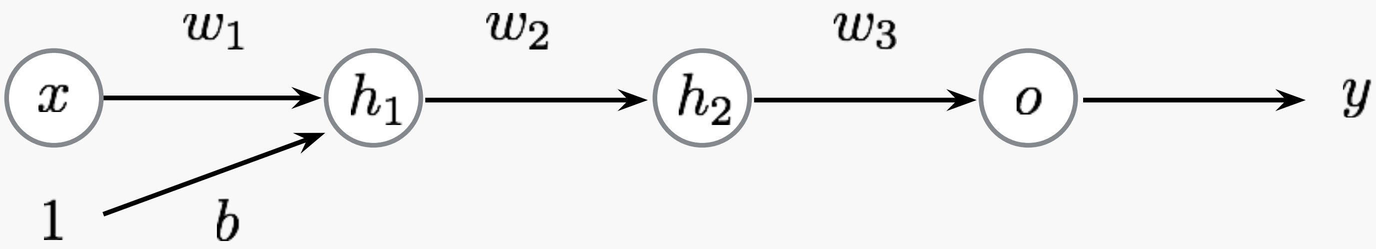
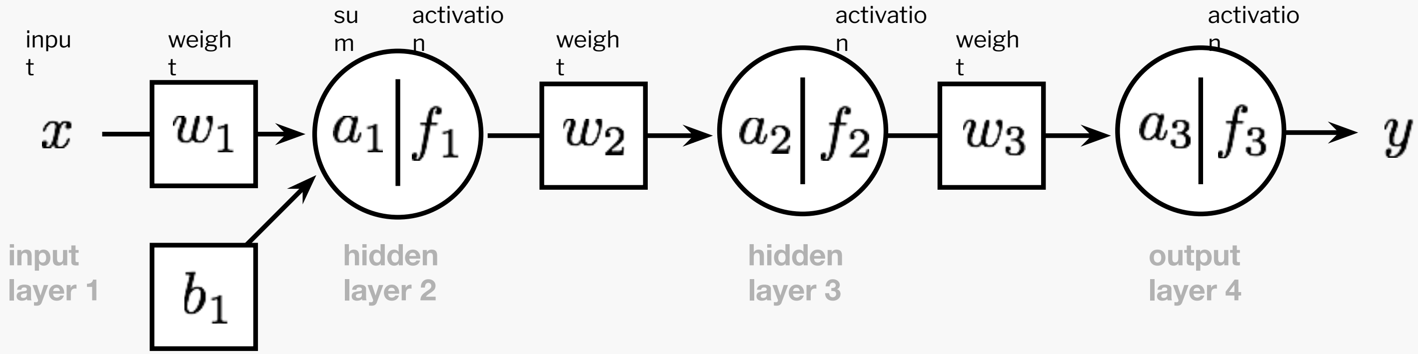
multi-layer perceptron



function of **FOUR** parameters and **FOUR** layers!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y
input
layer 1
b_1
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layer 2
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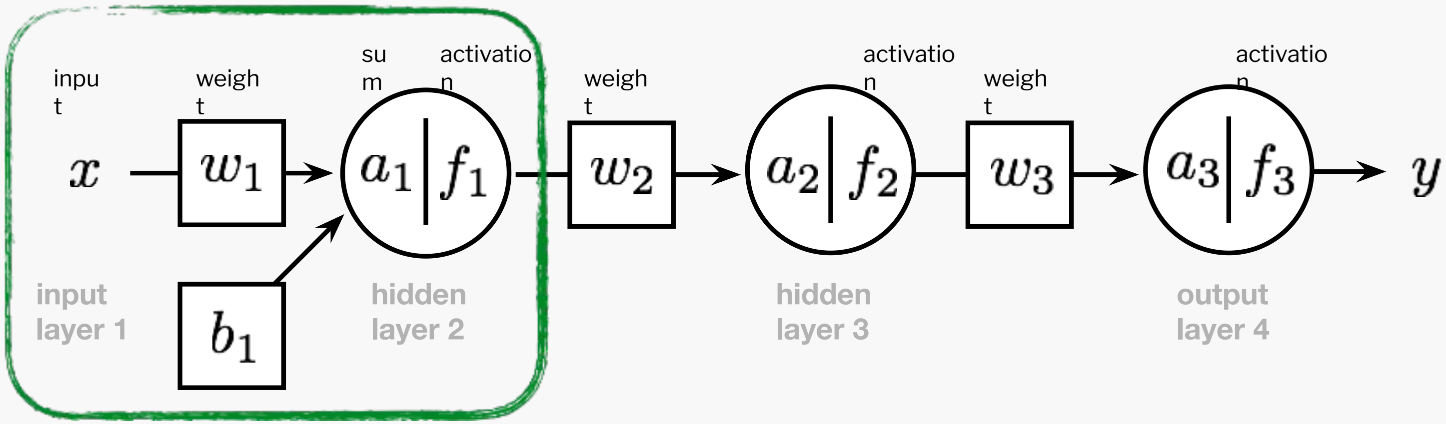
layer 3
output
layer 4


input
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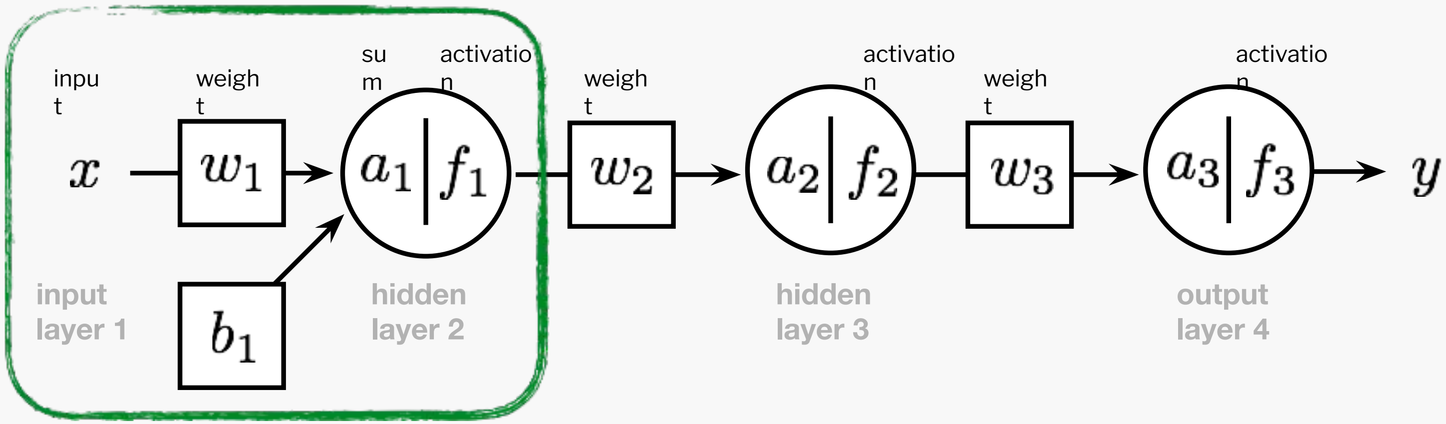
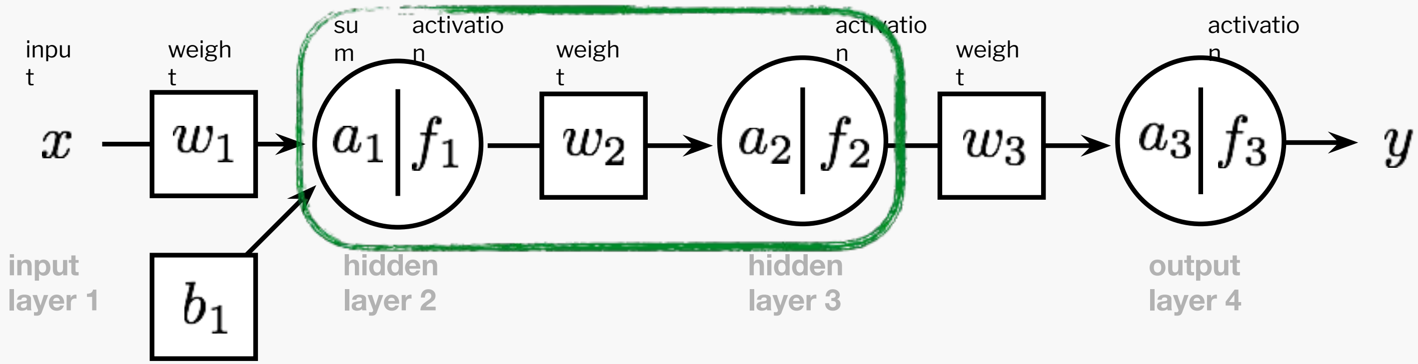
input layer 1
hidden layer 2
hidden layer 3
output layer 4



$$a_1 = w_1 \cdot x + b_1$$



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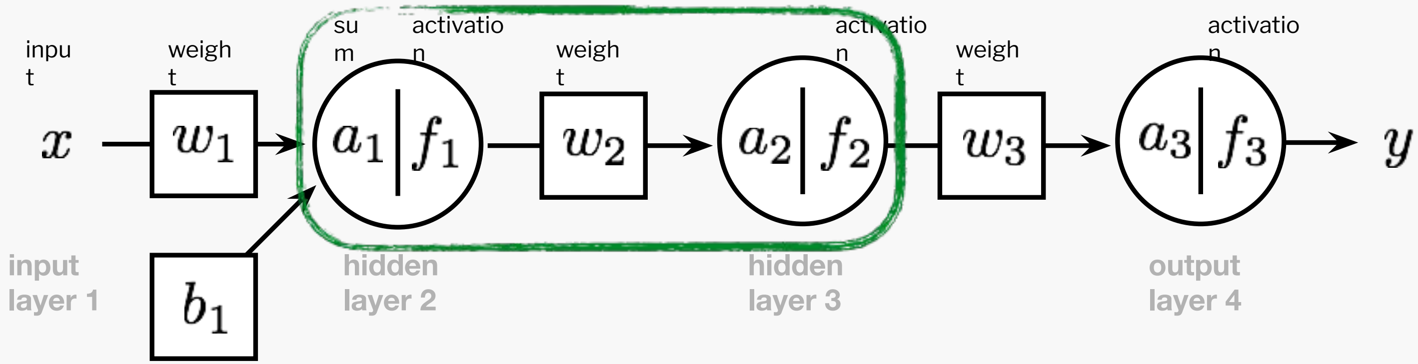
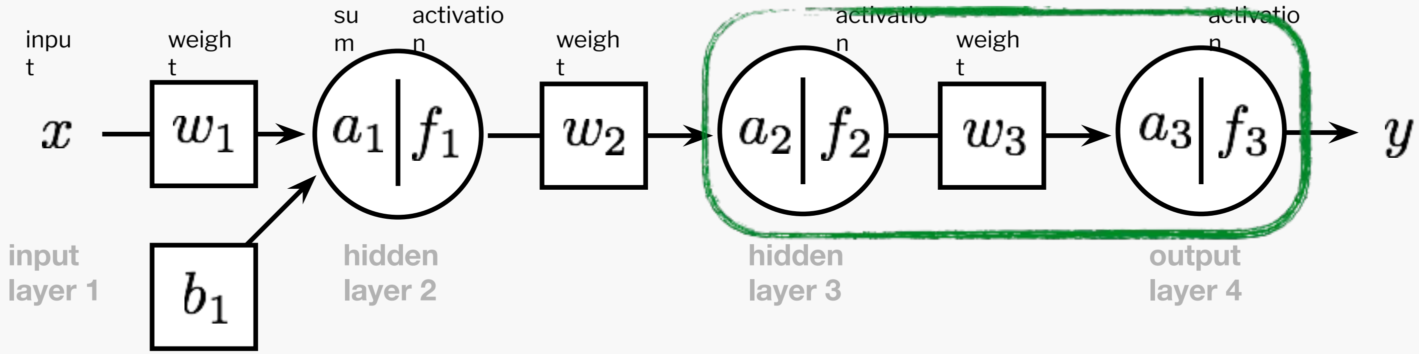


$$a_1 = w_1 \cdot x + b_1$$

$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$



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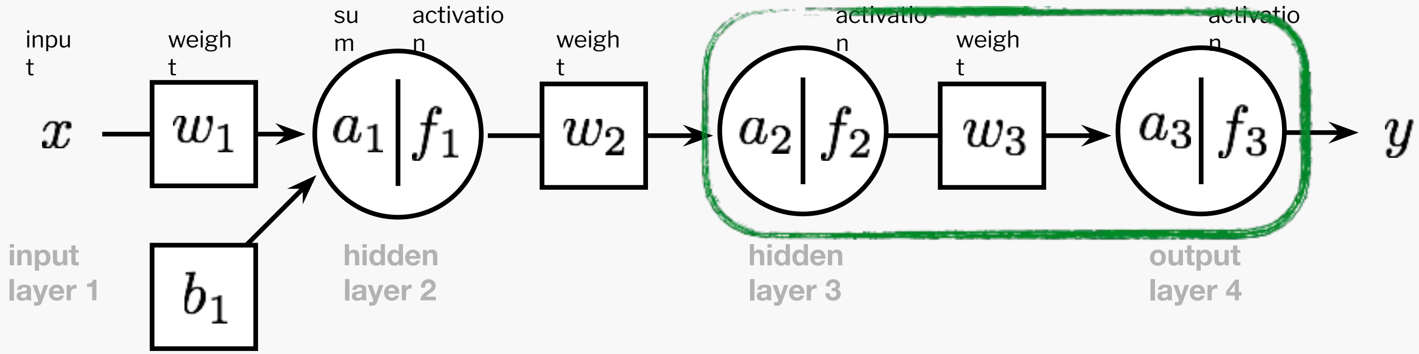

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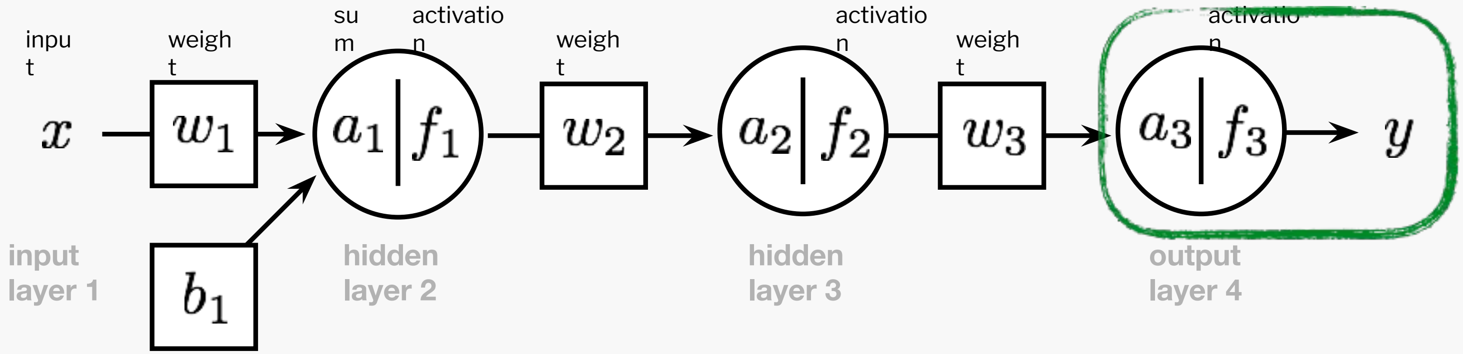

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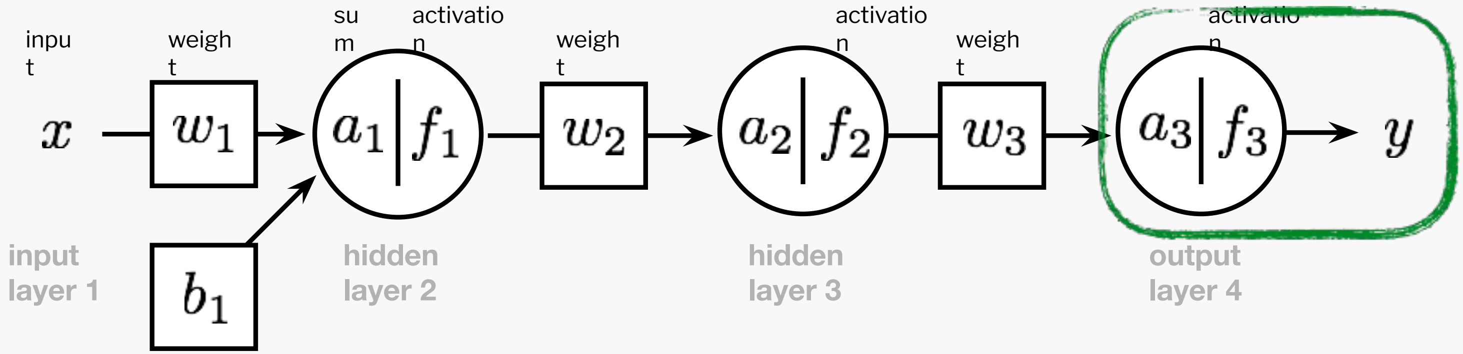

$$a_1 = w_1 \cdot x + b_1$$

$$a_2 = w_2 \cdot f_1(w_1 \cdot x + b_1)$$

$$a_3 = w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1))$$

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

Entire network can be written out as one long equation

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

We need to train the network:

What is known? What is unknown?

Entire network can be written out as a long equation

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known

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What is known? What is unknown?

Entire network can be written out as a long equation

$$y = f_3(w_3 \cdot f_2(w_2 \cdot f_1(w_1 \cdot x + b_1)))$$

activation function sometimes has parameters

unknown

We need to train the network:

What is known? What is unknown?

Learning an MLP

Given a set of samples and a MLP

$$\{x_i, y_i\}$$

$$y = f_{\mathrm{MLP}}(x; \theta)$$

Estimate the parameters of the MLP

$$\theta = \{f, w, b\}$$

Gradient Descent

For each **random** sample $\{x_i, y_i\}$

1. Predict
   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$
   b. Compute Loss
2. Update
   a. Back Propagation $\frac{\partial \mathcal{L}}{\partial \theta}$ vector of parameter partial derivatives
   b. Gradient update $\theta \leftarrow \theta - \eta \nabla \theta$ vector of parameter update equations

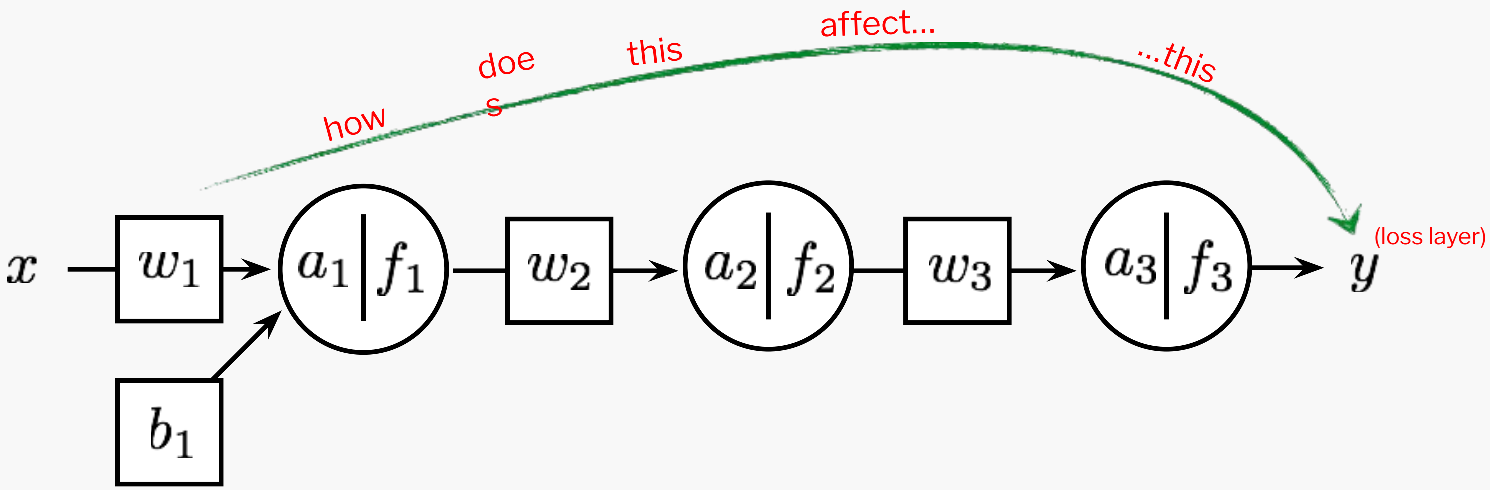
So we need to compute the partial derivatives

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \left[\frac{\partial \mathcal{L}}{\partial w_3} \frac{\partial \mathcal{L}}{\partial w_2} \frac{\partial \mathcal{L}}{\partial w_1} \frac{\partial \mathcal{L}}{\partial b} \right]$$

Remember,

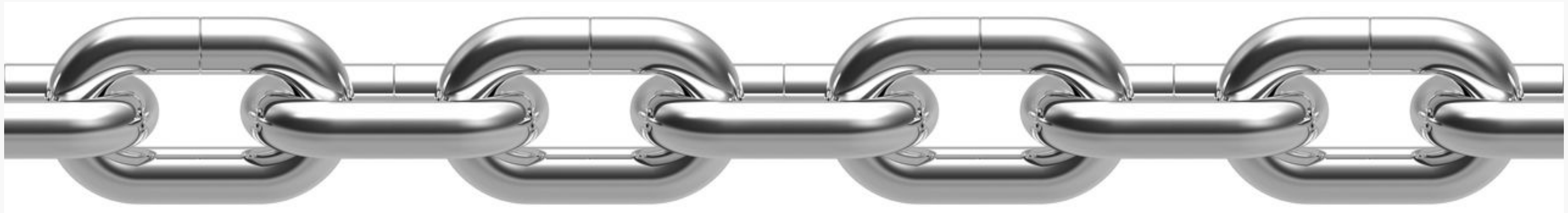
Partial derivative

$$\frac{\partial L}{\partial w_1}$$ describes ...



So, how do you compute it?

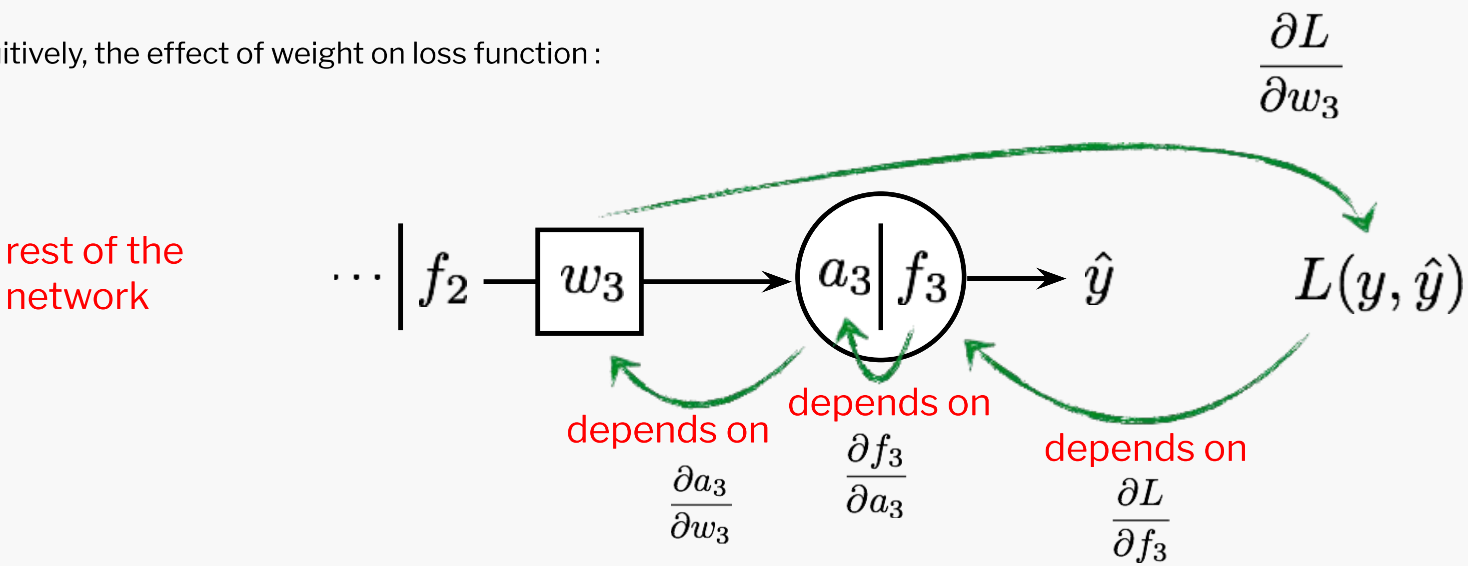
The Chain Rule



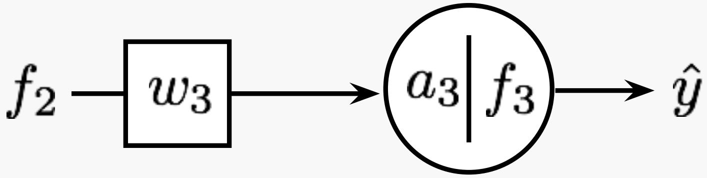
According to the chain rule...

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

Intuitively, the effect of weight on loss function :



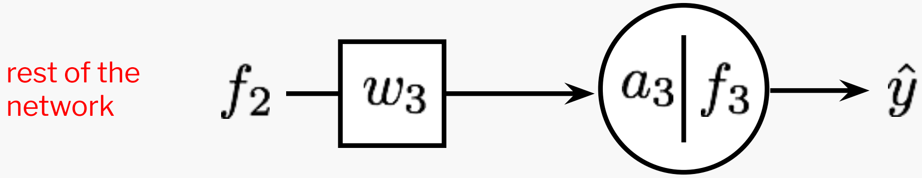
rest of the network



$L(y, \hat{y})$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3} \frac{\partial f_3}{\partial a_3} \frac{\partial a_3}{\partial w_3}$$

Chain Rule!

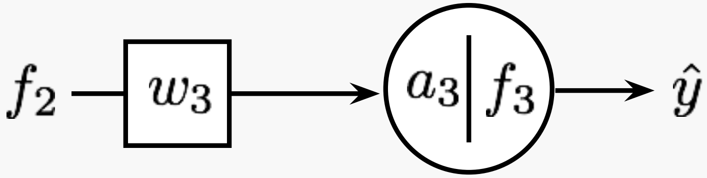


$$L(y, \hat{y})$$

$$
\begin{aligned}
\frac{\partial L}{\partial w_3} &= \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3} \\
&= -\eta(y-\hat{y})\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}
\end{aligned}
$$

Just the partial derivative of L2 loss

rest of the network



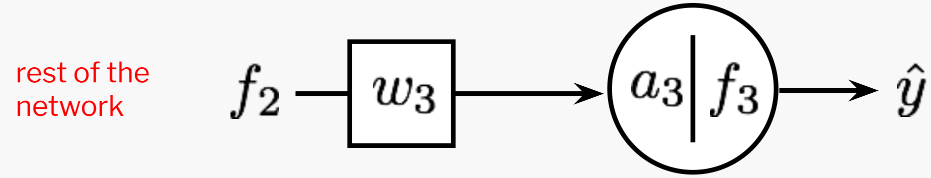
$$L(y, \hat{y})$$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$= -\eta(y - \hat{y})\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

Let's use a Sigmoid function

$$\frac{ds(x)}{dx} = s(x)(1 - s(x))$$



$L(y, \hat{y})$

$$\frac{\partial L}{\partial w_3} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$
$$= -\eta(y - \hat{y})\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$
$$= -\eta(y - \hat{y})f_3(1 - f_3)\frac{\partial a_3}{\partial w_3}$$

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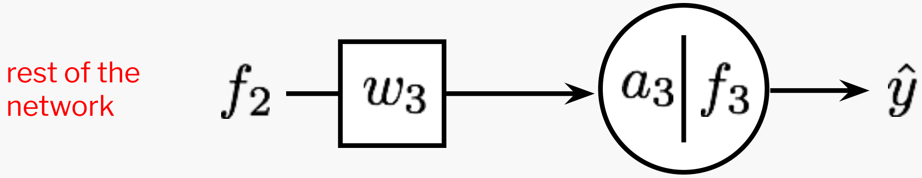
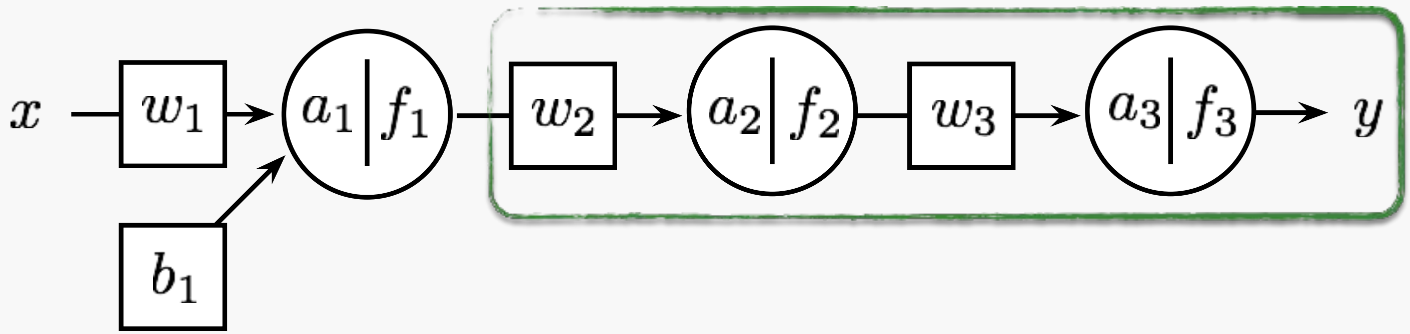
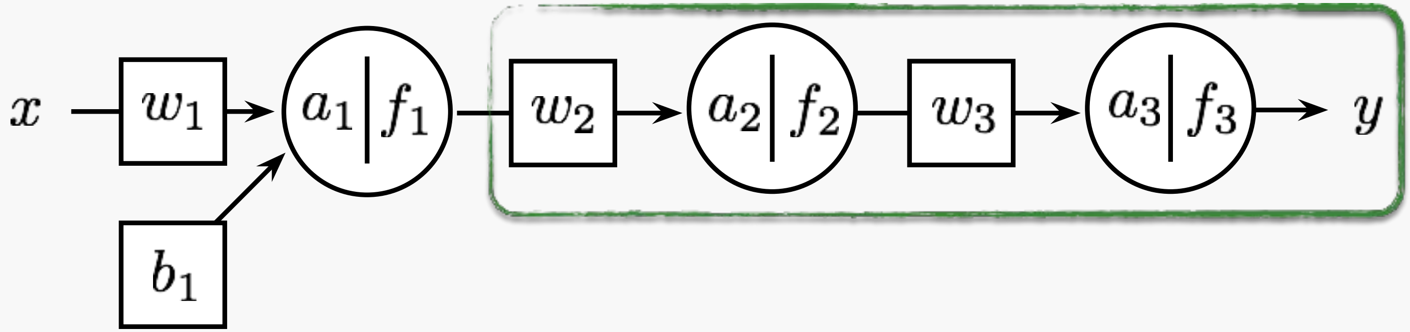


$L(y, \hat{y})$

$$
\begin{aligned}
\frac{\partial L}{\partial w_3} &= \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3} \\
&= -\eta(y - \hat{y})\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3} \\
&= -\eta(y - \hat{y})f_3(1 - f_3)\frac{\partial a_3}{\partial w_3} \\
&= -\eta(y - \hat{y})f_3(1 - f_3)f_2
\end{aligned}
$$



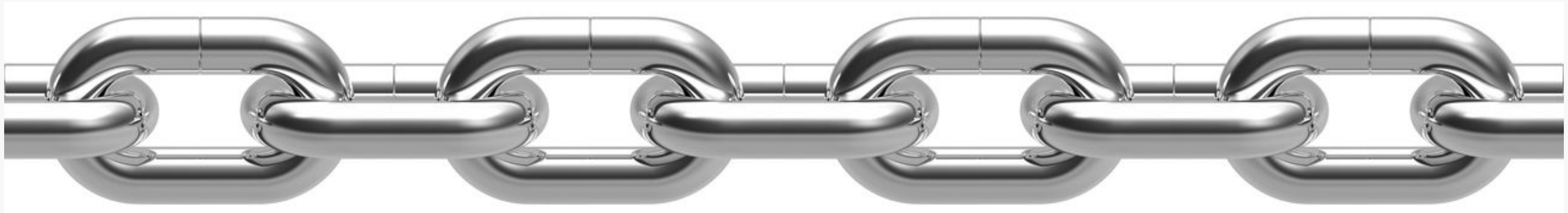
$$\frac{\partial L}{\partial w_2} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$



$$\frac{\partial L}{\partial w_2} = \boxed{\frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$

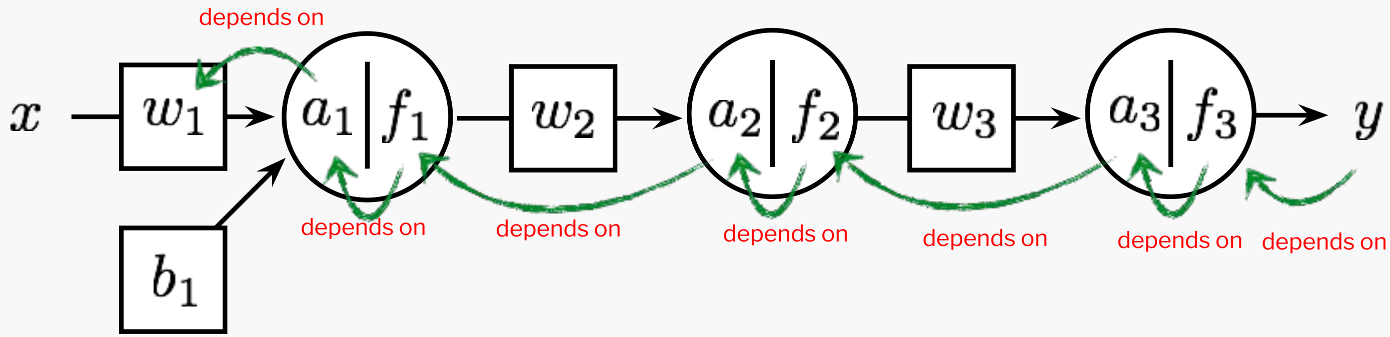
already computed. re-use(propagate)!

The Chain Rule



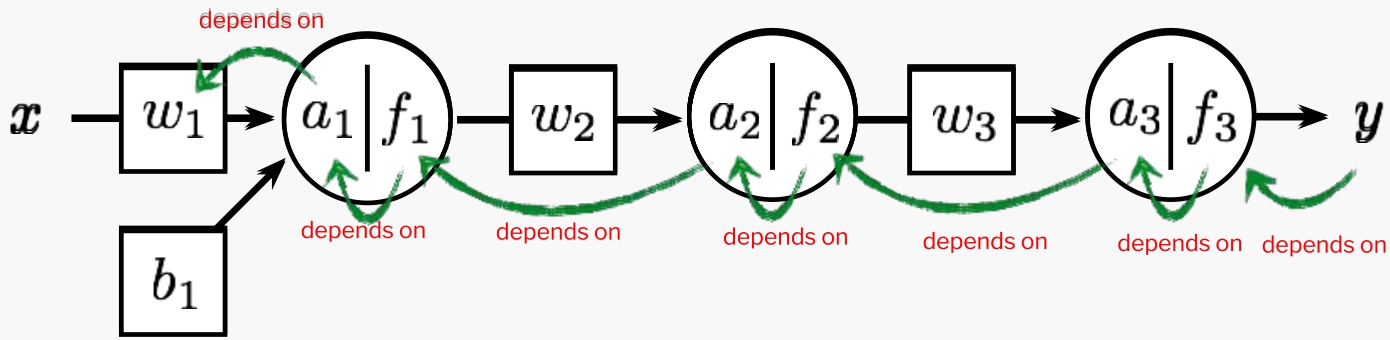
a.k.a. backpropagation

The chain rule says...



$$\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

The chain rule says...



$$\frac{\partial L}{\partial w_1} = \boxed{\frac{\partial L}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

already computed.
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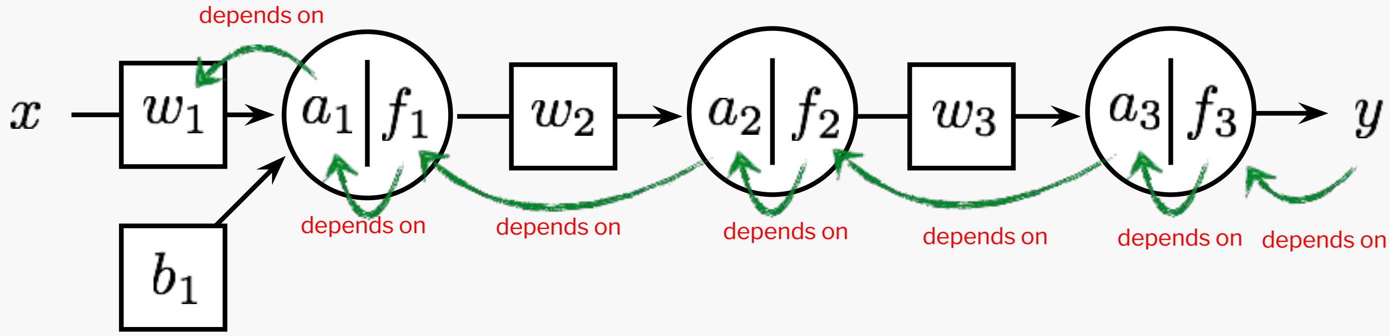
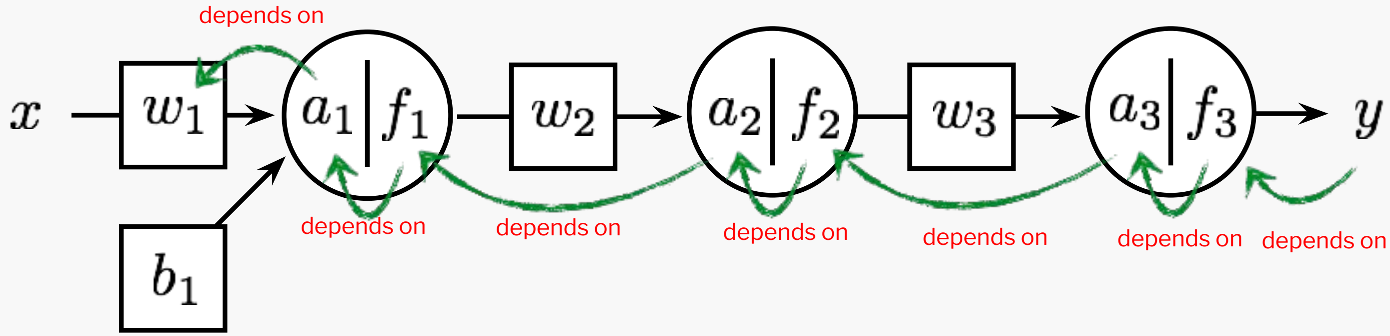


$$\frac{\partial \mathcal{L}}{\partial w_3} = \boxed{\frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}}\frac{\partial a_3}{\partial w_3}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = \boxed{\frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial b}$$

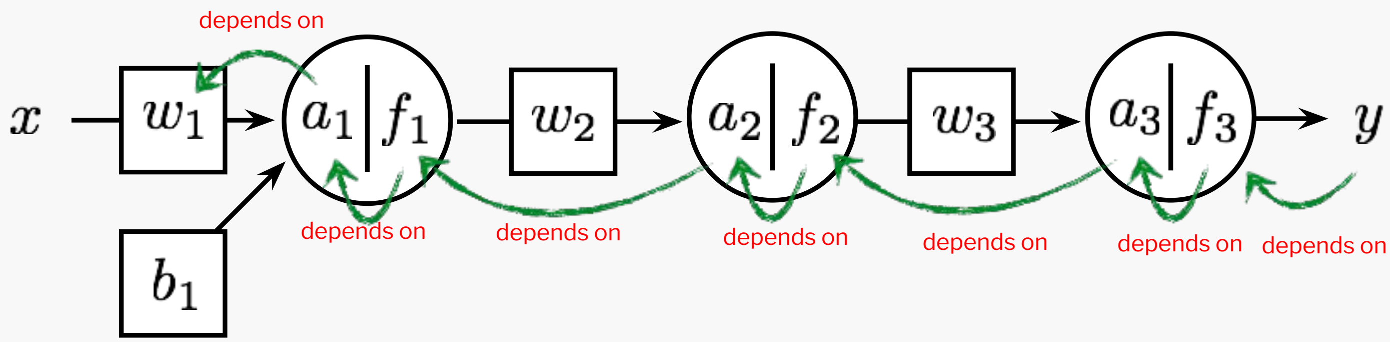


$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = \boxed{\frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}}\frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \boxed{\frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial b}$$



$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$

$$\frac{\partial \mathcal{L}}{\partial b} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial b}$$

Gradient Descent

For each example sample $\{x_i, y_i\}$

1. Predict

   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$

   b. Compute Loss $\mathcal{L}_i$

2. Update

   a. Back Propagation

$$\frac{\partial \mathcal{L}}{\partial w_3} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial w_3}$$
$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial w_2}$$
$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial f_3}\frac{\partial f_3}{\partial a_3}\frac{\partial a_3}{\partial f_2}\frac{\partial f_2}{\partial a_2}\frac{\partial a_2}{\partial f_1}\frac{\partial f_1}{\partial a_1}\frac{\partial a_1}{\partial w_1}$$
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   b. Gradient update

$$w_3 = w_3 - \eta \nabla w_3$$
$$w_2 = w_2 - \eta \nabla w_2$$
$$w_1 = w_1 - \eta \nabla w_1$$
$$b = b - \eta \nabla b$$

Gradient Descent

For each example sample $\{x_i, y_i\}$

1. Predict
   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$
   b. Compute Loss $\mathcal{L}_i$
2. Update
   a. Back Propagation $\frac{\partial \mathcal{L}}{\partial \theta}$

      vector of parameter partial derivatives

   b. Gradient update $\theta \leftarrow \theta + \eta \frac{\partial \mathcal{L}}{\partial \theta}$

      vector of parameter update equations

Stochastic gradient descent

What we are truly minimizing:

$$\min_{\theta} \sum_{i=1}^{N} L(y_i, f_{MLP}(x_i))$$

The gradient is:

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$$\min_{\theta} \sum_{i=1}^{N} L(y_i, f_{MLP}(x_i))$$

The gradient is:

$$\sum_{i=1}^{N} \frac{\partial L(y_i, f_{MLP}(x_i))}{\partial \theta}$$

What we use for gradient update is:

What we are truly minimizing:

$$\min_{\theta} \sum_{i=1}^{N} L(y_i, f_{MLP}(x_i))$$

The gradient is:

$$\sum_{i=1}^{N} \frac{\partial L(y_i, f_{MLP}(x_i))}{\partial \theta}$$

What we use for gradient update is:

$$\frac{\partial L(y_i, f_{MLP}(x_i))}{\partial \theta}$$

for some i

Stochastic Gradient Descent

For each example sample $\{x_i, y_i\}$

1. Predict

   a. Forward pass $\hat{y} = f_{\text{MLP}}(x_i; \theta)$

   b. Compute Loss $\mathcal{L}_i$

2. Update

   a. Back Propagation $\frac{\partial \mathcal{L}}{\partial \theta}$

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How do we select which sample?

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- Select randomly!

Do we need to use only one sample?

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- You can use a *minibatch* of size $B < N$.

Why not do gradient descent with all samples?

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Why not do gradient descent with all samples?

- It’s very expensive when N is large (big data).

Do I lose anything by using stochastic GD?

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- Select randomly!

Do we need to use only one sample?

- You can use a *minibatch* of size $B < N$.

Why not do gradient descent with all samples?

- It's very expensive when N is large (big data).

Do I lose anything by using stochastic GD?

- Same convergence guarantees and complexity!
- Better generalization.

BACK PROPAGATION VECTORIZED

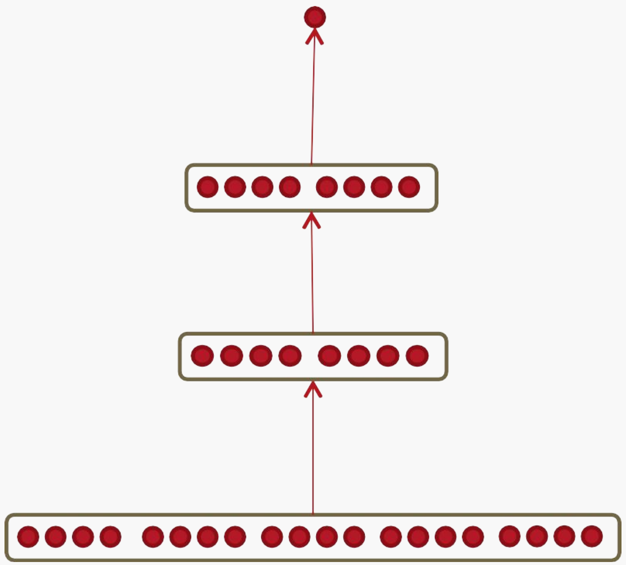
Two-layer Neural Net

$$s = \boldsymbol{u}^T \boldsymbol{h}_2$$

$$\boldsymbol{h}_2 = f(\boldsymbol{W_2} \boldsymbol{h}_1 + \boldsymbol{b}_2)$$

$$\boldsymbol{h}_1 = f(\boldsymbol{W}_1 \boldsymbol{x} + \boldsymbol{b}_1)$$

$$\boldsymbol{x} \quad \text{(input)}$$



Repeat as Needed!

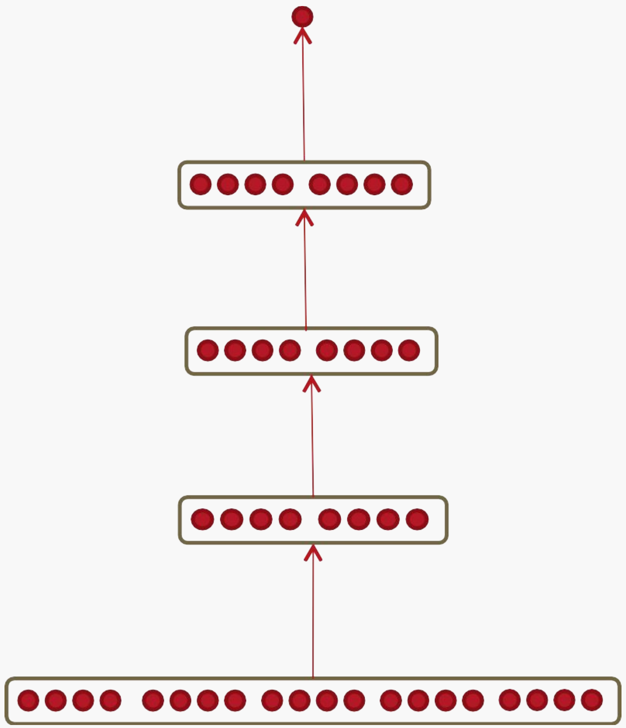
$$s = \boldsymbol{u}^T \boldsymbol{h}_3$$

$$\boldsymbol{h}_3 = f(\boldsymbol{W_3} \boldsymbol{h}_2 + \boldsymbol{b}_3)$$

$$\boldsymbol{h}_2 = f(\boldsymbol{W_2} \boldsymbol{h}_1 + \boldsymbol{b}_2)$$

$$\boldsymbol{h}_1 = f(\boldsymbol{W}_1 \boldsymbol{x} + \boldsymbol{b}_1)$$

$$\boldsymbol{x} \quad \text{(input)}$$



Remember: Stochastic Gradient Descent

- Update equation:

$$\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$$

$\boxed{\alpha = \textit{step size} \text{ or } \textit{learning rate}}$

Remember: Stochastic Gradient Descent

- Update equation:

$$\theta^{new} = \theta^{old} - \alpha \nabla_\theta J(\theta)$$

α = *step size* or *learning rate*

- This Lecture: How do we compute $\nabla_\theta J(\theta)$?
  - By hand
  - Algorithmically (the backpropagation algorithm)

Gradients

- Given a function with 1 output and *n* inputs

$$f(\boldsymbol{x}) = f(x_1, x_2, ..., x_n)$$

- Its gradient is a vector of partial derivatives

$$\frac{\partial f}{\partial \boldsymbol{x}} = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, ..., \frac{\partial f}{\partial x_n} \right]$$

Jacobian Matrix: Generalization of the Gradient

- Given a function with ***m* outputs** and *n* inputs

$$\boldsymbol{f}(\boldsymbol{x}) = [f_1(x_1, x_2, ..., x_n), ..., f_m(x_1, x_2, ..., x_n)]$$

- Its Jacobian is an ***m* x *n* matrix** of partial derivatives

$$\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

$$\boxed{\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)_{ij} = \frac{\partial f_i}{\partial x_j}}$$

Chain Rule For Jacobians

- For one-variable functions: multiply derivatives

$$z = 3y$$
$$y = x^2$$
$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx} = (3)(2x) = 6x$$

- For multiple variables: multiply Jacobians

$$\boldsymbol{h} = f(\boldsymbol{z})$$
$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$
$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} = \ldots$$

Example Jacobian: Activation Function

$$\boldsymbol{h} = f(\boldsymbol{z}), \text{what is } \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}? \qquad \boldsymbol{h}, \boldsymbol{z} \in \mathbb{R}^n$$

$$h_i = f(z_i)$$

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Function has *n* outputs and *n* inputs -> *n* by *n* Jacobian

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$$\left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}}\right)_{ij} = \frac{\partial h_i}{\partial z_j} = \frac{\partial}{\partial z_j} f(z_i) \qquad \text{definition of Jacobian}$$

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$$= \begin{cases} f'(z_i) & \text{if } i = j \\ 0 & \text{if otherwise} \end{cases} \qquad \text{regular 1-variable derivative}$$

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$$\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} = \begin{pmatrix} f'(z_1) & & 0 \\ & \ddots & \\ 0 & & f'(z_n) \end{pmatrix} = \operatorname{diag}(\boldsymbol{f}'(\boldsymbol{z}))$$

Other Jacobians

$$\frac{\partial}{\partial \boldsymbol{x}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{W}$$

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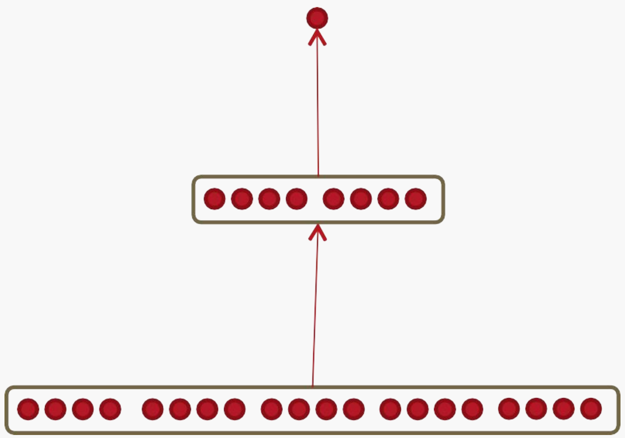
- Compute these at home for practice!
  - Check your answers with the lecture notes

Back to Neural Nets!

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad \text{(input)}$$



$x = [\ x_{museums} \quad x_{in} \quad x_{Paris} \quad x_{are} \quad x_{amazing}\ ]$

Back to Neural Nets!

- Let's find $\frac{\partial s}{\partial \boldsymbol{b}}$
  - In practice we care about the gradient of the loss, but we will compute the gradient of the score for simplicity

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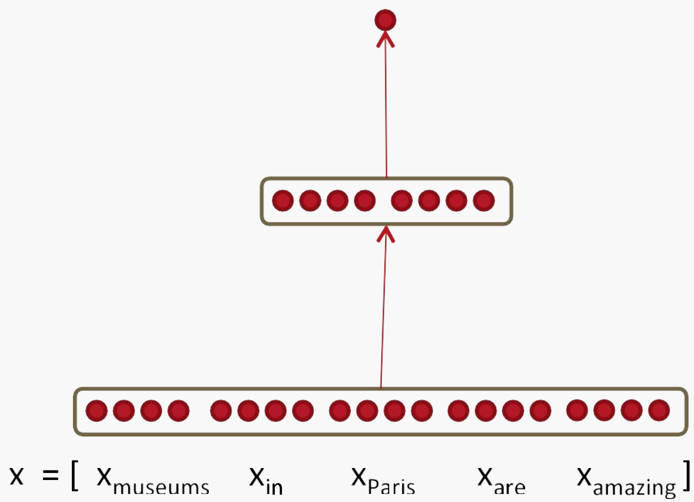

1. Break up equations into simple pieces

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})$$

$$\boldsymbol{x} \quad \text{(input)}$$

$$s = \boldsymbol{u}^T \boldsymbol{h}$$

$$\boldsymbol{h} = f(\boldsymbol{z})$$

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

$$\boldsymbol{x} \quad \text{(input)}$$

2. Apply the chain rule

$$
\begin{aligned}
s &= \boldsymbol{u}^T \boldsymbol{h} \\
\boldsymbol{h} &= f(\boldsymbol{z}) \\
\boldsymbol{z} &= \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b} \\
\boldsymbol{x} &\quad \text{(input)}
\end{aligned}
$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

2. Apply the chain rule

$$\boxed{s = \boldsymbol{u}^T \boldsymbol{h}}$$
$$\boldsymbol{h} = f(\boldsymbol{z})$$
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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \boxed{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}}$$

3. Write out the Jacobians

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$$\boldsymbol{x} \quad \text{(input)}$$

$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

Useful Jacobians from previous slide

$$\frac{\partial}{\partial \boldsymbol{h}}(\boldsymbol{u}^T \boldsymbol{h}) = \boldsymbol{u}^T$$
$$\frac{\partial}{\partial \boldsymbol{z}}(f(\boldsymbol{z})) = \text{diag}(f'(\boldsymbol{z}))$$
$$\frac{\partial}{\partial \boldsymbol{b}}(\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}) = \boldsymbol{I}$$

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$$\frac{\partial s}{\partial \boldsymbol{b}} = \frac{\partial s}{\partial \boldsymbol{h}} \quad \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{z}} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{b}}$$

$$= \boldsymbol{u}^T$$

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$$= \boldsymbol{u}^T \circ f'(\boldsymbol{z})$$

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