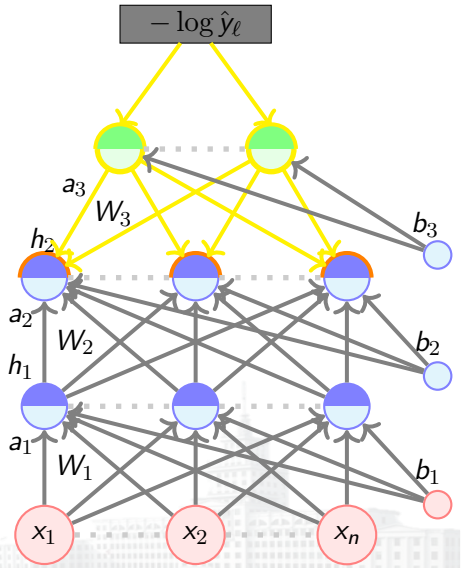
$$\nabla_{\mathbf{h_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial h_{i1}} \\ \\ \\ \\ \end{bmatrix} = \begin{bmatrix} \\ \\ \\ \\ \end{bmatrix}$$



$$\text{有,} \frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} = (W_{i+1,.,j})^T \nabla_{a_{i+1}} \mathscr{L}(\theta)$$

可以重写 gradient w.r.t. h_i

$$\nabla_{\mathbf{h_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial h_{i1}} \\ \\ \\ \end{bmatrix} = \begin{bmatrix} (W_{i+1,\cdot,1})^T \nabla_{a_{i+1}} \mathscr{L}(\theta) \\ \\ \\ \end{bmatrix}$$



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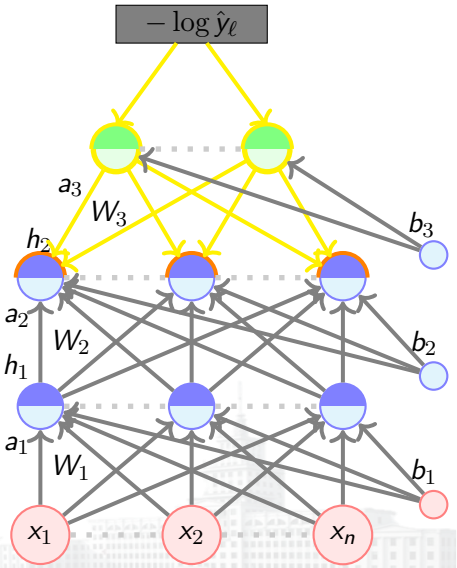

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可以重写 gradient w.r.t. h_i

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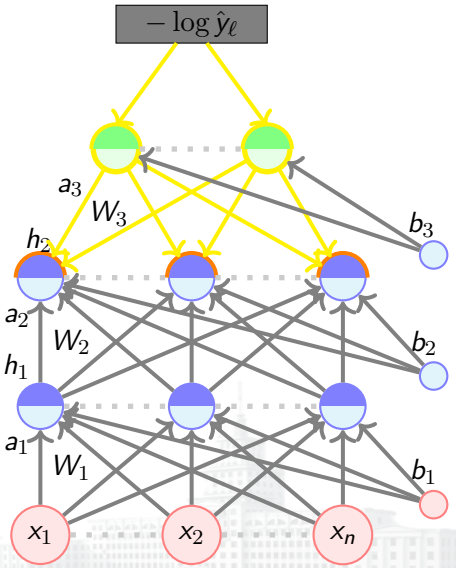

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可以重写 gradient w.r.t. h_i

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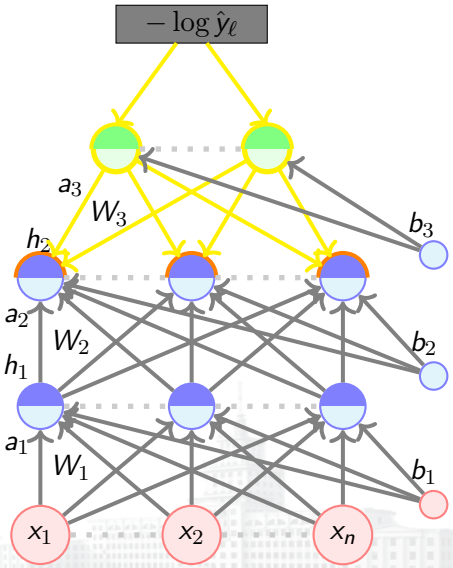

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可以重写 gradient w.r.t. h_i

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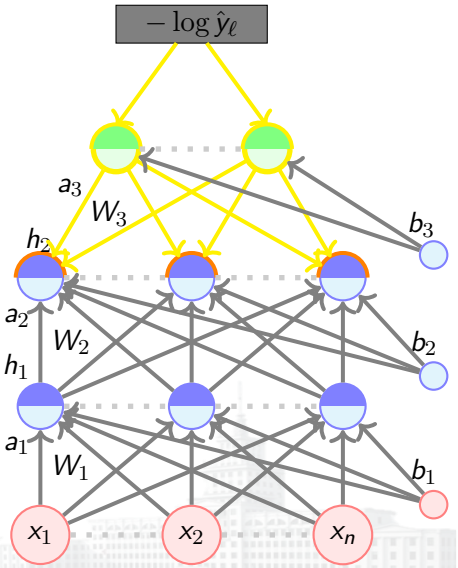

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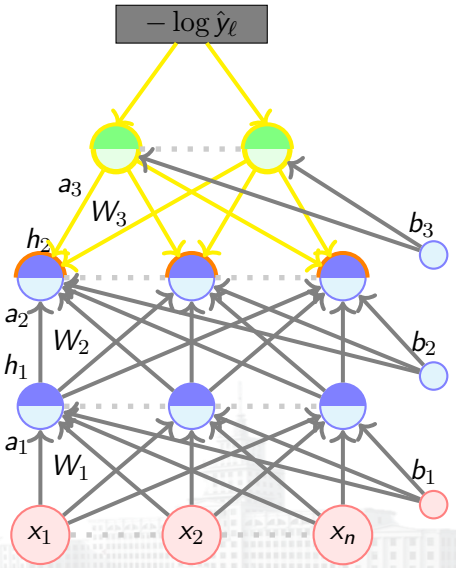

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可以重写 gradient w.r.t. h_i

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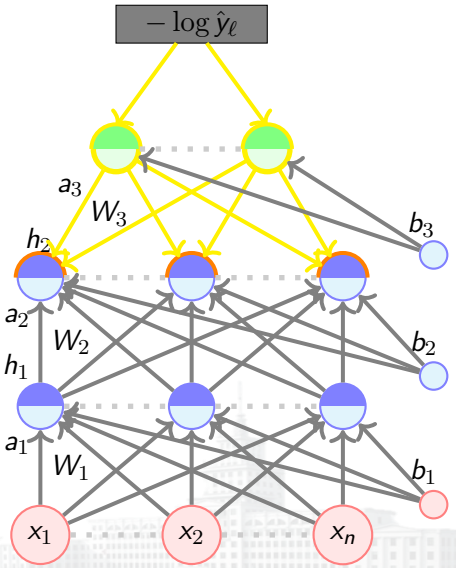
$$= (W_{i+1})^T (\nabla_{a_{i+1}} \mathscr{L}(\theta))$$



$$\text{有,} \frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} = (W_{i+1,.,j})^T \nabla_{a_{i+1}} \mathscr{L}(\theta)$$

可以重写 gradient w.r.t. h_i

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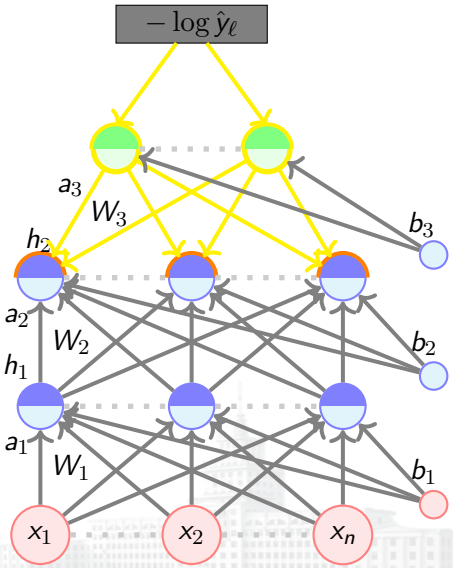
$$= (W_{i+1})^T (\nabla_{a_{i+1}} \mathscr{L}(\theta))$$

- 现在就差计算 $\nabla_{a_{i+1}} \mathscr{L}(\theta)$ for $i < L-1$ 就大功告成了



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可以重写 gradient w.r.t. h_i

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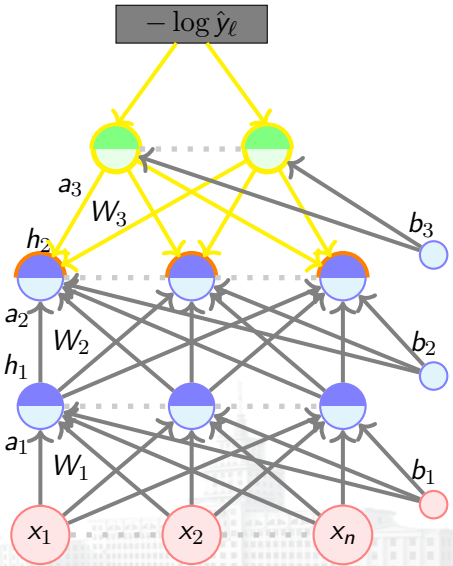
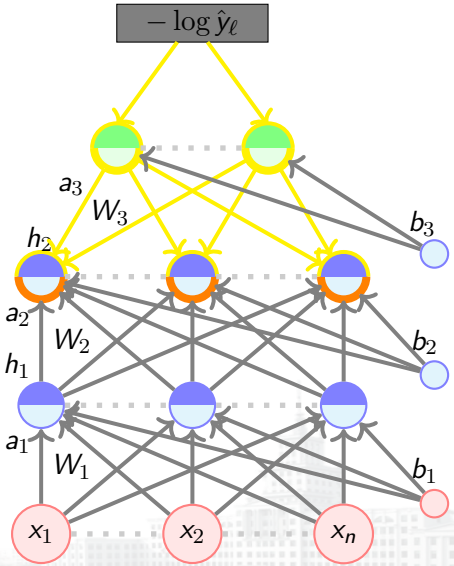
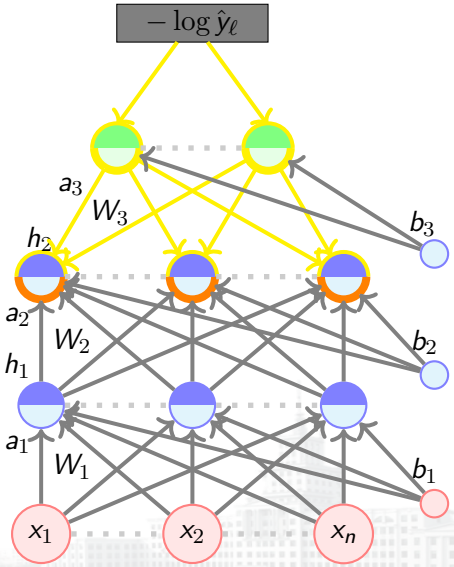
- 现在就差计算 $\nabla_{a_{i+1}} \mathscr{L}(\theta)$ for $i < L-1$ 就大功告成了
- 如何计算？



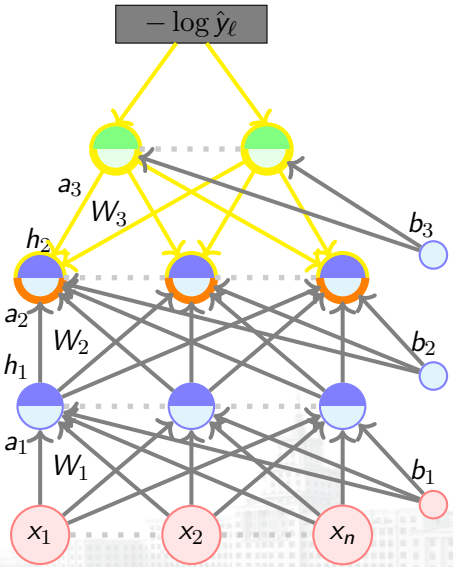
$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta)$



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



$$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{i1}} \\ \\ \\ \end{bmatrix}$$



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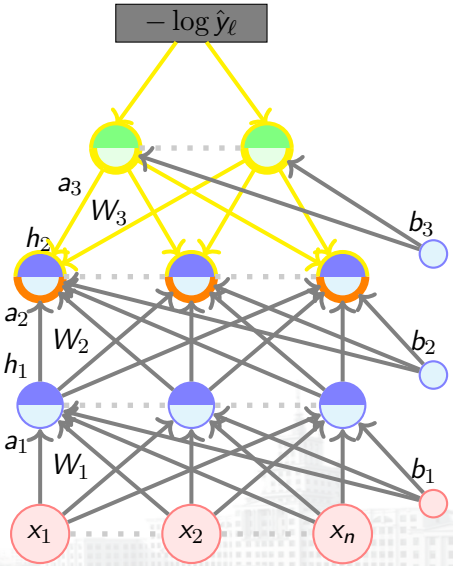
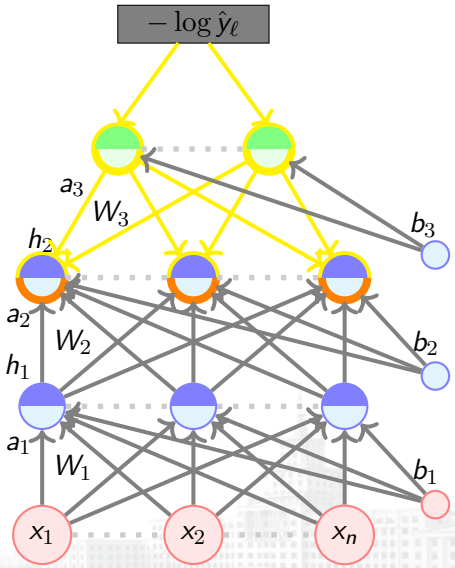
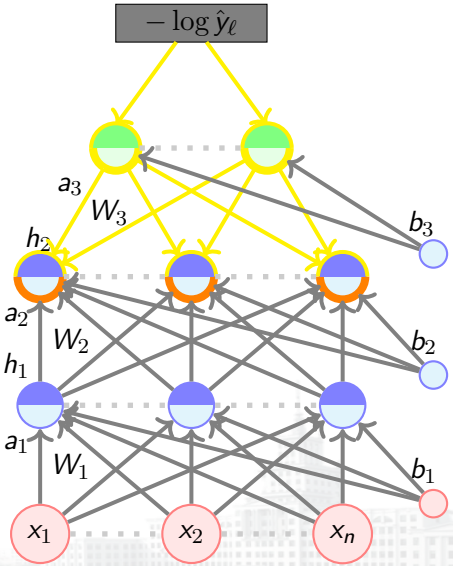


$$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{i1}} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial a_{in}} \end{bmatrix}$$



$$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{i1}} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial a_{in}} \end{bmatrix}$$

$$\frac{\partial \mathscr{L}(\theta)}{\partial a_{ij}}$$



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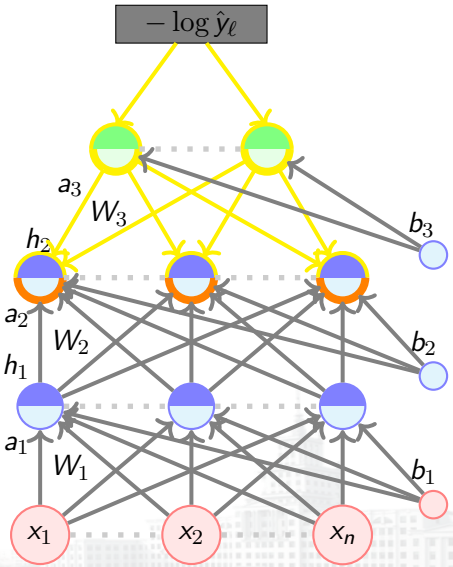
$$\frac{\partial \mathscr{L}(\theta)}{\partial a_{ij}} = \frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} \frac{\partial h_{ij}}{\partial a_{ij}}$$



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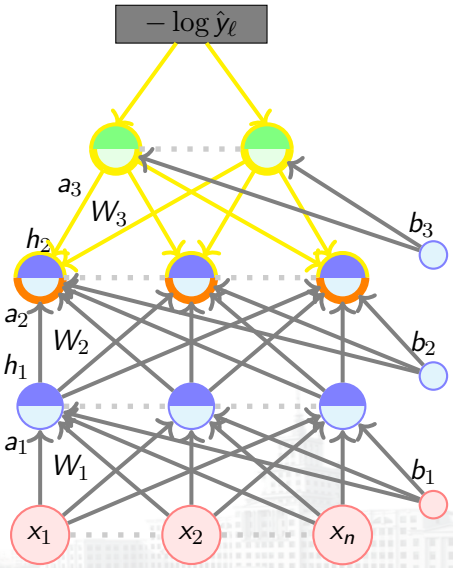
$$= \frac{\partial \mathscr{L}(\theta)}{\partial h_{ij}} g^{'}(a_{ij}) \quad [\because h_{ij} = g(a_{ij})]$$



$$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{i1}} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial a_{in}} \end{bmatrix}$$

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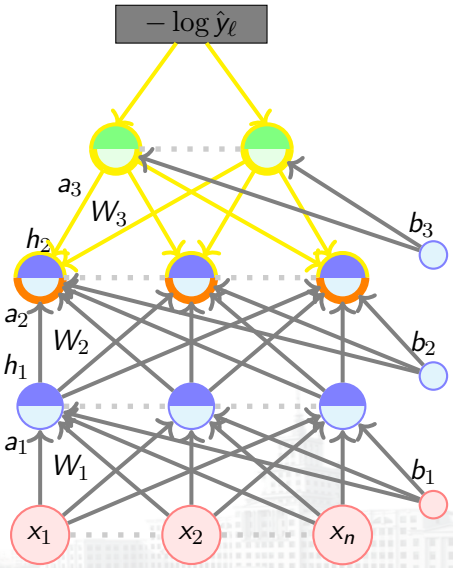
$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta)$



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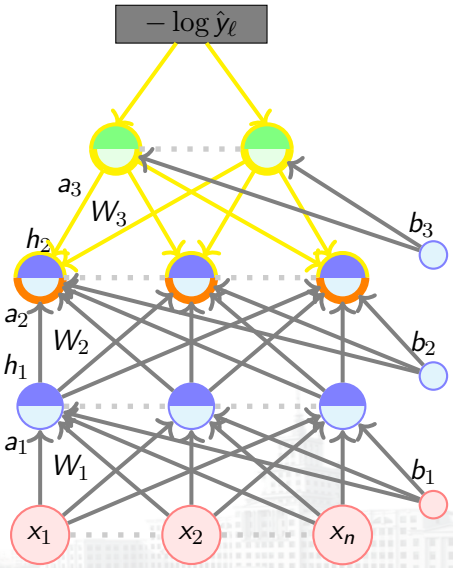

$$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial a_{i1}} \\ \vdots \\ \frac{\partial \mathscr{L}(\theta)}{\partial a_{in}} \end{bmatrix}$$

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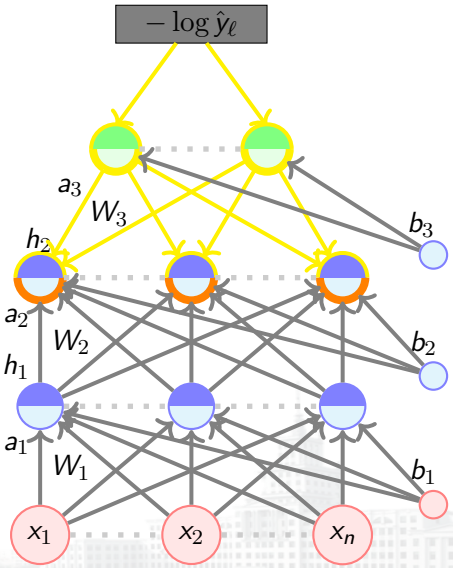
$$\nabla_{\mathbf{a_i}} \mathscr{L}(\theta) = \begin{bmatrix} \frac{\partial \mathscr{L}(\theta)}{\partial h_{i1}} g'(a_{i1}) \\ \\ \\ \end{bmatrix}$$



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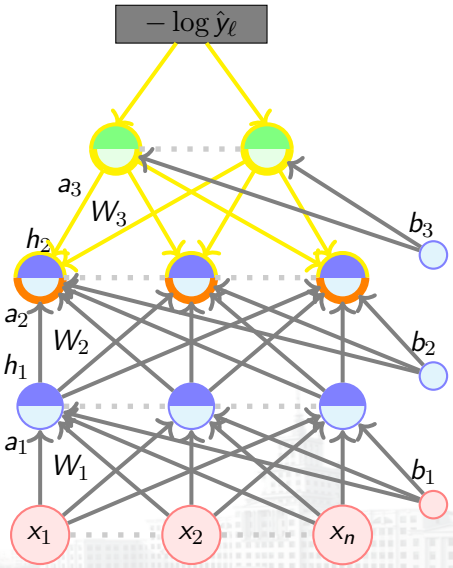

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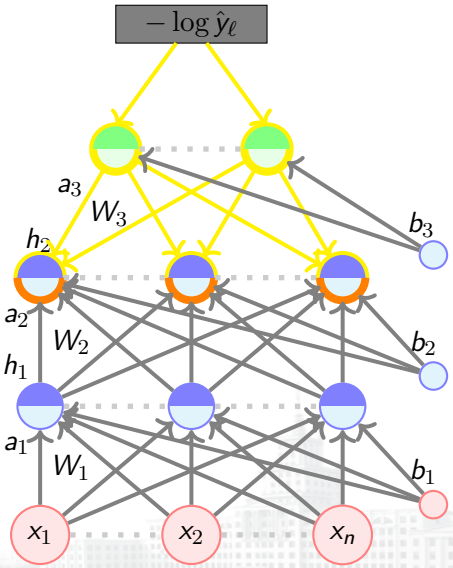

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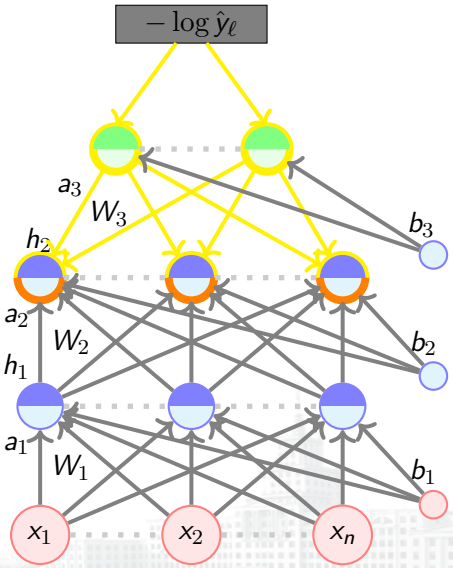
$$= \nabla_{h_i} \mathscr{L}(\theta) \odot [\ldots, g^{'}(a_{ik}), \ldots]$$



反向传播: 计算损失函数对参数的梯度（Computing Gradients w.r.t. Parameters）

需要计算的梯度:

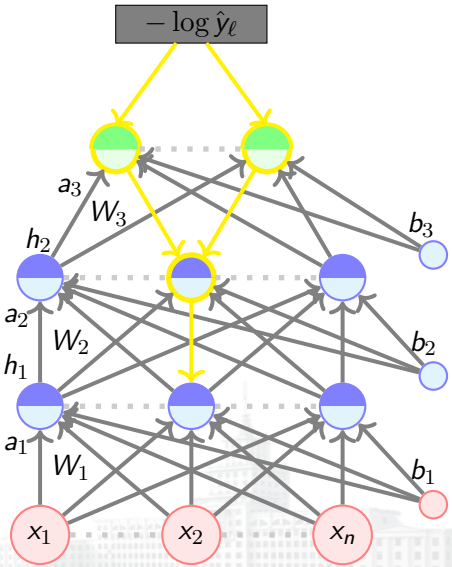
- Gradient w.r.t. output units
- Gradient w.r.t. hidden units
- Gradient w.r.t. weights and biases

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

- 我们关注 交叉熵损失函数和 *Softmax* 输出函数

回忆一下

$$\mathbf{a_k} = \mathbf{b_k} + W_k \mathbf{h_{k-1}}$$



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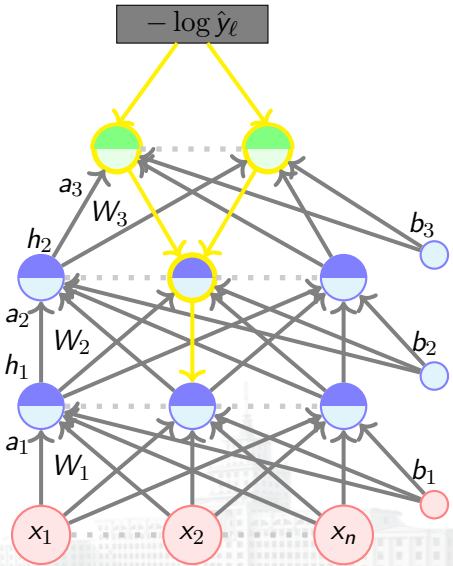

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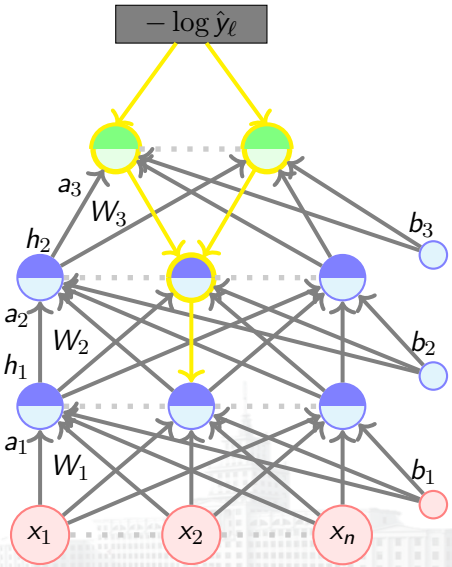

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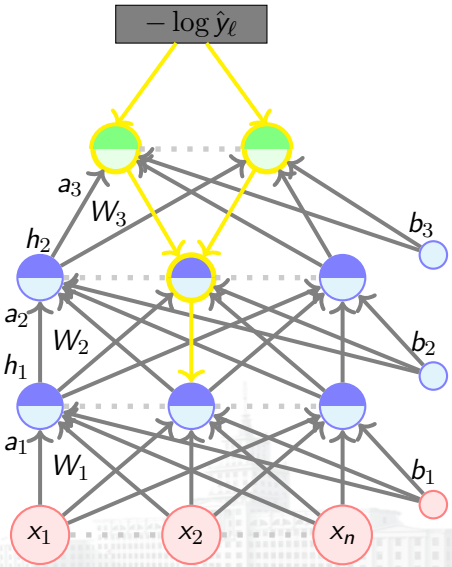

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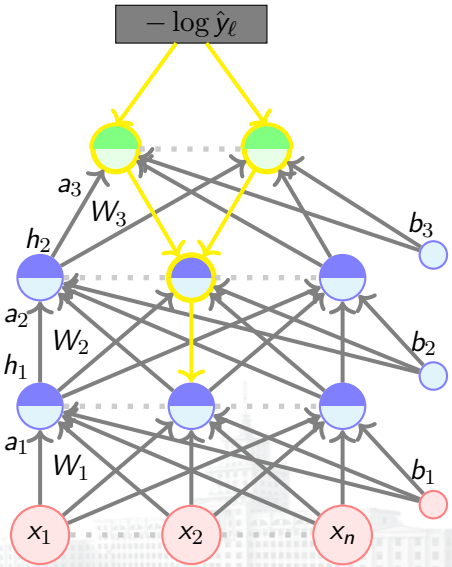

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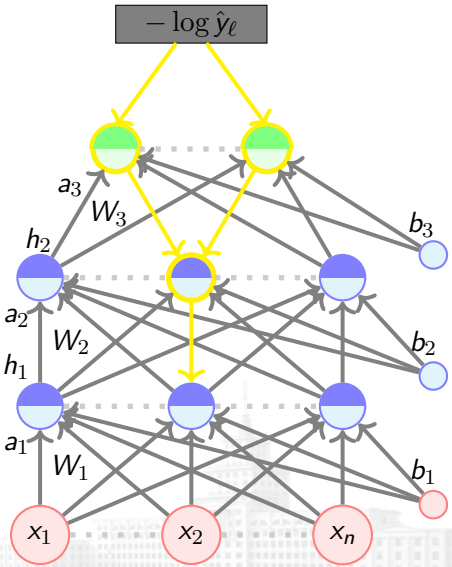
$$\nabla_{W_k} \mathscr{L}(\theta) =$$



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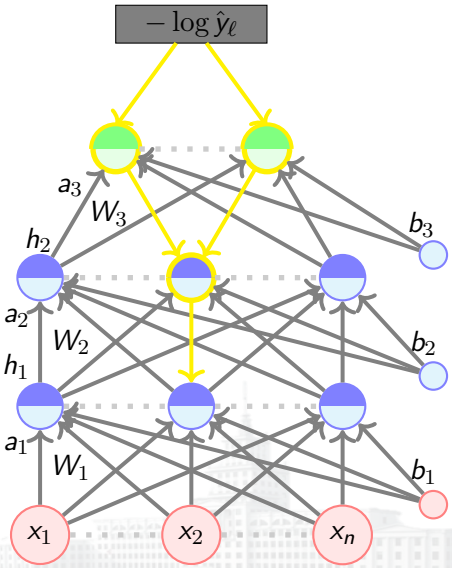

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举一个列子 $W_k \in \mathbb{R}^{3\times 3}$ 来看看如何计算

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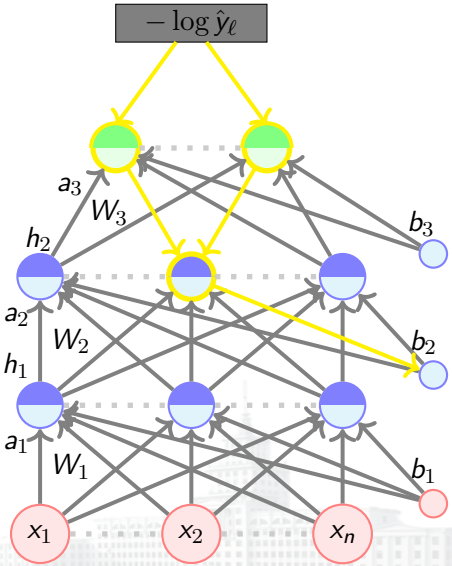
最后，看看对偏置的梯度



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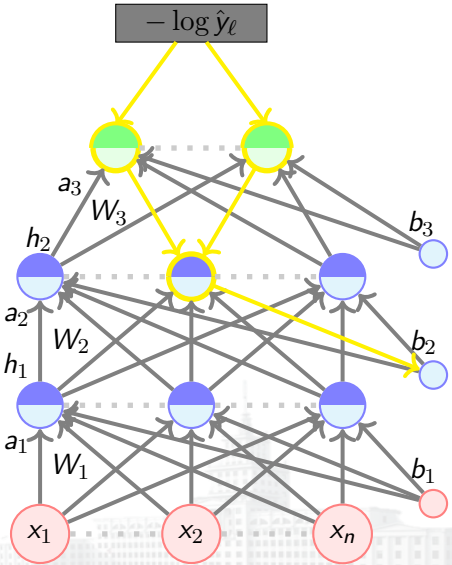

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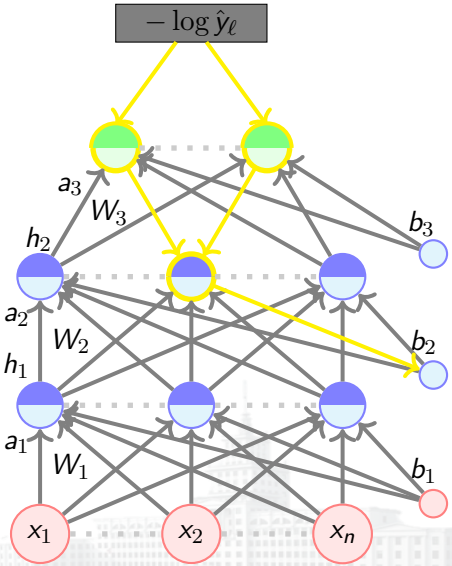

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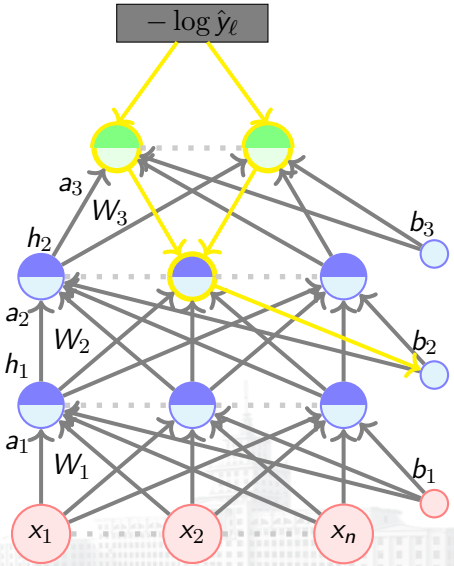

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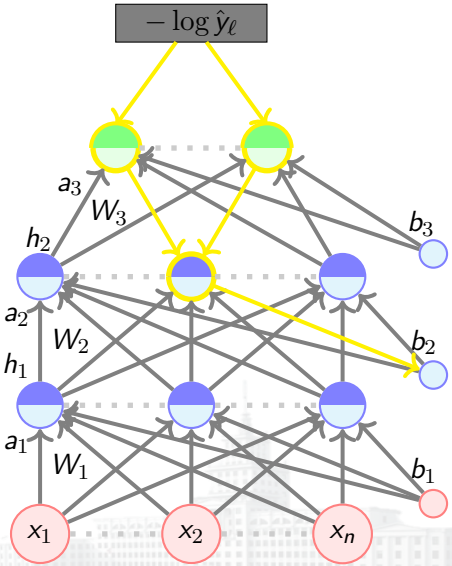
重写 gradient w.r.t. the vector b_k



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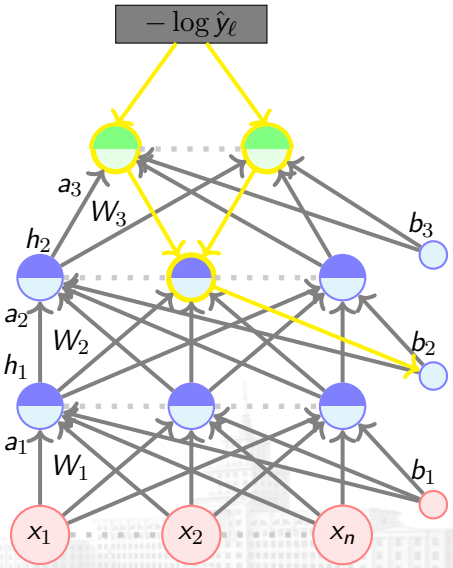

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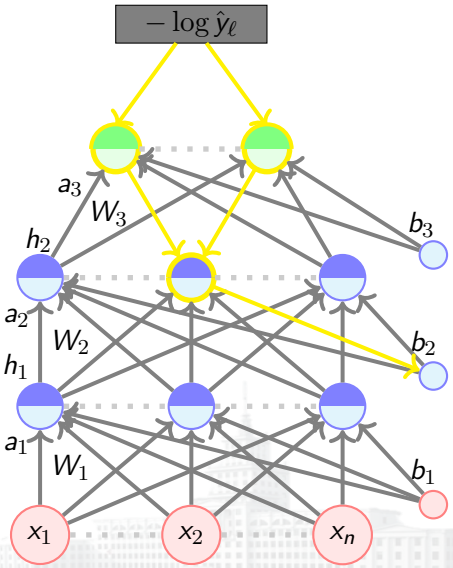

反向传播: Pseudo code

所有需要的梯度已经计算出来

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$$\nabla_{\mathbf{a_L}} \mathscr{L}(\theta) \quad \text{(gradient w.r.t. output layer)}$$

$$\nabla_{\mathbf{h_k}} \mathscr{L}(\theta), \nabla_{\mathbf{a_k}} \mathscr{L}(\theta) \quad \text{(gradient w.r.t. hidden layers, } 1 \leq k < L\text{)}$$

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$$\nabla_{W_k} \mathscr{L}(\theta), \nabla_{\mathbf{b_k}} \mathscr{L}(\theta) \quad \text{(gradient w.r.t. weights and biases, } 1 \leq k \leq L\text{)}$$

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$$\nabla_{W_k} \mathscr{L}(\theta), \nabla_{\mathbf{b_k}} \mathscr{L}(\theta) \quad \text{(gradient w.r.t. weights and biases, } 1 \leq k \leq L\text{)}$$

可以得出整个学习算法

Algorithm: gradient_descent()

$t \leftarrow 0$;
max_iterations $\leftarrow 1000$;
Initialize $\theta_0 = [W_1^0, ..., W_L^0, b_1^0, ..., b_L^0]$;

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while $t{+}{+} < max\_iterations$ **do**
    $h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, \hat{y} = forward\_propagation(\theta_t)$;
end

Algorithm: gradient_descent()

$t \leftarrow 0$;
$max\_iterations \leftarrow 1000$;
Initialize $\theta_0 = [W_1^0, ..., W_L^0, b_1^0, ..., b_L^0]$;
while $t{+}{+} < max\_iterations$ **do**
    $h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, \hat{y} = forward\_propagation(\theta_t)$;
    $\nabla\theta_t = backward\_propagation(h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, y, \hat{y})$;
end

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  $h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, \hat{y} = forward\_propagation(\theta_t)$;
  $\nabla\theta_t = backward\_propagation(h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, y, \hat{y})$;
  $\theta_{t+1} \leftarrow \theta_t - \eta\nabla\theta_t$;
end

Algorithm: forward_propagation(θ)

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for $k = 1$ *to* $L - 1$ **do**

end

Algorithm: forward_propagation(θ)

for $k = 1$ *to* $L - 1$ **do**

  $a_k = b_k + W_k h_{k-1}$;

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Algorithm: forward_propagation(θ)

for $k = 1$ *to* $L - 1$ **do**

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$h_k = g(a_k)$;

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Algorithm: forward_propagation(θ)

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$a_k = b_k + W_k h_{k-1}$;

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$a_L = b_L + W_L h_{L-1}$;

Algorithm: forward_propagation(θ)

for $k = 1$ *to* $L - 1$ **do**

$a_k = b_k + W_k h_{k-1}$;

$h_k = g(a_k)$;

end

$a_L = b_L + W_L h_{L-1}$;

$\hat{y} = O(a_L)$;

执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

Algorithm: back_propagation($h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, y, \hat{y}$)

//Compute output gradient ;

执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

Algorithm: back_propagation($h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, y, \hat{y}$)

//Compute output gradient ;
$\nabla_{a_L} \mathscr{L}(\theta) = -(e(y) - \hat{y})$;

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for $k = L$ *to* 1 **do**
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执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

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for $k = L$ *to* 1 **do**
    // Compute gradients w.r.t. parameters ;
    $\nabla_{W_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta) h_{k-1}^T$;

end

执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

Algorithm: back_propagation($h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, y, \hat{y}$)

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    $\nabla_{W_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta) h_{k-1}^T$;

    $\nabla_{b_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta)$;

end

执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

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    $\nabla_{W_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta) h_{k-1}^T$;

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    // Compute gradients w.r.t. layer below ;

end

执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

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$\nabla_{b_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta)$;

// Compute gradients w.r.t. layer below ;

$\nabla_{h_{k-1}} \mathscr{L}(\theta) = W_k^T (\nabla_{a_k} \mathscr{L}(\theta))$;

end

执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

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$\nabla_{a_L} \mathscr{L}(\theta) = -(e(y) - \hat{y})$;
for $k = L$ *to* 1 **do**
    // Compute gradients w.r.t. parameters ;
    $\nabla_{W_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta) h_{k-1}^T$;
    $\nabla_{b_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta)$;
    // Compute gradients w.r.t. layer below ;
    $\nabla_{h_{k-1}} \mathscr{L}(\theta) = W_k^T (\nabla_{a_k} \mathscr{L}(\theta))$;
    // Compute gradients w.r.t. layer below (pre-activation);
end

执行前向传播，计算所有的 h_i's, a_i's, and $\hat{y}$

Algorithm: back_propagation($h_1, h_2, ..., h_{L-1}, a_1, a_2, ..., a_L, y, \hat{y}$)

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$\nabla_{a_L} \mathscr{L}(\theta) = -(e(y) - \hat{y})$;

for $k = L$ *to* 1 **do**

  // Compute gradients w.r.t. parameters ;

  $\nabla_{W_k} \mathscr{L}(\theta) = \nabla_{a_k} \mathscr{L}(\theta) h_{k-1}^T$;

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  // Compute gradients w.r.t. layer below ;

  $\nabla_{h_{k-1}} \mathscr{L}(\theta) = W_k^T (\nabla_{a_k} \mathscr{L}(\theta))$;

  // Compute gradients w.r.t. layer below (pre-activation);

  $\nabla_{a_{k-1}} \mathscr{L}(\theta) = \nabla_{h_{k-1}} \mathscr{L}(\theta) \odot [\ldots, g'(a_{k-1,j}), \ldots]$;

end

激活函数的导数

最后需要解决的事情是如何计算 g'

最后需要解决的事情是如何计算 g'

Logistic function

$$\begin{aligned} g(z) &= \sigma(z) \\ &= \frac{1}{1+e^{-z}} \end{aligned}$$

最后需要解决的事情是如何计算 g'

Logistic function

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\begin{aligned}
g(z) &= \sigma(z) \\
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&= \frac{1}{1+e^{-z}}\left(\frac{1+e^{-z}-1}{1+e^{-z}}\right)
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g(z) &= \tanh(z) \\
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&= \frac{(e^{z}+e^{-z})^2-(e^{z}-e^{-z})^2}{(e^{z}+e^{-z})^2}
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&= \frac{(e^{z}+e^{-z})^2-(e^{z}-e^{-z})^2}{(e^{z}+e^{-z})^2} \\
&= 1-\frac{(e^{z}-e^{-z})^2}{(e^{z}+e^{-z})^2}
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&= \frac{(e^{z}+e^{-z})^2-(e^{z}-e^{-z})^2}{(e^{z}+e^{-z})^2} \\
&= 1-\frac{(e^{z}-e^{-z})^2}{(e^{z}+e^{-z})^2} \\
&= 1-(g(z))^2
\end{aligned}
$$