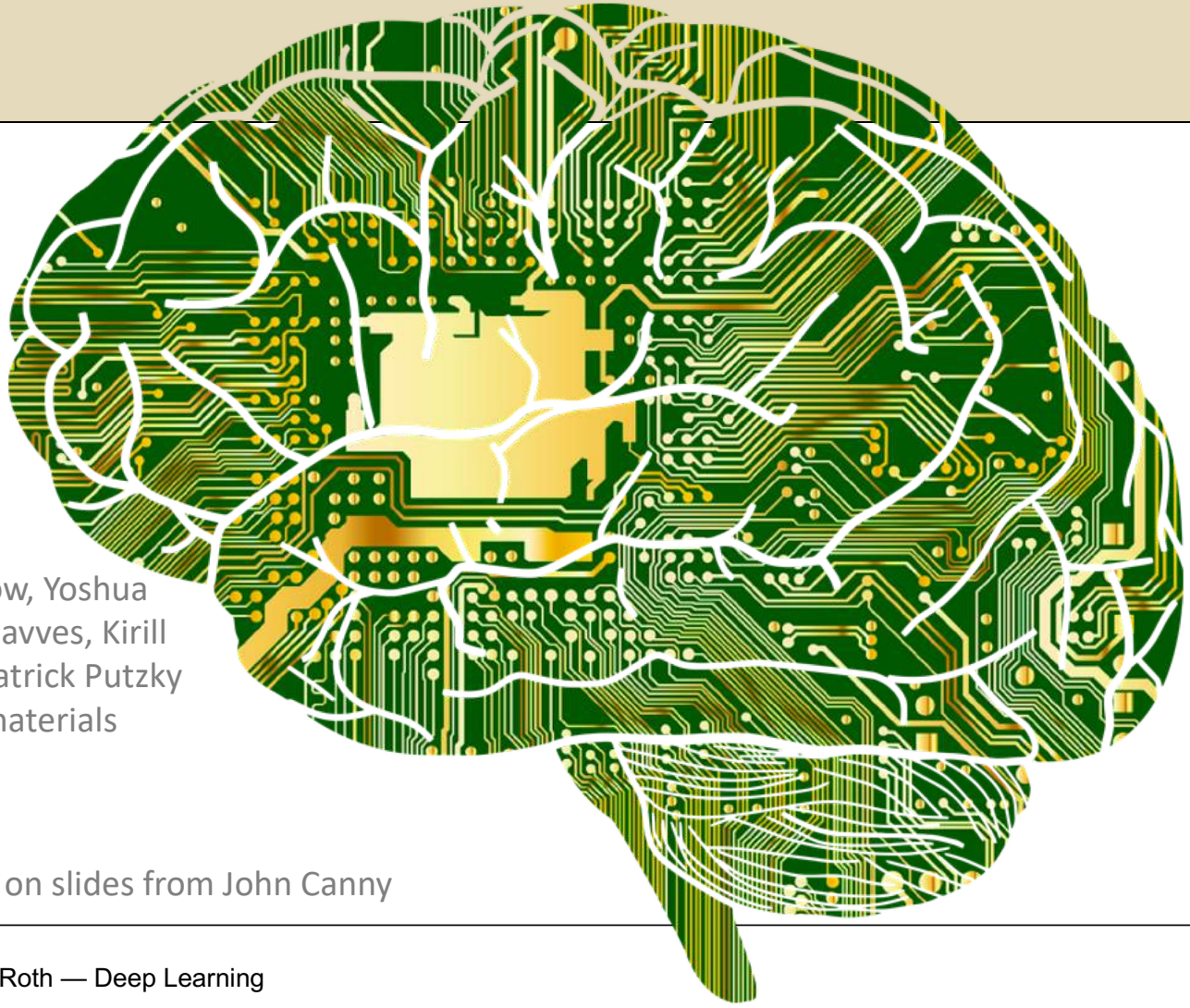
Deep Learning

Architectures and Methods:

Backpropagation



Thanks to John Canny, Ian Goodfellow, Yoshua Bengio, Aaron Courville, Efstratios Gavves, Kirill Gavrilyuk, Berkay Kicanaoglu, and Patrick Putzky and many others for making their materials publically available.

The present slides are mainly based on slides from John Canny

Where we are...

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$$s = f(x; W) = Wx$$ scores function

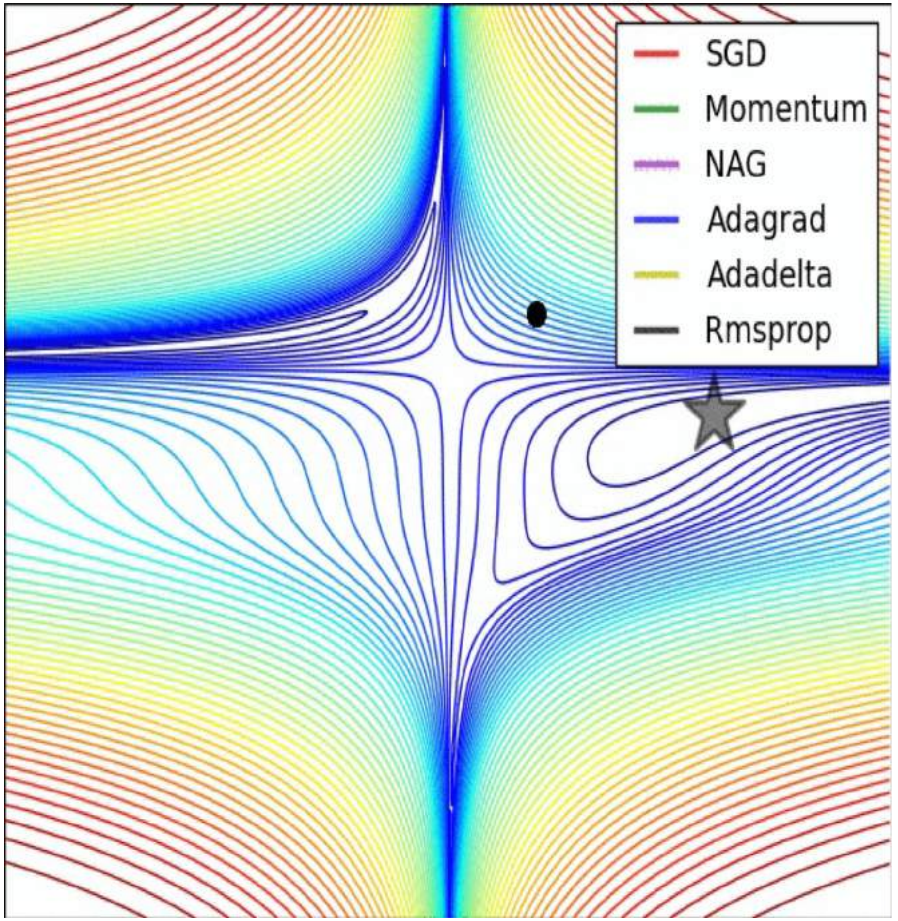
$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$ SVM loss

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \sum_k W_k^2$$ data loss + regularization

Compute gradients and steps to progressively improve the model via SGD and its variants.

i.e. want $\nabla_W L$

Optimization




```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```

(image credits to Alec Radford)

Gradient Descent

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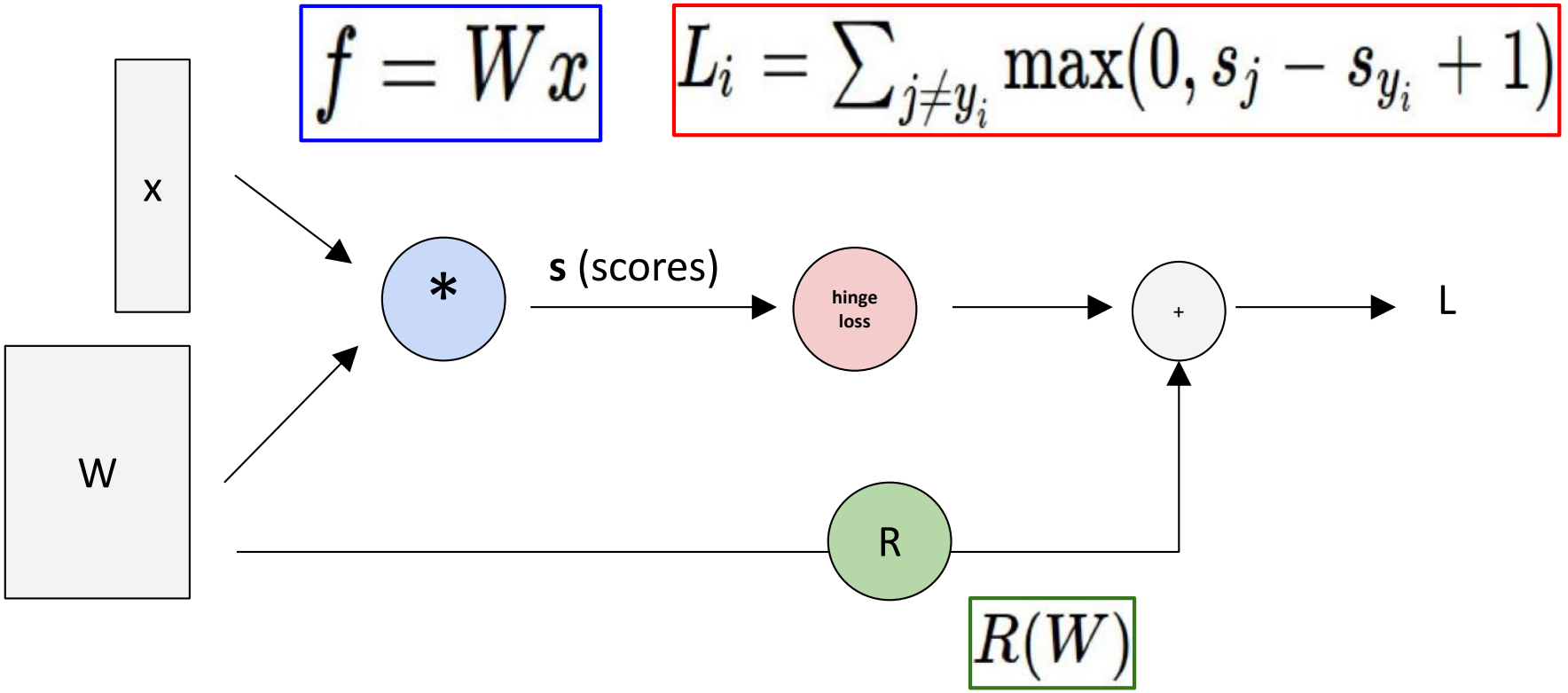
$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

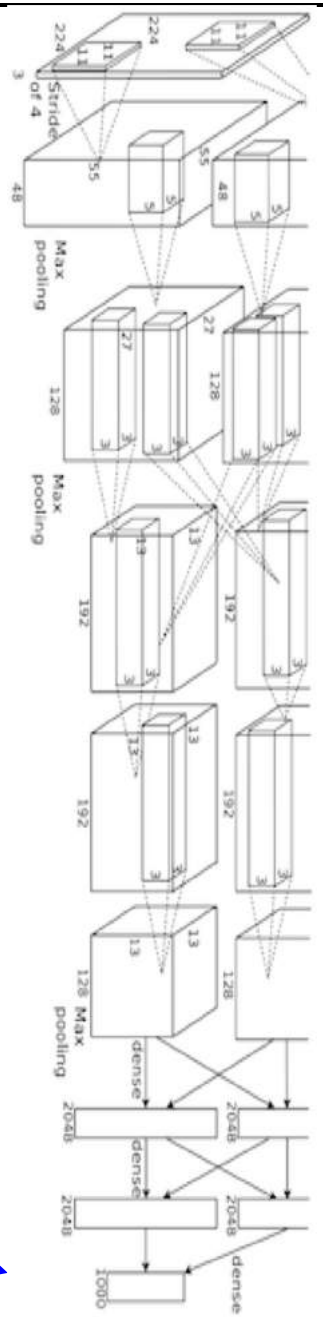
Numerical gradient: slow :(, approximate :(, easy to write :)
Analytic gradient: fast :), exact :), error-prone :(

In practice: Derive analytic gradient, check your implementation with numerical gradient

Computational Graph



Convolutional Network (AlexNet)



Differentiating a Computation Graph

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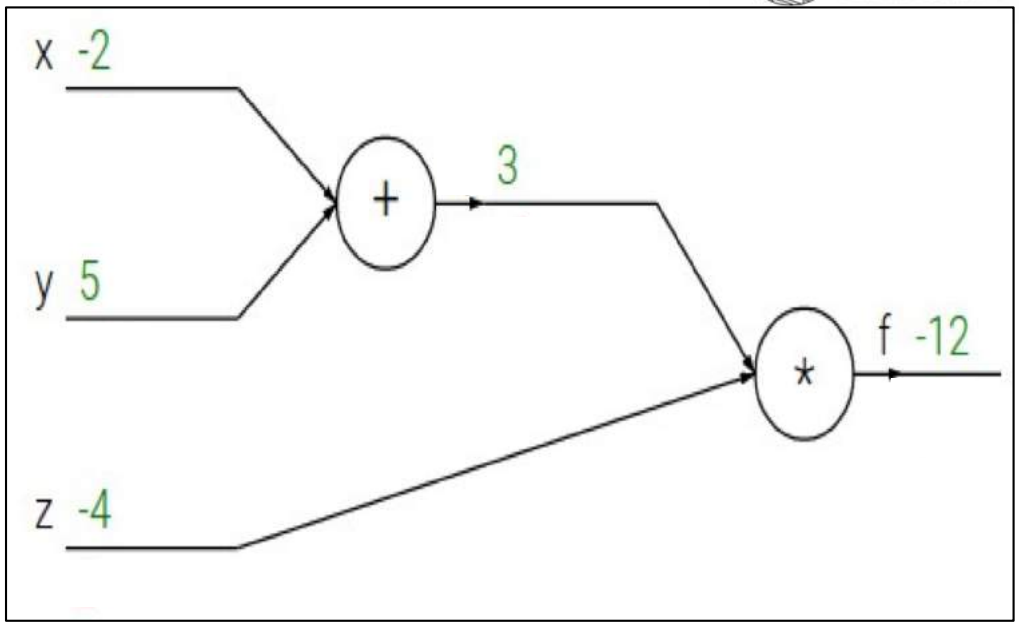
$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4



Chain rule

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We can write

$$\mathrm{f}(x, y, z) = g(h(x, y), z)$$

Where $h(x, y) = x + y$, and $g(a, b) = a * b$

By the chain rule, $\frac{df}{dx} = \frac{dg}{dh}\frac{dh}{dx}$ and $\frac{df}{dy} = \frac{dg}{dh}\frac{dh}{dy}$

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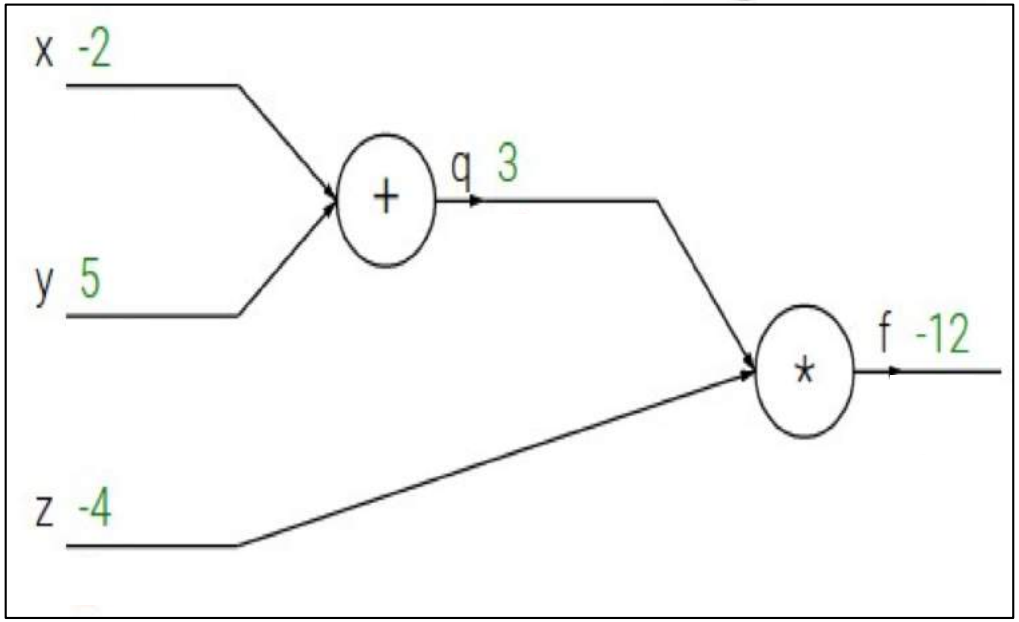

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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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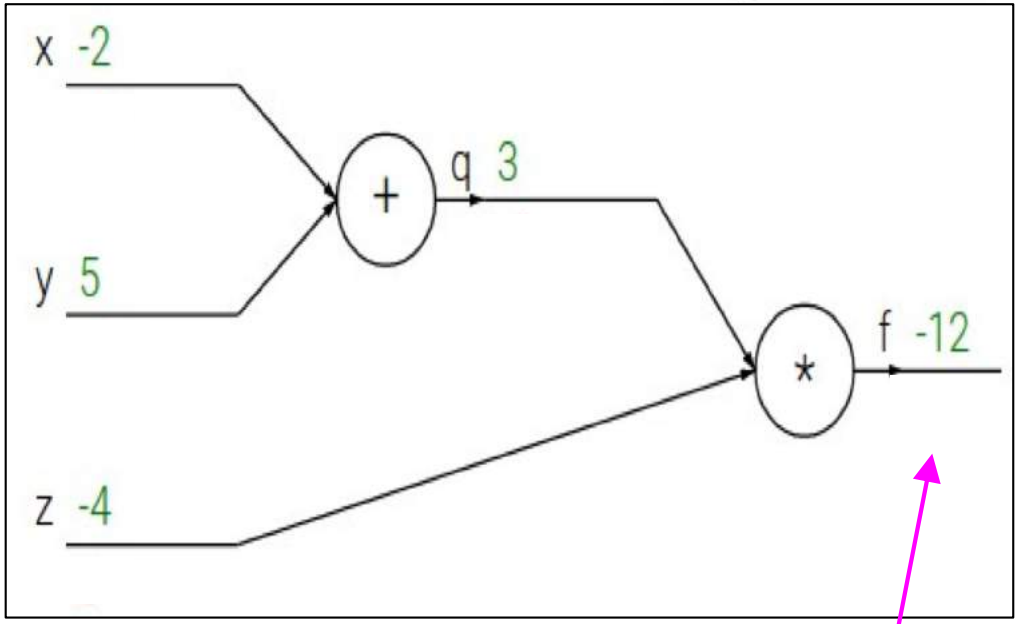

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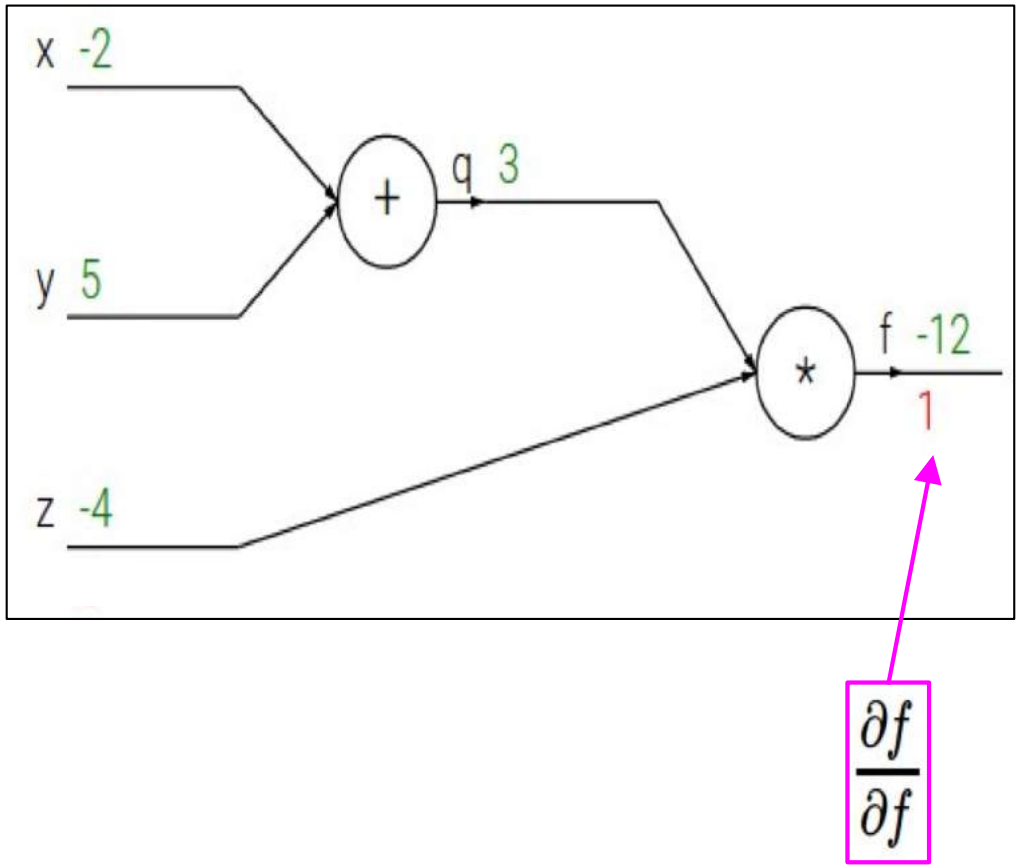

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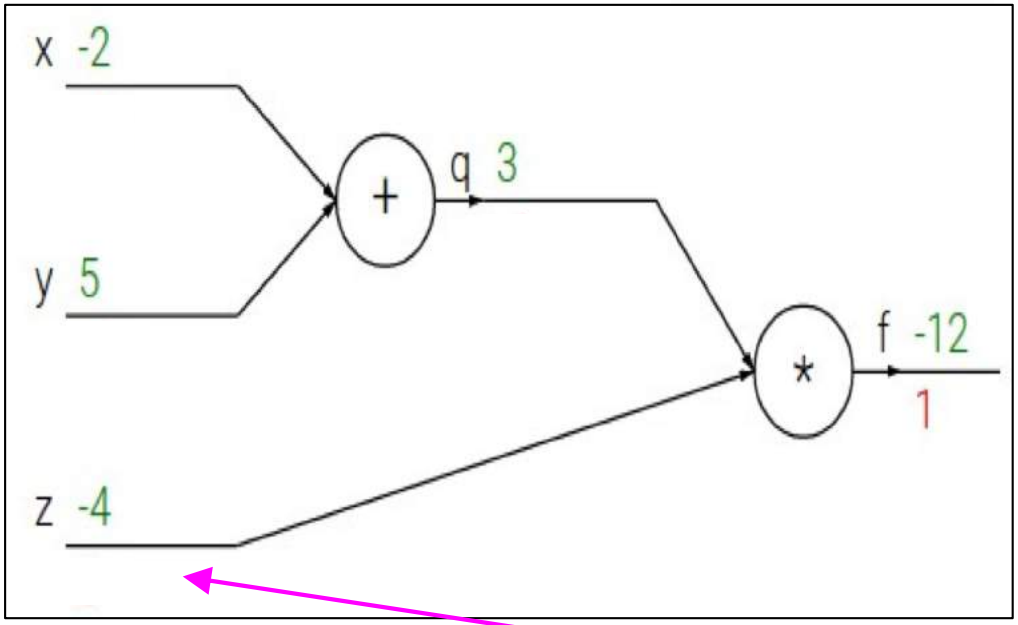

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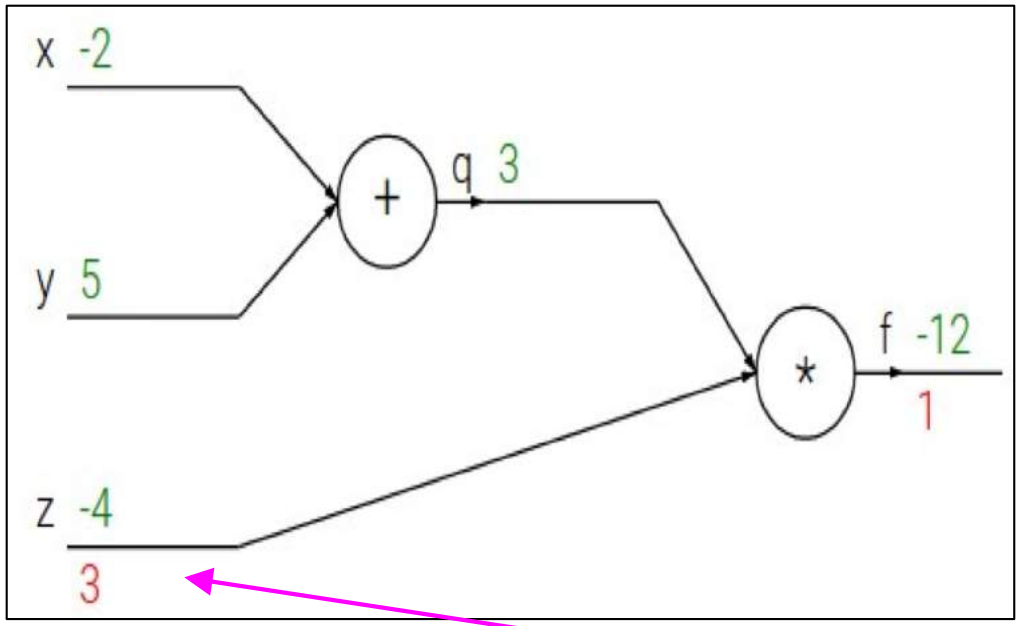

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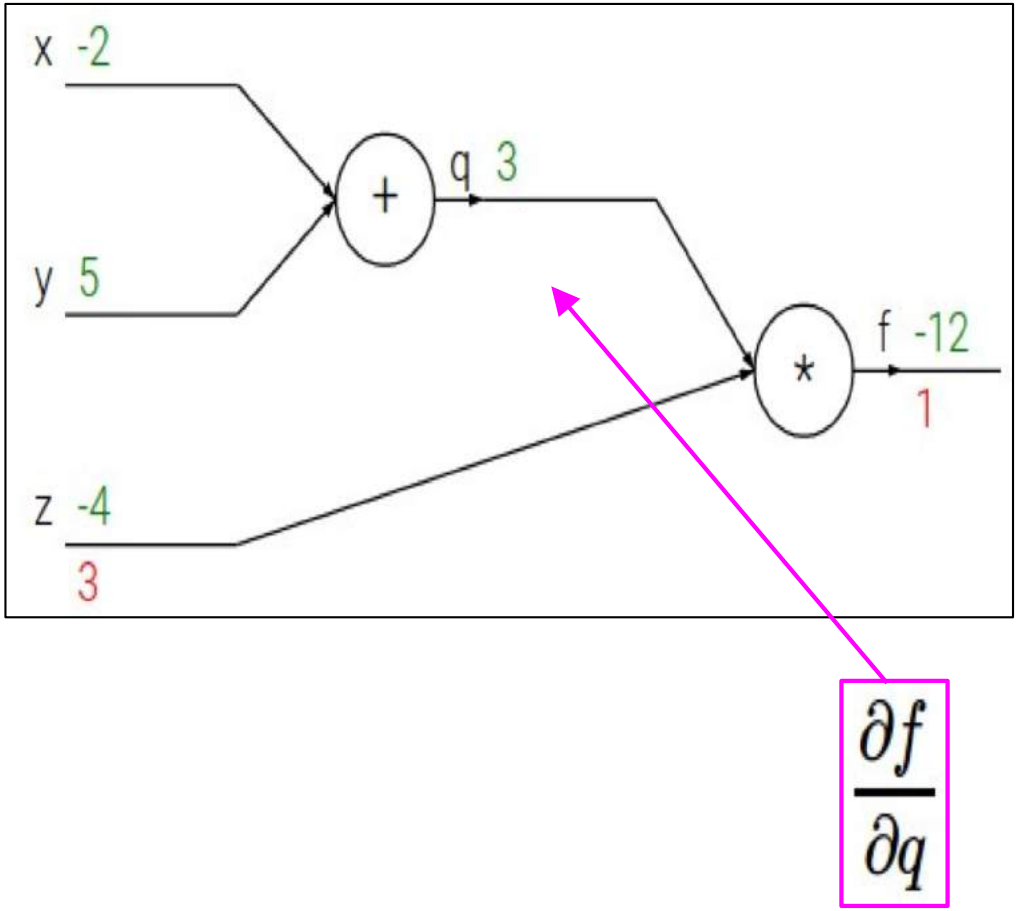

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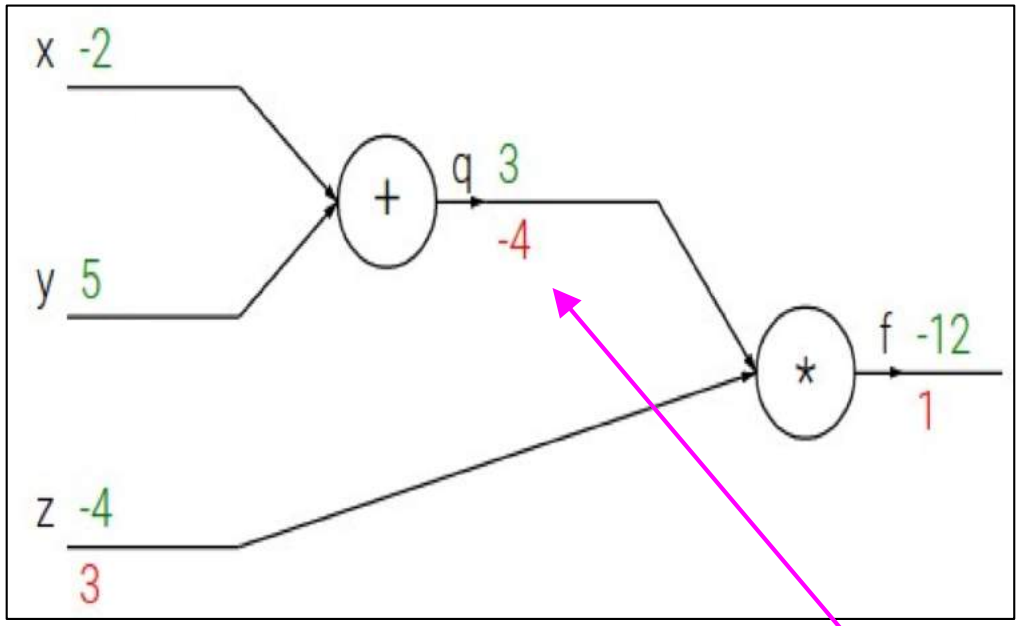

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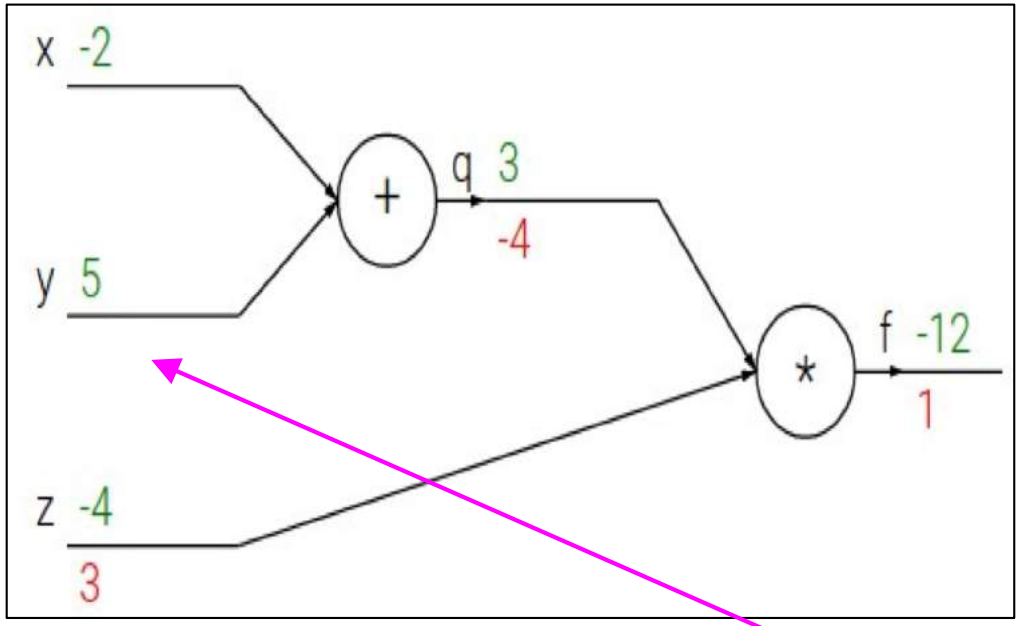

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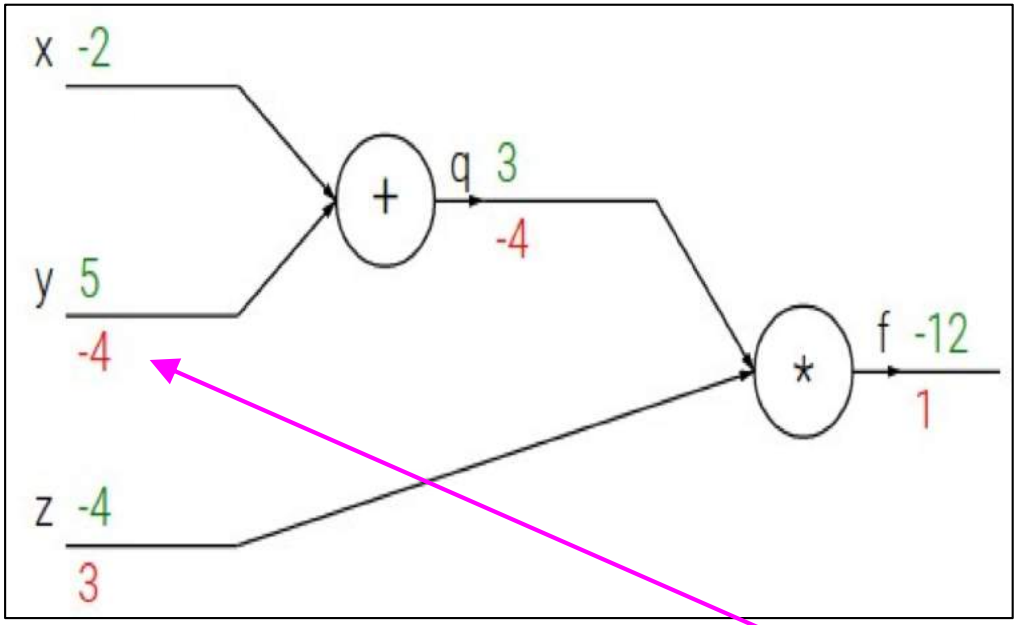

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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

$\frac{\partial f}{\partial y}$

Chain rule:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial y}$$

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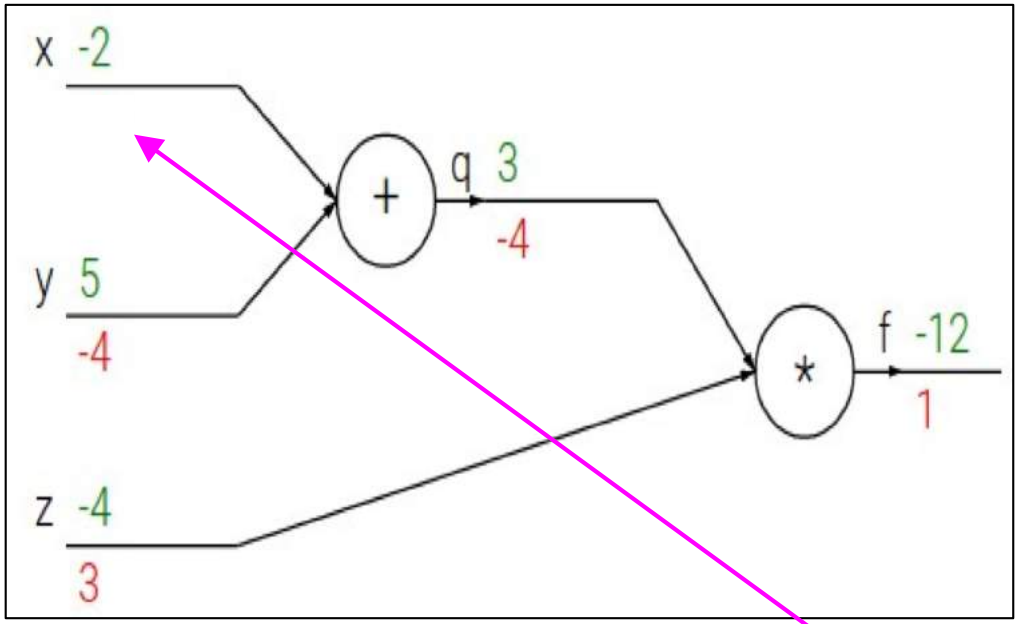

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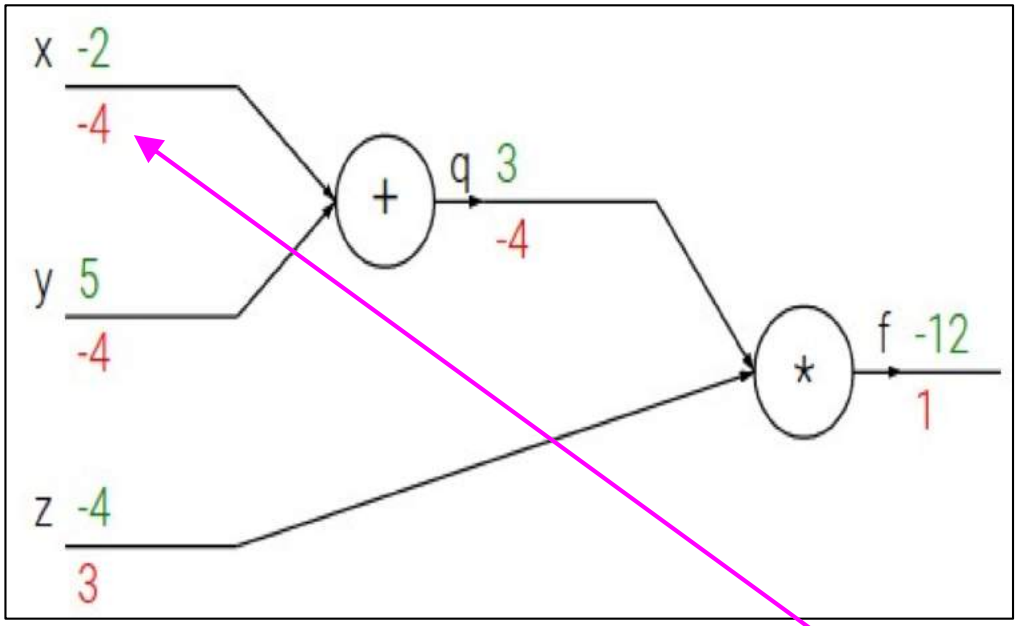

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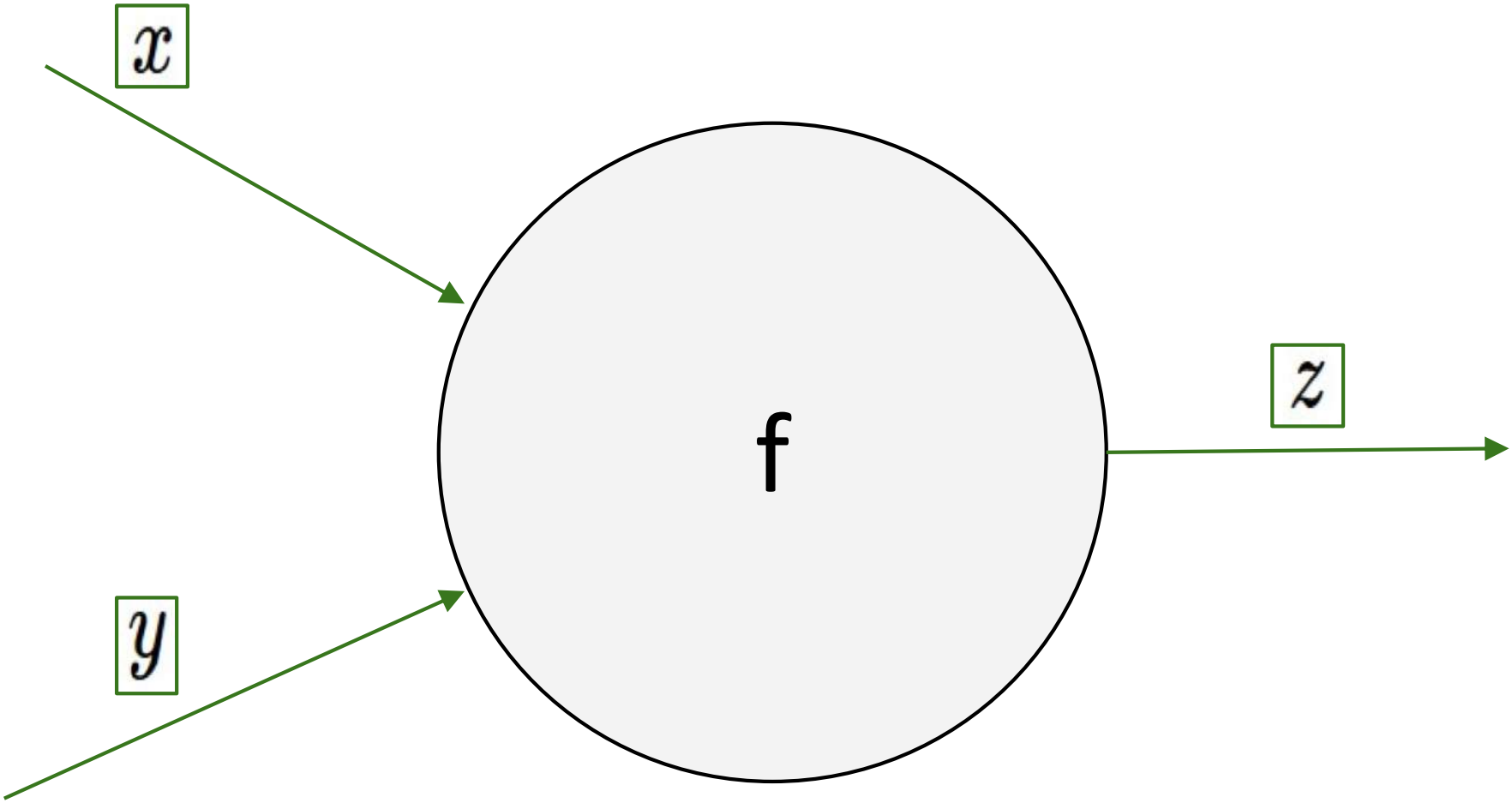
Activations



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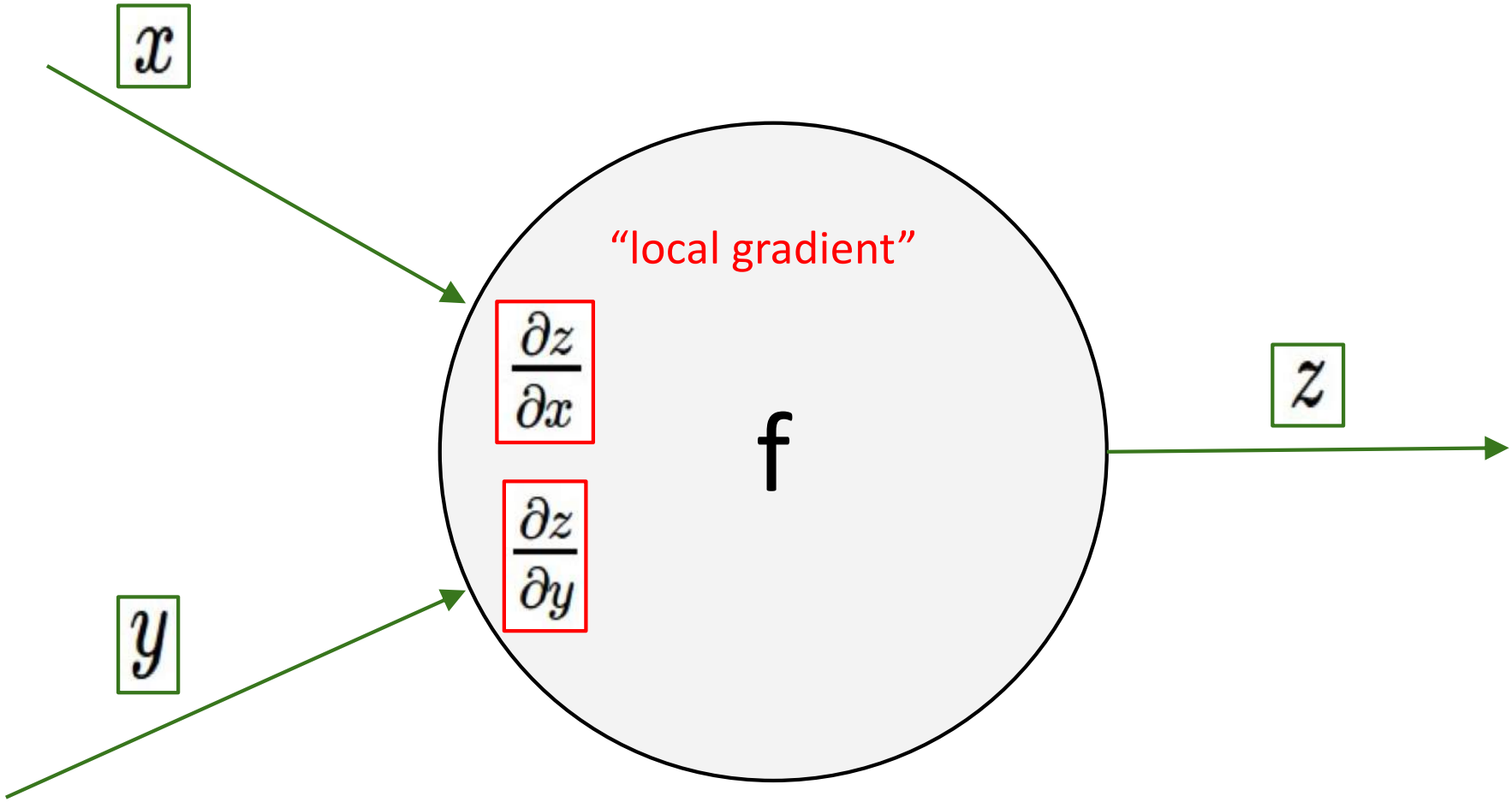

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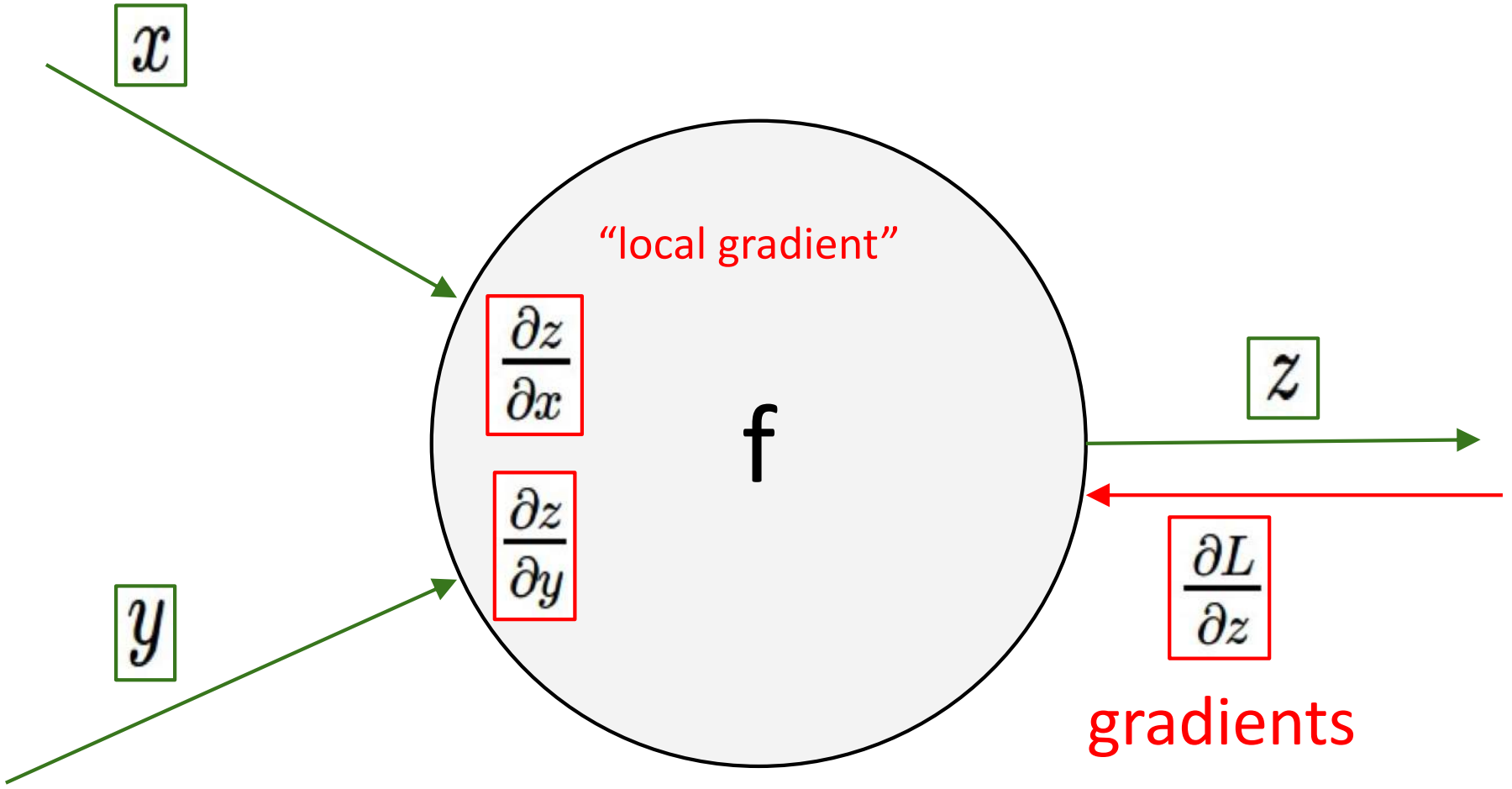

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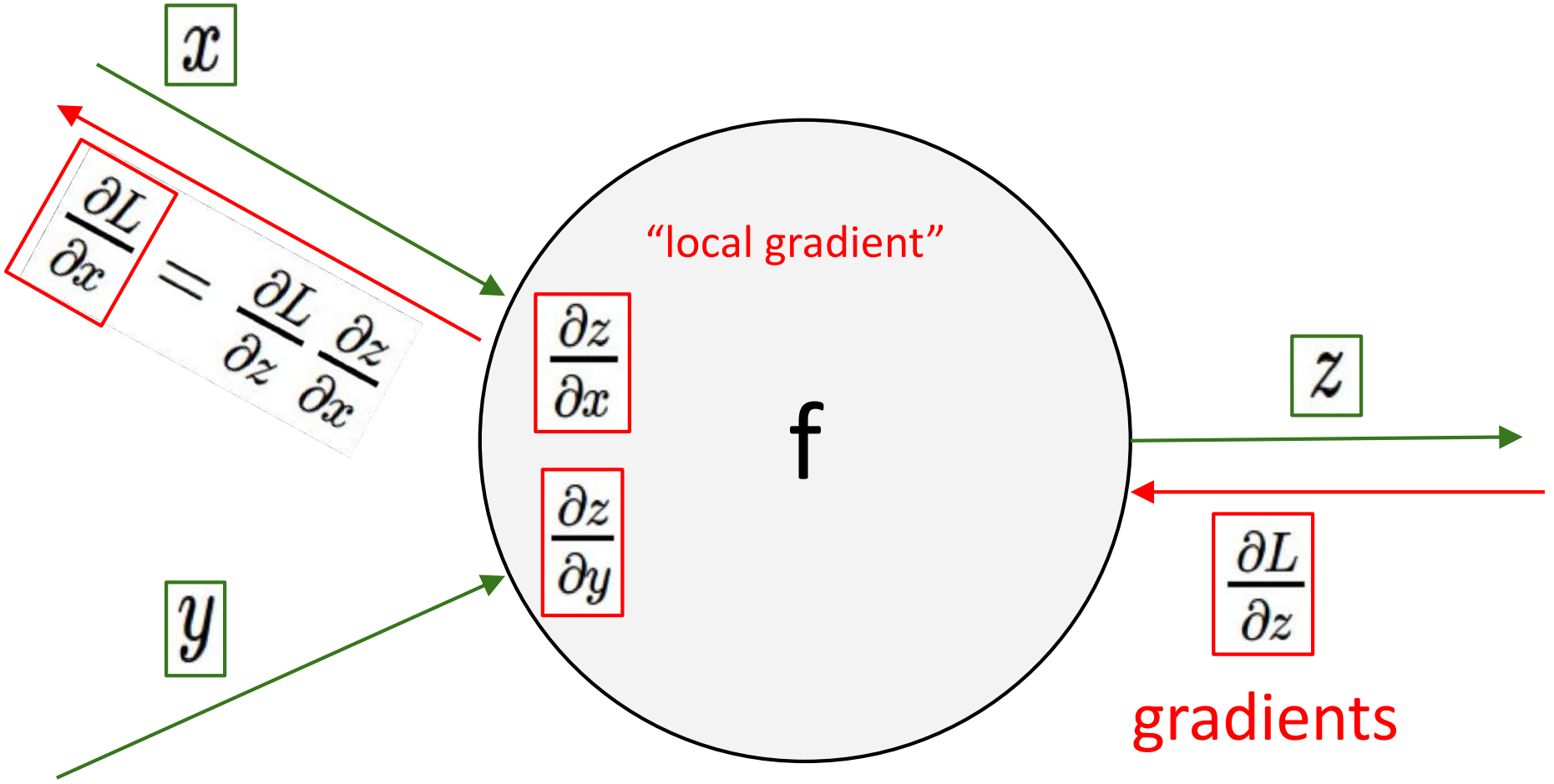

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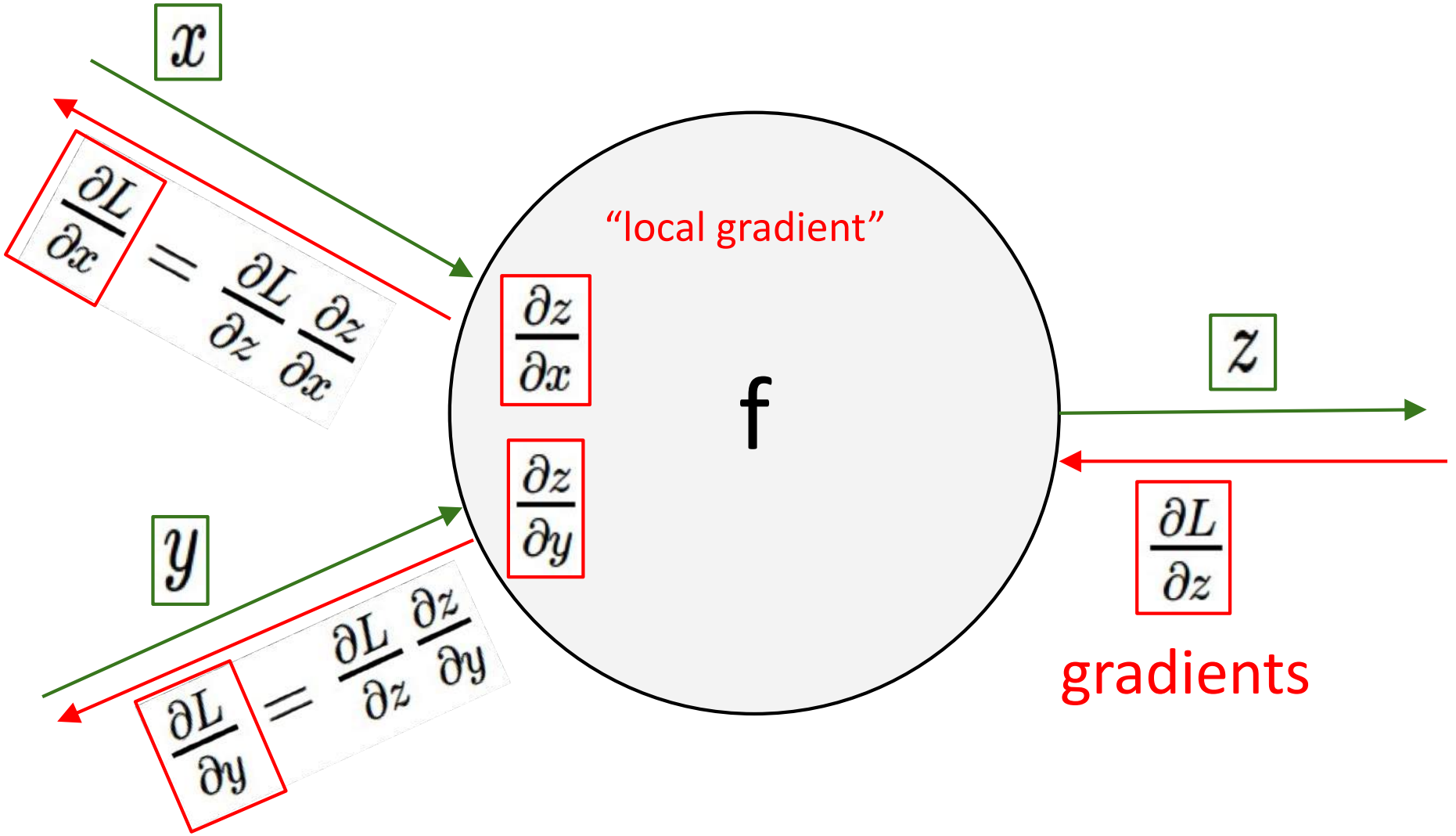

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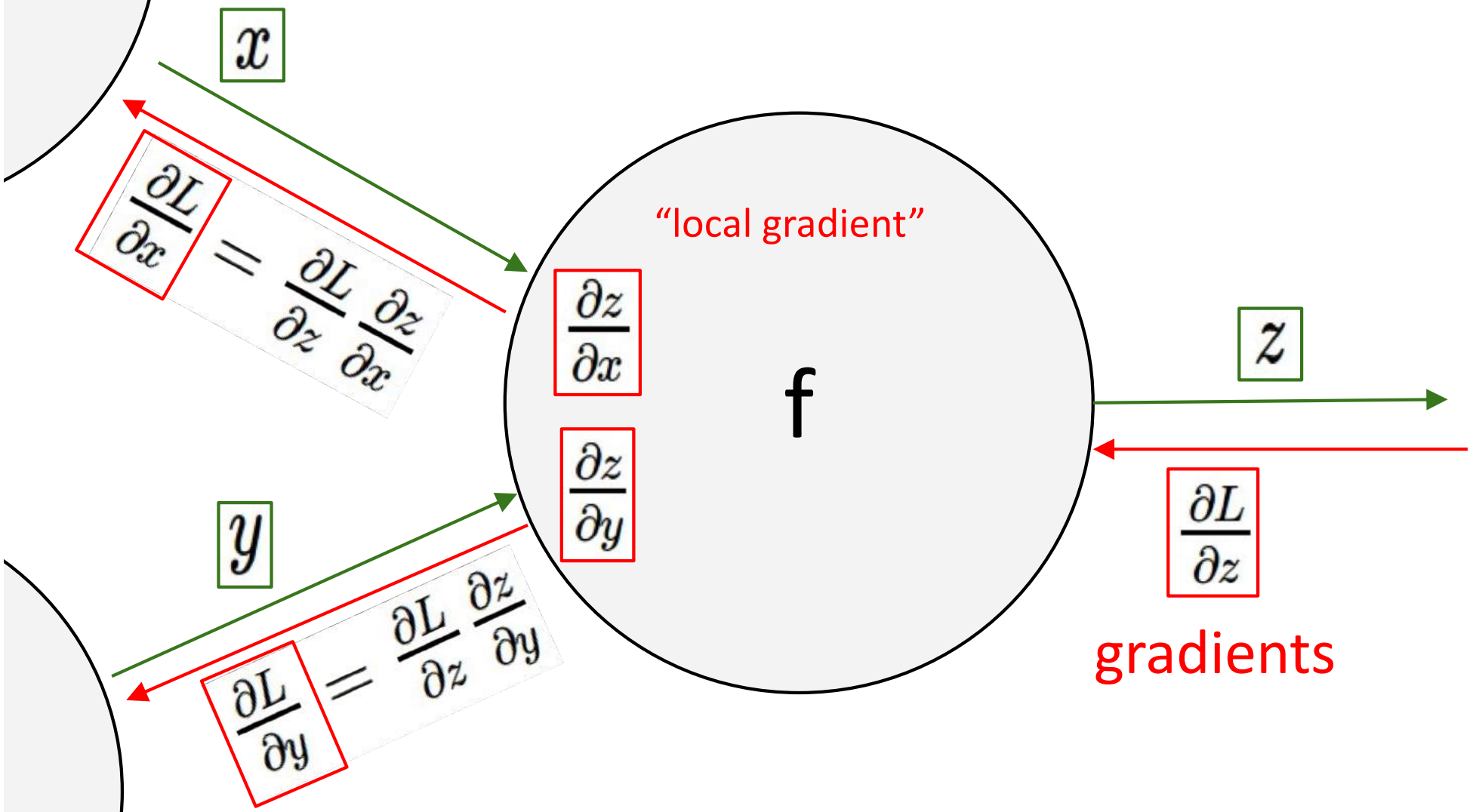
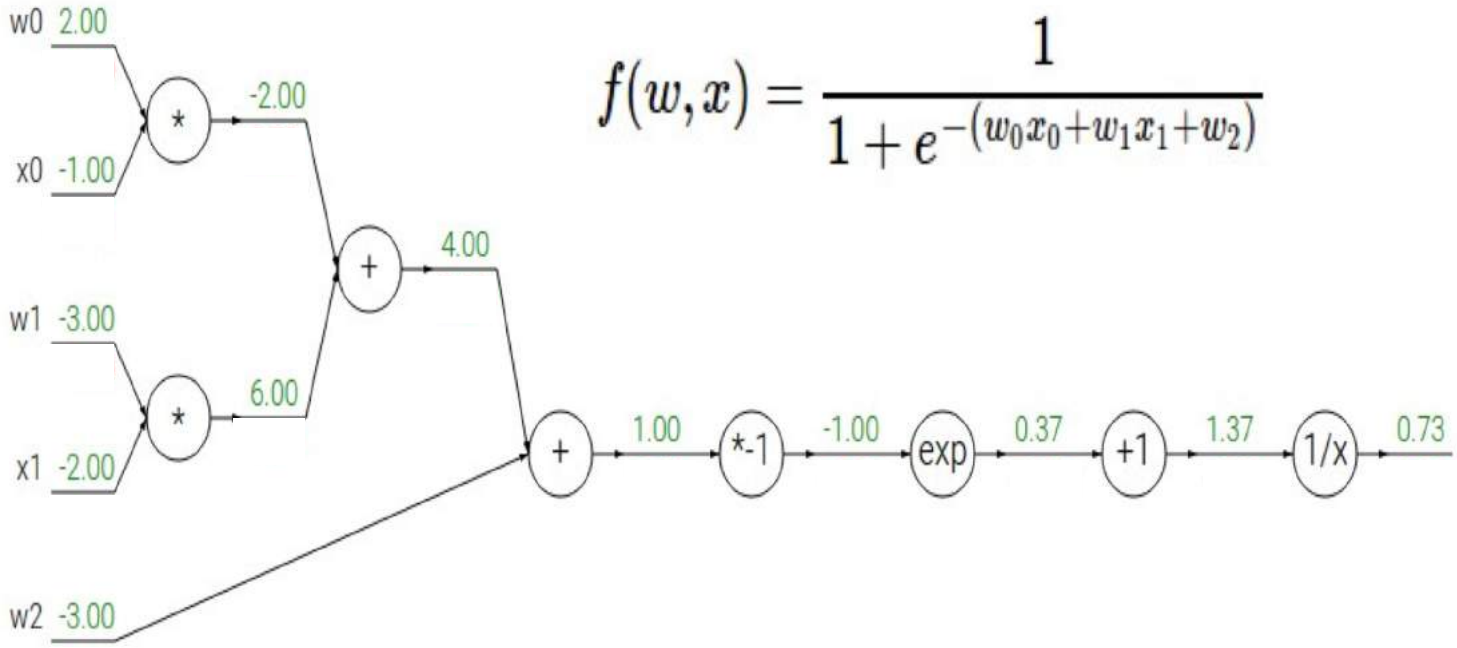


Another backprop example:



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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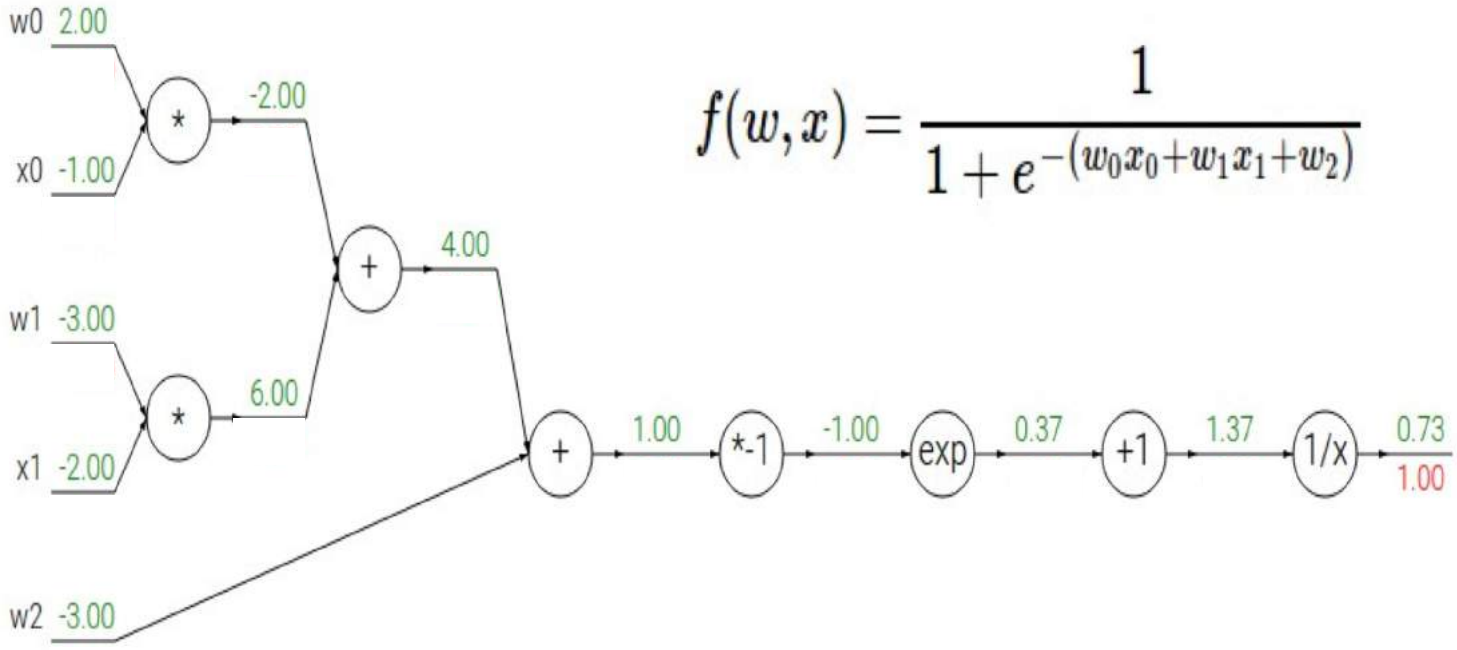

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$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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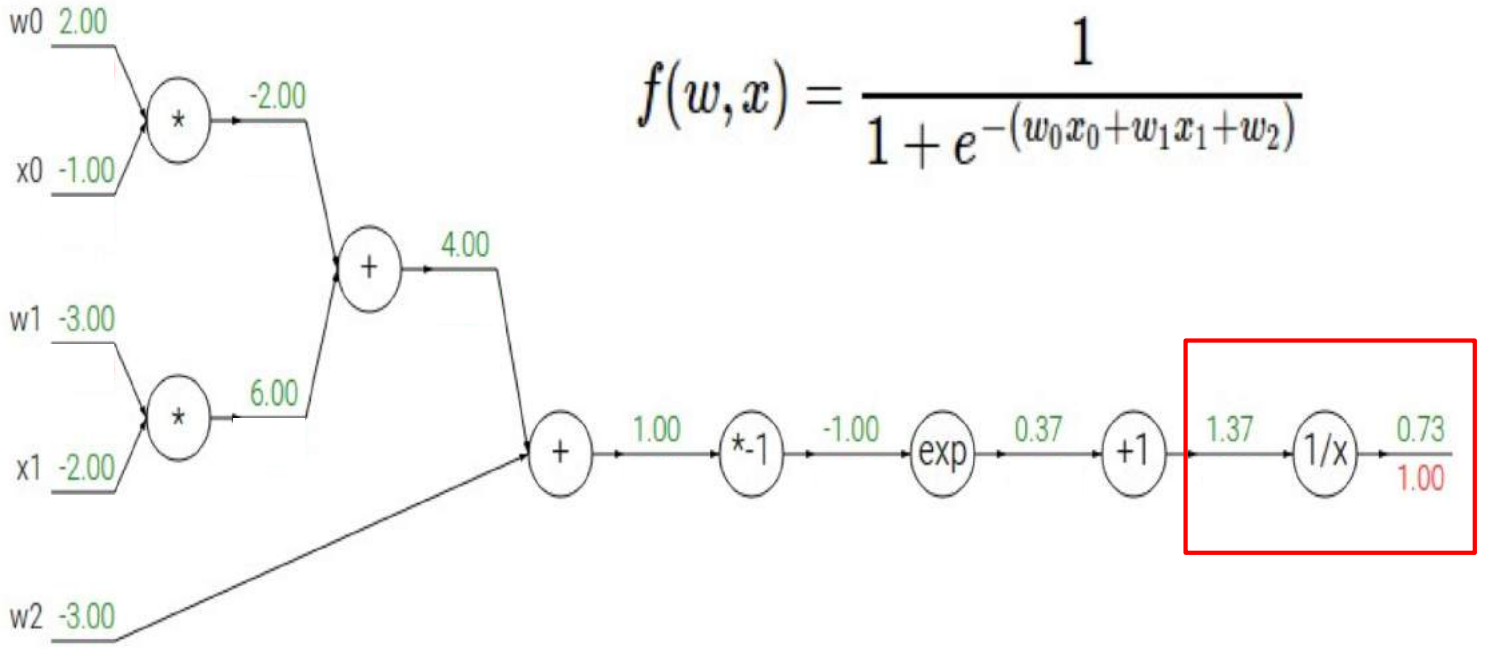

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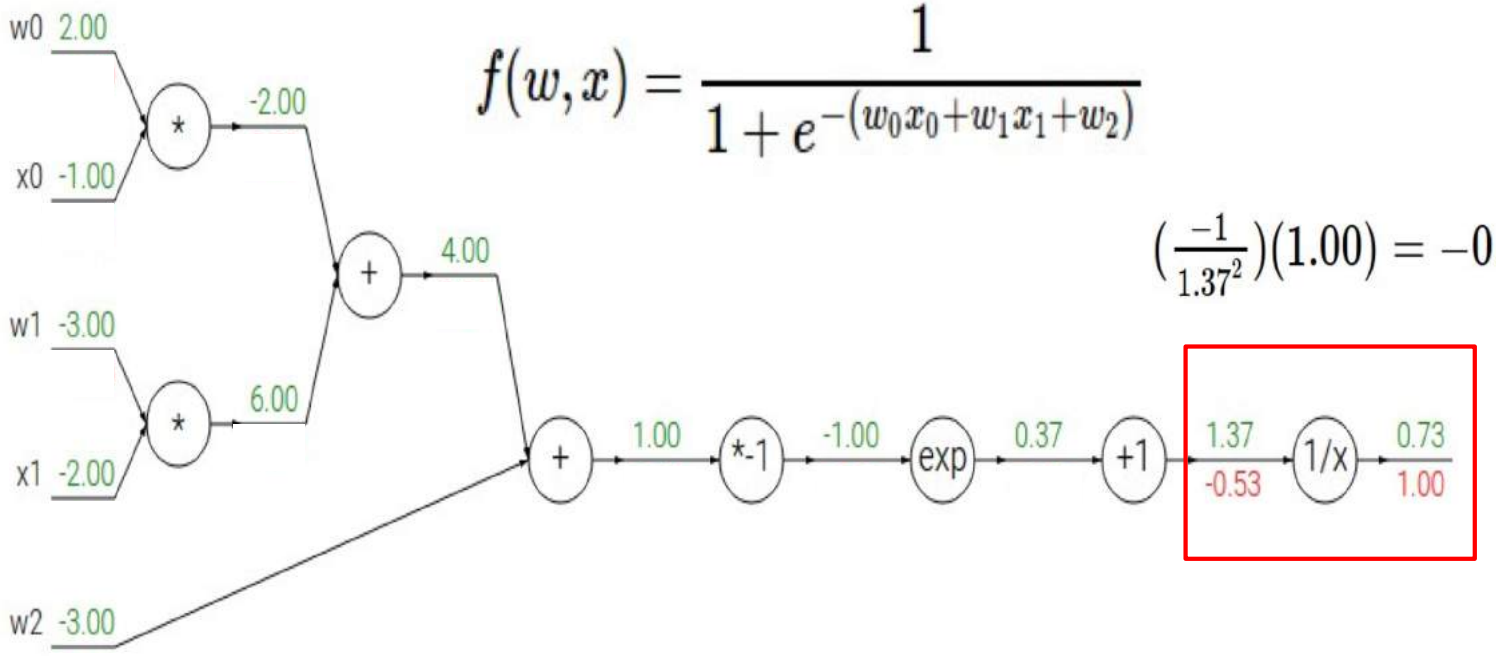

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$(\frac{-1}{1.37^2})(1.00) = -0.53$$

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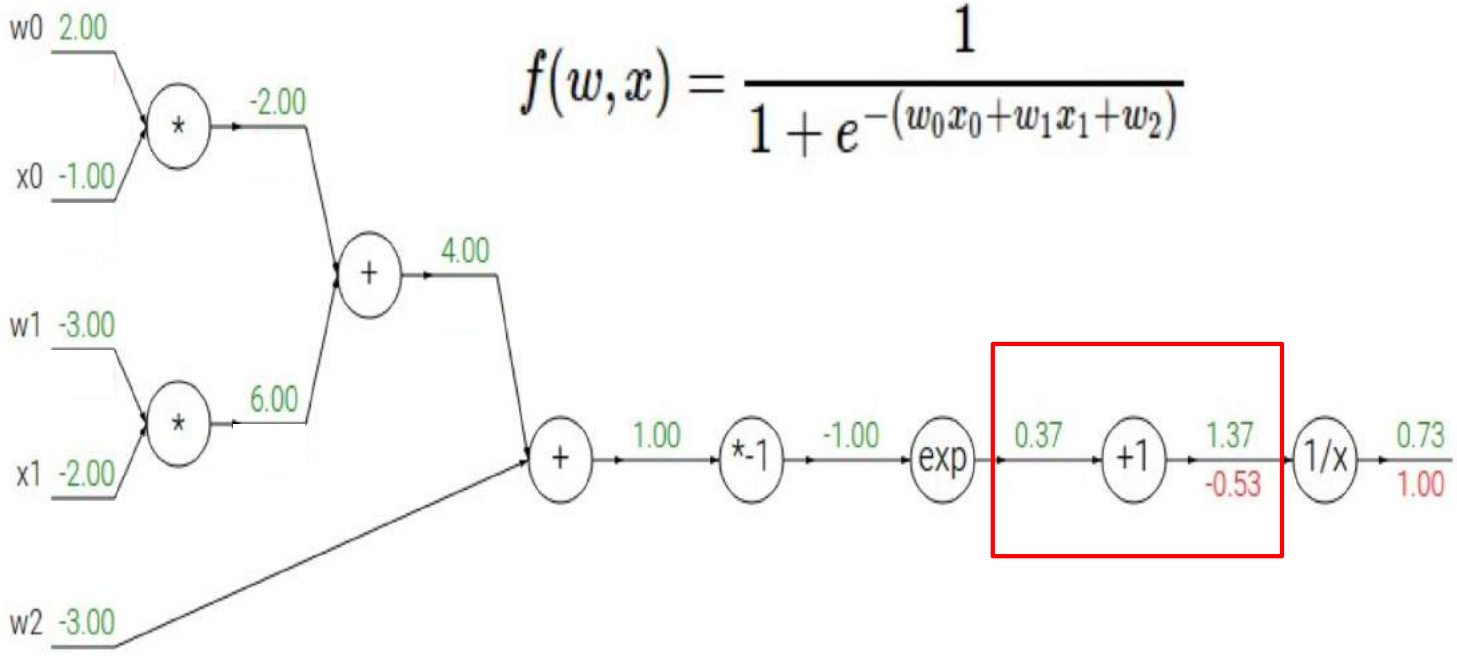

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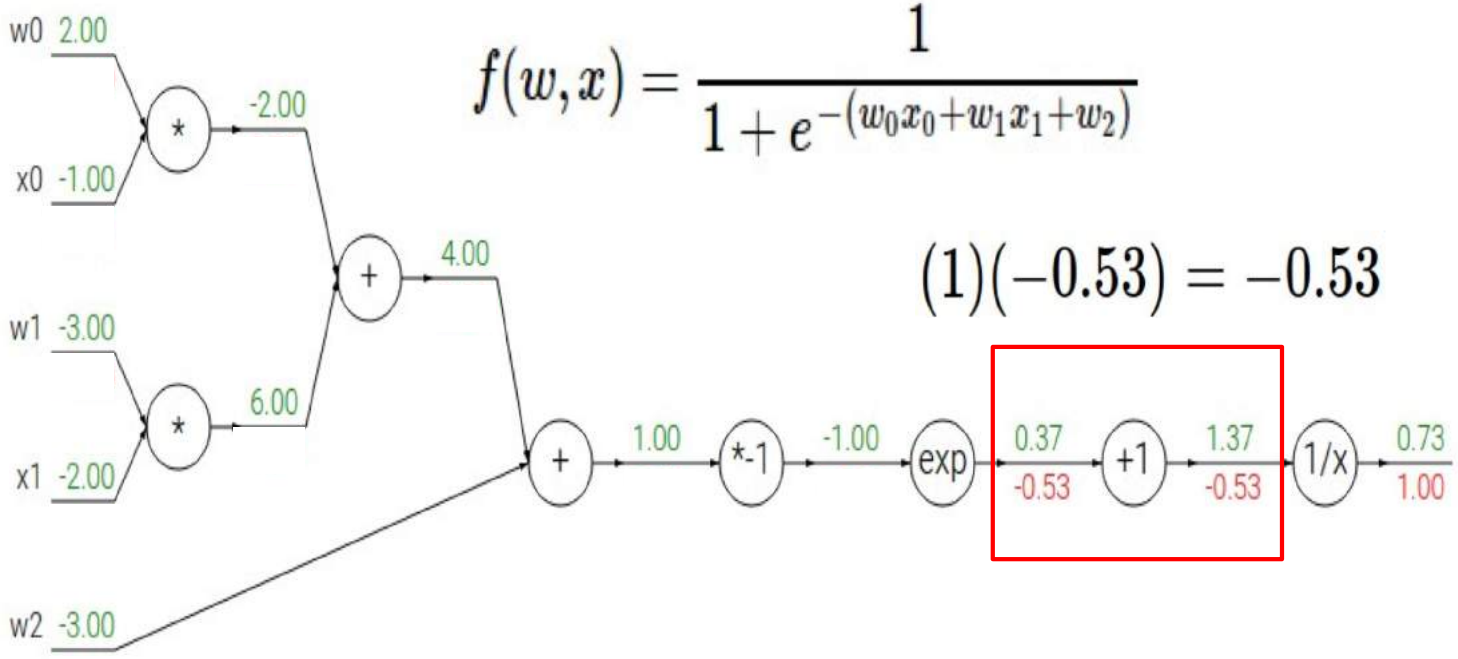

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$(1)(-0.53) = -0.53$$

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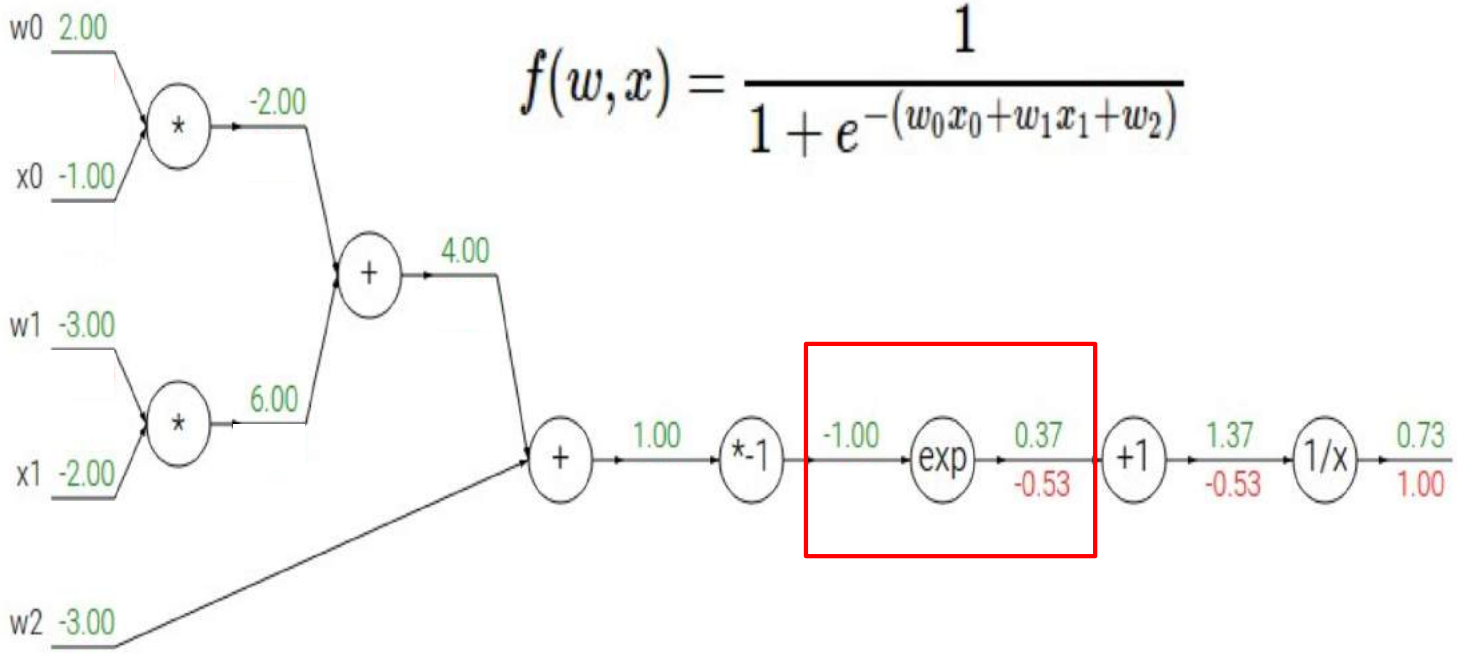

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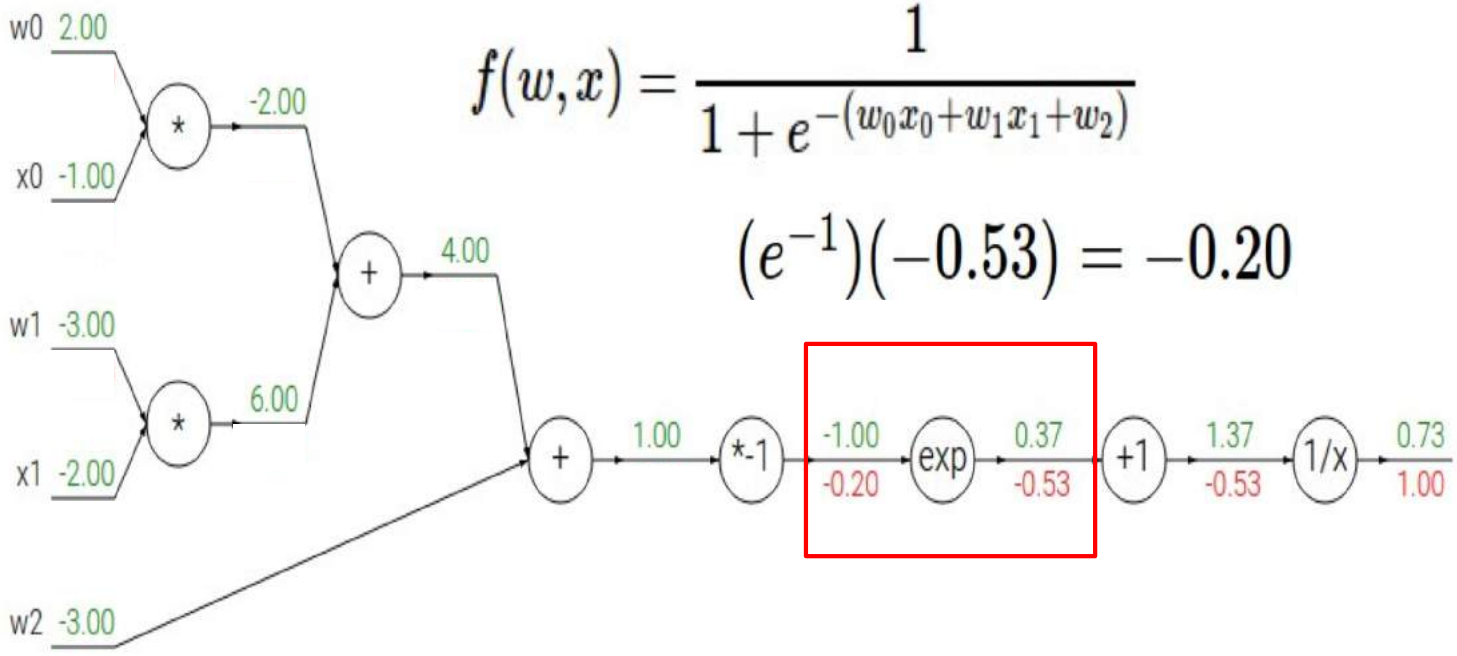

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$(e^{-1})(-0.53) = -0.20$$

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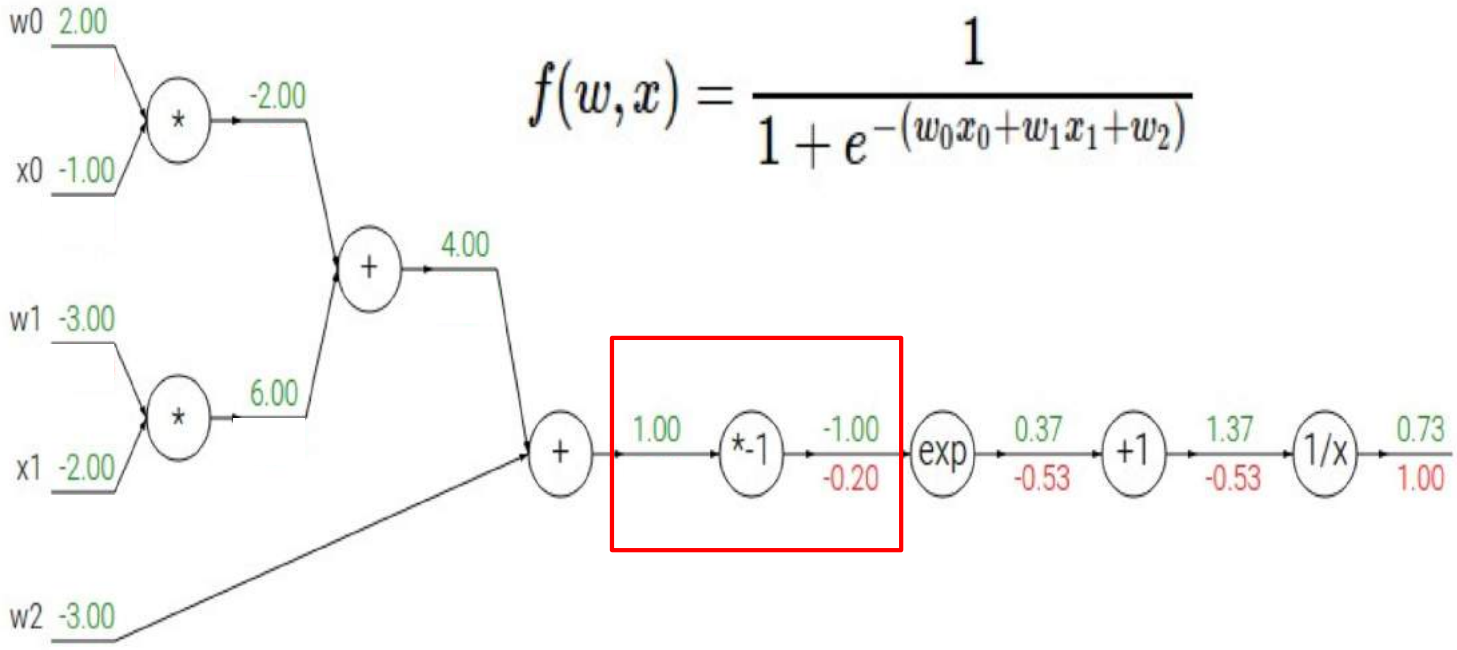

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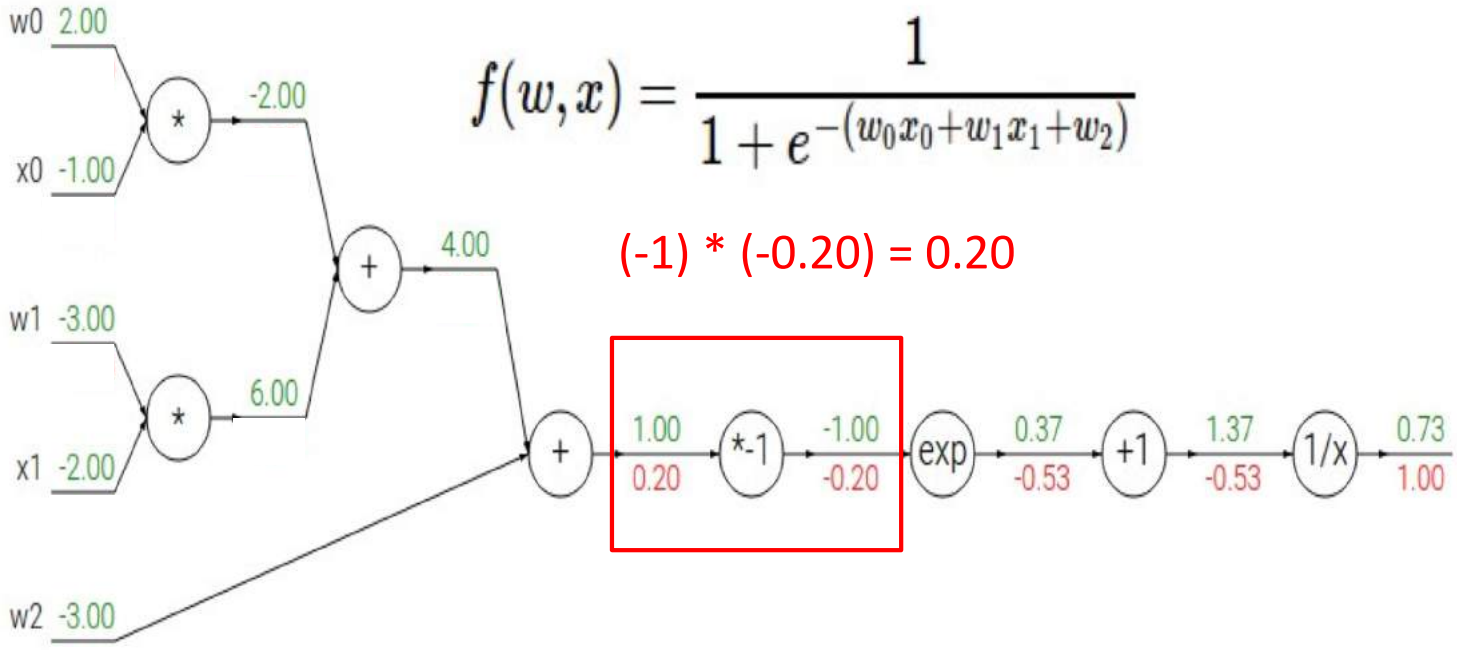

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(-1) * (-0.20) = 0.20

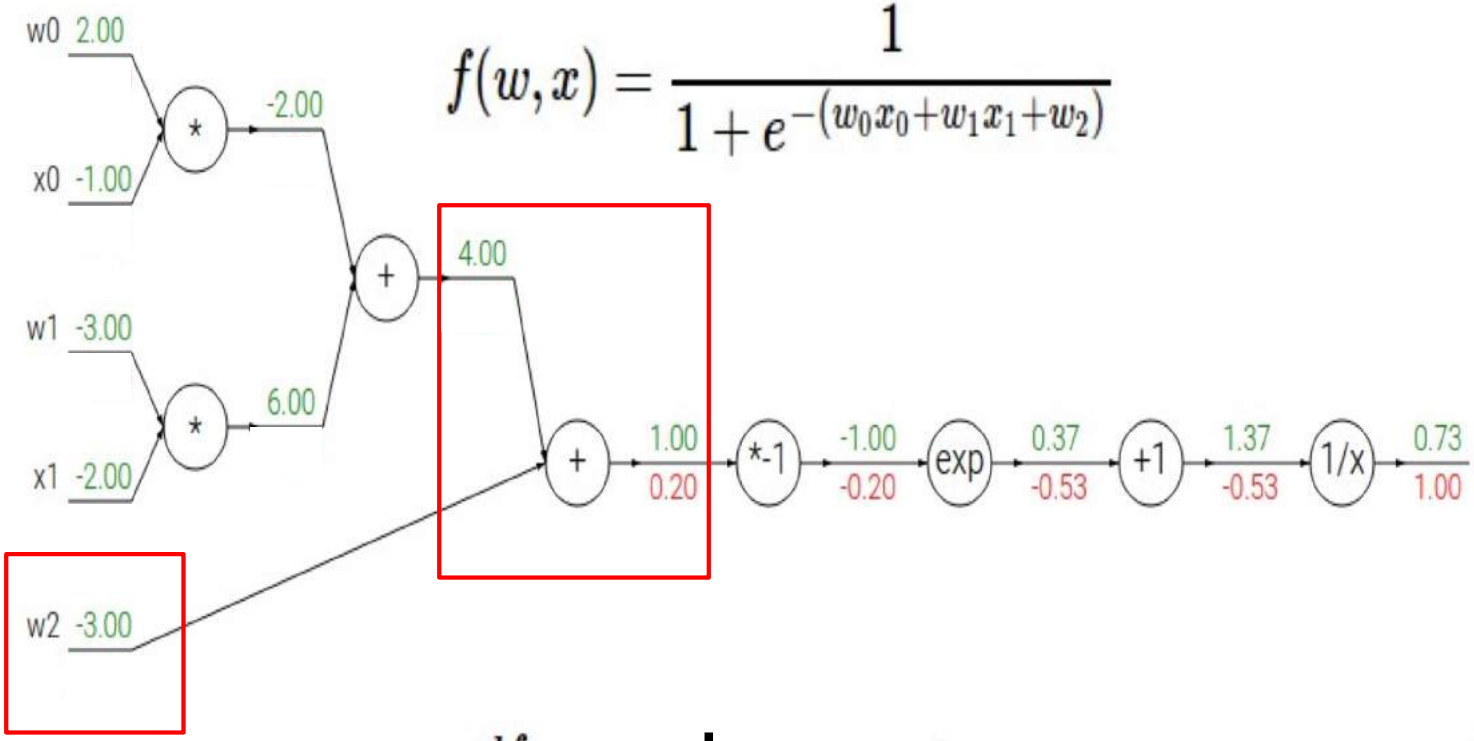
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Another backprop example:



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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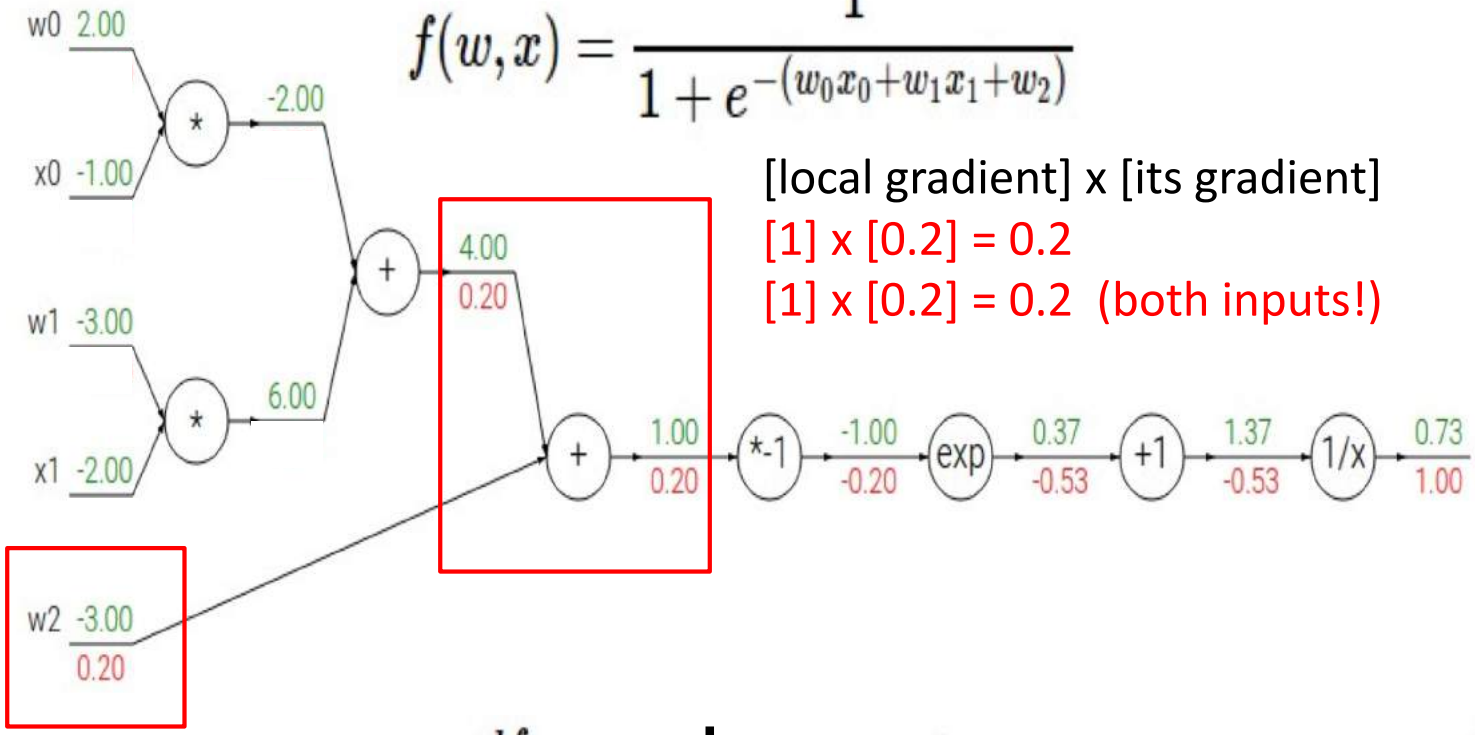
$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



[local gradient] x [its gradient]

[1] x [0.2] = 0.2

[1] x [0.2] = 0.2 (both inputs!)

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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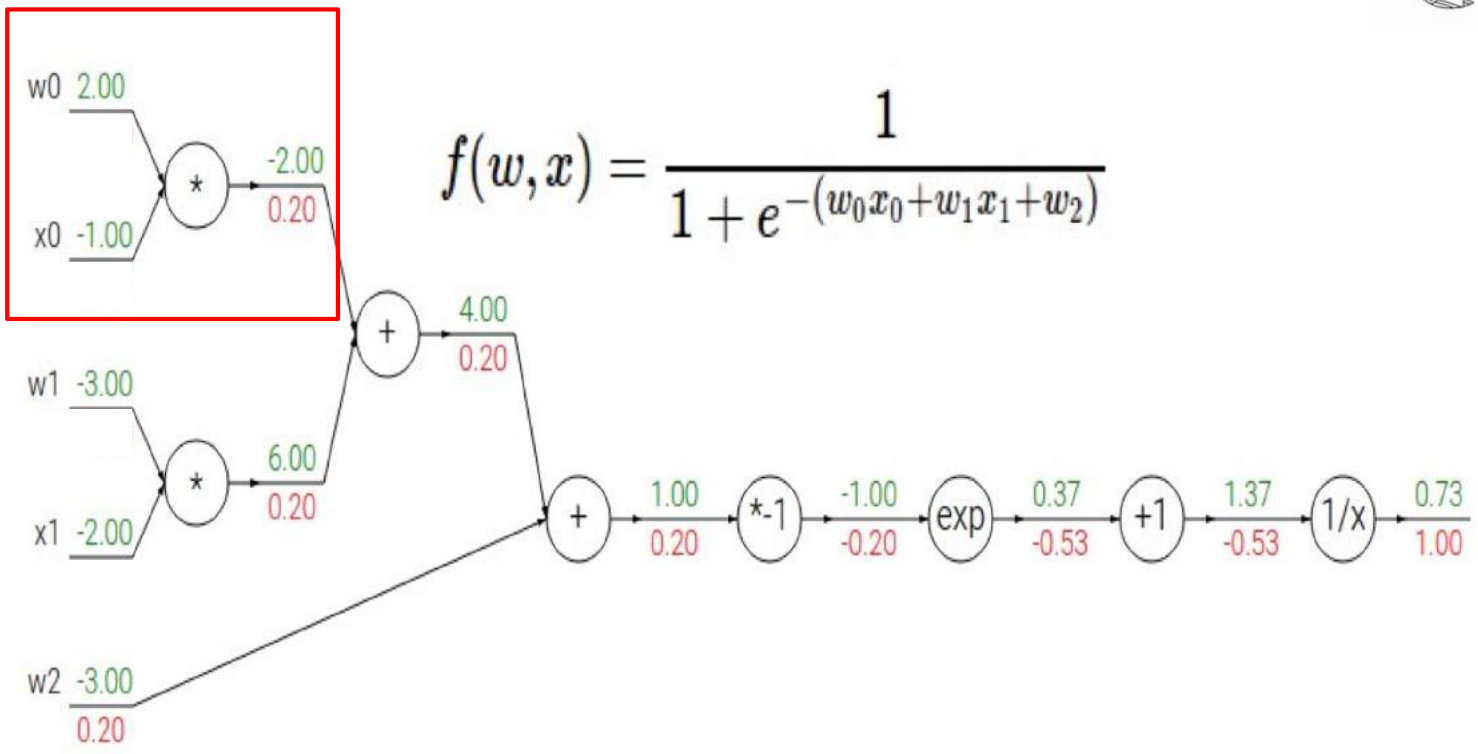
Another backprop example:



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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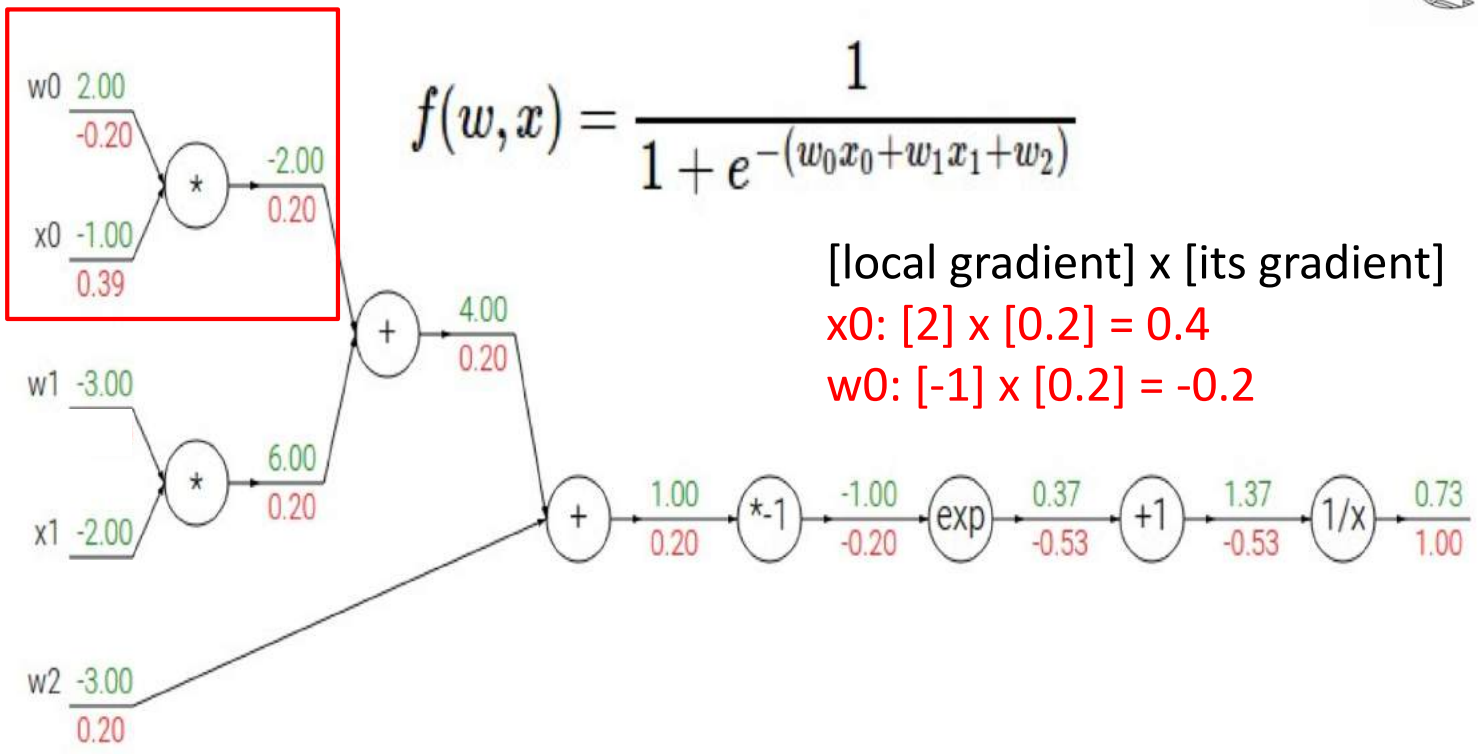
Another backprop example:



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

[local gradient] x [its gradient]

x0: [2] x [0.2] = 0.4

w0: [-1] x [0.2] = -0.2

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

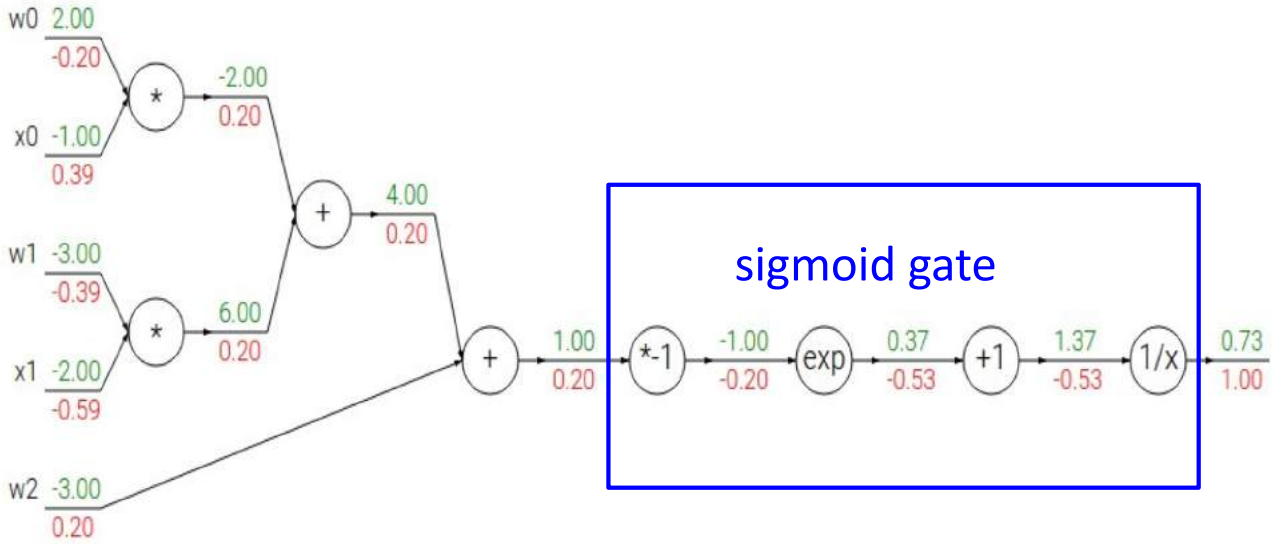
$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

sigmoid function

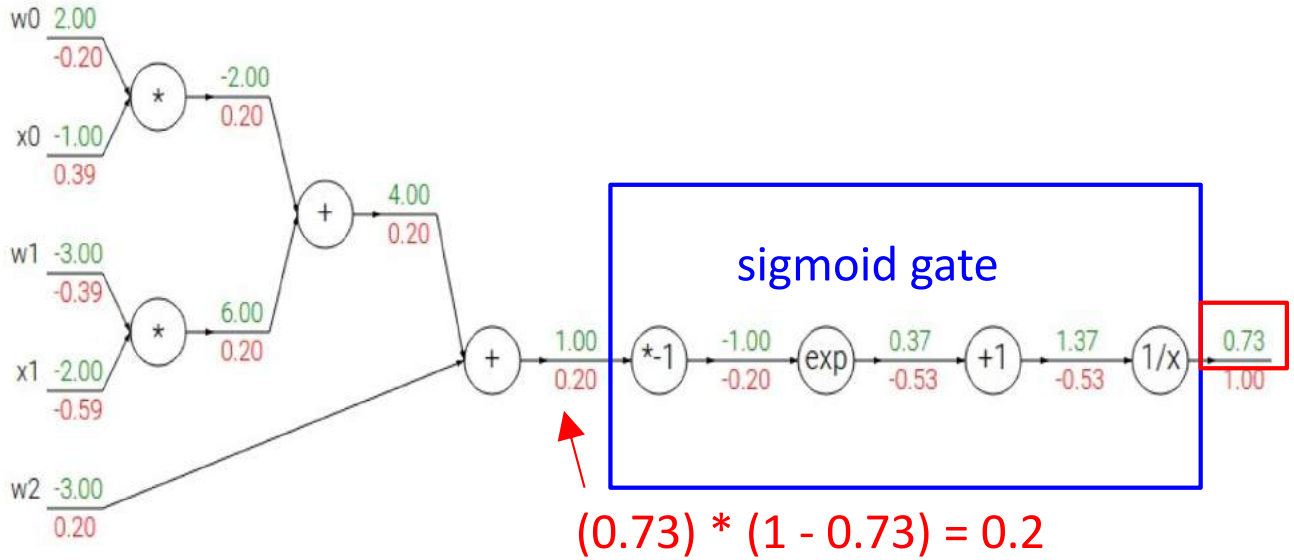
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}} \qquad \boxed{\sigma(x) = \frac{1}{1+e^{-x}}}$$

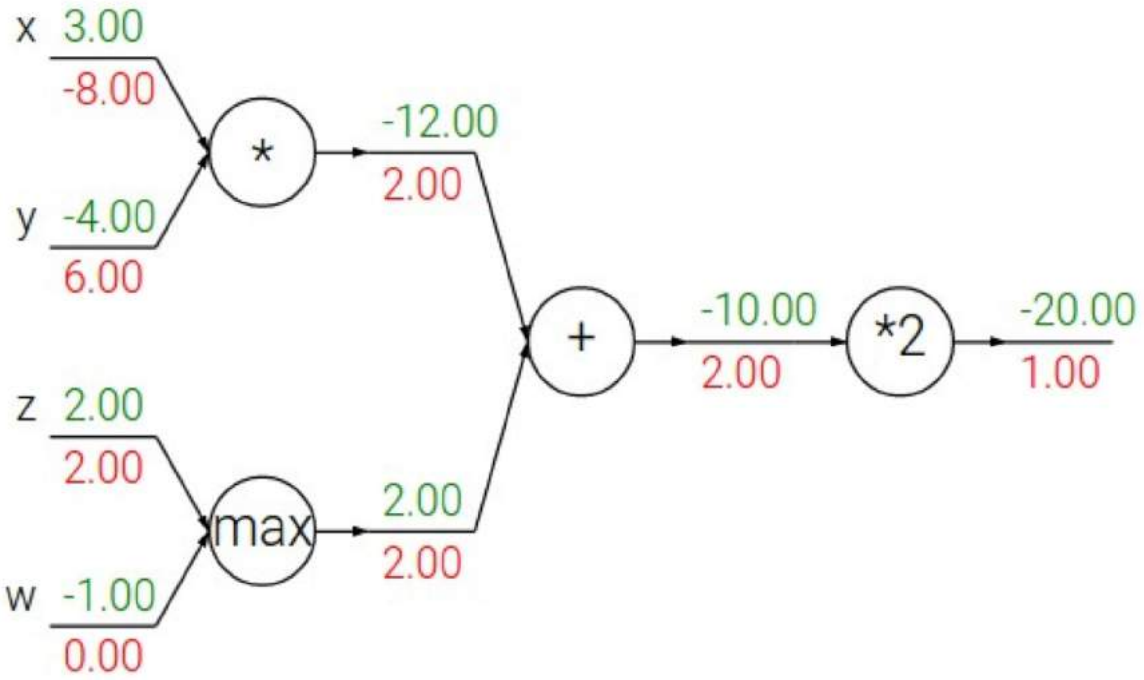
sigmoid function

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$

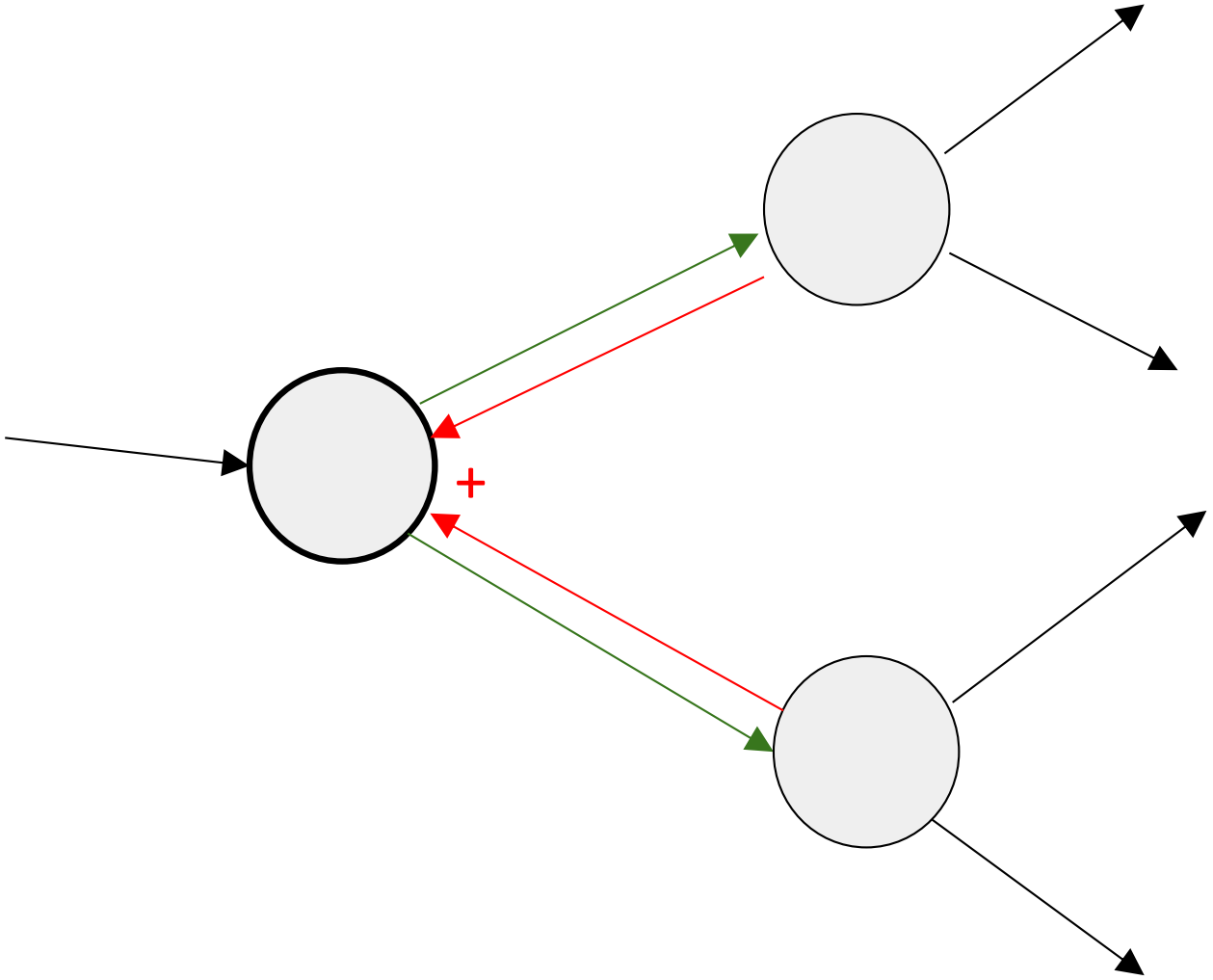


Patterns in backward flow

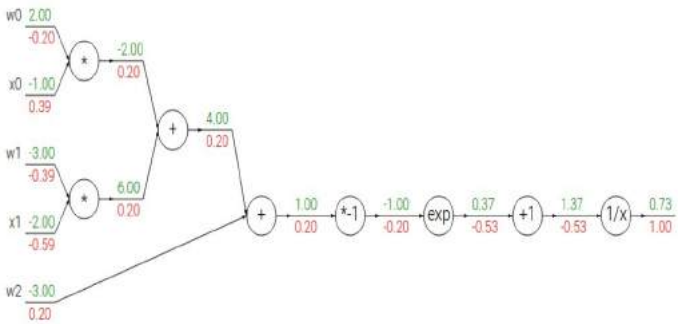
add gate: gradient distributor
max gate: gradient router
mul gate: gradient… “switcher”?



Gradients add at branches



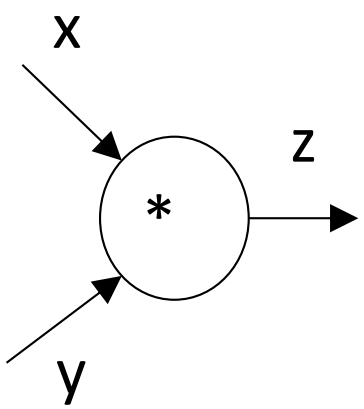
Implementation: forward/backward API



Graph (or Net) object. *(Rough psuedo code)*

```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
            gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```


Implementation: forward/backward API



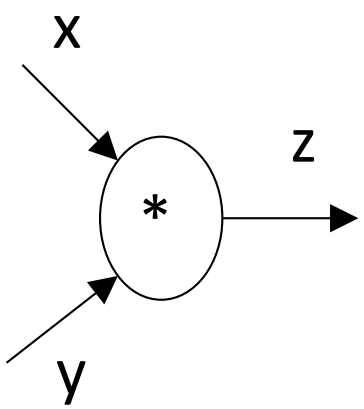
(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

$\frac{\partial L}{\partial z}$

$\frac{\partial L}{\partial x}$

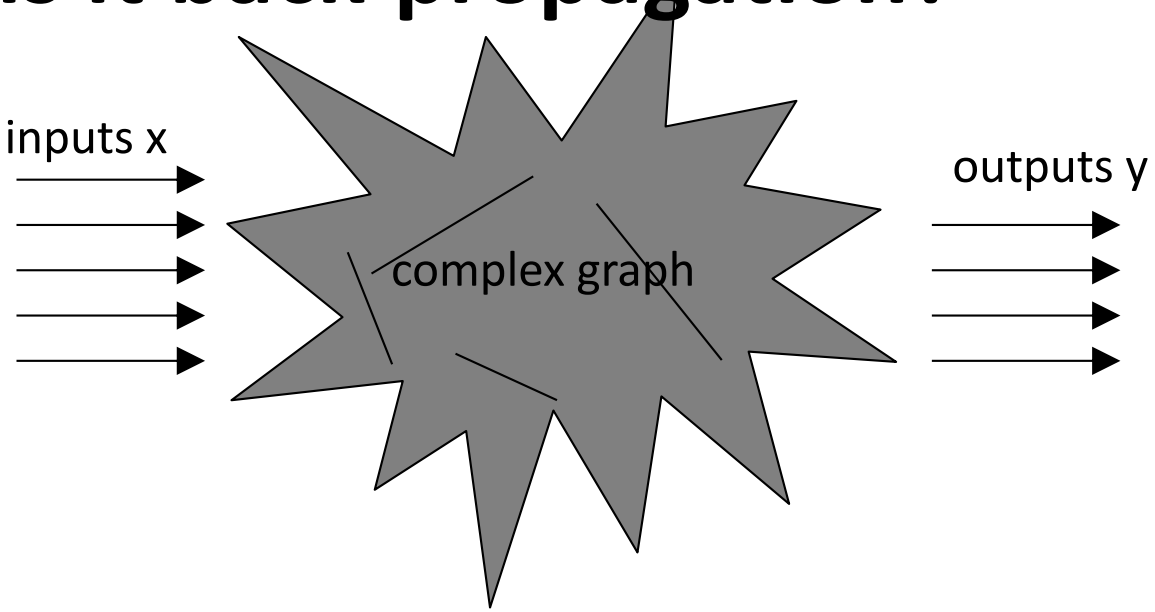
Implementation: forward/backward API



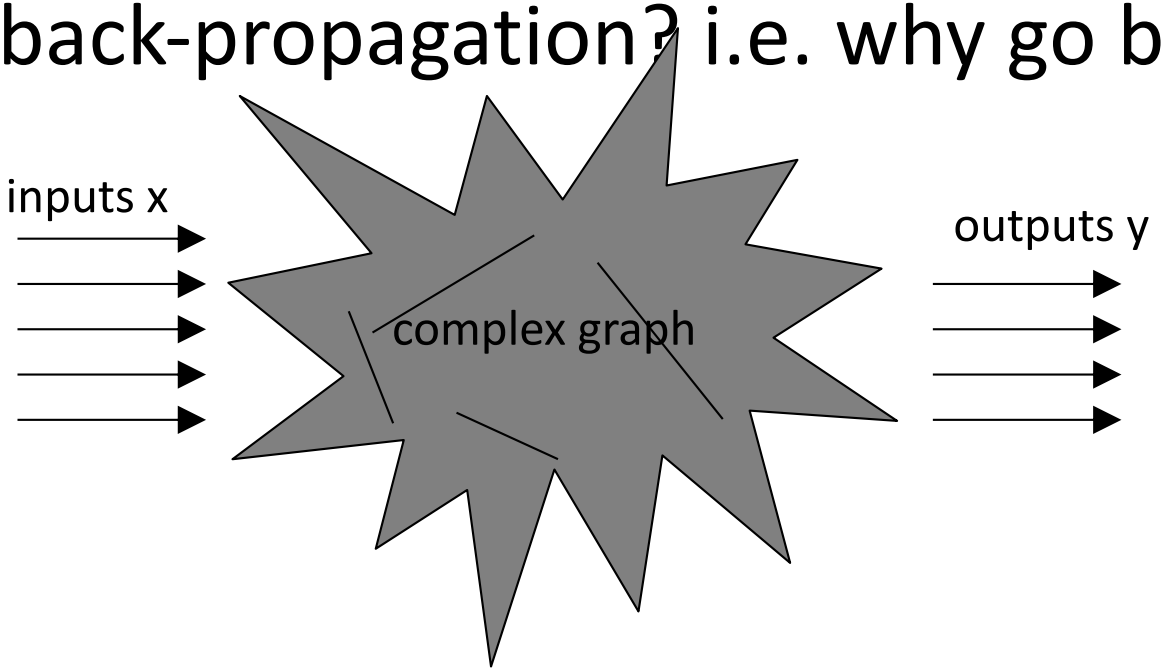

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

(x,y,z are scalars)

Q: Why is it back-propagation?



Why is it back-propagation? i.e. why go backwards?



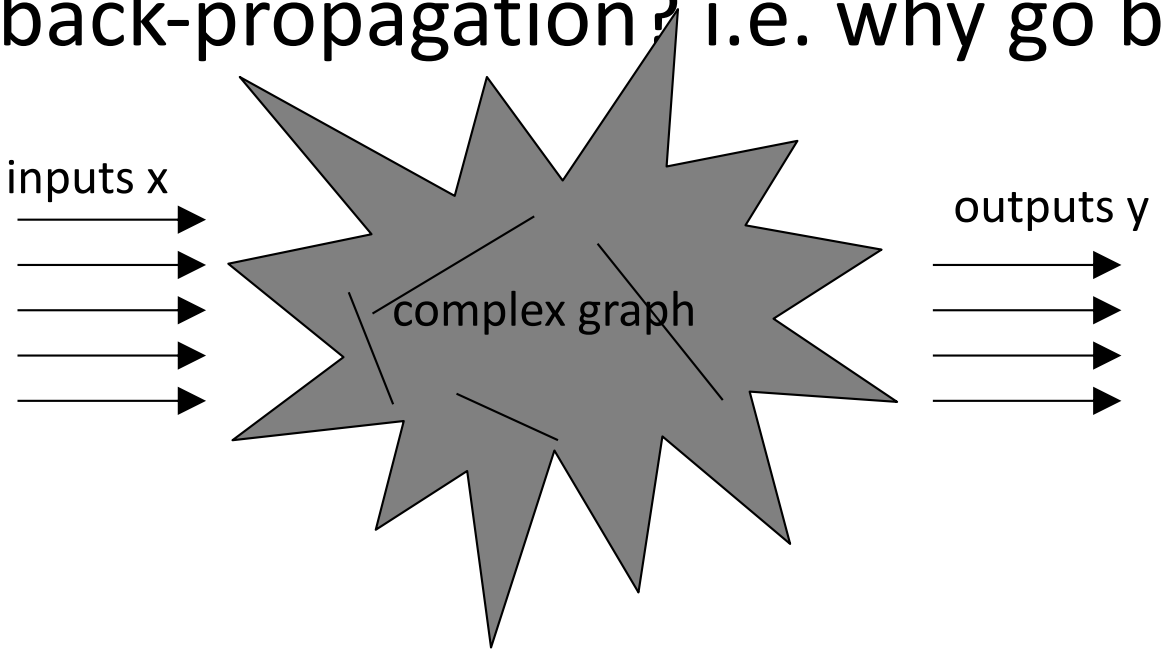
reverse-mode differentiation (if you want effect of many things on one thing)

$\frac{\partial y}{\partial x}$ for many different x

forward-mode differentiation (if you want effect of one thing on many things)

$\frac{\partial y}{\partial x}$ for many different y

Why is it back-propagation? i.e. why go backwards?



reverse-mode differentiation (if you want effect of many things on one thing)

$\frac{\partial y}{\partial x}$ for many different x

More common simply because many nets have a scalar loss function as output.

Example: Torch Layers

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Example: Torch Layers

=

Example: Torch MulConstant

```lua
local MulConstant, parent = torch.class('nn.MulConstant', 'nn.Module')

function MulConstant:__init(constant_scalar,ip)
  parent.__init(self)
  assert(type(constant_scalar) == 'number', 'input is not scalar!')
  self.constant_scalar = constant_scalar

  -- default for inplace is false
   self.inplace = ip or false
   if (ip and type(ip) ~= 'boolean') then
      error('in-place flag must be boolean')
   end
end

function MulConstant:updateOutput(input)
  if self.inplace then
    input:mul(self.constant_scalar)
    self.output = input
  else
    self.output:resizeAs(input)
    self.output:copy(input)
    self.output:mul(self.constant_scalar)
  end
  return self.output
end

function MulConstant:updateGradInput(input, gradOutput)
  if self.gradInput then
    if self.inplace then
      gradOutput:mul(self.constant_scalar)
      self.gradInput = gradOutput
      -- restore previous input value
      input:div(self.constant_scalar)
    else
      self.gradInput:resizeAs(gradOutput)
      self.gradInput:copy(gradOutput)
      self.gradInput:mul(self.constant_scalar)
    end
    return self.gradInput
  end
end
```

$$f(X) = aX$$

initialization

forward()

backward()

Example: Caffe Layers

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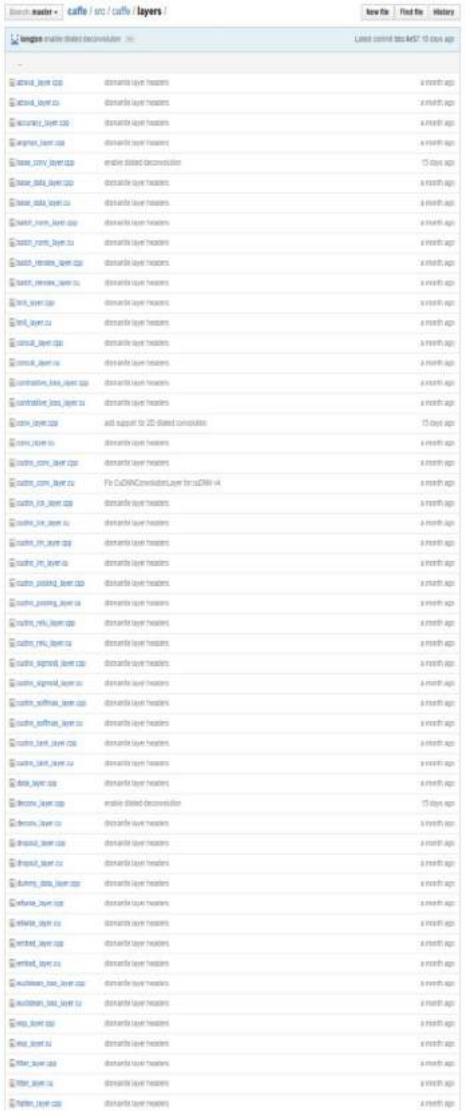

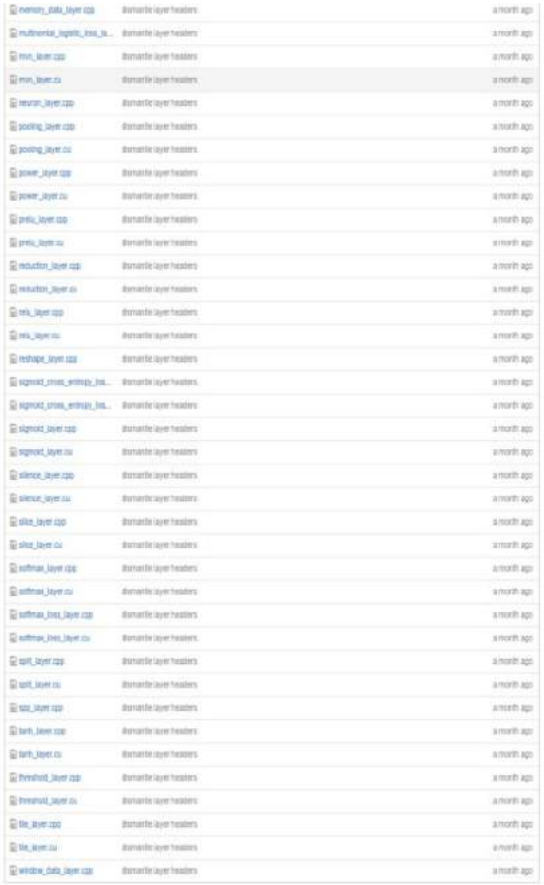

Caffe Sigmoid Layer

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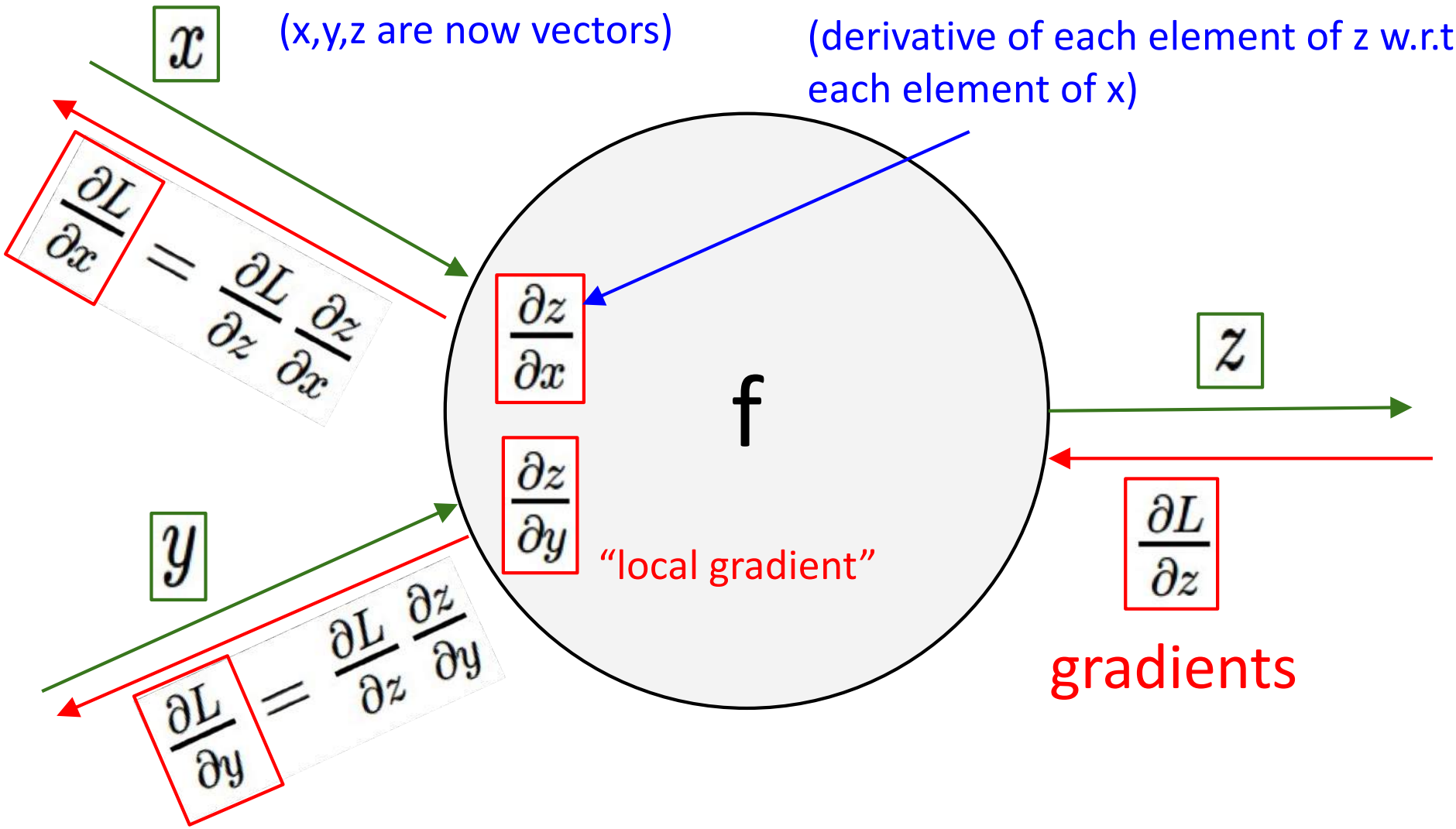
```cpp
#include <cmath>
#include <vector>

#include "caffe/layers/sigmoid_layer.hpp"

namespace caffe {

template <typename Dtype>
inline Dtype sigmoid(Dtype x) {
  return 1. / (1. + exp(-x));
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
    const vector<Blob<Dtype>*>& top) {
  const Dtype* bottom_data = bottom[0]->cpu_data();
  Dtype* top_data = top[0]->mutable_cpu_data();
  const int count = bottom[0]->count();
  for (int i = 0; i < count; ++i) {
    top_data[i] = sigmoid(bottom_data[i]);
  }
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
    const vector<bool>& propagate_down,
    const vector<Blob<Dtype>*>& bottom) {
  if (propagate_down[0]) {
    const Dtype* top_data = top[0]->cpu_data();
    const Dtype* top_diff = top[0]->cpu_diff();
    Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
    const int count = bottom[0]->count();
    for (int i = 0; i < count; ++i) {
      const Dtype sigmoid_x = top_data[i];
      bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x);
    }
  }
}

#ifdef CPU_ONLY
STUB_GPU(SigmoidLayer);
#endif

INSTANTIATE_CLASS(SigmoidLayer);


}  // namespace caffe
```

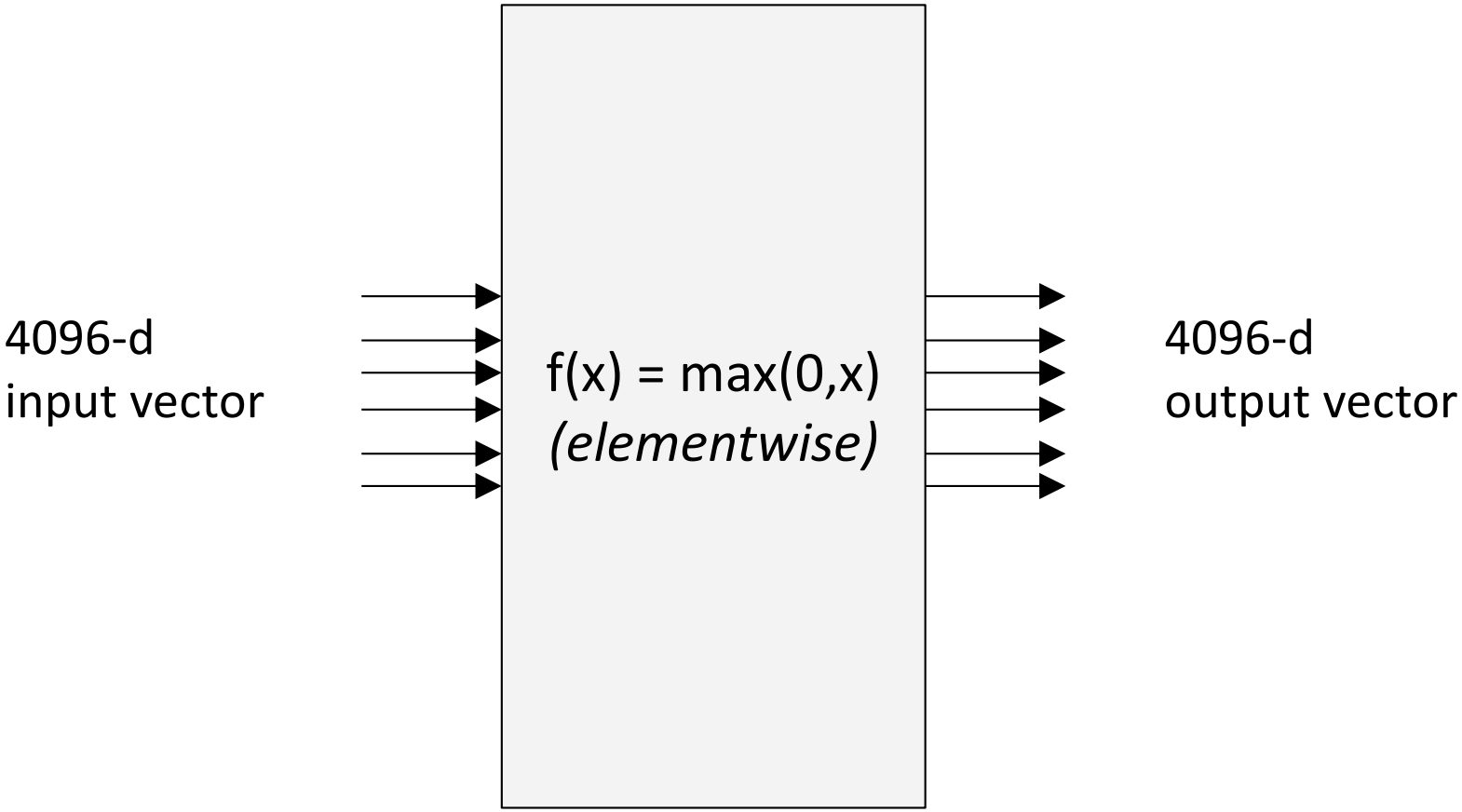
$$\sigma(x) = \frac{1}{1+e^{-x}}$$

$$(1-\sigma(x))\sigma(x)$$ *top_diff (chain rule)

Gradients for vector data



Vectorized operations



Vectorized operations

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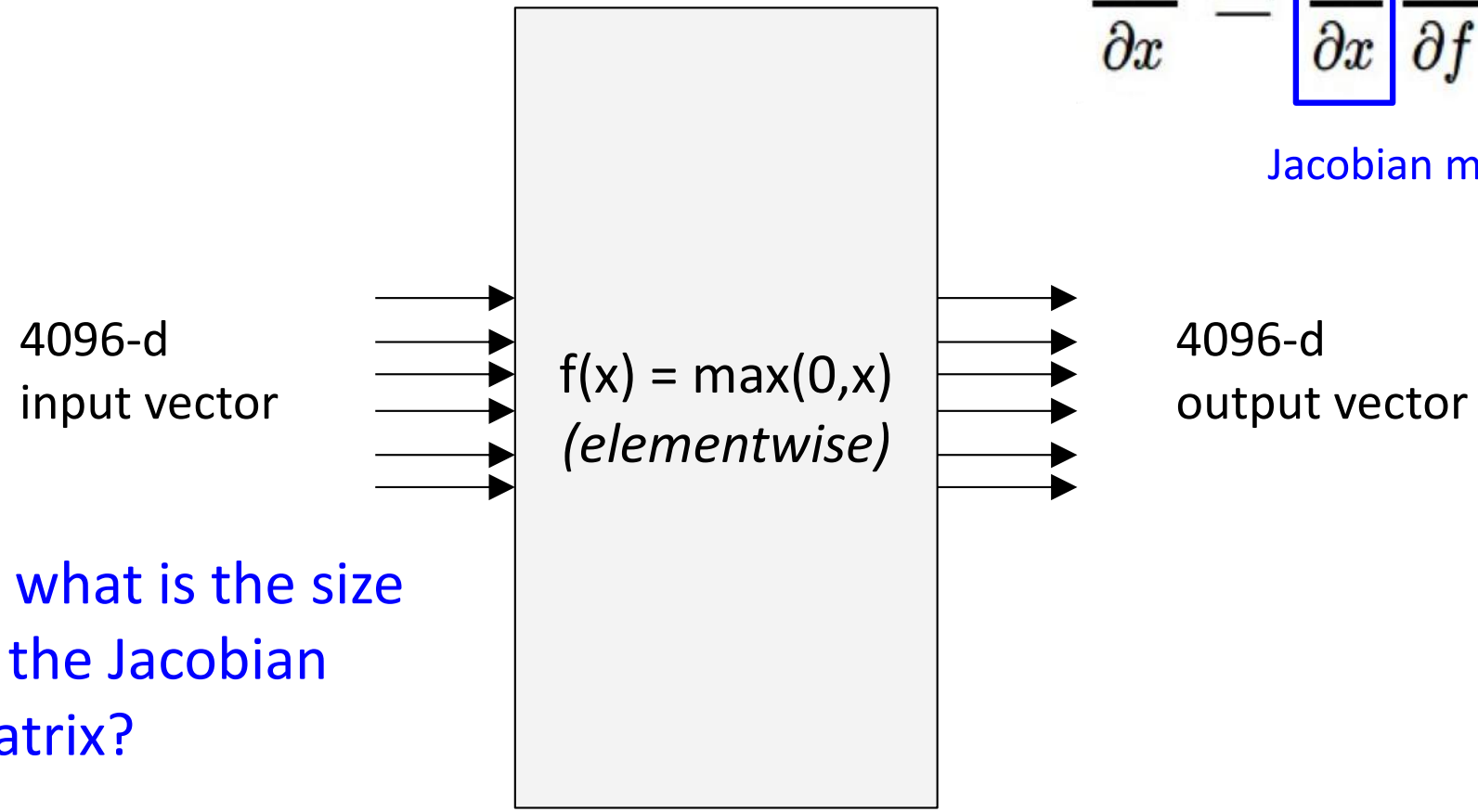
$$\frac{\partial L}{\partial x} = \boxed{\frac{\partial f}{\partial x}} \frac{\partial L}{\partial f}$$

Jacobian matrix



Q: what is the size of the Jacobian matrix?

Vectorized operations

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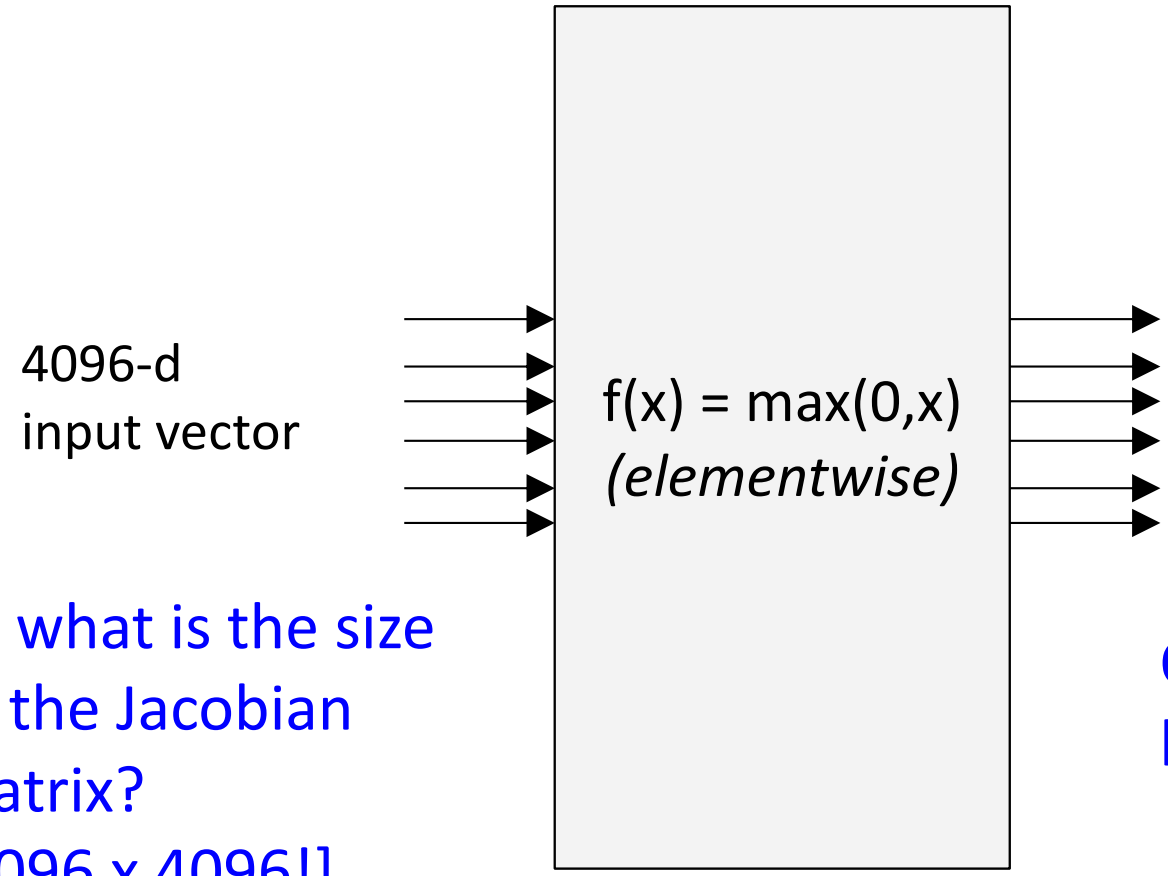
$$\frac{\partial L}{\partial x} = \boxed{\frac{\partial f}{\partial x}} \frac{\partial L}{\partial f}$$

Jacobian matrix



Q: what is the size of the Jacobian matrix?
[4096 x 4096!]

Q2: what does it look like?

Vectorized operations

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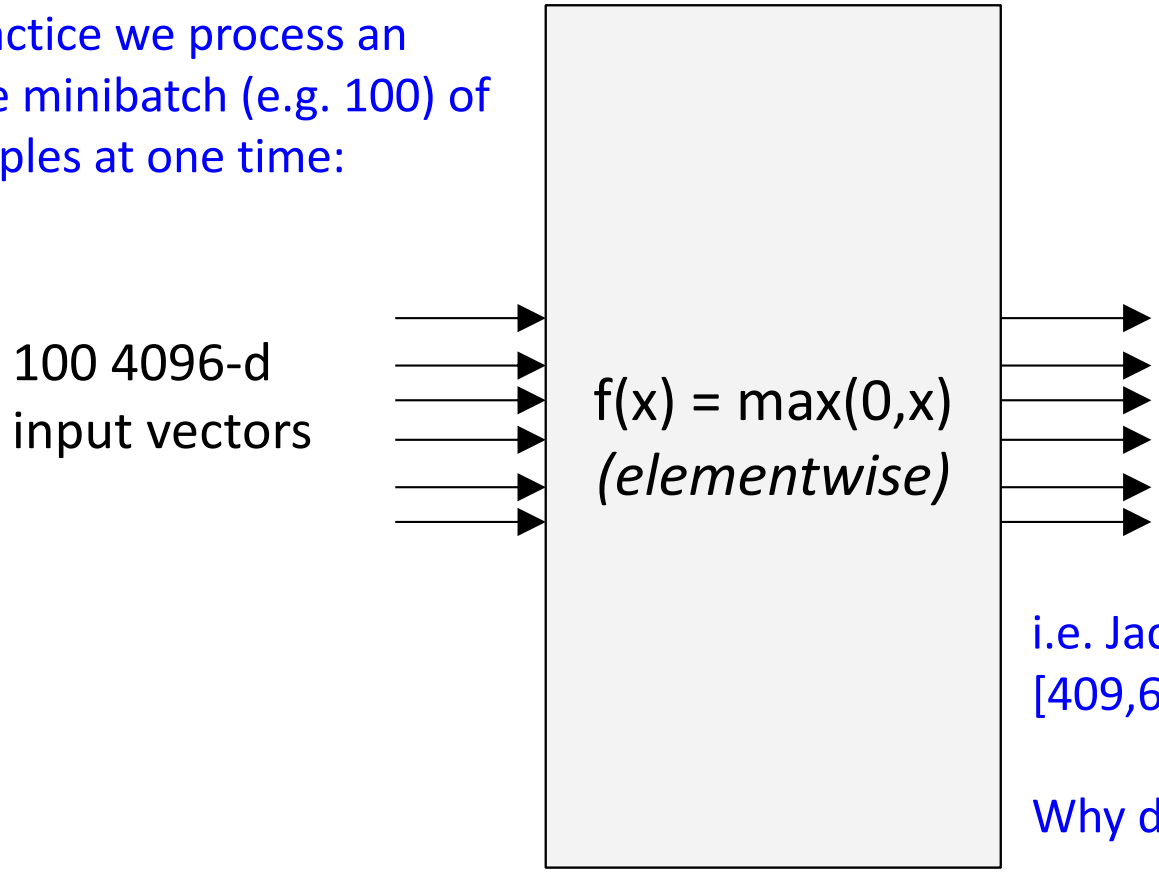
in practice we process an entire minibatch (e.g. 100) of examples at one time:



i.e. Jacobian would technically be a [409,600 x 409,600] matrix :\

Why don't we compute it that way?

And yes, since these are just computations, we can also implement SVMs

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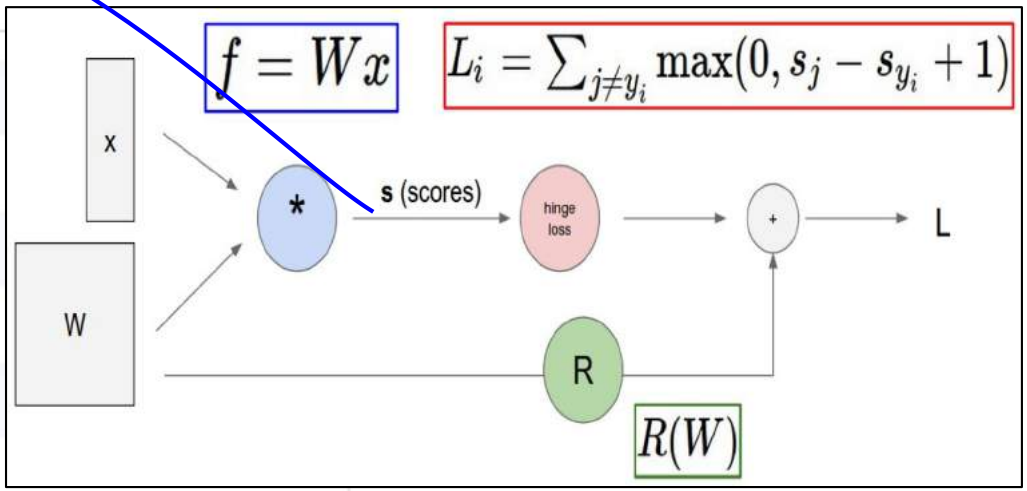
E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 8 lines)
scores = #...
margins = #...
data_loss = #...
reg_loss = #...
loss = data_loss + reg_loss
# backward pass (we have 5 lines)
dmargins = # ... (optionally, we go direct to dscores)
dscores = #...
dW = #...
```



What have you learnt so far?

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- neural nets will be very large: no hope of writing down gradient formula by hand for all parameters
- backpropagation = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates
- implementations maintain a graph structure, where the nodes implement the forward() / backward() API.
- forward: compute result of an operation and save any intermediates needed for gradient computation in memory
- backward: apply the chain rule to compute the gradient of the loss function with respect to the inputs.

Real Neural Networks

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Neural Network: without the brain stuff

(**Before**) Linear score function:

$$f = Wx$$

Neural Network: without the brain stuff

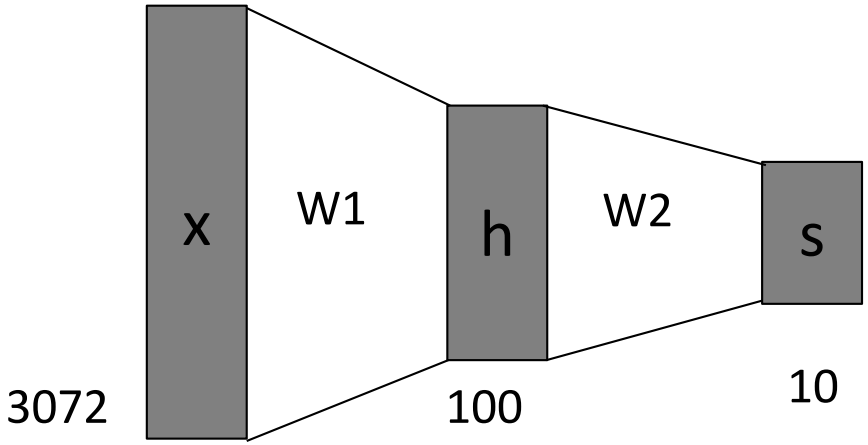
(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

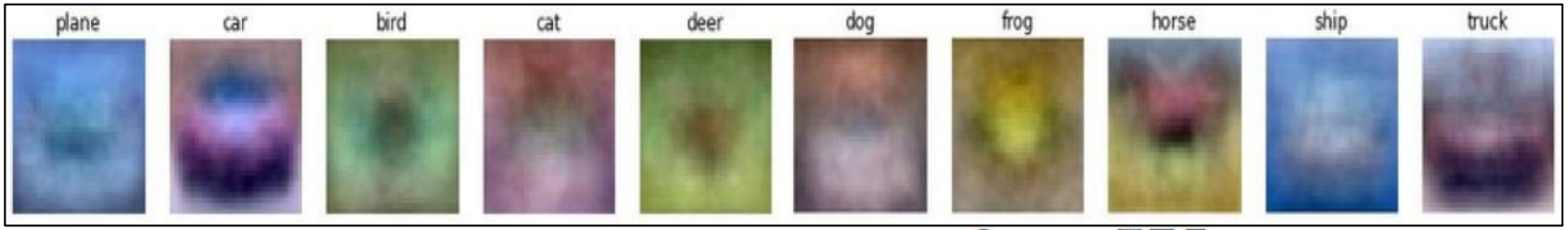
Neural Network: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

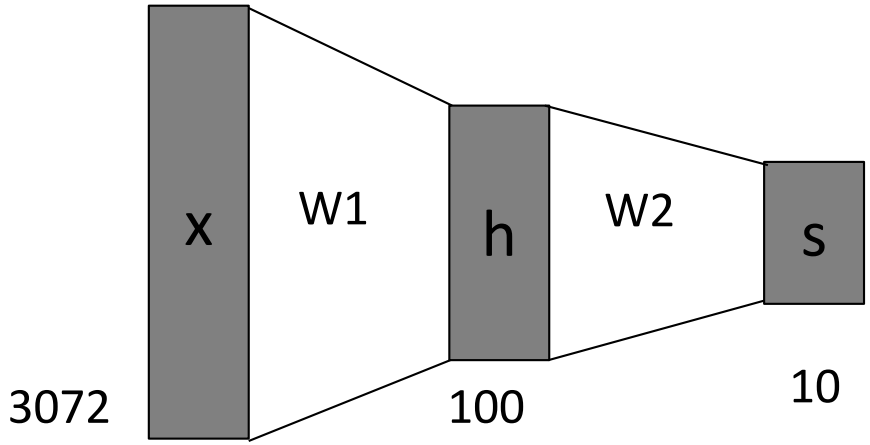


Neural Network: without the brain stuff



(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$



Neural Network: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

or 3-layer Neural Network

$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

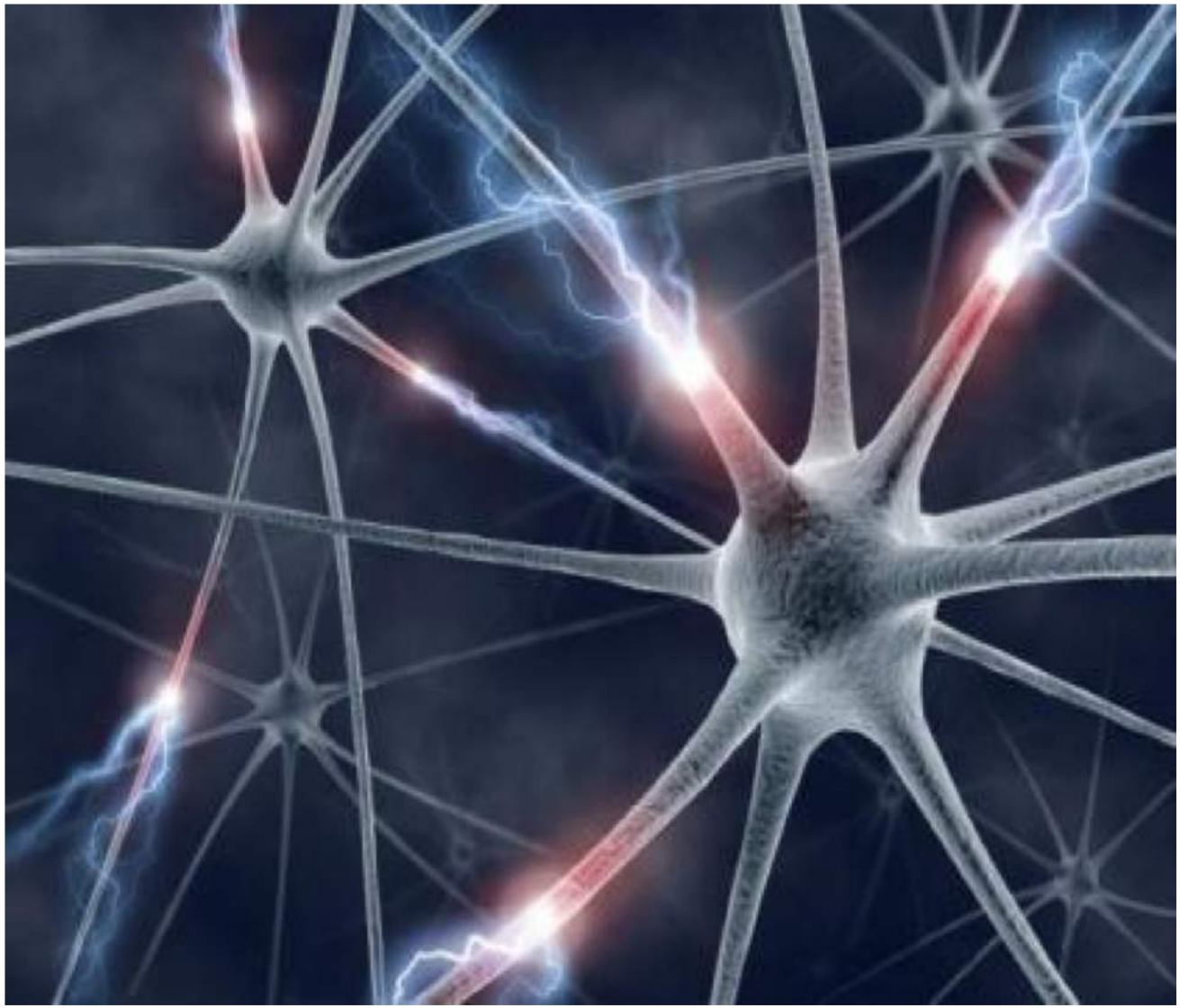
Full implementation of training a 2-layer Neural Network needs ~11 lines:

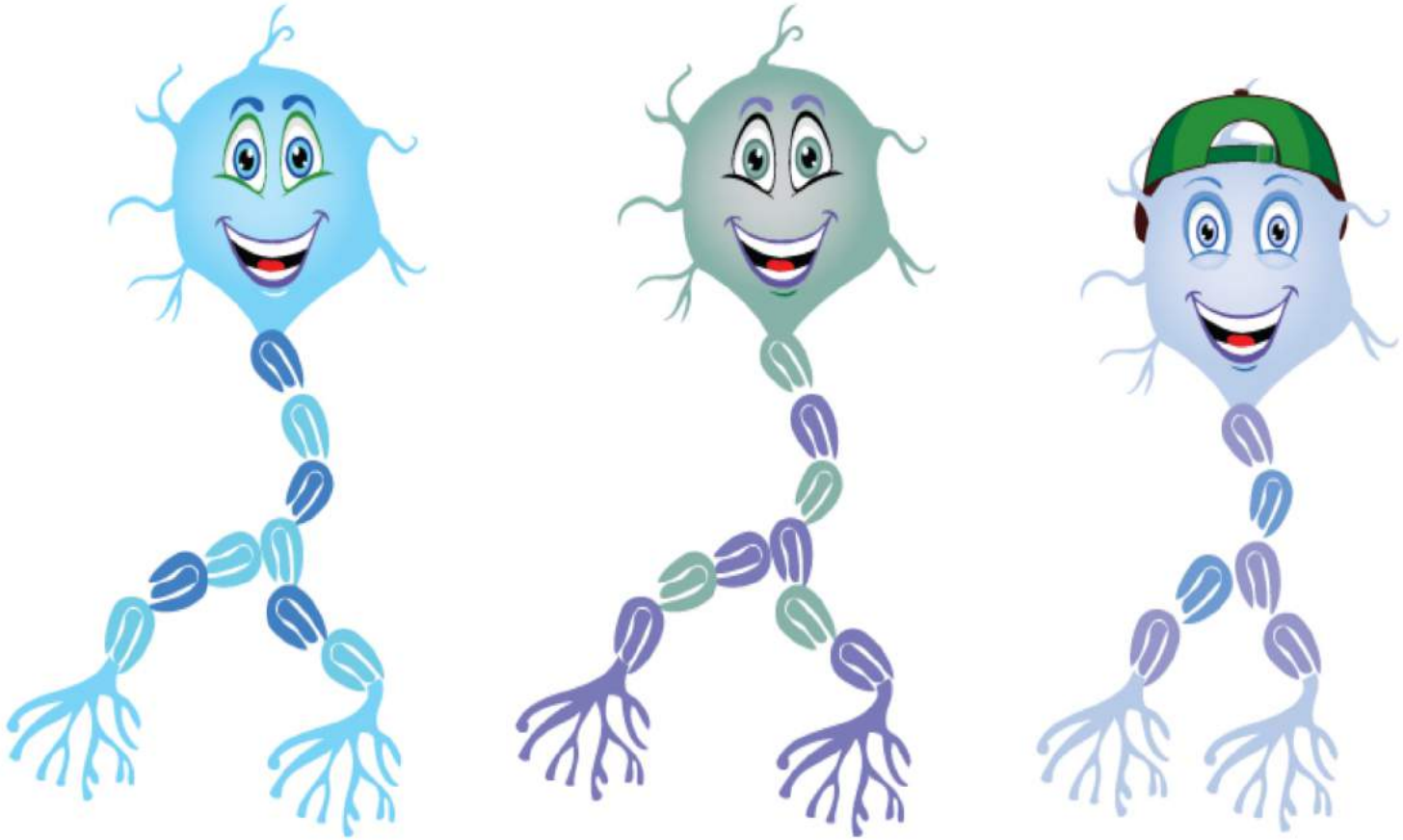
```
01. X = np.array([ [0,0,1],[0,1,1],[1,0,1],[1,1,1] ])
02. y = np.array([[0,1,1,0]]).T
03. syn0 = 2*np.random.random((3,4)) - 1
04. syn1 = 2*np.random.random((4,1)) - 1
05. for j in xrange(60000):
06.     l1 = 1/(1+np.exp(-(np.dot(X,syn0))))
07.     l2 = 1/(1+np.exp(-(np.dot(l1,syn1))))
08.     l2_delta = (y - l2)*(l2*(1-l2))
09.     l1_delta = l2_delta.dot(syn1.T) * (l1 * (1-l1))
10.     syn1 += l1.T.dot(l2_delta)
11.     syn0 += X.T.dot(l1_delta)
```

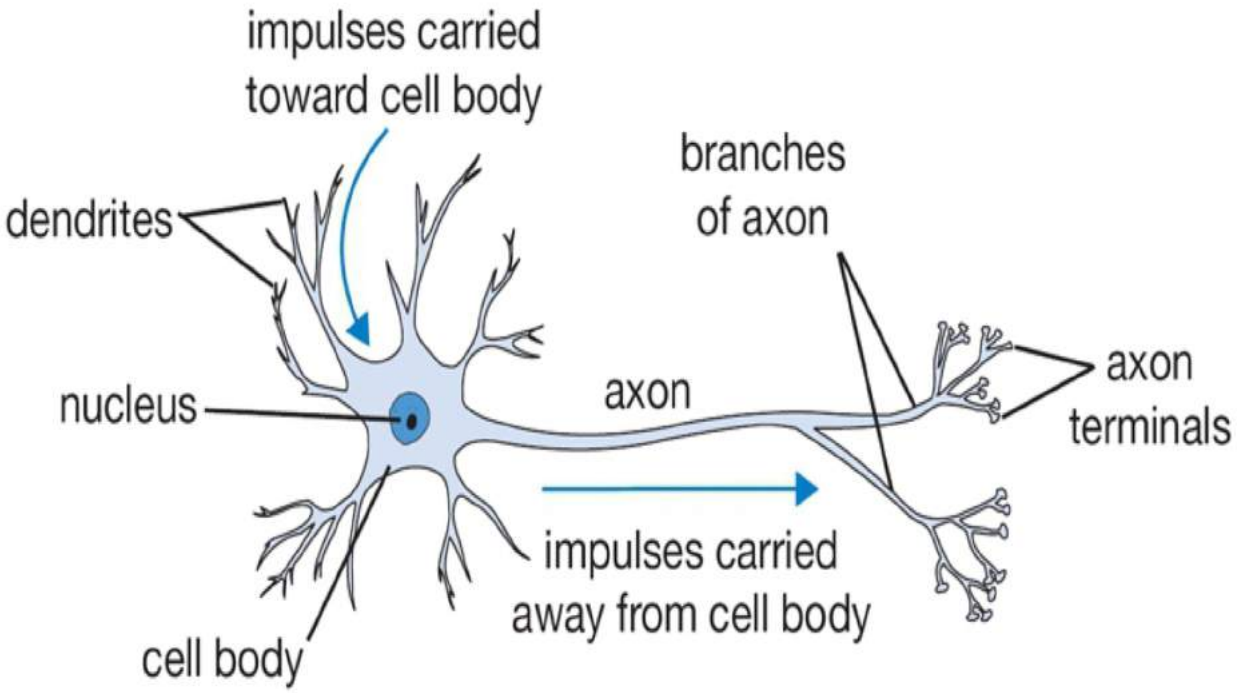
from @iamtrask, http://iamtrask.github.io/2015/07/12/basic-python-network/

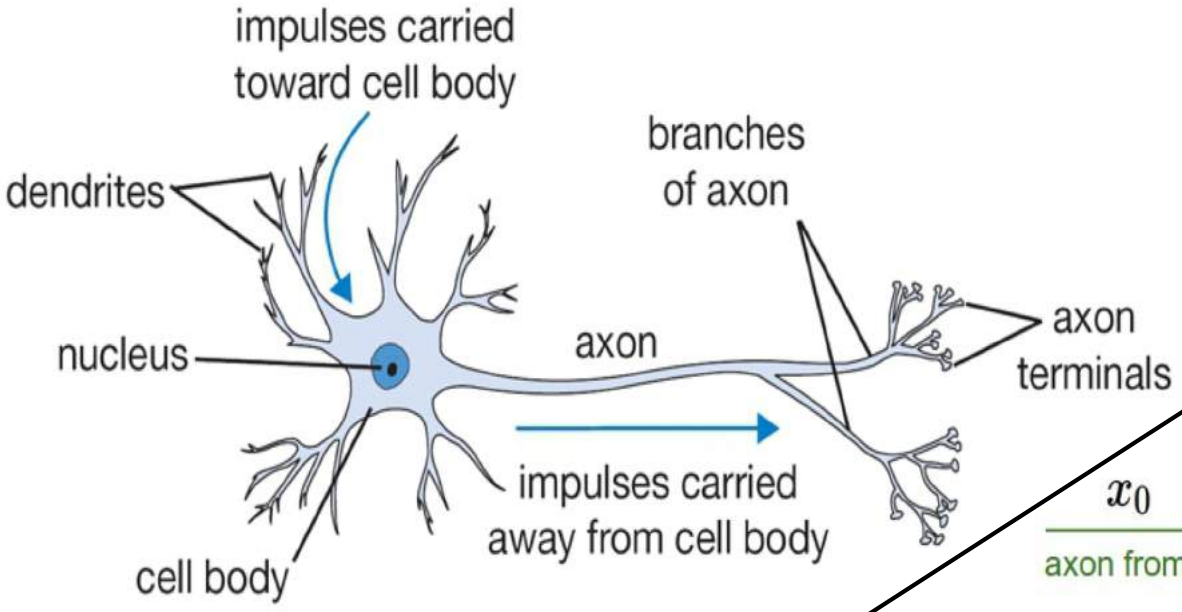
Stage your forward/backward computation!

```
# receive W1,W2,b1,b2 (weights/biases), X (data)
# forward pass:
h1 = #... function of X,W1,b1
scores = #... function of h1,W2,b2
loss = #... (several lines of code to evaluate Softmax loss)
# backward pass:
dscores = #...
dh1,dW2,db2 = #...
dW1,db1 = #...
```




impulses carried
toward cell body
dendrites
branches
of axon
nucleus
axon
axon
terminals
impulses carried
away from cell body
cell body


impulses carried
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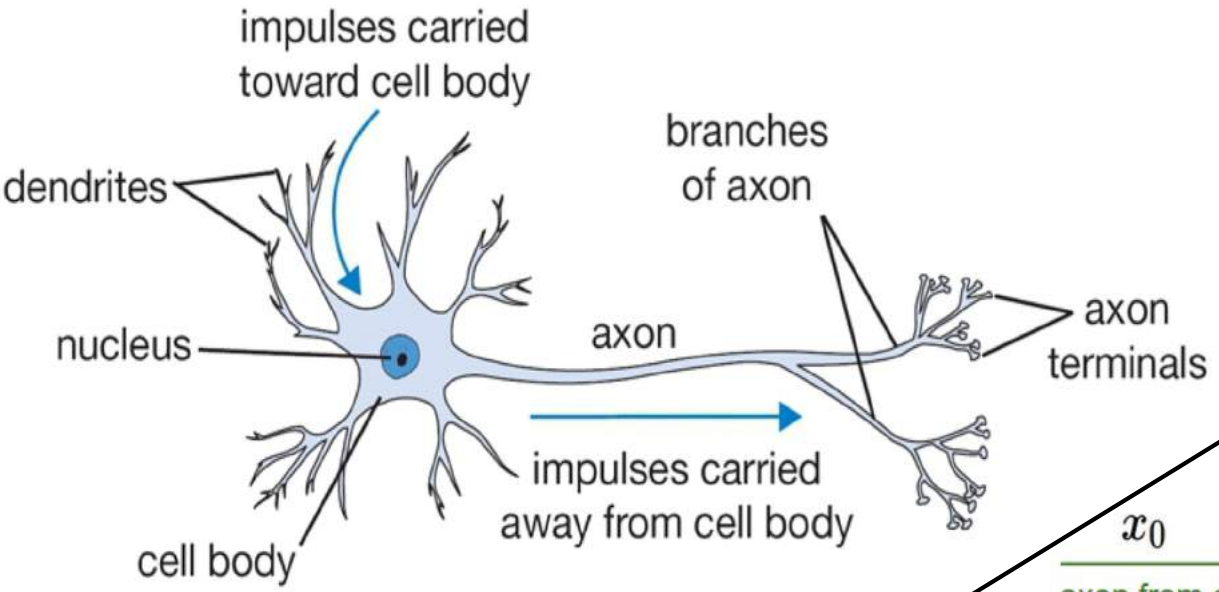
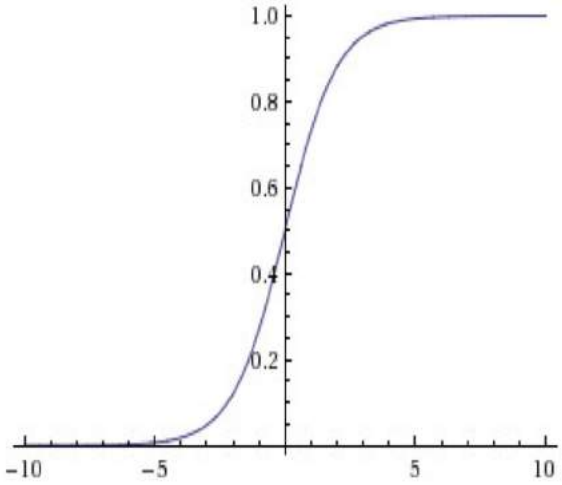
of axon
nucleus
axon
axon
terminals
impulses carried
away from cell body
cell body

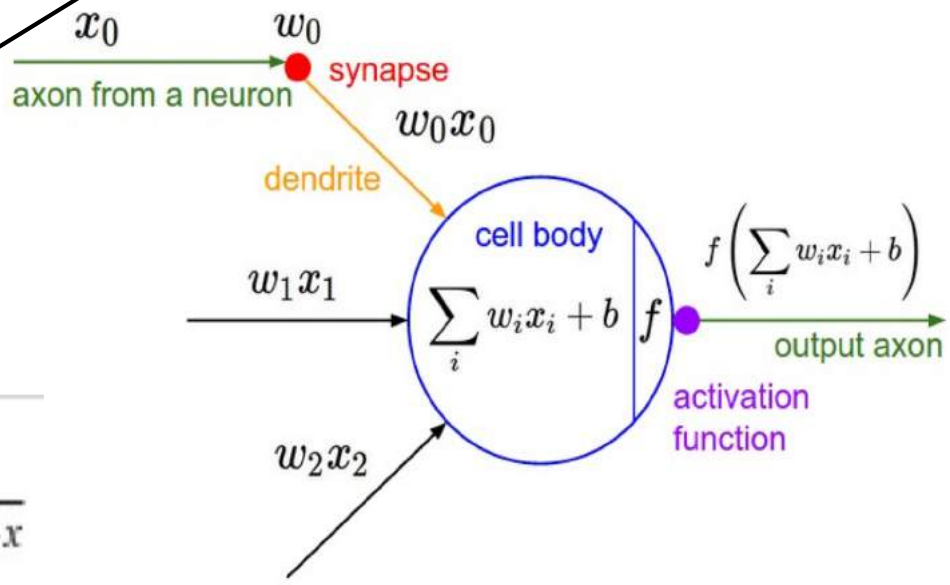
x_0
w_0
axon from a neuron
synapse
$w_0 x_0$
dendrite
cell body
$w_1 x_1$
$\sum_i w_i x_i + b$
f
$f\left(\sum_i w_i x_i + b\right)$
output axon
activation
function
$w_2 x_2$

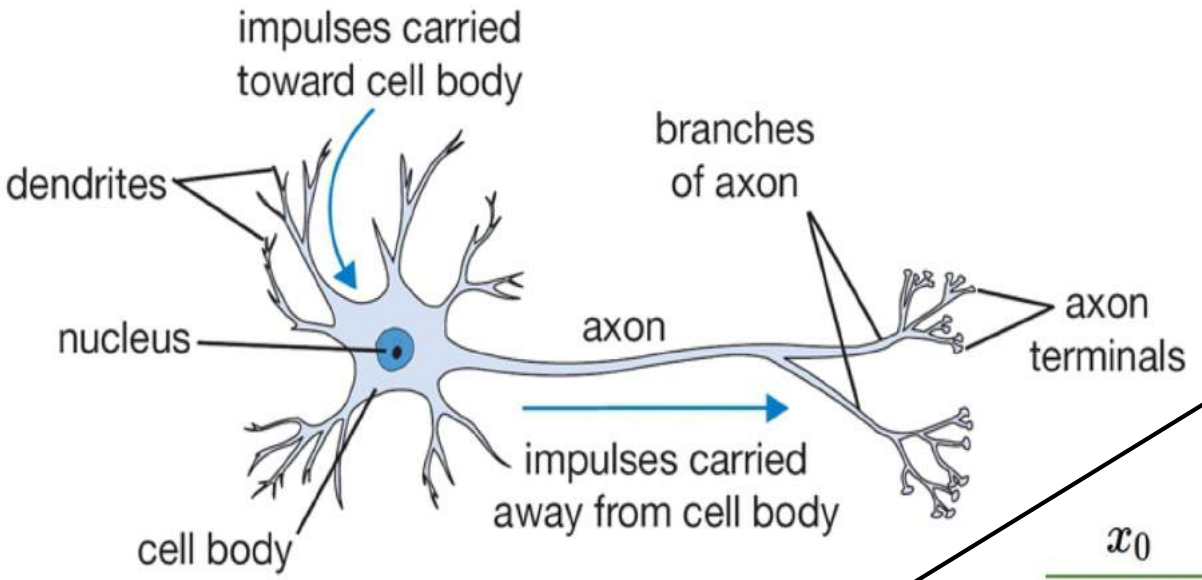


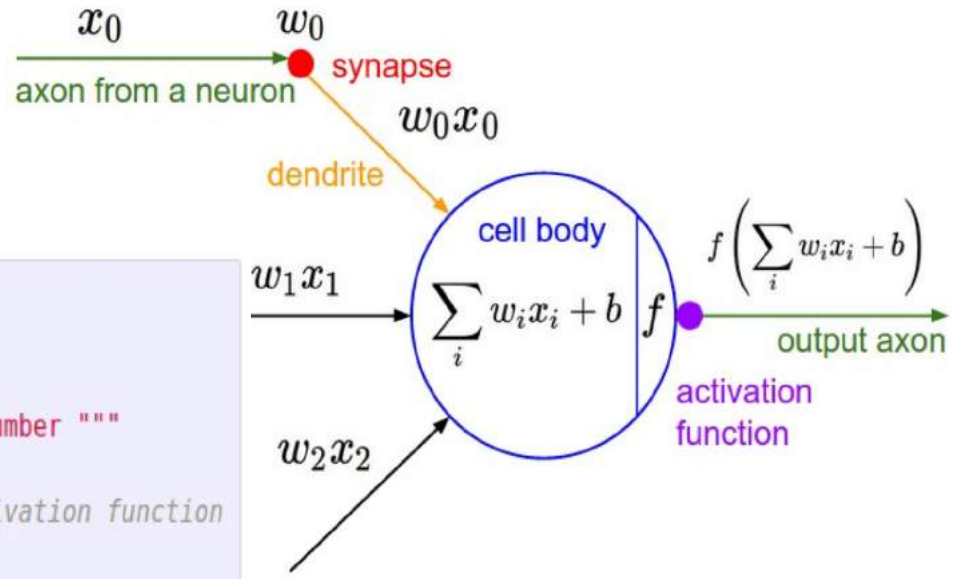


sigmoid activation function

$$\frac{1}{1+e^{-x}}$$





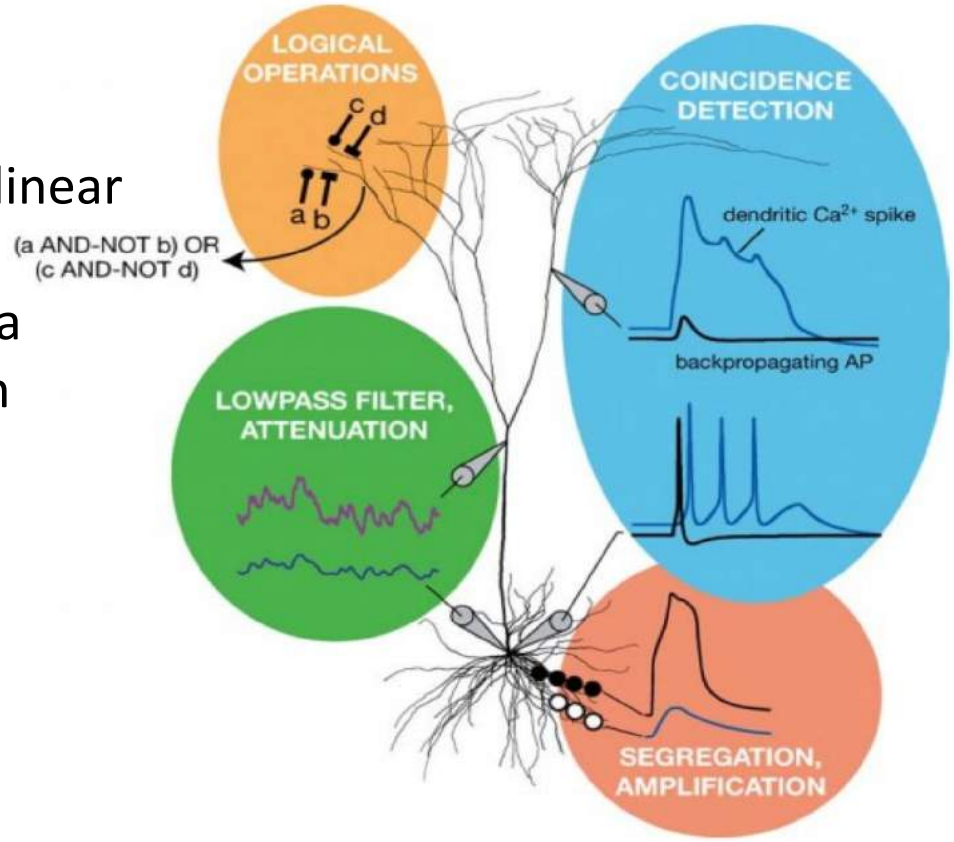



```python
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation function
    return firing_rate
```

Be very careful with your Brain analogies:

Biological Neurons:

- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate

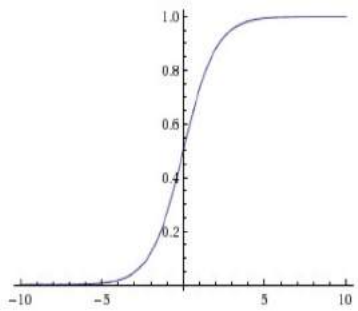


[Dendritic Computation. London and Hausser]

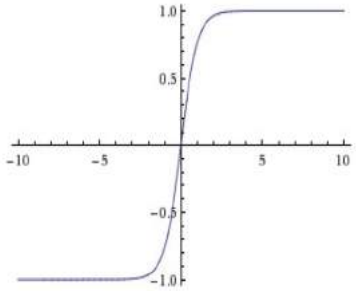
Activation Functions

Sigmoid

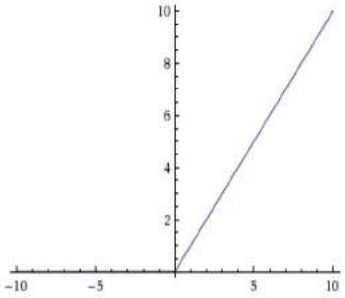
$$\sigma(x) = 1/(1+e^{-x})$$



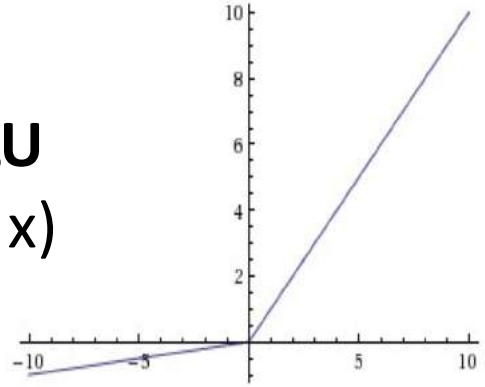
tanh tanh(x)



ReLU max(0,x)



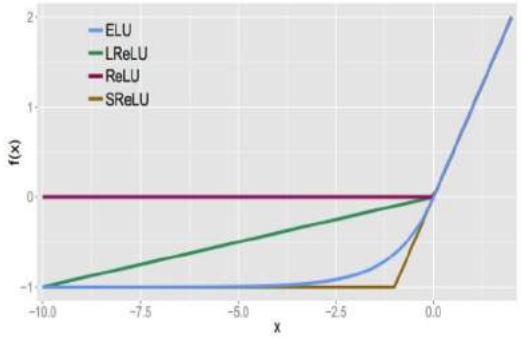
Leaky ReLU
max(0.1x, x)



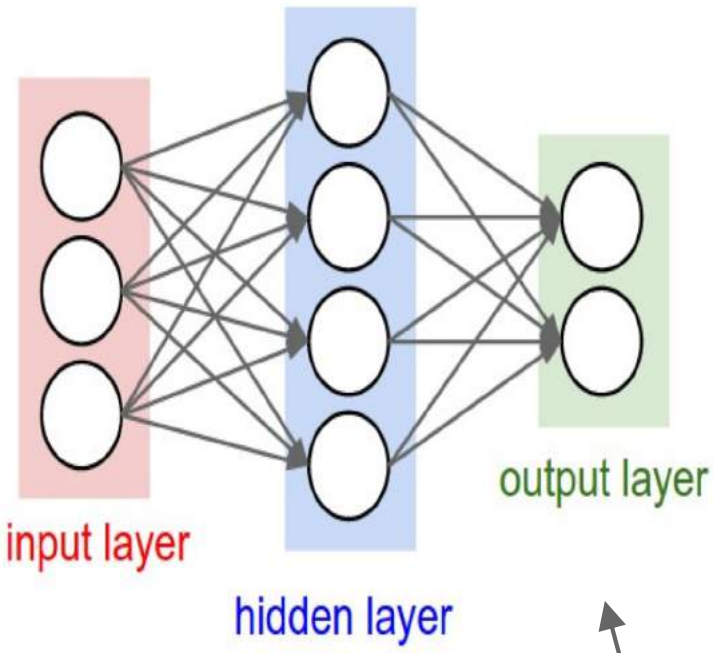
Maxout $\max(w_1^T x + b_1, w_2^T x + b_2)$

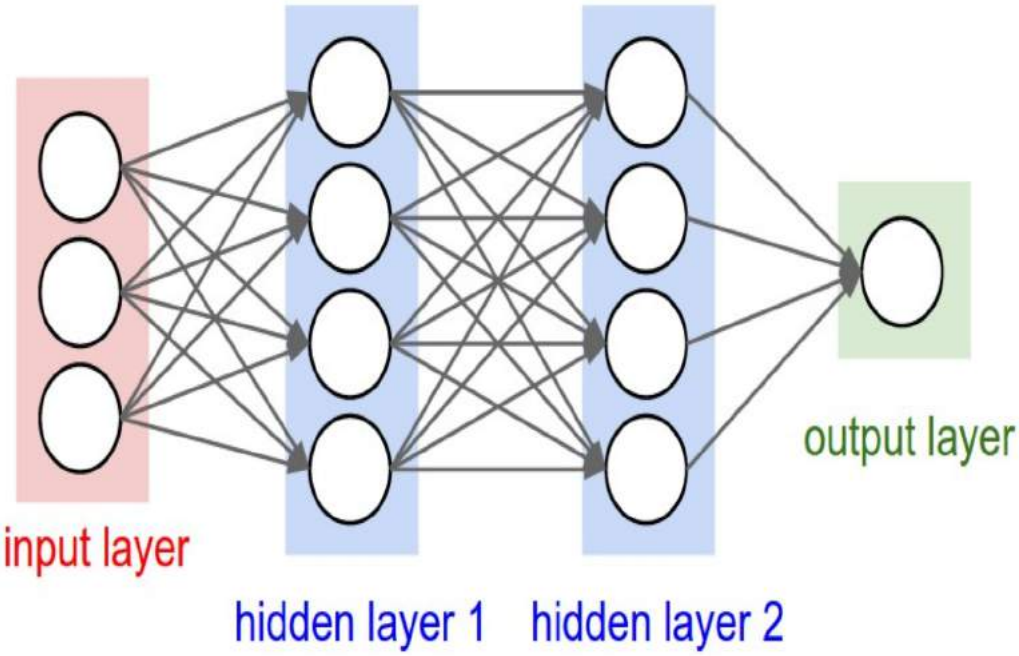
ELU

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$



Neural Networks: Architectures





"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

"Fully-connected" layers

Example Feed-forward computation of a Neural Network

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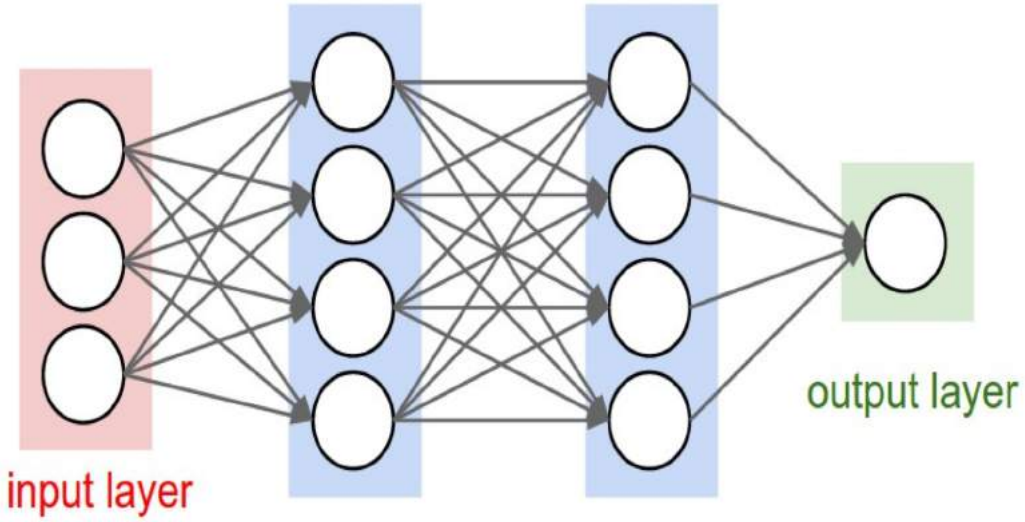
```
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation function
    return firing_rate
```

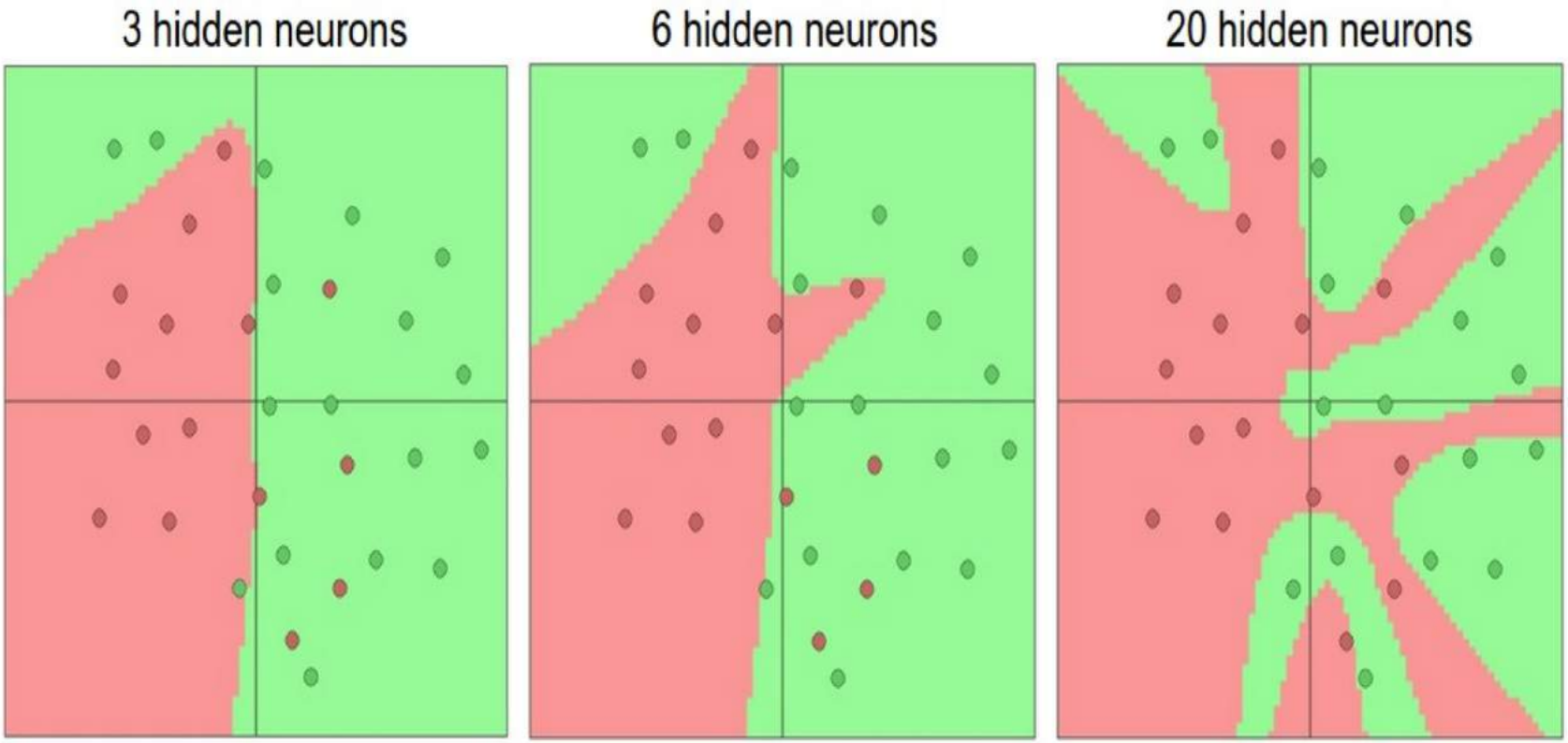
We can efficiently evaluate an entire layer of neurons.

Example Feed-forward computation of a Neural Network



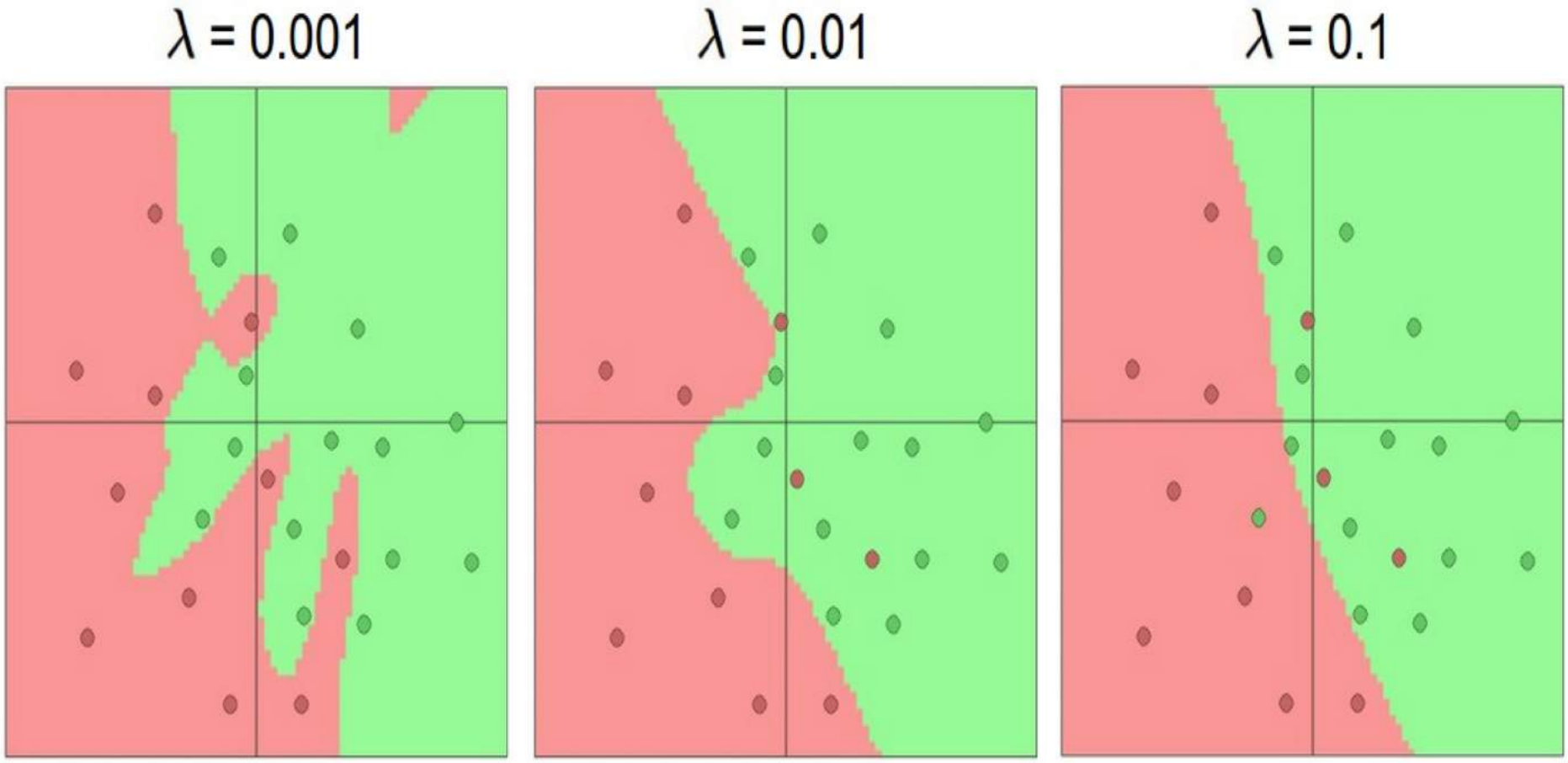

```
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```

Setting the number of layers and their sizes



more neurons = more capacity

Do not use size of neural network as a regularizer. Use stronger regularization instead:



(you can play with this demo over at ConvNetJS: http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html)

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What have you learnt?

- we arrange neurons into fully-connected layers
- the abstraction of a **layer** has the nice property that it allows us to use efficient vectorized code (e.g. matrix multiplies)
- neural networks are not really *neural*
- neural networks: bigger = better (but might have to regularize more strongly)

More than you ever wanted to know about Neural Networks and how to train them.