Lecture 10

Backpropagation

Spring 2022

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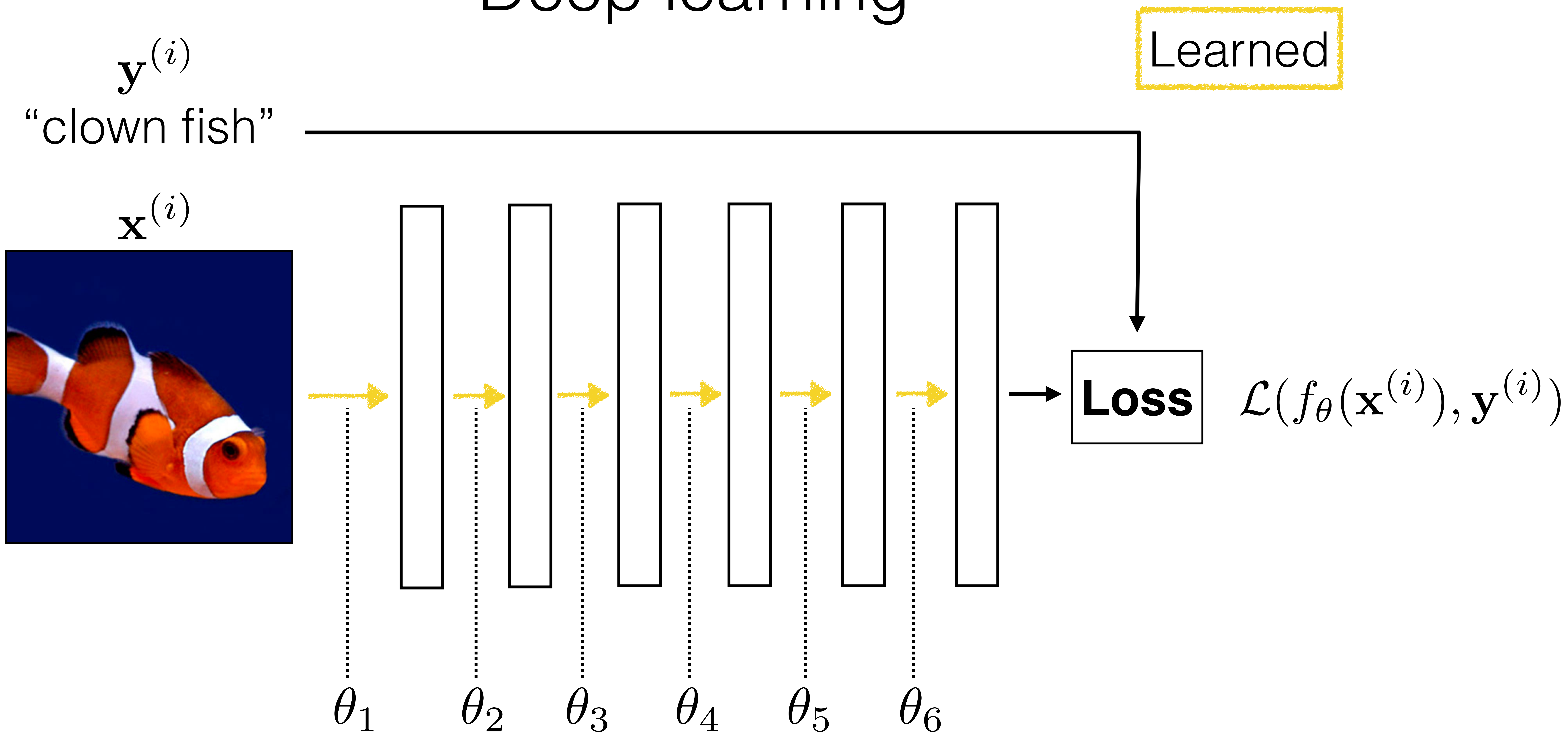
2. Backprop and Differentiable Programming

- Review of gradient descent, SGD
- Forward propagation
- Computing gradients
- Backward propagation
- Computation graphs and differentiable programming

Deep learning



Learned

$\mathbf{y}^{(i)}$

“clown fish”

$\mathbf{x}^{(i)}$

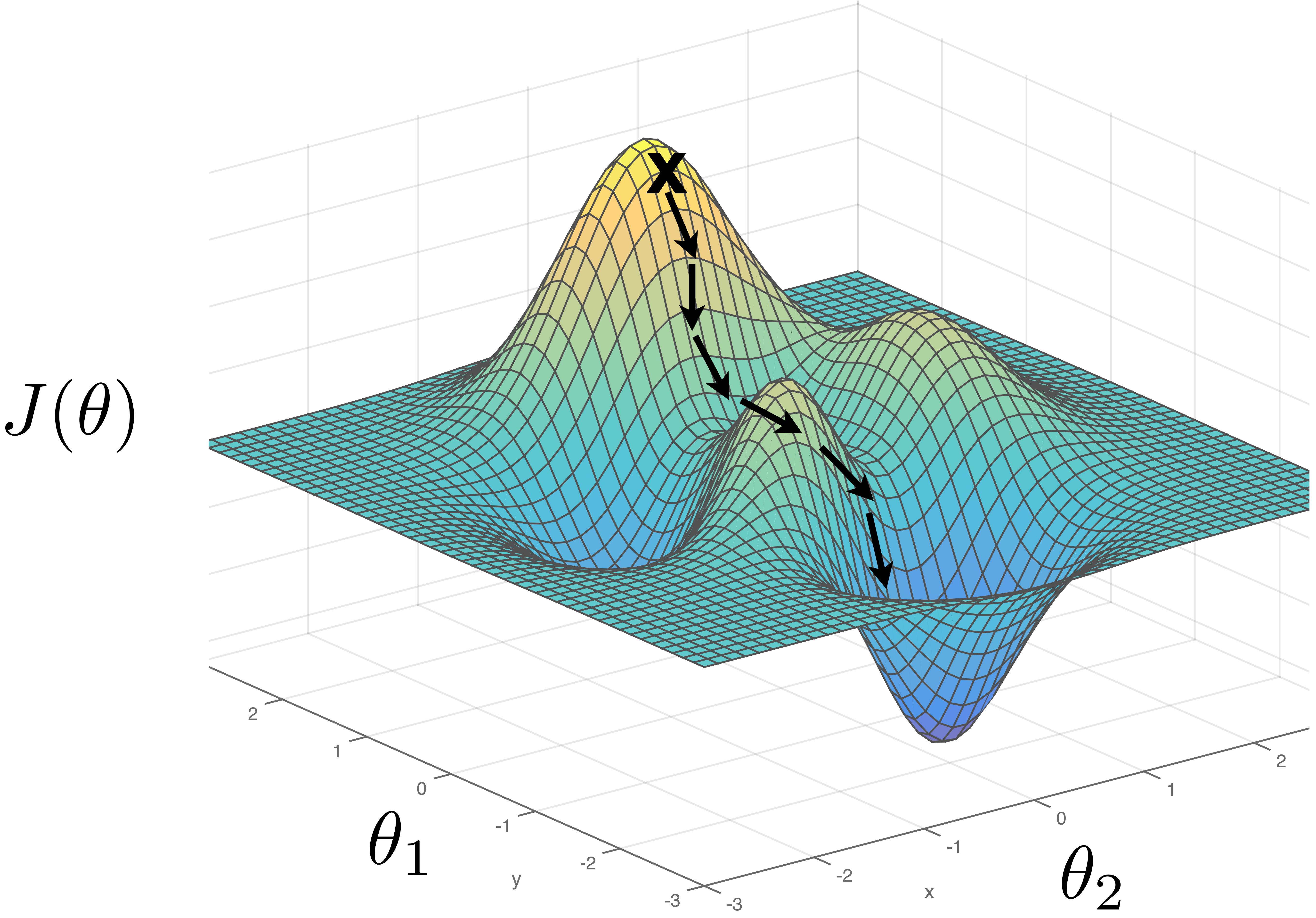
θ_1 θ_2 θ_3 θ_4 θ_5 θ_6

Loss

$\mathcal{L}(f_\theta(\mathbf{x}^{(i)}), \mathbf{y}^{(i)})$

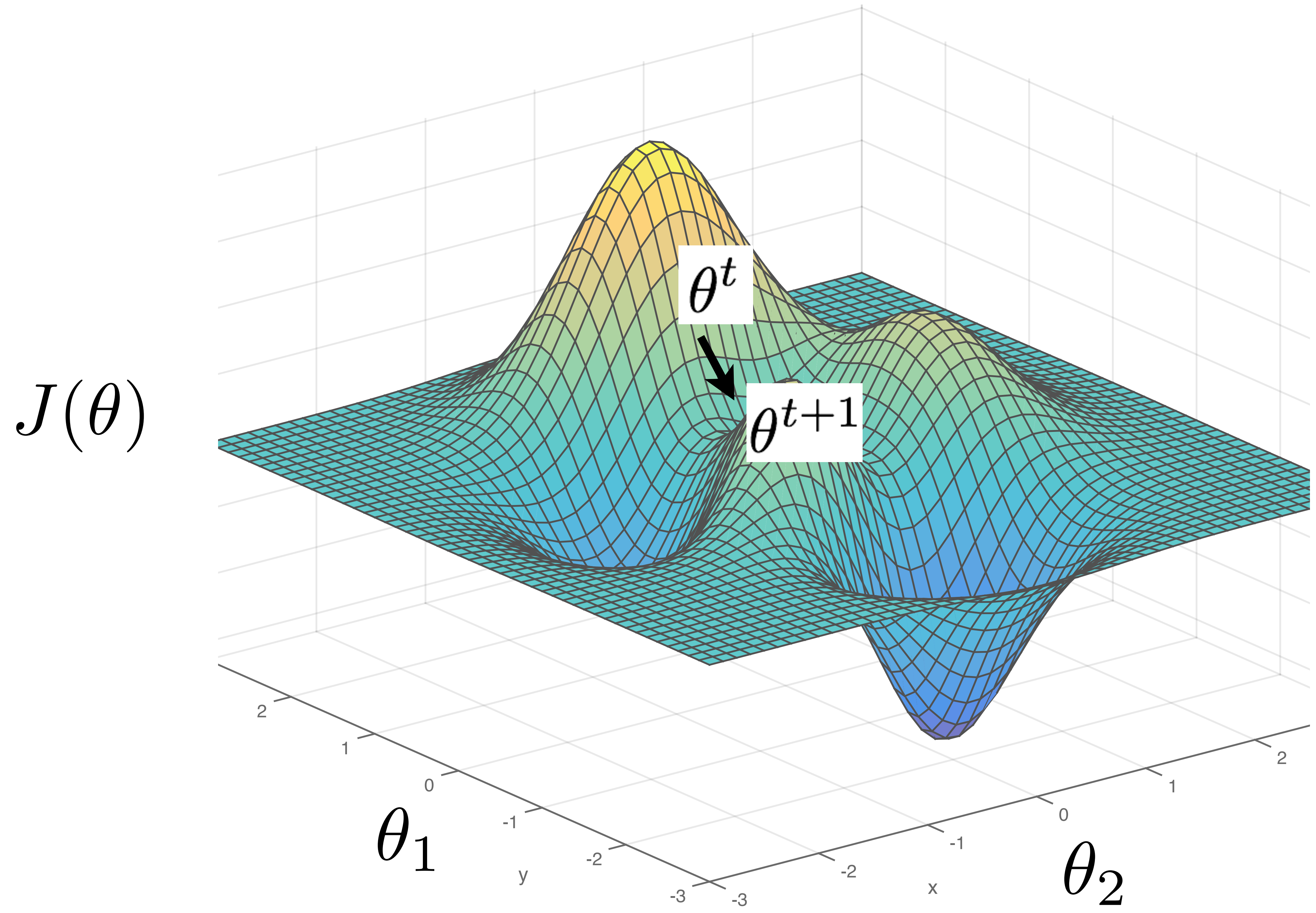
$$\theta^* = \arg\min_\theta \sum_{i=1}^{N} \mathcal{L}(f_\theta(\mathbf{x}^{(i)}), \mathbf{y}^{(i)})$$

Gradient descent



$$\theta^* = \arg\min_{\theta} J(\theta)$$

Gradient descent



$$\boxed{\theta^* = \arg\min_{\theta} \underbrace{\sum_{i=1}^{N} \mathcal{L}(f_\theta(\mathbf{x}^{(i)}), \mathbf{y}^{(i)})}_{J(\theta)}}$$

One iteration of gradient descent:

$$\theta^{t+1} = \theta^t - \eta_t \frac{\partial J(\theta)}{\partial \theta}\bigg|_{\theta=\theta^t}$$

learning rate

Stochastic gradient descent (SGD)

- Want to minimize overall loss function **J**, which is sum of individual losses over each example.
- In Stochastic gradient descent, compute gradient on sub-set (batch) of data.

  If batchsize=1 then θ is updated after each example.

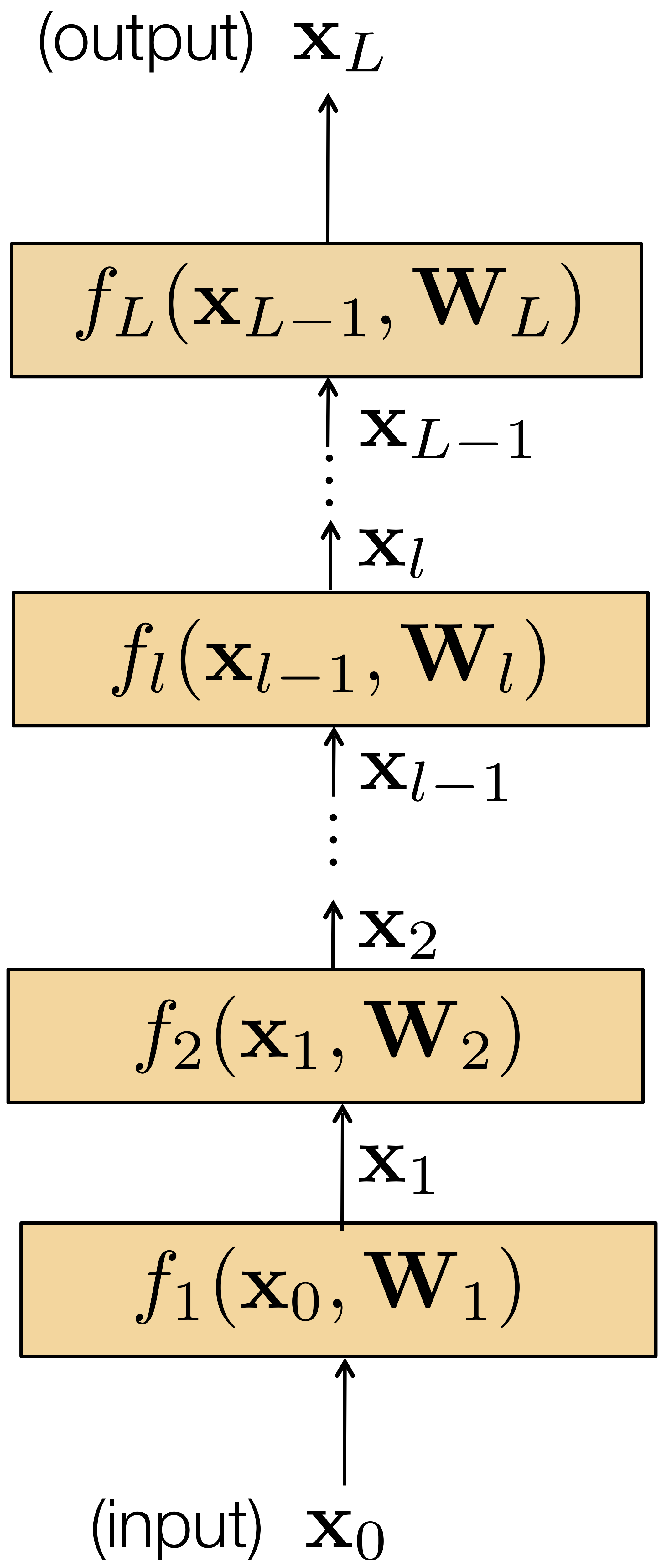
  If batchsize=N (full set) then this is standard gradient descent.
- Gradient direction is noisy, relative to average over all examples (standard gradient descent).
- Advantages
  - Faster: approximate total gradient with small sample
  - Implicit regularizer
- Disadvantages
  - High variance, unstable updates

Forward pass

- Consider model with L layers. Layer l has vector of weights $\mathbf{W}_l$
- **Forward pass**: takes input $\mathbf{x}_{l-1}$ and passes it through each layer f_l :

$$\mathbf{x}_l = f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)$$

- Output of layer l is $\mathbf{x}_l$.
- Network output (top layer) is $\mathbf{x}_L$.



Forward pass

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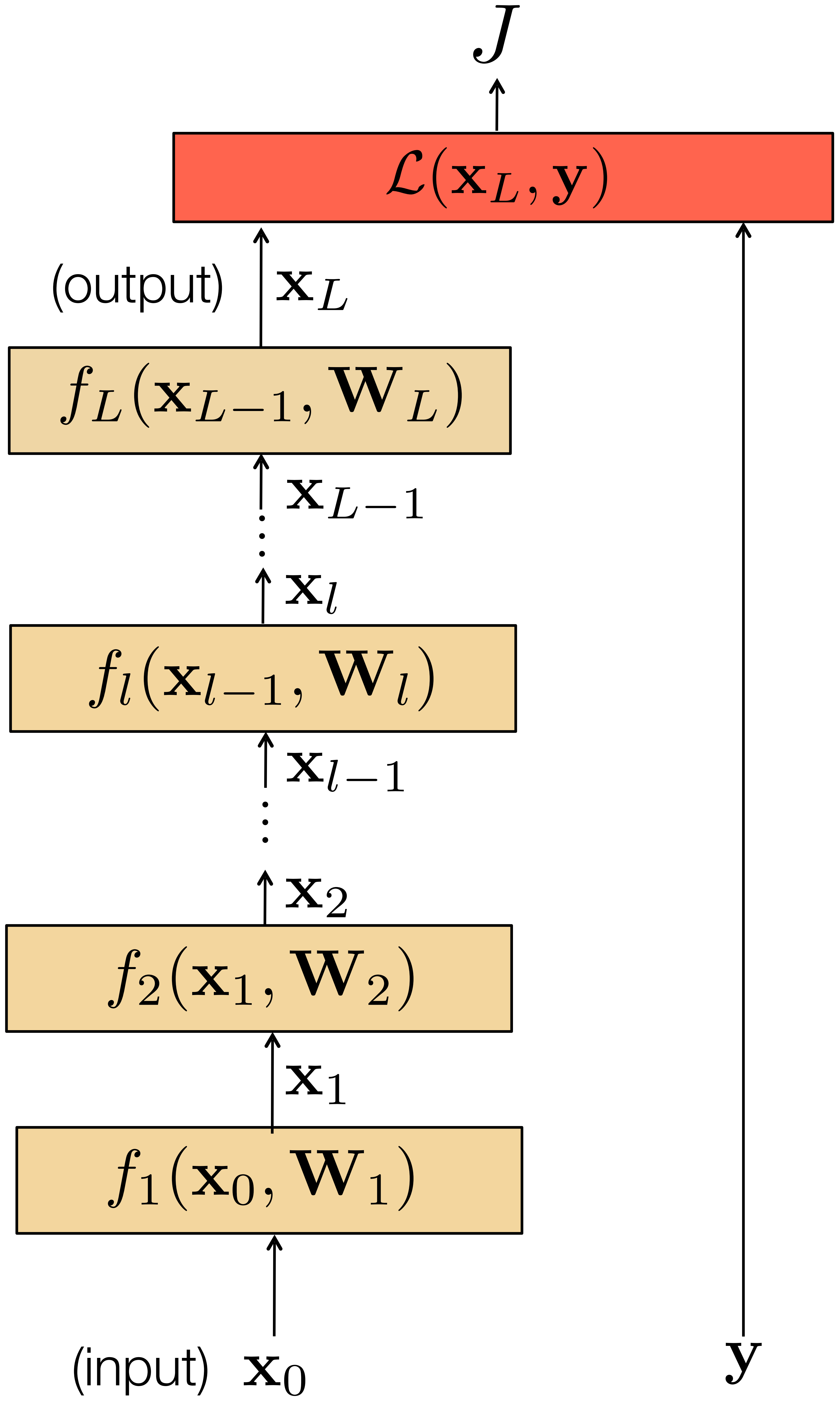
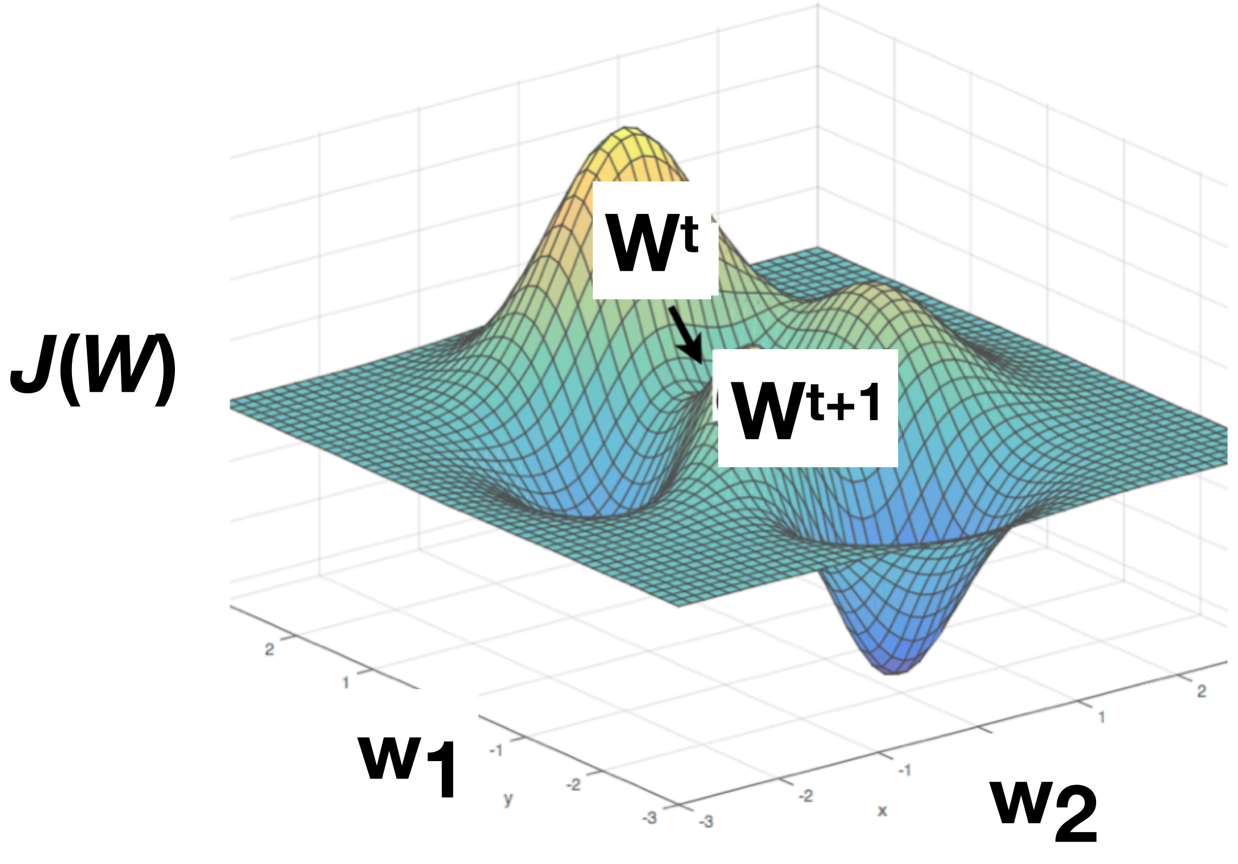
- **Forward pass**: takes input $\mathbf{x}_{l-1}$ and passes it through each layer f_l :

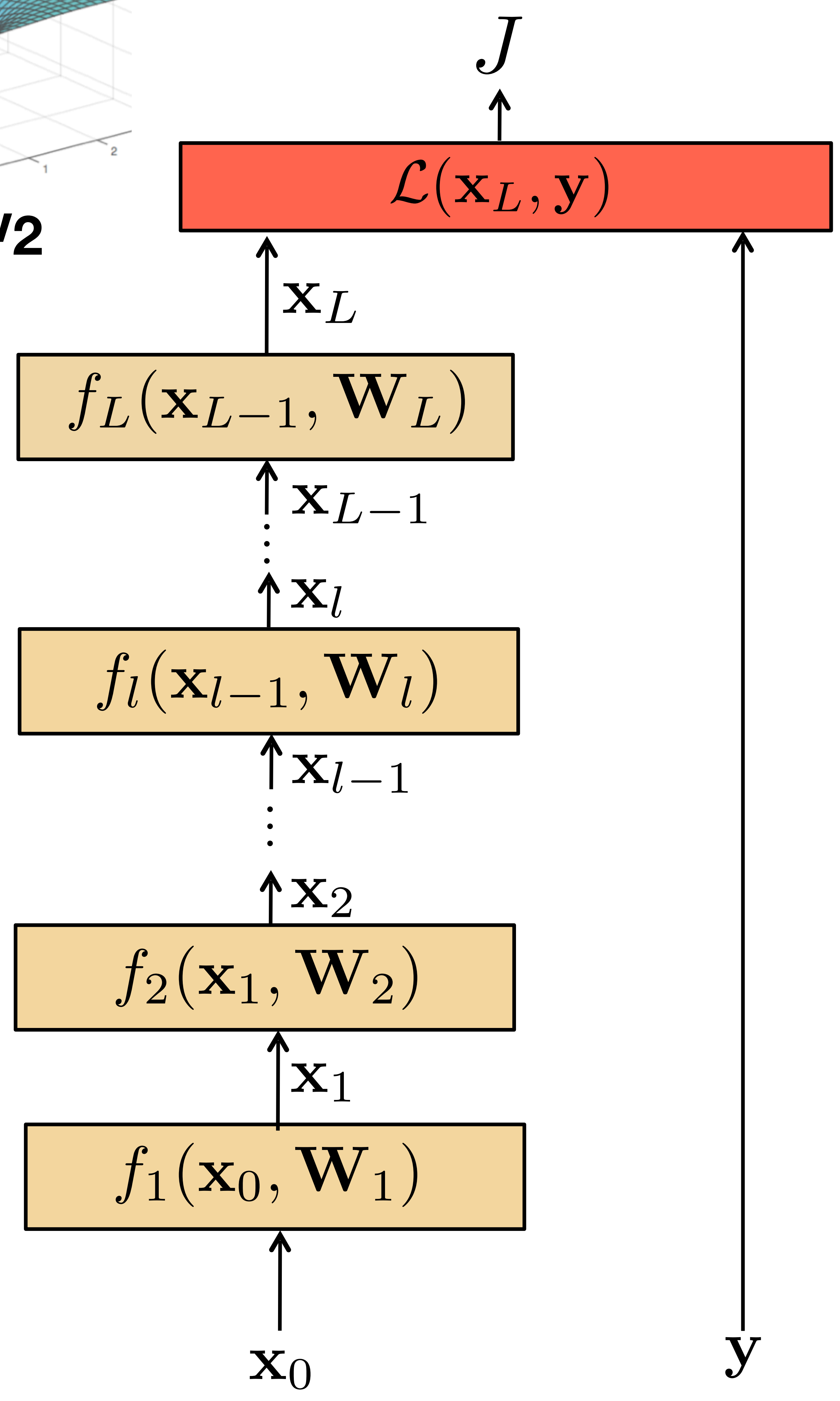
$$\mathbf{x}_l = f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)$$

- Output of layer l is $\mathbf{x}_l$.
- Network output (top layer) is $\mathbf{x}_L$.
- **Loss function** $\mathcal{L}$ compares $\mathbf{x}_L$ to $\mathbf{y}$.
- Overall cost is the sum of the losses over all training examples: $J = \sum_{i=1}^{N} \mathcal{L}(\mathbf{x}_L^{(i)}, \mathbf{y}^{(i)})$



Gradient descent





- We need to compute gradients of the cost with respect to model parameters $\mathbf{W}_l$.
- By design, each layer is differentiable with respect to its parameters and input.

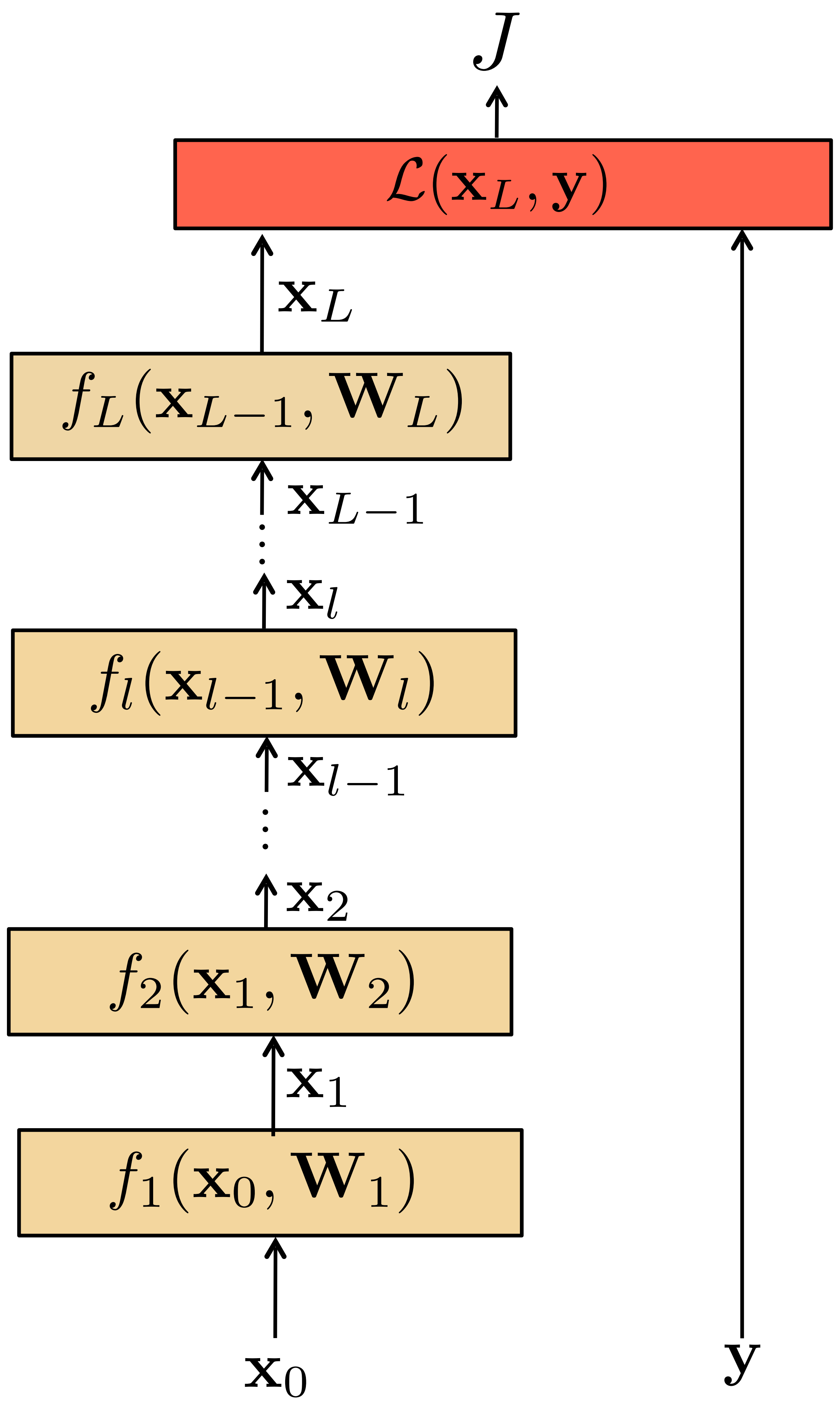
Computing gradients

To compute the gradients, we could start by writing the full energy J as a function of the network parameters.

$$J(\mathbf{W}) = \sum_{i=1} \mathcal{L}(f_L(\ldots f_2(f_1(\mathbf{x}_0^{(i)}, \mathbf{W}_1), \mathbf{W}_2), \ldots \mathbf{W}_L), \mathbf{y}^{(i)})$$

And then compute the partial derivatives…

$$\frac{\partial J}{\partial \mathbf{W}_l}$$



instead, we can use the chain rule to derive a compact algorithm: **backpropagation**

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Matrix calculus

- $\mathbf{x}$ column vector of size $[n \times 1]$:

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

- We now define a function on vector $\mathbf{x}$: $\mathbf{y} = f(\mathbf{x})$
- If y is a scalar, then

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial y}{\partial x_1} & \frac{\partial y}{\partial x_2} & \cdots & \frac{\partial y}{\partial x_n} \end{pmatrix}$$

The derivative of y is a row vector of size $[1 \times n]$

- If $\mathbf{y}$ is a vector $[m \times 1]$, then (*Jacobian formulation*):

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

The derivative of y is a matrix of size $[m \times n]$

(m rows and n columns)

Matrix calculus

- If y is a scalar and $\mathbf{X}$ is a matrix of size $[n \times m]$, then

$$\frac{\partial y}{\partial \mathbf{X}} = \begin{pmatrix} \frac{\partial y}{\partial x_{11}} & \frac{\partial y}{\partial x_{21}} & \cdots & \frac{\partial y}{\partial x_{n1}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial y}{\partial x_{1m}} & \frac{\partial y}{\partial x_{2m}} & \cdots & \frac{\partial y}{\partial x_{nm}} \end{pmatrix}$$

The output is a matrix of size $[m \times n]$

Wikipedia: The three types of derivatives that have not been considered are those involving vectors-by-matrices, matrices-by-vectors, and matrices-by-matrices. These are not as widely considered and a notation is not widely agreed upon.

Matrix calculus

- Chain rule:

For the function: $h(\mathbf{x}) = f(g(\mathbf{x}))$

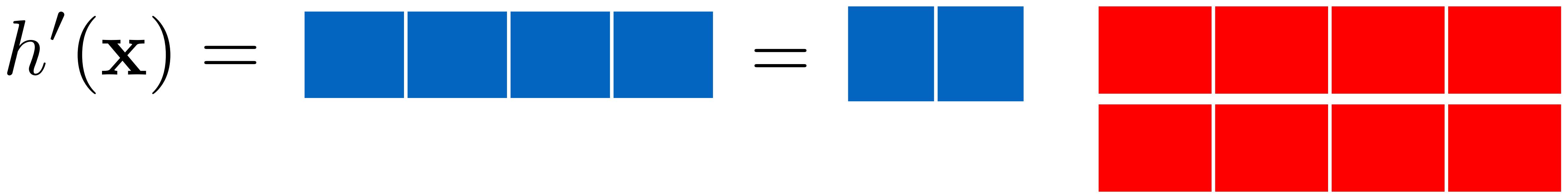
Its derivative is: $h'(\mathbf{x}) = f'(g(\mathbf{x}))g'(\mathbf{x})$

and writing $\mathbf{z} = f(\mathbf{u})$, and $\mathbf{u} = g(\mathbf{x})$:

$$\underset{[m \times n]}{\left.\frac{\partial \mathbf{z}}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{a}}} = \underset{[m \times p]}{\left.\frac{\partial \mathbf{z}}{\partial \mathbf{u}}\right|_{\mathbf{u}=g(\mathbf{a})}} \cdot \underset{[p \times n]}{\left.\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{a}}}$$

with $p =$ length of vector $\mathbf{u}$ $= |\mathbf{u}|$, $m = |\mathbf{z}|$, and $n = |\mathbf{x}|$

Example, if $|\mathbf{z}| = 1\,, |\mathbf{u}| = 2\,, |\mathbf{x}| = 4$



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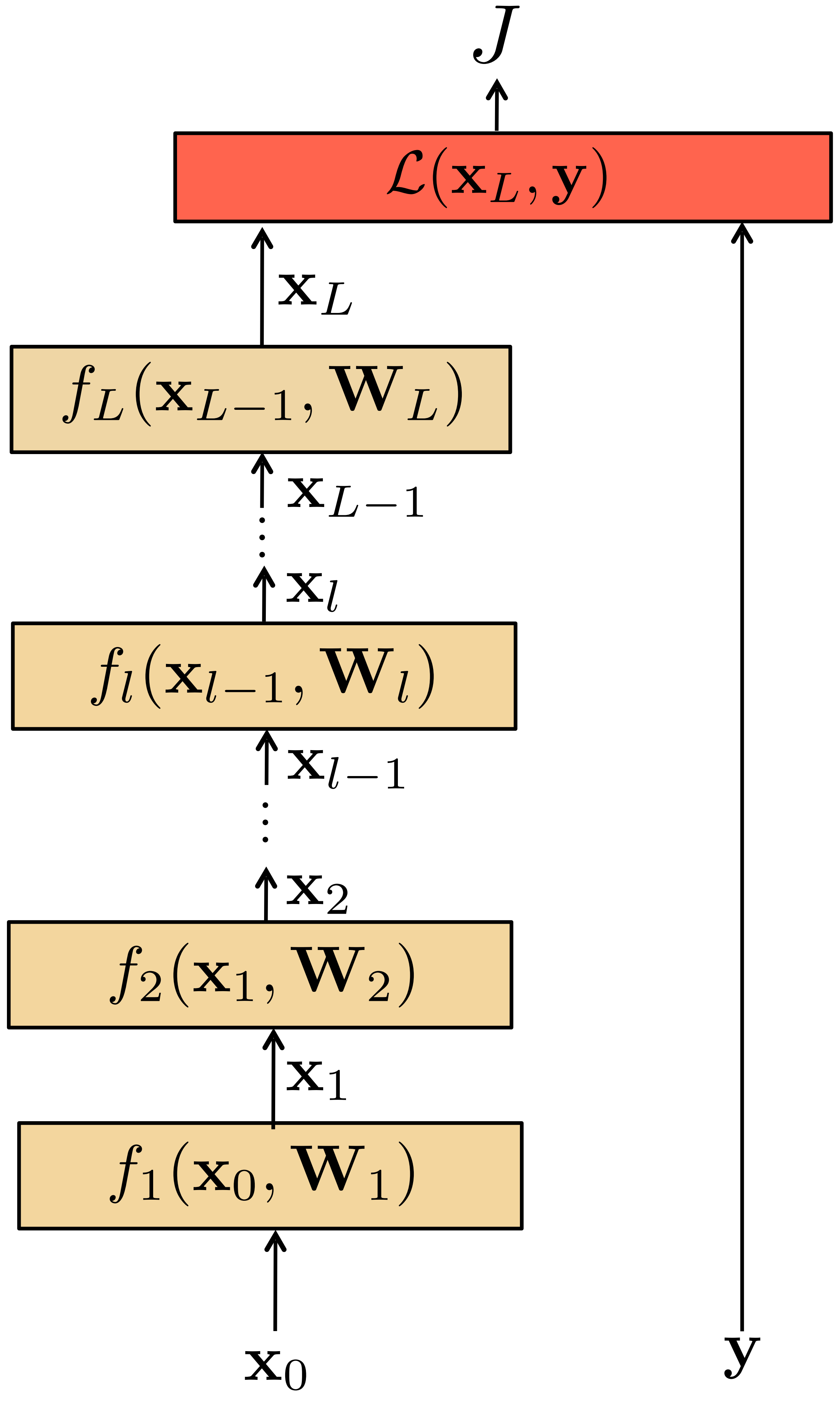
Computing gradients

To compute the gradients, we could start by writing the full energy J as a function of the network parameters.

$$J(\mathbf{W}) = \sum_{i=1} \mathcal{L}(f_L(\dots f_2(f_1(\mathbf{x}_0^{(i)}, \mathbf{W}_1), \mathbf{W}_2), \dots \mathbf{W}_L), \mathbf{y}^{(i)})$$

And then compute the partial derivatives… instead, we can use the chain rule to derive a compact algorithm: **backpropagation**



Computing gradients

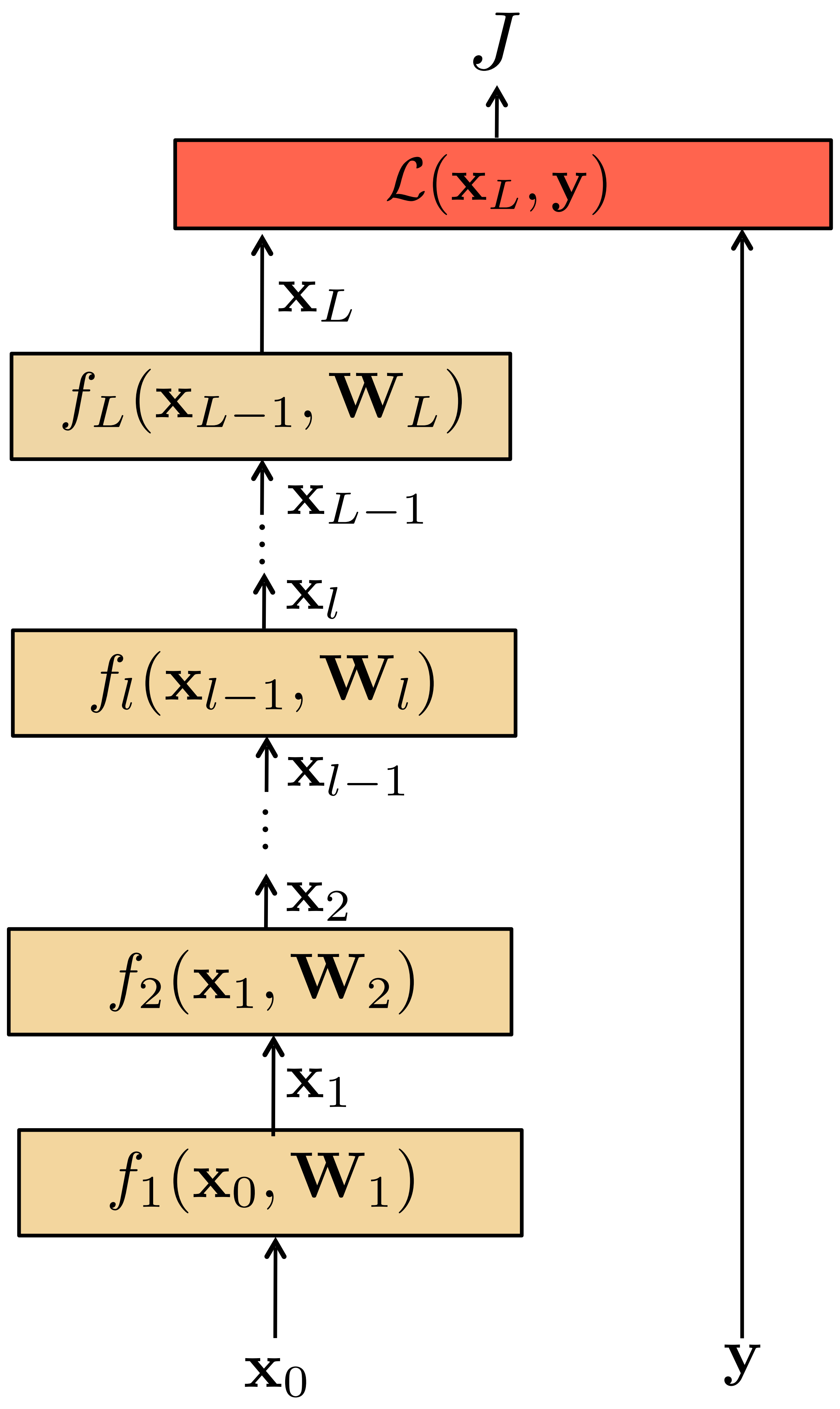
The loss J is the sum of the losses associated with each training example $\{\mathbf{x}_0^{(i)}, \mathbf{y}^{(i)}\}$

$$J(\mathbf{W}) = \sum_{i=1}^{N} \mathcal{L}(\mathbf{x}_L^{(i)}, \mathbf{y}^{(i)}; \mathbf{W})$$

Its gradient with respect to each of the network's parameters w is:

$$\frac{\partial J(\mathbf{W})}{\partial w} = \sum_{i=1}^{N} \frac{\partial \mathcal{L}(\mathbf{x}_L^{(i)}, \mathbf{y}^{(i)}; \mathbf{W})}{\partial w}$$

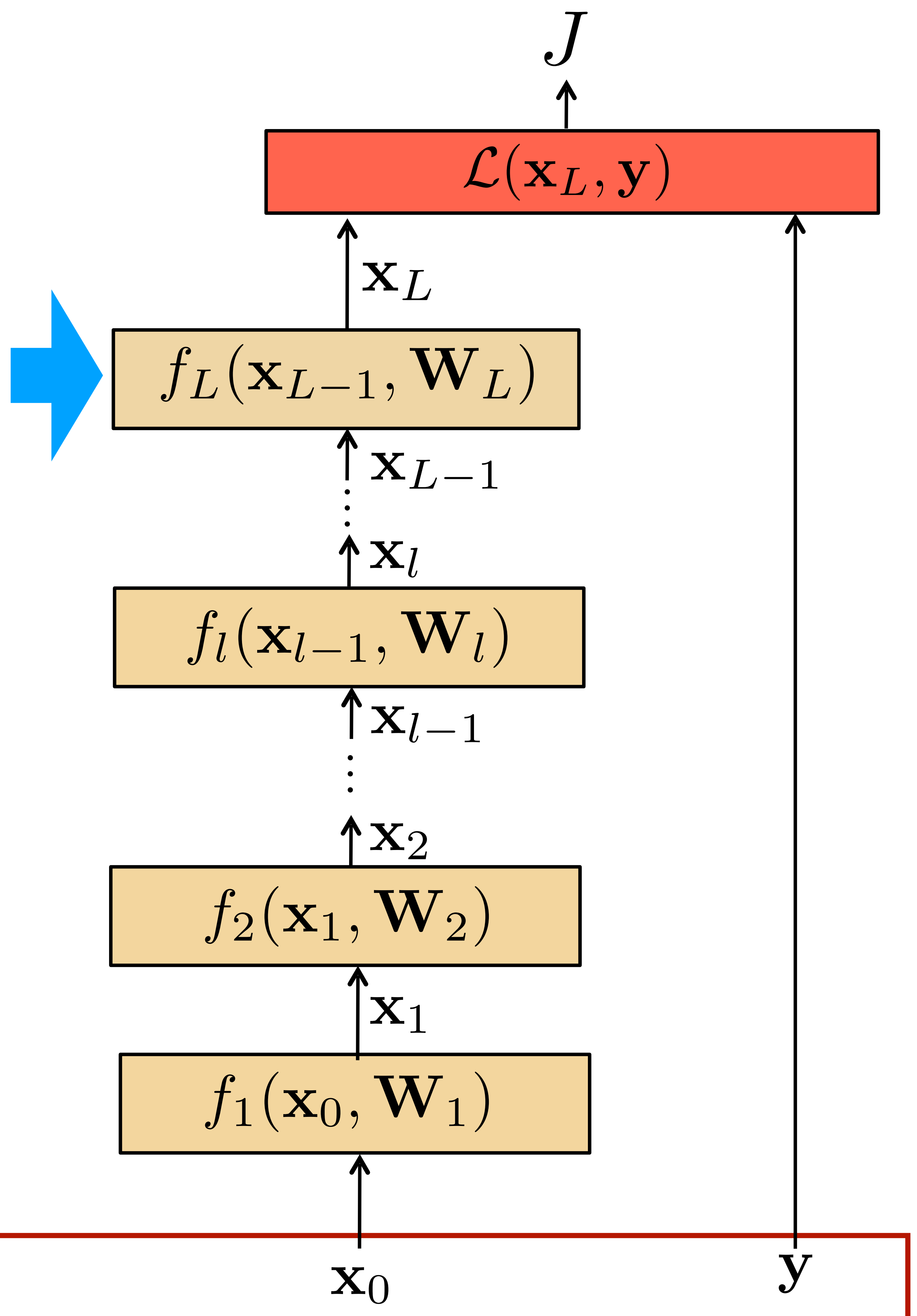
is how much J varies when the parameter w is varied.



Computing gradients

We could write the loss function to get the gradients as:

$$\mathcal{L}(\mathbf{x}_L, \mathbf{y}; \mathbf{W}) = \mathcal{L}(f_L(\mathbf{x}_{L-1}, \mathbf{W}_L), \mathbf{y})$$



If we compute the gradient with respect to the parameters of the last layer (output layer) W_L, using the **chain rule**:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_L} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_L} \cdot \frac{\partial \mathbf{x}_L}{\partial \mathbf{W}_L} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_L} \cdot \frac{\partial f_L(\mathbf{x}_{L-1}, \mathbf{W}_L)}{\partial \mathbf{W}_L}$$

How much the loss changes when we change W_L?

The change is the product between how much the loss changes when we change the output of the last layer and how much the output changes when we change the layer parameters.

Computing gradients: loss layer

If we compute the gradient with respect to the parameters of the last layer (output layer) W_L, using the chain rule:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_L} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_L} \cdot \frac{\partial \mathbf{x}_L}{\partial \mathbf{W}_L} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_L} \cdot \frac{\partial f_L(\mathbf{x}_{L-1}, \mathbf{W}_L)}{\partial \mathbf{W}_L}$$

For example, for an Euclidean loss:

$$\mathcal{L}(\mathbf{x}_L, \mathbf{y}) = \frac{1}{2} \left\| \mathbf{x}_L - \mathbf{y} \right\|_2^2$$

The gradient is:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_L} = \mathbf{x}_L - \mathbf{y}$$

Will depend on the layer structure and non-linearity.

Computing gradients: layer l

We could write the full loss function to get the gradients:

$$\mathcal{L}(\mathbf{x}_L, \mathbf{y}; \mathbf{W}) = \mathcal{L}(f_L(\dots f_2(f_1(\mathbf{x}_0, \mathbf{W}_1), \mathbf{W}_2), \dots \mathbf{W}_L), \mathbf{y})$$

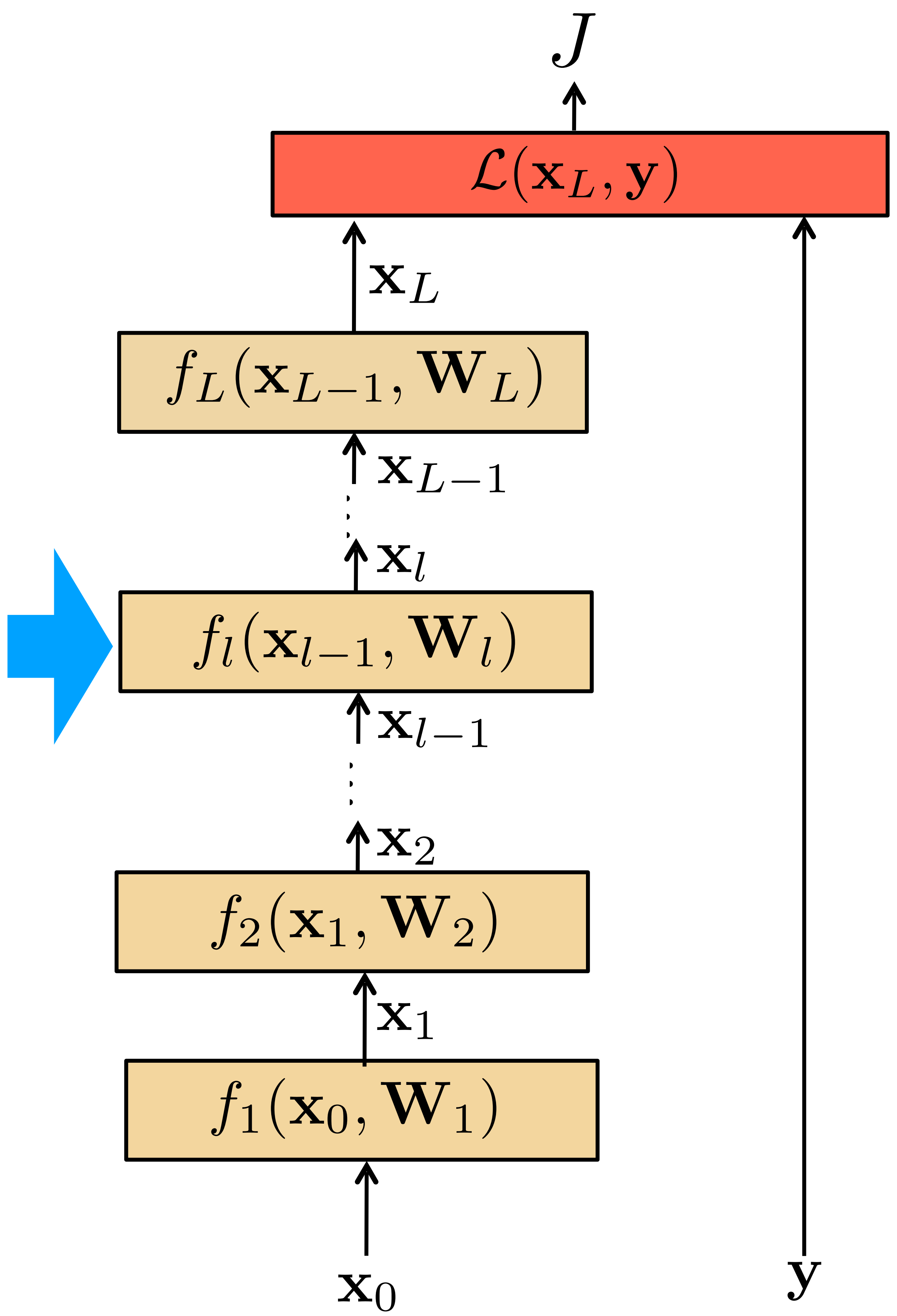
If we compute the gradient with respect to $\mathbf{W}_l$, using the chain rule:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_l} = \underbrace{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_L} \cdot \frac{\partial \mathbf{x}_L}{\partial \mathbf{x}_{L-1}} \cdot \frac{\partial \mathbf{x}_{L-1}}{\partial \mathbf{x}_{L-2}} \cdots \frac{\partial \mathbf{x}_{l+1}}{\partial \mathbf{x}_l}}_{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_l}} \cdot \frac{\partial \mathbf{x}_l}{\partial \mathbf{W}_l}$$

And this can be computed iteratively!

$$\frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{W}_l}$$

This is easy.



Backpropagation

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l+1}} \rightarrow \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l}} \rightarrow \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l-1}}$$

And this can be computed iteratively. We start at the top (L) and we can compute the gradient at layer l-1

If we have the value of $\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l}}$ we can compute the gradient at the layer below as:

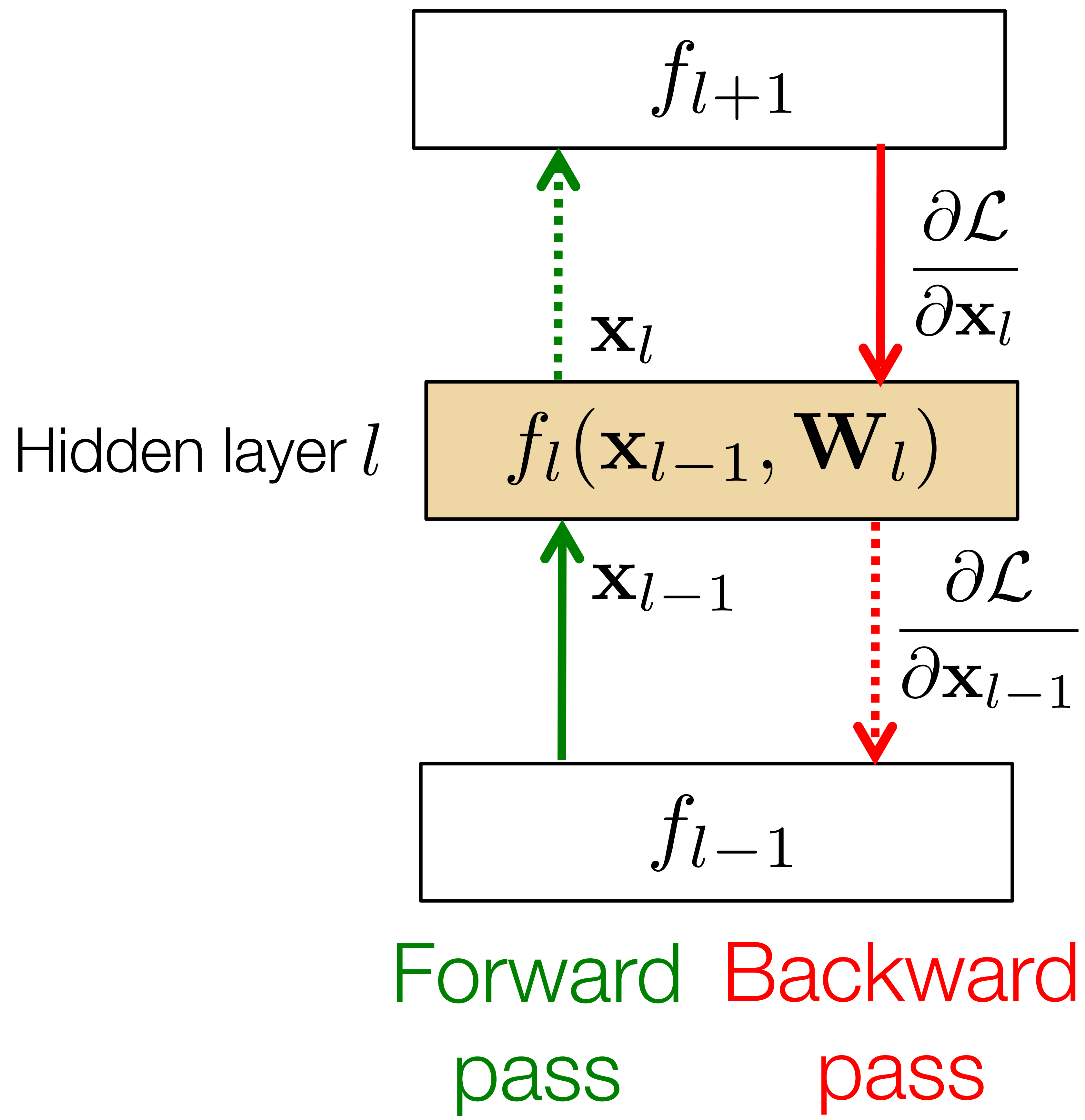
$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l-1}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l}} \cdot \frac{\partial \mathbf{x}_{l}}{\partial \mathbf{x}_{l-1}}$$

Gradient layer l-1

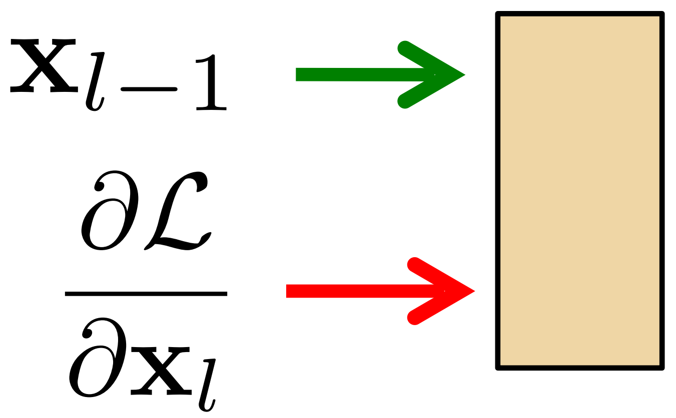
Gradient layer l

$$\frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{x}_{l-1}}$$

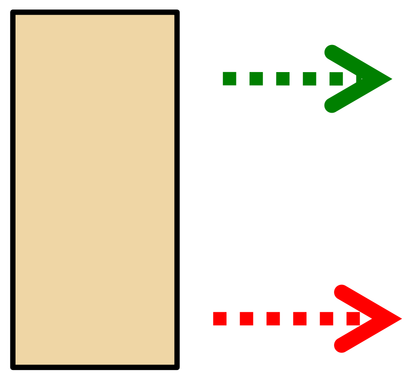
Backpropagation — Goal: to update parameters of layer l



- Layer l has two inputs (during training)



- We compute the outputs



$$\mathbf{x}_l = f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l-1}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_l} \cdot \frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{x}_{l-1}}$$

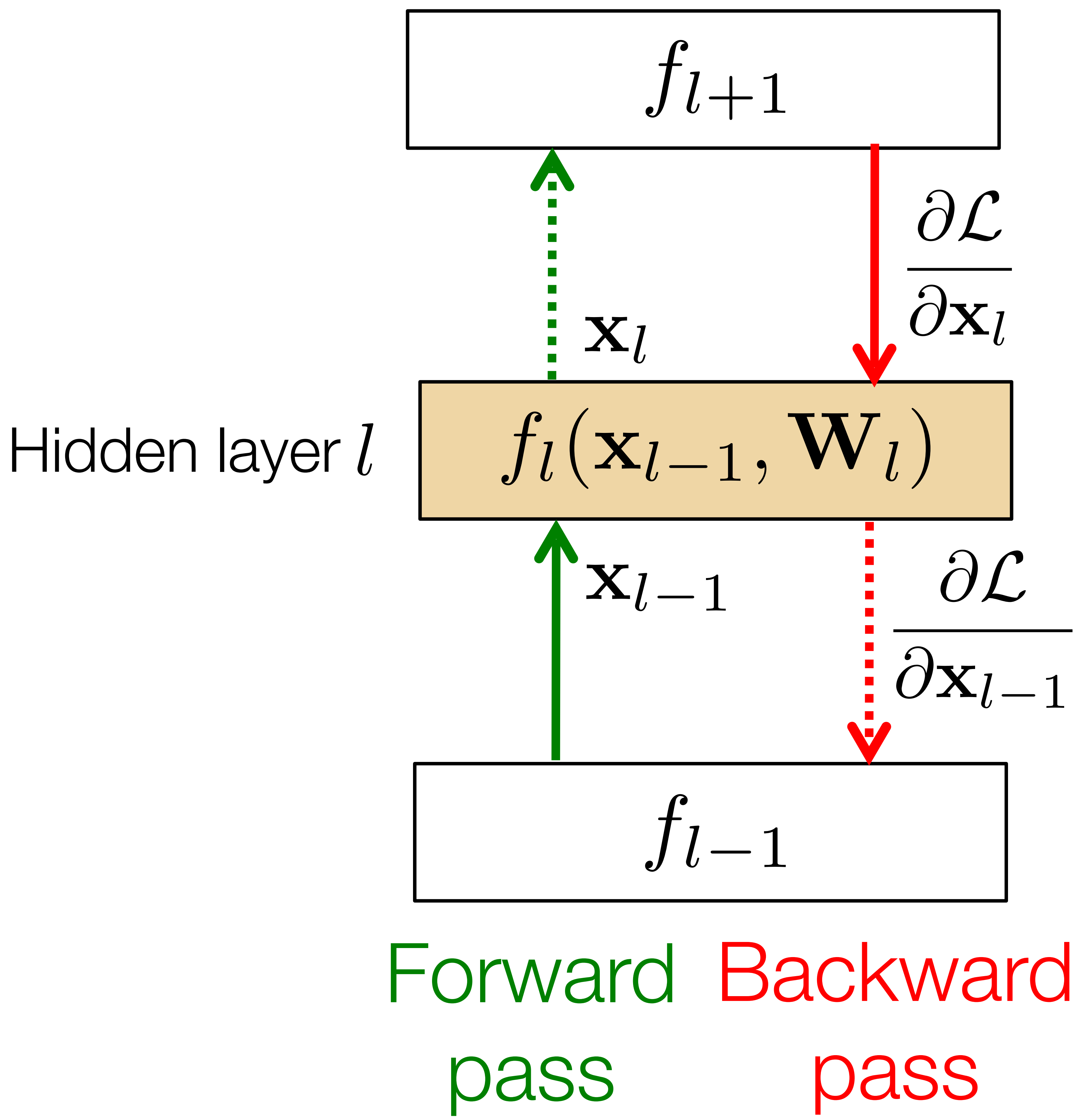
- To compute the output, we need:

$$\frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{x}_{l-1}}$$

- To compute the weight update, we need:

$$\frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{W}_l}$$

Backpropagation — Goal: to update parameters of layer l



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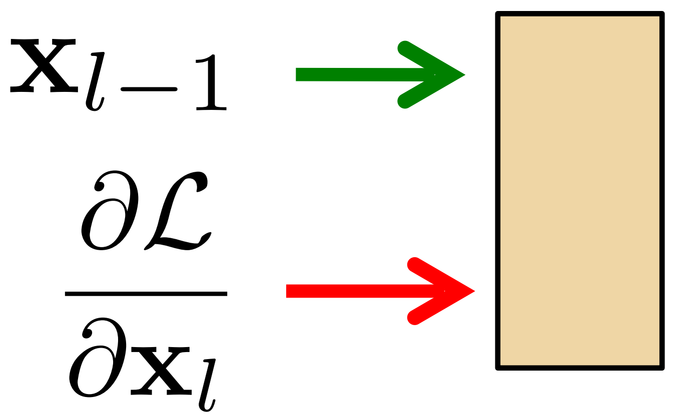
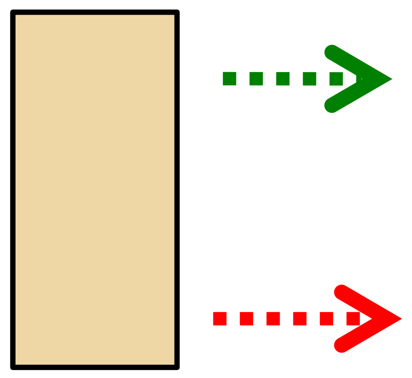


- We compute the outputs



$$\mathbf{x}_l = f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l-1}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_l} \cdot \frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{x}_{l-1}}$$

- The weight update equation is:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_l} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_l} \cdot \frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{W}_l}$$

$$\boxed{\mathbf{W}_l \leftarrow \mathbf{W}_l + \eta \left(\frac{\partial J}{\partial \mathbf{W}_l} \right)^T}$$

(sum over all training examples to get J)

Backpropagation Summary

- Forward pass: for each training example, compute the outputs for all layers:

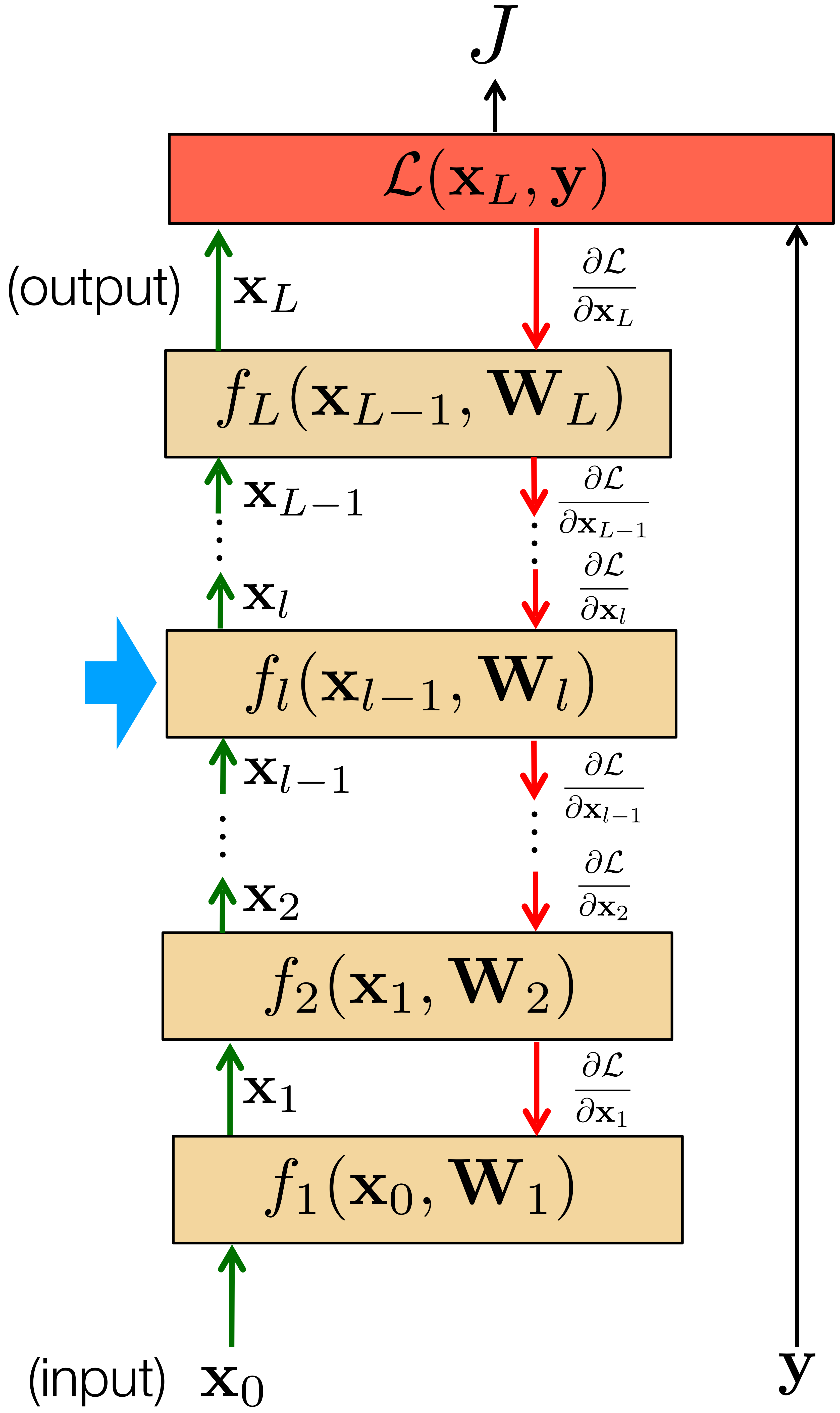
$$\mathbf{x}_l = f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)$$

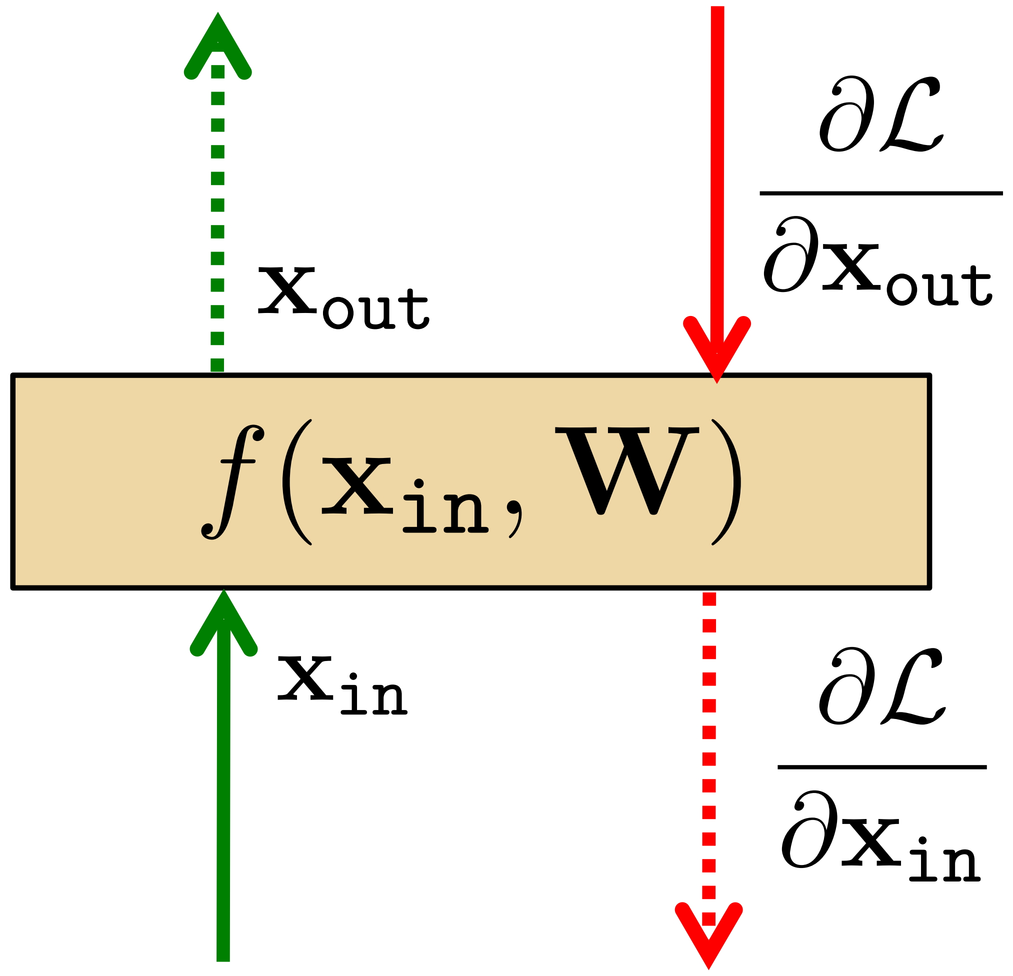
- Backwards pass: compute loss derivatives iteratively from top to bottom:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{l-1}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_l} \cdot \frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{x}_{l-1}}$$

- Compute gradients w.r.t. weights, and update weights:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_l} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_l} \cdot \frac{\partial f_l(\mathbf{x}_{l-1}, \mathbf{W}_l)}{\partial \mathbf{W}_l}$$





Linear Module

- Forward propagation: $\mathbf{x}_{\mathtt{out}} = f(\mathbf{x}_{\mathtt{in}}, \mathbf{W}) = \mathbf{W}\mathbf{x}_{\mathtt{in}}$

With W being a matrix of size $|x_{out}| \times |x_{in}|$

- Backprop to input:

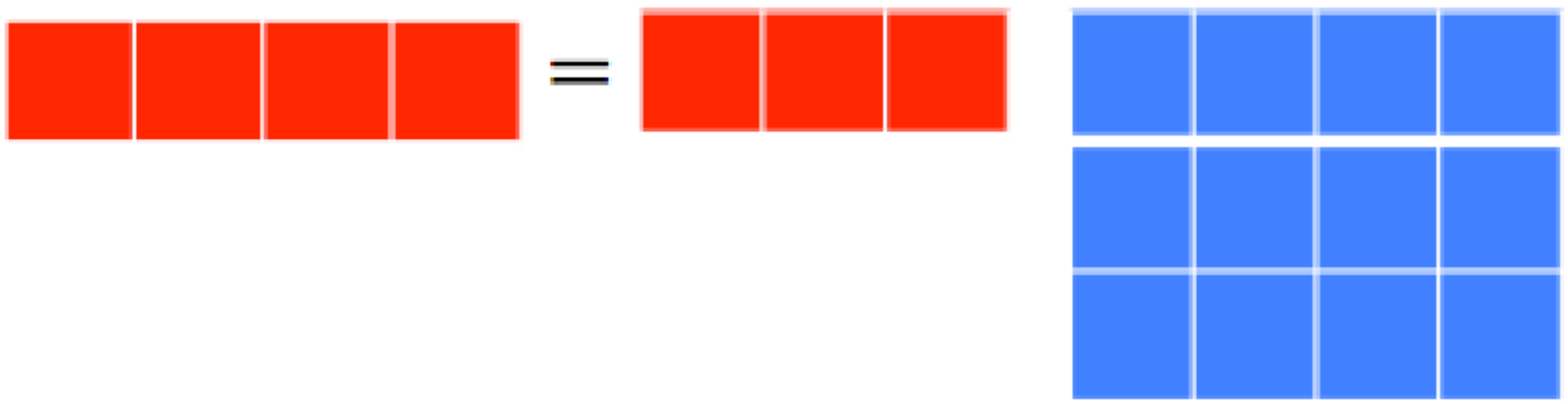
$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{in}}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{out}}} \cdot \frac{\partial f(\mathbf{x}_{\mathtt{in}}, \mathbf{W})}{\partial \mathbf{x}_{\mathtt{in}}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{out}}} \cdot \frac{\partial \mathbf{x}_{\mathtt{out}}}{\partial \mathbf{x}_{\mathtt{in}}}$$

If we look at the j component of output x_{out}, with respect to the i component of the input, x_{in}:

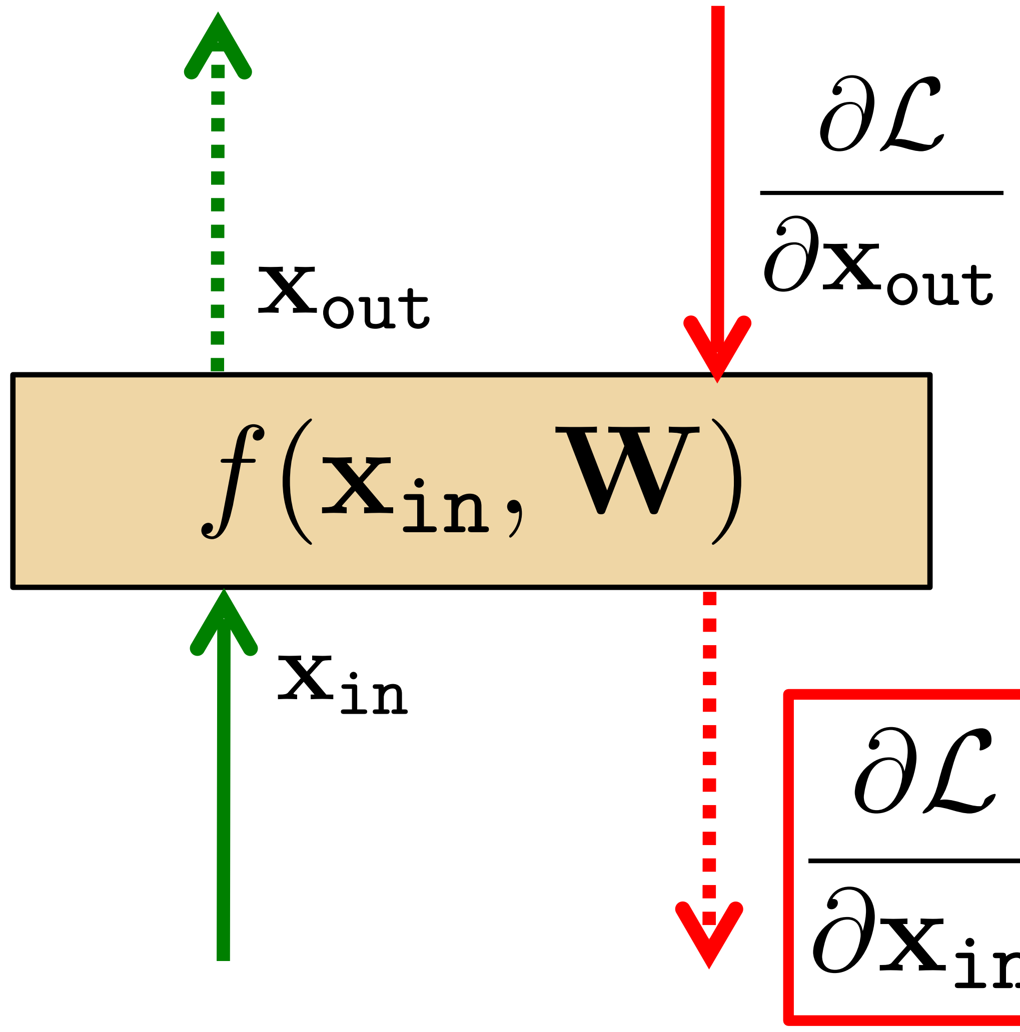
$$\frac{\partial \mathbf{x}_{\mathtt{out}_i}}{\partial \mathbf{x}_{\mathtt{in}_j}} = \mathbf{W}_{ij} \longrightarrow \frac{\partial f(\mathbf{x}_{\mathtt{in}}, \mathbf{W})}{\partial \mathbf{x}_{\mathtt{in}}} = \mathbf{W}$$

Therefore:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{in}}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{out}}} \cdot \mathbf{W}}$$

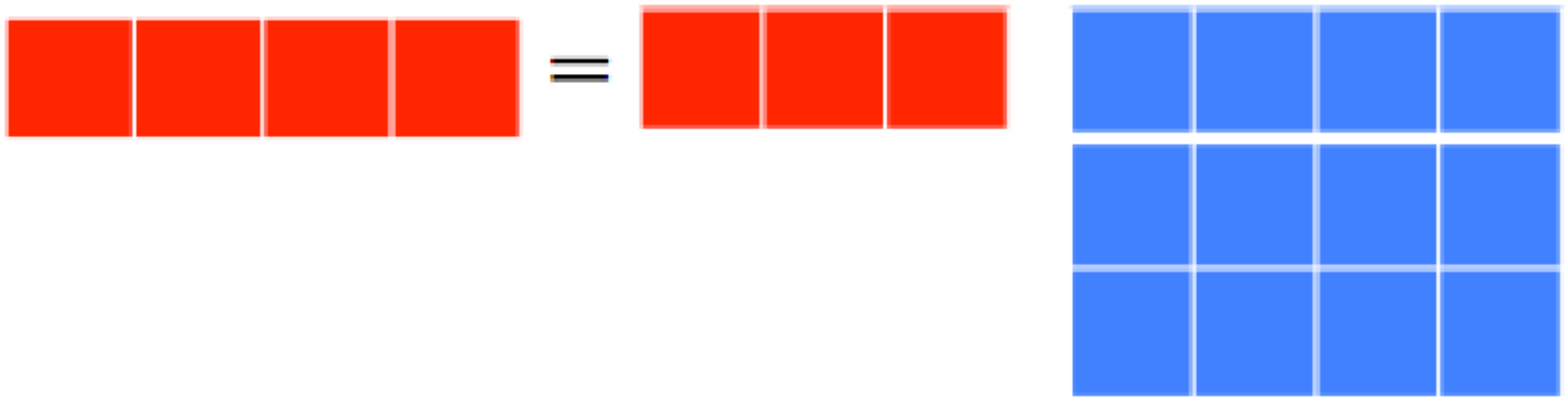


Linear Module

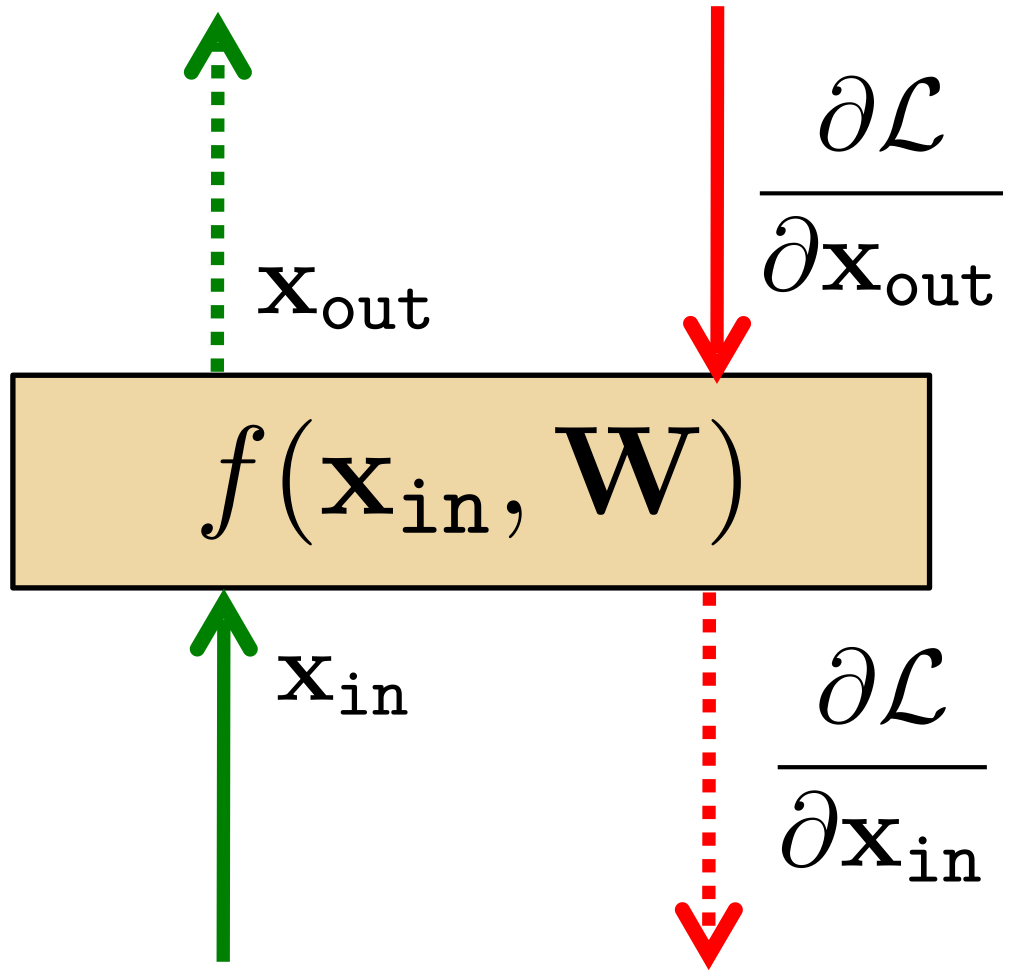


- Forward propagation: $\mathbf{x}_{\text{out}} = f(\mathbf{x}_{\text{in}}, \mathbf{W}) = \mathbf{W}\mathbf{x}_{\text{in}}$
- Backprop to input:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{in}}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}}} \cdot \mathbf{W}}$$



Now let’s see how we use the set of outputs to compute the weights update equation (backprop to the weights).



Linear Module

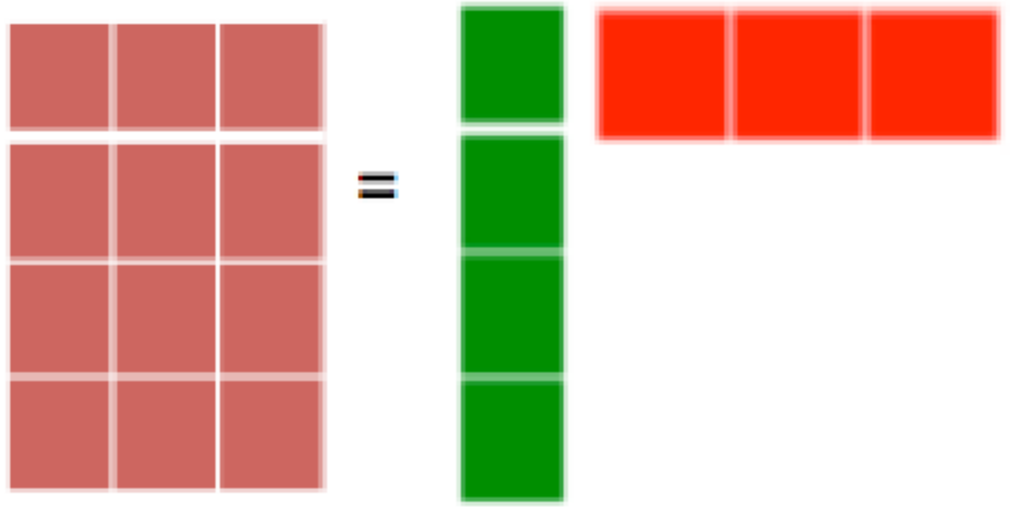
- Forward propagation: $\mathbf{x}_{\text{out}} = f(\mathbf{x}_{\text{in}}, \mathbf{W}) = \mathbf{W}\mathbf{x}_{\text{in}}$
- Backprop to weights:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}}} \cdot \frac{\partial f(\mathbf{x}_{\text{in}}, \mathbf{W})}{\partial \mathbf{W}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}}} \cdot \frac{\partial \mathbf{x}_{\text{out}}}{\partial \mathbf{W}}$$

If we look at how the parameter W_{ij} changes the cost, only the i component of the output will change, therefore:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_{ij}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}_i}} \cdot \frac{\partial \mathbf{x}_{\text{out}_i}}{\partial \mathbf{W}_{ij}} \underset{\underset{\displaystyle \frac{\partial \mathbf{x}_{\text{out}_i}}{\partial \mathbf{W}_{ij}} = \mathbf{x}_{\text{in}_j}}{\uparrow}}{=} \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}_i}} \cdot \mathbf{x}_{\text{in}_j}$$

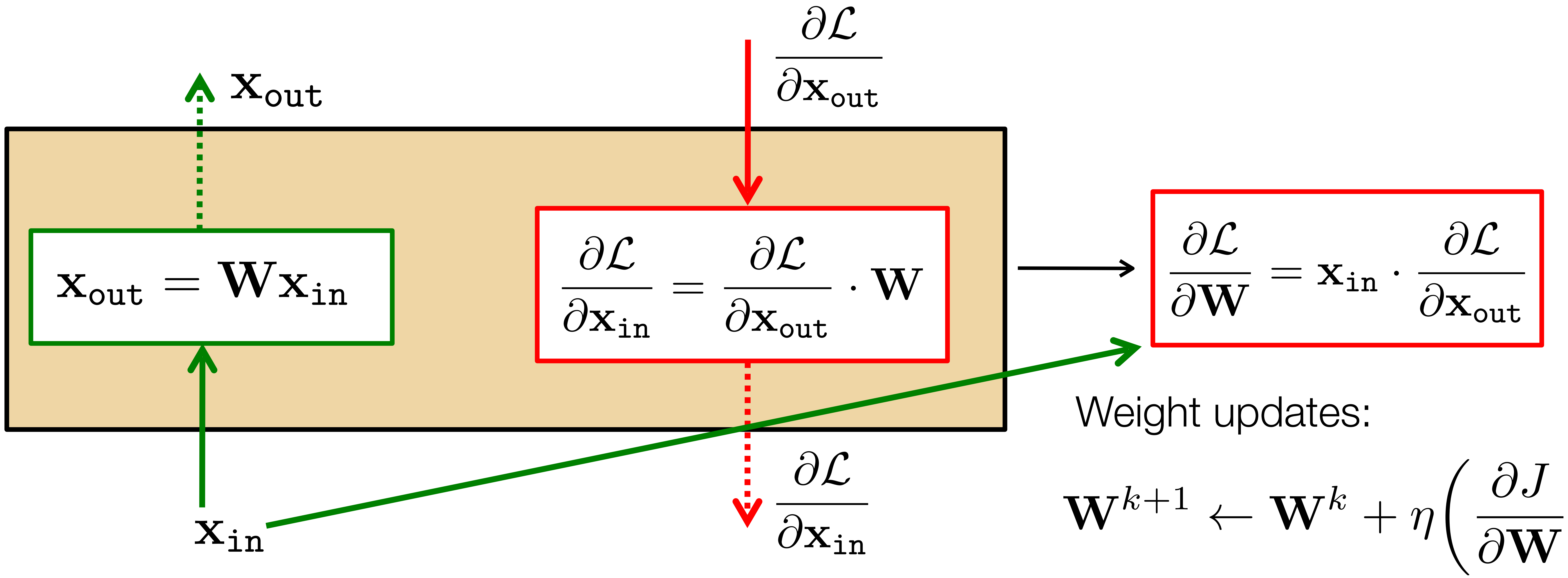
$$\boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{W}} = \mathbf{x}_{\text{in}} \cdot \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}}}}$$



And now we can update the weights (by summing over all the training examples):

$$\boxed{\mathbf{W}^{k+1} \leftarrow \mathbf{W}^{k} + \eta \left(\frac{\partial J}{\partial \mathbf{W}} \right)^{T} \quad \text{(sum over all training examples to get J)}}$$

Linear Module



$$\mathbf{x}_{\texttt{out}}$$

$$\mathbf{x}_{\texttt{out}} = \mathbf{W}\mathbf{x}_{\texttt{in}}$$

$$\mathbf{x}_{\texttt{in}}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}}}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{in}}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}}} \cdot \mathbf{W}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{in}}}$$

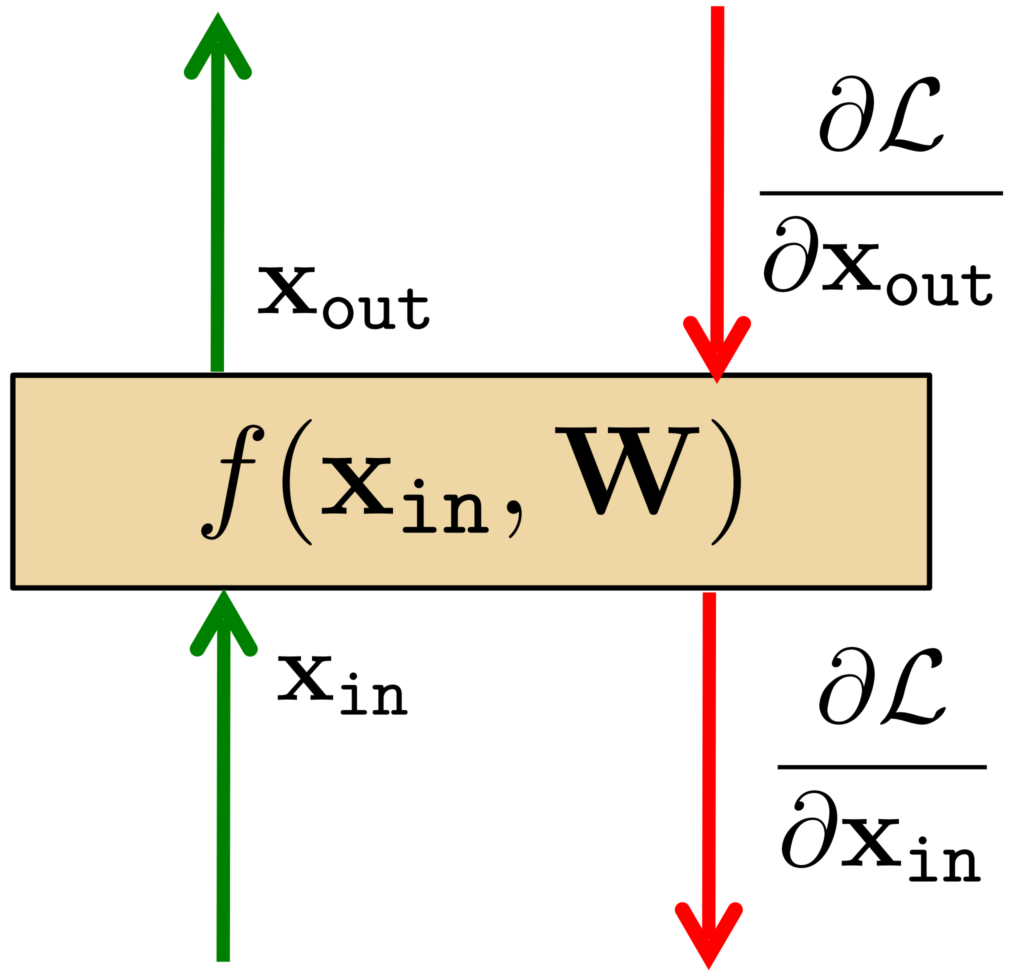
$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}} = \mathbf{x}_{\texttt{in}} \cdot \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}}}$$

Weight updates:

$$\mathbf{W}^{k+1} \leftarrow \mathbf{W}^{k} + \eta \left(\frac{\partial J}{\partial \mathbf{W}} \right)^{T}$$

$$J = \sum_{i=1}^{N} \mathcal{L}(\mathbf{x}^{(i)}, \mathbf{y}^{(i)}) \longrightarrow \frac{\partial J}{\partial \mathbf{W}} = \sum_{i=1}^{N} \mathbf{x}_{\texttt{in}} \cdot \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}}} \bigg|_{\mathbf{x}^{(i)}, \mathbf{y}^{(i)}}$$

Sum over N training pairs



Pointwise function

- Forward propagation:

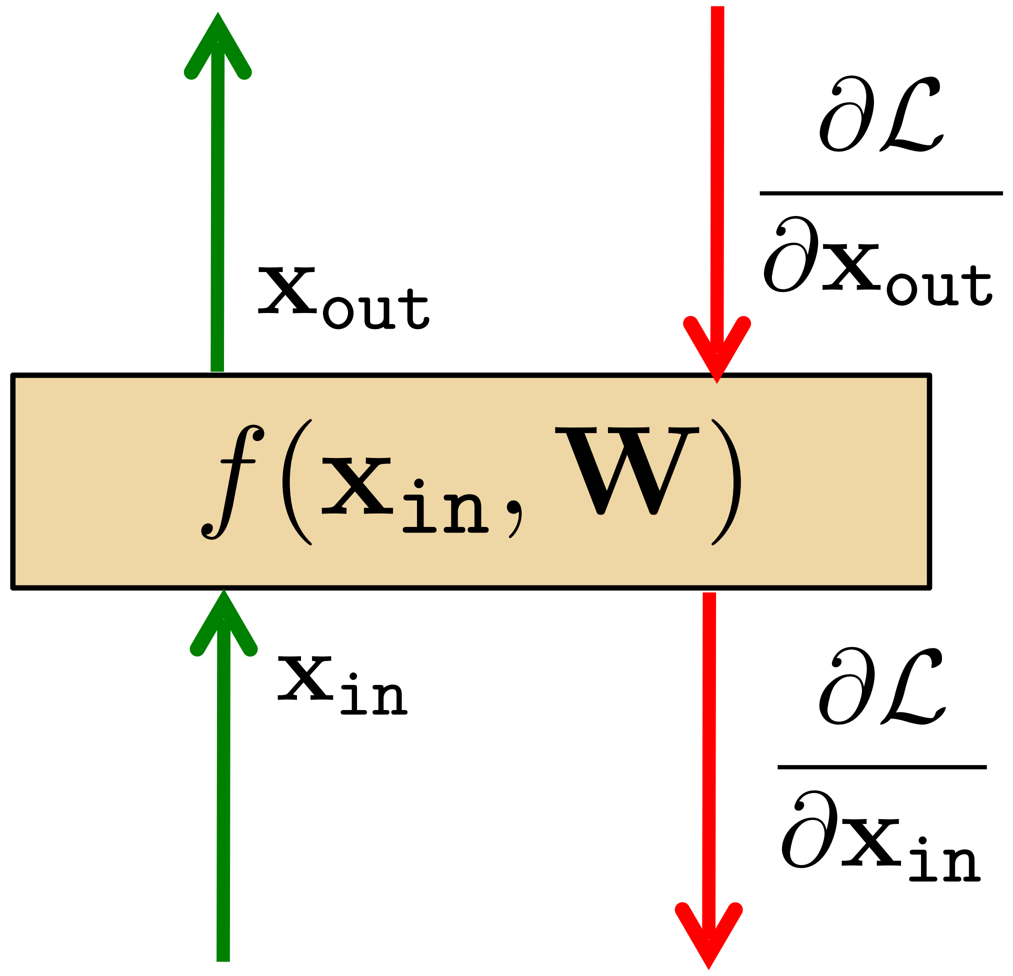
$$\mathbf{x}_{\texttt{out}_i} = h(\mathbf{x}_{\texttt{in}_i} + b_i)$$

h = an arbitrary function, b_i is a bias term.

- Backprop to input: $\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{in}_i}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}_i}} \cdot \frac{\partial \mathbf{x}_{\texttt{out}_i}}{\partial \mathbf{x}_{\texttt{in}_i}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}_i}} \cdot \frac{\partial h(\mathbf{x}_{\texttt{in}_i} + b_i)}{\partial \mathbf{x}_{\texttt{in}_i}}$

- Backprop to bias: $\frac{\partial \mathcal{L}}{\partial b_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}_i}} \cdot \frac{\partial \mathbf{x}_{\texttt{out}_i}}{\partial b_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}_i}} \cdot \frac{\partial h(\mathbf{x}_{\texttt{in}_i} + b_i)}{\partial b_i}$

We use this last expression to update the bias.



Pointwise function

- Forward propagation:

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- Backprop to bias: $\frac{\partial \mathcal{L}}{\partial b_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}_i}} \cdot \frac{\partial \mathbf{x}_{\text{out}_i}}{\partial b_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\text{out}_i}} \cdot h'(\mathbf{x}_{\text{in}_i} + b_i)$

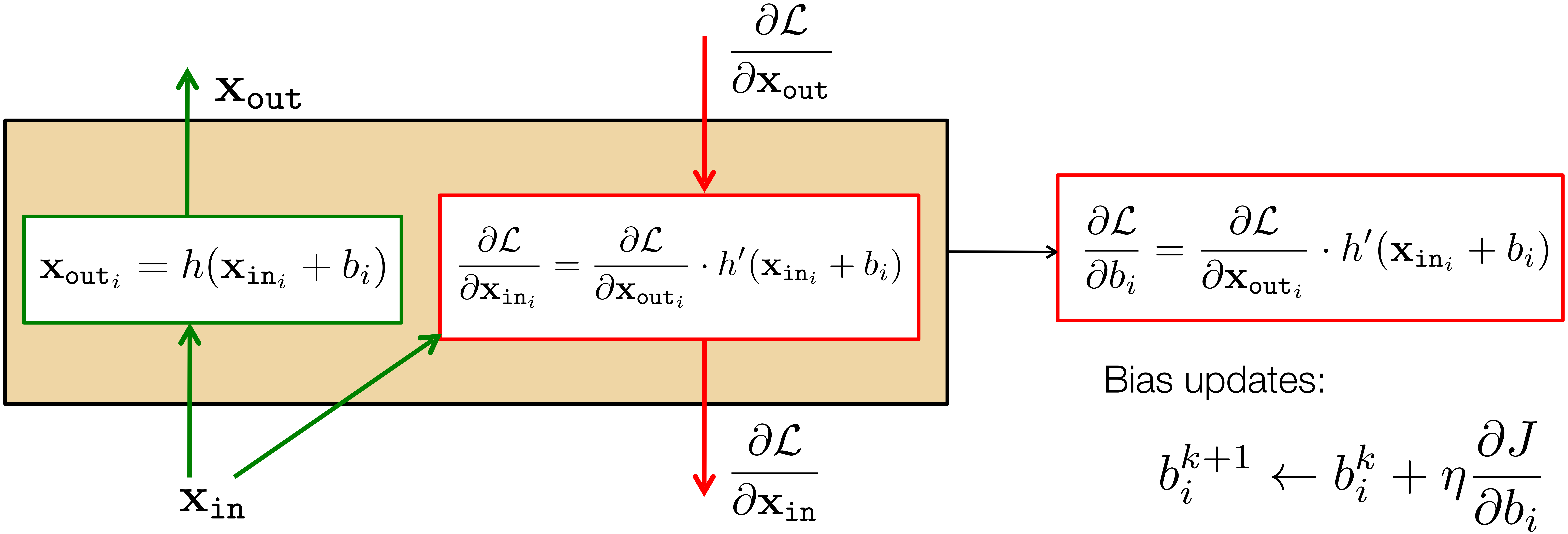
We use this last expression to update the bias.

Some useful derivatives:

For hyperbolic tangent: $\tanh'(x) = 1 - \tanh^2(x)$

For ReLU: $h(x) = \max(0, x), \quad h'(x) = \mathbb{1}(x \geq 0)$

Pointwise function



$\mathbf{x}_{\mathtt{out}}$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{out}}}$

$$\mathbf{x}_{\mathtt{out}_i} = h(\mathbf{x}_{\mathtt{in}_i} + b_i)$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{in}_i}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{out}_i}} \cdot h'(\mathbf{x}_{\mathtt{in}_i} + b_i)$$

$$\frac{\partial \mathcal{L}}{\partial b_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{out}_i}} \cdot h'(\mathbf{x}_{\mathtt{in}_i} + b_i)$$

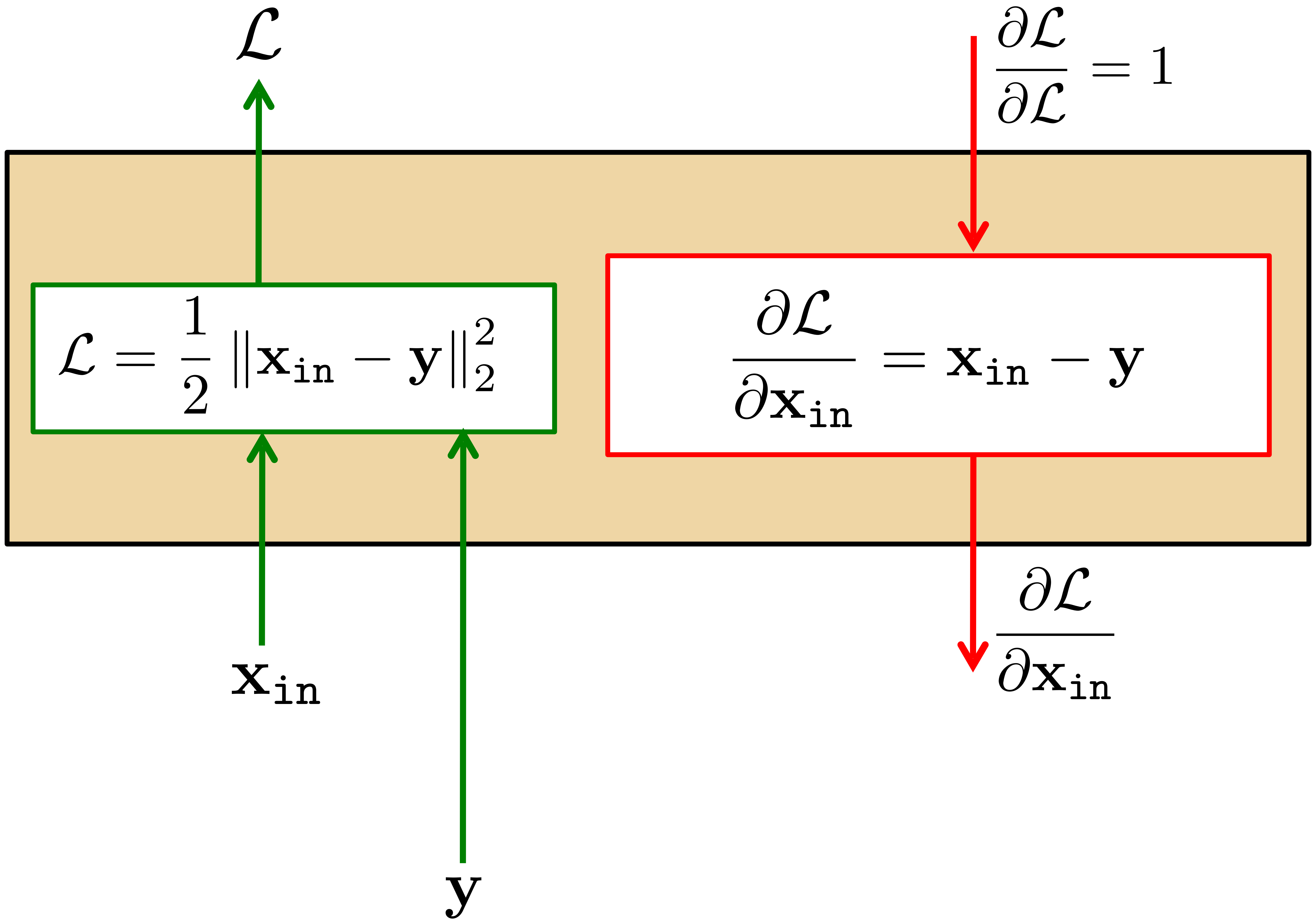
$\mathbf{x}_{\mathtt{in}}$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathtt{in}}}$

Bias updates:

$$b_i^{k+1} \leftarrow b_i^k + \eta \frac{\partial J}{\partial b_i}$$

Euclidean loss module



$\mathcal{L}$

$\frac{\partial \mathcal{L}}{\partial \mathcal{L}} = 1$

$\mathcal{L} = \frac{1}{2} \|\mathbf{x}_{\texttt{in}} - \mathbf{y}\|_2^2$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{in}}} = \mathbf{x}_{\texttt{in}} - \mathbf{y}$

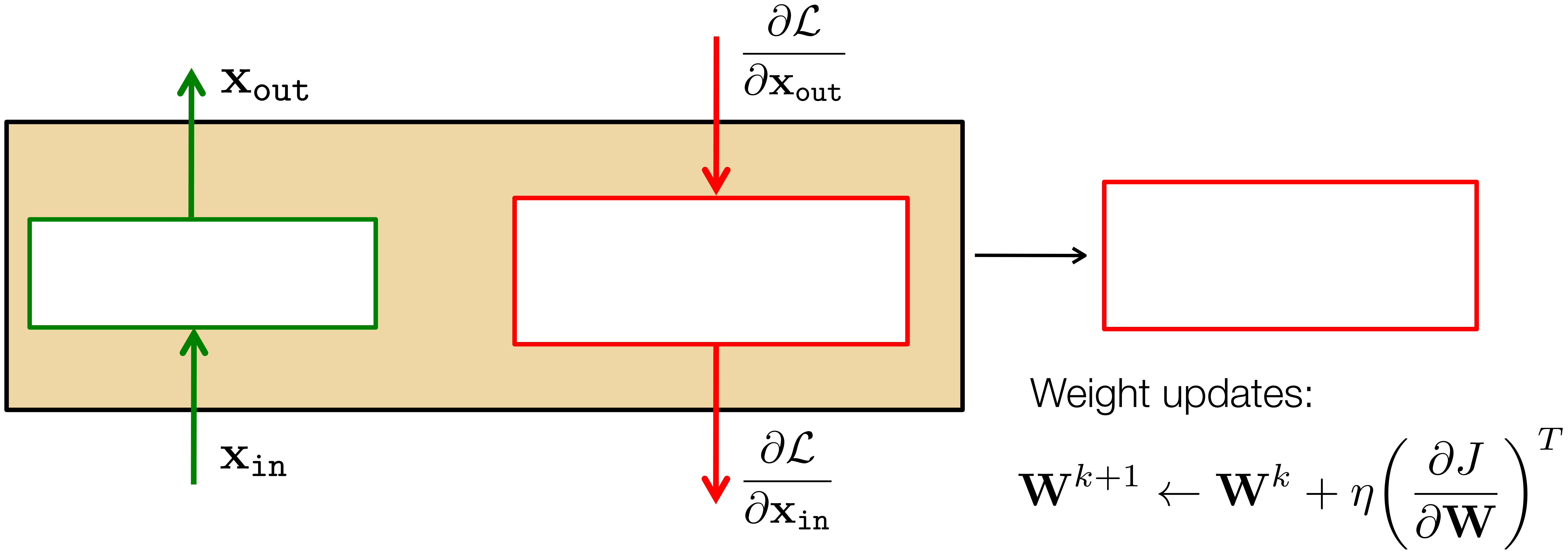
$\mathbf{x}_{\texttt{in}}$

$\mathbf{y}$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{in}}}$

Homework: Convolution Module

Assume the input x_{in} and output x_{out} are 1D signals of the same length N.
The convolution kernel is W, and has length k < N



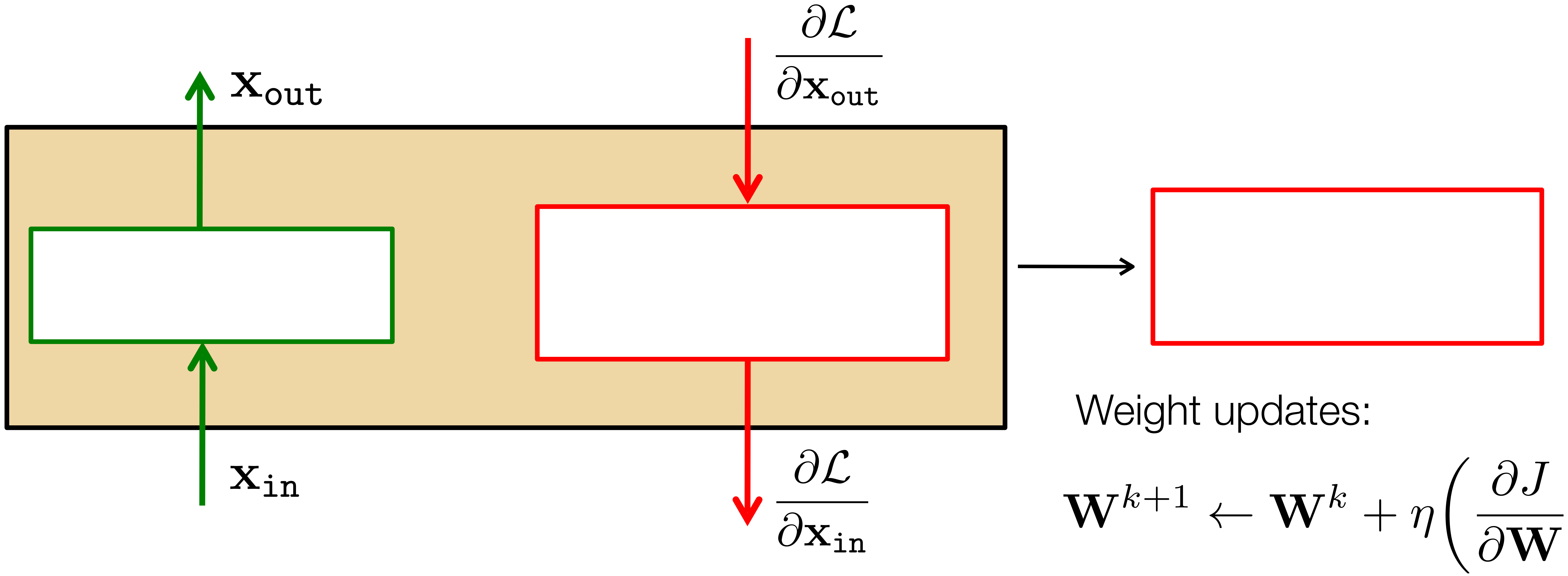
Weight updates:

$$\mathbf{W}^{k+1} \leftarrow \mathbf{W}^{k} + \eta \left(\frac{\partial J}{\partial \mathbf{W}} \right)^{T}$$

Derive the equations that go inside each box.
Discuss how you handle the boundaries.

Homework: max pooling module

Assume the input x_{in} and output x_{out} are 1D signals of different lengths.



$\mathbf{x}_{\texttt{out}}$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{out}}}$

$\mathbf{x}_{\texttt{in}}$

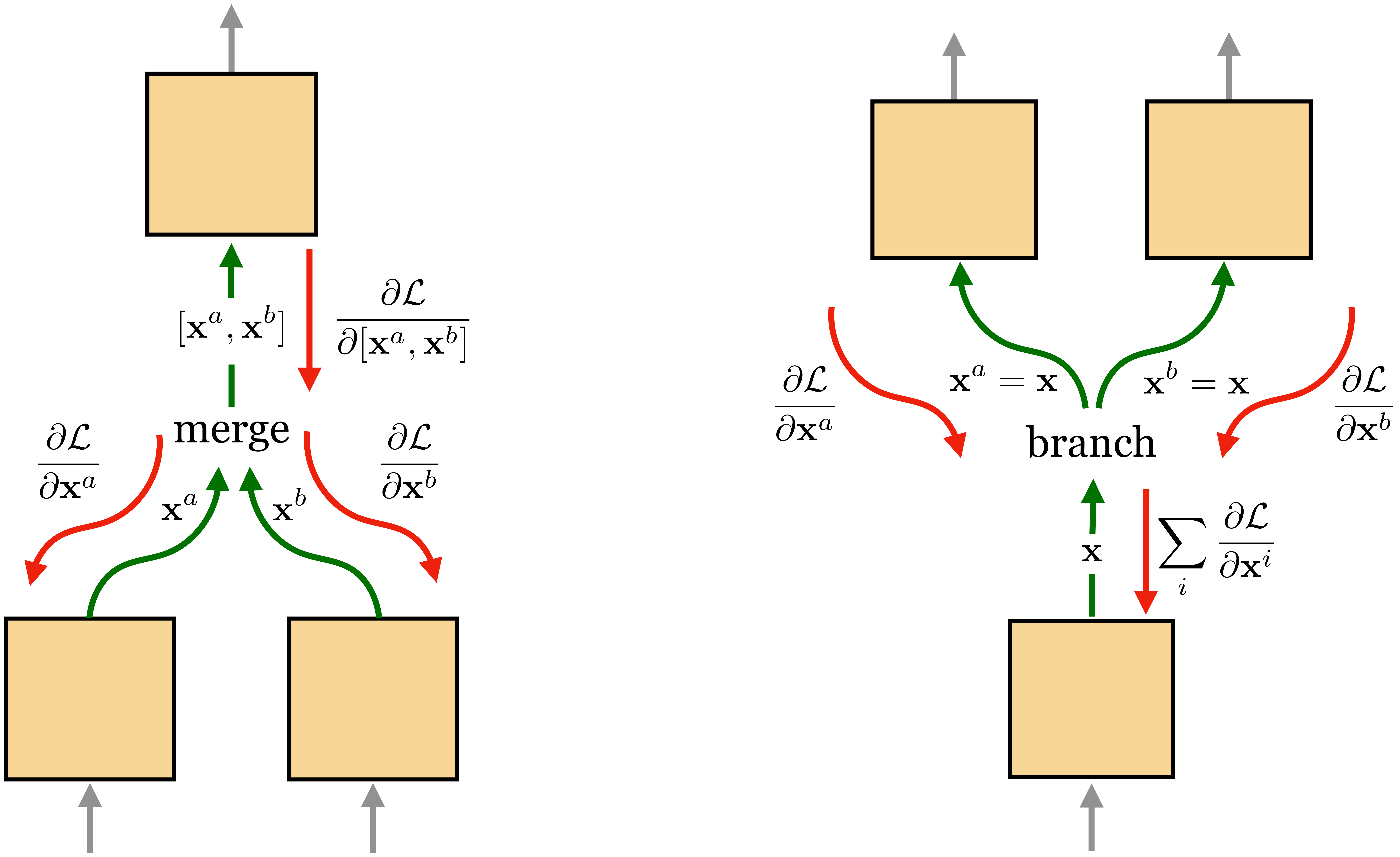
$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\texttt{in}}}$

Weight updates:

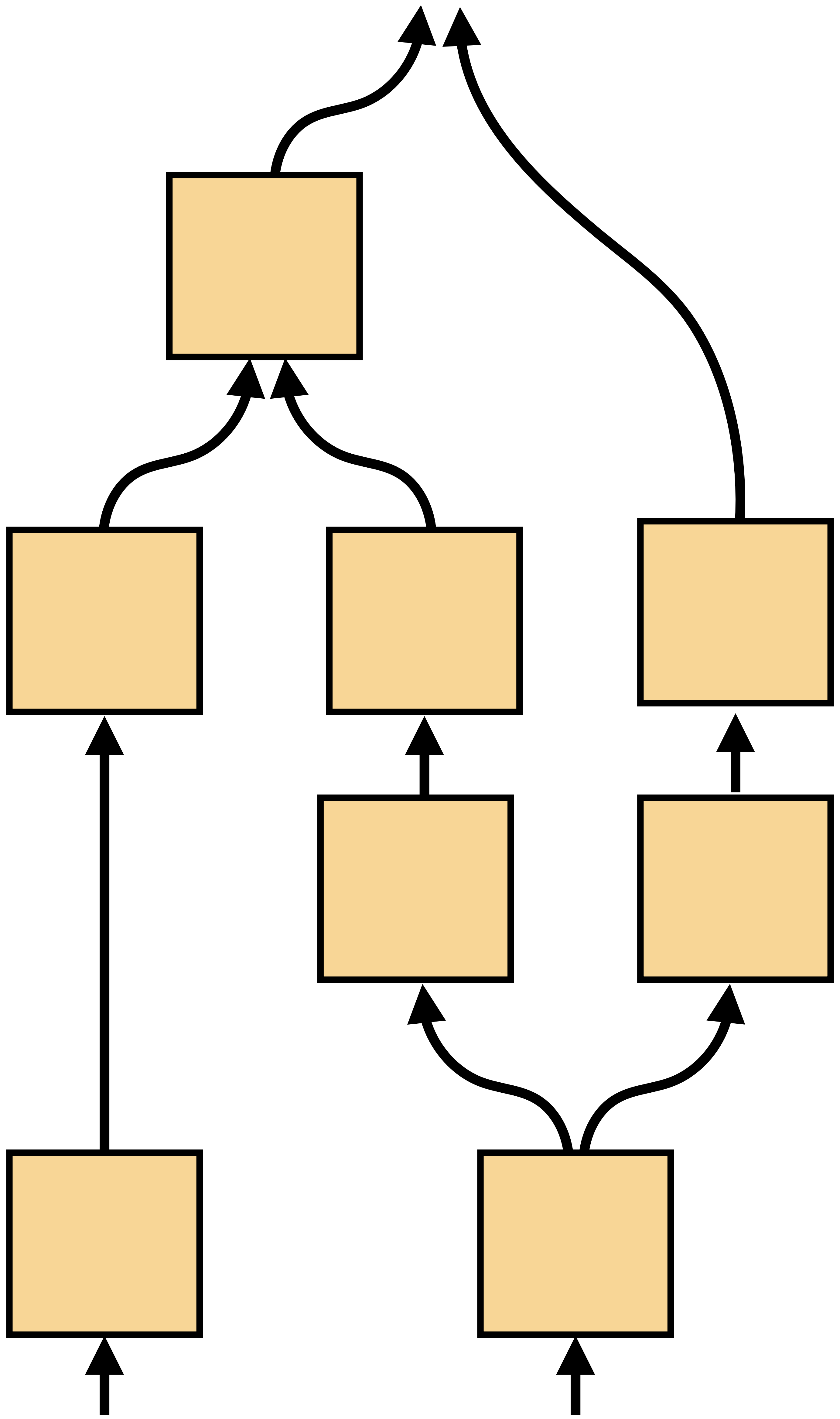
$$\mathbf{W}^{k+1} \leftarrow \mathbf{W}^{k} + \eta \left(\frac{\partial J}{\partial \mathbf{W}} \right)^{T}$$

Derive the equations that go inside each box.
Discuss how you handle the boundaries.

Branching and Merging



Computation Graphs



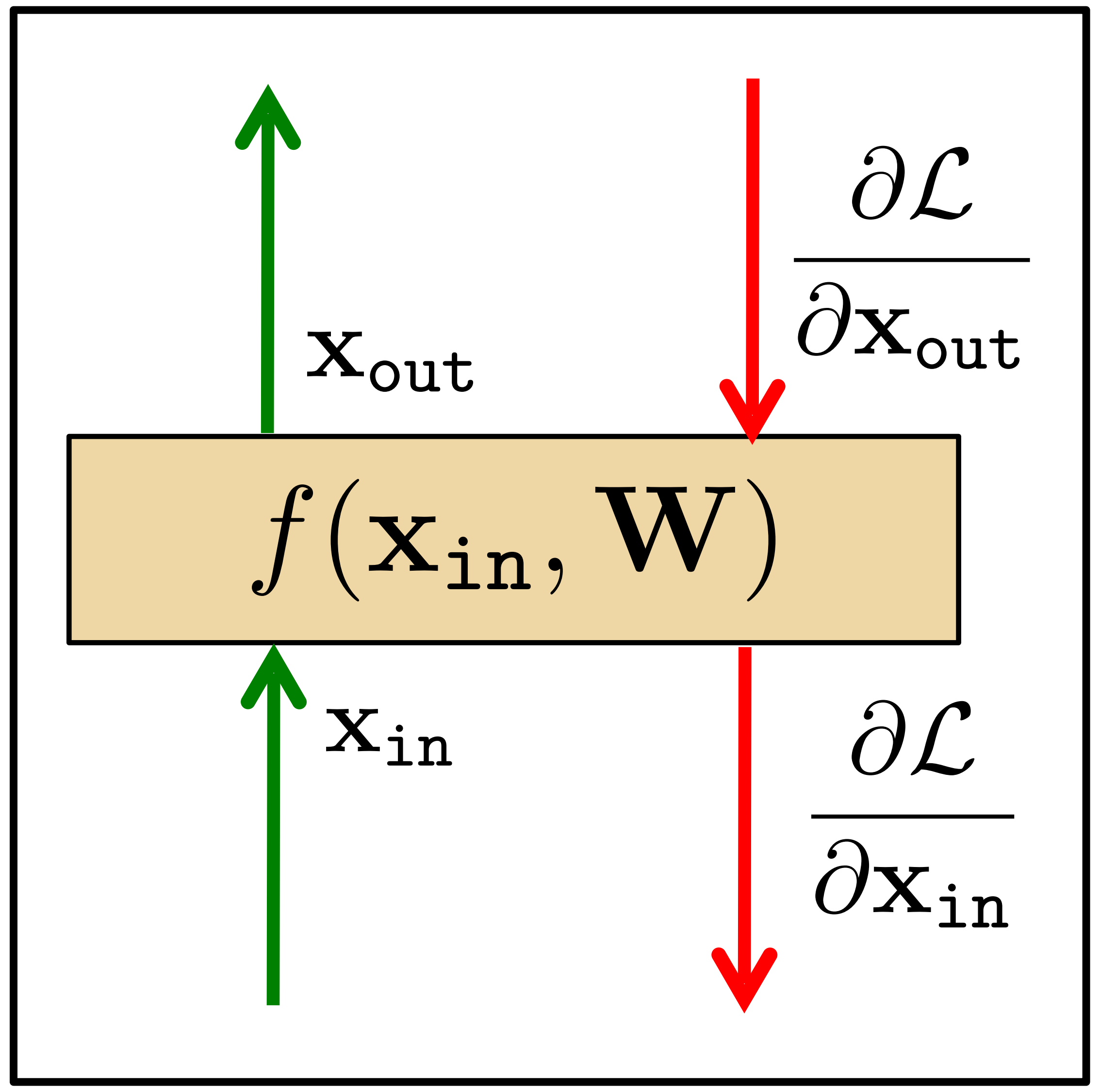
If all the modules (🟨) are differentiable, and they are connected to form a Directed Acyclic Graph (**DAG**), then you can use backprop to train this whole system!

This is an example of a **computation graph**.

Many programs can be represented with differentiable DAGs, not just “neural nets”.

Differentiable programming

Deep learning



$\mathbf{x}_{\mathrm{out}}$

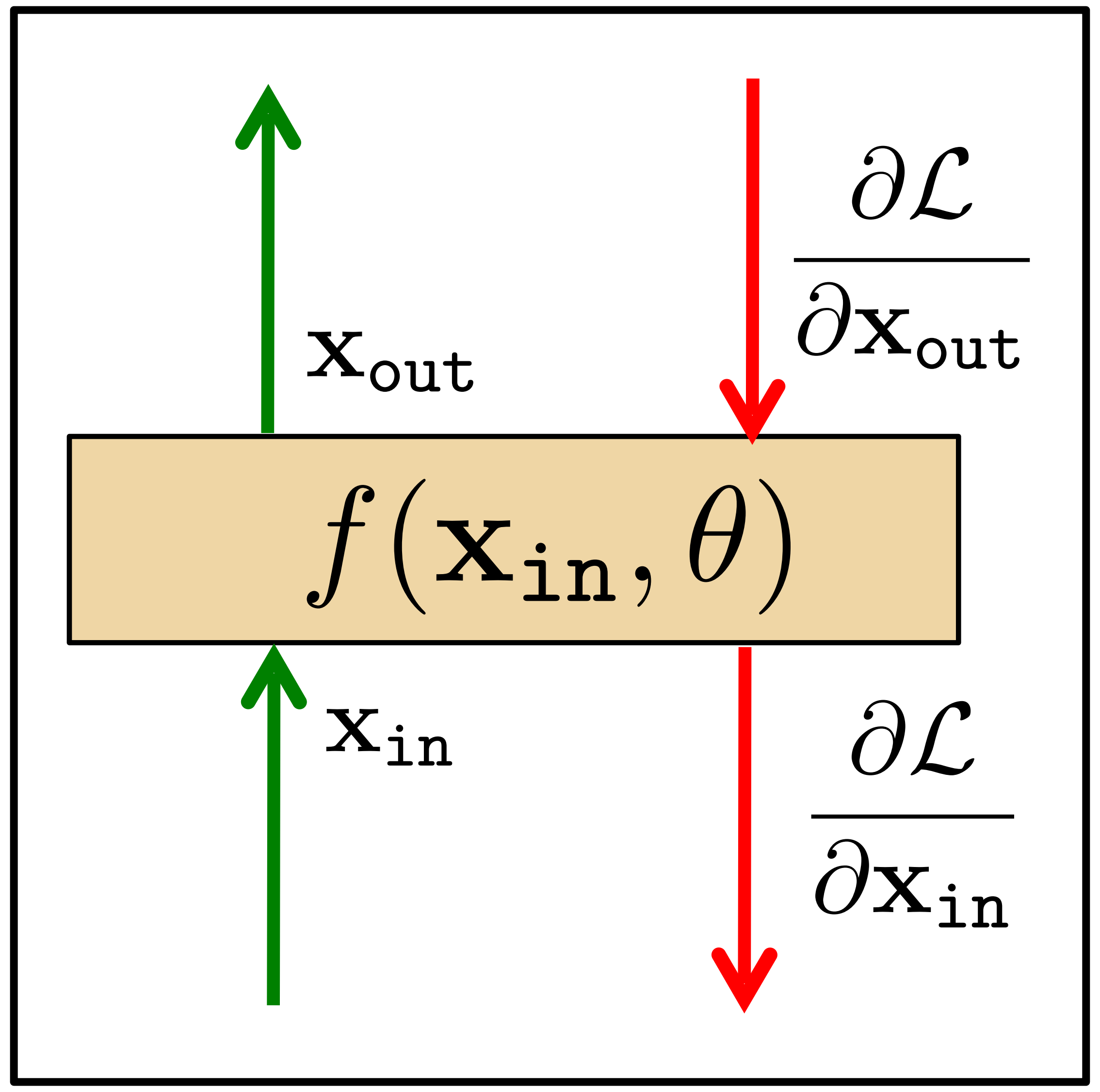
$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathrm{out}}}$

$f(\mathbf{x}_{\mathrm{in}}, \mathbf{W})$

$\mathbf{x}_{\mathrm{in}}$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathrm{in}}}$

Differentiable programming



$\mathbf{x}_{\mathrm{out}}$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathrm{out}}}$

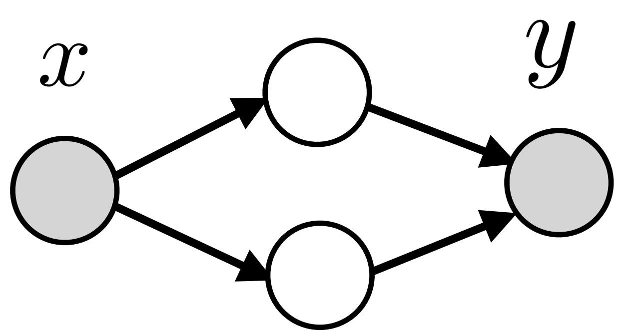
$f(\mathbf{x}_{\mathrm{in}}, \theta)$

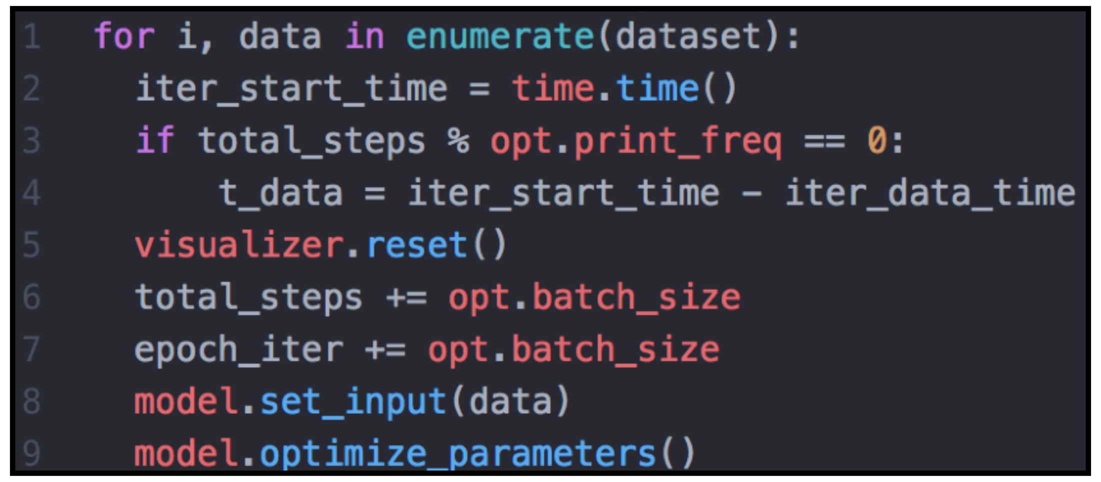
$\mathbf{x}_{\mathrm{in}}$

$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_{\mathrm{in}}}$

PyTorch

TensorFlow ™





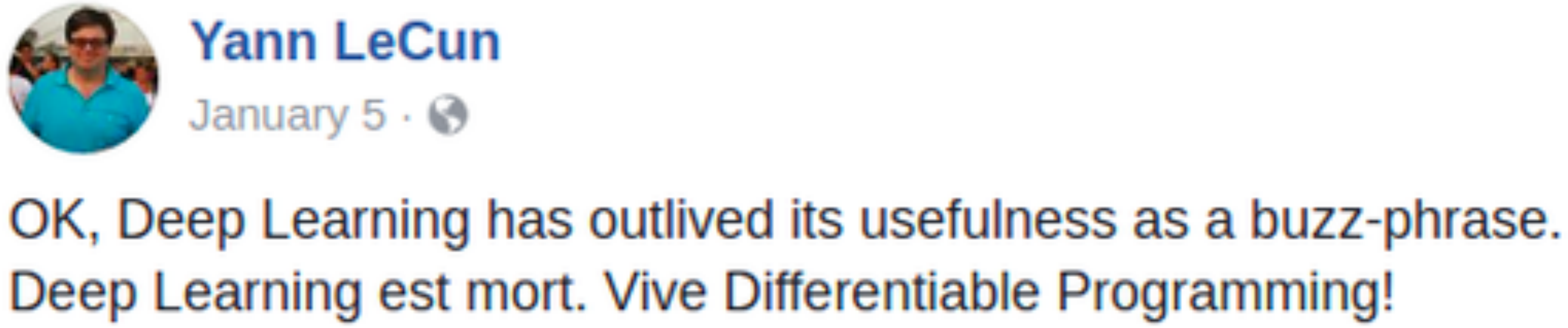
```
for i, data in enumerate(dataset):
  iter_start_time = time.time()
  if total_steps % opt.print_freq == 0:
      t_data = iter_start_time - iter_data_time
  visualizer.reset()
  total_steps += opt.batch_size
  epoch_iter += opt.batch_size
  model.set_input(data)
  model.optimize_parameters()
```

Differentiable programming

Deep nets are popular for a few reasons:

1. Easy to optimize (differentiable)
2. Compositional “block based programming”

An emerging term for general models with these properties is **differentiable programming**.



Yann LeCun
January 5 ·

OK, Deep Learning has outlived its usefulness as a buzz-phrase.
Deep Learning est mort. Vive Differentiable Programming!

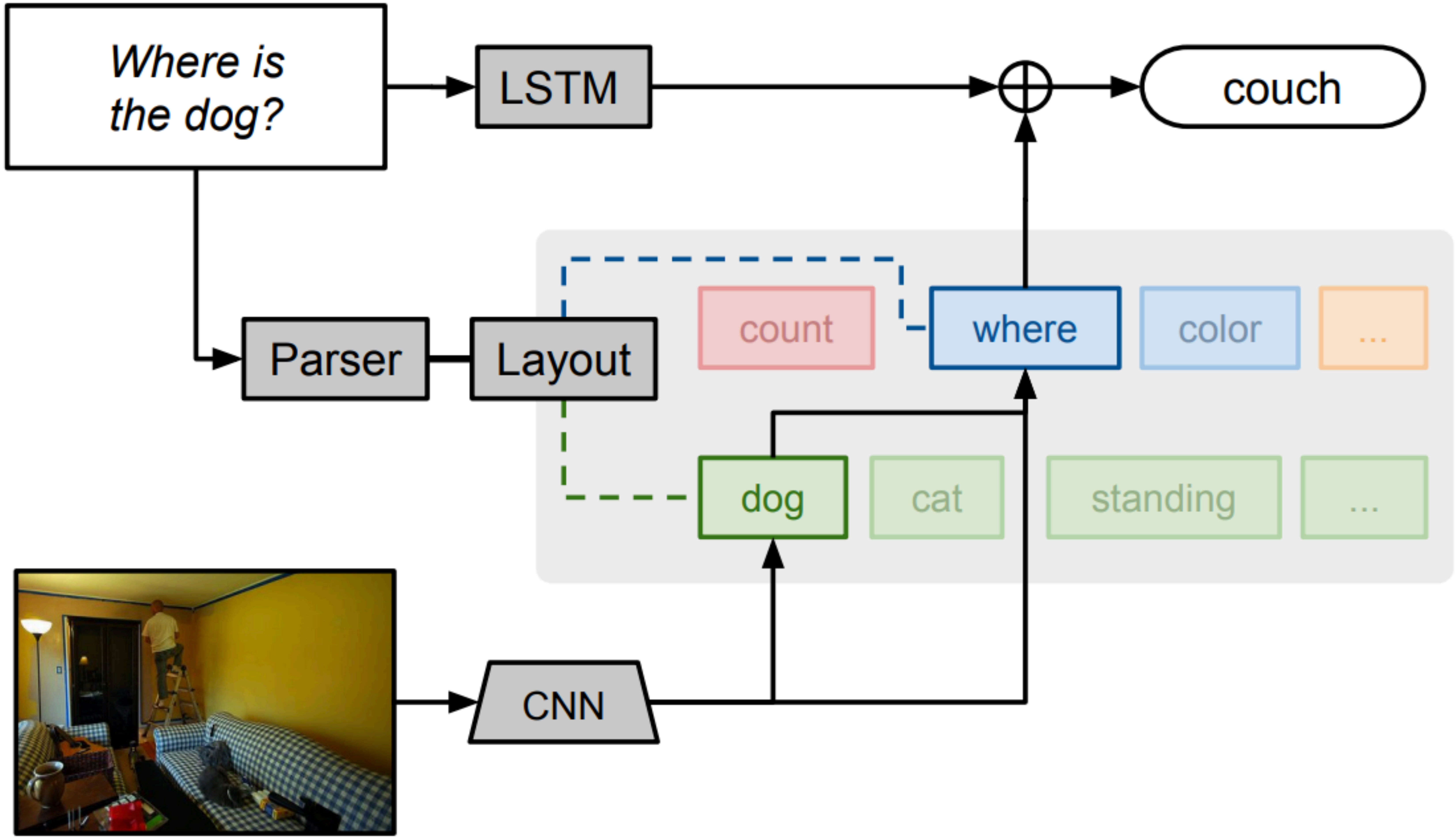
Thomas G. Dietterich
@tdietterich

DL is essentially a new style of programming--"differentiable programming"--and the field is trying to work out the reusable constructs in this style. We have some: convolution, pooling, LSTM, GAN, VAE, memory units, routing units, etc. 8/

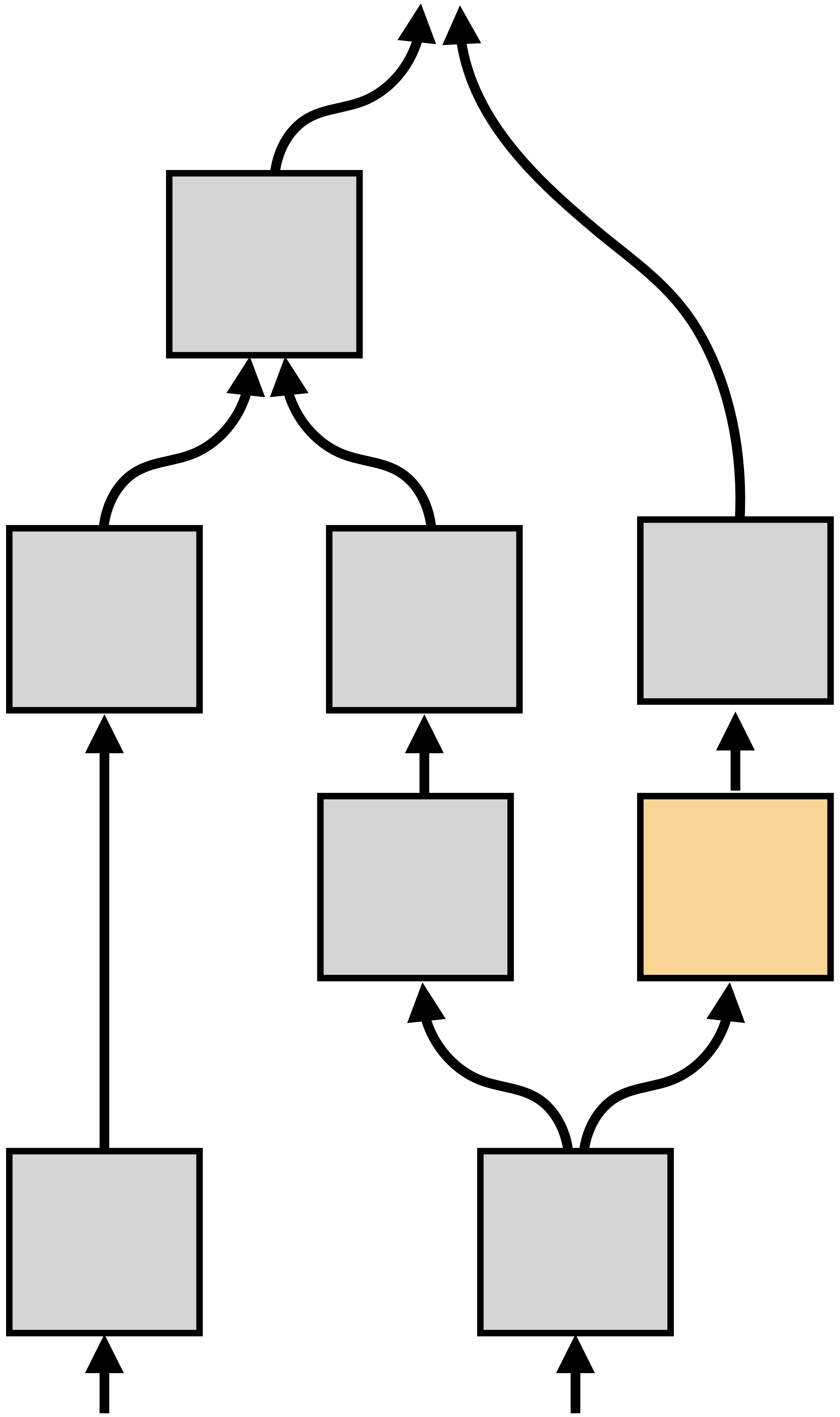
8:02 AM - 4 Jan 2018

65 Retweets **194** Likes

Differentiable programming



[Figure from "Neural Module Networks", Andreas et al. 2017]

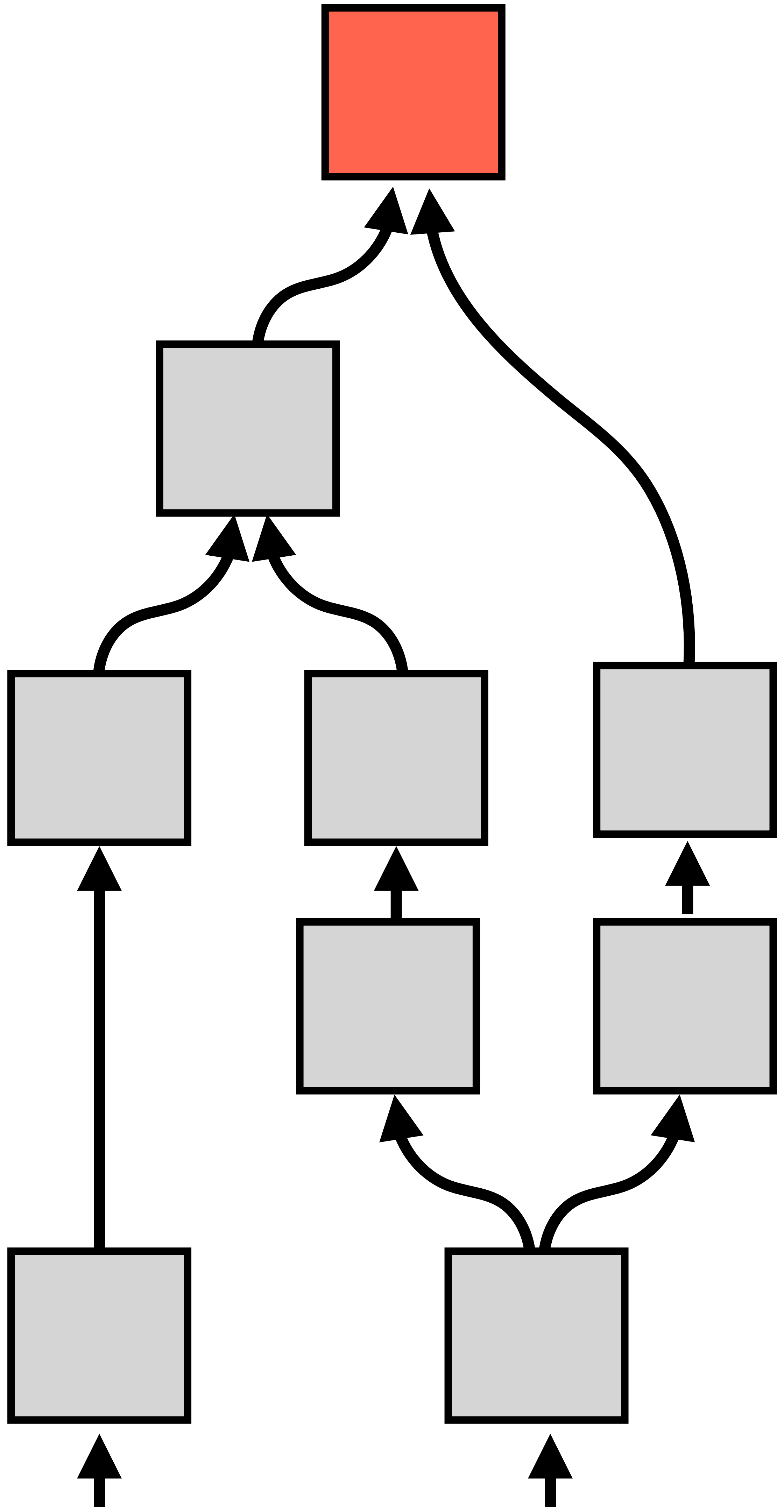


Programmed by a human

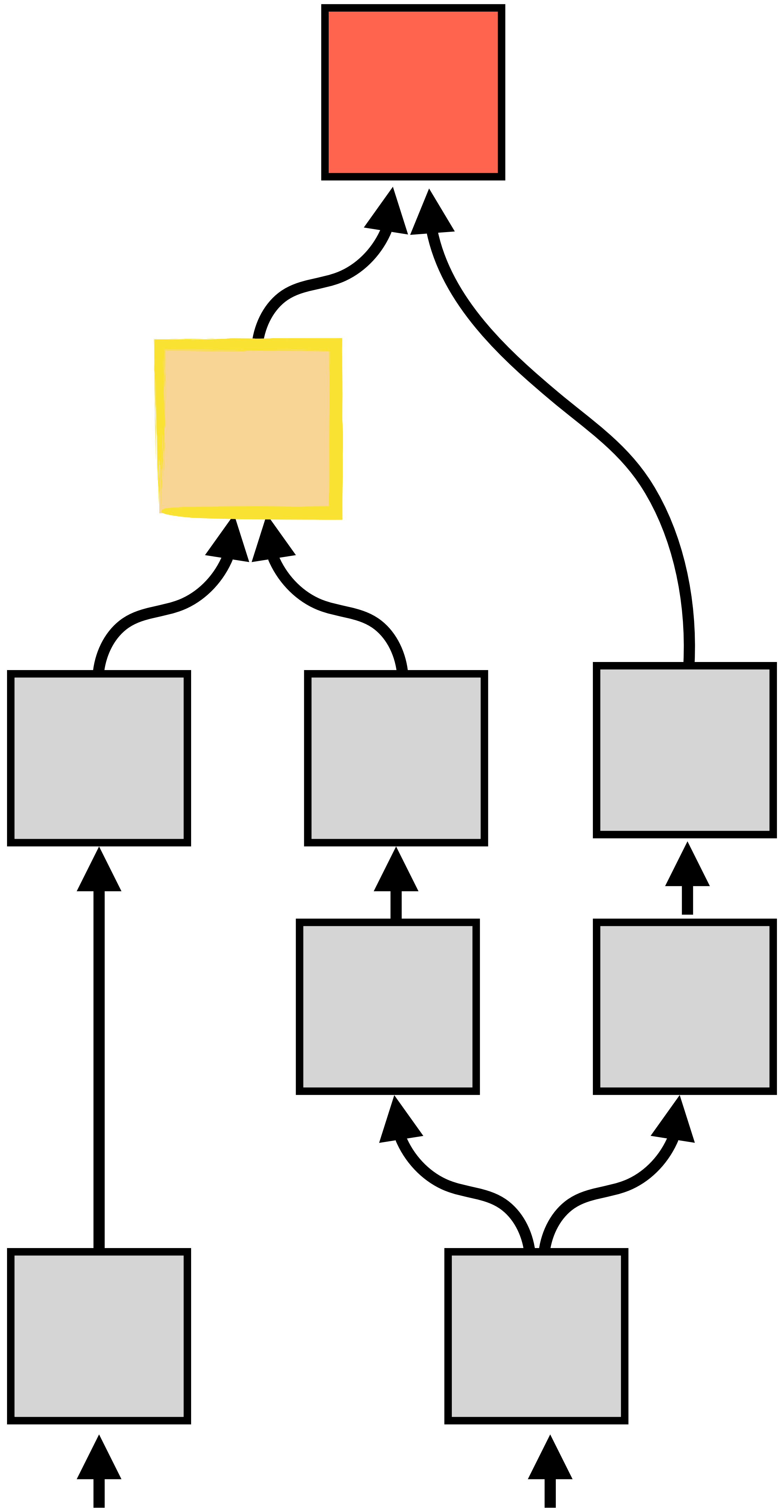
Programmed by backprop

e.g., programmed by tuning behavior to match training examples

Backprop lets you optimize any node (function) or edge (variable) in your computation graph w.r.t. to any scalar cost



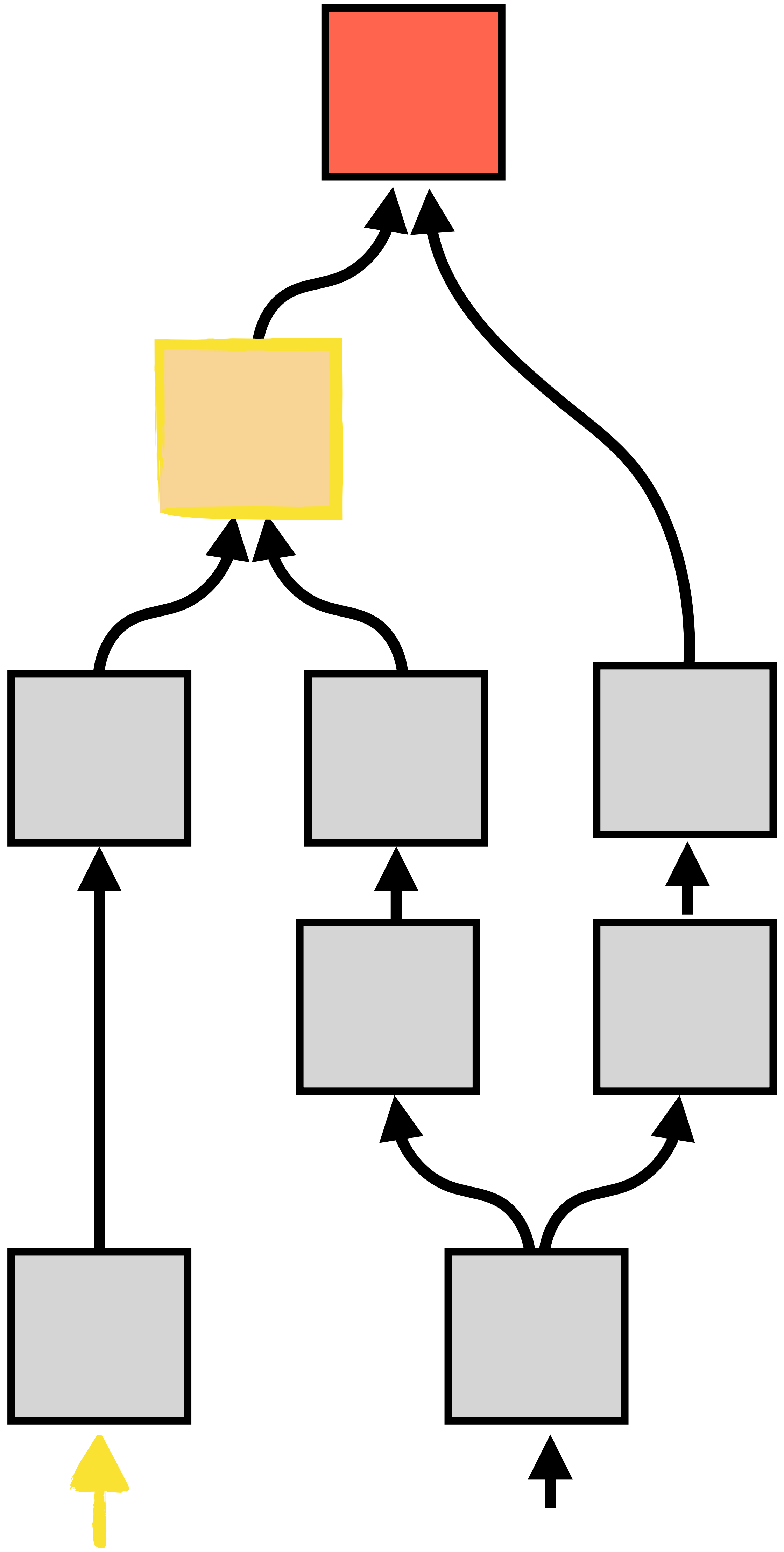
Backprop lets you optimize any node (function) or edge (variable) in your computation graph w.r.t. to any scalar cost



$$\frac{\partial\,\text{🟥}}{\partial\,\text{🟧}}$$

How the loss changes when the functional node highlighted changes

Backprop lets you optimize any node (function) or edge (variable) in your computation graph w.r.t. to any scalar cost



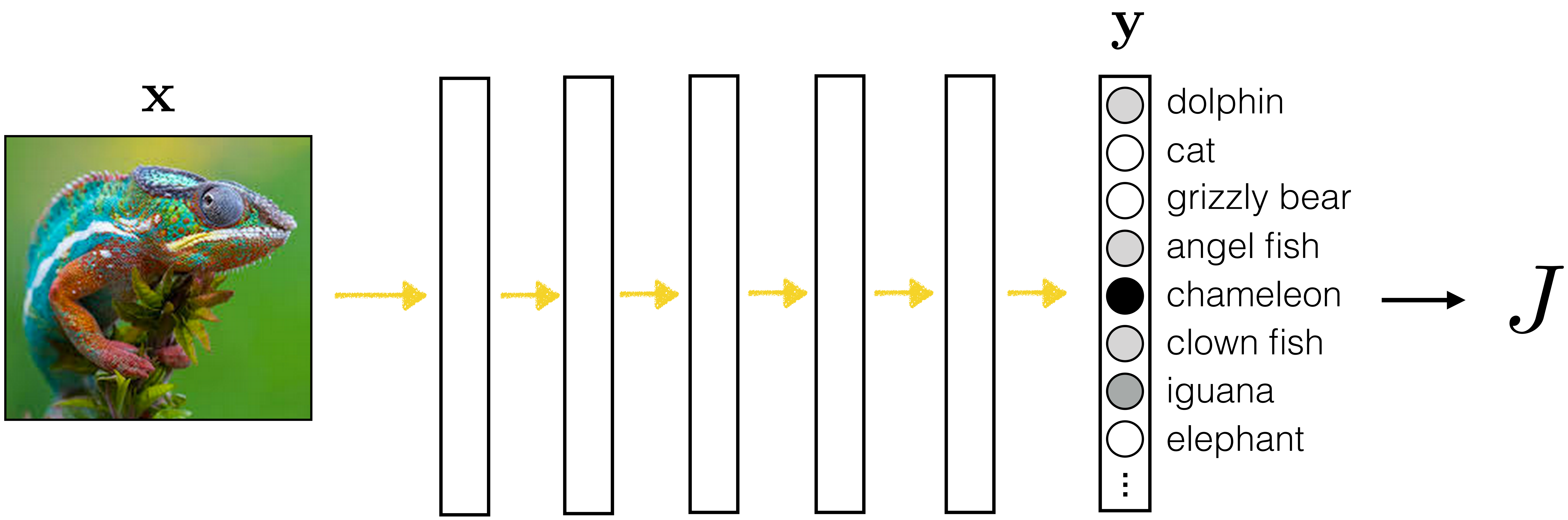
$$\frac{\partial\, 🟥}{\partial\, 🟨}$$

How the loss changes when the functional node highlighted changes

$$\frac{\partial\, 🟥}{\partial\, \uparrow}$$

How the cost changes when the input data changes

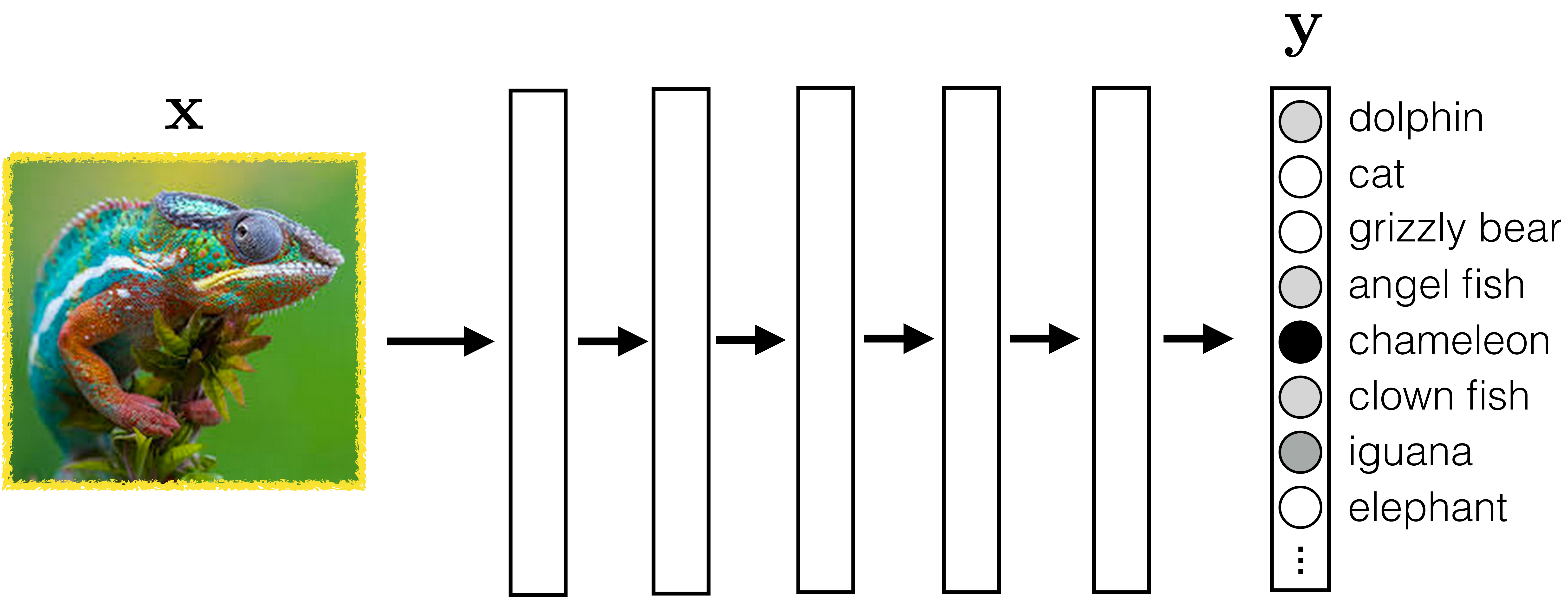
Optimizing parameters versus optimizing inputs



$$\frac{\partial J}{\partial \theta} \leftarrow$$

How much the total cost is increased or decreased by changing the parameters.

Optimizing parameters versus optimizing inputs



$\mathbf{x}$

$\mathbf{y}$

dolphin
cat
grizzly bear
angel fish
chameleon
clown fish
iguana
elephant
⋮

$$\frac{\partial y_j}{\partial \mathbf{x}} \leftarrow$$

How much the “chameleon” score is increased or decreased by changing the image pixels.

Unit visualization via backprop

$$\arg\max_{\mathbf{x}} y_j$$

$$\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k + \eta \frac{\partial y_j(\mathbf{x})}{\partial \mathbf{x}}\bigg|_{\mathbf{x}=\mathbf{x}^k}$$

Unit visualization

$$\arg\max_{\mathbf{x}} y_j + \lambda R(\mathbf{x})$$

$$\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k + \eta \frac{\partial(y_j(\mathbf{x}) + \lambda R(\mathbf{x}))}{\partial \mathbf{x}}\Bigg|_{\mathbf{x}=\mathbf{x}^k}$$

Make an image that maximizes the “cat” output neuron:

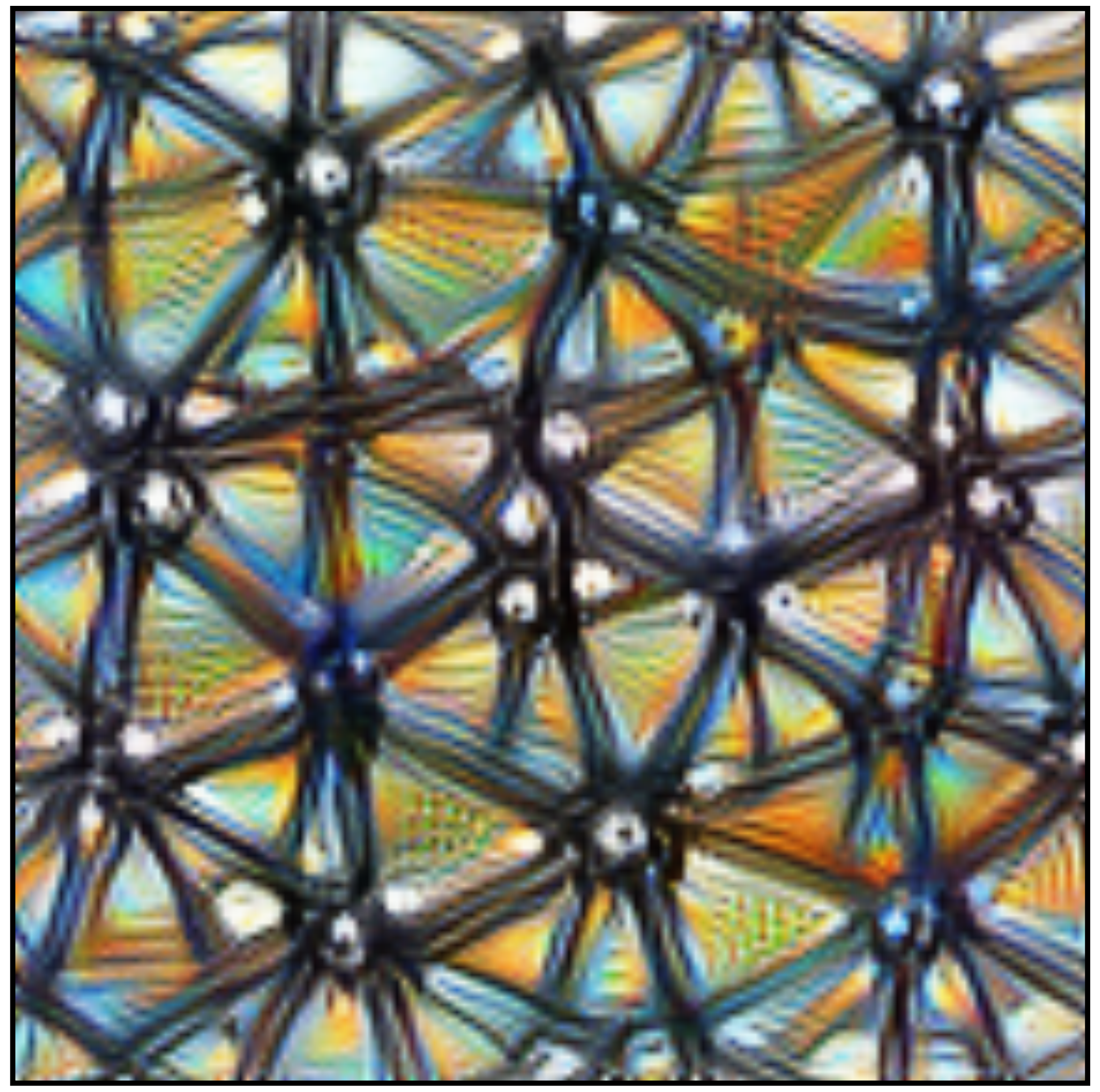
[https://distill.pub/2017/feature-visualization/]

Unit visualization

$$\arg\max_{\mathbf{x}} h_{l_j} + \lambda R(\mathbf{x})$$

$$\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k + \eta \frac{\partial(h_{l_j}(\mathbf{x}) + \lambda R(\mathbf{x}))}{\partial \mathbf{x}} \Bigg|_{\mathbf{x}=\mathbf{x}^k}$$

Make an image that maximizes the value of neuron j on layer l of the network:

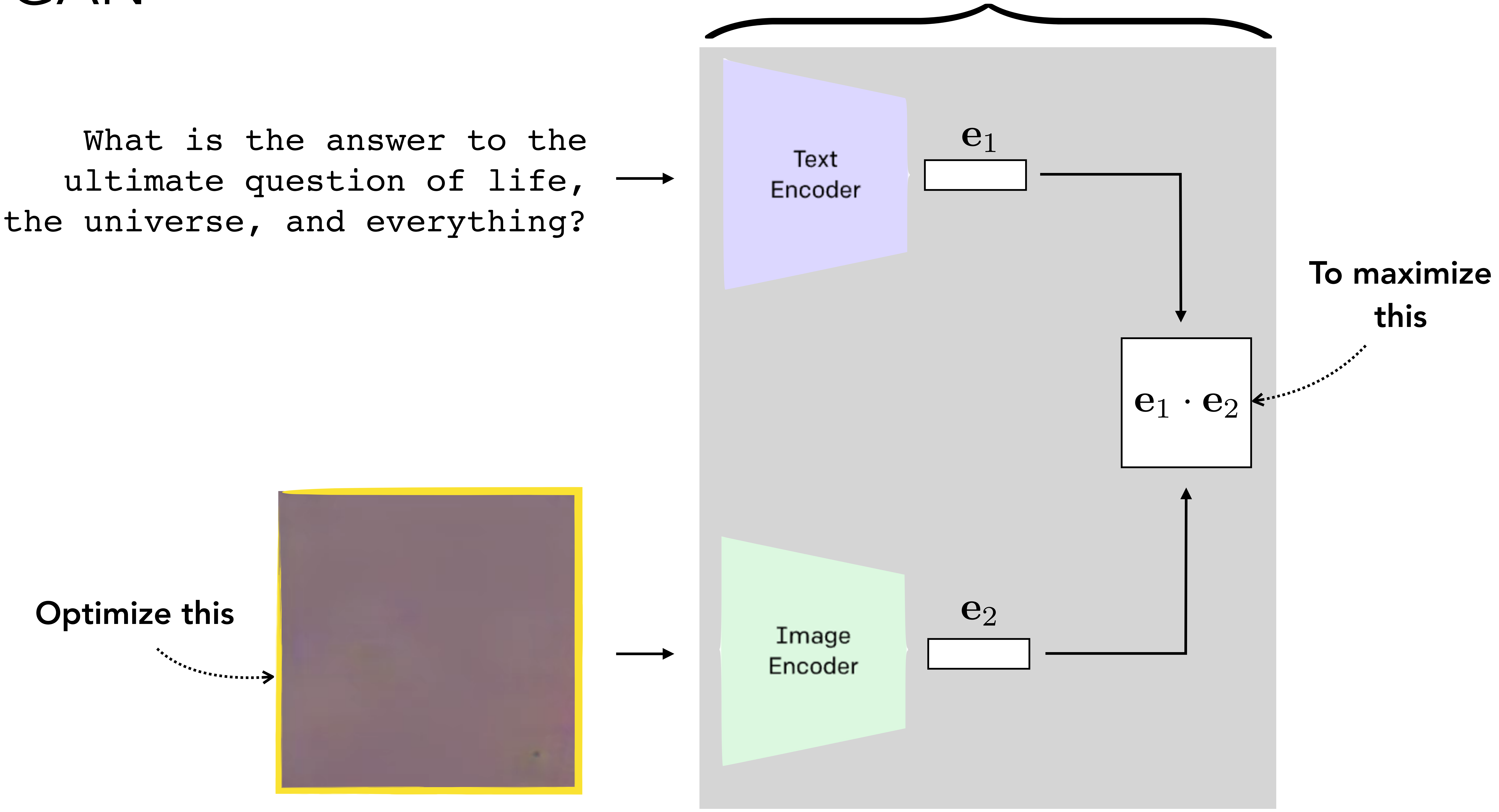


[https://distill.pub/2017/feature-visualization/]

“Deep dream” [https://ai.googleblog.com/2015/06/inceptionism-going-deeper-into-neural.html]

CLIP+GAN

Differentiable program that measures the similarity between text and images



`What is the answer to the ultimate question of life, the universe, and everything?`

Text Encoder

$\mathbf{e}_1$

Image Encoder

$\mathbf{e}_2$

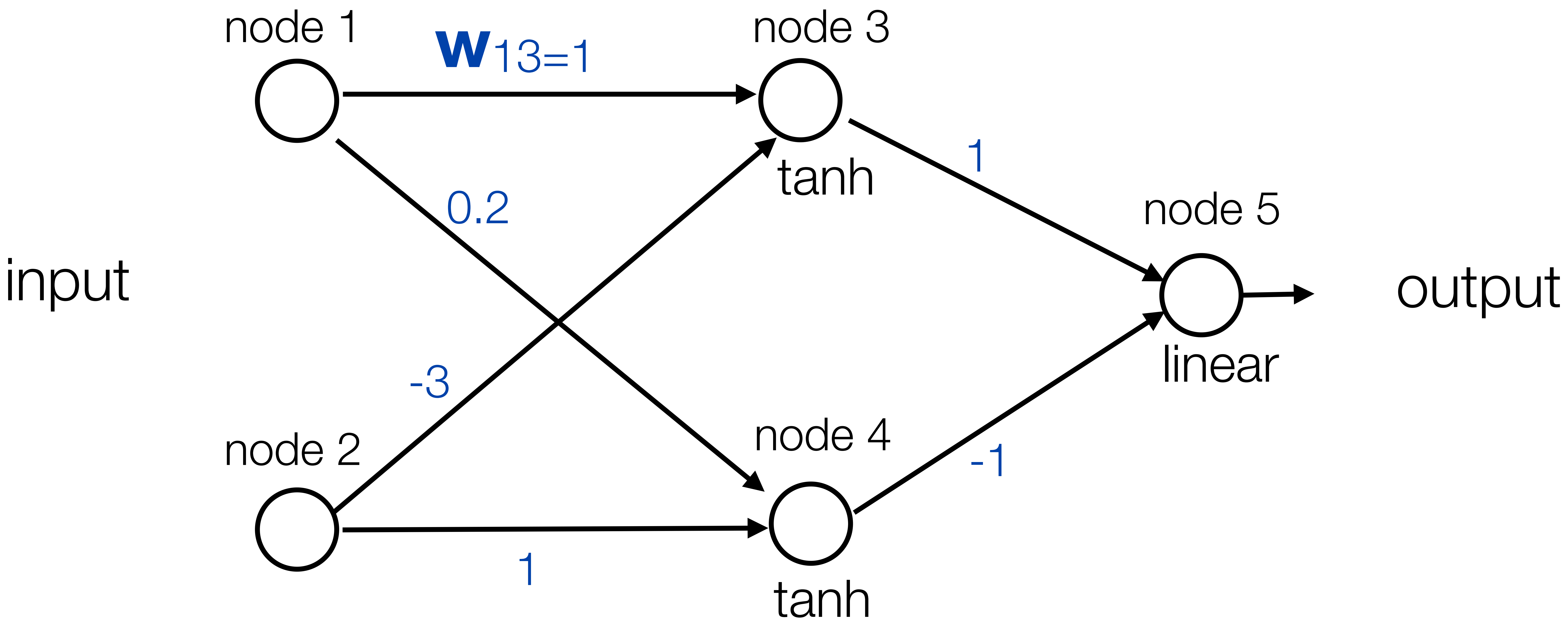
$\mathbf{e}_1 \cdot \mathbf{e}_2$

To maximize this

Optimize this

Code: https://colab.research.google.com/drive/1_4PQqzM_0KKytCzWtn-ZPi4cCa5bwK2F?usp=sharing

Backpropagation example



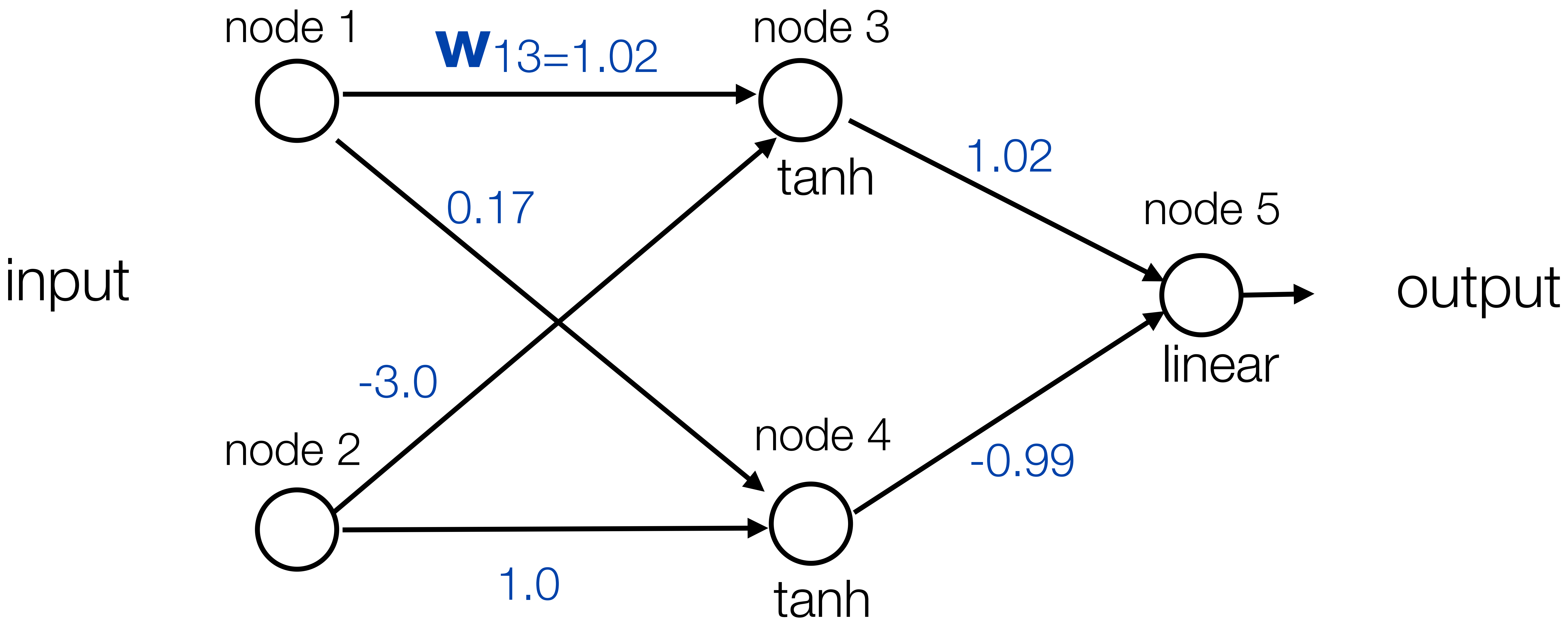
Learning rate η = -0.2 (because we used positive increments)

Euclidean loss

Training data:	input		desired output
	node 1	node 2	node 5
	1.0	0.1	0.5

Exercise: run one iteration of back propagation

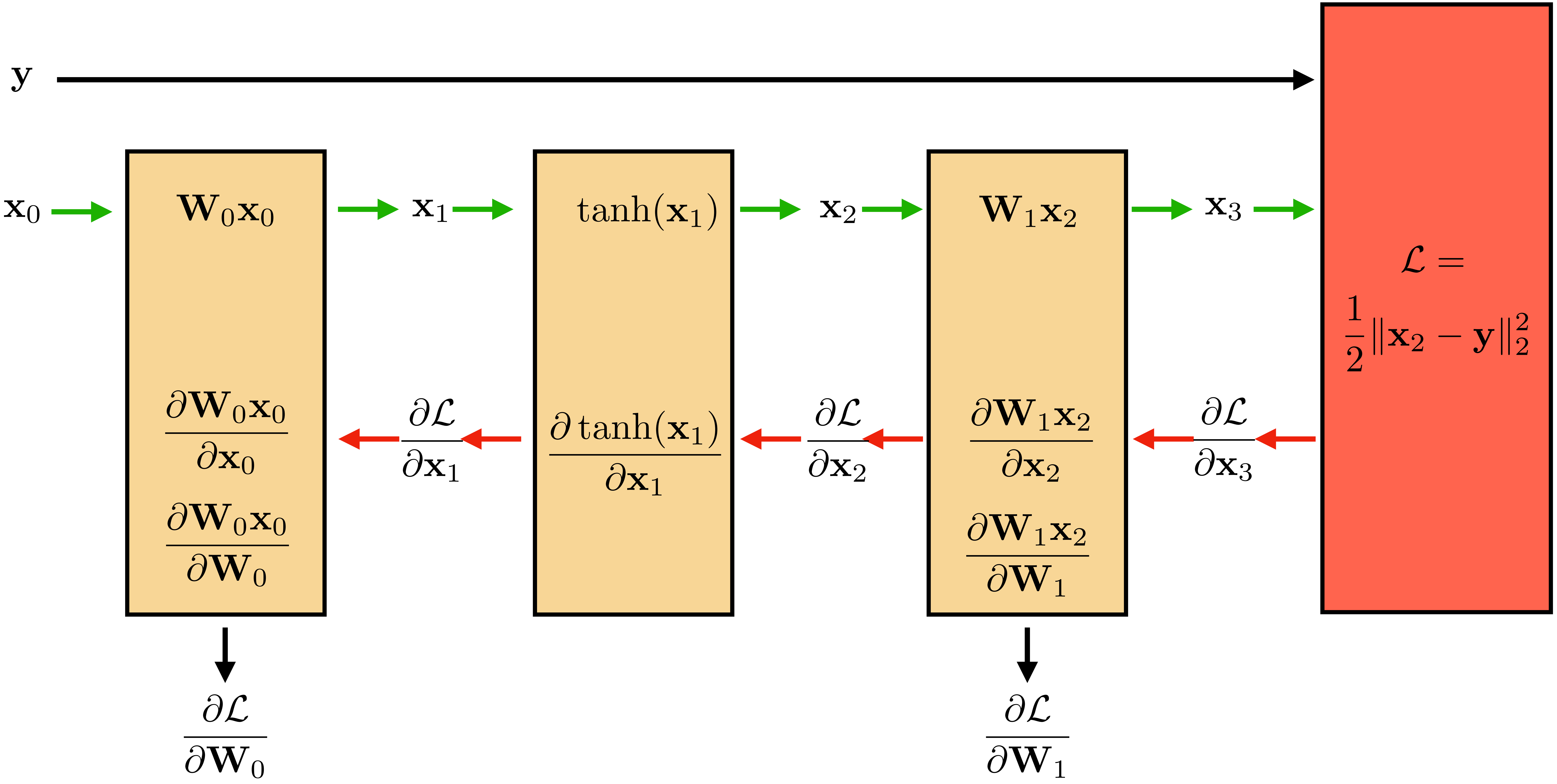
Backpropagation example



After one iteration (rounding to two digits)

Step by step solution

First, let’s rewrite the network using the modular block notation:



$\mathbf{y}$

$\mathbf{x}_0$

$\mathbf{W}_0\mathbf{x}_0$

$\dfrac{\partial \mathbf{W}_0\mathbf{x}_0}{\partial \mathbf{x}_0}$

$\dfrac{\partial \mathbf{W}_0\mathbf{x}_0}{\partial \mathbf{W}_0}$

$\dfrac{\partial \mathcal{L}}{\partial \mathbf{W}_0}$

$\mathbf{x}_1$

$\dfrac{\partial \mathcal{L}}{\partial \mathbf{x}_1}$

$\tanh(\mathbf{x}_1)$

$\dfrac{\partial \tanh(\mathbf{x}_1)}{\partial \mathbf{x}_1}$

$\mathbf{x}_2$

$\dfrac{\partial \mathcal{L}}{\partial \mathbf{x}_2}$

$\mathbf{W}_1\mathbf{x}_2$

$\dfrac{\partial \mathbf{W}_1\mathbf{x}_2}{\partial \mathbf{x}_2}$

$\dfrac{\partial \mathbf{W}_1\mathbf{x}_2}{\partial \mathbf{W}_1}$

$\dfrac{\partial \mathcal{L}}{\partial \mathbf{W}_1}$

$\mathbf{x}_3$

$\dfrac{\partial \mathcal{L}}{\partial \mathbf{x}_3}$

$\mathcal{L} =$

$\frac{1}{2}\|\mathbf{x}_2 - \mathbf{y}\|_2^2$

We need to compute all these terms simply so we can find the weight updates at the bottom.

Our goal is to perform the following two updates:

$$\mathbf{W}_0^{k+1} = \mathbf{W}_0^k + \eta \left(\frac{\partial \mathcal{L}}{\partial \mathbf{W}_0} \right)^T$$

$$\mathbf{W}_1^{k+1} = \mathbf{W}_1^k + \eta \left(\frac{\partial \mathcal{L}}{\partial \mathbf{W}_1} \right)^T$$

where W^k are the weights at some iteration k of gradient descent given by the first slide:

$$\mathbf{W}_0^k = \begin{pmatrix} 1 & -3 \\ 0.2 & 1 \end{pmatrix} \qquad \mathbf{W}_1^k = \begin{pmatrix} 1 & -1 \end{pmatrix}$$

First we compute the derivative of the loss with respect to the output:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_3}} = \mathbf{x}_3 - \mathbf{y}$$

Now, by the chain rule, we can derive equations, working *backwards*, for each remaining term we need:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_2}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_3} \frac{\partial \mathbf{x}_3}{\partial \mathbf{x}_2} = \boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_3}} \mathbf{W}_1$$

$$\boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_1}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_2} \frac{\partial \mathbf{x}_2}{\partial \mathbf{x}_1} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_2} \frac{\partial \tanh(\mathbf{x}_1)}{\partial \mathbf{x}_1} = \boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_2}} (1 - \tanh^2(\mathbf{x}_1))$$

ending up with our two gradients needed for the weight update:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_0} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_1} \frac{\partial \mathbf{x}_1}{\partial \mathbf{W}_0} = \mathbf{x}_0 \boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_1}}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_1} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_3} \frac{\partial \mathbf{x}_3}{\partial \mathbf{W}_1} = \mathbf{x}_2 \boxed{\frac{\partial \mathcal{L}}{\partial \mathbf{x}_3}}$$

Notice the ordering of the two terms being multiplied here. The notation hides the details but you can write out all the indices to see that this is the correct ordering — or just check that the dimensions work out.

The values for input vector x_0 and target y are also given by the first slide:

$$\mathbf{x}_0 = \begin{pmatrix} 1.0 \\ 0.1 \end{pmatrix} \qquad \mathbf{y} = 0.5$$

Finally, we simply plug these values into our equations and compute the numerical updates:

Forward pass:

$$\mathbf{x}_1 = \mathbf{W}_0 \mathbf{x}_0 = \begin{pmatrix} 1 & -3 \\ 0.2 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0.1 \end{pmatrix} = \begin{pmatrix} 0.7 \\ 0.3 \end{pmatrix}$$

$$\mathbf{x}_2 = \tanh(\mathbf{x}_1) = \begin{pmatrix} 0.604 \\ 0.291 \end{pmatrix}$$

$$\mathbf{x}_3 = \mathbf{W}_1 \mathbf{x}_2 = \begin{pmatrix} 1 & -1 \end{pmatrix} \begin{pmatrix} 0.604 \\ 0.291 \end{pmatrix} = 0.313$$

$$\mathcal{L} = \frac{1}{2}(\mathbf{x}_3 - \mathbf{y})^2 = 0.017$$

Backward pass:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_3} = \mathbf{x}_3 - \mathbf{y} = -0.1869$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_2} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_3} \mathbf{W}_1 = -0.1869 \begin{pmatrix} 1 & -1 \end{pmatrix} = \begin{pmatrix} -0.1869 & 0.1869 \end{pmatrix}$$

diagonal matrix because tanh is a pointwise operation

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}_1} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}_2} (1 - \tanh^2(\mathbf{x}_1)) = \begin{pmatrix} -0.1869 & 0.1869 \end{pmatrix} \begin{pmatrix} 1 - \tanh^2(0.7) & 0 \\ 0 & 1 - \tanh^2(0.3) \end{pmatrix} = \begin{pmatrix} -0.1186 & 0.171 \end{pmatrix}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_0} = \mathbf{x}_0 \frac{\partial \mathcal{L}}{\partial \mathbf{x}_1} = \begin{pmatrix} 1.0 \\ 0.1 \end{pmatrix} \begin{pmatrix} -0.1186 & 0.171 \end{pmatrix} = \begin{pmatrix} -0.1186 & 0.171 \\ -0.01186 & 0.0171 \end{pmatrix}$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}_1} = \mathbf{x}_2 \frac{\partial \mathcal{L}}{\partial \mathbf{x}_3} = \begin{pmatrix} 0.604 \\ 0.291 \end{pmatrix} \begin{pmatrix} -0.1186 \end{pmatrix} = \begin{pmatrix} -0.113 \\ -0.054 \end{pmatrix}$$

Gradient updates:

$$\begin{aligned}\mathbf{W}_0^{k+1} &= \mathbf{W}_0^k + \eta\left(\frac{\partial\mathcal{L}}{\partial\mathbf{W}_0}\right)^T\\ &= \begin{pmatrix}1 & -3\\ 0.2 & 1\end{pmatrix} - 0.2\begin{pmatrix}-0.1186 & 0.171\\ -0.01186 & 0.0171\end{pmatrix}\\ &= \begin{pmatrix}1.02 & -3.0\\ 0.17 & 1.0\end{pmatrix}\end{aligned}$$

$$\begin{aligned}\mathbf{W}_1^{k+1} &= \mathbf{W}_1^k + \eta\left(\frac{\partial\mathcal{L}}{\partial\mathbf{W}_1}\right)^T\\ &= \begin{pmatrix}1 & -1\end{pmatrix} - 0.2\begin{pmatrix}-0.113 & -0.054\end{pmatrix}\\ &= \begin{pmatrix}1.02 & -0.989\end{pmatrix}\end{aligned}$$