Training FeedForward Networks

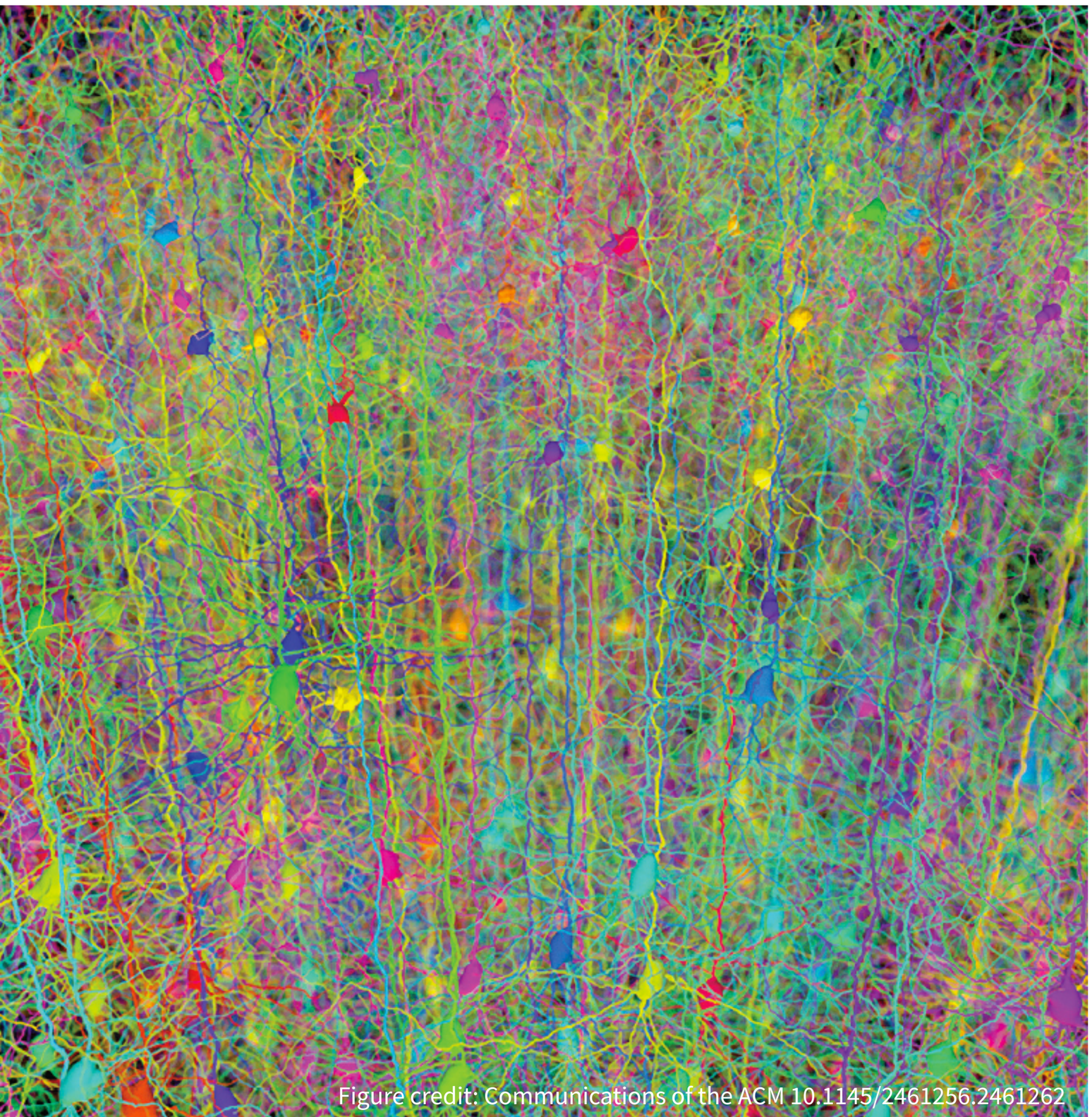

Figure credit: Communications of the ACM 10.1145/2461256.2461262

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Empirical Risk Minimization

A framework to design learning algorithms:

$$\tilde{J}(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) = J(\boldsymbol{\theta}; \boldsymbol{X}, \boldsymbol{y}) + \alpha\Omega(\boldsymbol{\theta})$$

regularized objective objective function regularizer (penalizes certain values of $\boldsymbol{\theta}$)

Learning cast as optimization:

$$\arg\min_{\boldsymbol{\theta}} \frac{1}{m} \sum_{i=1}^{m} L\left(f\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right), y^{(i)}\right) + \alpha\Omega(\boldsymbol{\theta})$$

Note: loss function is typically
a surrogate for what we truly should optimize

Stochastic Gradient Descent

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An algorithm that performs parameter updates after each example:

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- initialize: $\boldsymbol{\theta}$ $\left(\boldsymbol{\theta} \equiv \{\boldsymbol{W}^{(1)}, \boldsymbol{b}^{(1)}, \ldots, \boldsymbol{W}^{(l)}, \boldsymbol{b}^{(l)}\}\right)$
- while stopping criterion not met, do:
  - for each minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with targets $y^{(i)}$
    - Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L\left(f\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right), y^{(i)}\right) + \alpha \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$
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To apply this algorithm to neural network training, we need:

- the loss function $L\left(f\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right), y^{(i)}\right)$
- a procedure to compute parameter gradients $\nabla_{\boldsymbol{\theta}} L\left(f\left(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}\right), y^{(i)}\right)$
- the regularizer $\Omega(\boldsymbol{\theta})$ (and the gradient $\nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$)
- an initialization method

Loss Function

Regression (Mean-squared error):

$$L_{MSE} = \frac{1}{2}\left(f(\boldsymbol{x}) - y\right)^2$$

Classification:

- Let neural network estimate $f(\boldsymbol{x})_c = p(y = c|\boldsymbol{x})$
  - We could maximize the probabilities of $y^{(i)}$ given $x^{(i)}$ in the training set
- To frame as minimization, minimize the negative log-likelihood

$$L_{CE} = -\sum_c 1_{(y=c)} \log f(\boldsymbol{x})_c = -\log f(\mathbf{x})_y$$

"cross-entropy"

  - take the log to simplify numerical stability and mathematical simplicity

Forward and Back-propagation

- The process of propagating $\boldsymbol{x}$ through a feedforward neural network to produce an output $\hat{\boldsymbol{y}}$ is called forward propagation

- During training, forward propagation continues to produce a scalar cost $J(\boldsymbol{\theta})$

- The back-propagation algorithm (backprop) allows the cost to flow backward through the net to compute the gradient

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- Another algorithm, such as stochastic gradient descent (SGD) is used to perform learning, using this gradient

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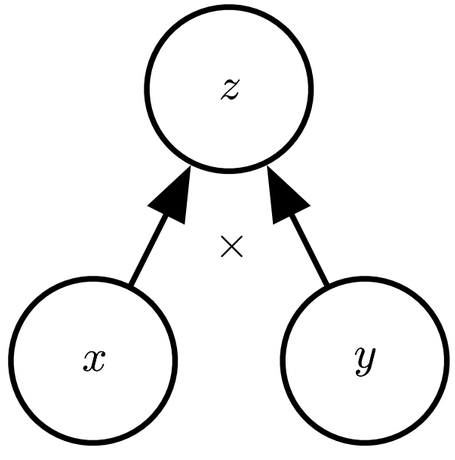
Terminology: backprop computes gradient $\nabla_{\boldsymbol{x}} f(\boldsymbol{x}, \boldsymbol{y})$

- for an arbitrary function f
- where $\boldsymbol{x}$ is a set of variables whose derivatives are desired
- and $\boldsymbol{y}$ are inputs to the function whose derivatives are not desired

Operations

- To introduce the computational graph language, we need to introduce the idea of an operation
- An operation is a simple function of one or more variables
- A graph language is accompanied by a set of allowable operations
- More complicated functions are made by composing many operations
- Without loss of generality, we define an operation to return only a single variable (the output can have multiple entries)

Example: Computational Graphs



Reproduced from Goodfellow et al.

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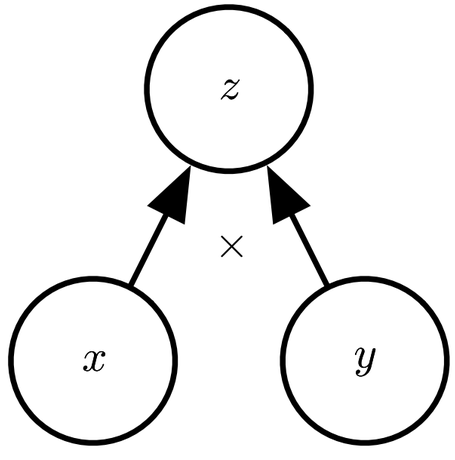

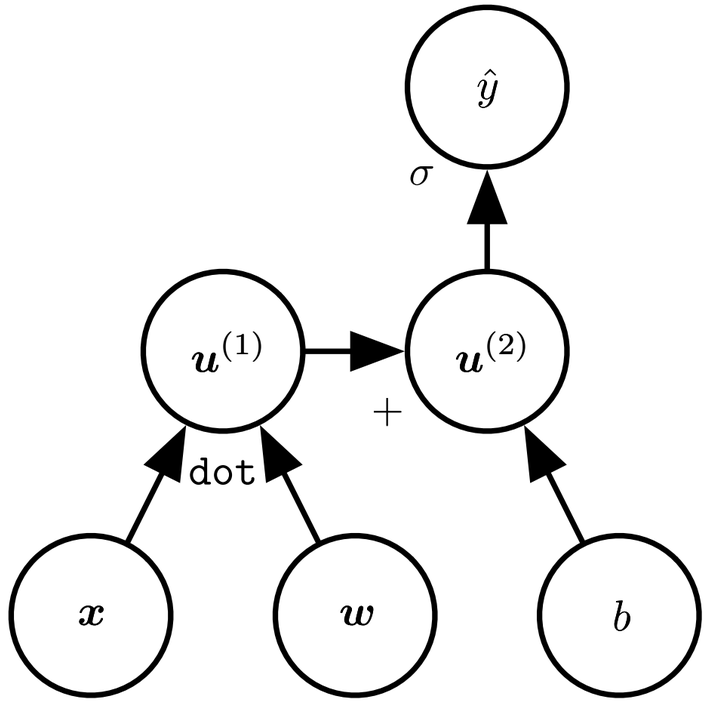

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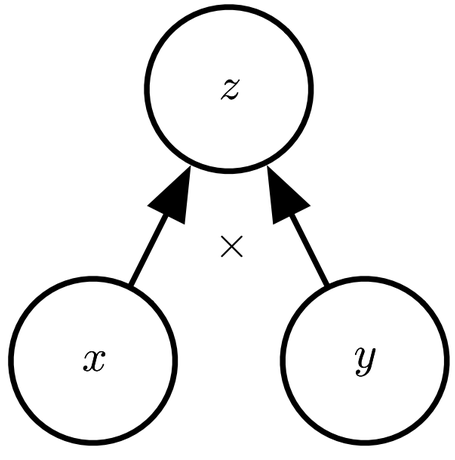

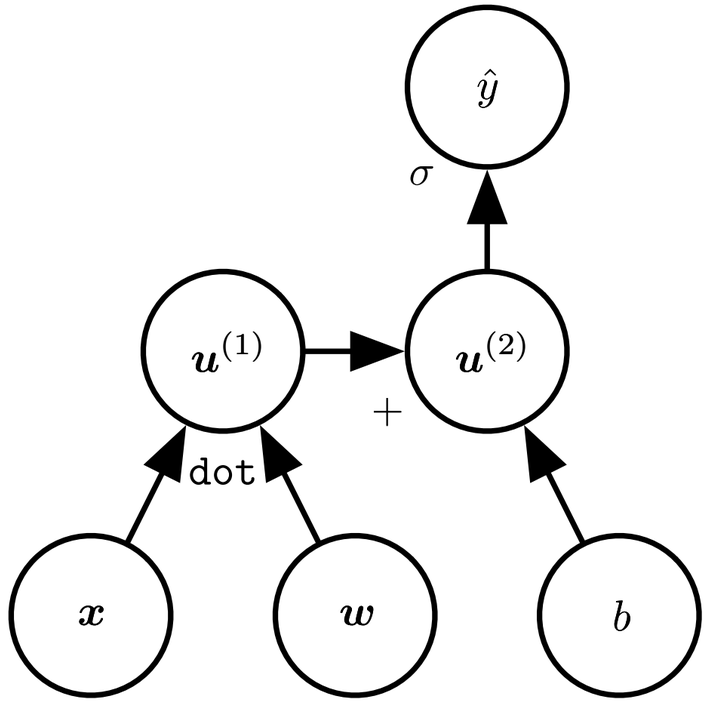

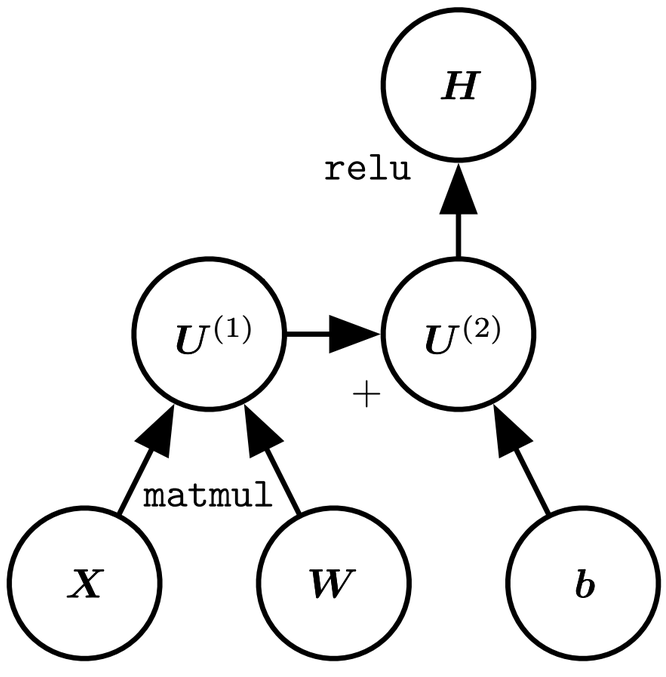

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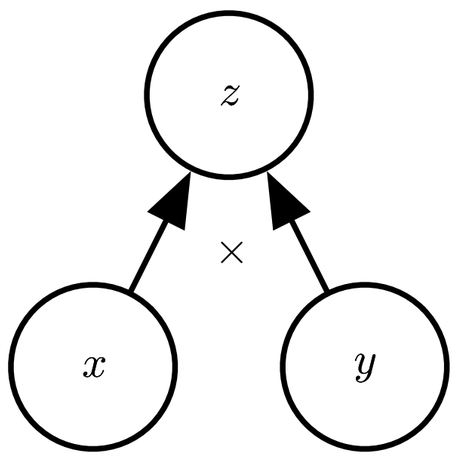

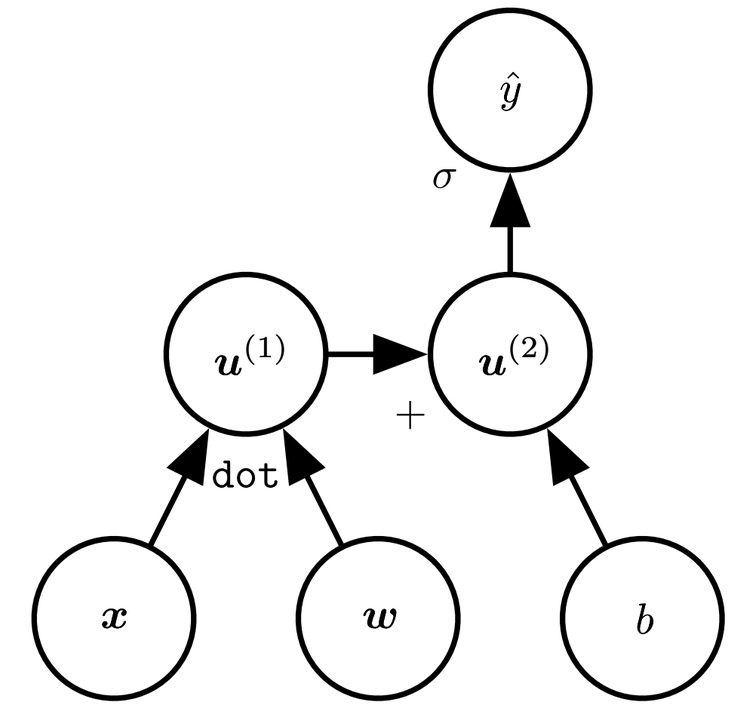

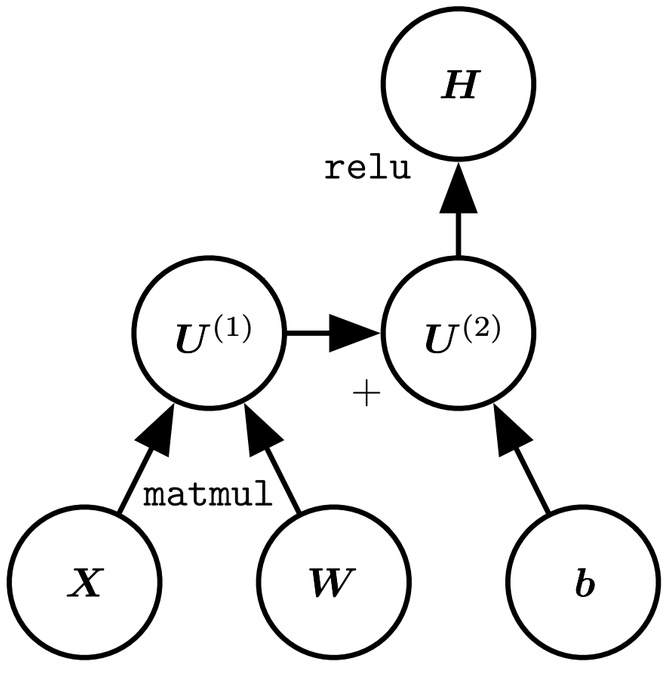

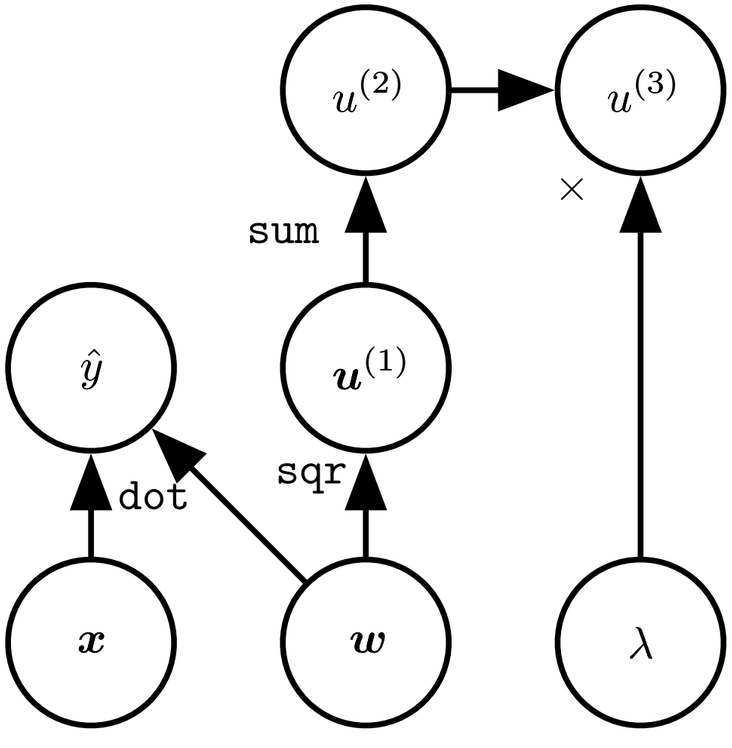

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Chain Rule of Calculus

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Used to compute the derivatives of functions formed by composing other functions whose derivatives are known

- Suppose that $y = g(x)$ and $z = f(g(x)) = f(y)$
- Then the chain rule states that:

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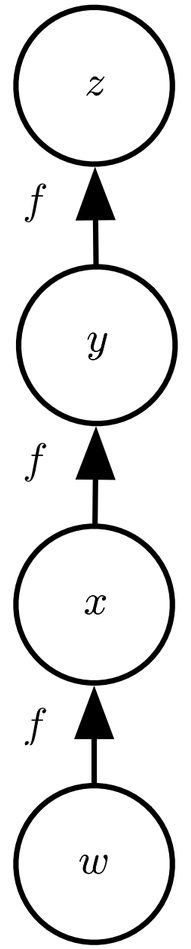
Back-propagation consists of performing one Jacobian-gradient product for each operation in the graph

Back-propagation as Recursive Chain Rule

- Using the chain rule, it is straightforward to write down an expression for the gradient of a scalar w.r.t. any node in the graph

- Actually evaluating that expression involves some extra considerations

- Specifically, many subexpressions may be repeated several times within overall expression for gradient



$$\frac{\partial z}{\partial w} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}\frac{\partial x}{\partial w} = f'(y)f'(x)f'(w) = f'(f(f(w)))f'(f(w))f'(w)$$

Reproduced from Goodfellow et al.

Back-propagation in a Computational Graph

- Consider a computational graph describing how to compute a single scalar $u^{(n)}$ (e.g. the loss on a single example)

- This scalar is the quantity whose gradient we want to obtain, w.r.t. the n_i input nodes, $\{u^{(1)}, \ldots, u^{(n_i)}\}$ (e.g. the parameters of a model)

  - In other words, we wish to compute $\frac{\partial u^{(n)}}{\partial u^{(i)}} \forall i \in \{1, 2, \ldots, n_i\}$

- Assume that the nodes of the graph are ordered in such a way that we can compute their output one after another, starting at $u^{(n_i+1)}$ and going up to $u^{(n)}$

- Each node $u^{(i)}$ is associated with an operation $f^{(i)}$ and is computed by evaluating:

$$u^{(i)} = f^{(i)}(\mathbb{A}^{(i)})$$

set of all nodes that are parents of $u^{(i)}$

- Back-propagation computes each derivative $\frac{\partial u^{(n)}}{\partial u^{(i)}}$ associated with the respective forward graph node $u^{(i)}$, via the chain rule:

$$\frac{\partial u^{(n)}}{\partial u^{(j)}} = \sum_{i:j \in Pa(u^{(i)})} \frac{\partial u^{(n)}}{\partial u^{(i)}} \frac{\partial u^{(i)}}{\partial u^{(j)}}$$

Simplified Forward Pass

(See Algorithm 6.1 in Goodfellow et al.)

Simplified Backward Pass

(See Algorithm 6.2 in Goodfellow et al.)

Forward Propagation in MLP

Example of a 2 hidden layer (or 4 layer) network …

$\boldsymbol{x}$	input
$\boldsymbol{h}^{(1)}$	1st layer hidden units
$\boldsymbol{h}^{(2)}$	2nd layer hidden units
$\hat{\boldsymbol{y}}$	output (prediction)

Forward Propagation (L1)

Forward propagation is the process of computing the output of the network given its input

$$\boldsymbol{x} \in \mathbb{R}^d \qquad \boldsymbol{W}^{(1)} \in \mathbb{R}^{n_1 \times d} \qquad \boldsymbol{b}^{(1)} \in \mathbb{R}^{n_1} \qquad \boldsymbol{h}^{(1)} \in \mathbb{R}^{n_1}$$

$$\boldsymbol{a}^{(1)} = \boldsymbol{b}^{(1)} + \boldsymbol{W}^{(1)}\boldsymbol{x}$$

$$\boldsymbol{h}^{(1)} = g(\boldsymbol{a}^{(1)})$$

$\boldsymbol{W}^{(1)}$ 1st layer weights

$\boldsymbol{b}^{(1)}$ 1st layer biases

$g(\cdot)$ activation function (e.g. ReLU)

Forward Propagation (L2)

$$\boldsymbol{h}^{(1)} \in \mathbb{R}^{n_1} \qquad \boldsymbol{W}^{(2)} \in \mathbb{R}^{n_2 \times n_1} \qquad \boldsymbol{b}^{(2)} \in \mathbb{R}^{n_2} \qquad \boldsymbol{h}^{(2)} \in \mathbb{R}^{n_2}$$

$$\boldsymbol{a}^{(2)} = \boldsymbol{b}^{(2)} + \boldsymbol{W}^{(2)} \boldsymbol{h}^{(1)}$$

$$\boldsymbol{h}^{(2)} = g(\boldsymbol{a}^{(2)})$$

$\boldsymbol{W}^{(2)}$ 2nd layer weights

$\boldsymbol{b}^{(2)}$ 2nd layer biases

Forward Propagation (Out)

$\boldsymbol{h}^{(2)} \in \mathbb{R}^{n_2}$ $\boldsymbol{W}^{(3)} \in \mathbb{R}^{n_3 \times n_2}$ $\boldsymbol{b}^{(3)} \in \mathbb{R}^{n_3}$ $\hat{\boldsymbol{y}} \in \mathbb{R}^{n_3}$

$$\boldsymbol{a}^{(3)} = \boldsymbol{b}^{(3)} + \boldsymbol{W}^{(3)}\boldsymbol{h}^{(2)}$$

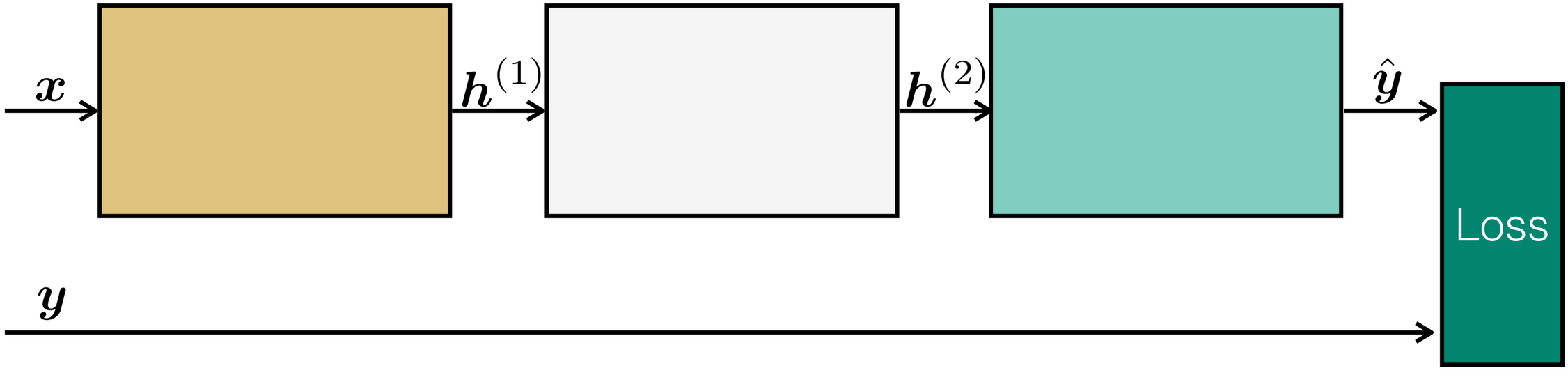
$$\hat{\boldsymbol{y}} = g(\boldsymbol{a}^{(3)})$$

$\boldsymbol{W}^{(3)}$ 3rd layer weights

$\boldsymbol{b}^{(3)}$ 3rd layer biases

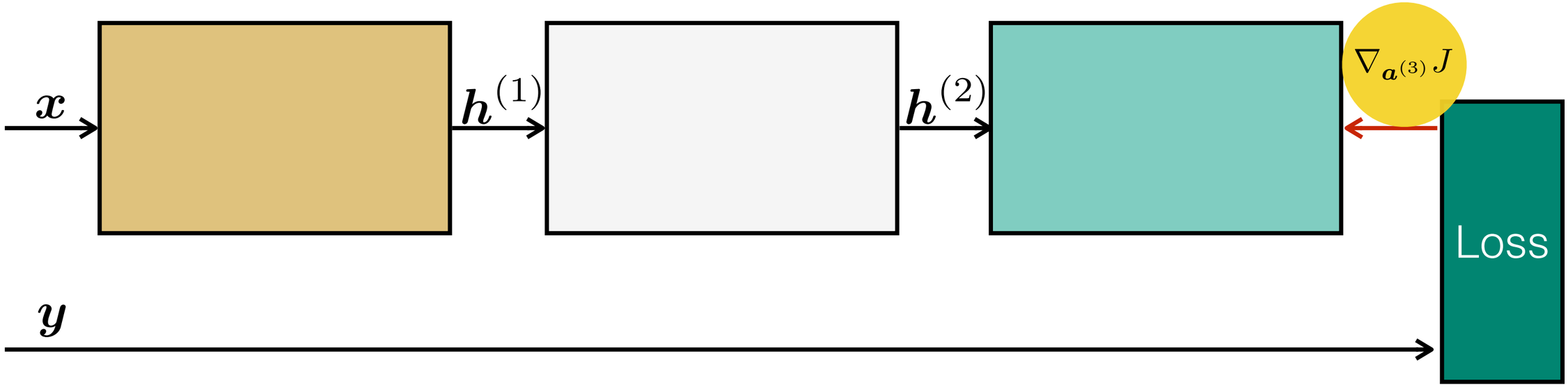
Note: $g(\cdot)$ is usually different at the output layer

How Good is a Network?



y	target (ground truth)
$\theta \equiv \{W^{(1)}, b^{(1)}, \ldots, W^{(l)}, b^{(l)}\}$	parameters
$L(\hat{y}, y)$	loss function
$J = L(\hat{y}, y) + \alpha\Omega(\theta)$	regularized cost

Backward Propagation (Out)



After the forward computation, compute the gradient on the output layer

$$g \leftarrow \nabla_{\hat{y}} J = \nabla_{\hat{y}} L(\hat{y}, y)$$

Then, convert the gradient on the layer's output into a gradient on the pre-activation:

$$g \leftarrow \nabla_{a^{(3)}} J$$

Derivative w.r.t. Input of Softmax

First convert the discrepancy between each output and its target value into an error derivative

$$\hat{y}_k = p(c_k = 1|\boldsymbol{x}) = \frac{e^{a_k}}{\sum_{j=1}^{C} e^{a_j}}$$

Note: layer superscript has been left off for simplicity, i.e. $a_j = (\boldsymbol{a}^{(3)})_j$

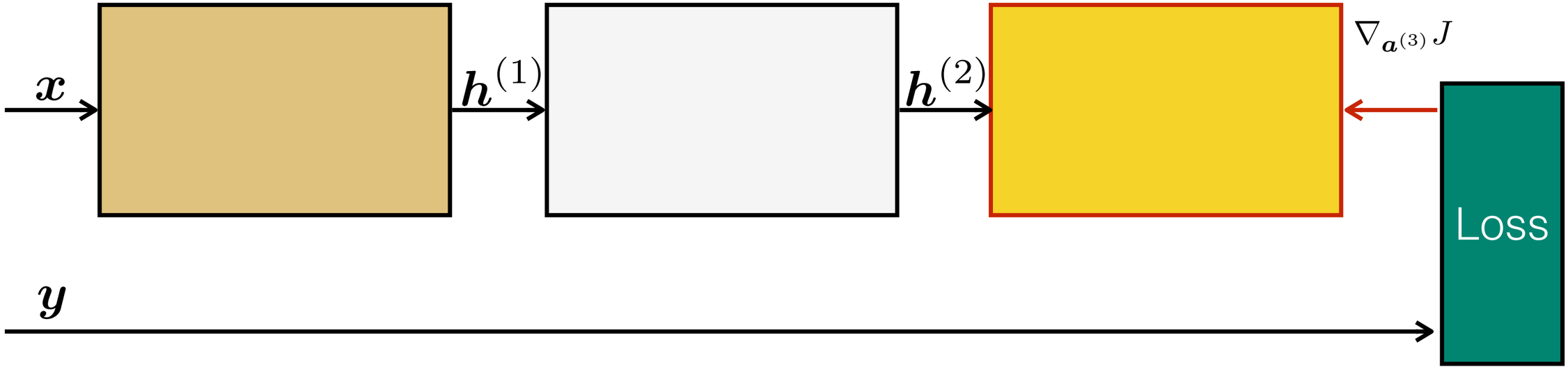
$$L(\hat{\boldsymbol{y}}, \boldsymbol{y}) = -\sum_j y_j \log p(c_j|\boldsymbol{x})$$

$$\boldsymbol{y} = [00 \ldots 010 \ldots 0]$$

By substituting the first formula into the second, and taking the derivative w.r.t. a we get:

$$\frac{\partial L}{\partial a_j} = p(c_j|\boldsymbol{x}) - y_j$$

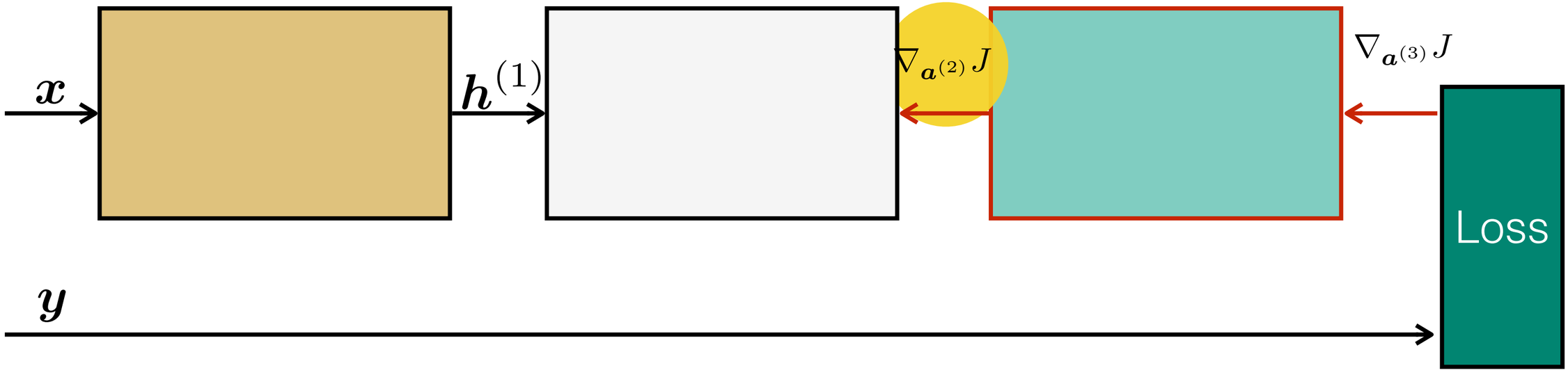
Backward Propagation (Update)



Compute gradients on weights and biases:

$$\nabla_{\boldsymbol{b}^{(3)}} J = \boldsymbol{g} + \alpha \nabla_{\boldsymbol{b}^{(3)}} \Omega(\boldsymbol{\theta}) \qquad \nabla_{\boldsymbol{W}^{(3)}} J = \boldsymbol{g}\, \boldsymbol{h}^{(2)\top} + \alpha \nabla_{\boldsymbol{W}^{(3)}} \Omega(\boldsymbol{\theta})$$

Backward Propagation (L2)



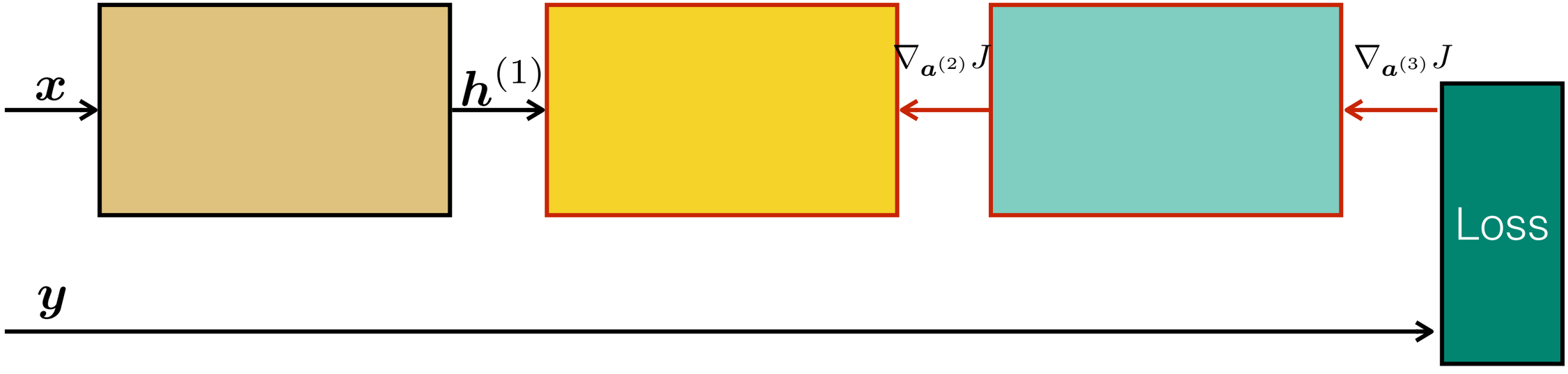
Propagate the gradients w.r.t. the next lower-level hidden layer's activation

$$\boldsymbol{g} \leftarrow \nabla_{\boldsymbol{h}^{(2)}} J = \boldsymbol{W}^{(3)\top} \boldsymbol{g}$$

Then, convert the gradient on the layer's output into a gradient on the pre-activation (element-wise nonlinearity):

$$\boldsymbol{g} \leftarrow \nabla_{\boldsymbol{a}^{(2)}} J = \boldsymbol{g} \odot g'(\boldsymbol{a}^{(2)})$$

Backward Propagation (Update)



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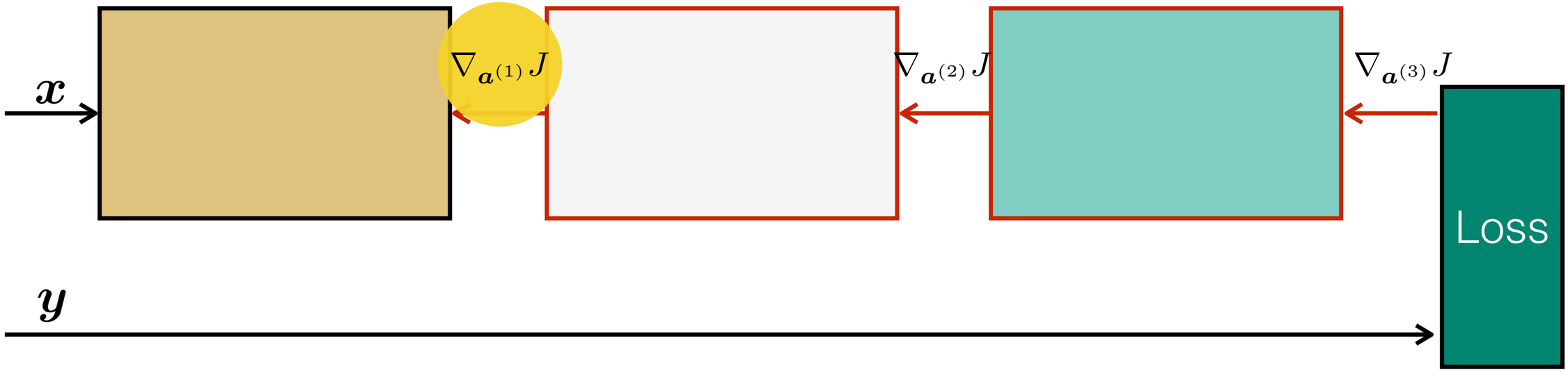
Backward Propagation (L1)



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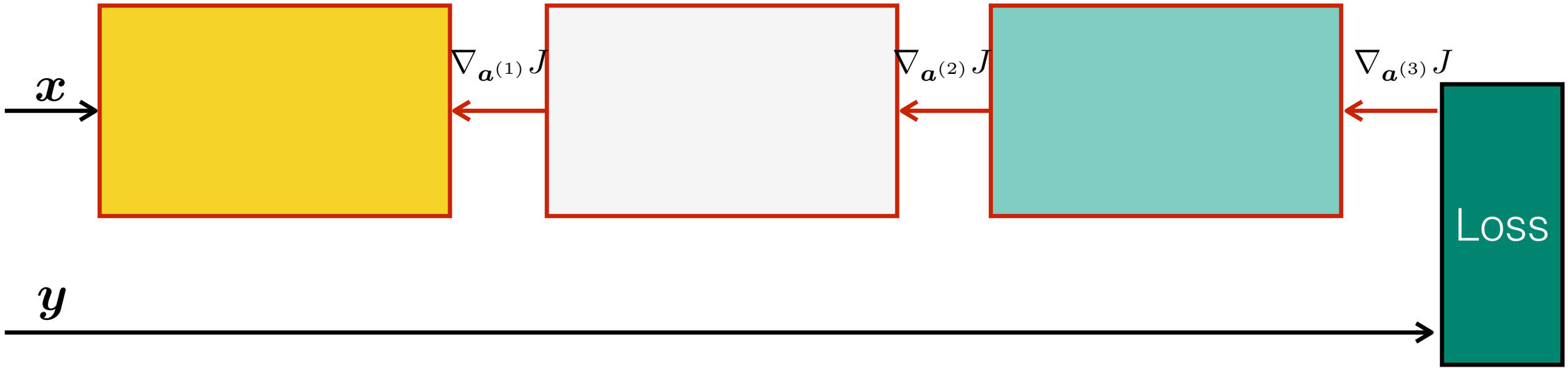

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