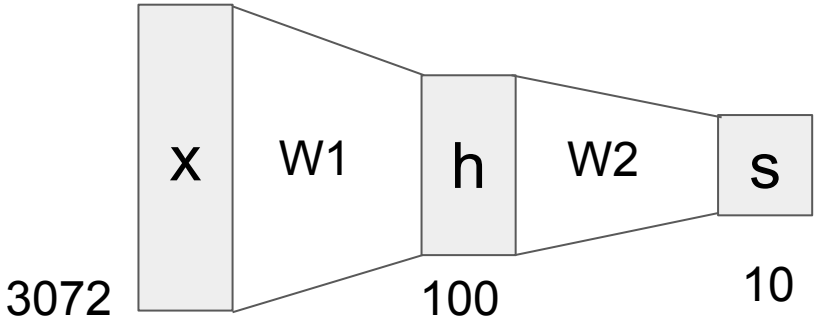
Lecture 6: Neural Networks Backpropagation

Neural networks: hierarchical computation

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

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



$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural networks: learning 100s of templates

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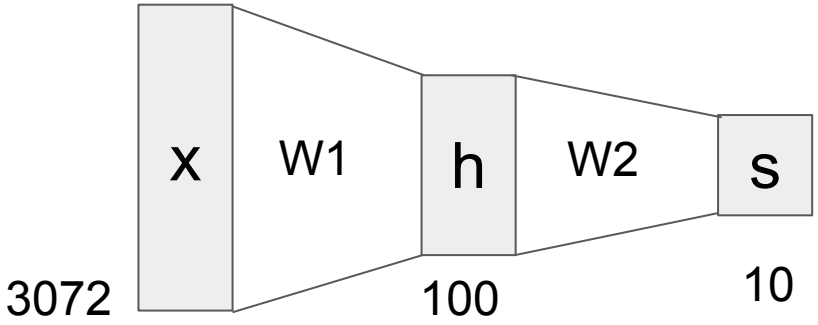
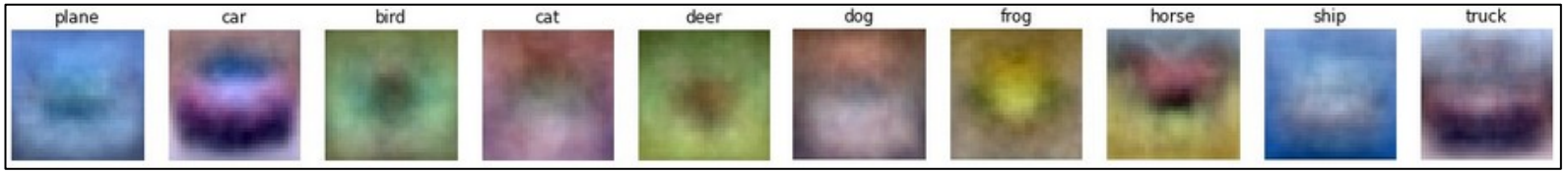
(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$





Learn 100 templates instead of 10.

Share templates between classes

Plugging in neural networks with loss functions

$$s = f(x; W_1, W_2) = W_2 \max(0, W_1 x)$$ Nonlinear score function

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

$$R(W) = \sum_k W_k^2$$ Regularization

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda R(W_1) + \lambda R(W_2)$$ Total loss: data loss + regularization

Problem: How to compute gradients?

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If we can compute $\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}$ then we can learn W_1 and W_2

(Bad) Idea: Derive $\nabla_W L$ on paper

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

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

$$= \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1)$$

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

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2$$

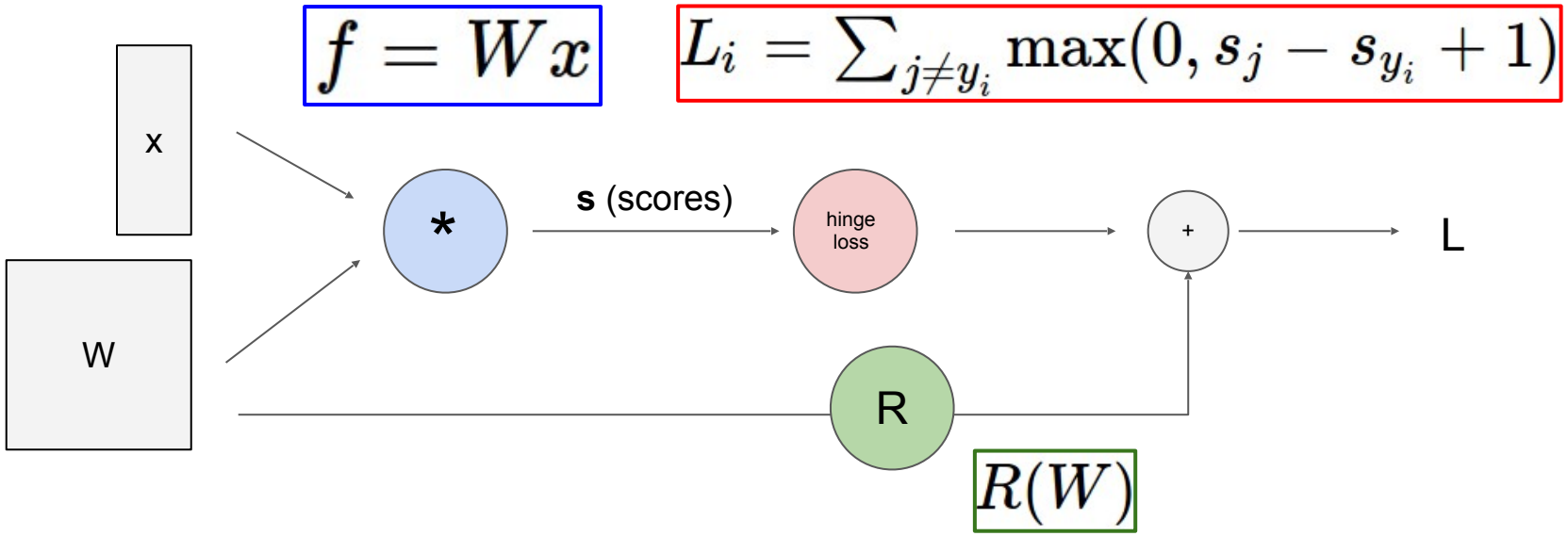
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

Problem: Very tedious: Lots of matrix calculus, need lots of paper

Problem: What if we want to change loss? E.g. use softmax instead of SVM? Need to re-derive from scratch =(

Problem: Not feasible for very complex models!

Better Idea: Computational graphs + Backpropagation

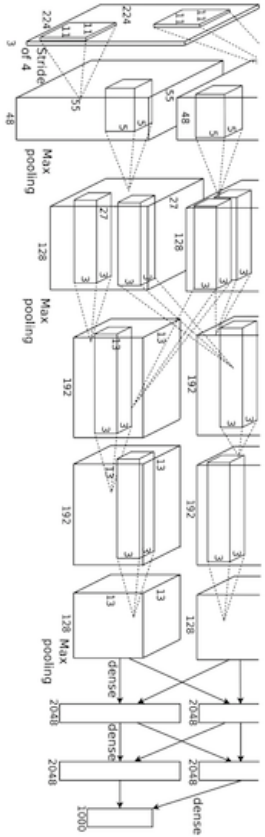


Convolutional network
(AlexNet)

input image

weights

loss



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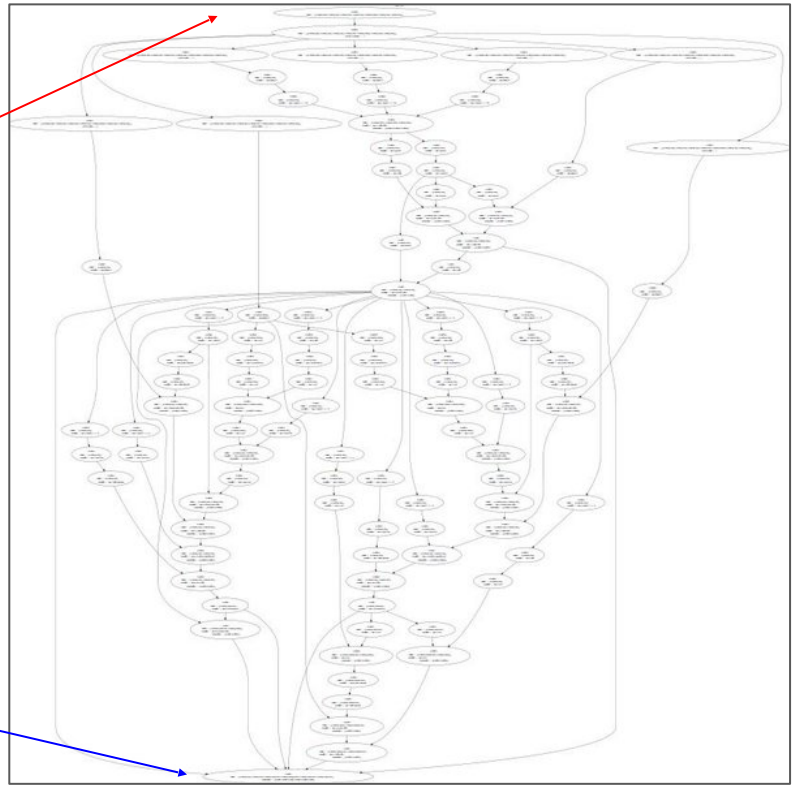
Really complex neural networks!!

input image

loss



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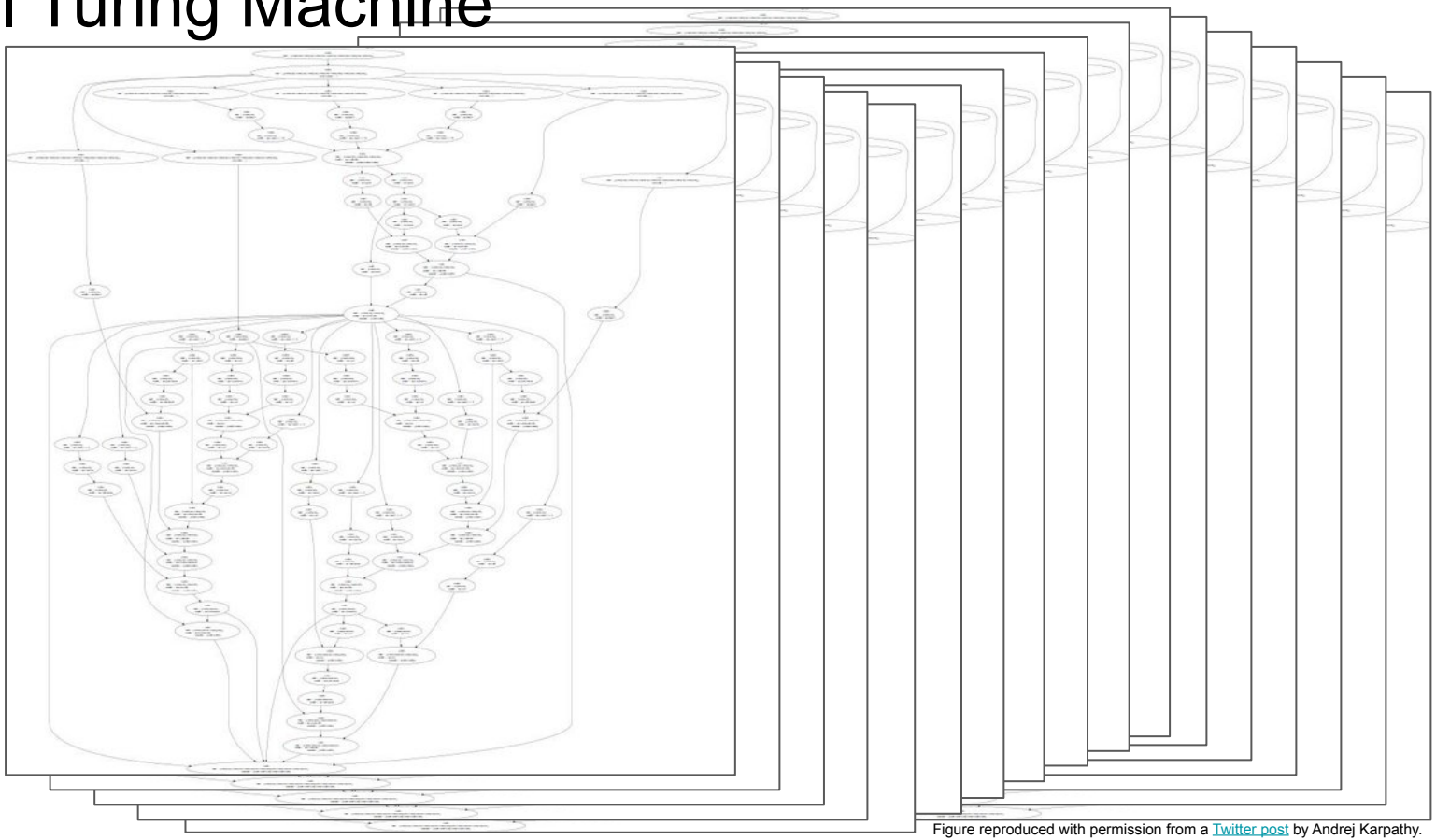
Neural Turing Machine



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Solution: Backpropagation

Backpropagation: a simple example

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

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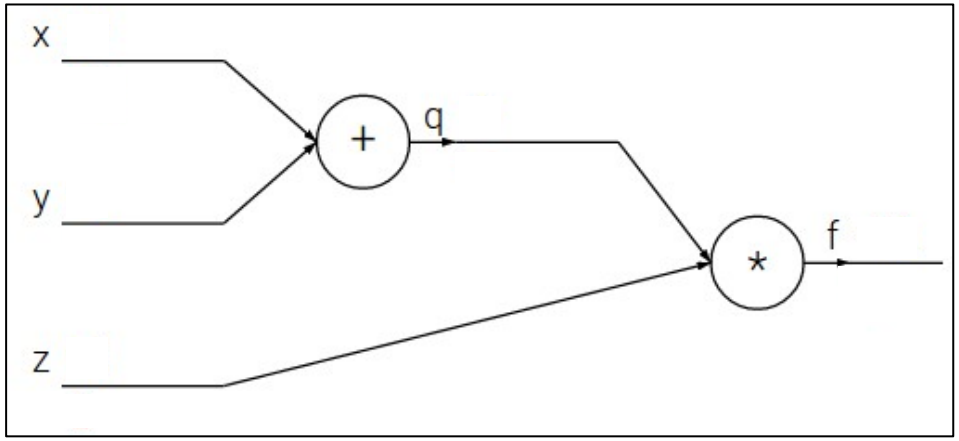
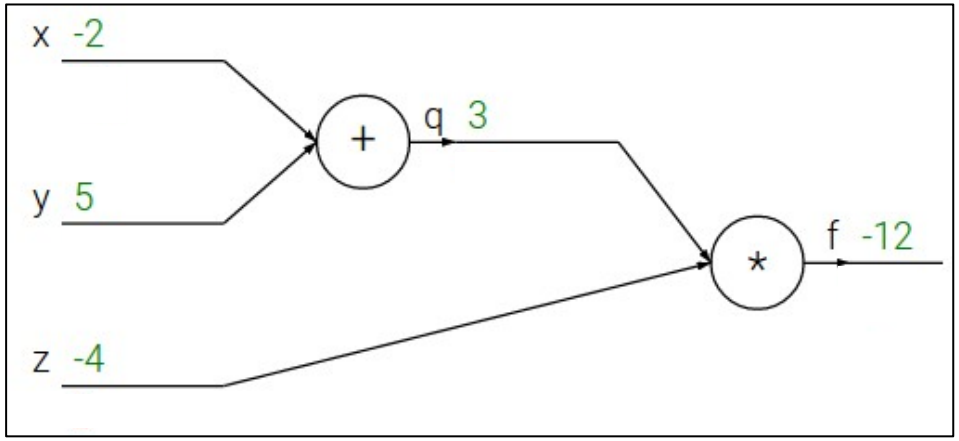


Backpropagation: a simple example

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

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



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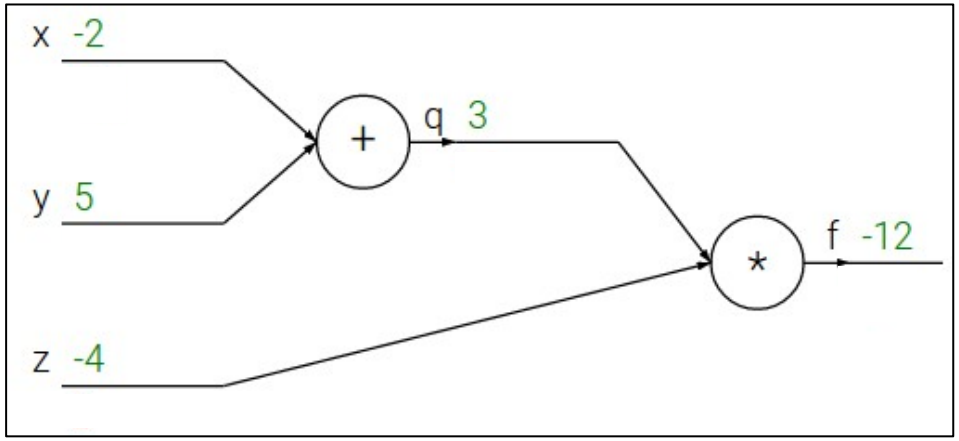

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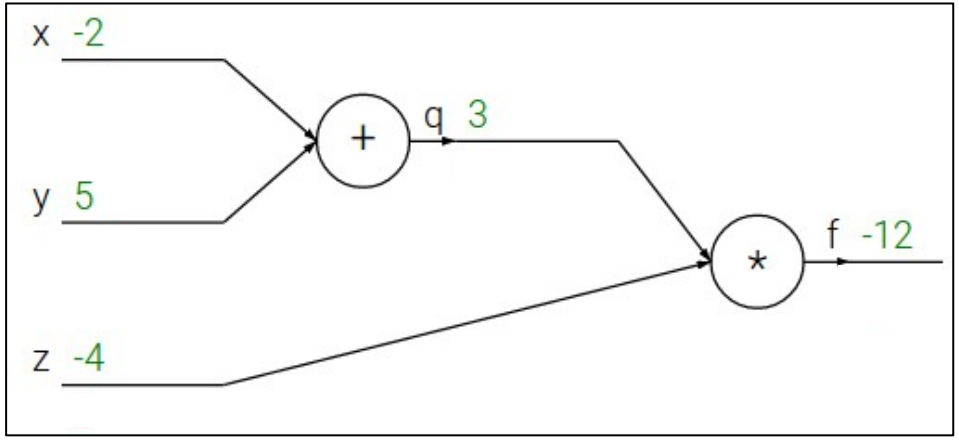

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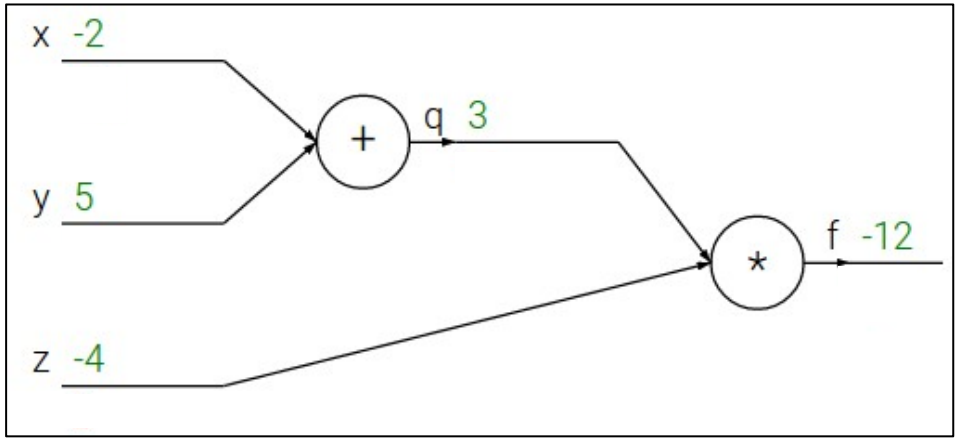

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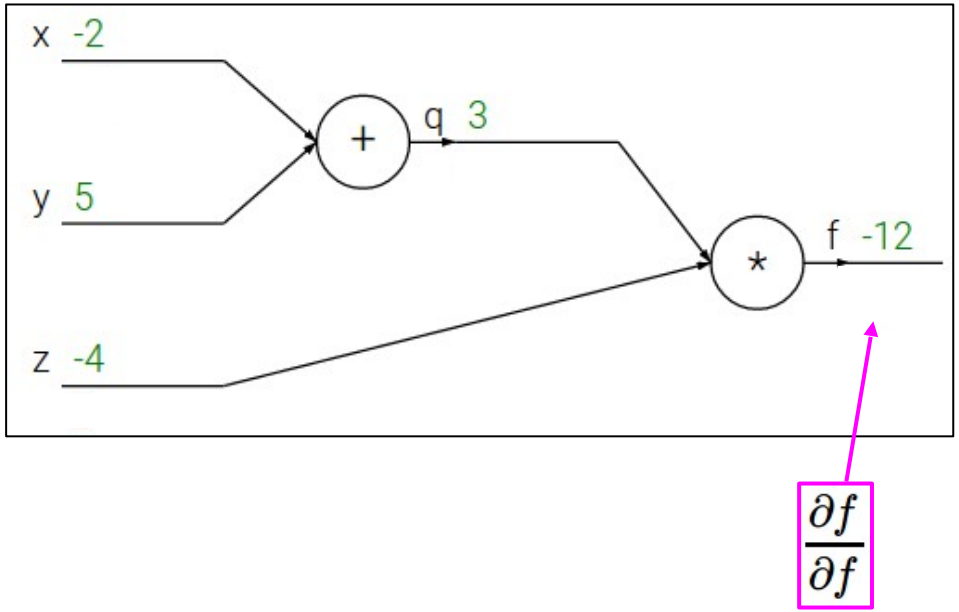

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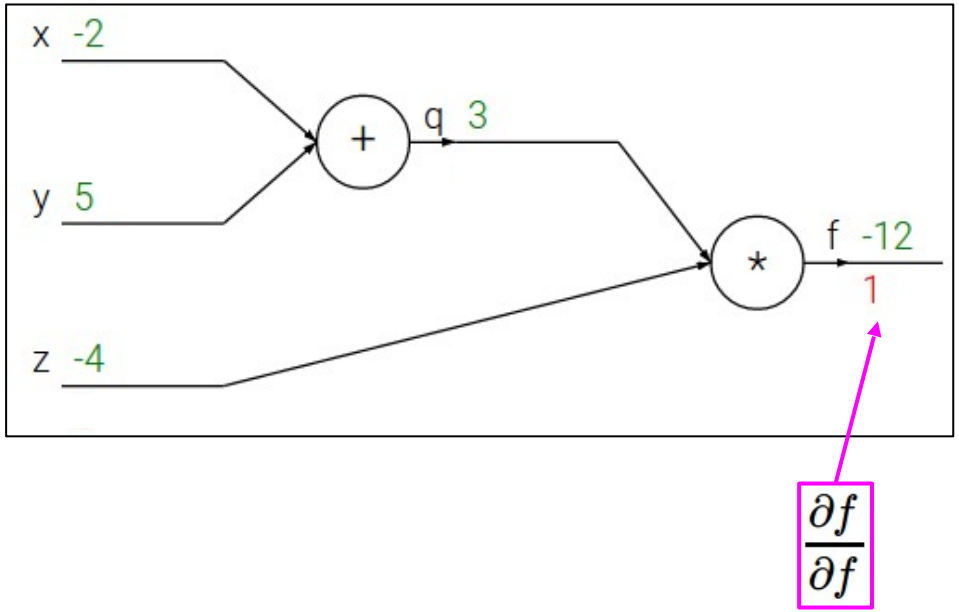

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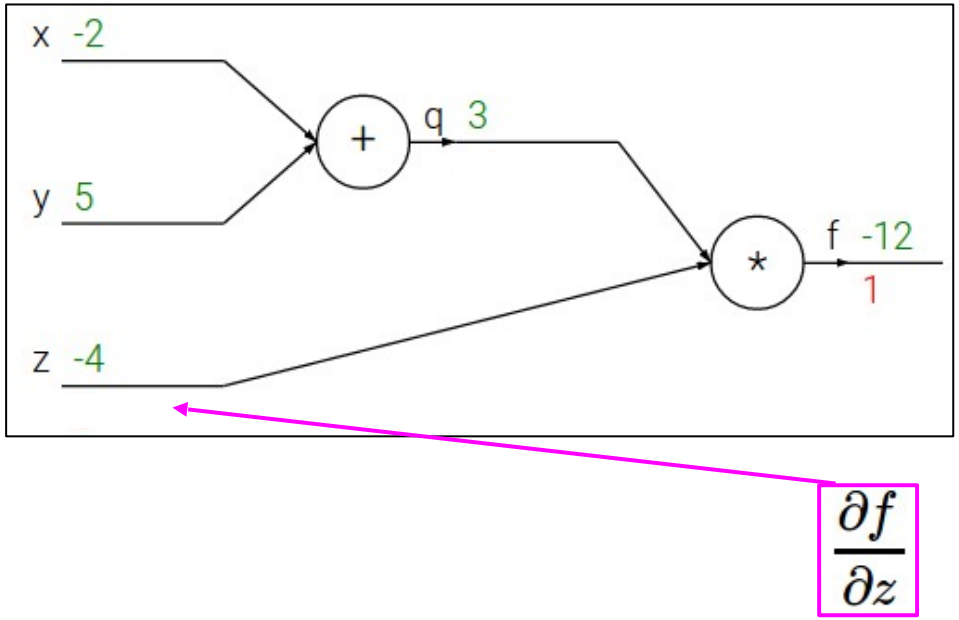

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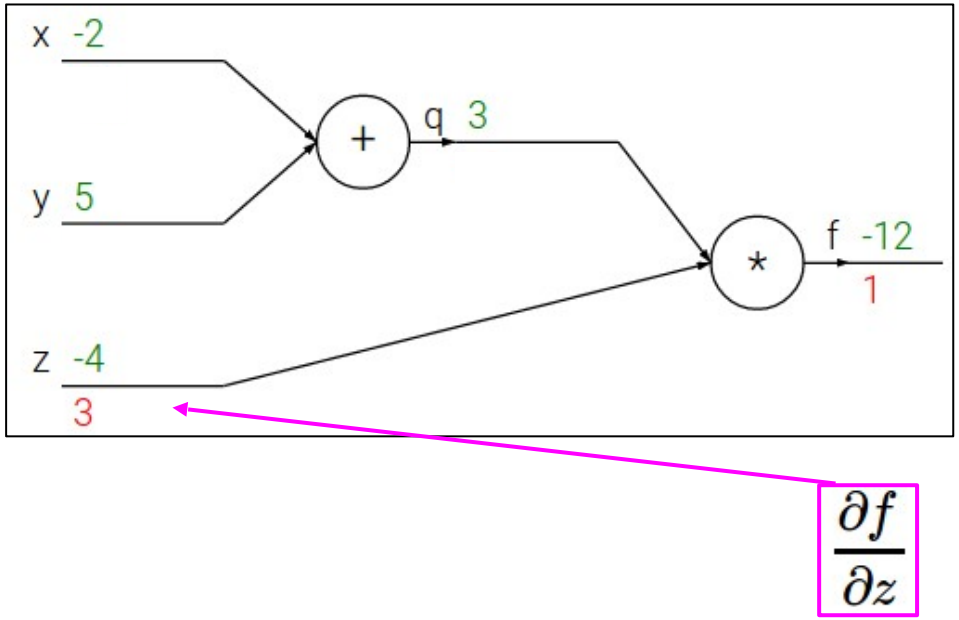

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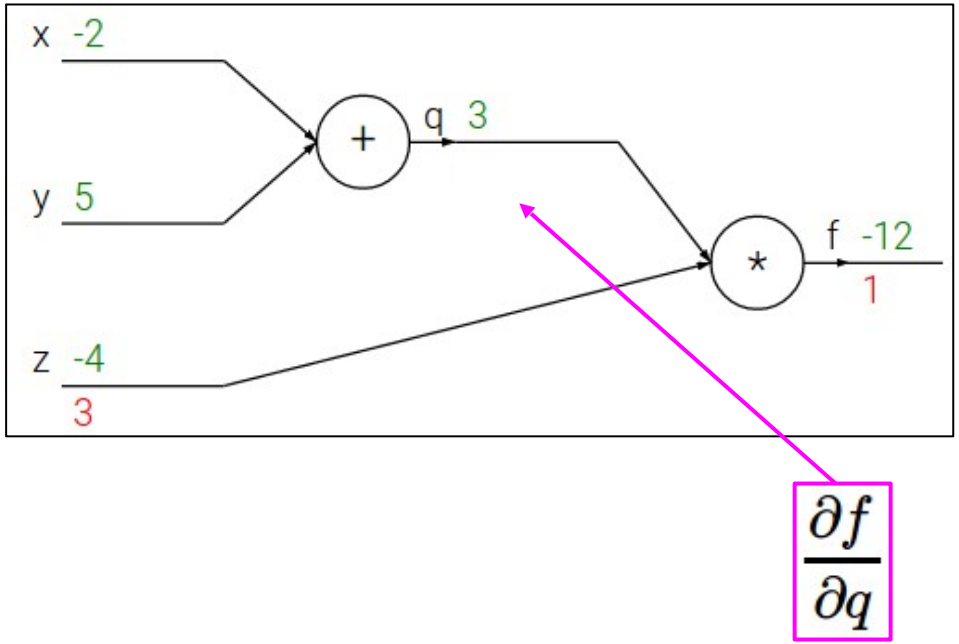

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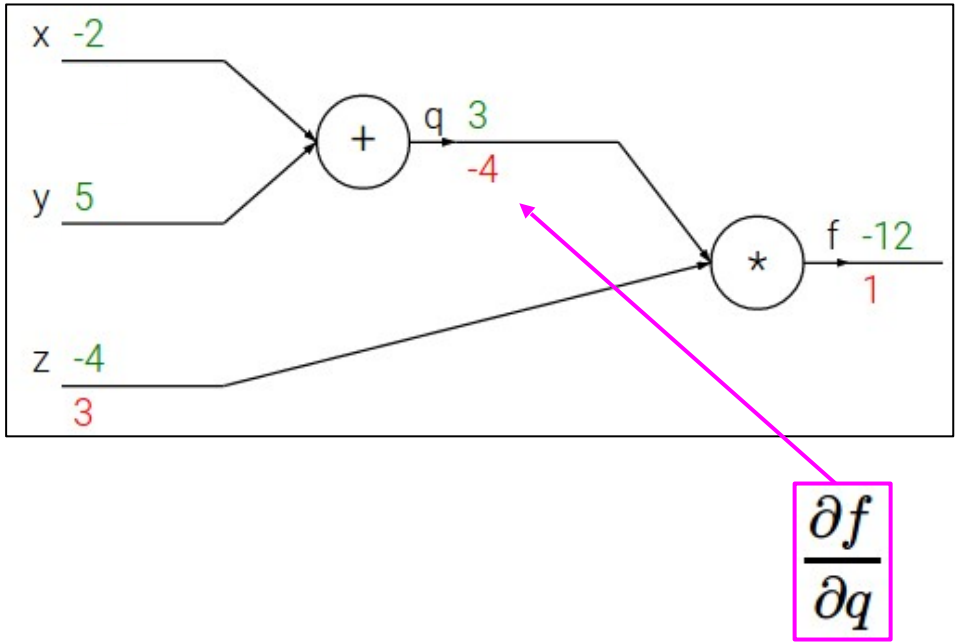

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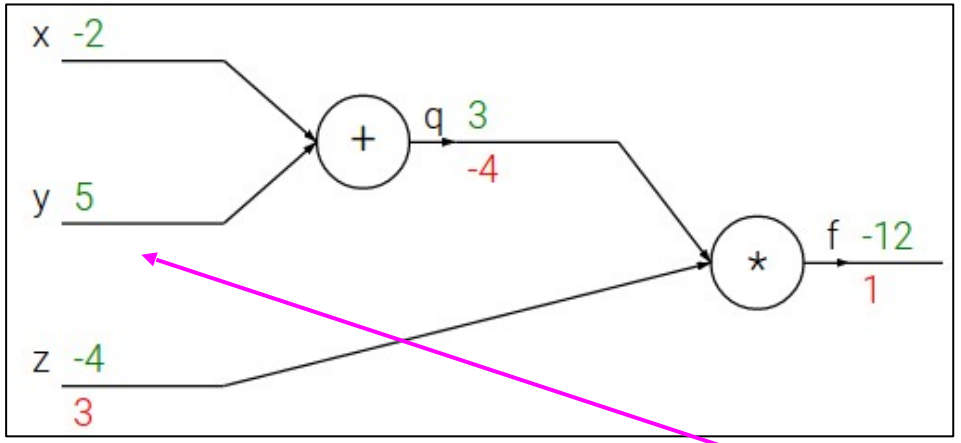

Chain rule:

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

Upstream gradient

Local gradient

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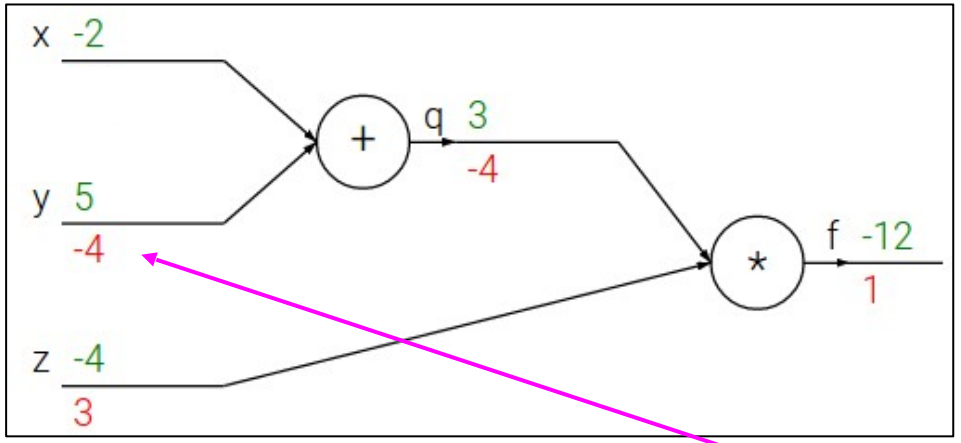

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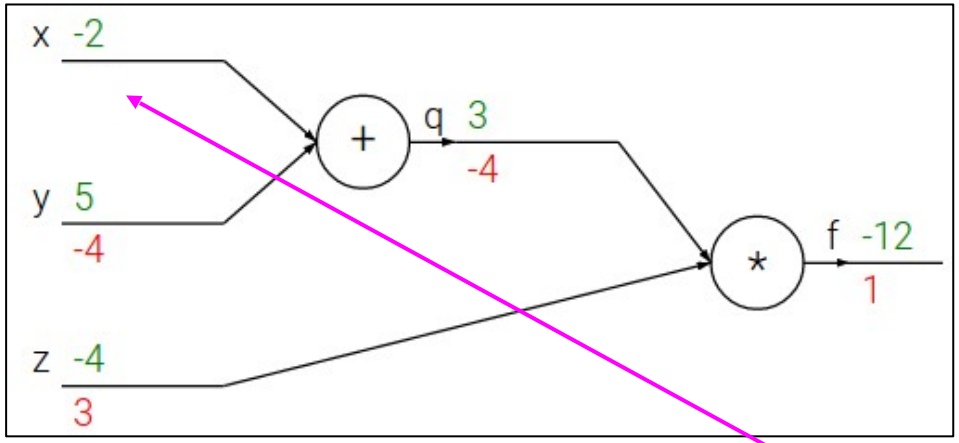

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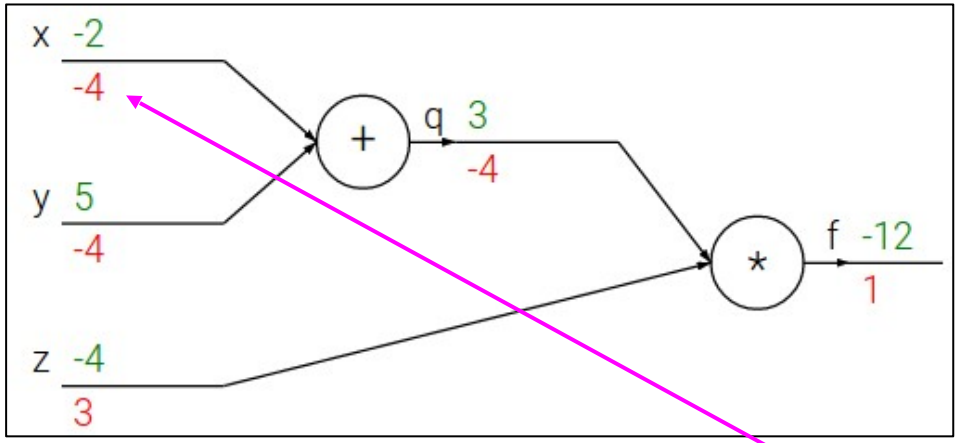

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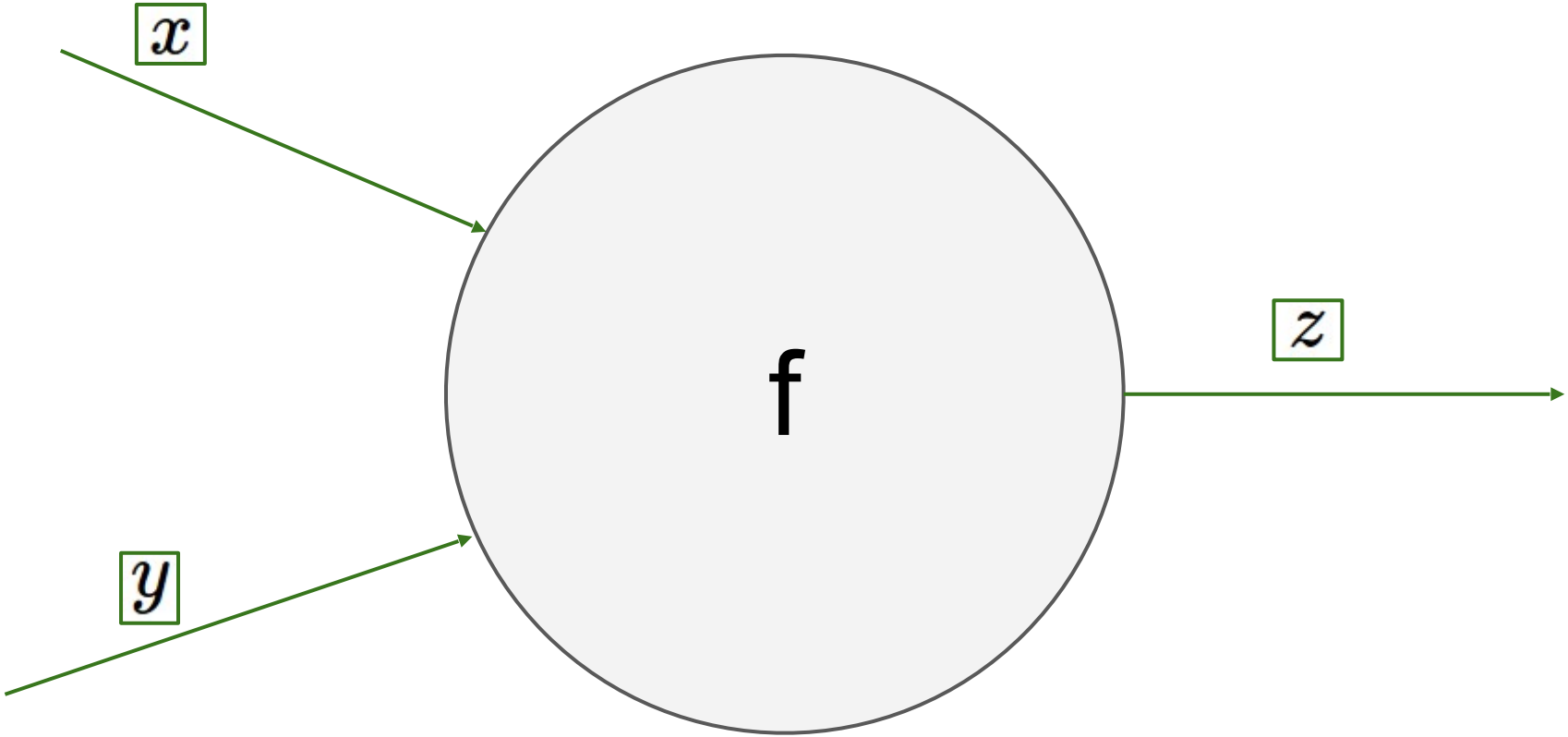
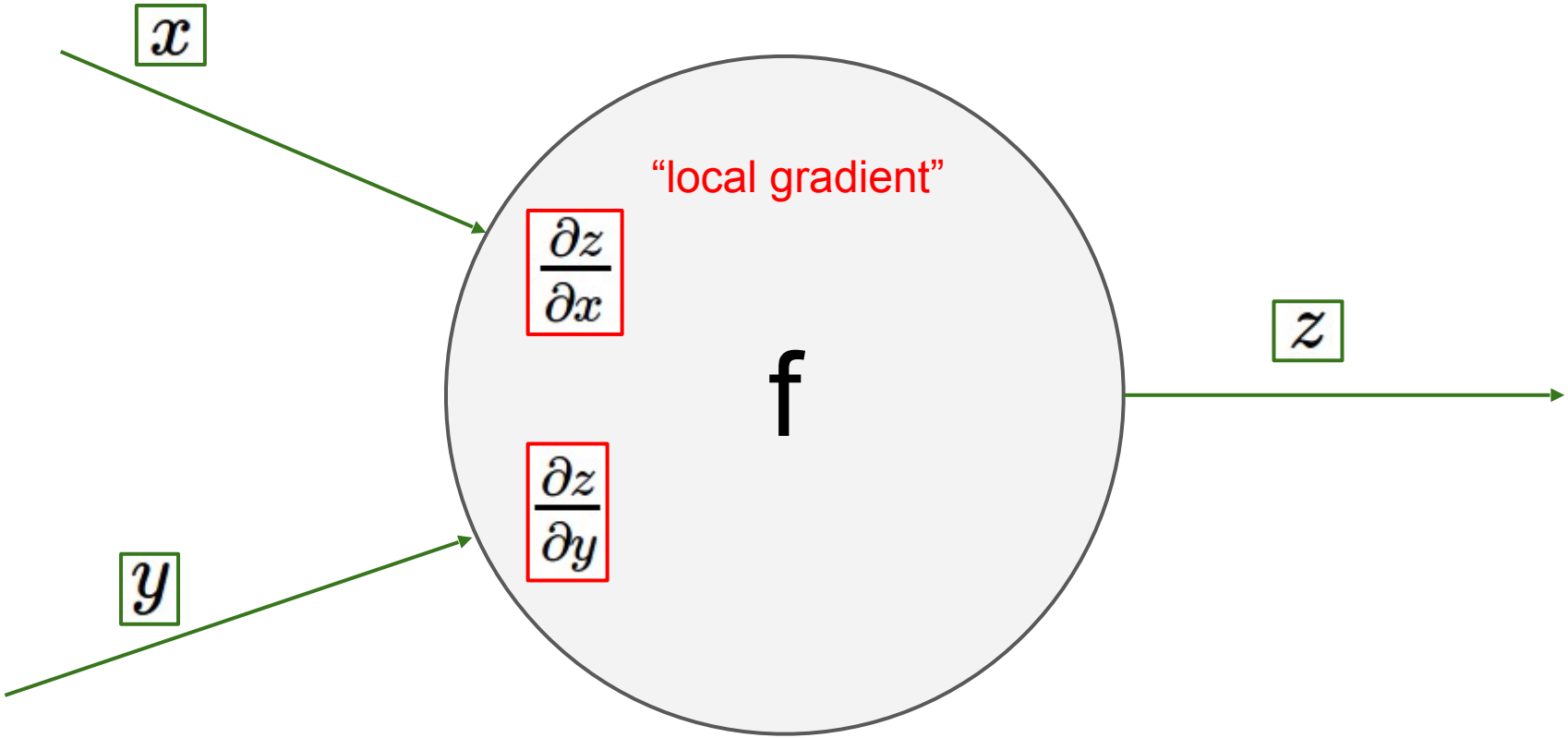
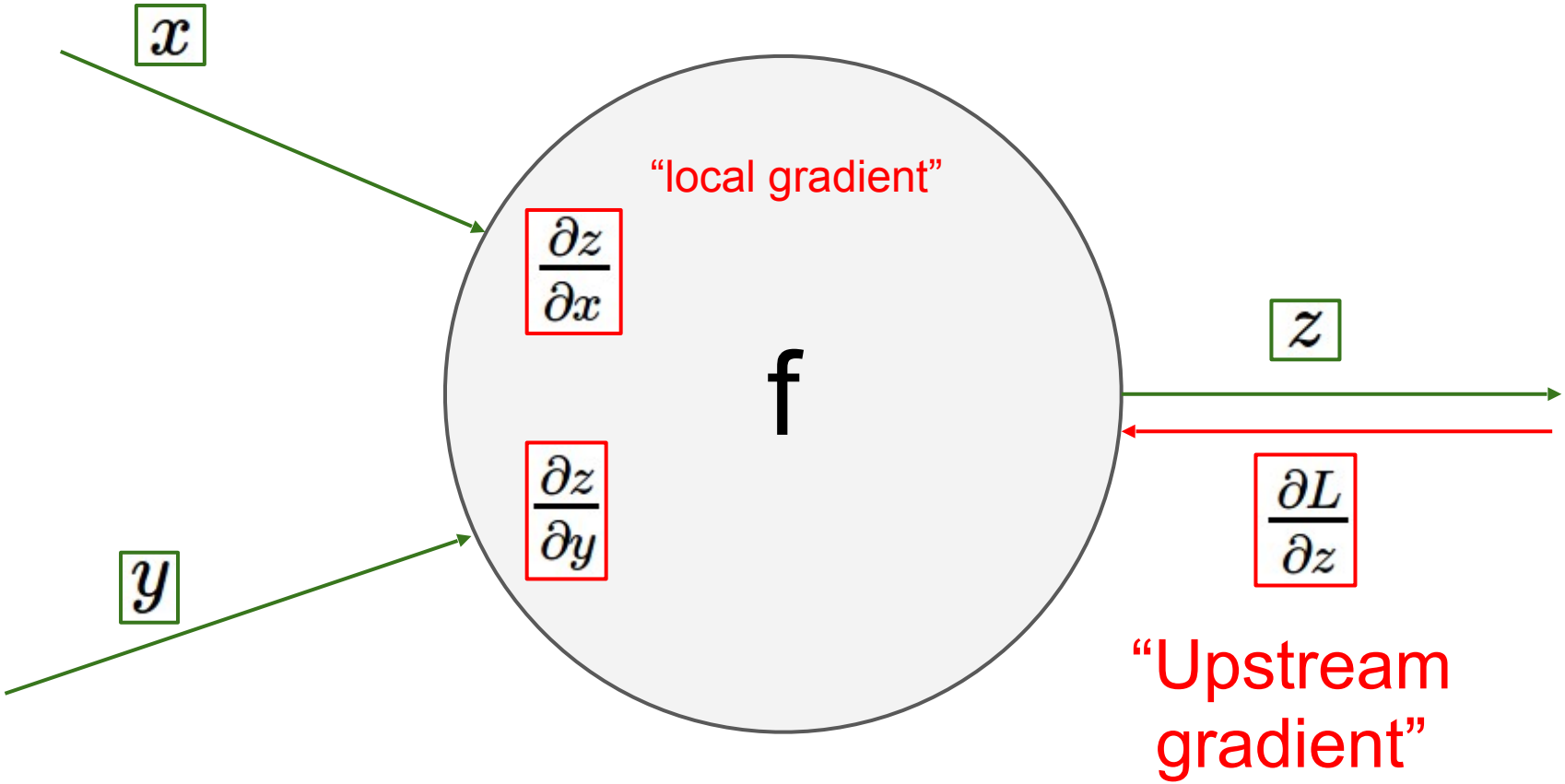

x
y
f
z


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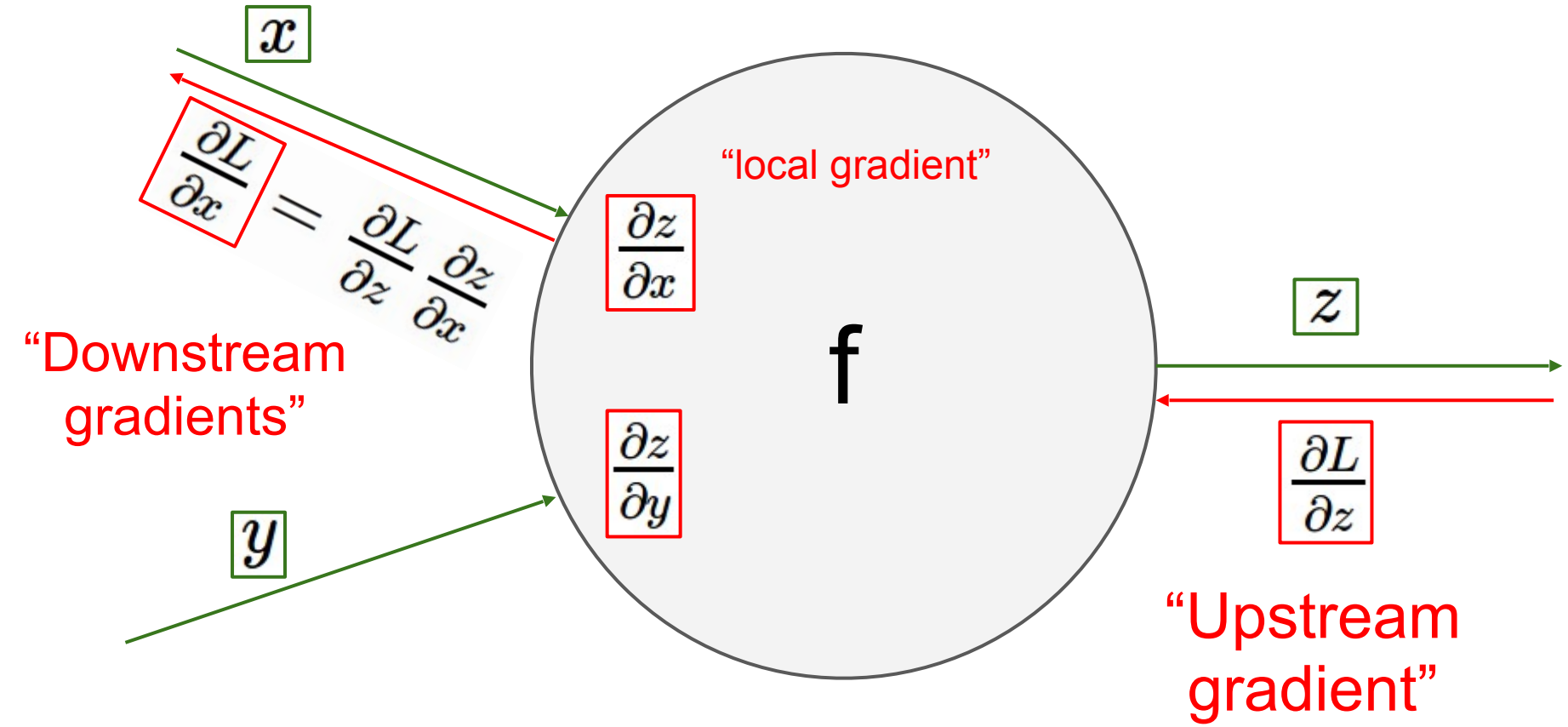
x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
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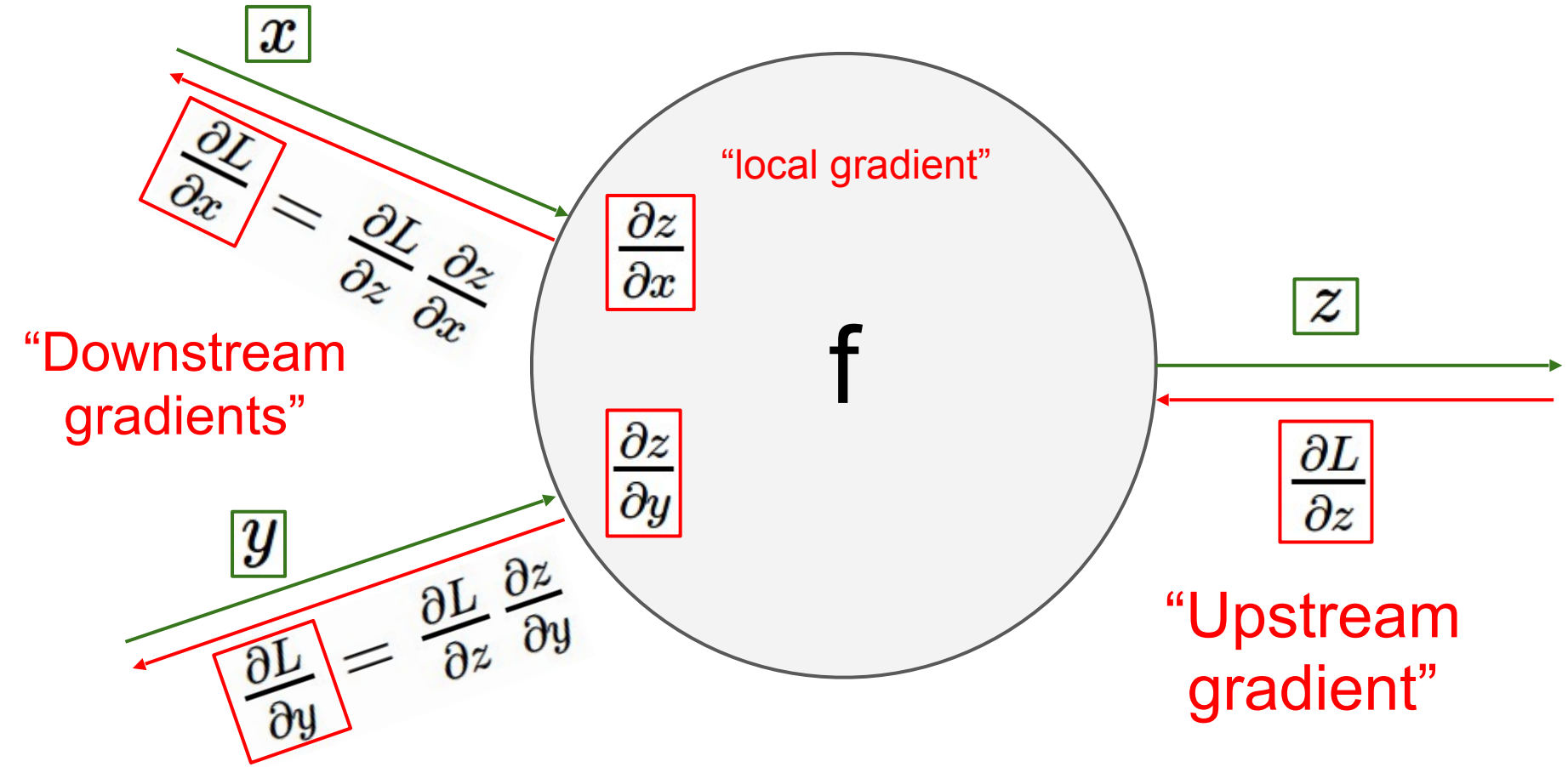
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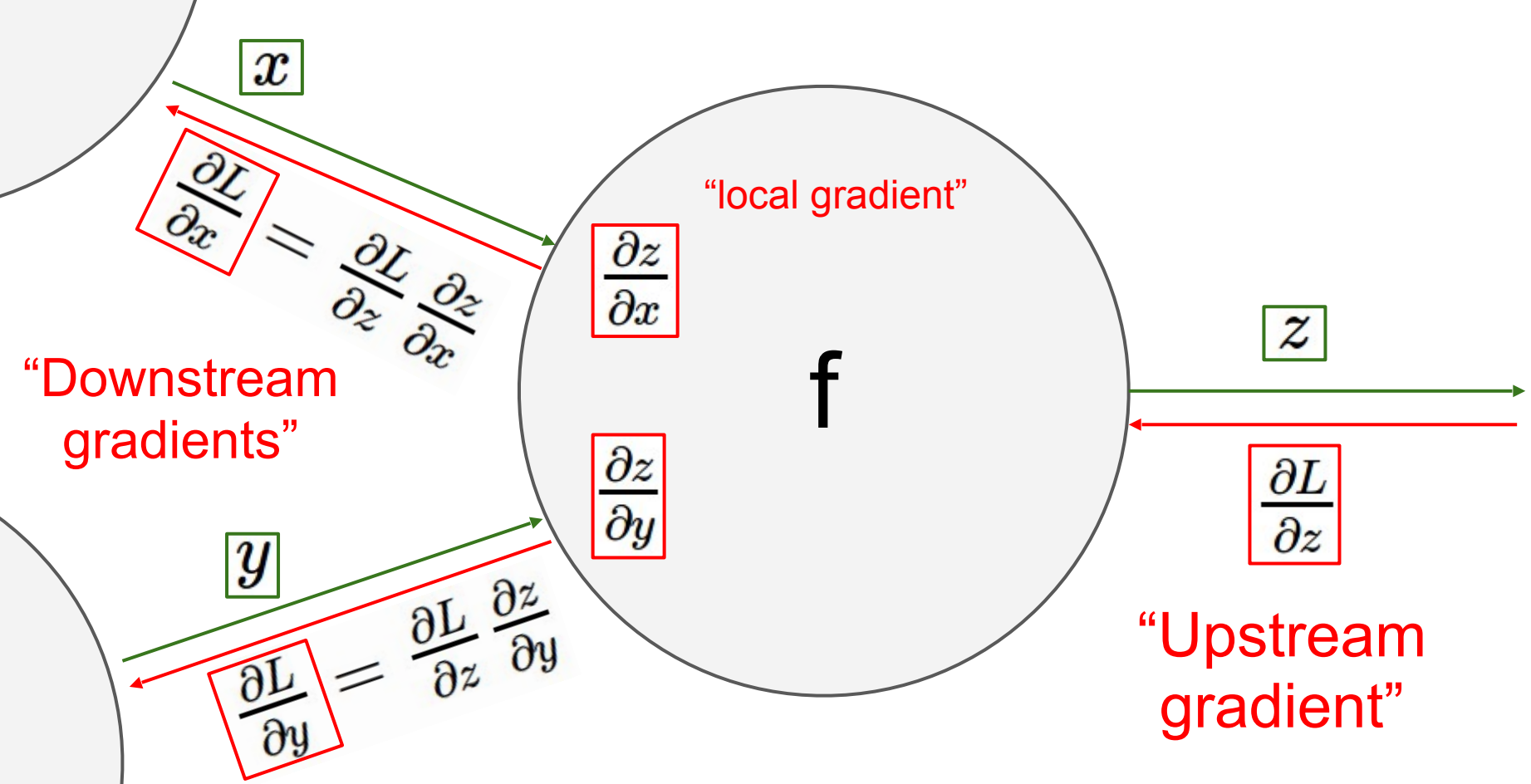
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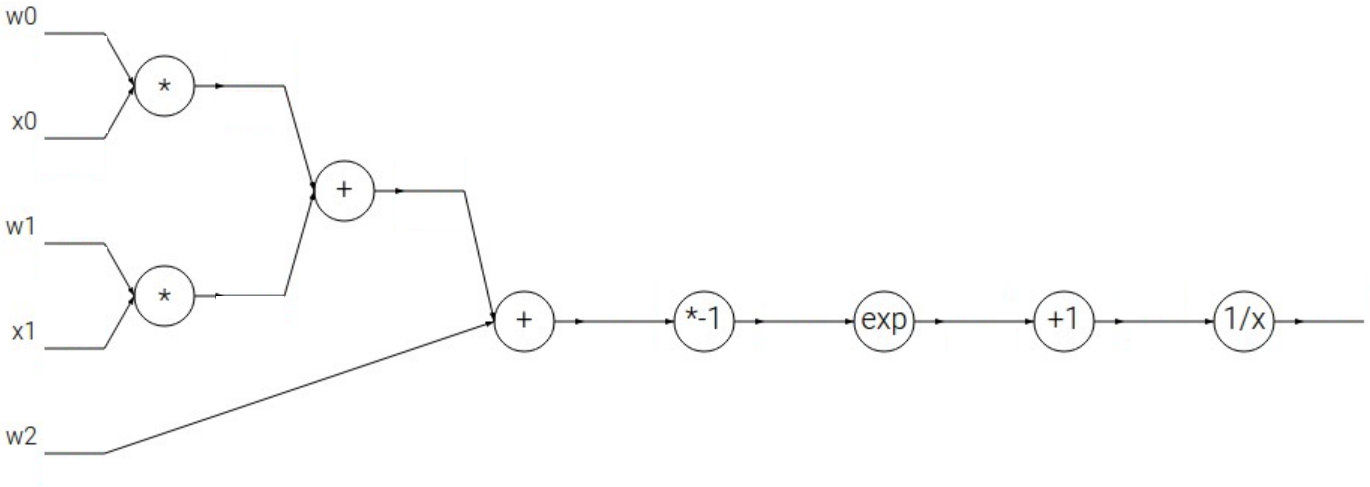
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$

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



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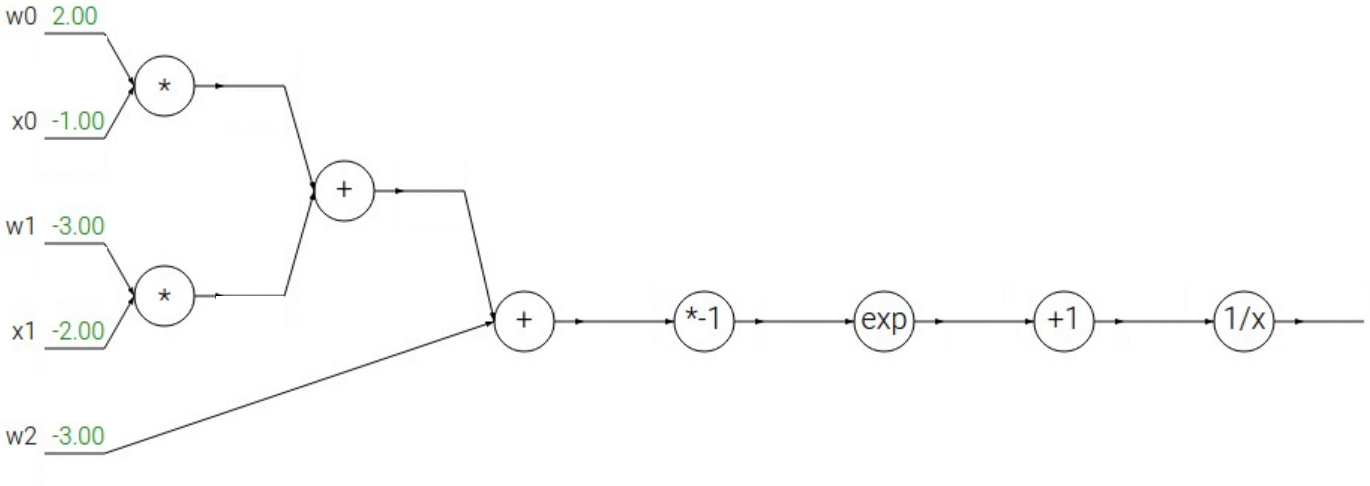

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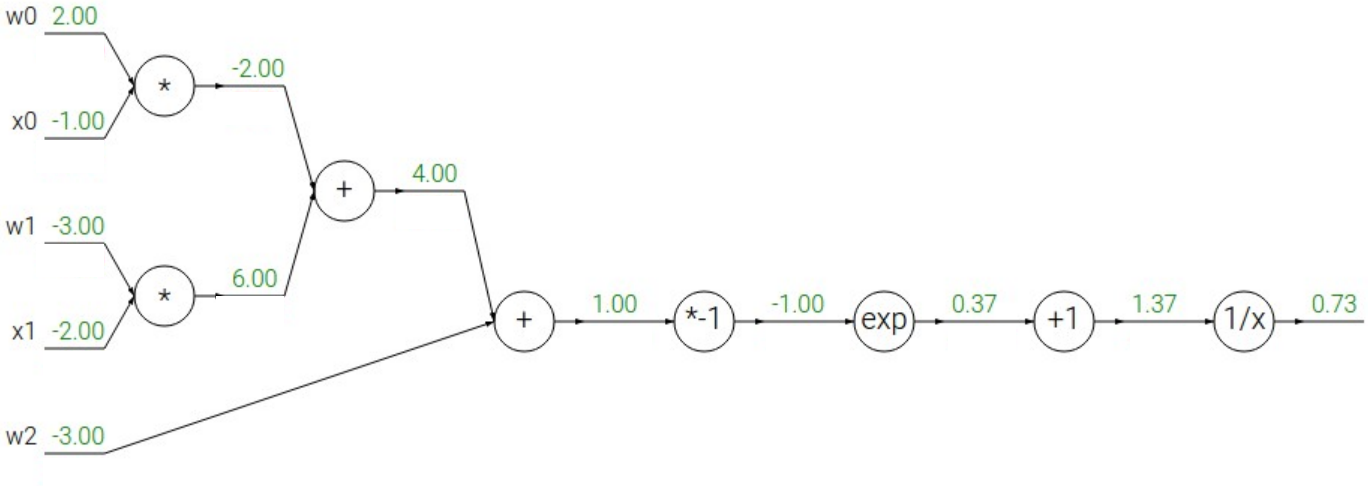

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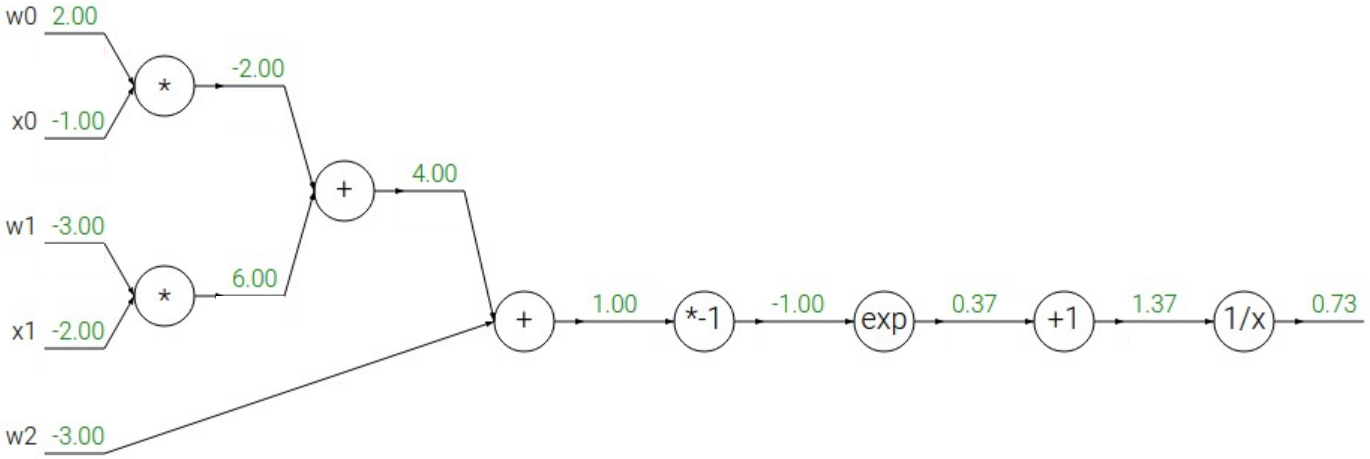

$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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

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

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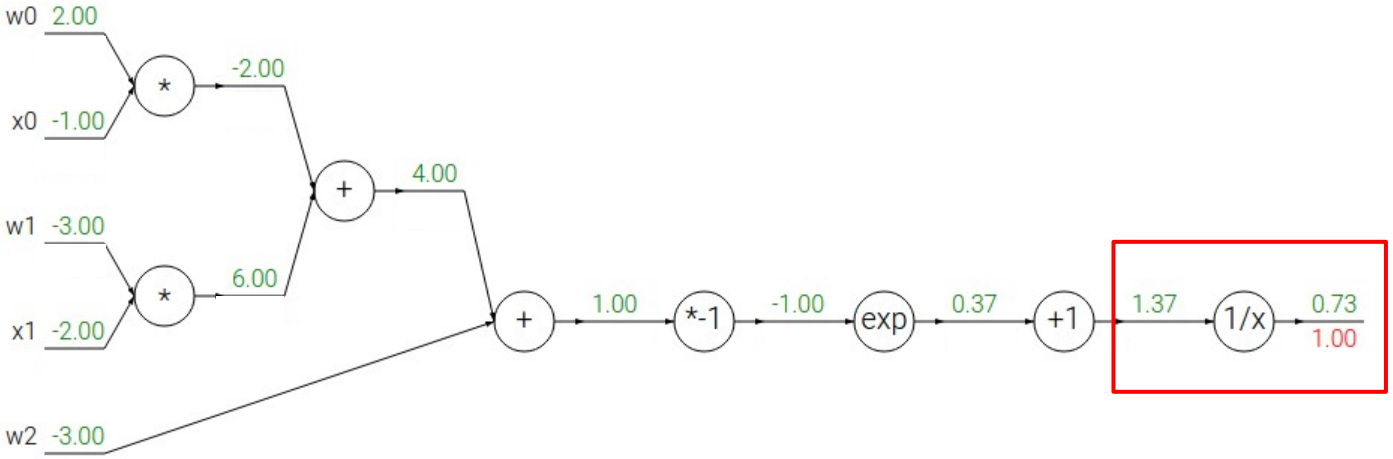

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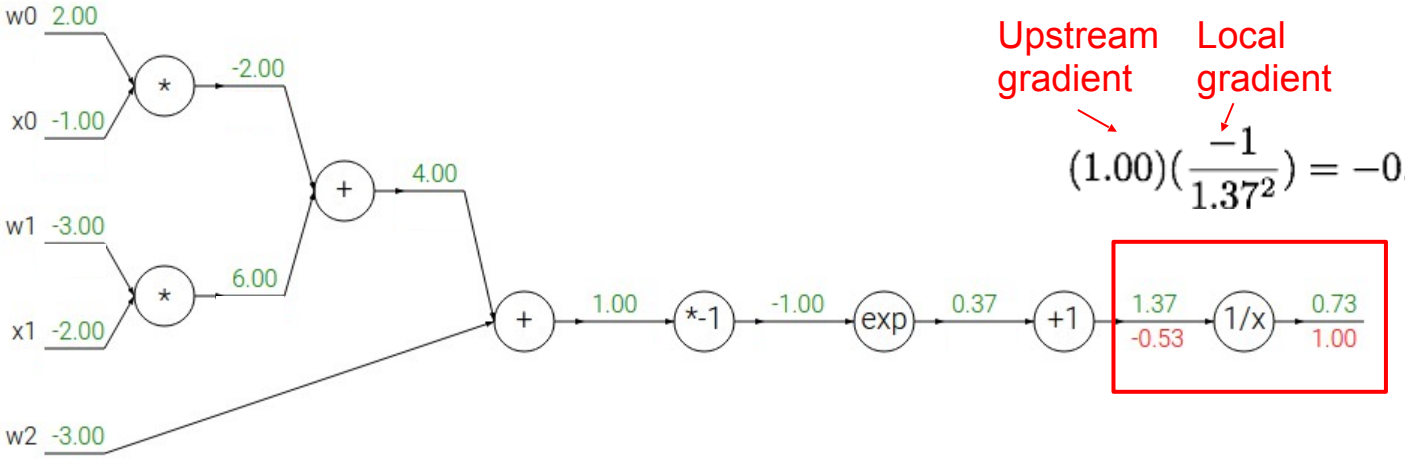

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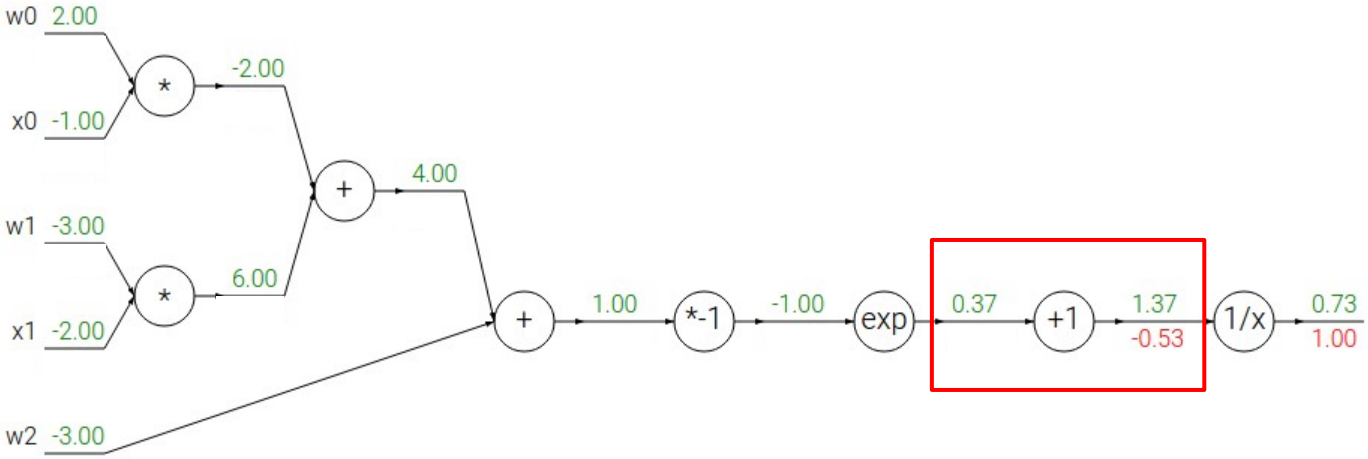

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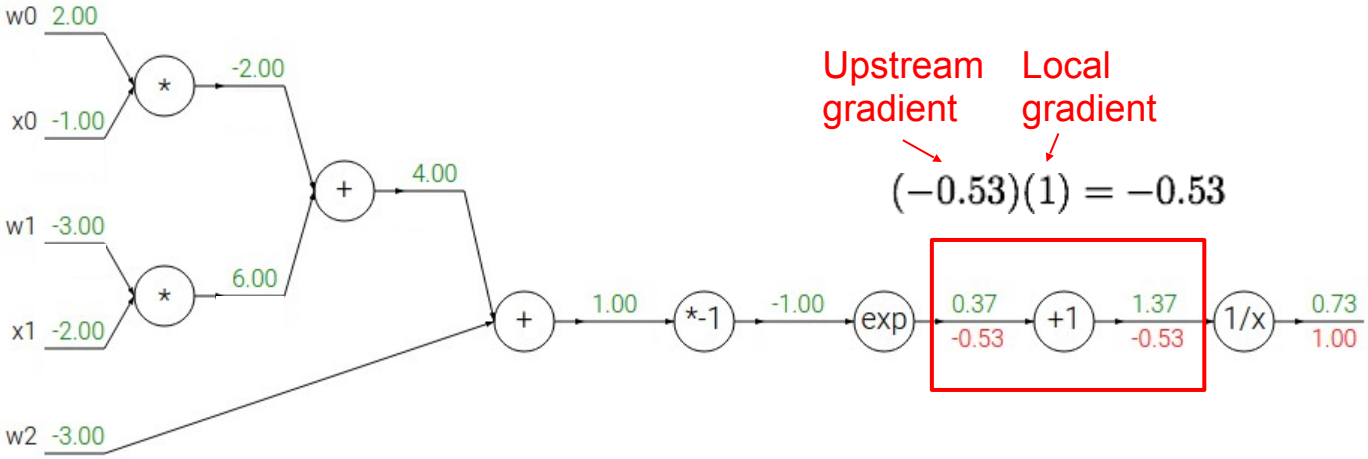

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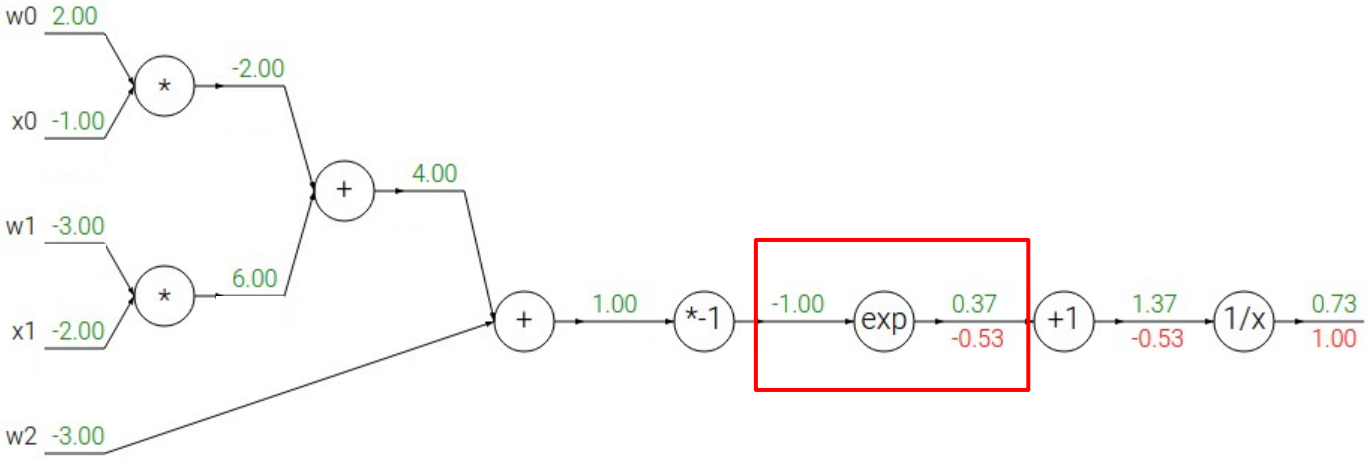

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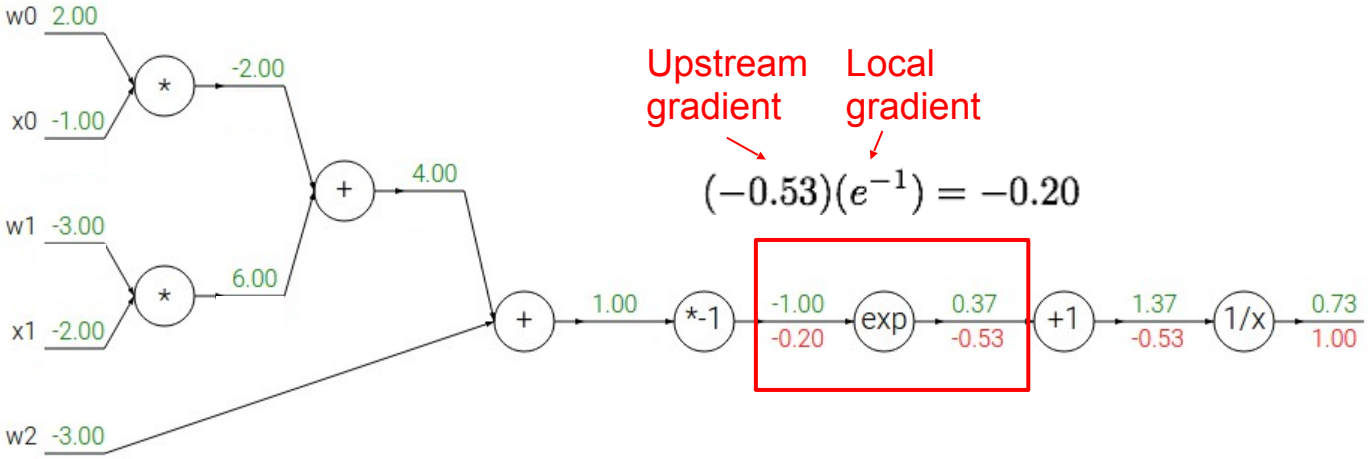

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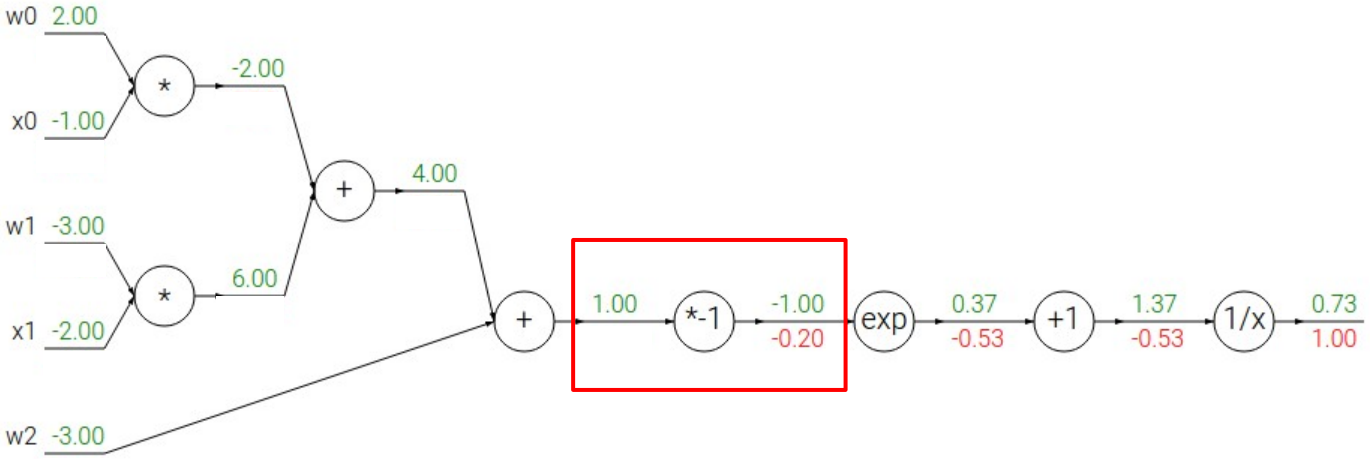

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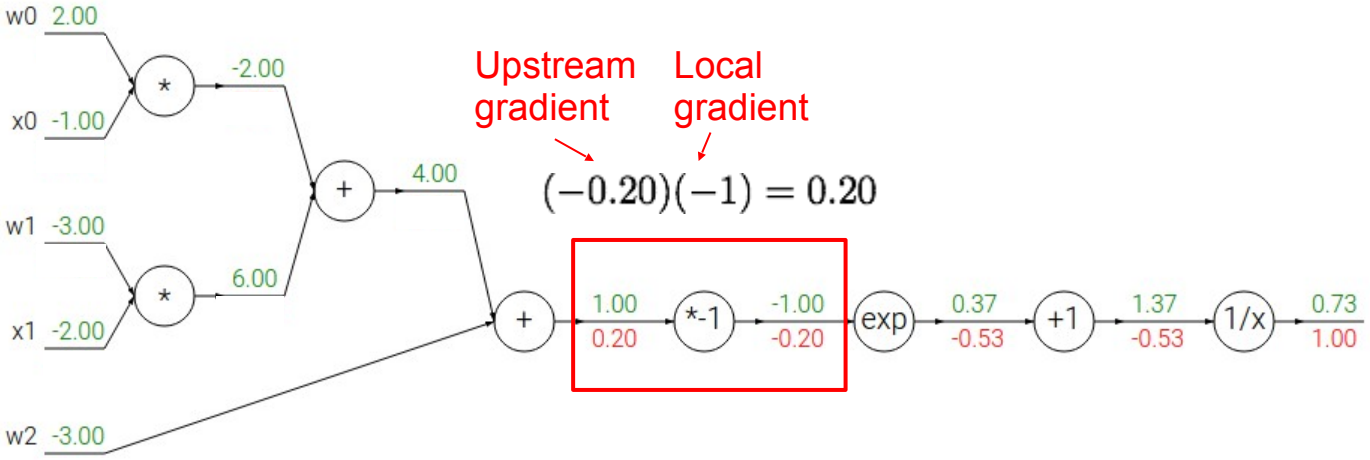

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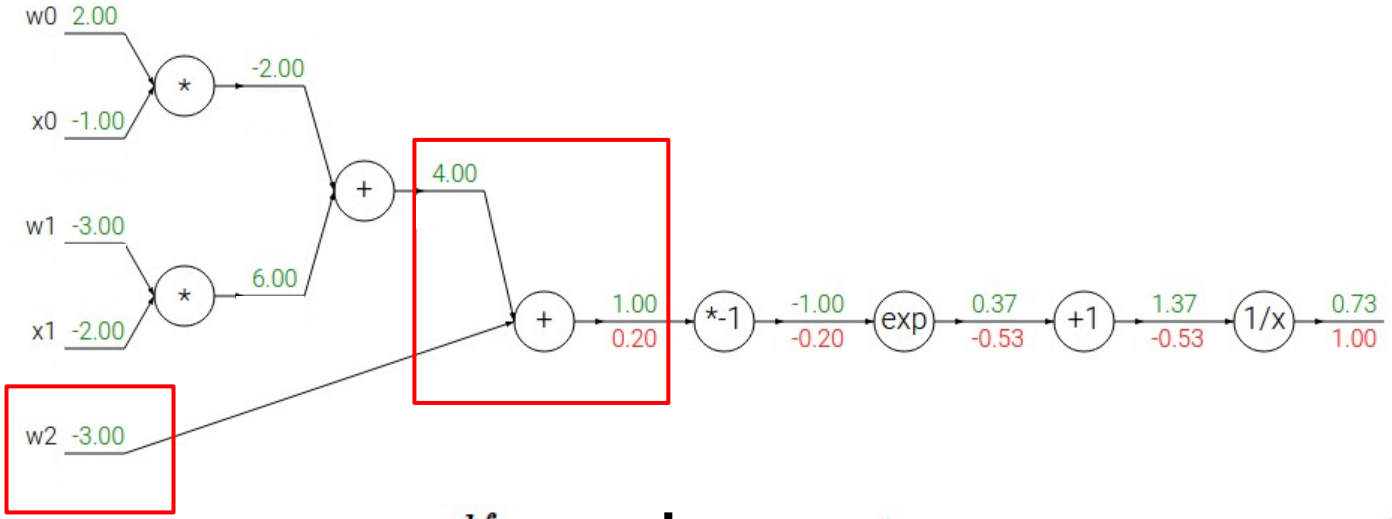

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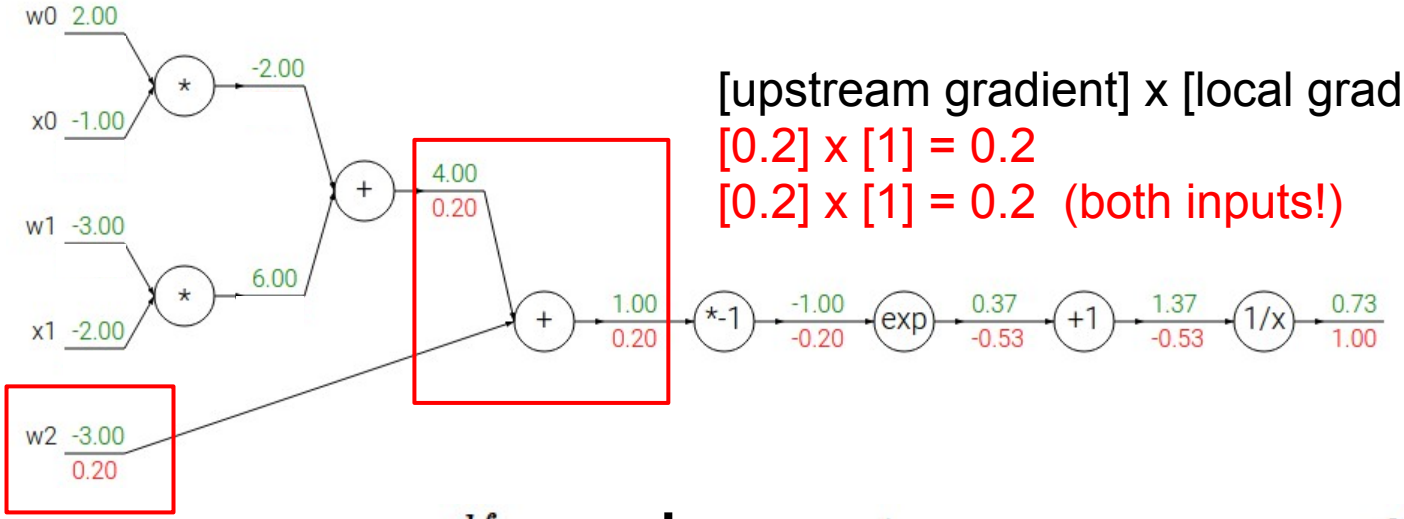

[upstream gradient] x [local gradient]

[0.2] x [1] = 0.2

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

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

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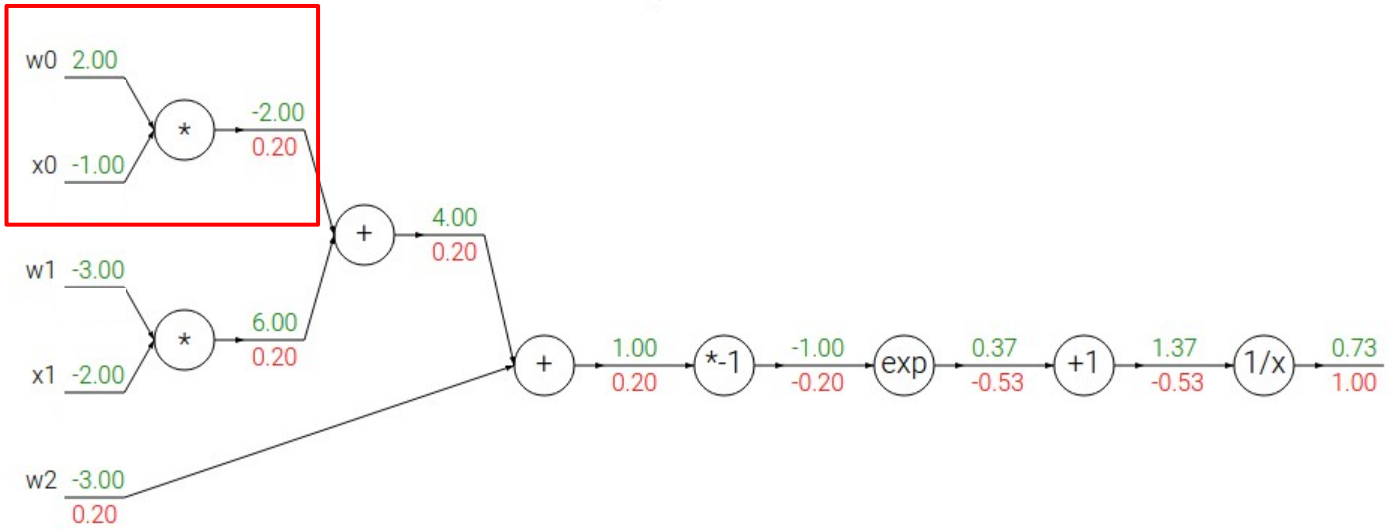

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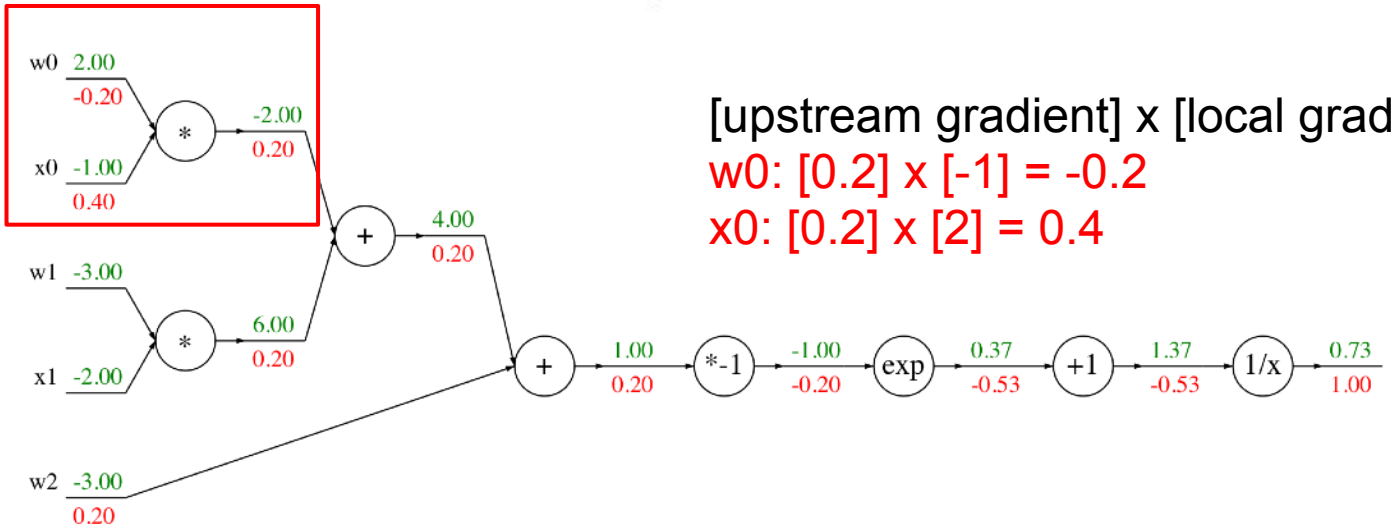

[upstream gradient] x [local gradient]

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

x0: [0.2] x [2] = 0.4

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

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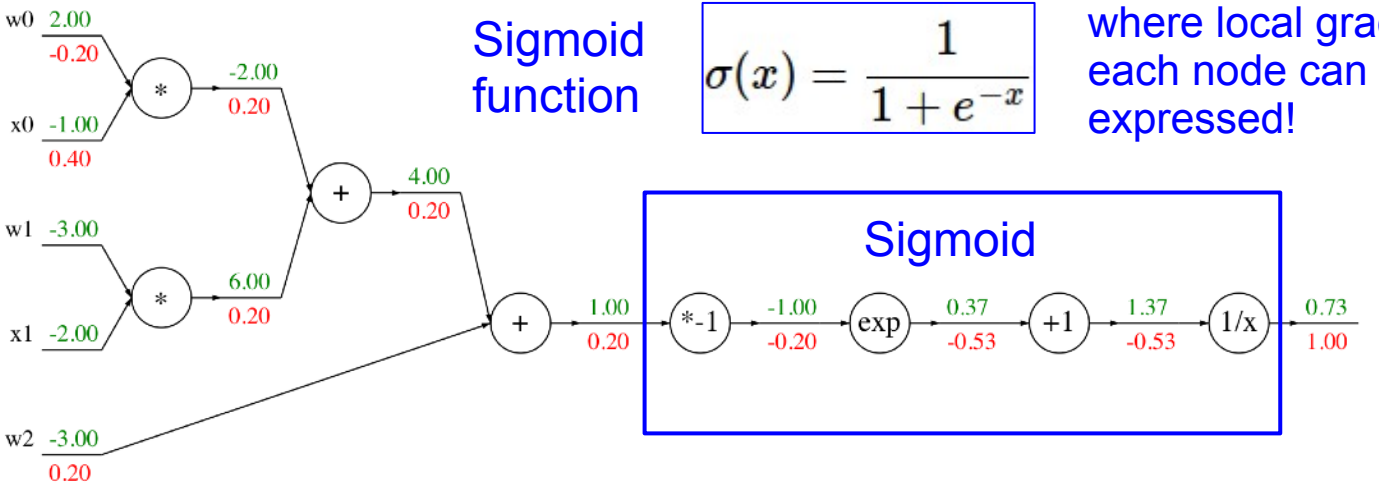
Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!



Sigmoid function

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

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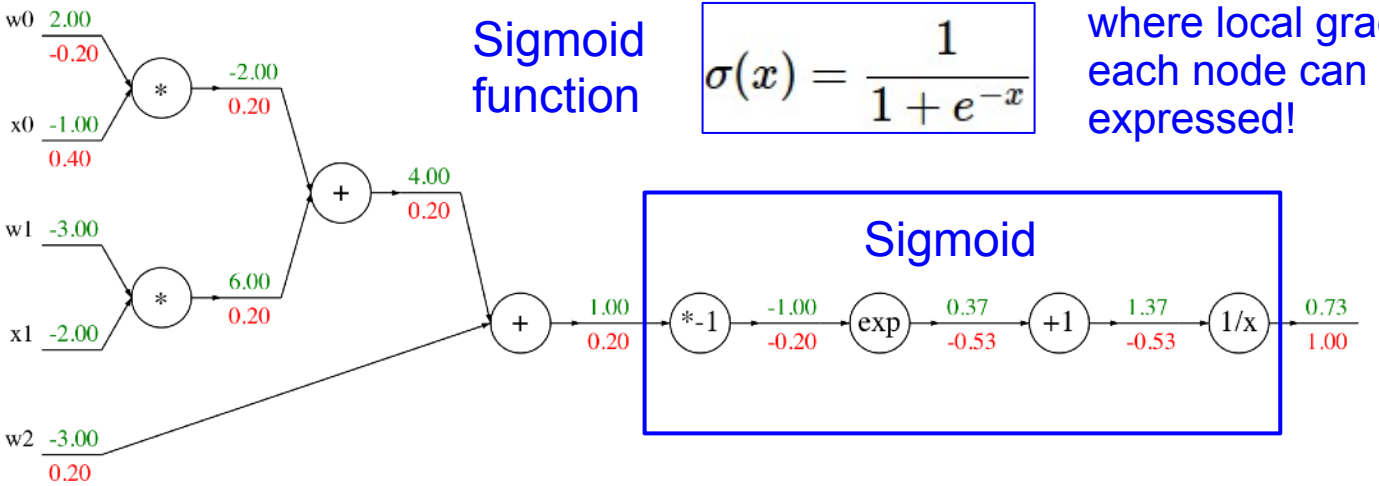

Sigmoid function

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

Sigmoid local gradient:

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

Another example:

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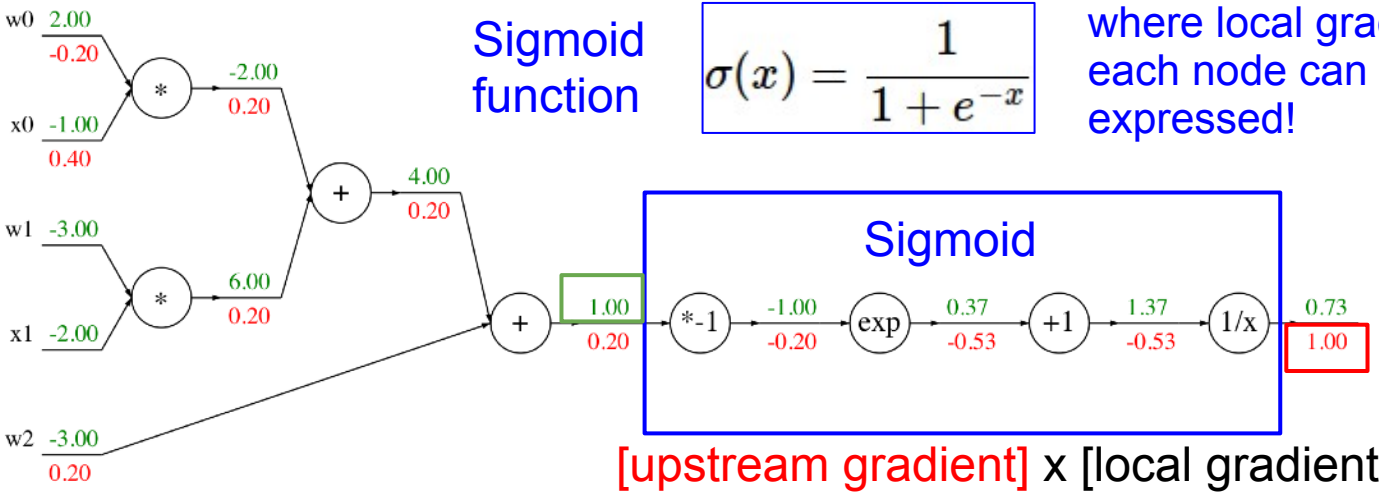

Sigmoid function

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

[upstream gradient] x [local gradient]

[1.00] x [(1 - 1/(1+e^{-1})) (1/(1+e^{-1}))] = 0.2

Sigmoid local gradient:

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

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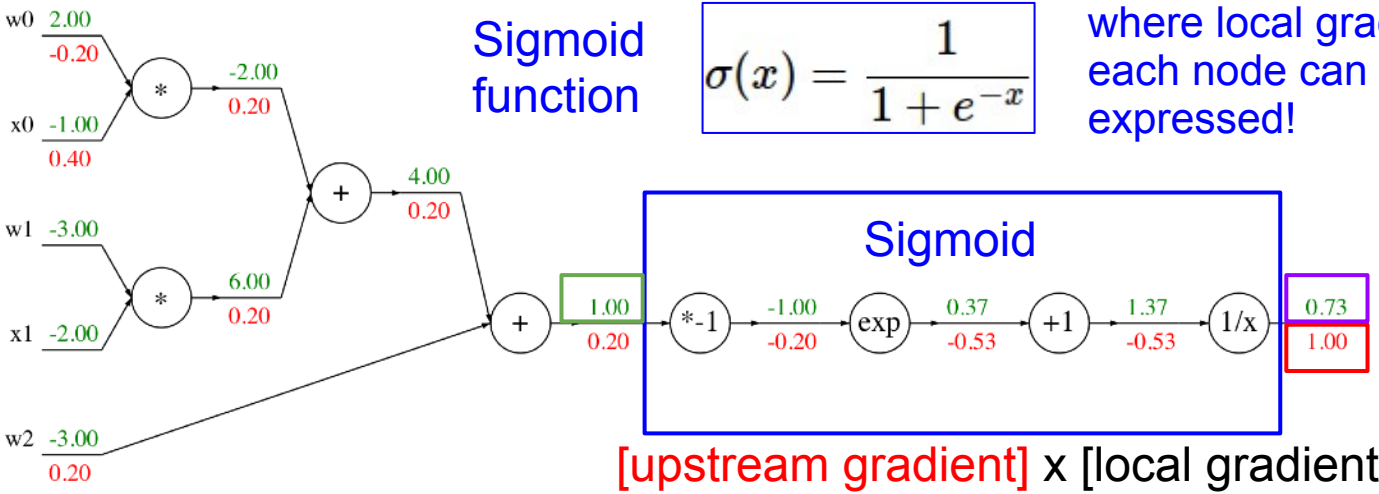


Sigmoid function

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

[upstream gradient] x [local gradient]

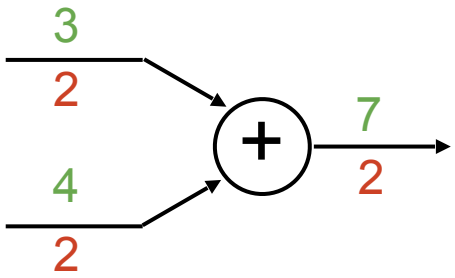
[1.00] x [(1 - 0.73) (0.73)] = 0.2

Sigmoid local gradient:

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

Patterns in gradient flow

add gate: gradient distributor



Patterns in gradient flow

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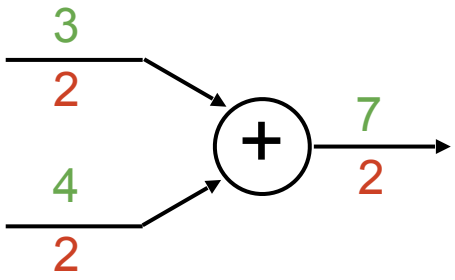
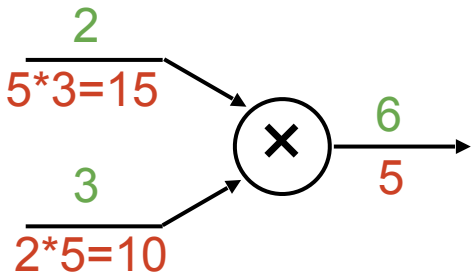


mul gate: “swap multiplier”



Patterns in gradient flow

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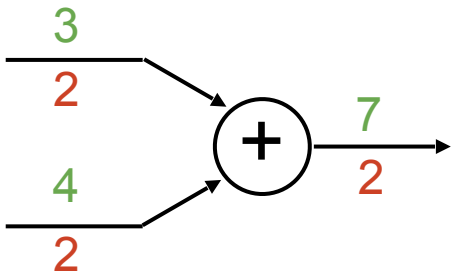

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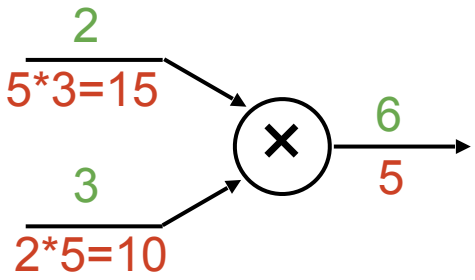
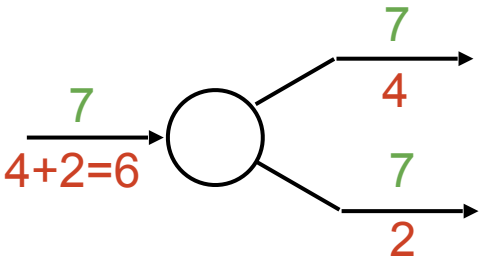
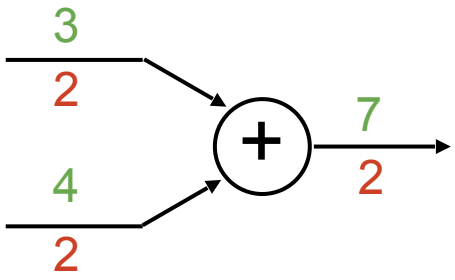


copy gate: gradient adder



Patterns in gradient flow

add gate: gradient distributor



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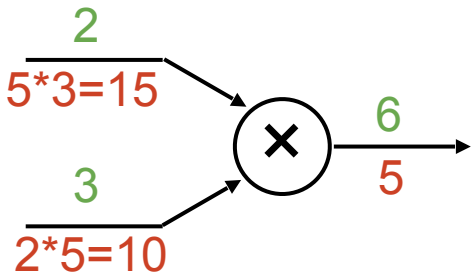
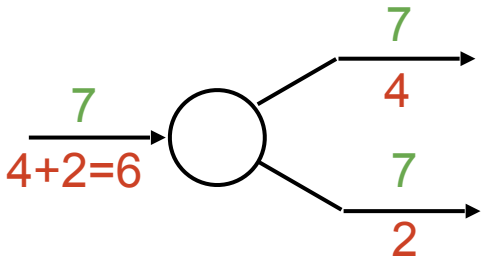
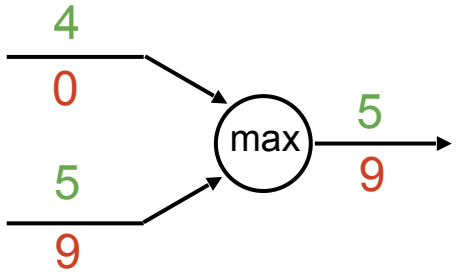


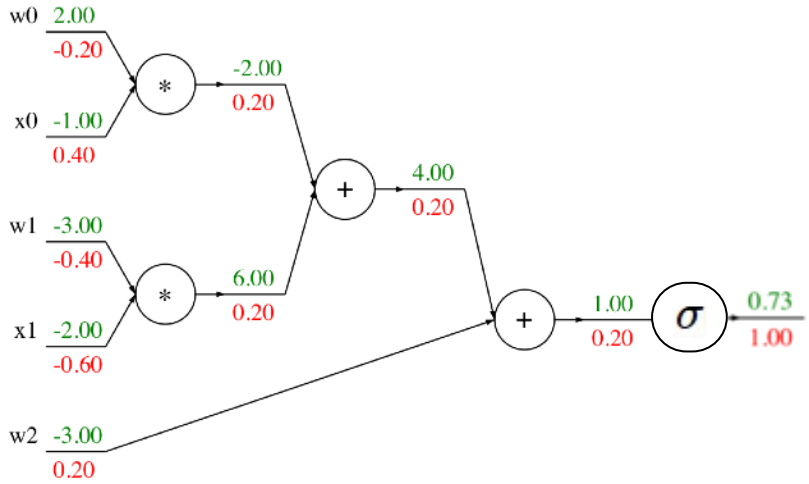
copy gate: gradient adder



max gate: gradient router



Backprop Implementation: "Flat" code



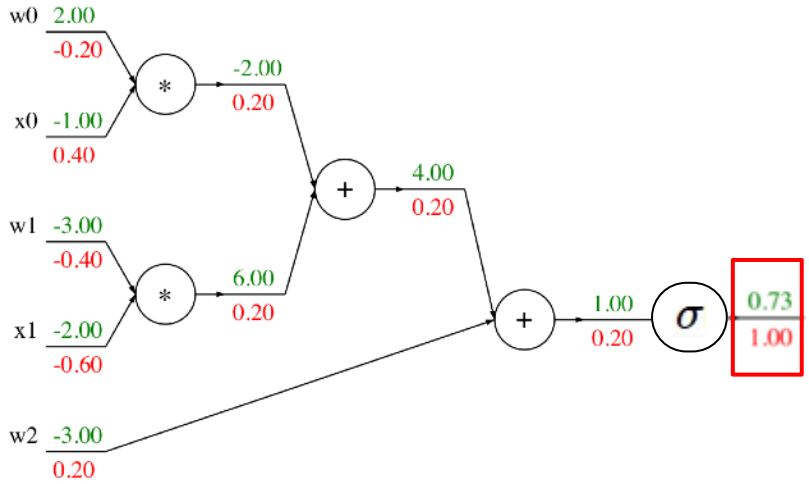
Forward pass: Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Backward pass: Compute grads

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" code



Forward pass: Compute output

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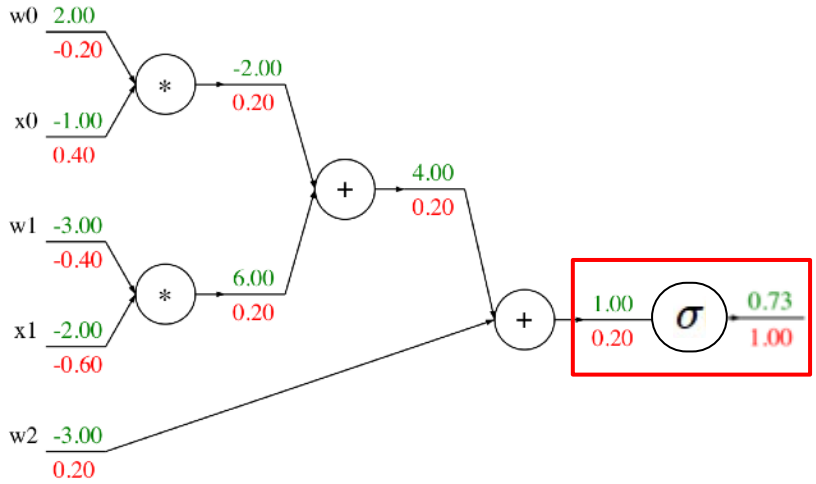
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Base case

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" code



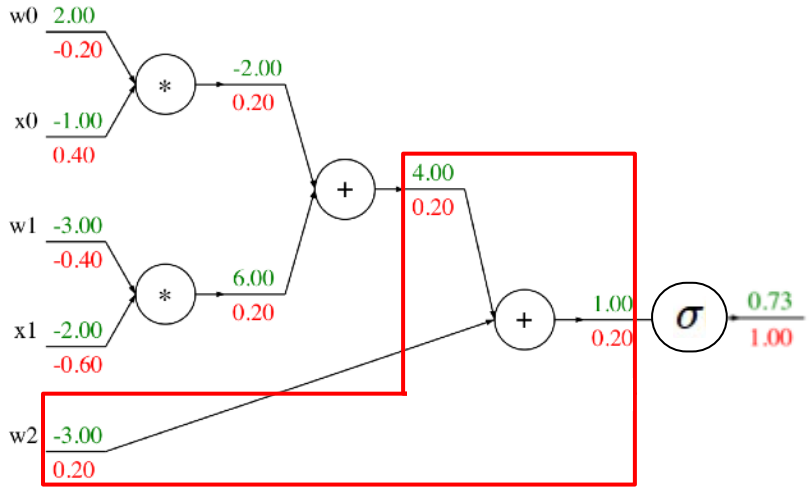
Forward pass: Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Sigmoid

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" code



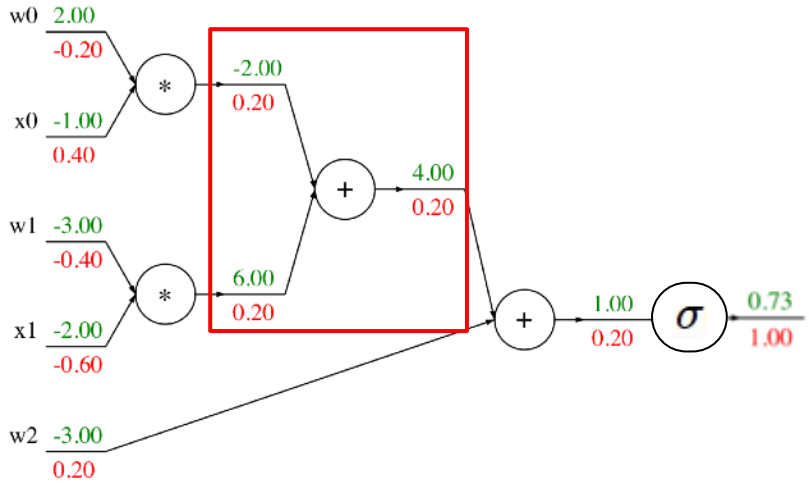
Forward pass: Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Add gate

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" code



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```
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  s0 = w0 * x0
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```

Add gate

```
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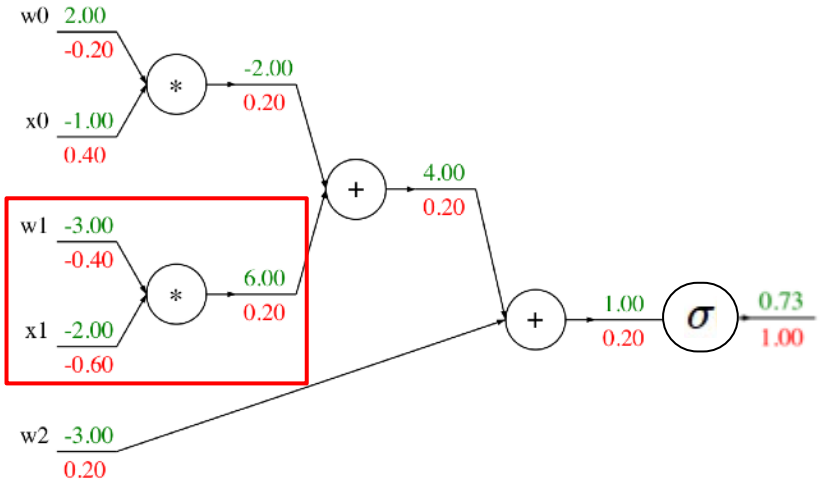
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" code



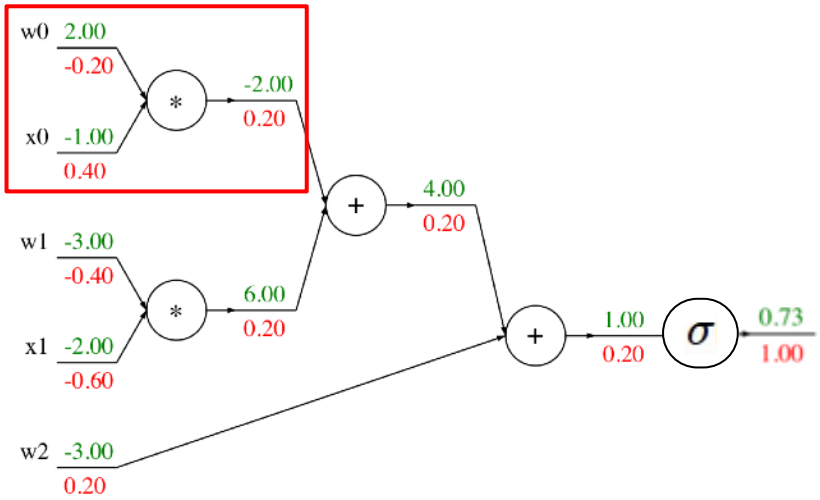
Forward pass: Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Multiply gate

Backprop Implementation: "Flat" code



Forward pass: Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Multiply gate

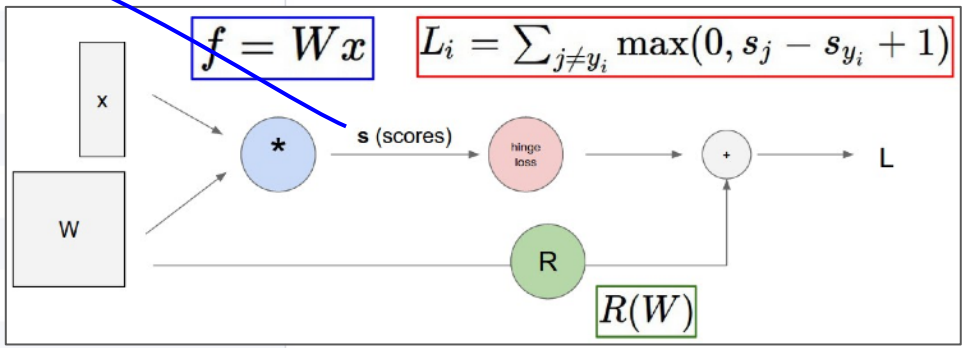
```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

“Flat” Backprop: Do this for assignment 1!

Stage your forward/backward computation!

E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 6 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 = #...
```

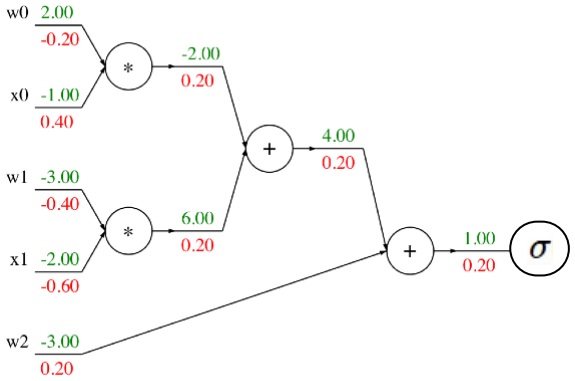


“Flat” Backprop: Do this for assignment 1!

E.g. for two-layer neural net:

```
# 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 = #...
```

Backprop Implementation: Modularized API

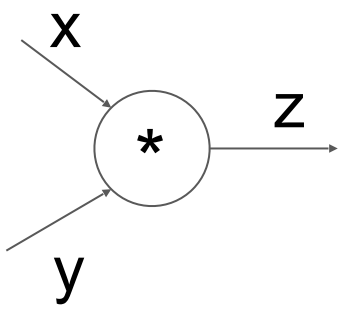


Graph (or Net) object *(rough pseudo code)*

```
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
```

Modularized implementation: forward / backward API

Gate / Node / Function object: Actual PyTorch code



(x,y,z are scalars)

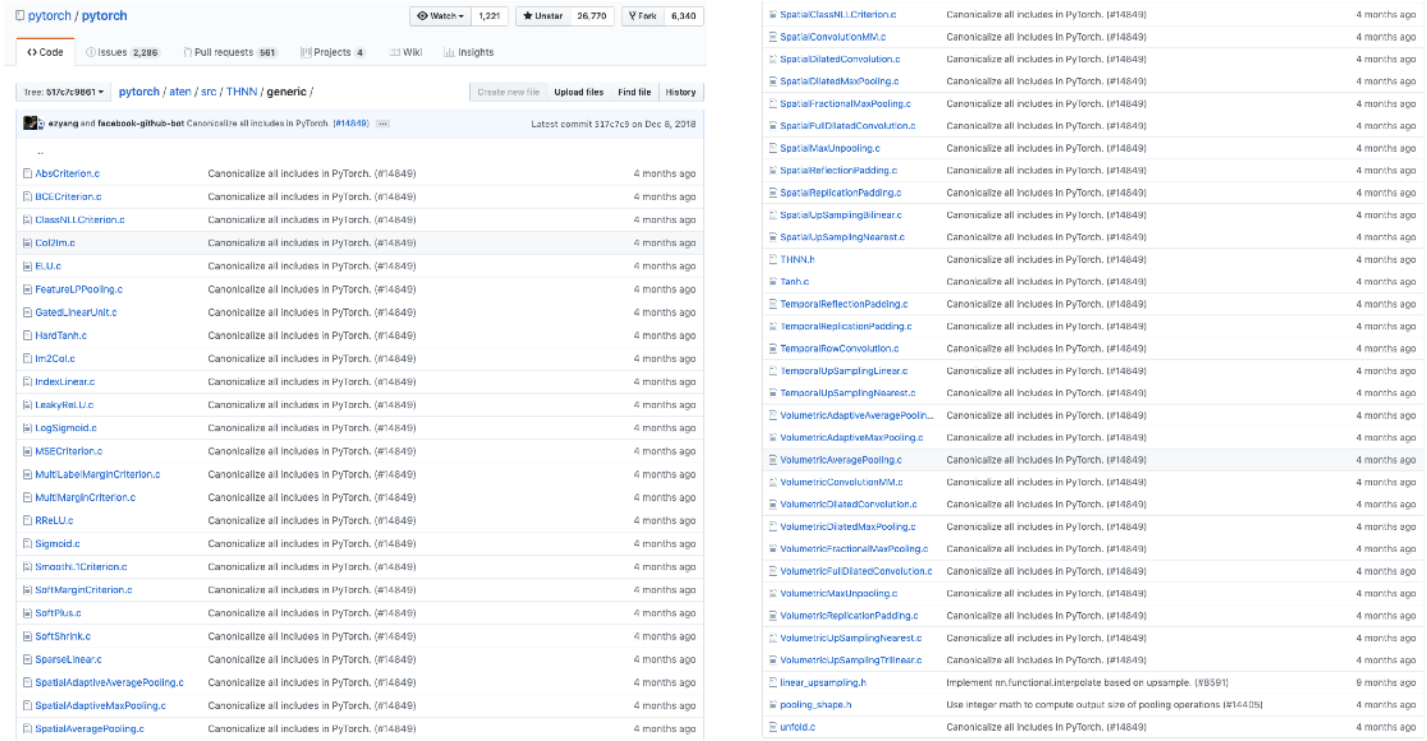
```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z    # dz/dx * dL/dz
    grad_y = x * grad_z    # dz/dy * dL/dz
    return grad_x, grad_y
```

Need to cash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

Example: PyTorch operators



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Tree: 517c7c9861 | pytorch / aten / src / THNN / generic / | Create new file | Upload files | Find file | History

ezyang and facebook-github-bot Canonicalize all includes in PyTorch. (#14849) | Latest commit 517c7c9 on Dec 8, 2018

AbsCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
BCECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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linear_upsampling.h	Implement nn.functional.interpolate based on upsample. (#8591)	9 months ago
pooling_shape.h	Use integer math to compute output size of pooling operations (#14405)	4 months ago
unfold.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago

PyTorch sigmoid layer

```
#ifndef TH_GENERIC_FILE
#define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
#else

void THNN_(Sigmoid_updateOutput)(
          THNNState *state,
          THTensor *input,
          THTensor *output)
{
  THTensor_(sigmoid)(output, input);
}

void THNN_(Sigmoid_updateGradInput)(
          THNNState *state,
          THTensor *gradOutput,
          THTensor *gradInput,
          THTensor *output)
{
  THNN_CHECK_NELEMENT(output, gradOutput);
  THTensor_(resizeAs)(gradInput, output);
  TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
    scalar_t z = *output_data;
    *gradInput_data = *gradOutput_data * (1. - z) * z;
  );
}

#endif
```

Forward

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

Source

PyTorch sigmoid layer

```
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}

void THNN_(Sigmoid_updateGradInput)(
          THNNState *state,
          THTensor *gradOutput,
          THTensor *gradInput,
          THTensor *output)
{
  THNN_CHECK_NELEMENT(output, gradOutput);
  THTensor_(resizeAs)(gradInput, output);
  TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
    scalar_t z = *output_data;
    *gradInput_data = *gradOutput_data * (1. - z) * z;
  );
}

#endif
```

Forward

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

```
static void sigmoid_kernel(TensorIterator& iter) {
  AT_DISPATCH_FLOATING_TYPES(iter.dtype(), "sigmoid_cpu", [&]() {
    unary_kernel_vec(
        iter,
        [=](scalar_t a) -> scalar_t { return (1 / (1 + std::exp((-a)))); },
        [=](Vec256<scalar_t> a) {
          a = Vec256<scalar_t>((scalar_t)(0)) - a;
          a = a.exp();
          a = Vec256<scalar_t>((scalar_t)(1)) + a;
          a = a.reciprocal();
          return a;
        });
  });
}
```

Forward actually defined elsewhere...

```
return (1 / (1 + std::exp((-a))));
```

Source

PyTorch sigmoid layer

```
#ifndef TH_GENERIC_FILE
#define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
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          THTensor *output)
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  THTensor_(sigmoid)(output, input);
}

void THNN_(Sigmoid_updateGradInput)(
          THNNState *state,
          THTensor *gradOutput,
          THTensor *gradInput,
          THTensor *output)
{
  THNN_CHECK_NELEMENT(output, gradOutput);
  THTensor_(resizeAs)(gradInput, output);
  TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
    scalar_t z = *output_data;
    *gradInput_data = *gradOutput_data * (1. - z) * z;
  );
}

#endif
```

Forward

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```
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  AT_DISPATCH_FLOATING_TYPES(iter.dtype(), "sigmoid_cpu", [&]() {
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          a = a.exp();
          a = Vec256<scalar_t>((scalar_t)(1)) + a;
          a = a.reciprocal();
          return a;
        });
  });
}
```

Forward actually defined elsewhere...

Backward

$$(1-\sigma(x))\,\sigma(x)$$

Source

So far: backprop with scalars

What about vector-valued functions?

Recap: Vector derivatives

Scalar to Scalar

$$x \in \mathbb{R}, y \in \mathbb{R}$$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

Recap: Vector derivatives

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Vector to Scalar

$x \in \mathbb{R}^N, y \in \mathbb{R}$

Derivative is **Gradient**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^N \quad \left(\frac{\partial y}{\partial x}\right)_n = \frac{\partial y}{\partial x_n}$$

For each element of x, if it changes by a small amount then how much will y change?

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For each element of x, if it changes by a small amount then how much will y change?

Vector to Vector

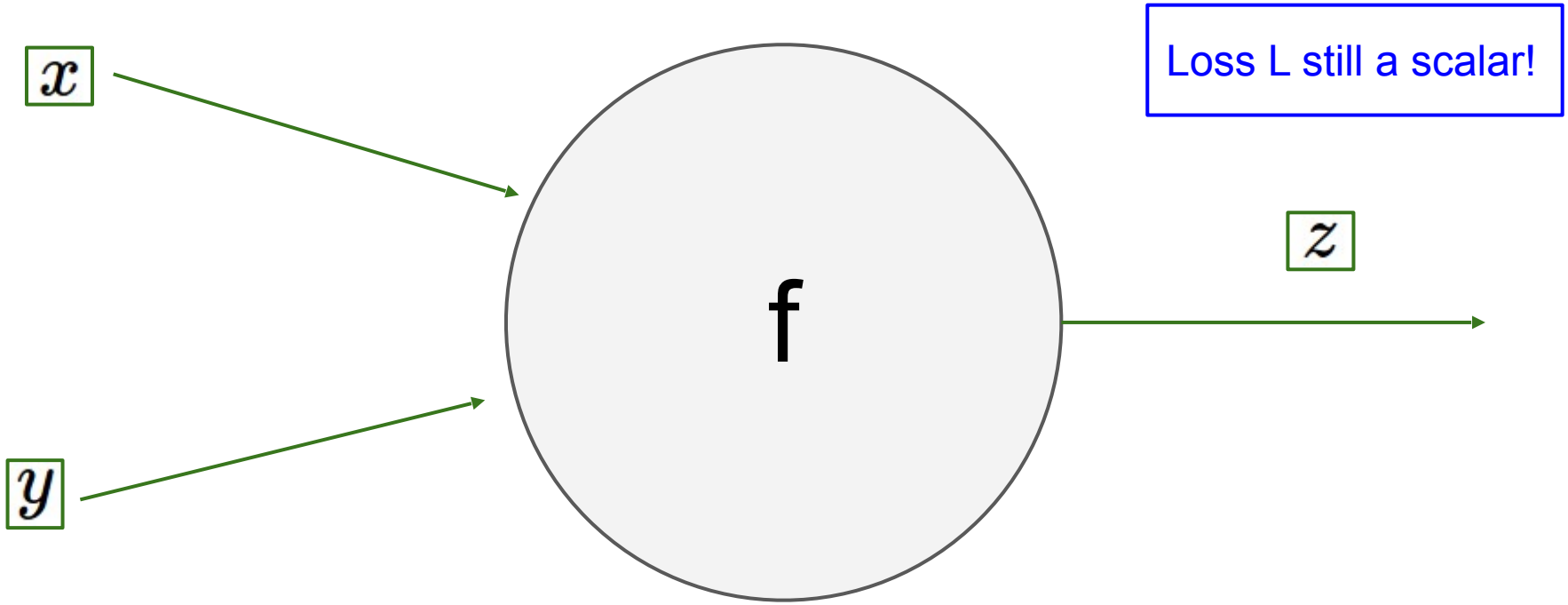
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

For each element of x, if it changes by a small amount then how much will each element of y change?

Backprop with Vectors



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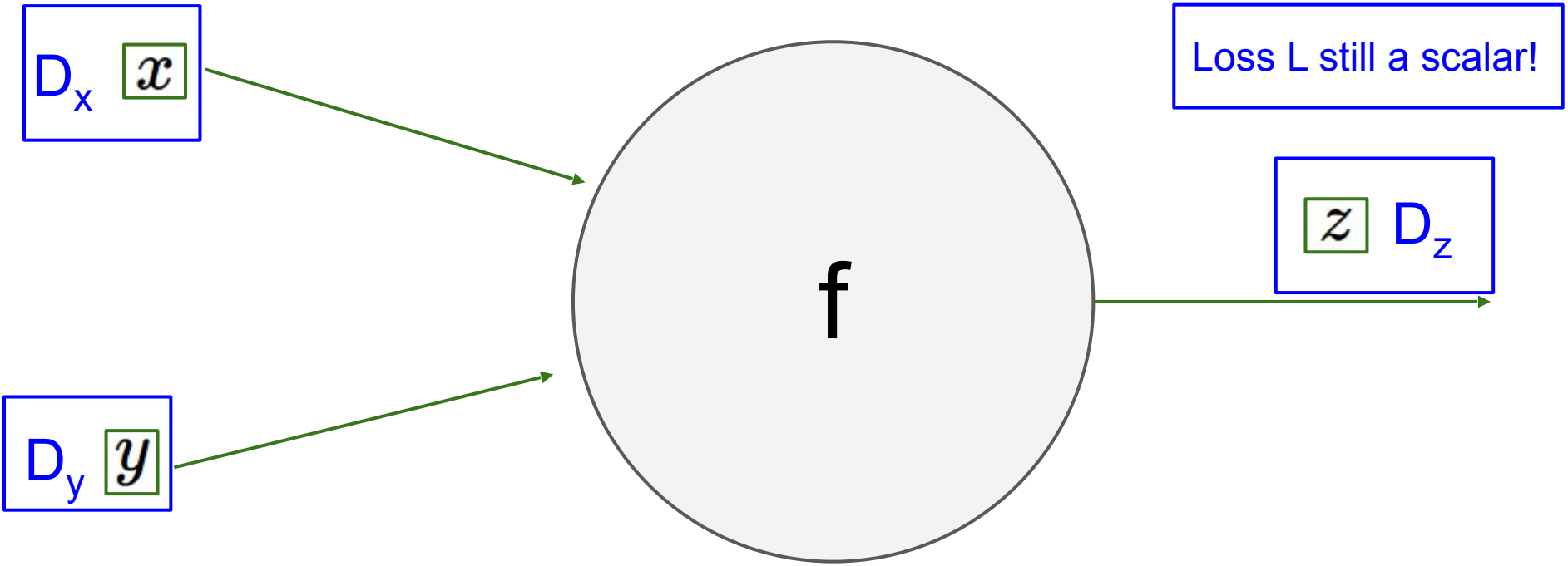

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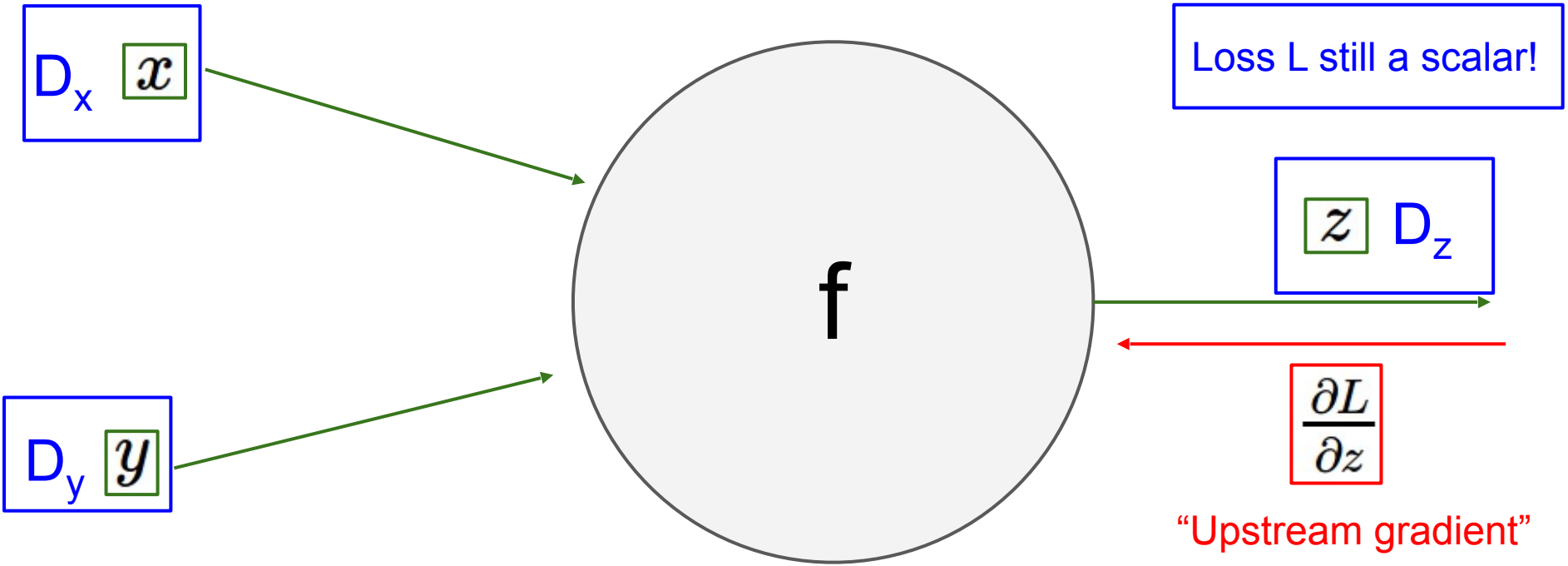
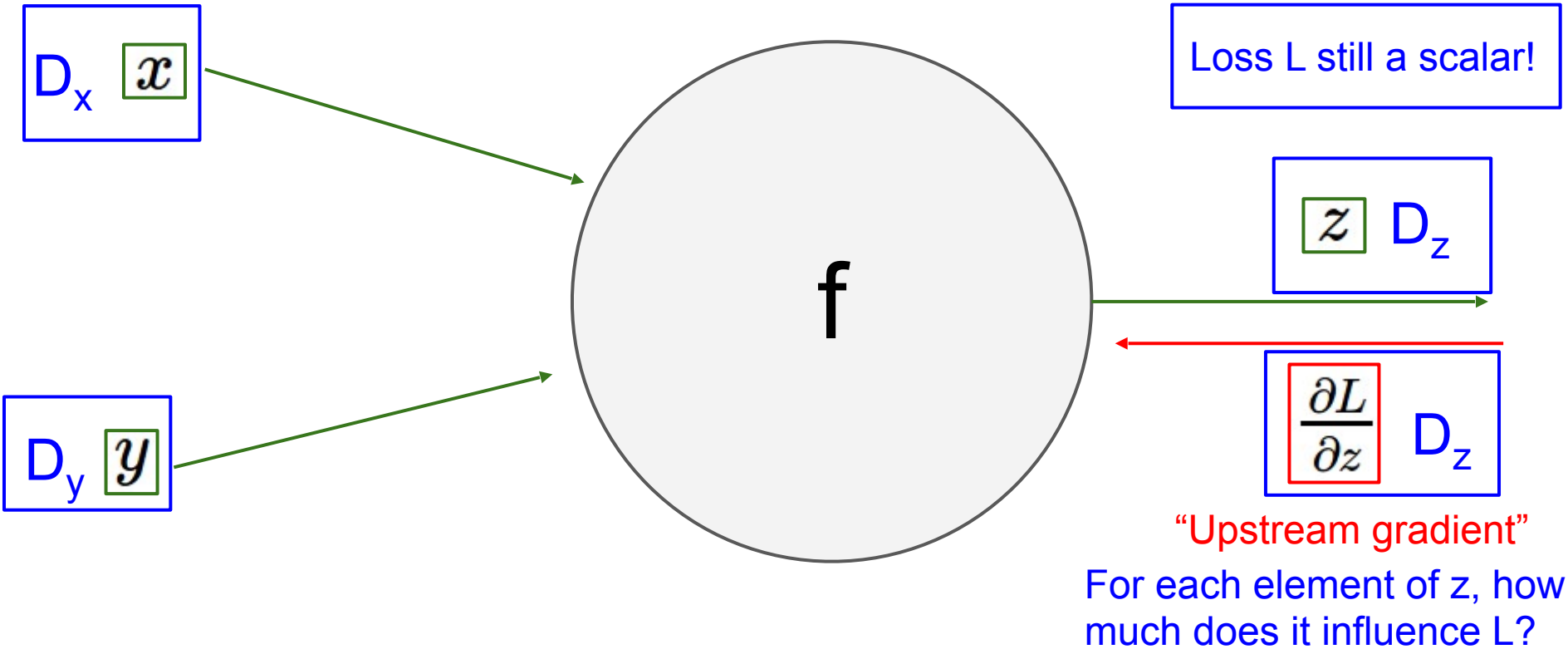
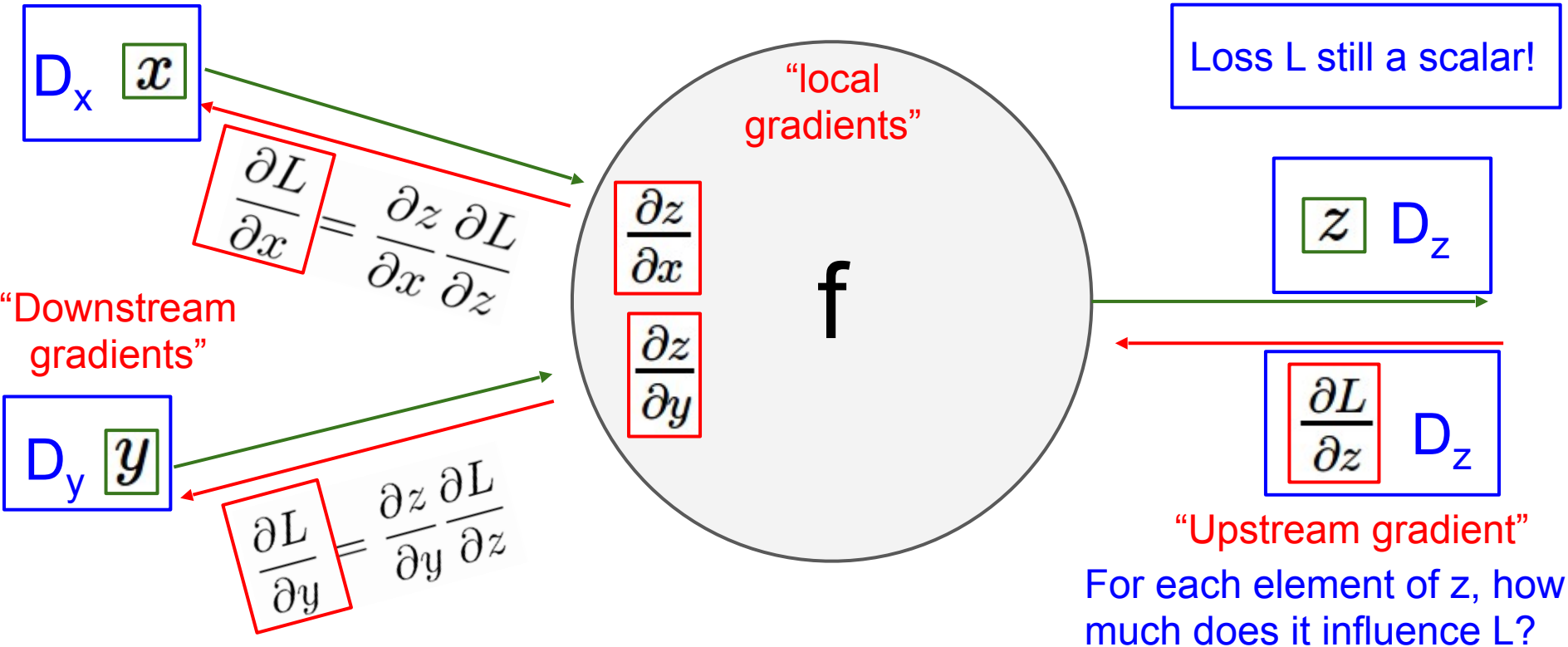


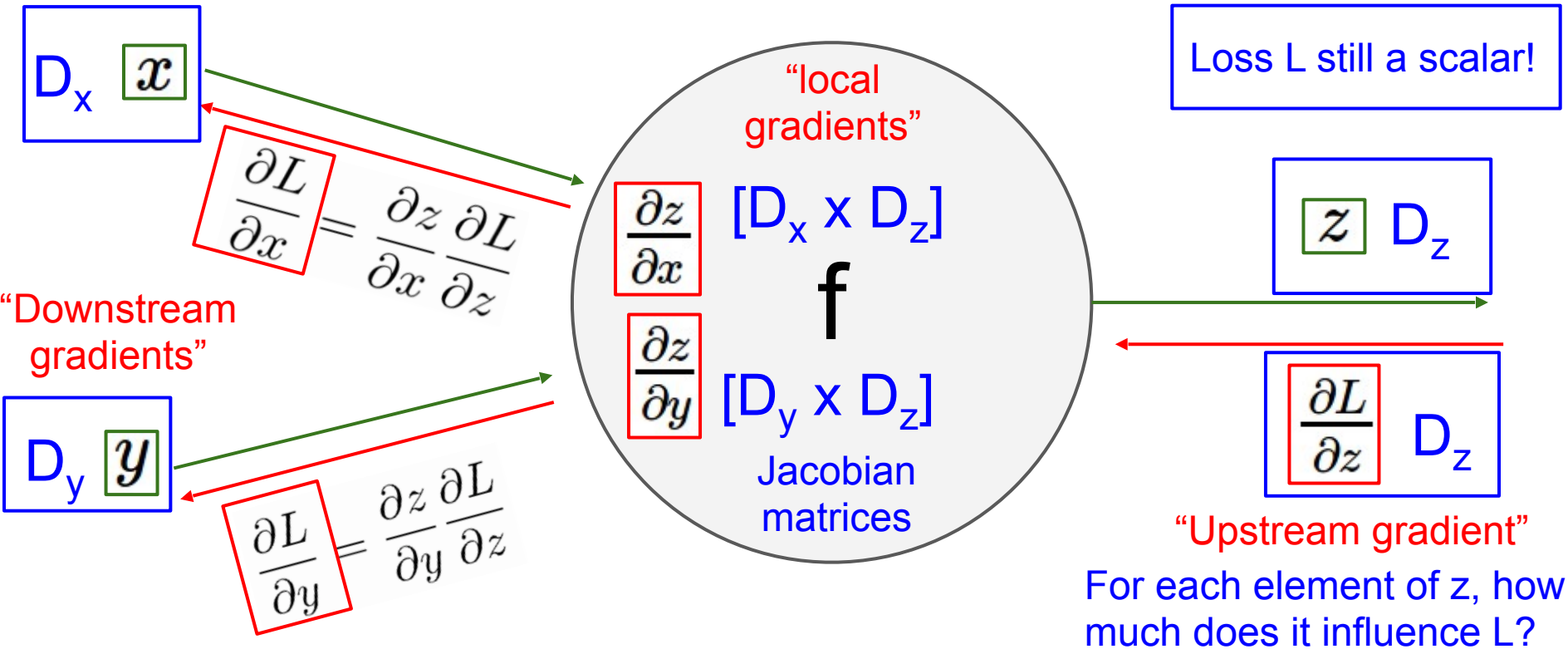
Backprop with Vectors



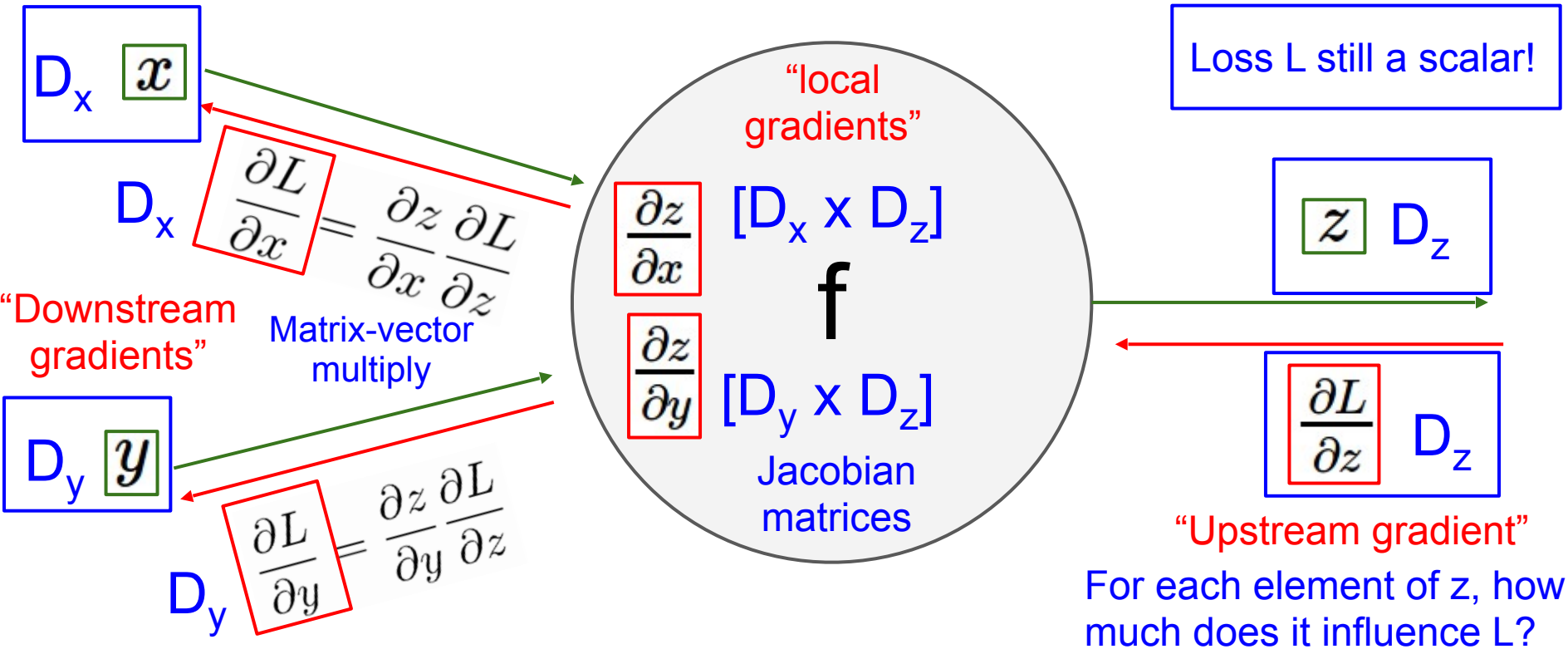
Backprop with Vectors



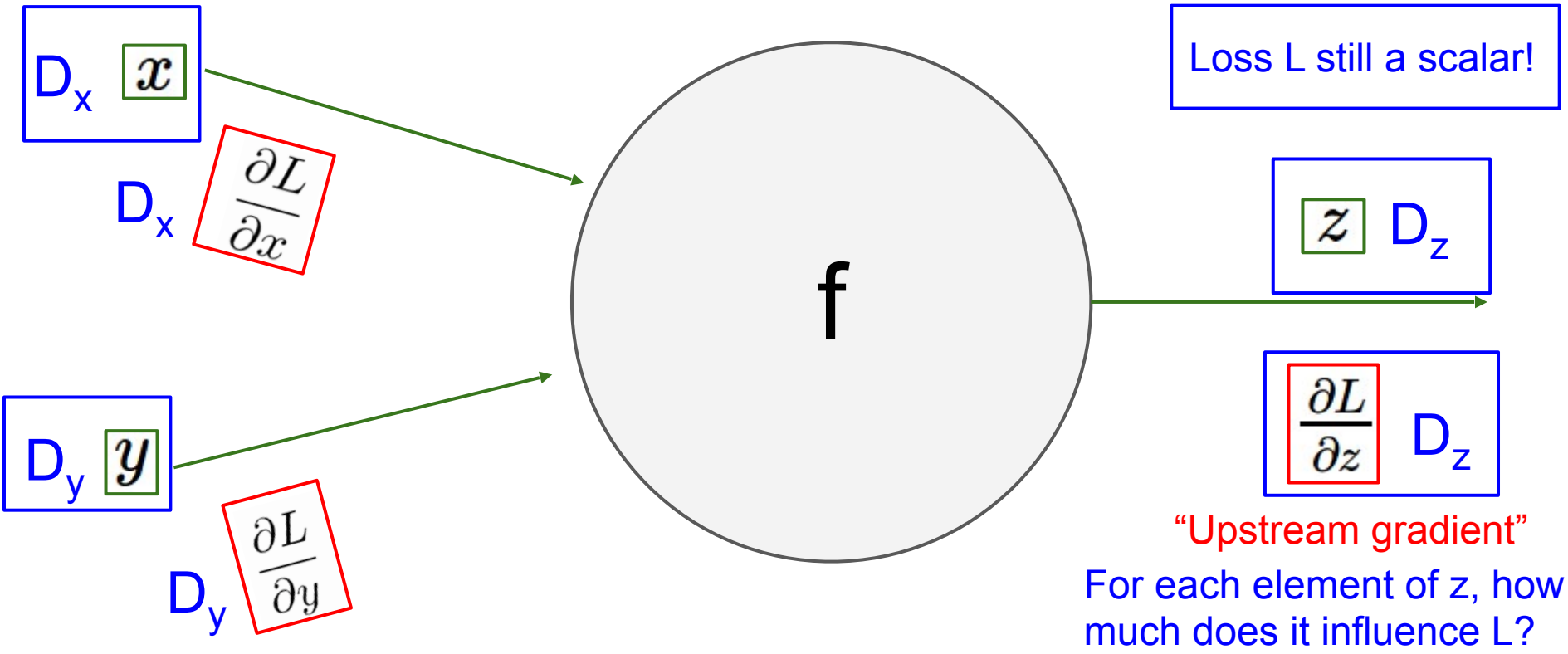
Backprop with Vectors



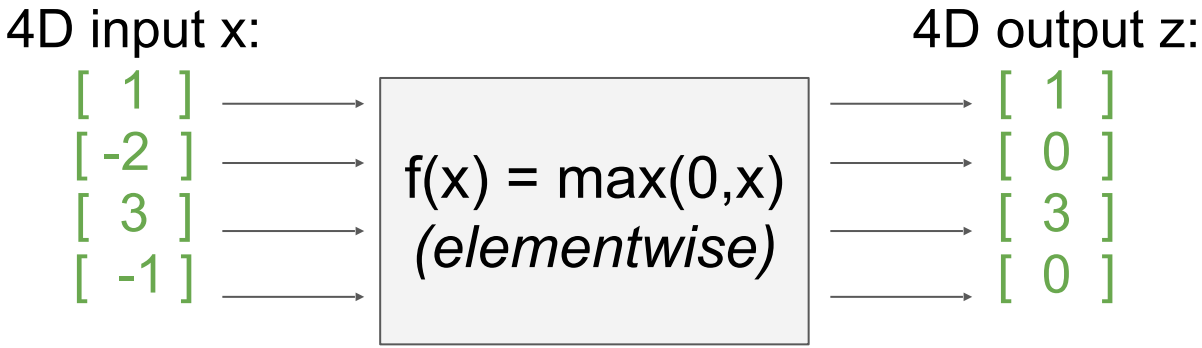
Backprop with Vectors



Gradients of variables wrt loss have same dims as the original variable



Backprop with Vectors



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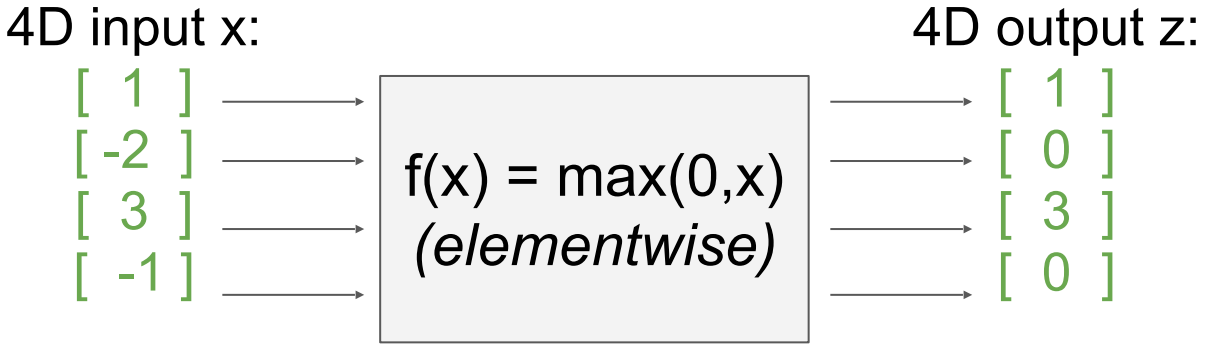

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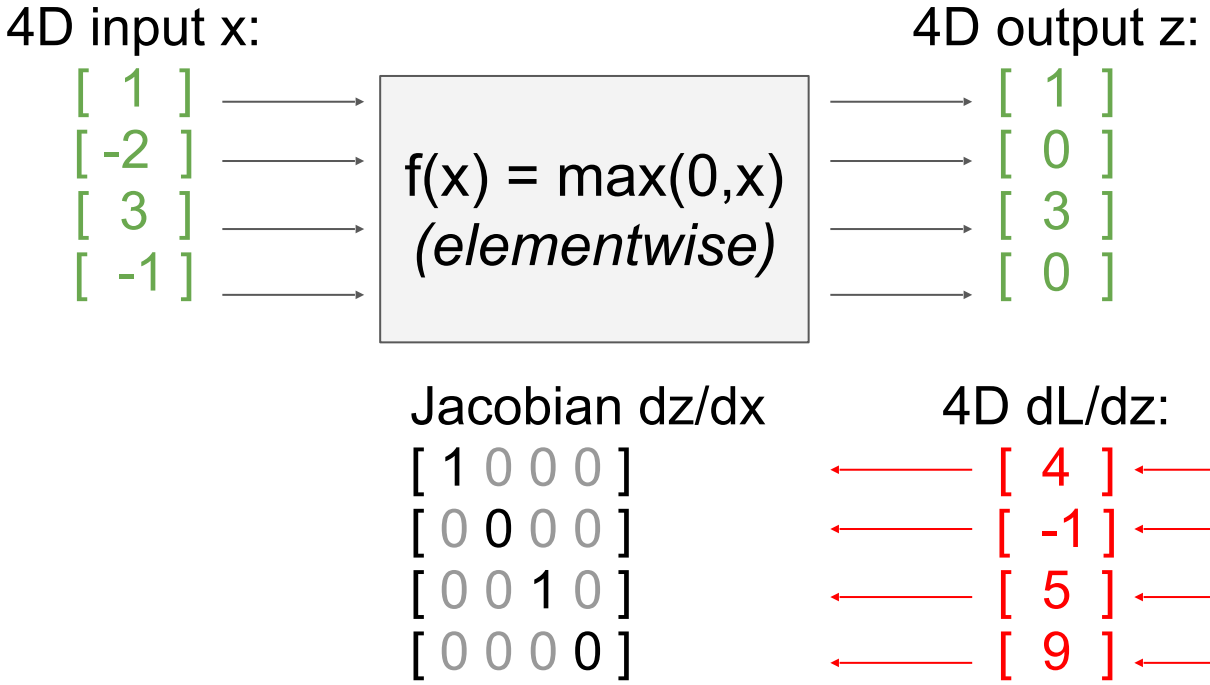
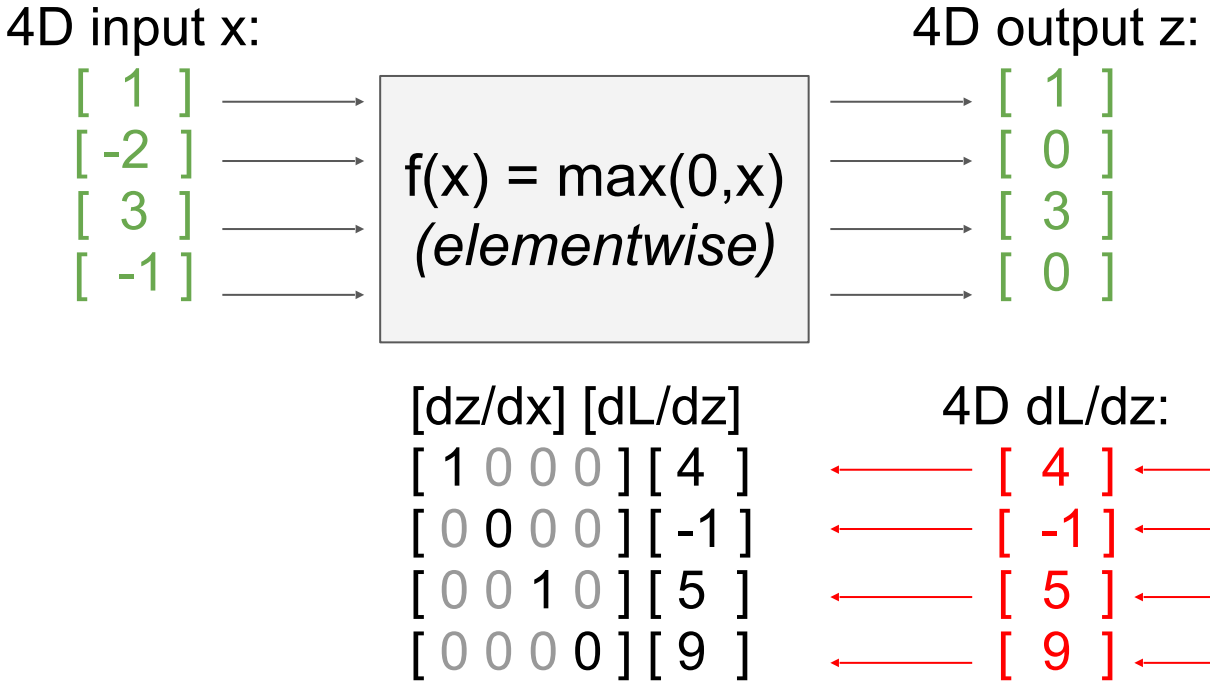
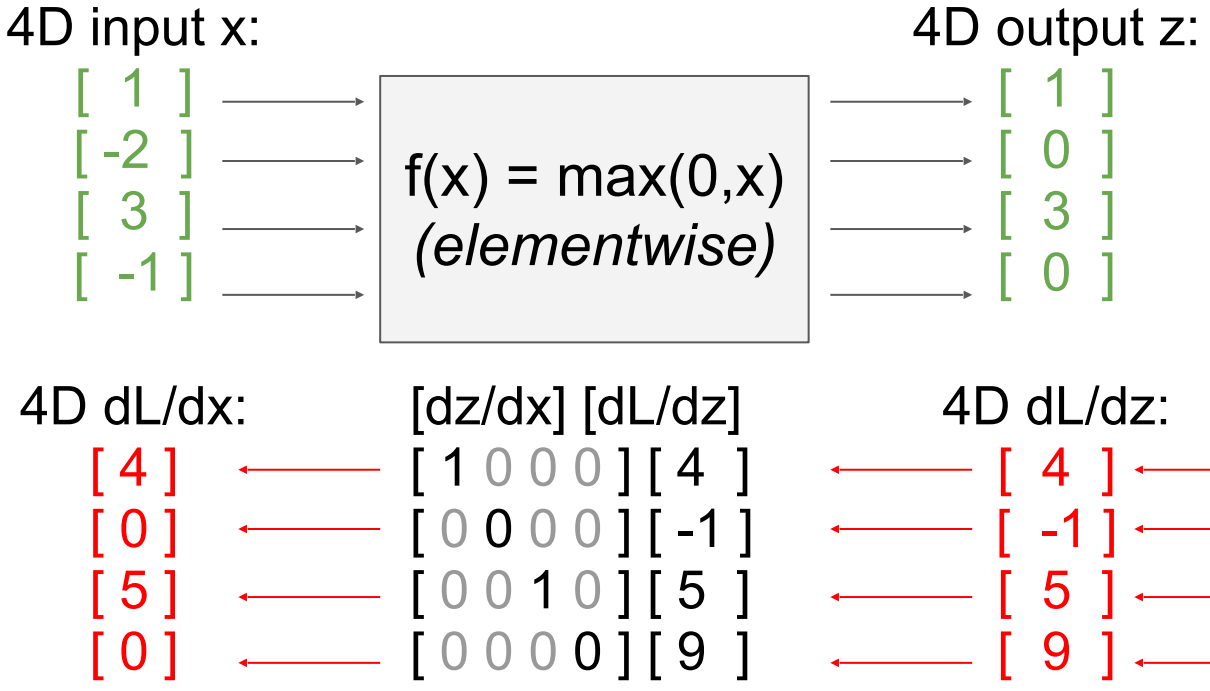


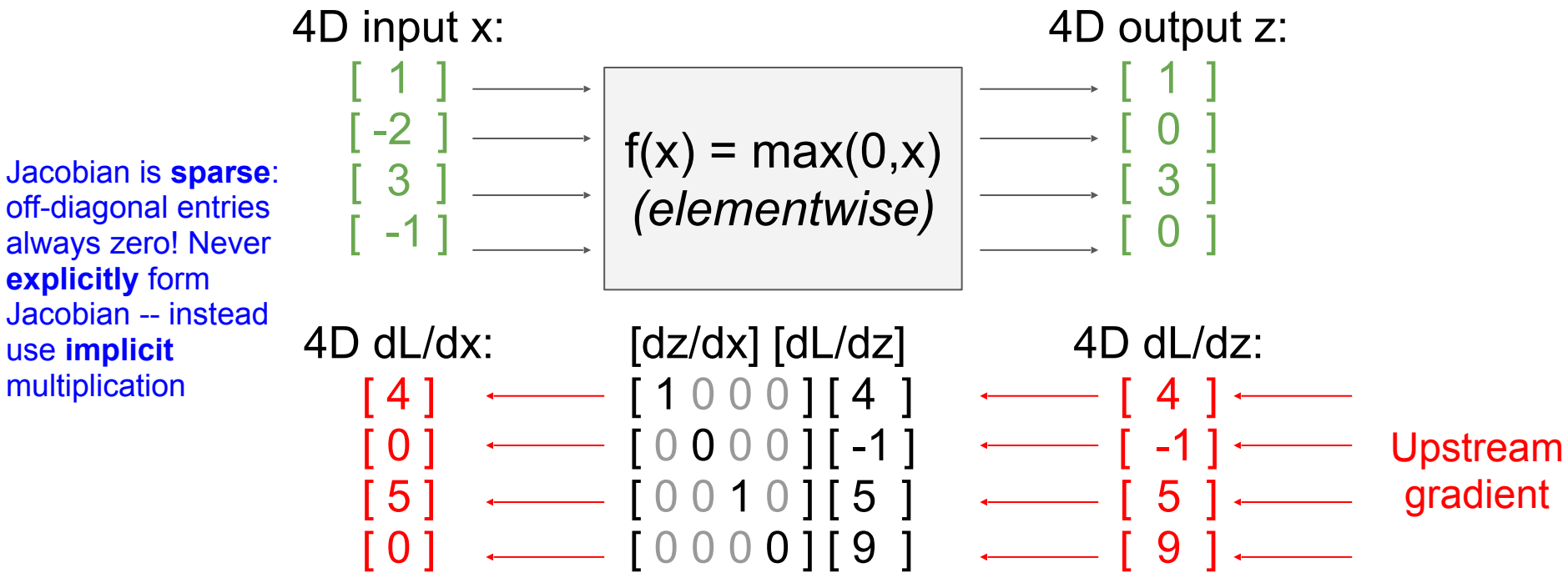
Backprop with Vectors



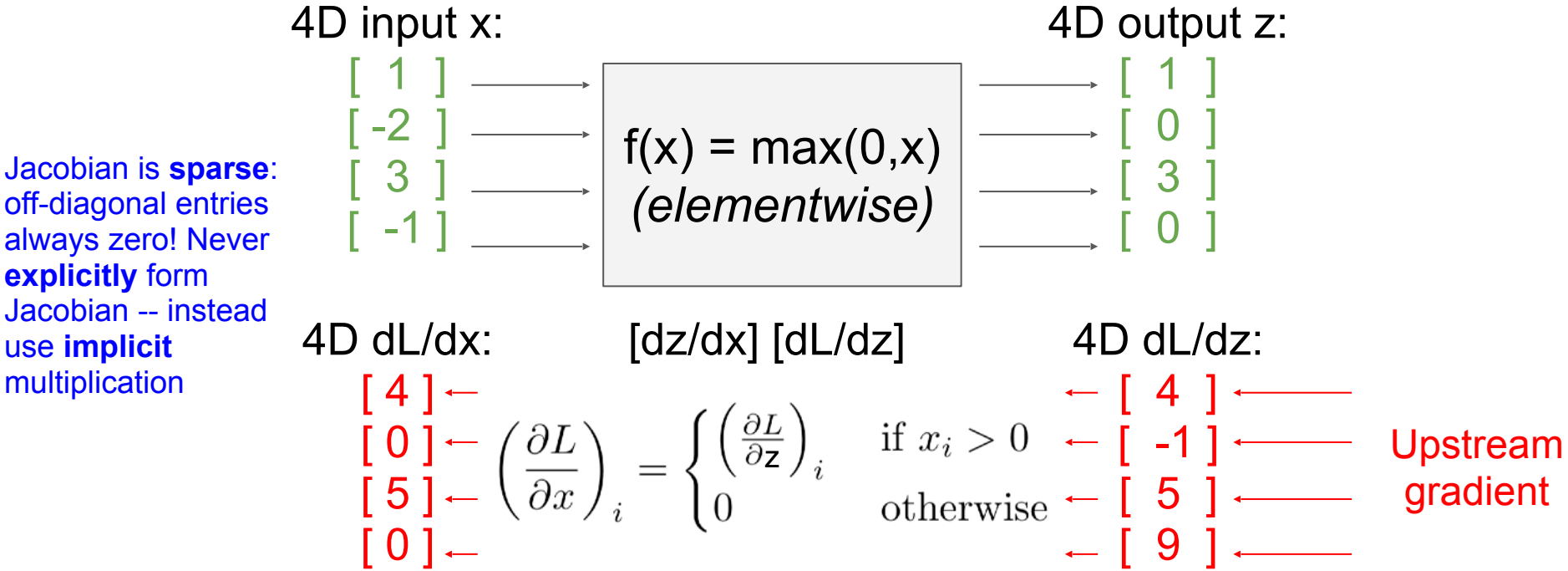
Backprop with Vectors



Backprop with Vectors



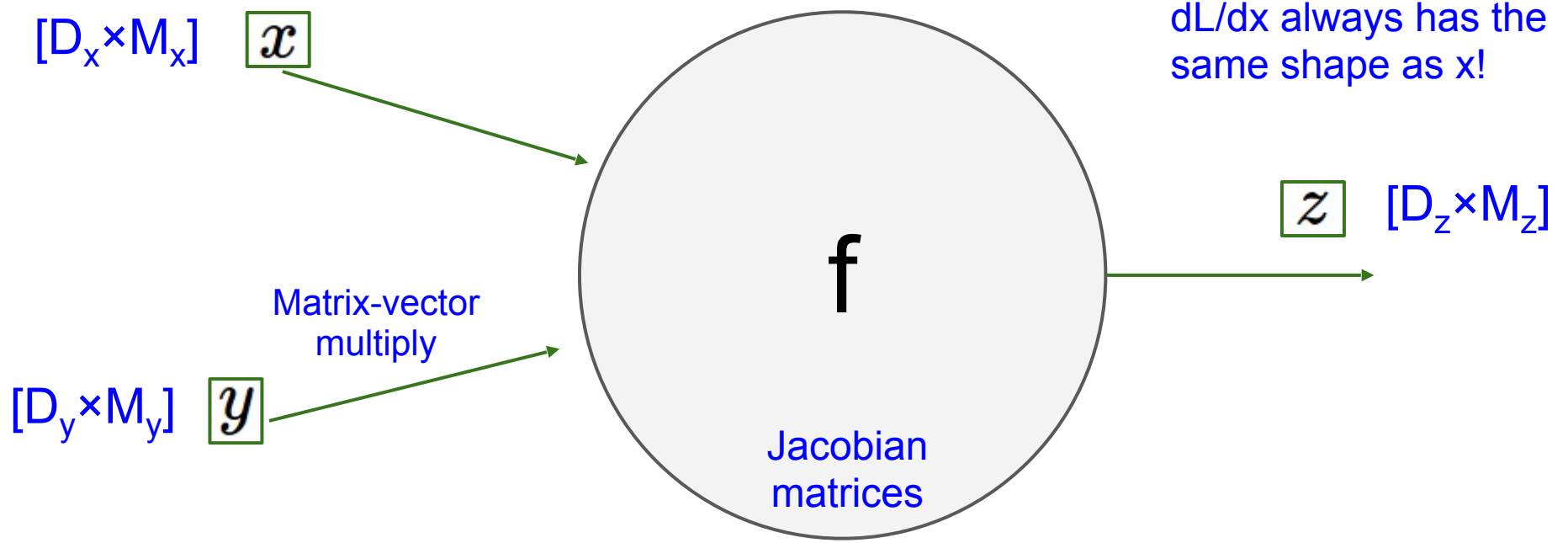
Backprop with Vectors



Backprop with Matrices (or Tensors)

Loss L still a scalar!

dL/dx always has the same shape as x!



Backprop with Matrices (or Tensors)

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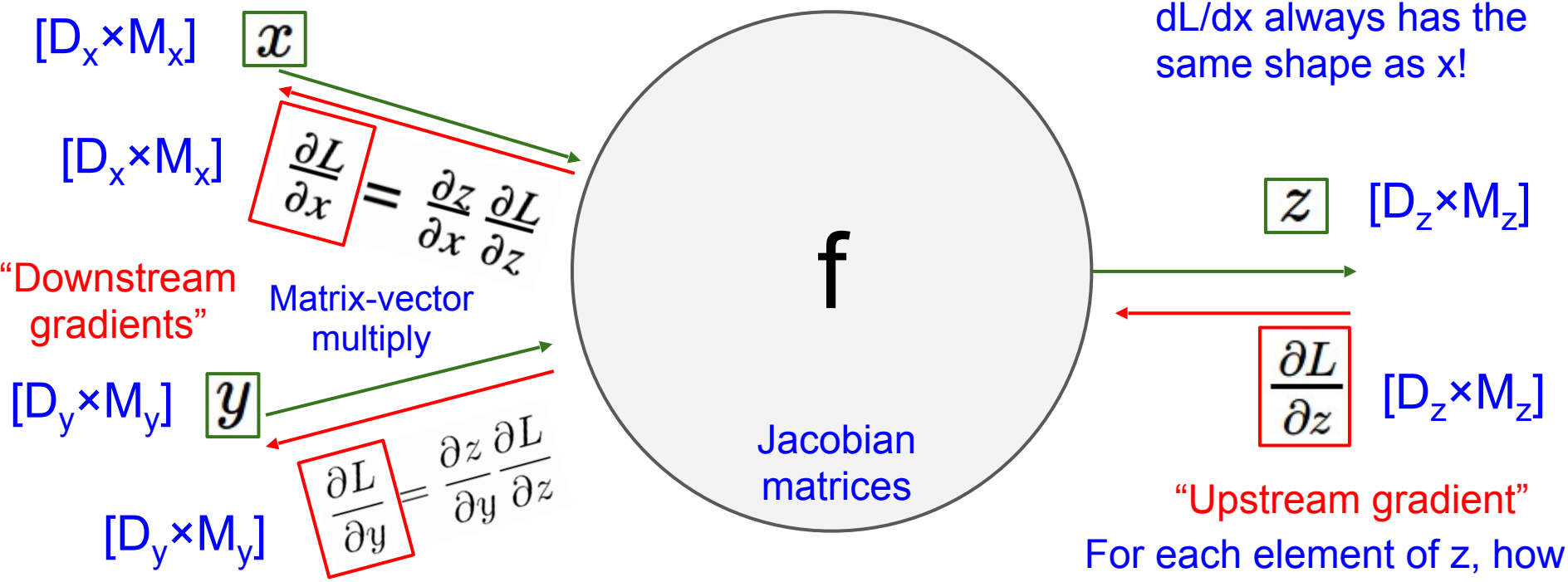


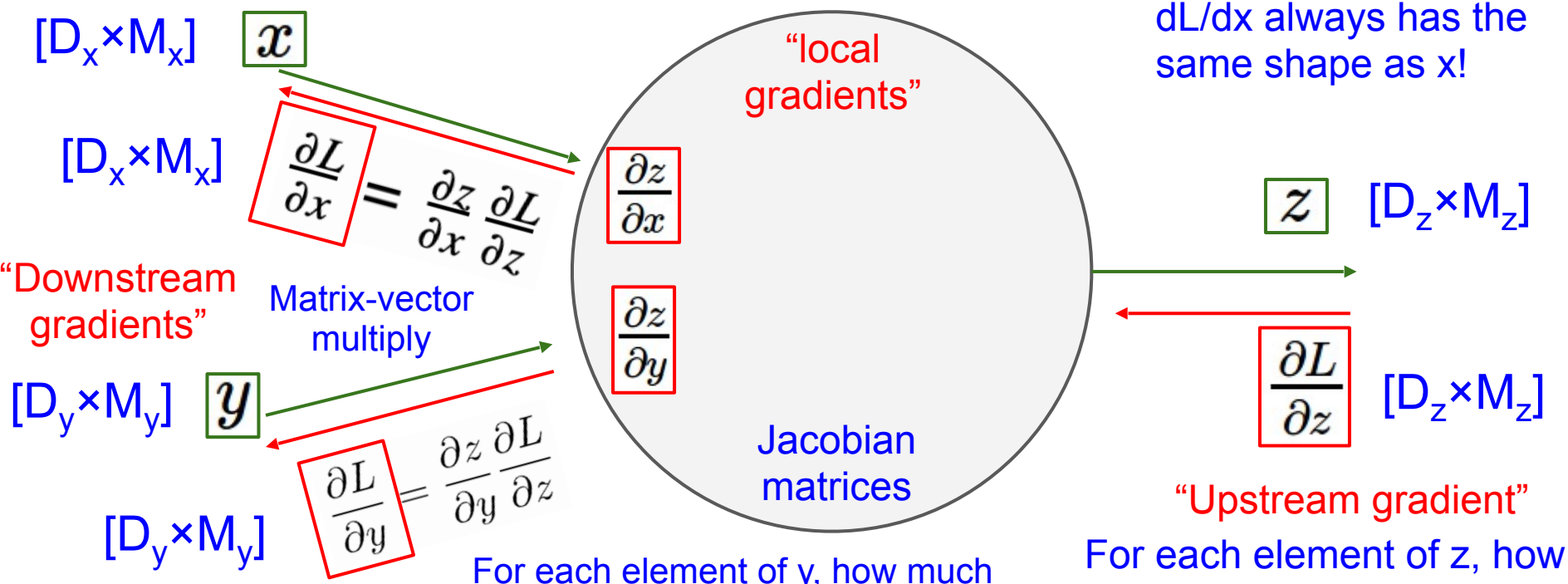
"Upstream gradient"

For each element of z, how much does it influence L?

Backprop with Matrices (or Tensors)

Loss L still a scalar!

dL/dx always has the same shape as x!



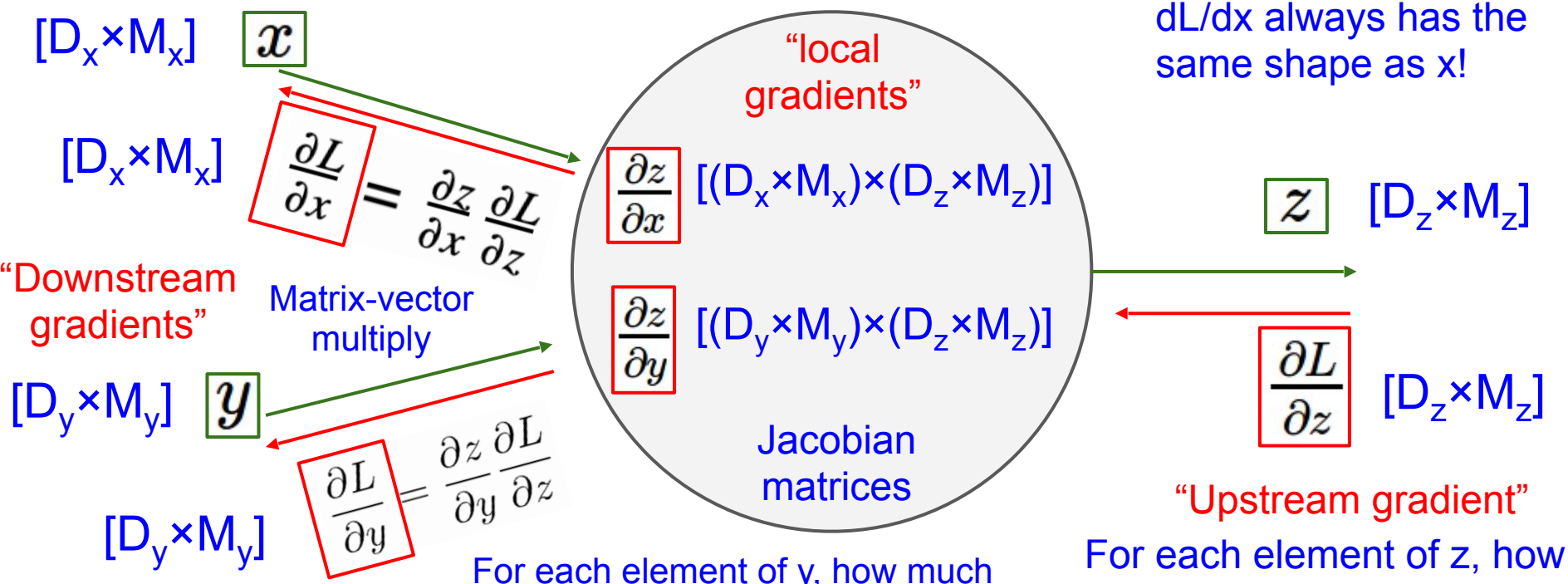
For each element of y, how much does it influence each element of z?

For each element of z, how much does it influence L?

Backprop with Matrices (or Tensors)

Loss L still a scalar!

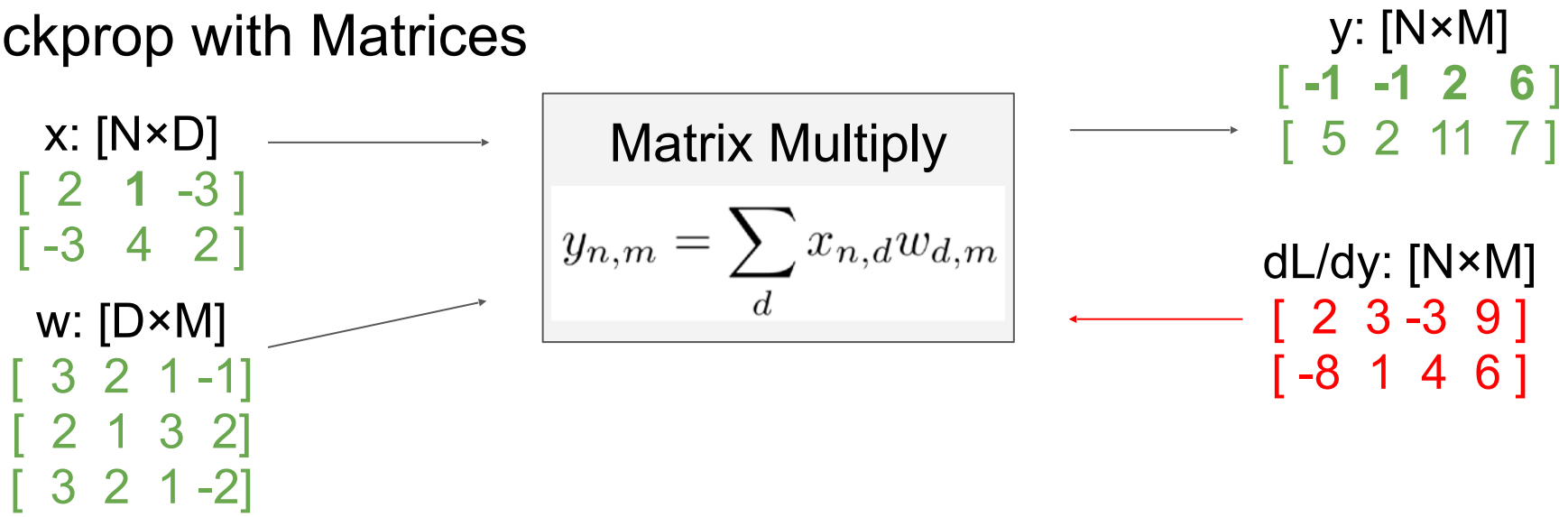
dL/dx always has the same shape as x!



For each element of y, how much does it influence each element of z?

For each element of z, how much does it influence L?

Backprop with Matrices



Also see derivation in the course notes:
http://cs231n.stanford.edu/handouts/linear-backprop.pdf

Backprop with Matrices

x: [N×D]
[2 **1** -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]
[**-1 -1 2 6**]
[5 2 11 7]

dL/dy: [N×M]
[2 3 -3 9]
[-8 1 4 6]

Jacobians:
dy/dx: [(N×D)×(N×M)]
dy/dw: [(D×M)×(N×M)]

For a neural net we may have
N=64, D=M=4096
Each Jacobian takes ~256 GB of
memory! Must work with them implicitly!

Backprop with Matrices

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Q: What parts of y are affected by one element of x?

Backprop with Matrices

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[2 **1** -3]
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[**-1 -1 2 6**]
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dL/dy: [N×M]

[2 3 -3 9]
[-8 1 4 6]

Q: What parts of y are affected by one element of x?

A: $x_{n,d}$ affects the whole row $y_{n,.}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}}$$

Backprop with Matrices

x: [N×D]

[2 **1** -3]
[-3 4 2]

w: [D×M]

[3 2 1 -1]
[2 1 3 2]
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Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

[**-1** **-1** **2** **6**]
[5 2 11 7]

dL/dy: [N×M]

[2 3 -3 9]
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Q: What parts of y are affected by one element of x?
A: $x_{n,d}$ affects the whole row $y_{n,.}$

Q: How much does $x_{n,d}$ affect $y_{n,m}$?

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}}$$

Backprop with Matrices

x: [N×D]

[2 1 -3]
[-3 4 2]

w: [D×M]

[3 2 1 -1]
[2 1 3 2]
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Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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dL/dy: [N×M]

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A: $w_{d,m}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m}$$

Backprop with Matrices

x: [N×D]
[2 1 -3]
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w: [D×M]
[3 2 1 -1]
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Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]
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Q: What parts of y are affected by one element of x?
A: $x_{n,d}$ affects the whole row $y_{n,.}$

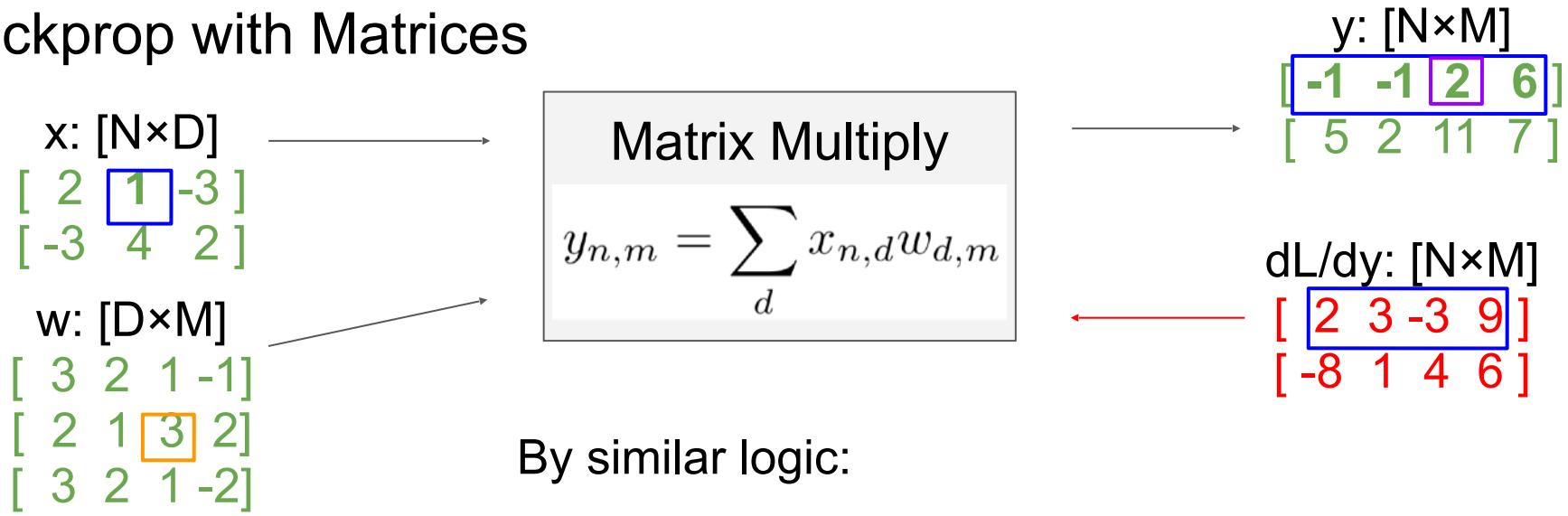
Q: How much does $x_{n,d}$ affect $y_{n,m}$?
A: $w_{d,m}$

[N×D] [N×M] [M×D]

$$\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T$$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m}$$

Backprop with Matrices



By similar logic:

[N×D] [N×M] [M×D]

$$\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T$$

[D×M] [D×N] [N×M]

$$\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y}\right)$$

These formulas are easy to remember: they are the only way to make shapes match up!

Summary for today:

- **Fully-connected neural networks** are stacks of linear functions and nonlinear activation functions; they have much more representational power than linear classifiers
- **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