Lecture 6: Backpropagation Vector, Matrix and Tensor Derivatives

Where we are ...

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

scores function

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

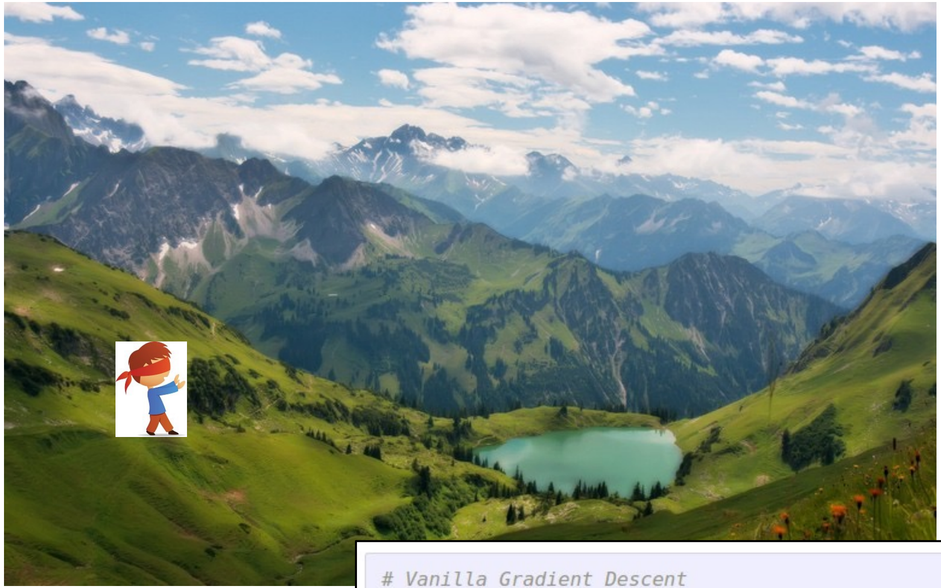
SVM loss

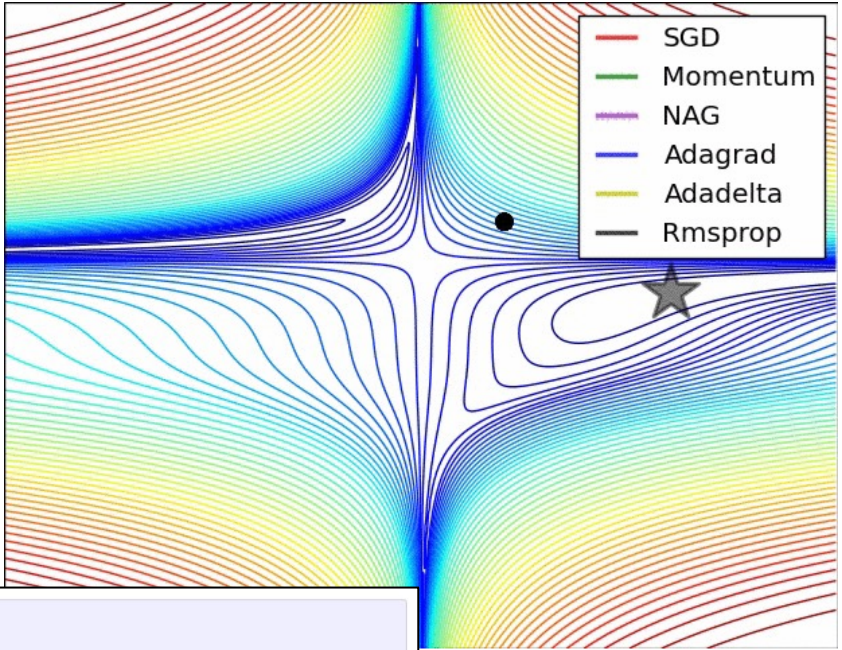
$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \sum_k W_k^2$$

data loss + regularization

want $\boxed{\nabla_W L}$

Optimization






```python
# 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

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

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

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

Overview of where we're going

- We want to **evaluate** the gradient of a Loss function L(x,W,...), with respect to the parameters (weights) of a neural network, at the "point" represented by the arguments to the function (x,W,...).
    - We are **not interested** in an **algebraic expression** for the gradient, but rather only in the **evaluation of that gradient at the current value of the function** arguments.

Consider the function

$$z(x, y) = x^2 + y^2,$$

and suppose we are interested in evaluating the gradient of this function at the point

$$(x, y) = (5, 3).$$

Evaluate the gradient:

$$\frac{\partial z}{\partial x} = 2x.$$

$$\frac{\partial z}{\partial y} = 2y.$$

The algebraic expression of the gradient is just the collection of these partials into a "vector":

$$\nabla z = \begin{bmatrix} 2x \\ 2y \end{bmatrix}.$$

Don't care about this

The evaluation of this gradient at the point $(x, y) = (5, 3)$ is simply

Do care about this

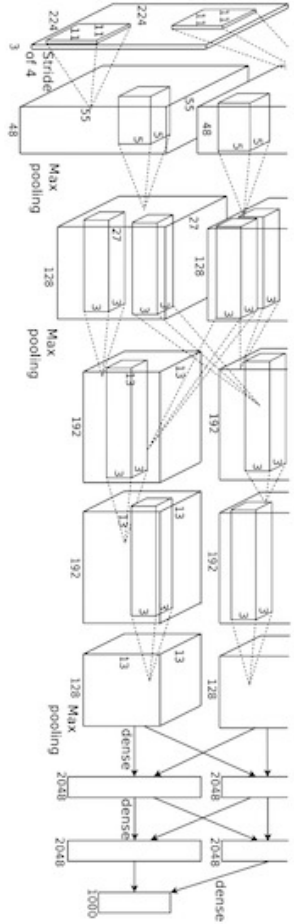
$$\nabla z(5, 3) = \begin{bmatrix} 2 \times 5 \\ 2 \times 3 \end{bmatrix} = \begin{bmatrix} 10 \\ 6 \end{bmatrix}.$$

Convolutional Network (AlexNet)

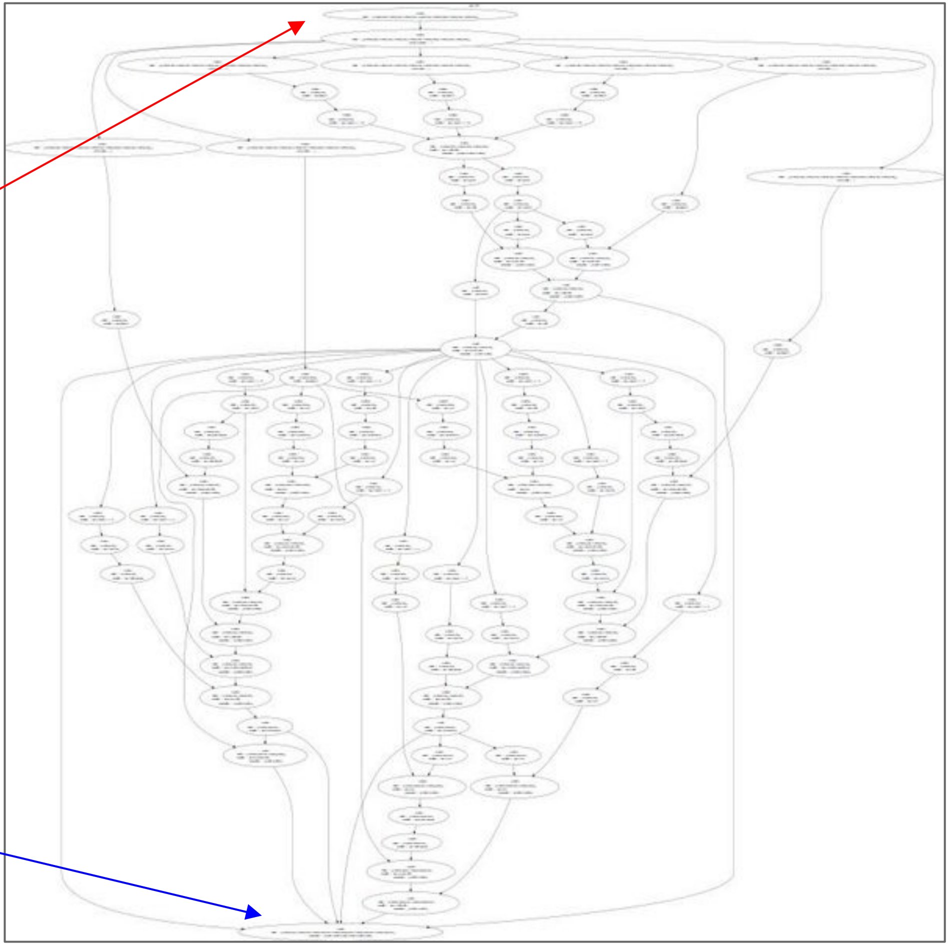
input image

weights

loss



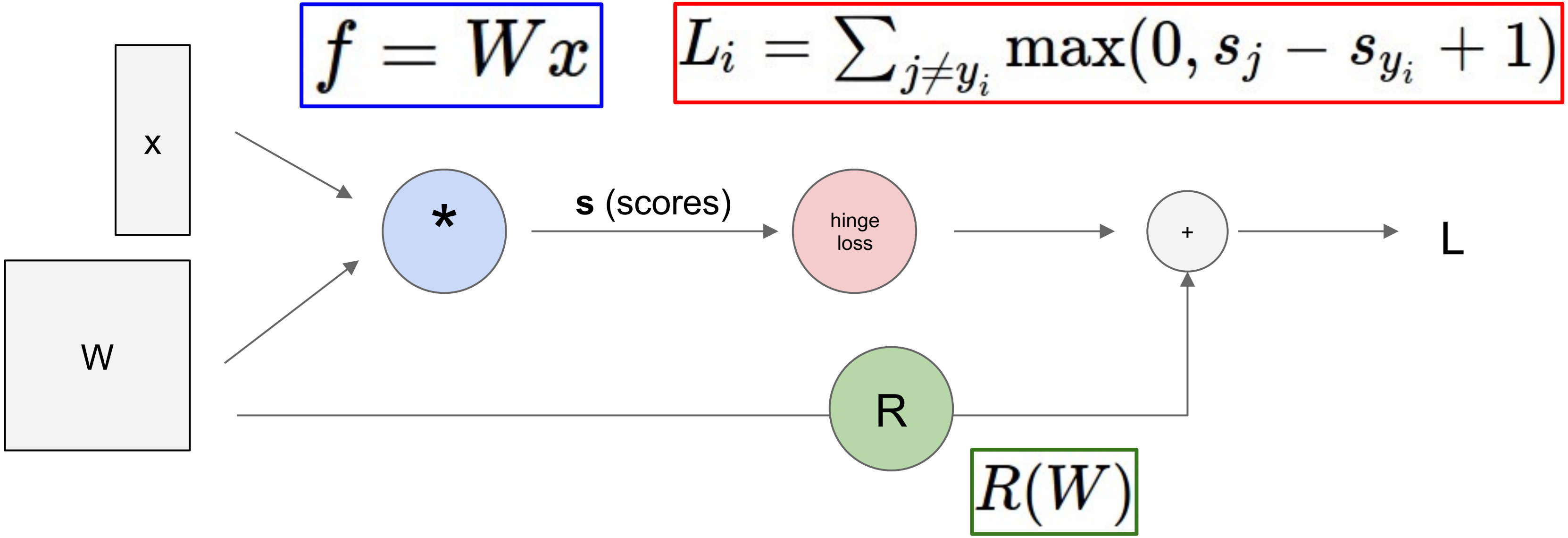
Neural Turing Machine



input tape

loss

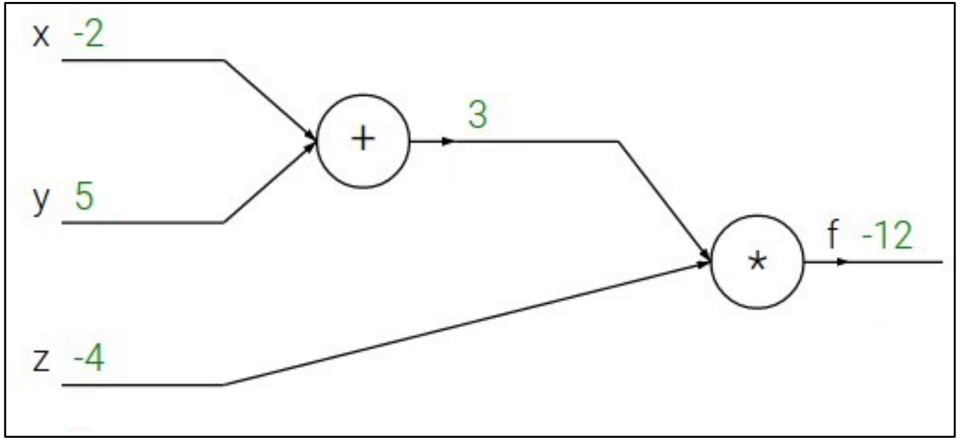
Computational Graph



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

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

Forward pass: evaluating each expression in the computational graph from the inputs to the final output (or outputs). The results of each forward step are shown in green.



```
# set some inputs
x = -2; y = 5; z = -4

# perform the forward pass
q = x + y # q becomes 3
f = q * z # f becomes -12

# perform the backward pass (backpropagation) in reverse order:
# first backprop through f = q * z
dfdz = q # df/dz = q, so gradient on z becomes 3
dfdq = z # df/dq = z, so gradient on q becomes -4
# now backprop through q = x + y
dfdx = 1.0 * dfdq # dq/dx = 1. And the multiplication here is the chain rule!
dfdy = 1.0 * dfdq # dq/dy = 1
```

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

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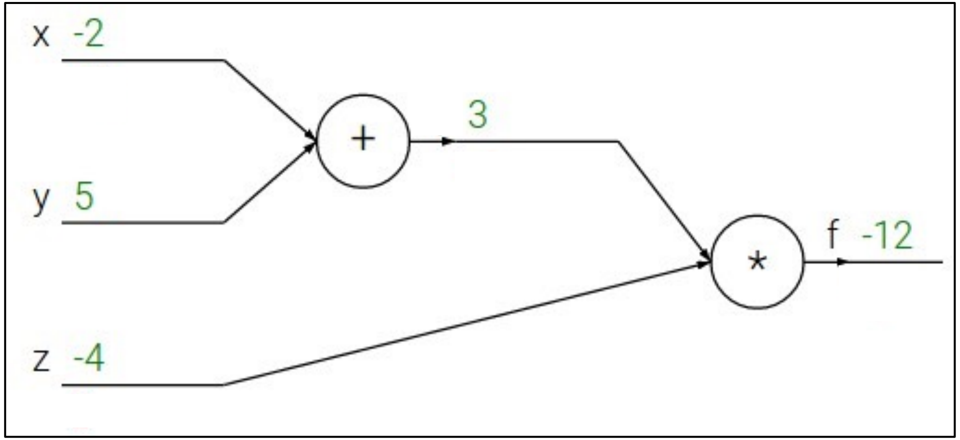
Backward pass: evaluating the partial derivative of each **parameter** or **intermediate result** in the computational graph from the outputs back to the inputs.The results of each backward step are shown in red.



Goal is to calculate

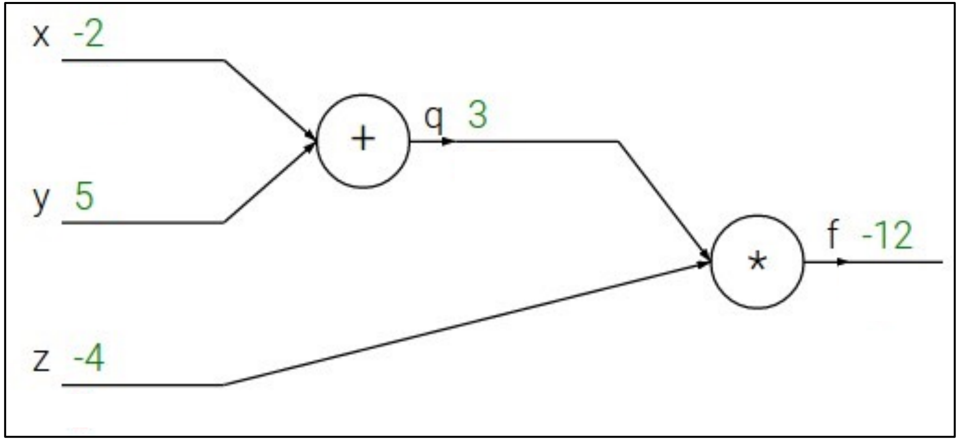
$$\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$

evaluated at the point

$$[x = -2, y = 5, z = -4].$$

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

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



$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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

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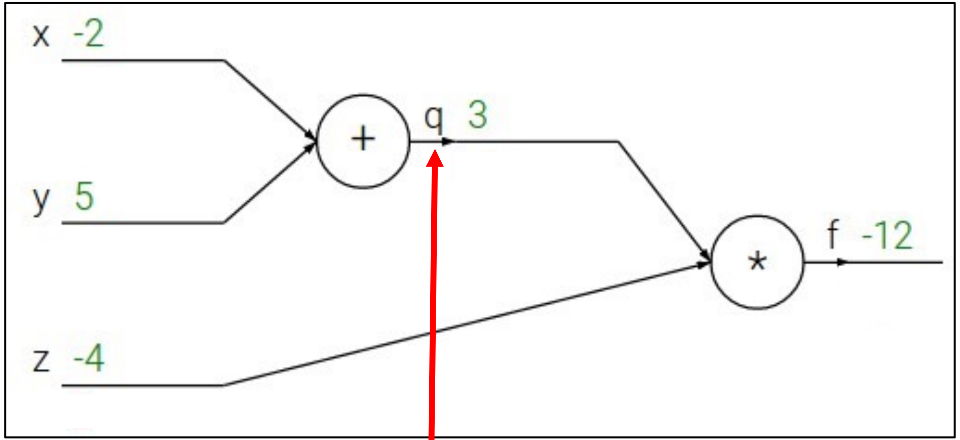

Important: name the intermediate quantities

Compute some **local partial derivatives.** These are derivatives of the outputs of a node with respect to the inputs....

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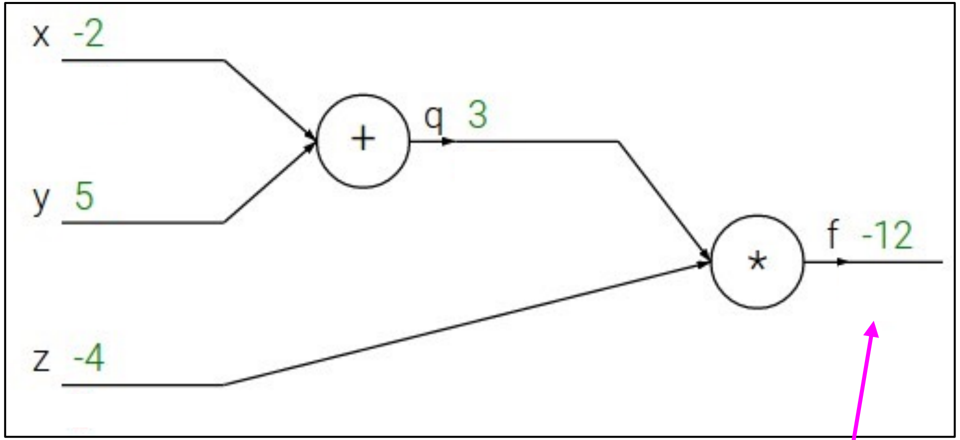

$$\frac{\partial f}{\partial f}$$

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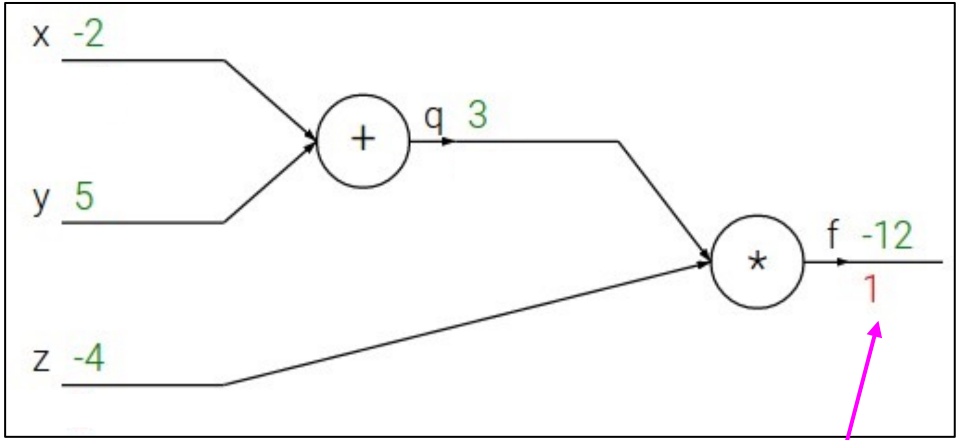

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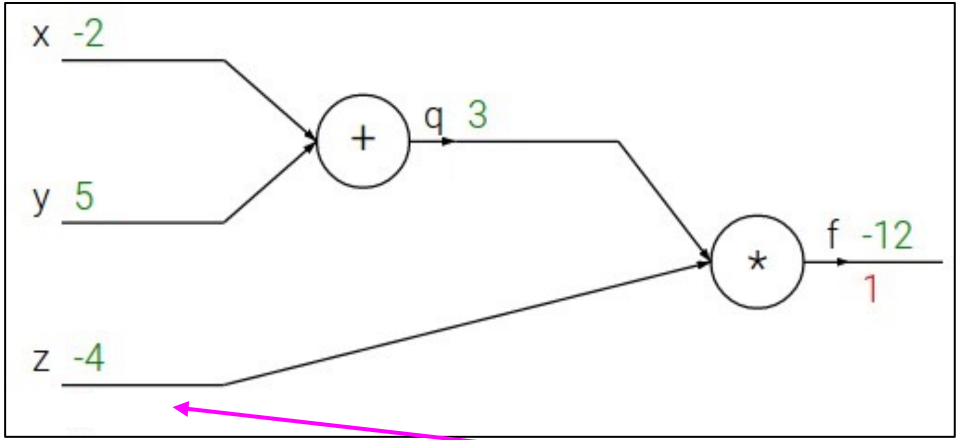

$\frac{\partial f}{\partial z}$

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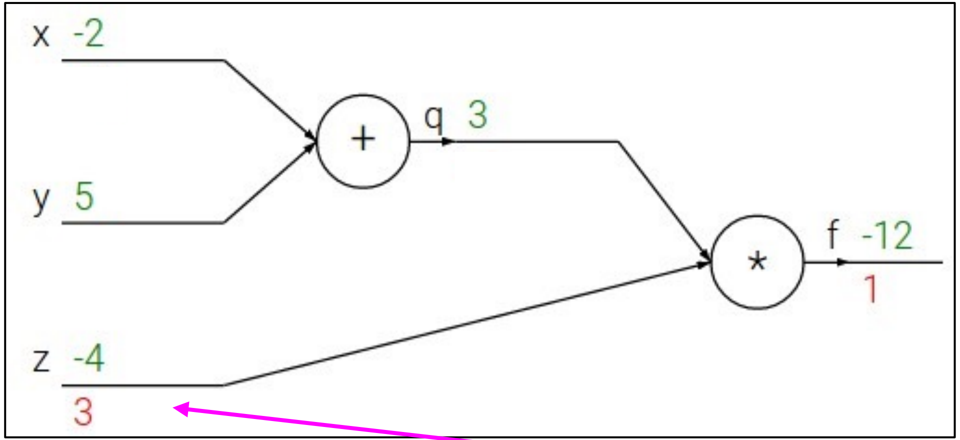

$$\boxed{\frac{\partial f}{\partial z}}$$

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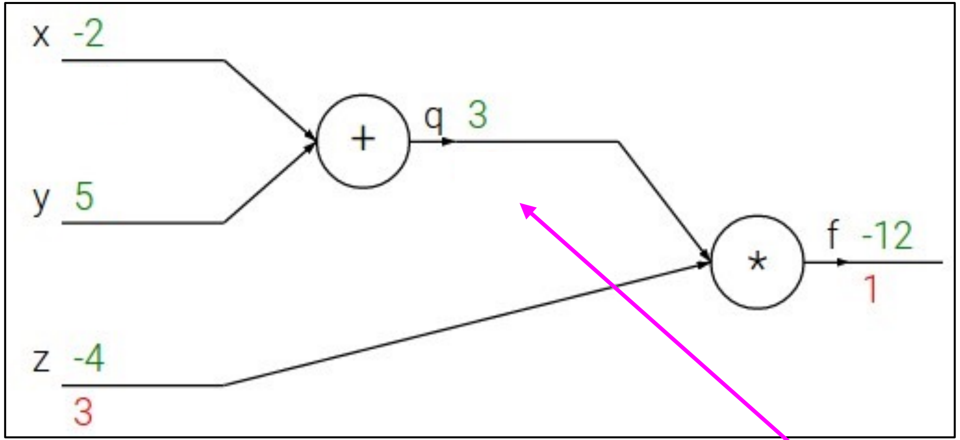

$$\boxed{\frac{\partial f}{\partial q}}$$

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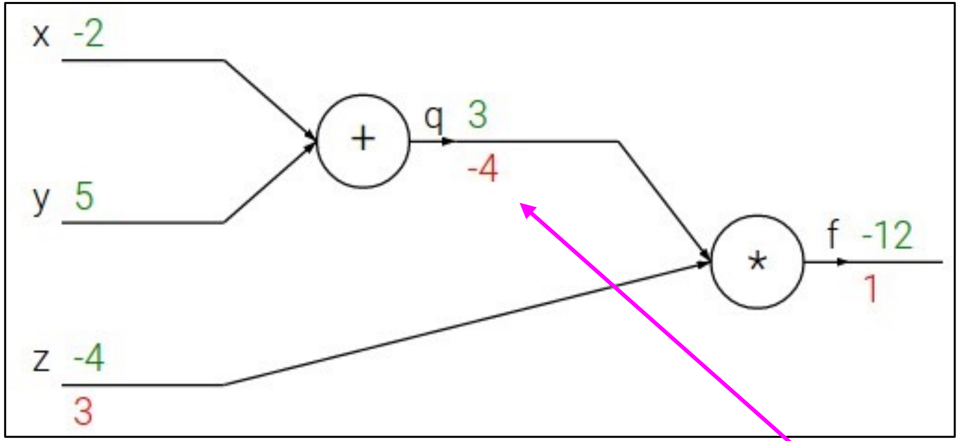

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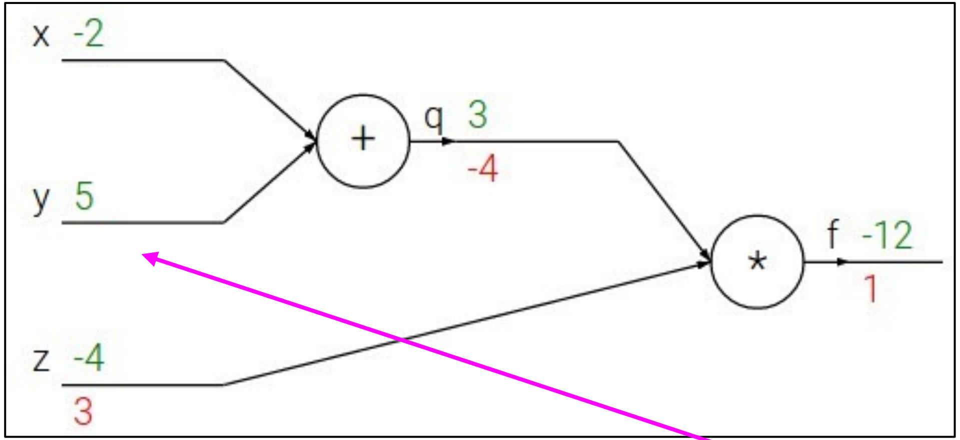

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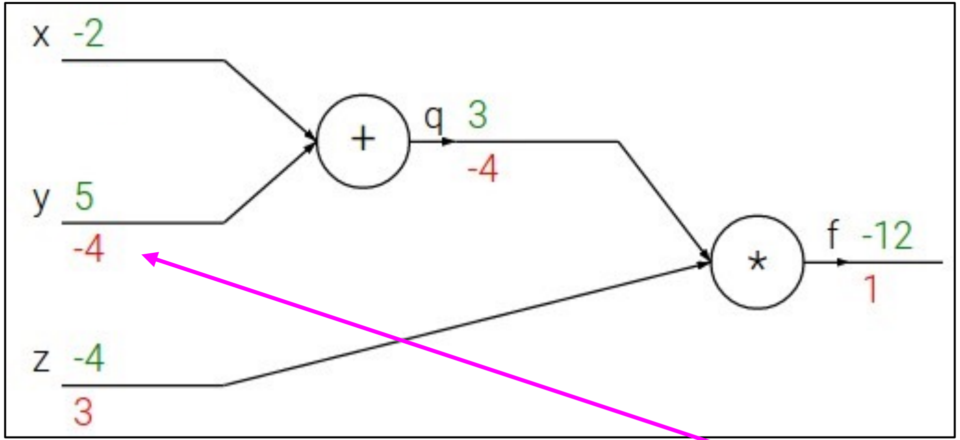

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$$\frac{\partial f}{\partial y}$$

Chain rule:

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

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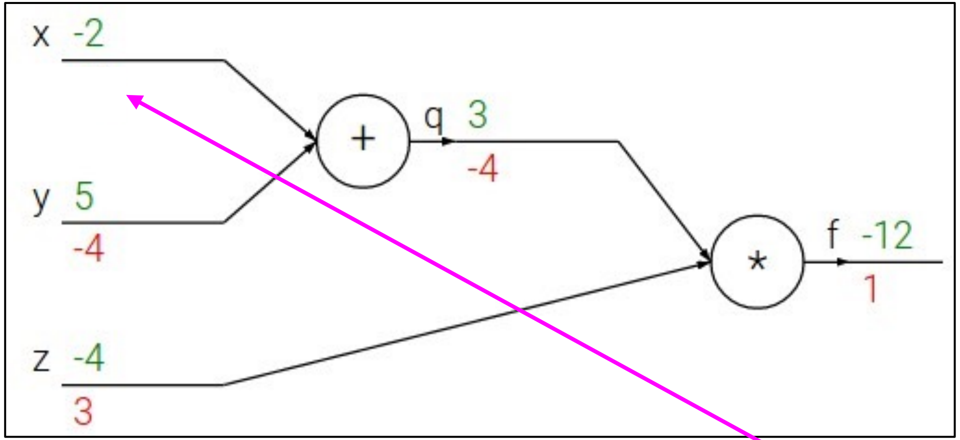

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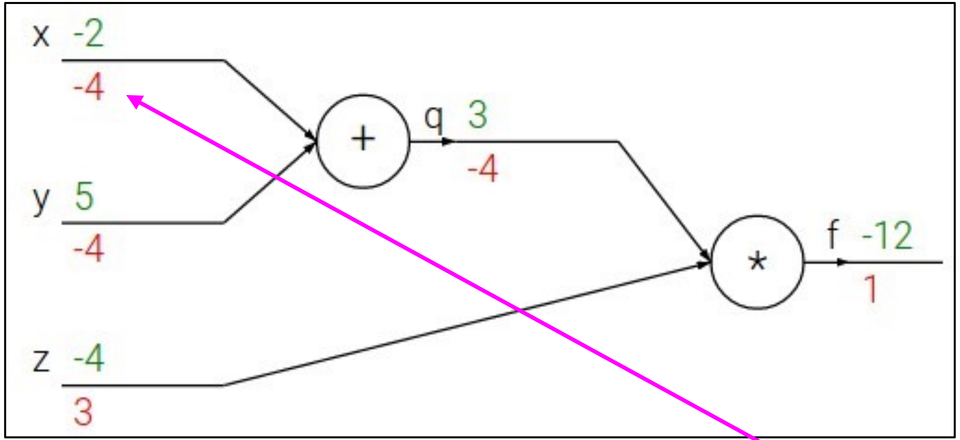

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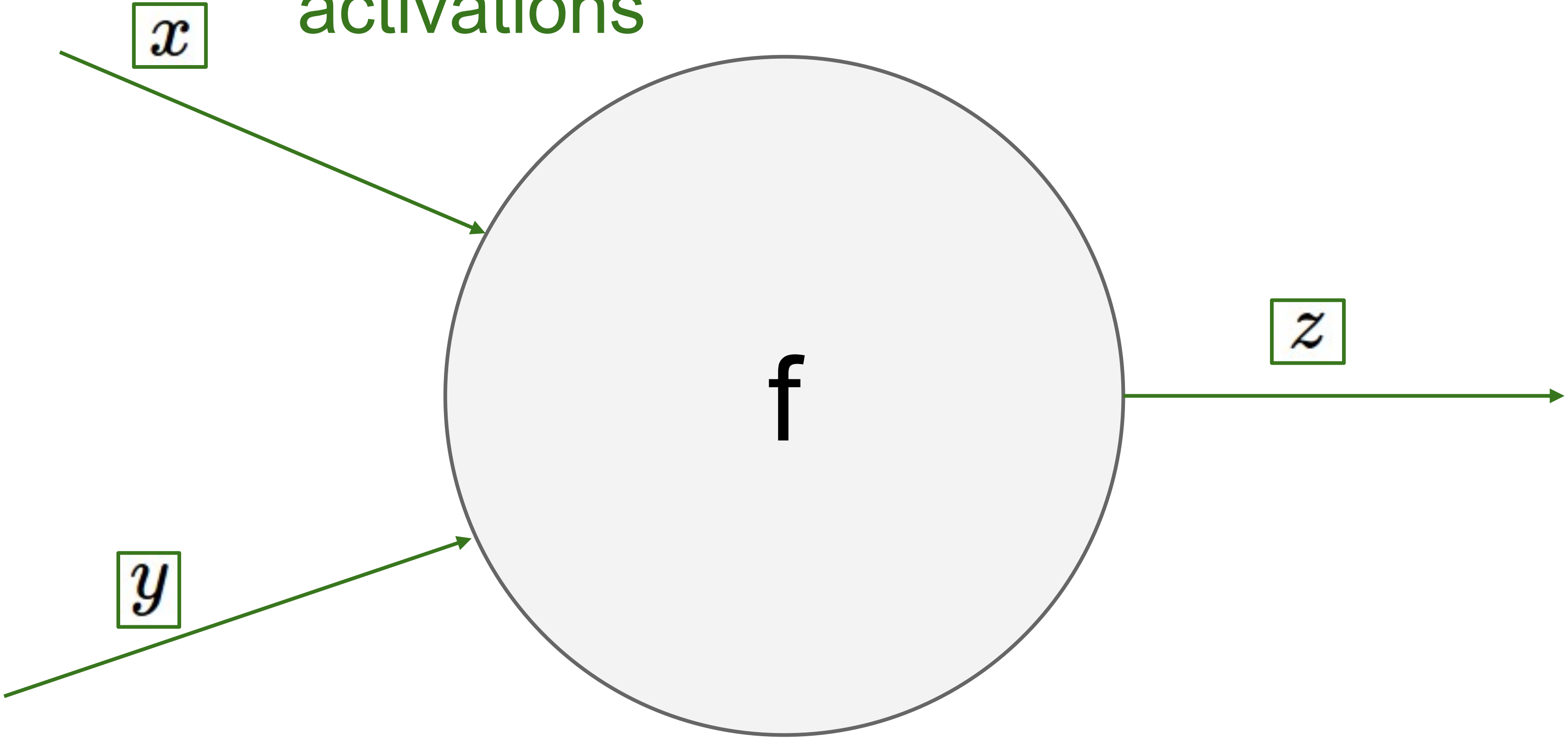
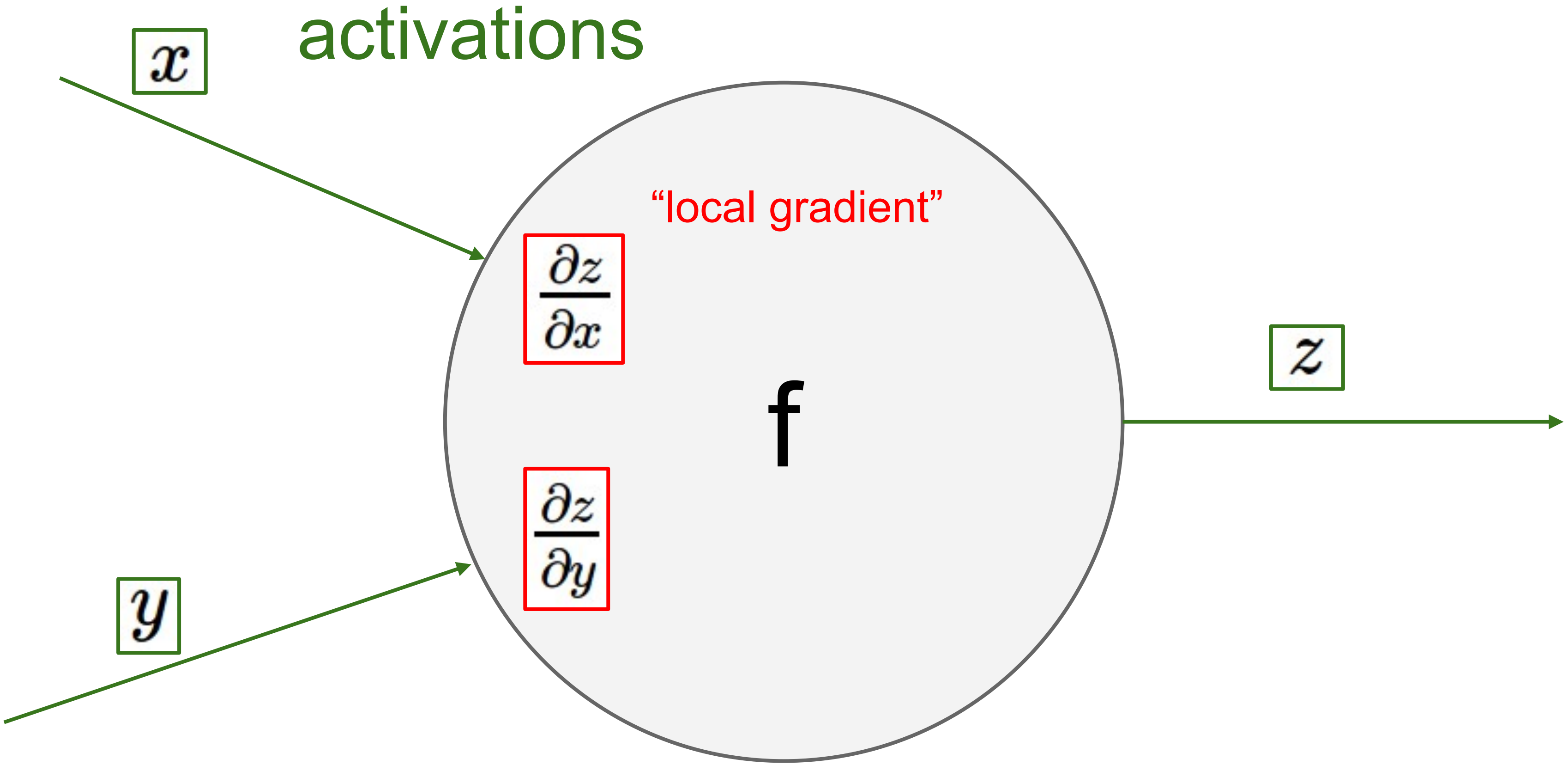
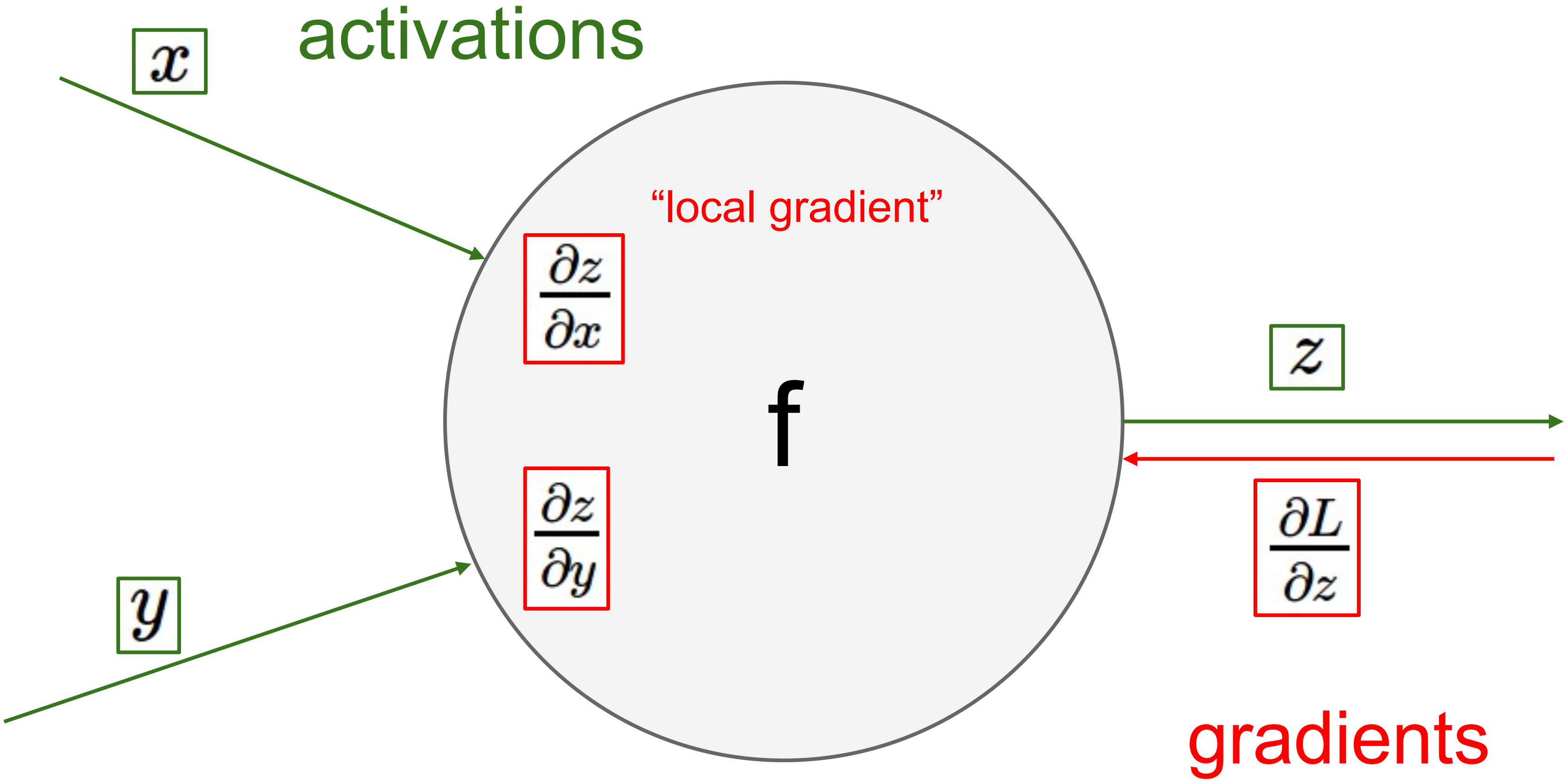
```

activations





activations
x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y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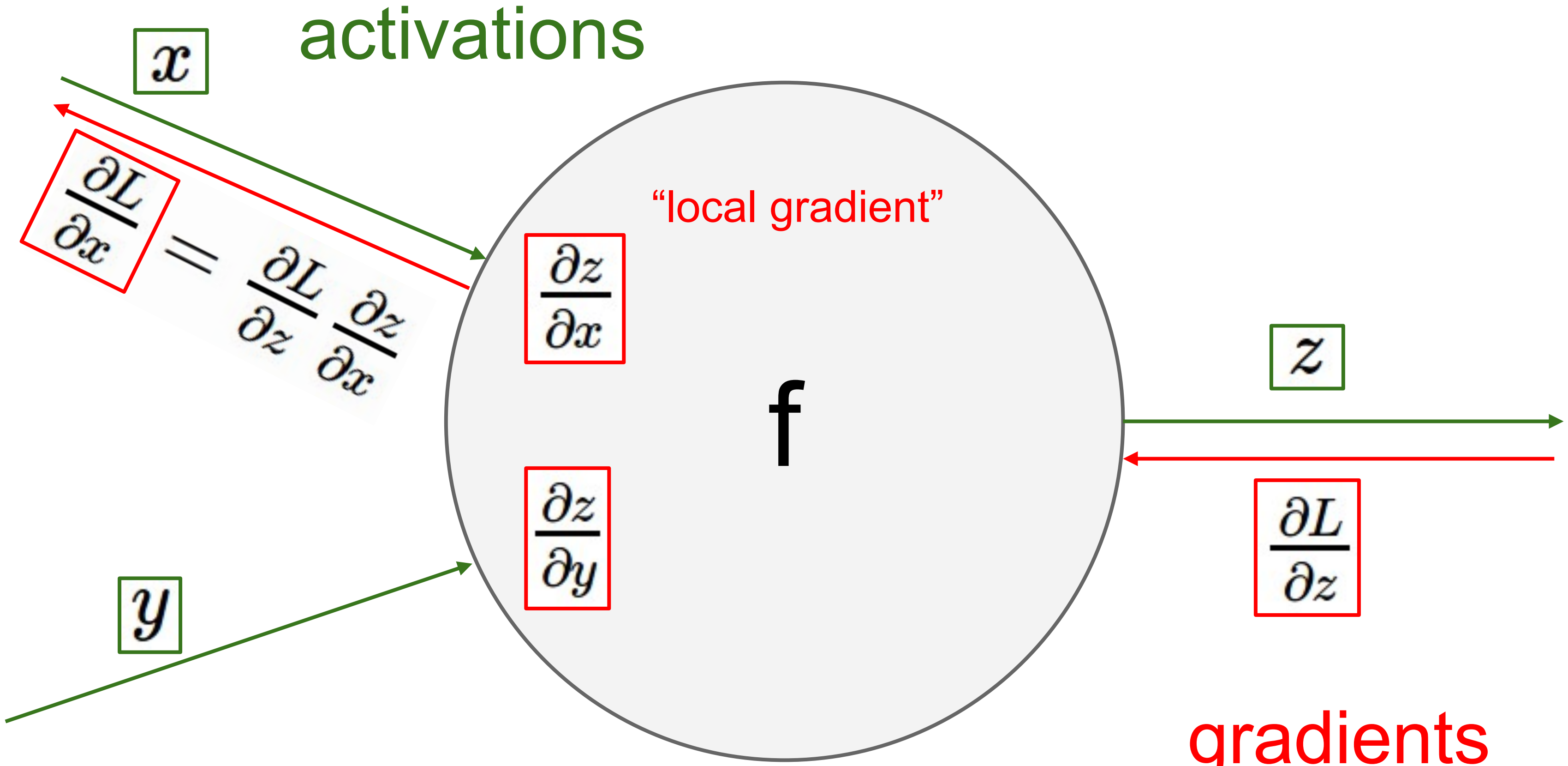
$\frac{\partial L}{\partial z}$
y
gradients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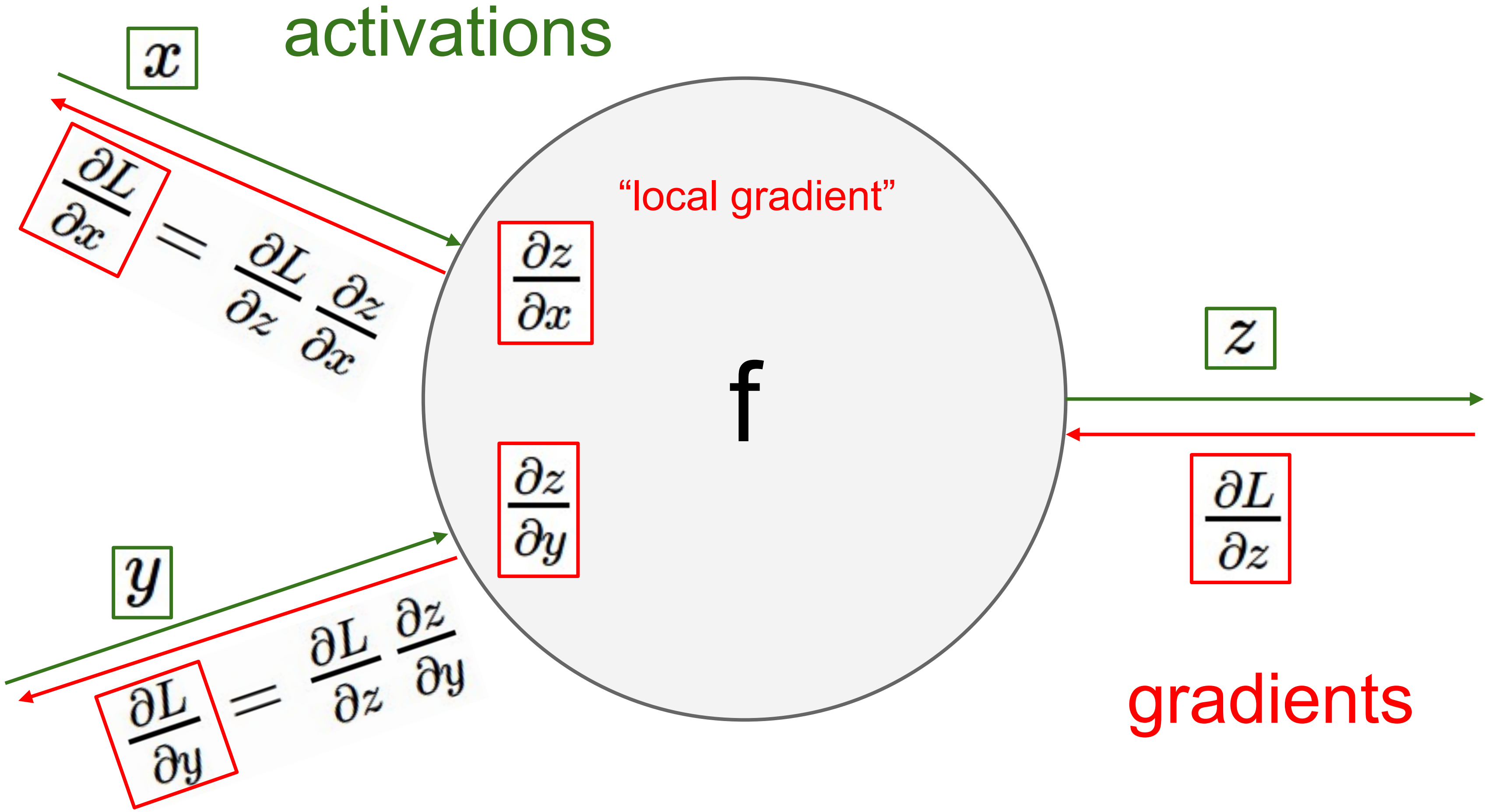
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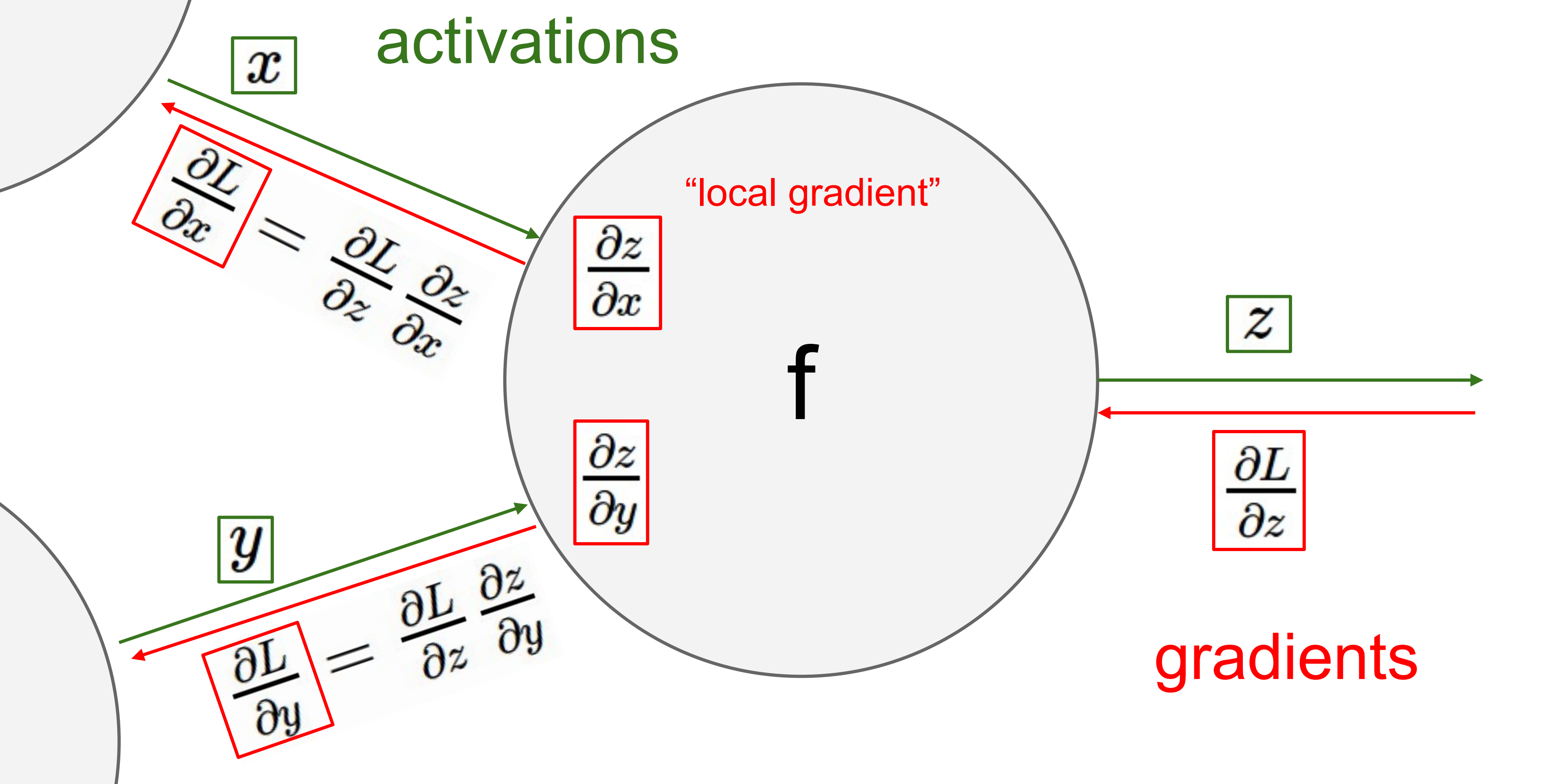
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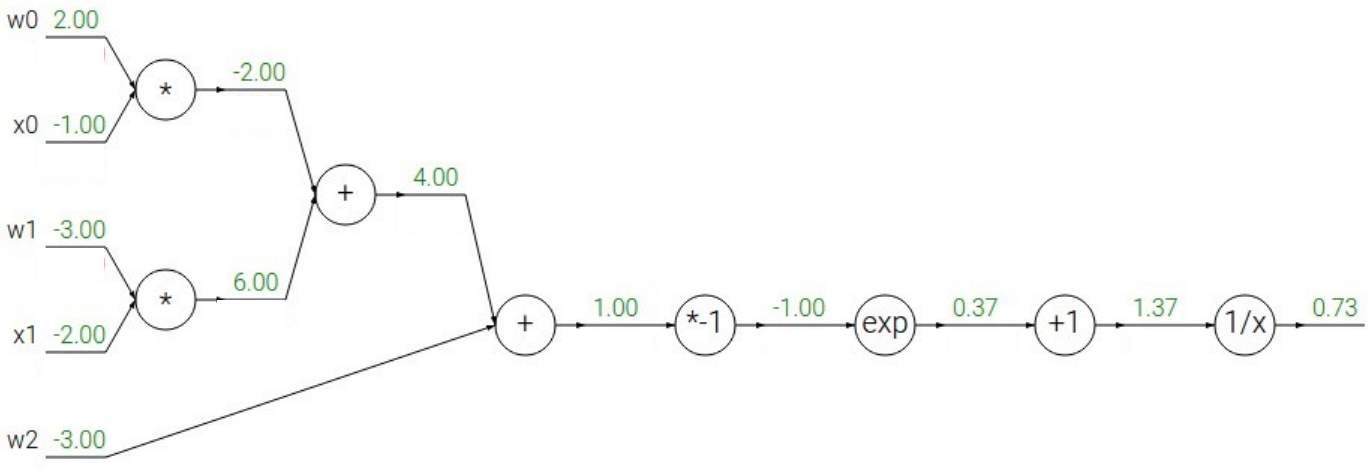
gradients

Another example:

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

"sigmoid function"



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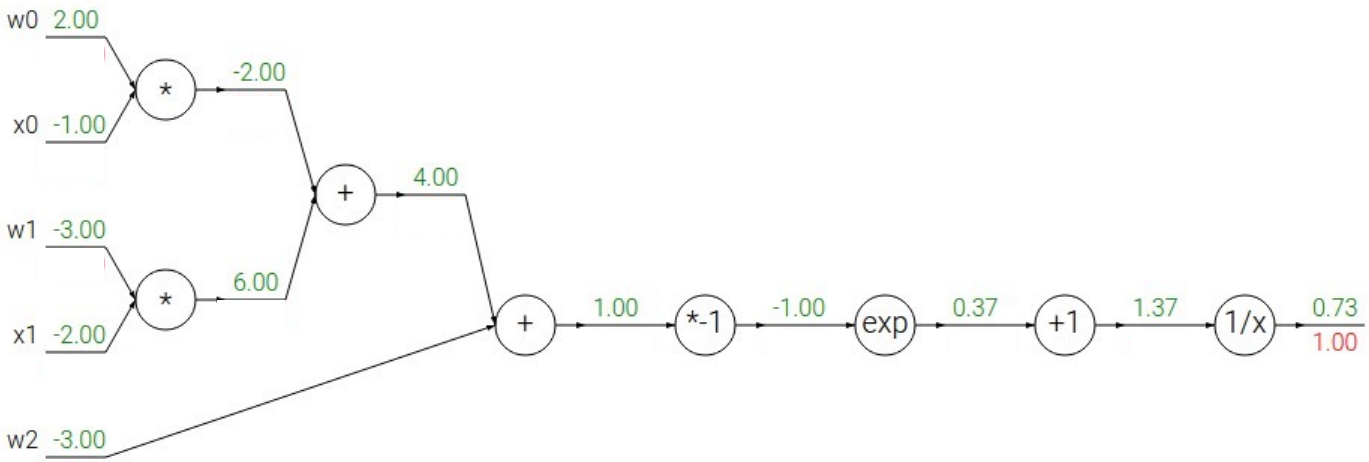

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x \qquad\qquad f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

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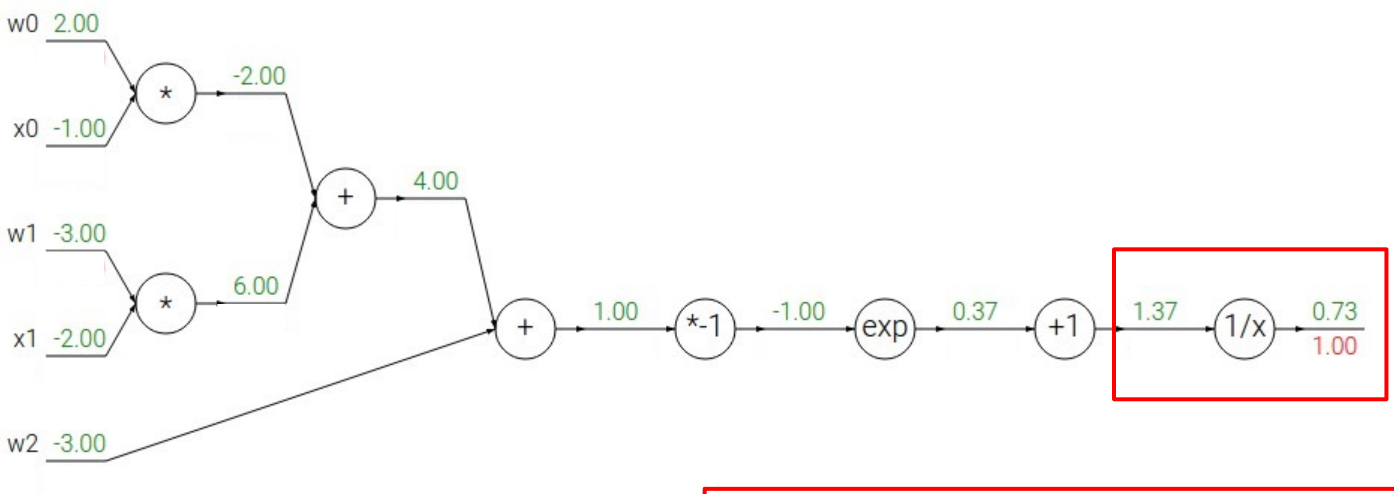

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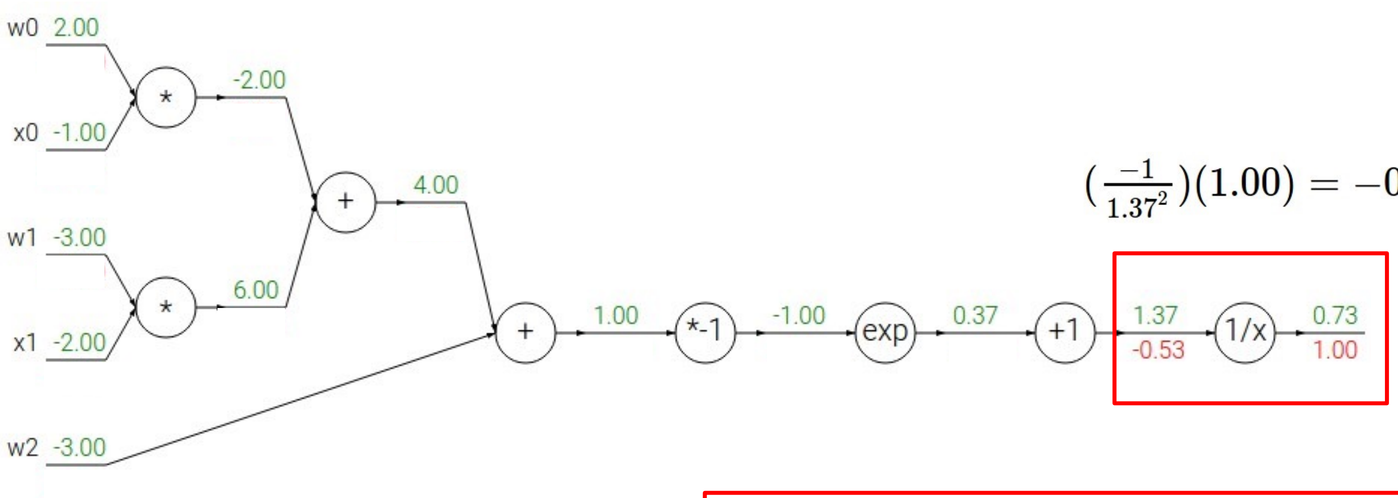

$$\left(\frac{-1}{1.37^2}\right)(1.00) = -0.53$$

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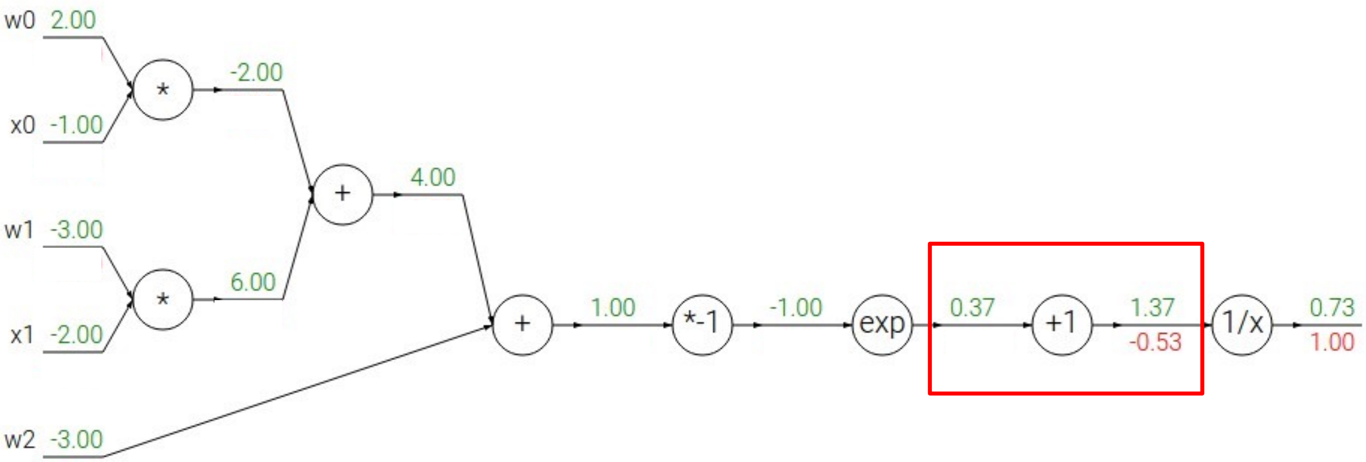

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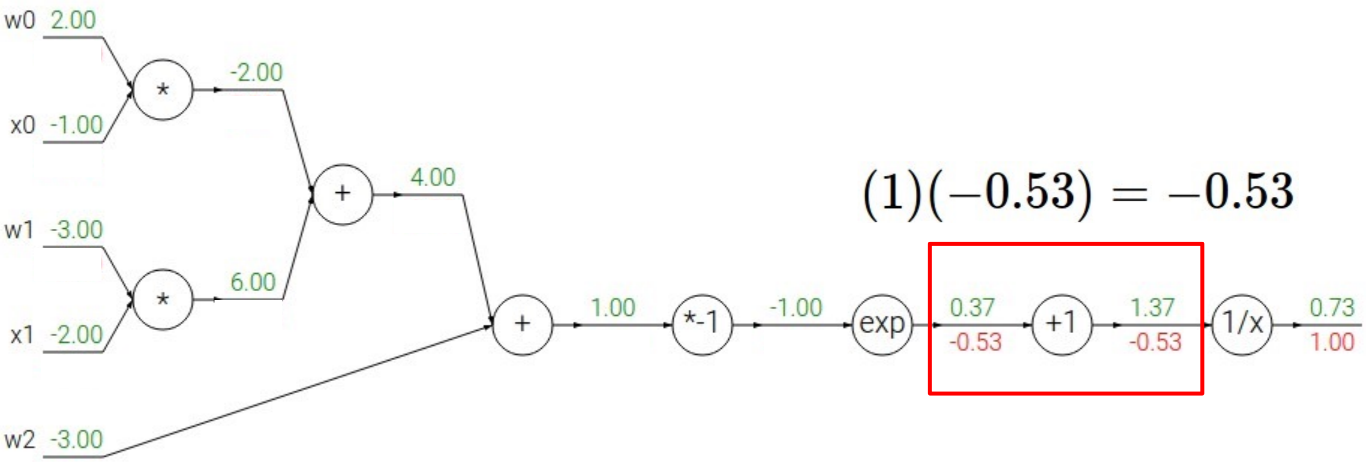

$$(1)(-0.53) = -0.53$$

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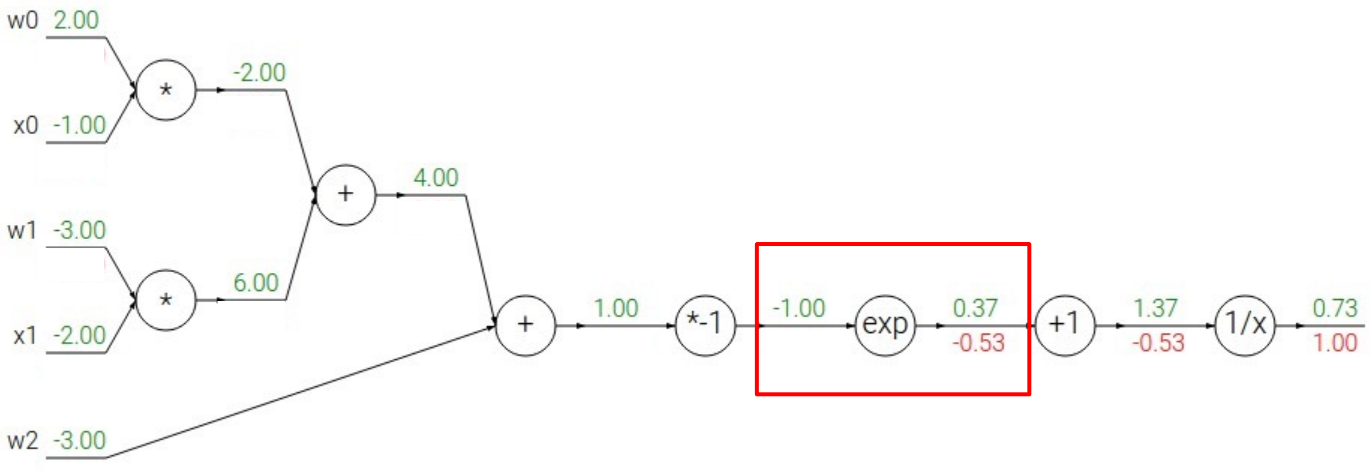

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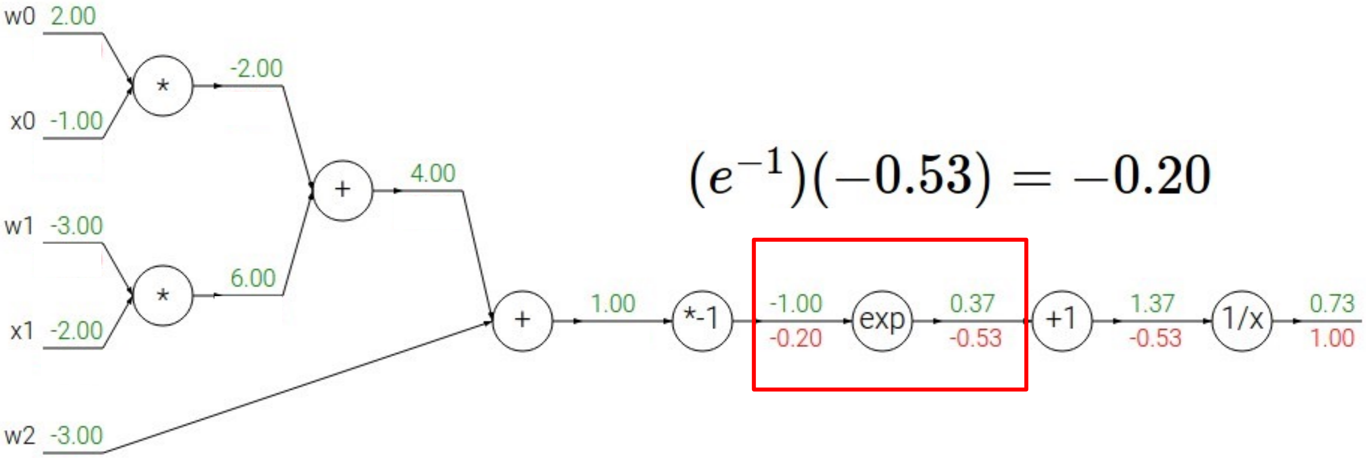


$$(e^{-1})(-0.53) = -0.20$$

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

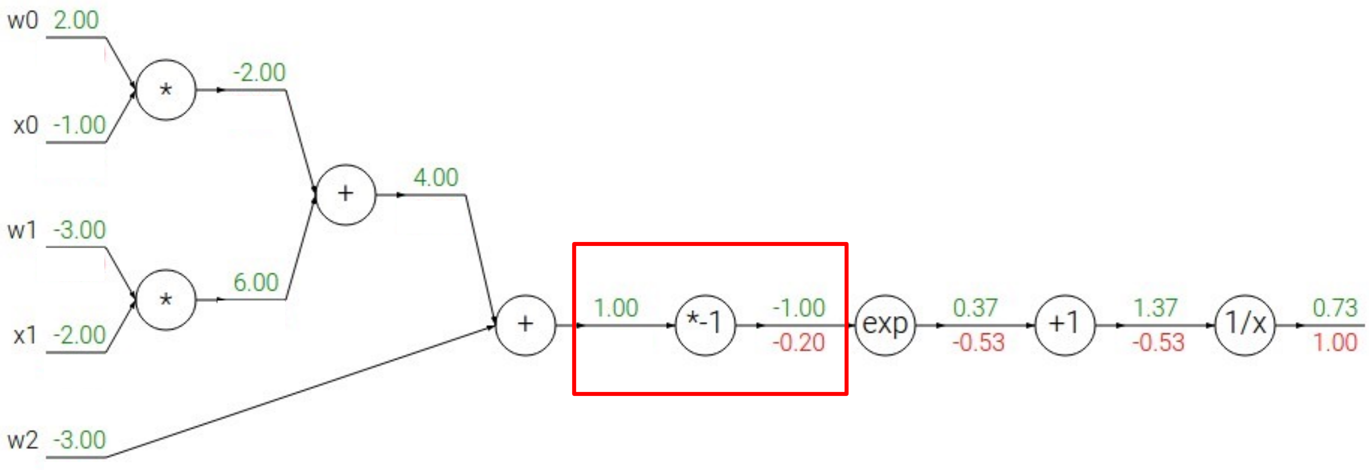
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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

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

Another example:

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



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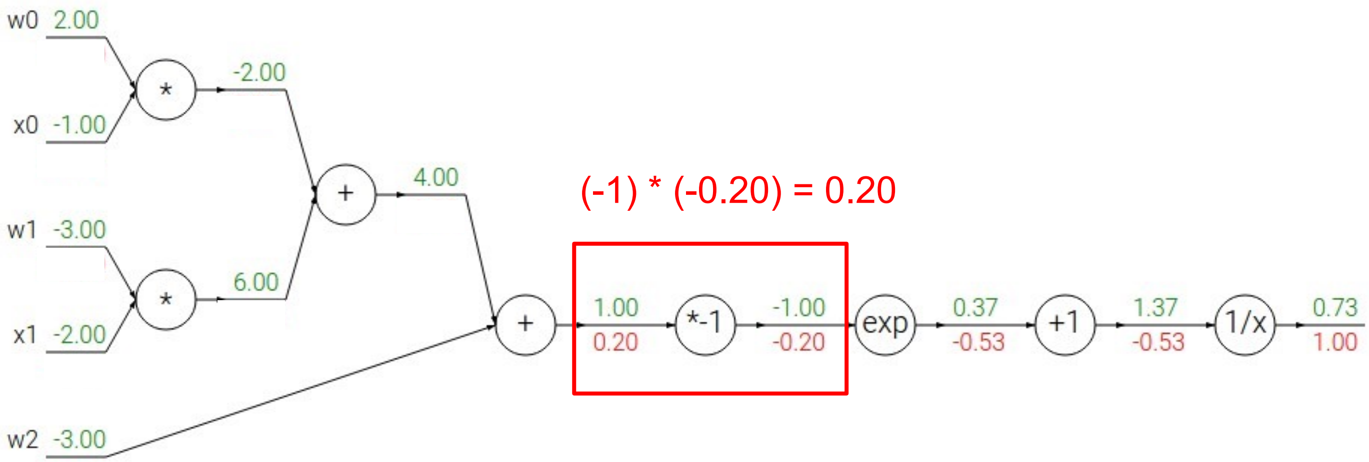

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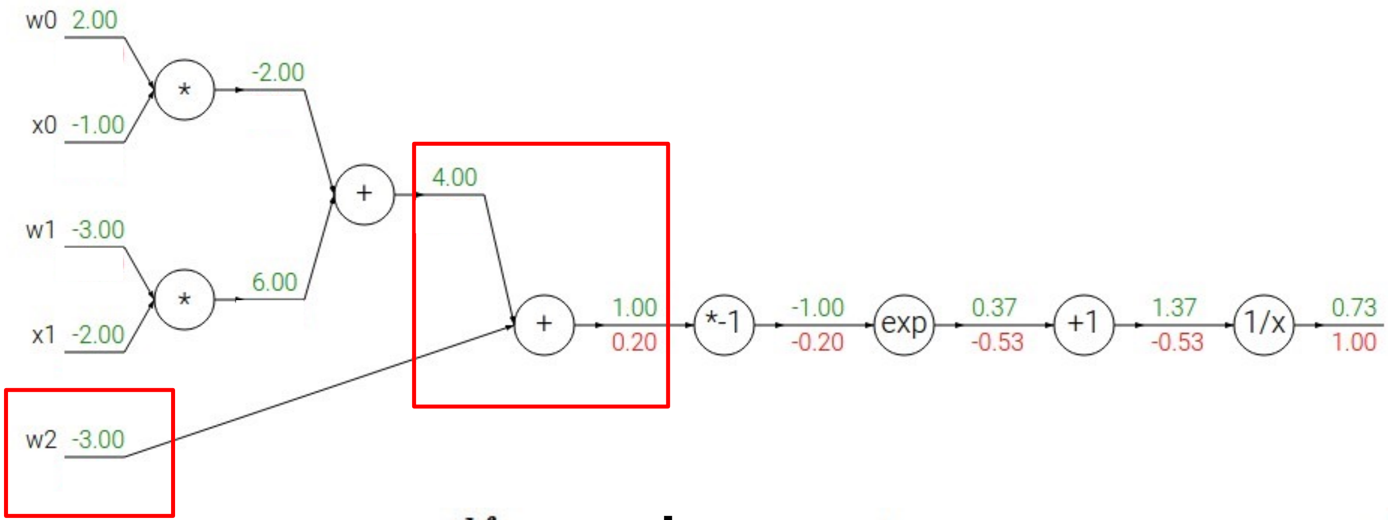

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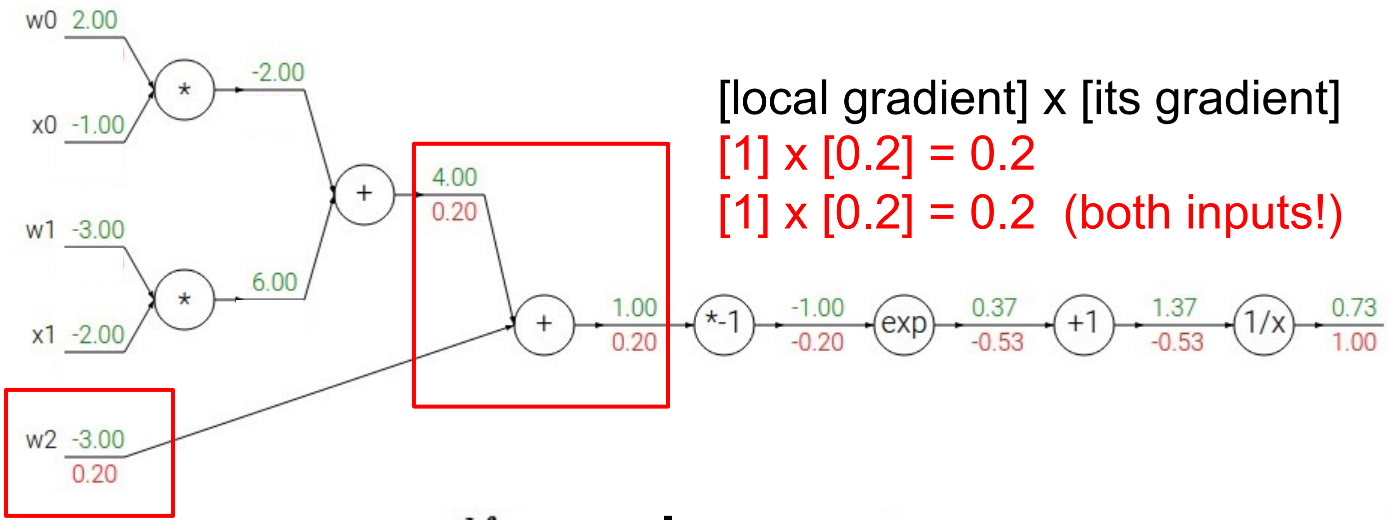

[local gradient] x [its gradient]
[1] x [0.2] = 0.2
[1] x [0.2] = 0.2 (both inputs!)

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

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

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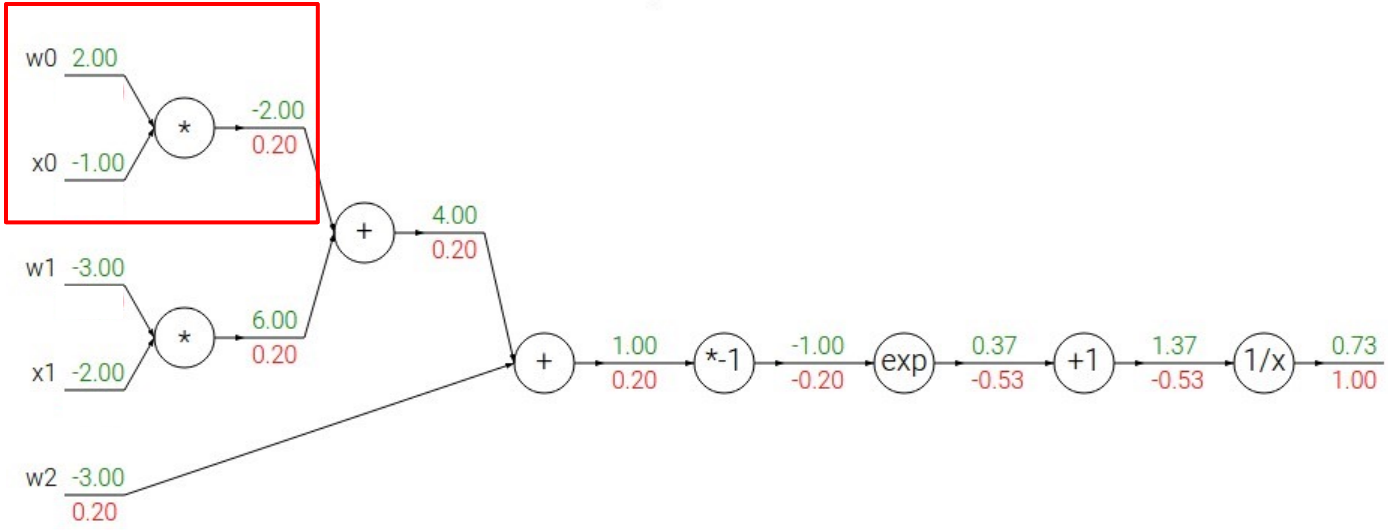

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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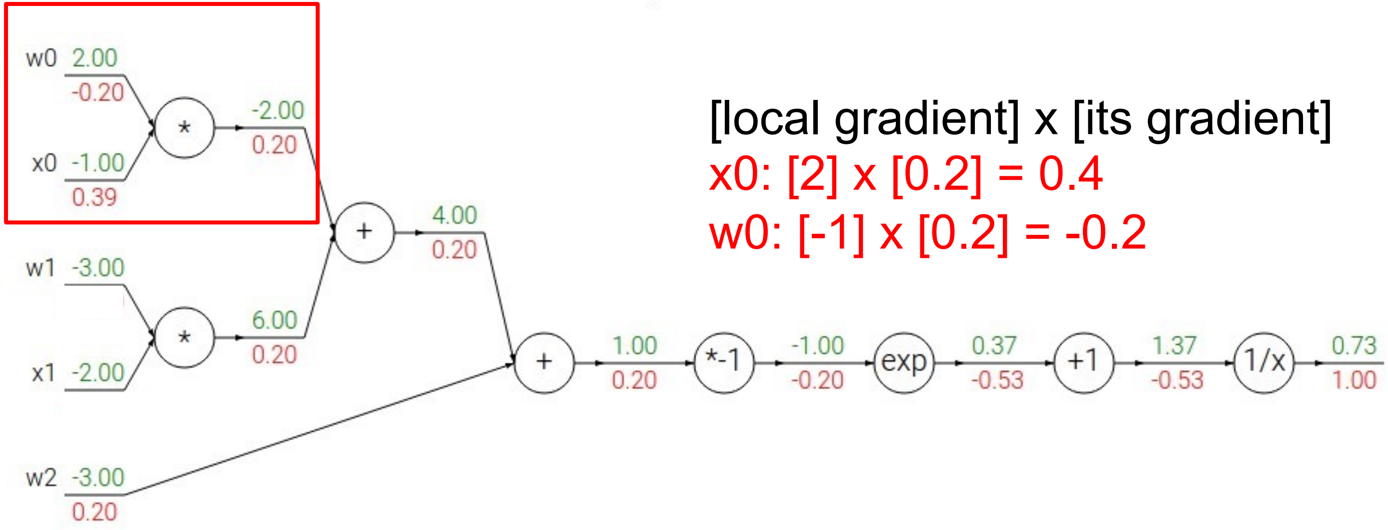


[local gradient] x [its gradient]
x0: [2] x [0.2] = 0.4
w0: [-1] x [0.2] = -0.2

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

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

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

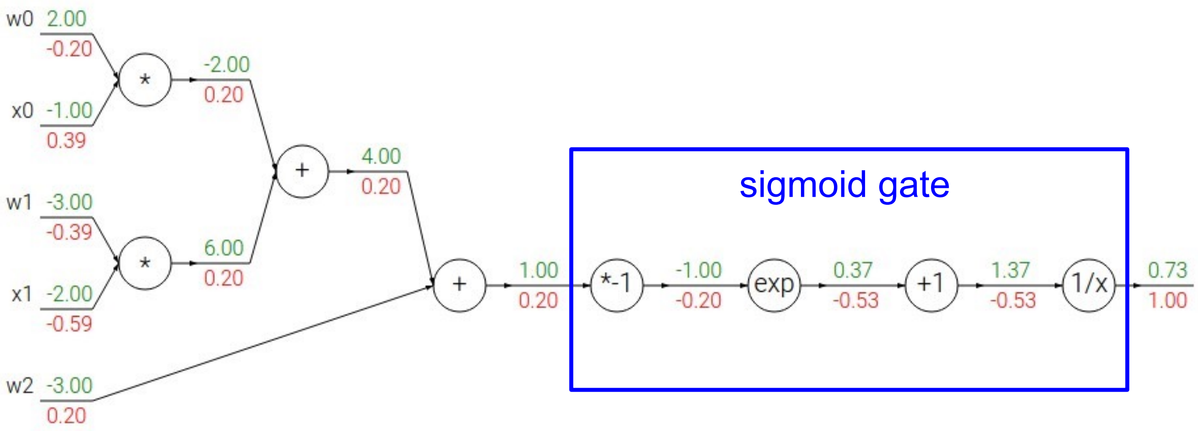
$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

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

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

sigmoid function

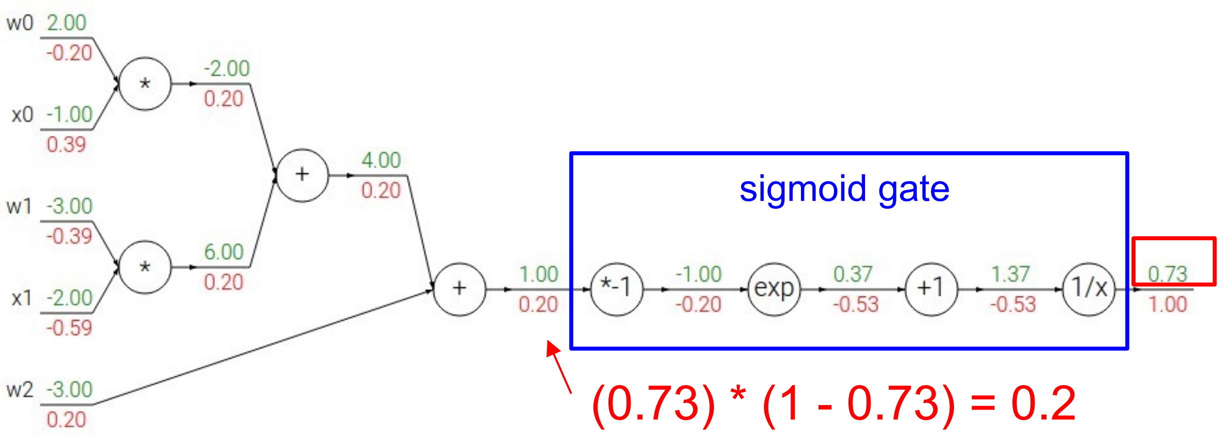
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



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

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

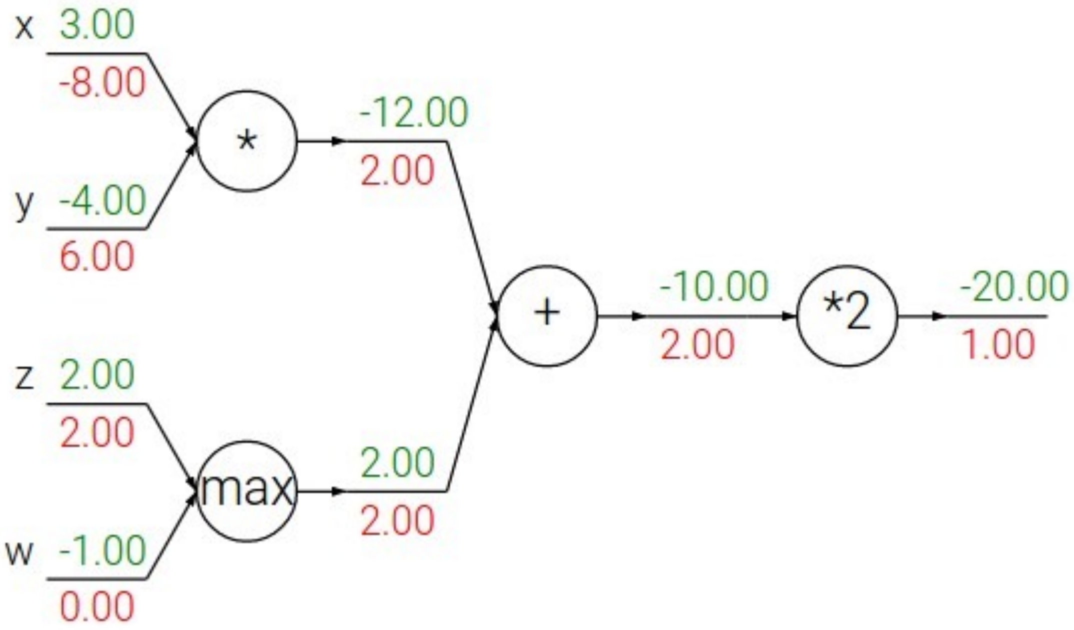
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



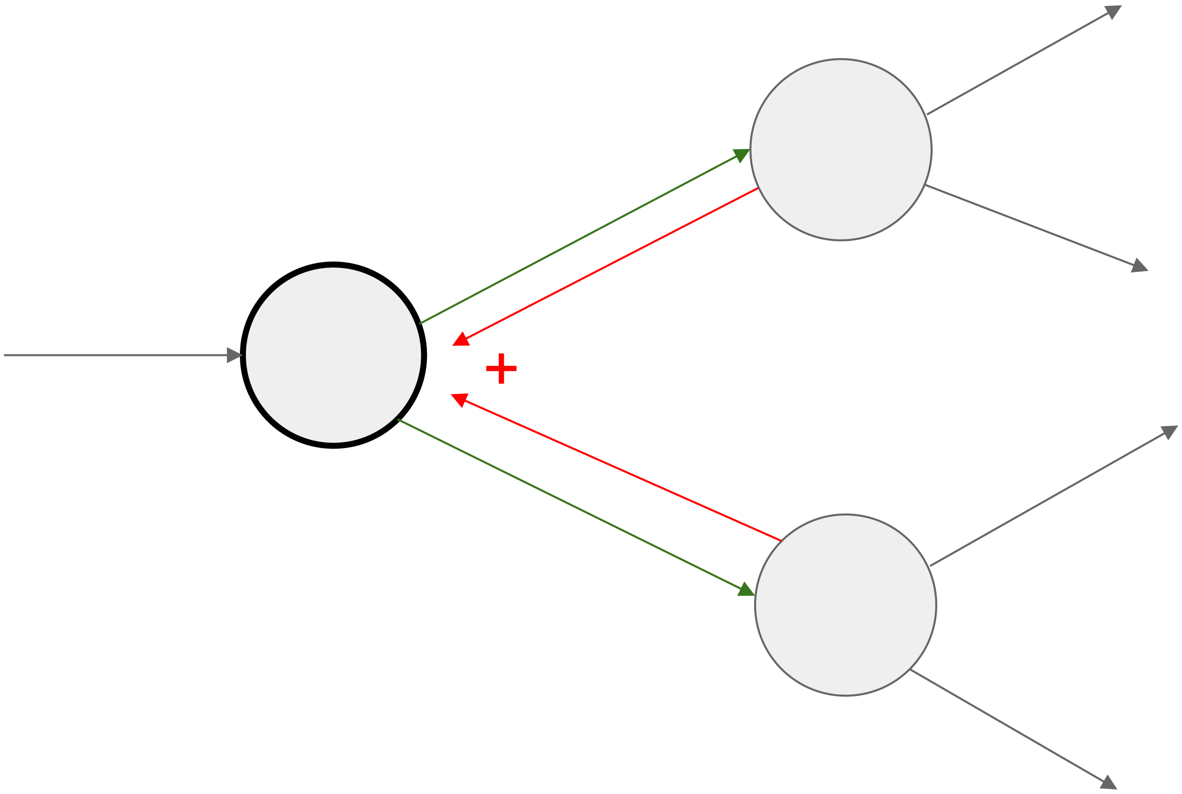
```python
w = [2,-3,-3] # assume some random weights and data
x = [-1, -2]

# forward pass
dot = w[0]*x[0] + w[1]*x[1] + w[2]
f = 1.0 / (1 + math.exp(-dot)) # sigmoid function

# backward pass through the neuron (backpropagation)
ddot = (1 - f) * f # gradient on dot variable, using the sigmoid gradient derivation
dx = [w[0] * ddot, w[1] * ddot] # backprop into x
dw = [x[0] * ddot, x[1] * ddot, 1.0 * ddot] # backprop into w
# we're done! we have the gradients on the inputs to the circuit
```

Patterns in backward flow

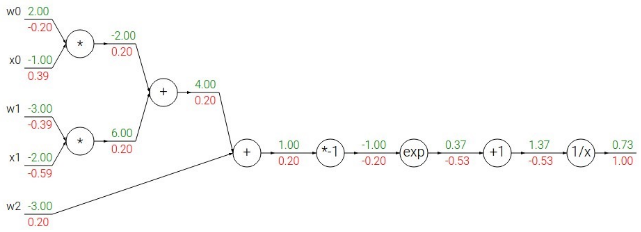
add gate: gradient distributor
max gate: gradient router
mul gate: gradient… “switcher”?



Gradients add at branches



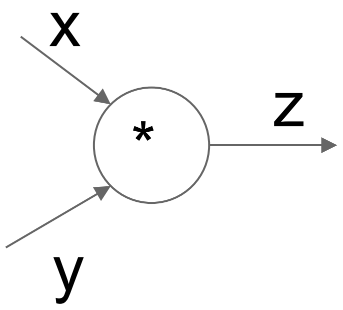
Implementation: forward/backward API



Graph (or Net) object. *(Rough pseudo 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



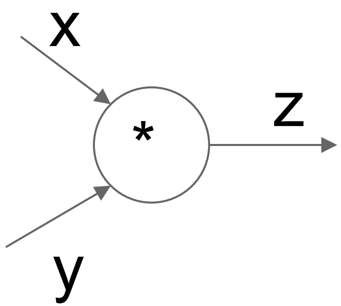
(x,y,z are scalars)

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

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

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

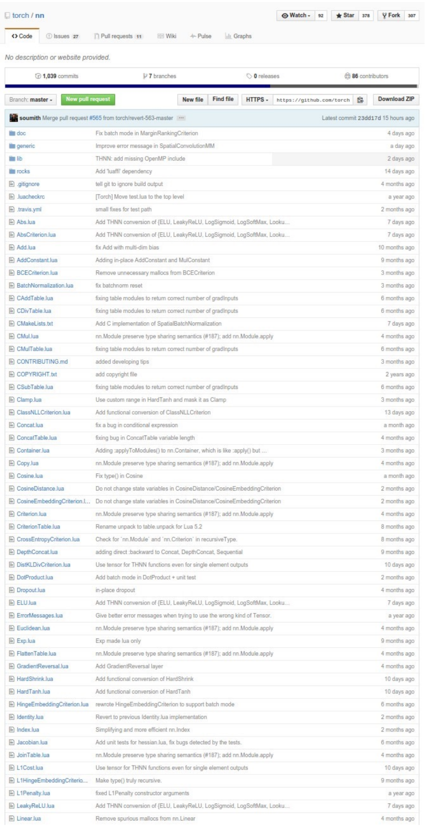
Implementation: forward/backward API

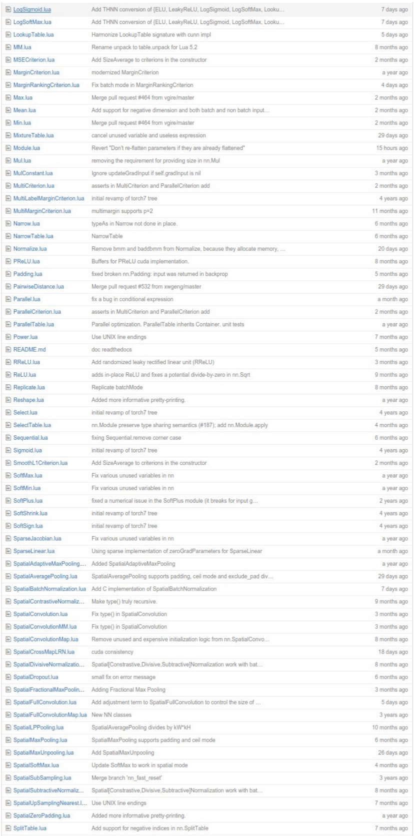



```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

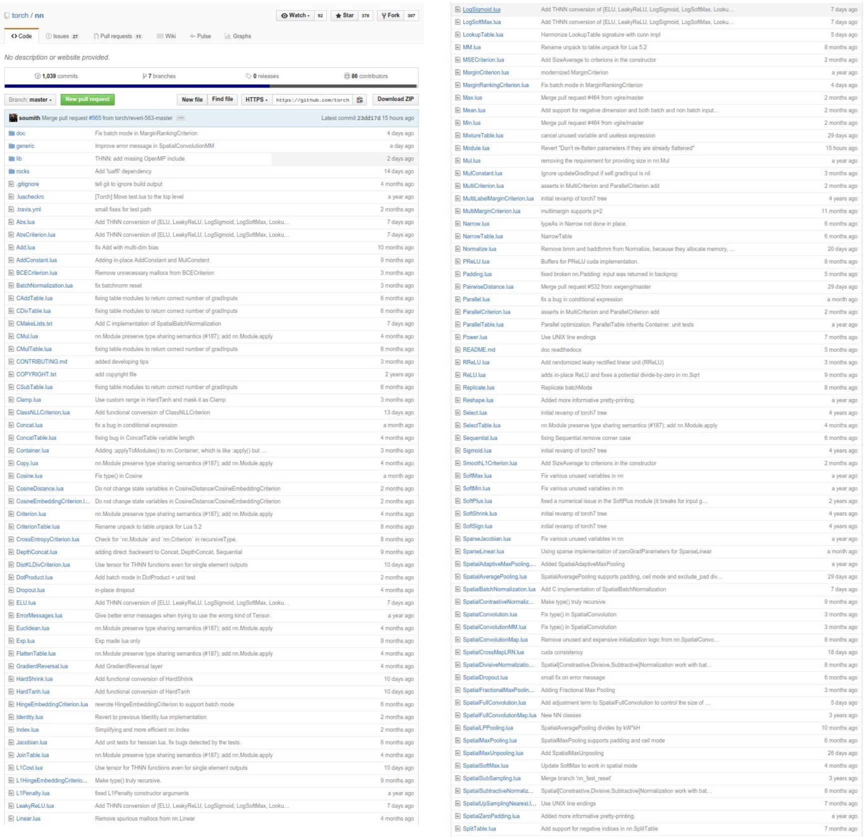
(x,y,z are scalars)

Example: Torch Layers





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
```

$$f(X) = aX$$

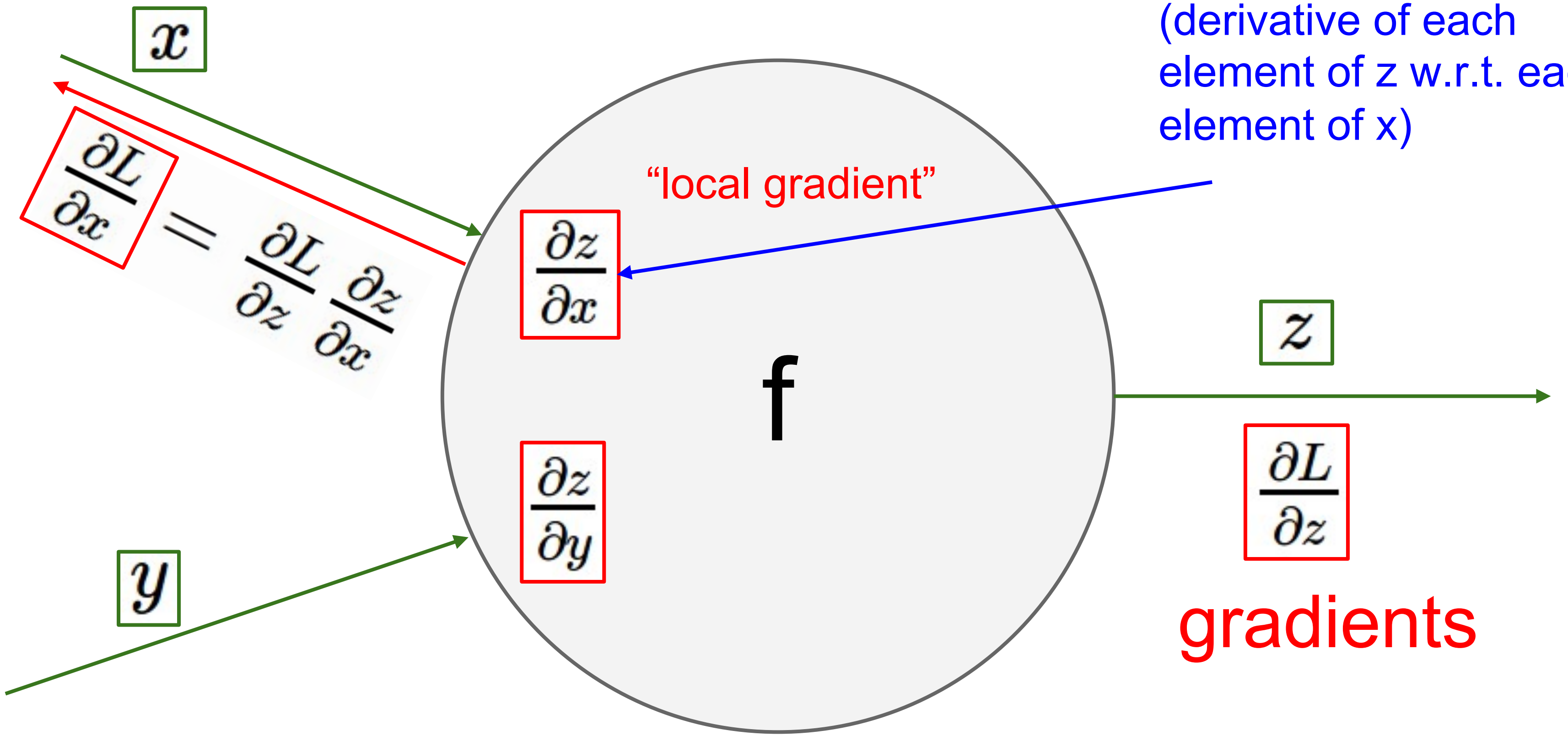
initialization

forward()

backward()

Gradients for vectorized code (x,y,z are now vectors)

This is now the **Jacobian matrix** (derivative of each element of z w.r.t. each element of x)

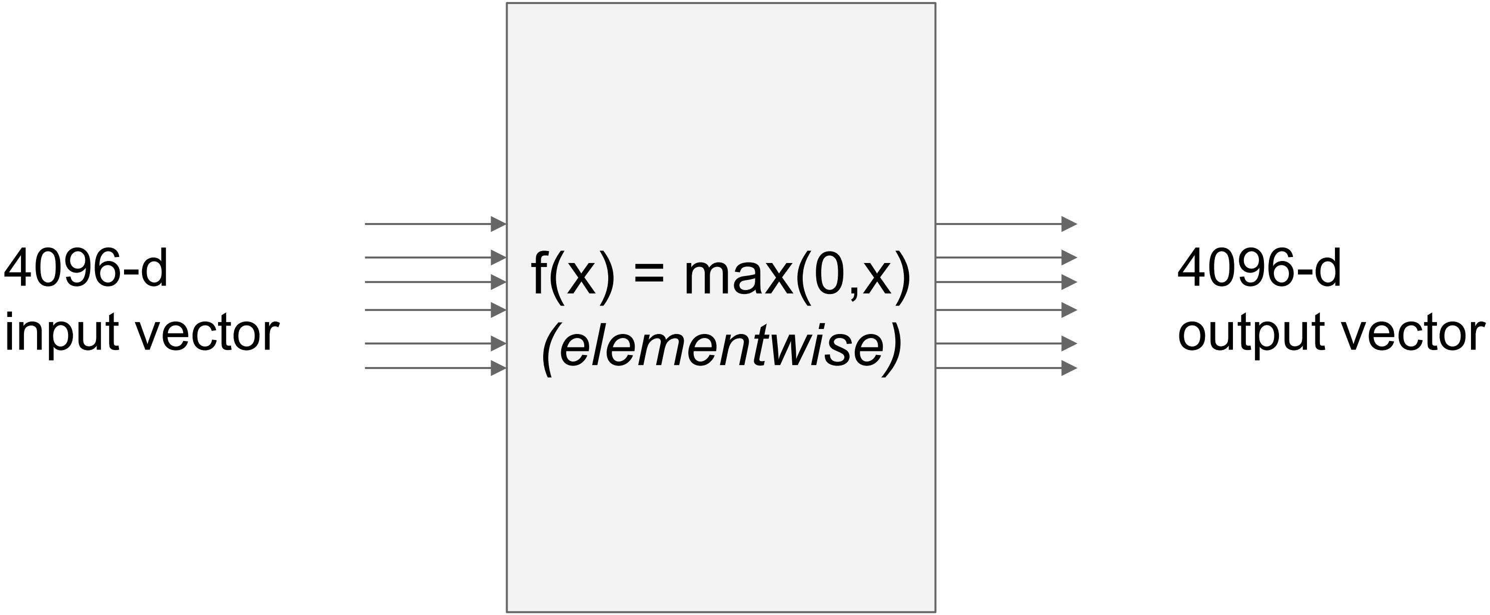


[slides]
[backprop notes]
[Efficient BackProp] (optional)
related: [1], [2], [3] (optional)

[slides]
handout 1: Vector, Matrix, and Tensor Derivatives
handout 2: Derivatives, Backpropagation, and Vectorization
Deep Learning [Nature] (optional)

[slides]
tips/tricks: [1], [2] (optional)

Vectorized operations

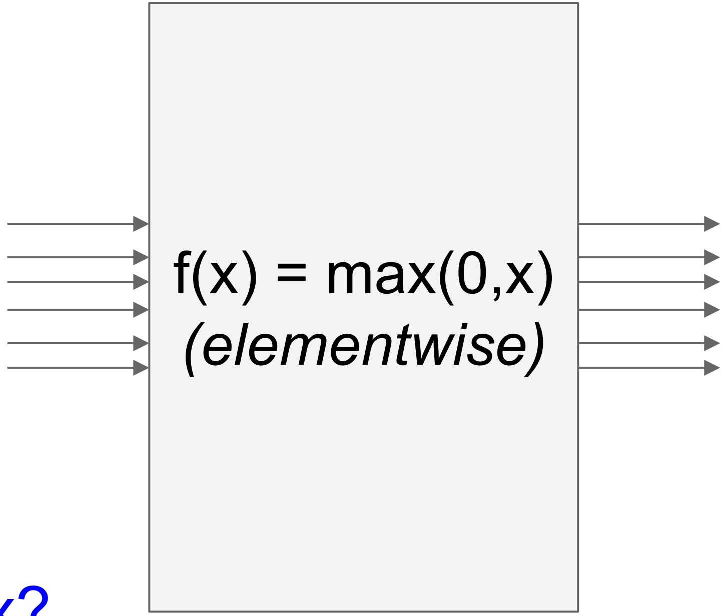


Vectorized operations

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

Jacobian matrix

4096-d
input vector



4096-d
output vector

Q: what is the size of the Jacobian matrix?

Vectorized operations

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

Jacobian matrix

4096-d
input vector

f(x) = max(0,x)
(elementwise)

4096-d
output vector

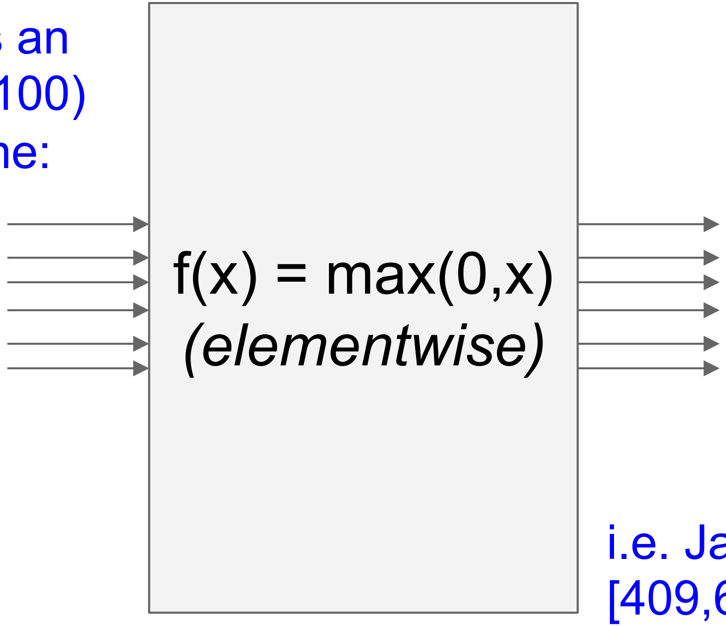
Q: what is the size of the Jacobian matrix?
[4096 x 4096!]

Q2: what does it look like?

Vectorized operations

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

100 4096-d input vectors



100 4096-d output vectors

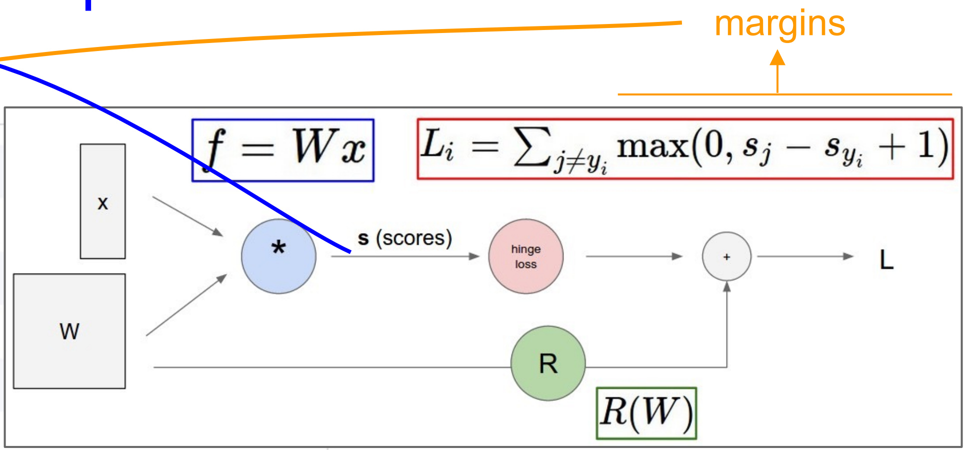
i.e. Jacobian would technically be a [409,600 x 409,600] matrix :\

Assignment: Writing SVM/Softmax

Stage your forward/backward computation!

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 = #...
```



Summary so far

- 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.