Lecture 8: Deep Learning, Autoencoder, Word2Vec

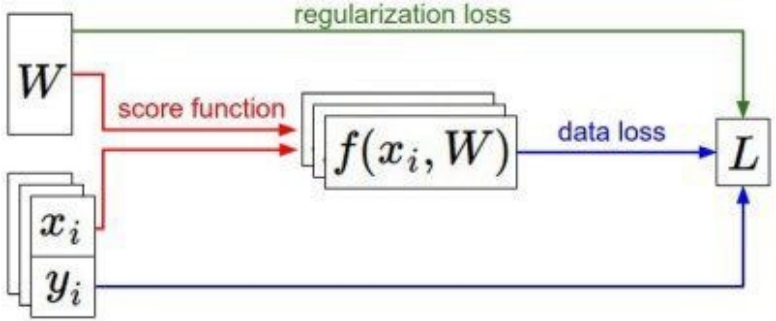
Recap

- We have some dataset of (x,y)
- We have a **score function:** $s = f(x; W) \overset{\text{e.g.}}{=} Wx$
- We have a **loss function**:

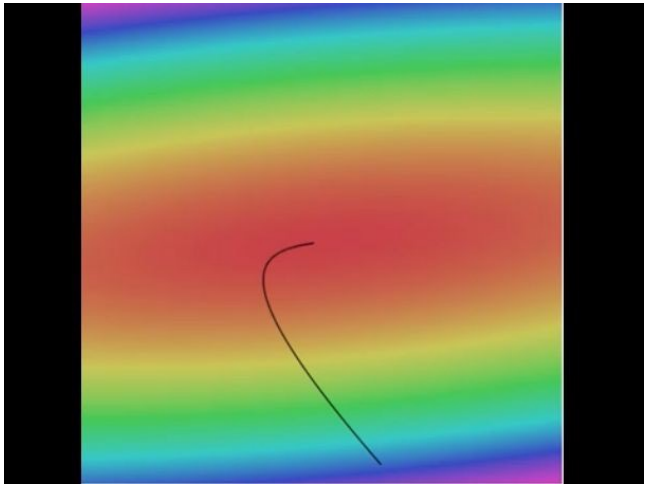
$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{s_j}}\right)$$ Softmax

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

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i + R(W)$$ Full loss



Finding the best W: Optimize with Gradient Descent



```
# Vanilla Gradient Descent

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

Landscape image is CC0 1.0 public domain
Walking man image is CC0 1.0 public domain

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

Stochastic Gradient Descent (SGD)

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

$$\nabla_W L(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

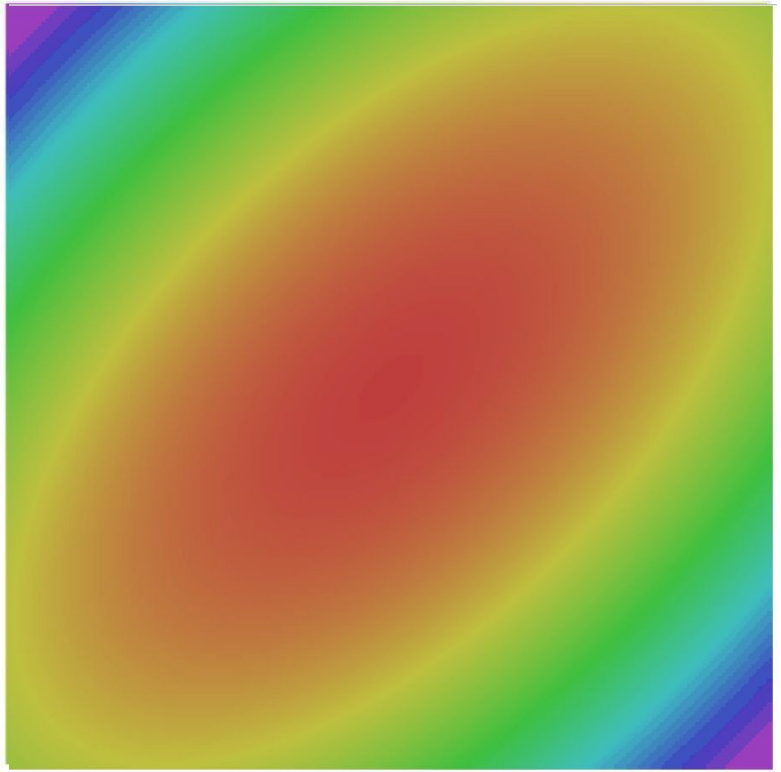
Full sum expensive when N is large!

Approximate sum using a **minibatch** of examples
32 / 64 / 128 common

```
# Vanilla Minibatch Gradient Descent

while True:
  data_batch = sample_training_data(data, 256) # sample 256 examples
  weights_grad = evaluate_gradient(loss_fun, data_batch, weights)
  weights += - step_size * weights_grad # perform parameter update
```

Last time: fancy optimizers



SGD

SGD+Momentum

RMSProp

Adam

Deep Learning

dall-e-2

“Teddy bears working on new AI research on the moon in the 1980s.”

“Rabbits attending a college seminar on human anatomy.

“A wise cat meditating in the Himalayas searching for enlightenment.”

Image source: Sam Altman, https://openai.com/dall-e-2/, https://twitter.com/sama/status/1511724264629678084

Neural Networks

Neural networks: the original linear classifier

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

$$x \in \mathbb{R}^D, W \in \mathbb{R}^{C \times D}$$

Neural networks: 2 layers

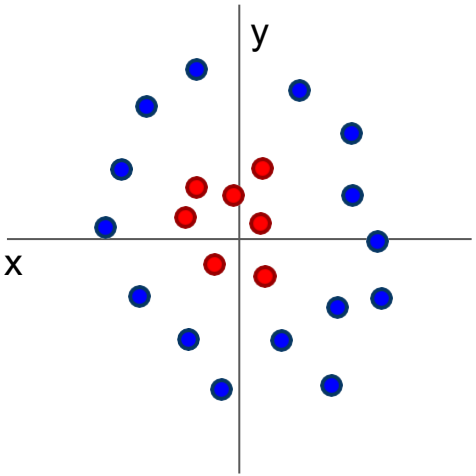
(**Before**) Linear score function: $f = Wx$

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

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

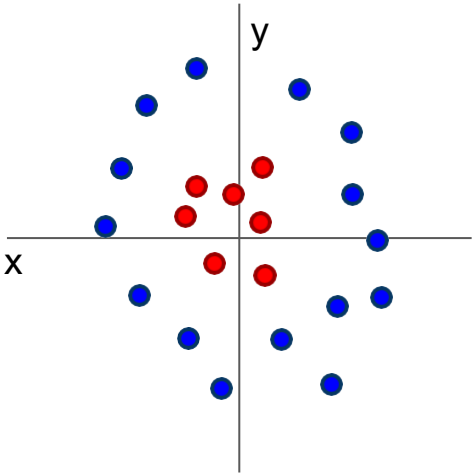
(In practice we will usually add a learnable bias at each layer as well)

Why do we want non-linearity?



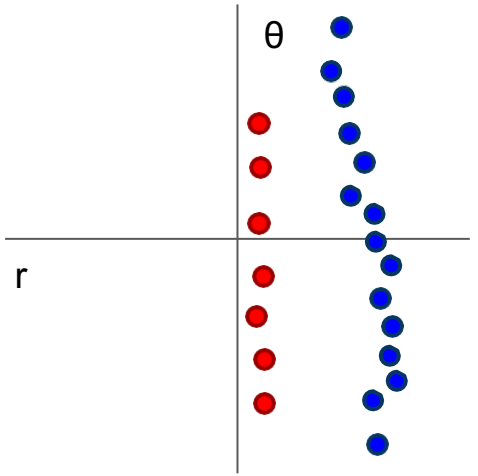
Cannot separate red and blue points with linear classifier

Why do we want non-linearity?



Cannot separate red and blue points with linear classifier

$$f(x, y) = (r(x, y), \theta(x, y))$$



After applying feature transform, points can be separated by linear classifier

Neural networks: also called fully connected network

(**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 Network" is a very broad term; these are more accurately called "fully-connected networks" or sometimes "multi-layer perceptrons" (MLP)

(In practice we will usually add a learnable bias at each layer as well)

Neural networks: 3 layers

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

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

or 3-layer Neural Network

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

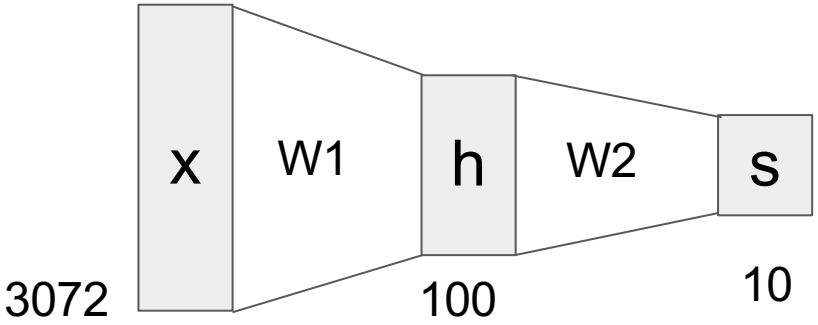
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

(In practice we will usually add a learnable bias at each layer as well)

Neural networks: hierarchical computation

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

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

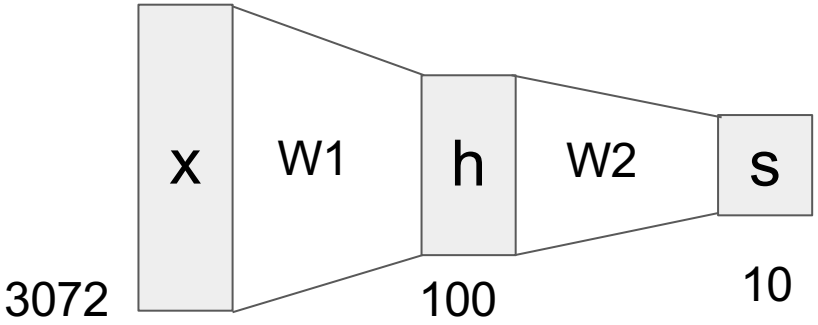


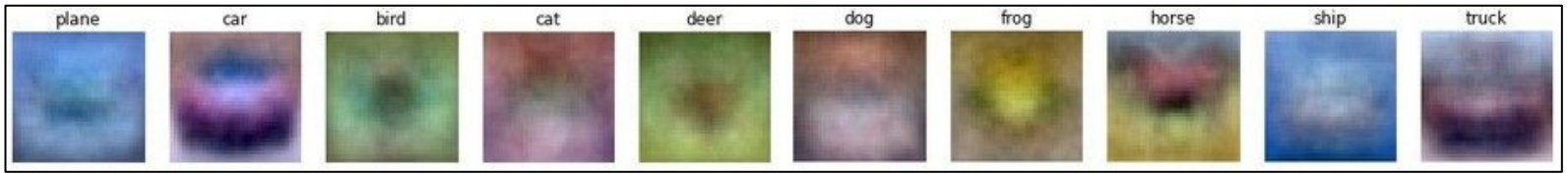
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural networks: learning 100s of templates

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

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





Learn 100 templates instead of 10.

Share templates between classes

Neural networks: why is max operator important?

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

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

The function $\max(0, z)$ is called the **activation function.**

Q: What if we try to build a neural network without one?

$$f = W_2 W_1 x$$

Neural networks: why is max operator important?

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

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

The function $\max(0, z)$ is called the **activation function.**

Q: What if we try to build a neural network without one?

$$f = W_2 W_1 x \qquad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

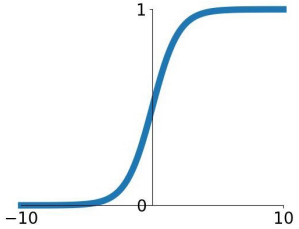
A: We end up with a linear classifier again!

Activation functions

ReLU is a good default choice for most problems

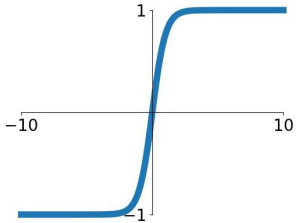
Sigmoid

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



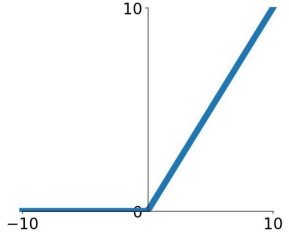
tanh

$$\tanh(x)$$



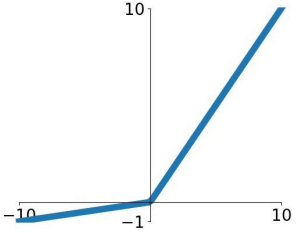
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

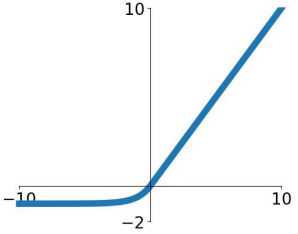


Maxout

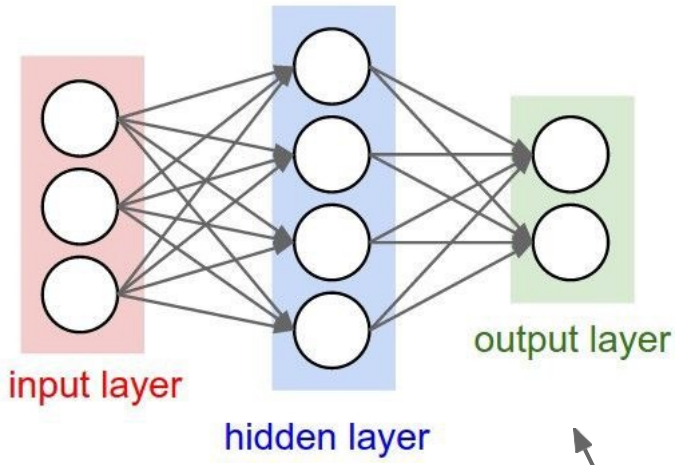
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

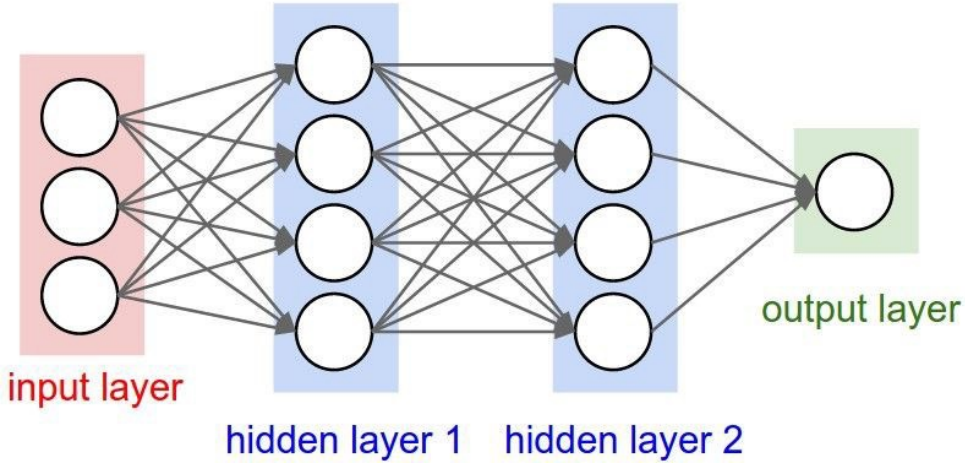
ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Neural networks: Architectures



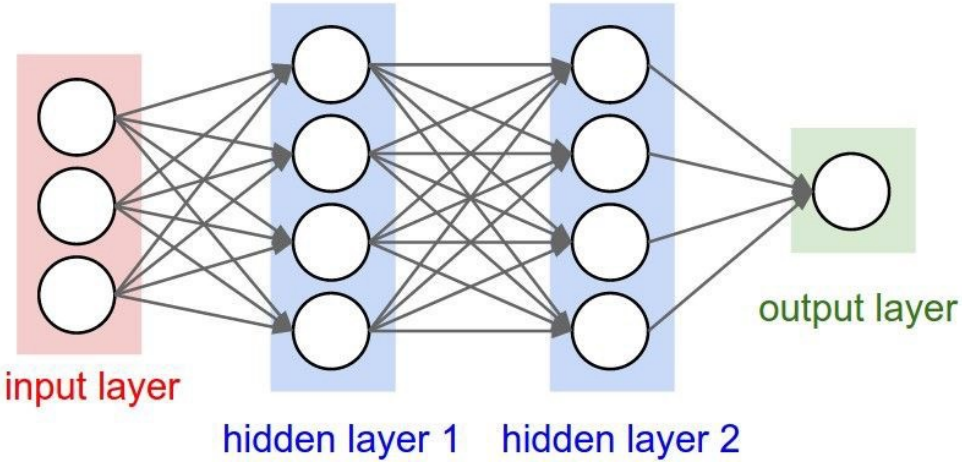


“2-layer Neural Net”, or
“1-hidden-layer Neural Net”

“3-layer Neural Net”, or
“2-hidden-layer Neural Net”

“Fully-connected” layers

Example feed-forward computation of a neural network




```
# 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)
```

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
import numpy as np
from numpy.random import randn

N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)

for t in range(2000):
  h = 1 / (1 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  print(t, loss)

  grad_y_pred = 2.0 * (y_pred - y)
  grad_w2 = h.T.dot(grad_y_pred)
  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))

  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
import numpy as np
from numpy.random import randn

N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)

for t in range(2000):
  h = 1 / (1 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  print(t, loss)

  grad_y_pred = 2.0 * (y_pred - y)
  grad_w2 = h.T.dot(grad_y_pred)
  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))

  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```

Define the network

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9    h = 1 / (1 + np.exp(-x.dot(w1)))
10   y_pred = h.dot(w2)
11   loss = np.square(y_pred - y).sum()
12   print(t, loss)
13
14   grad_y_pred = 2.0 * (y_pred - y)
15   grad_w2 = h.T.dot(grad_y_pred)
16   grad_h = grad_y_pred.dot(w2.T)
17   grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19   w1 -= 1e-4 * grad_w1
20   w2 -= 1e-4 * grad_w2
```

Define the network

Forward pass

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9    h = 1 / (1 + np.exp(-x.dot(w1)))
10   y_pred = h.dot(w2)
11   loss = np.square(y_pred - y).sum()
12   print(t, loss)
13
14   grad_y_pred = 2.0 * (y_pred - y)
15   grad_w2 = h.T.dot(grad_y_pred)
16   grad_h = grad_y_pred.dot(w2.T)
17   grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19   w1 -= 1e-4 * grad_w1
20   w2 -= 1e-4 * grad_w2
```

Define the network

Forward pass

Calculate the analytical gradients

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9    h = 1 / (1 + np.exp(-x.dot(w1)))
10   y_pred = h.dot(w2)
11   loss = np.square(y_pred - y).sum()
12   print(t, loss)
13
14   grad_y_pred = 2.0 * (y_pred - y)
15   grad_w2 = h.T.dot(grad_y_pred)
16   grad_h = grad_y_pred.dot(w2.T)
17   grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19   w1 -= 1e-4 * grad_w1
20   w2 -= 1e-4 * grad_w2
```

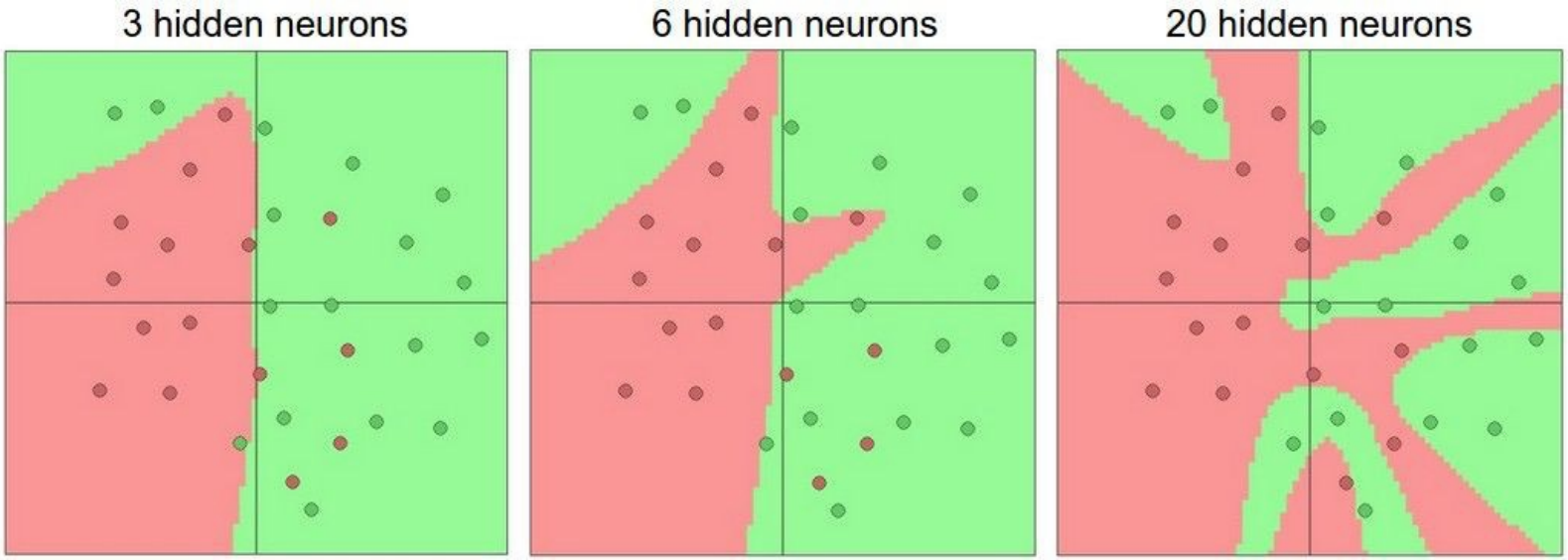
Define the network

Forward pass

Calculate the analytical gradients

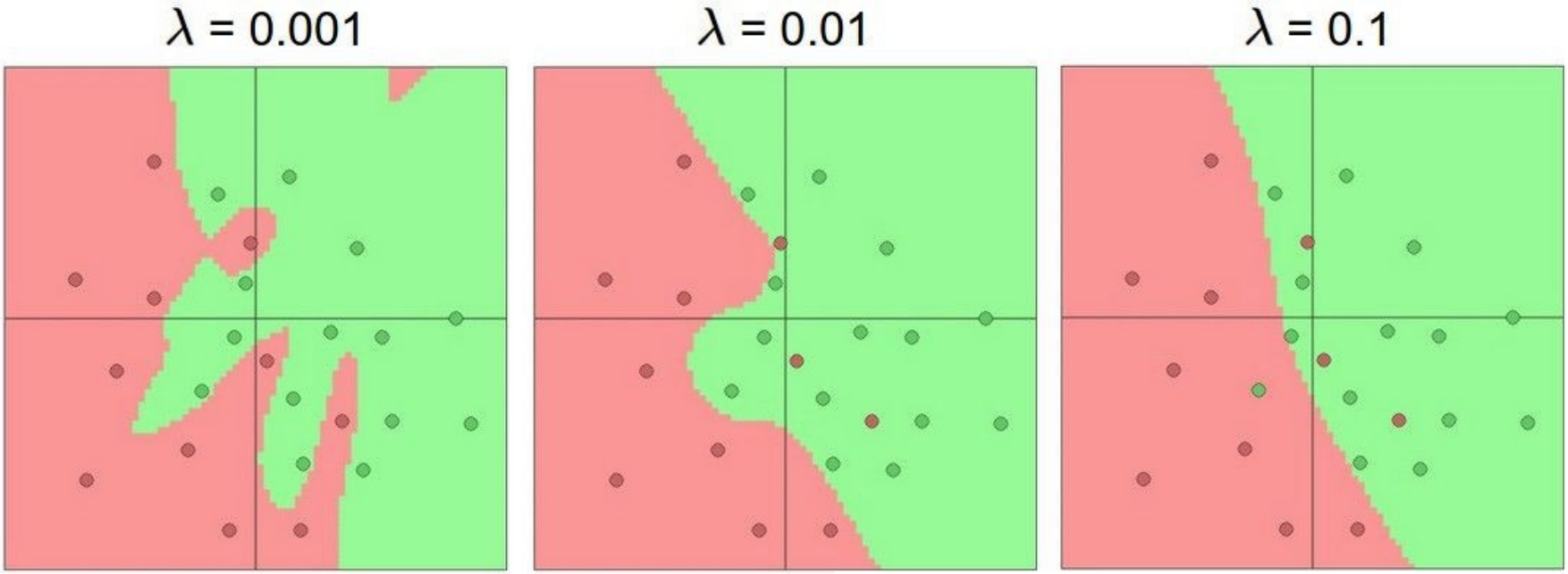
Gradient descent

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:



$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

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?

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

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

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

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

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

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

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

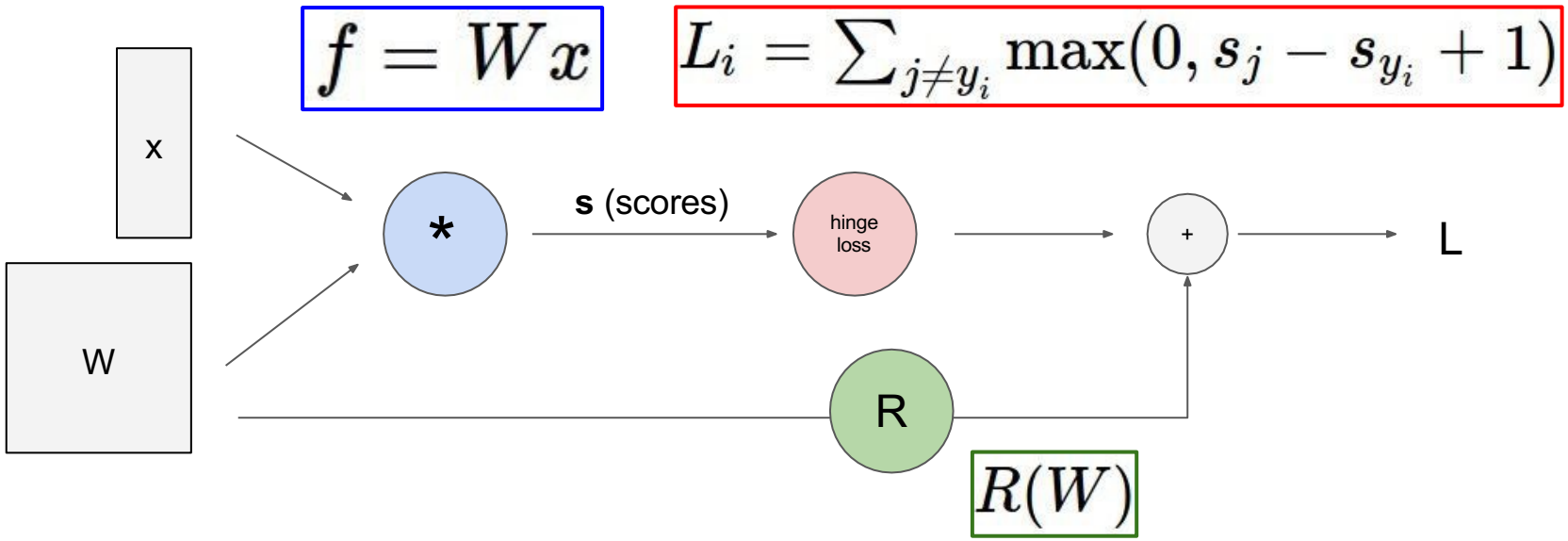
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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

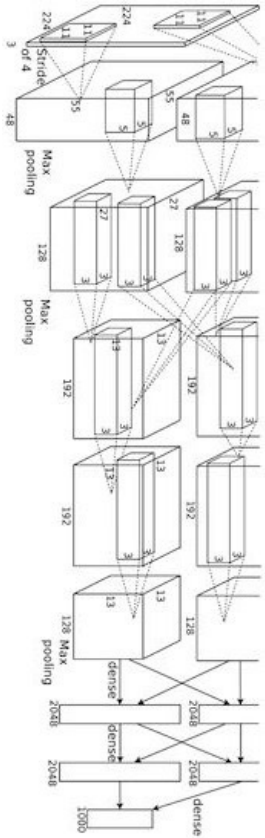


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Really complex neural networks!!

input image

loss

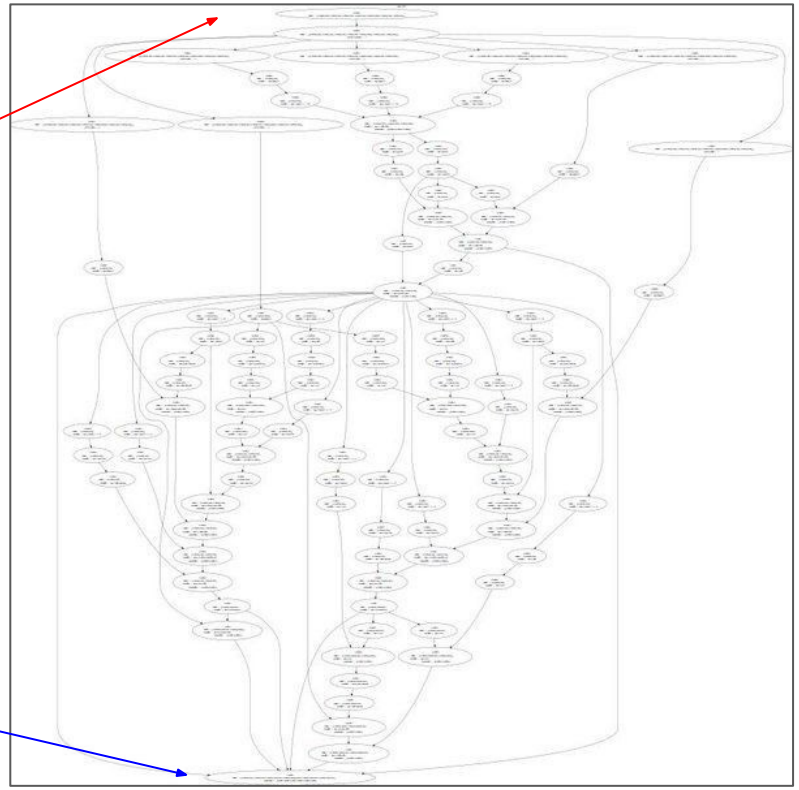


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

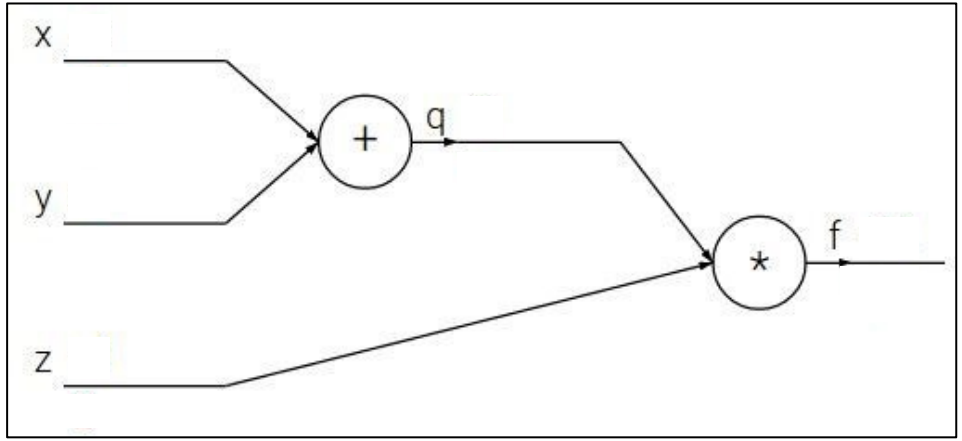
Solution: Backpropagation

Backpropagation: a simple example

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

Backpropagation: a simple example

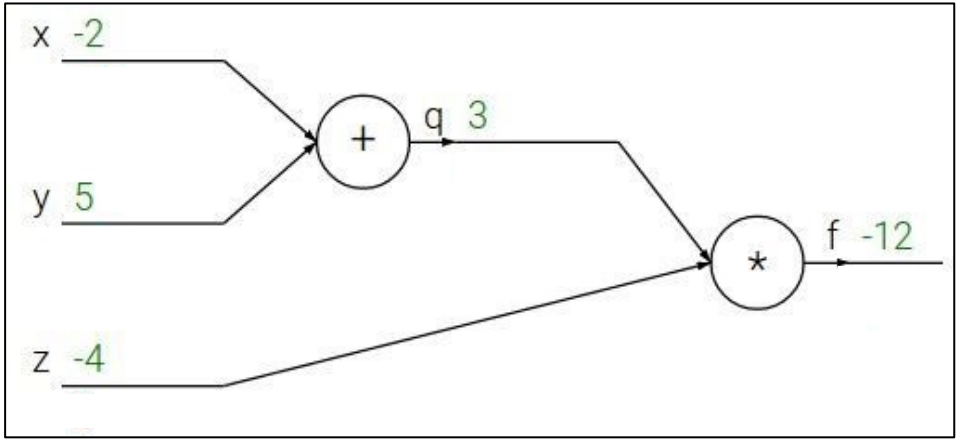
$$f(x, y, z) = (x + y)z$$



Backpropagation: a simple example

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

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

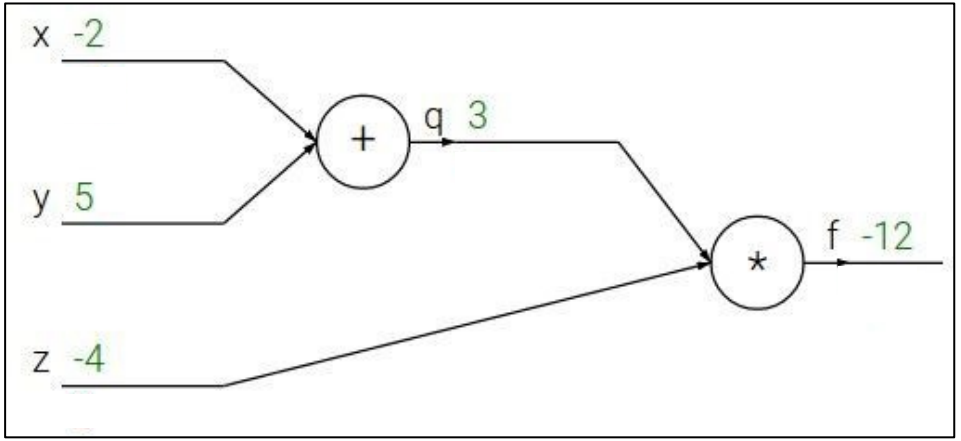


Backpropagation: a simple example

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

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

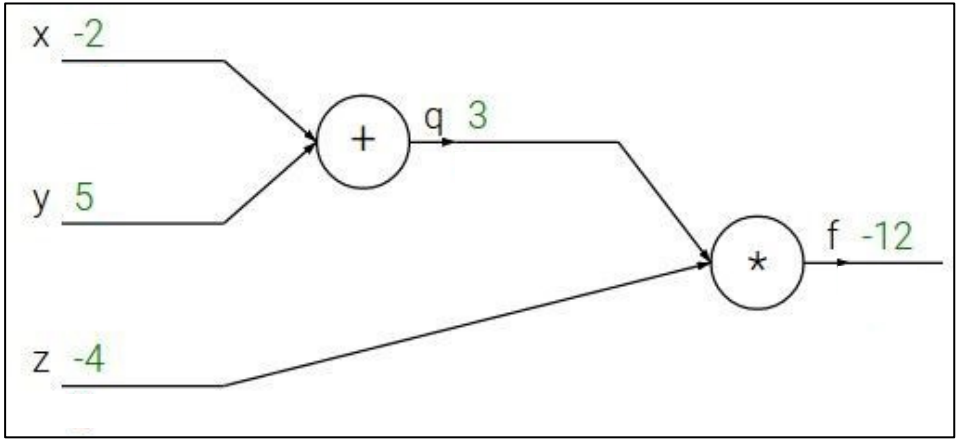
$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$



Backpropagation: a simple example

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

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



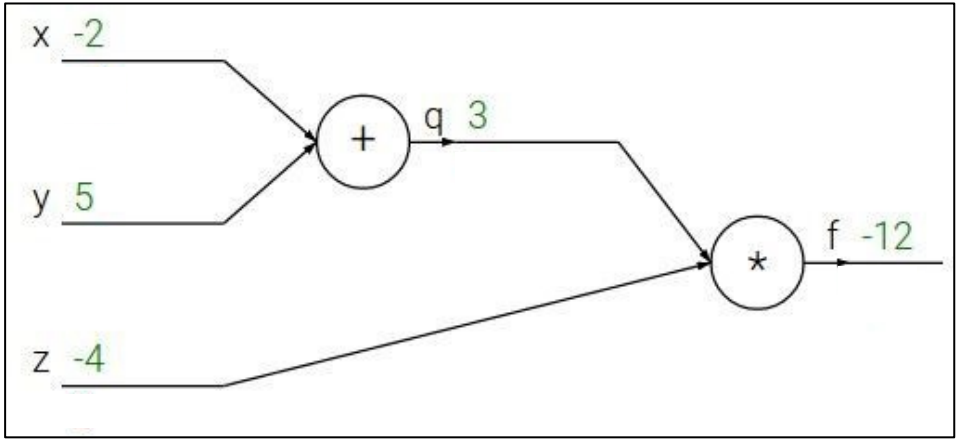
$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

Backpropagation: a simple example

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

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

Backpropagation: a simple example

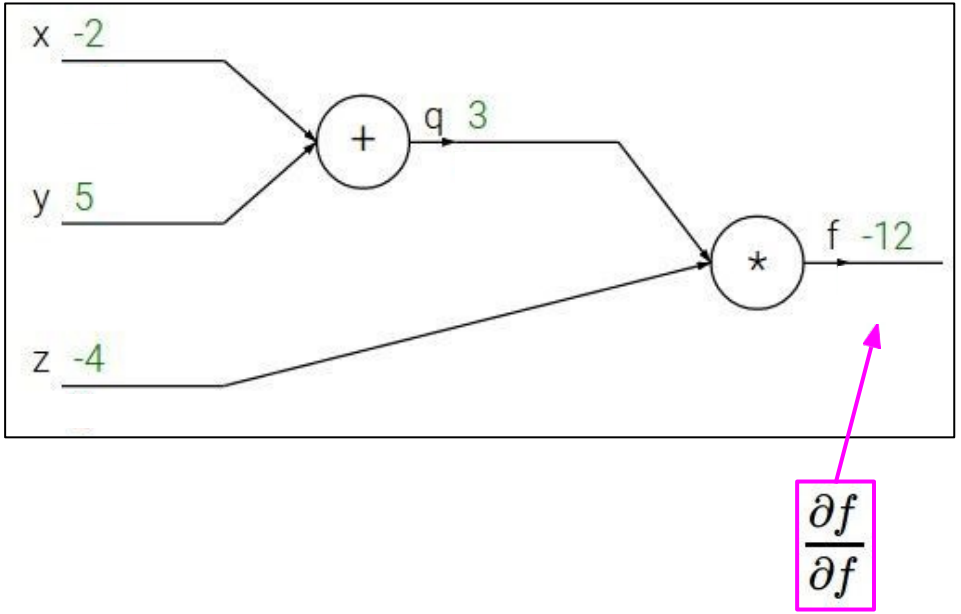
$$f(x, y, z) = (x + y)z$$

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



Backpropagation: a simple example

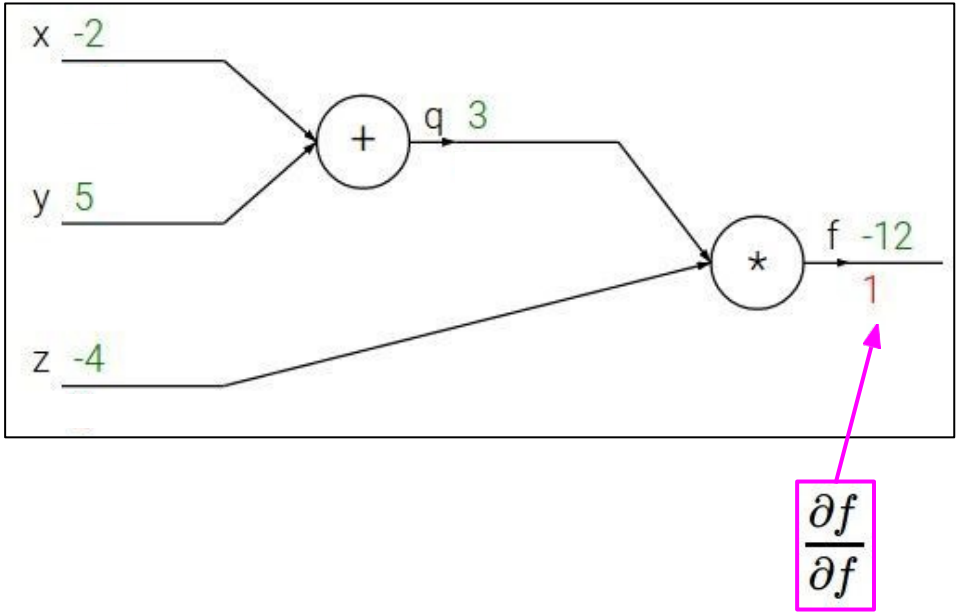
$$f(x, y, z) = (x + y)z$$

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



Backpropagation: a simple example

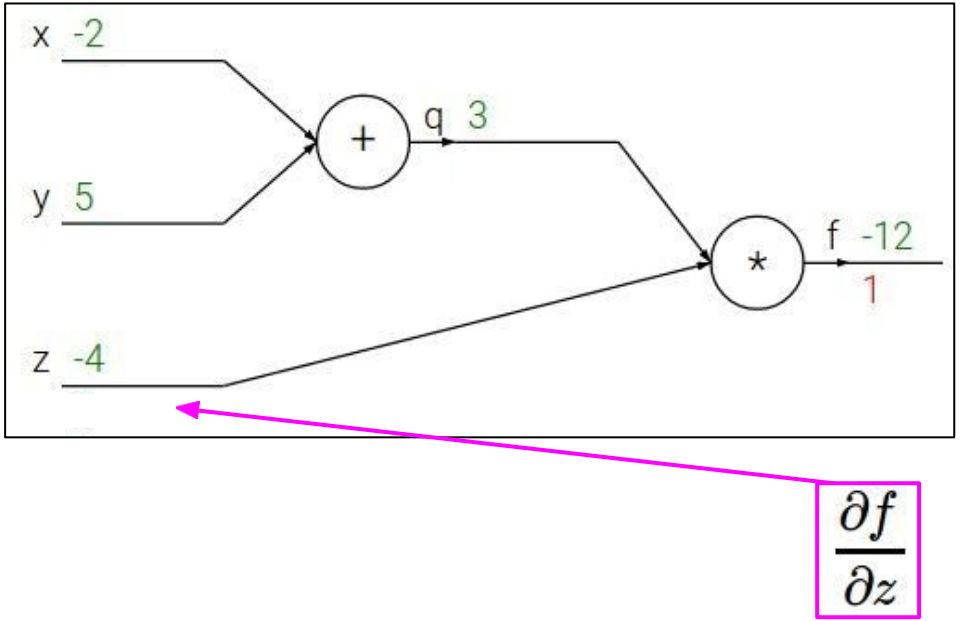
$$f(x, y, z) = (x + y)z$$

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



Backpropagation: a simple example

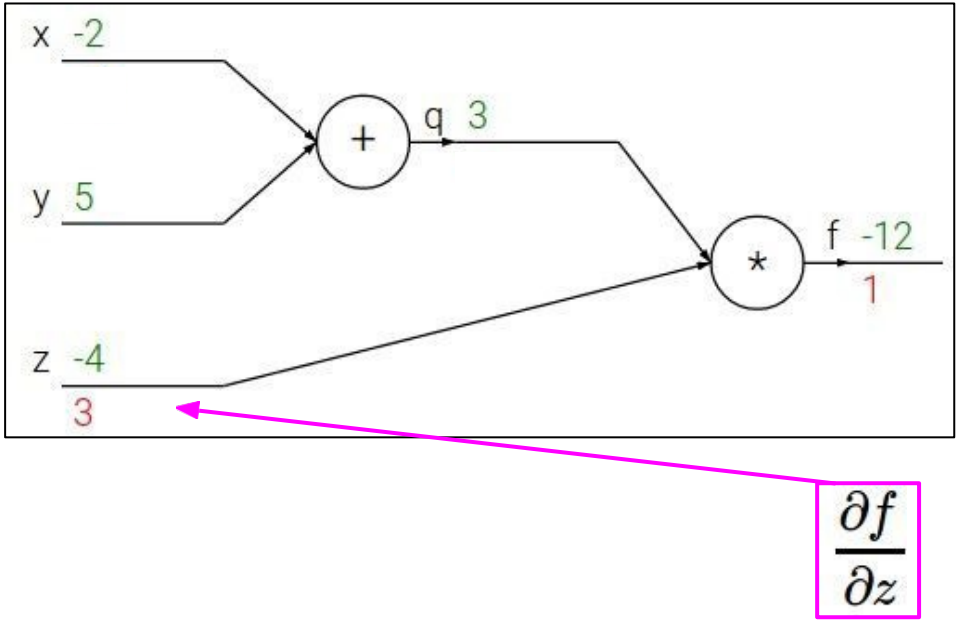
$$f(x, y, z) = (x + y)z$$

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



Backpropagation: a simple example

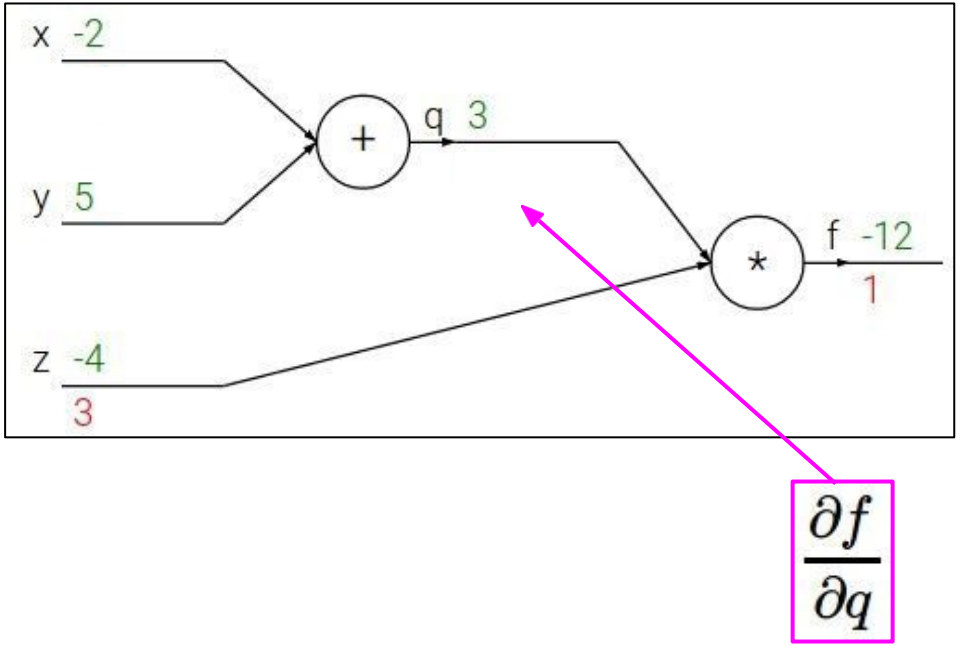
$$f(x, y, z) = (x + y)z$$

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



Backpropagation: a simple example

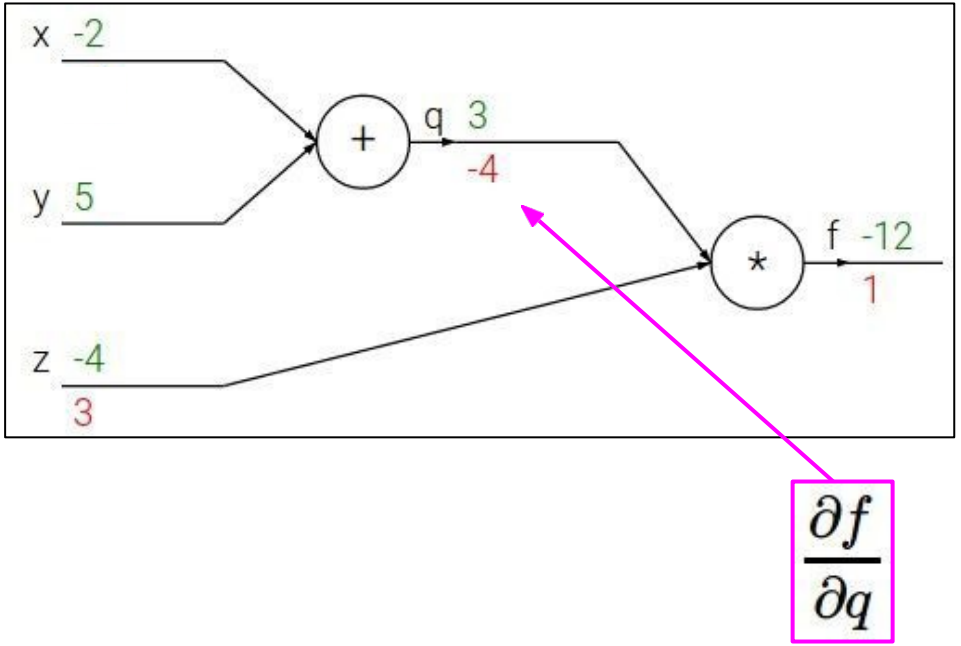
$$f(x, y, z) = (x + y)z$$

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



Backpropagation: a simple example

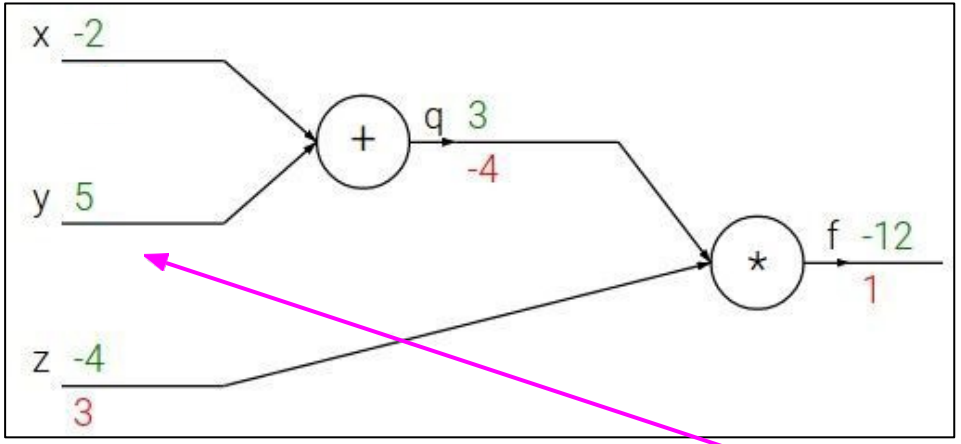
$$f(x, y, z) = (x + y)z$$

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



Chain rule:

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

Upstream gradient

Local gradient

Backpropagation: a simple example

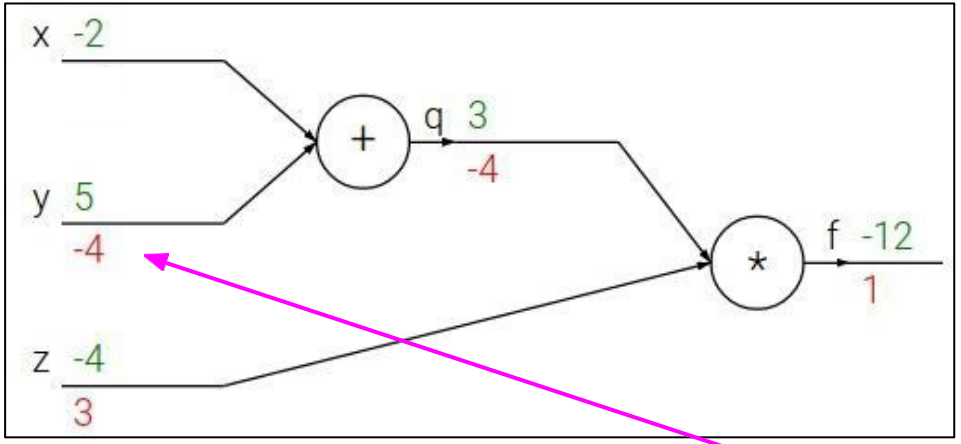
$$f(x, y, z) = (x + y)z$$

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



Chain rule:

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

Upstream gradient

Local gradient

Backpropagation: a simple example

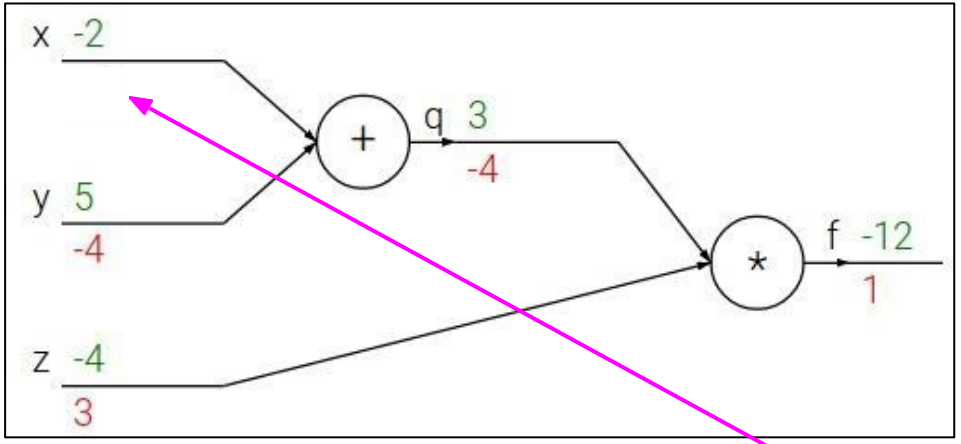
$$f(x, y, z) = (x + y)z$$

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



Chain rule:

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

Upstream gradient

Local gradient

Backpropagation: a simple example

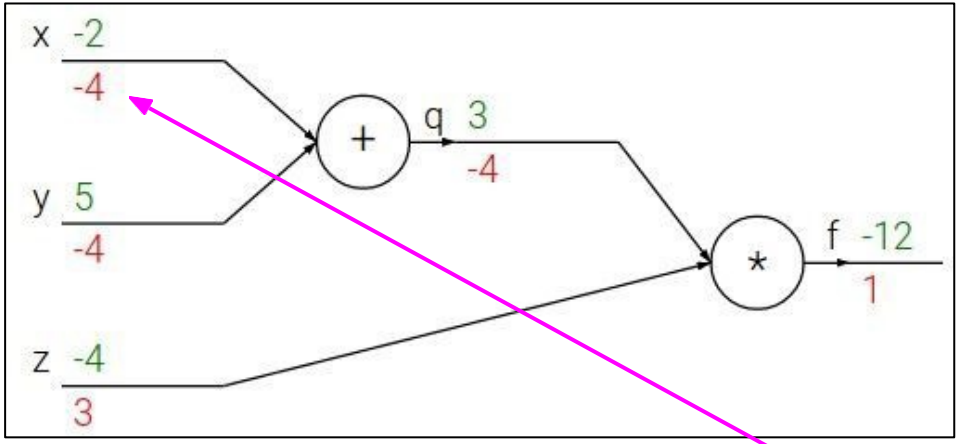
$$f(x, y, z) = (x + y)z$$

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

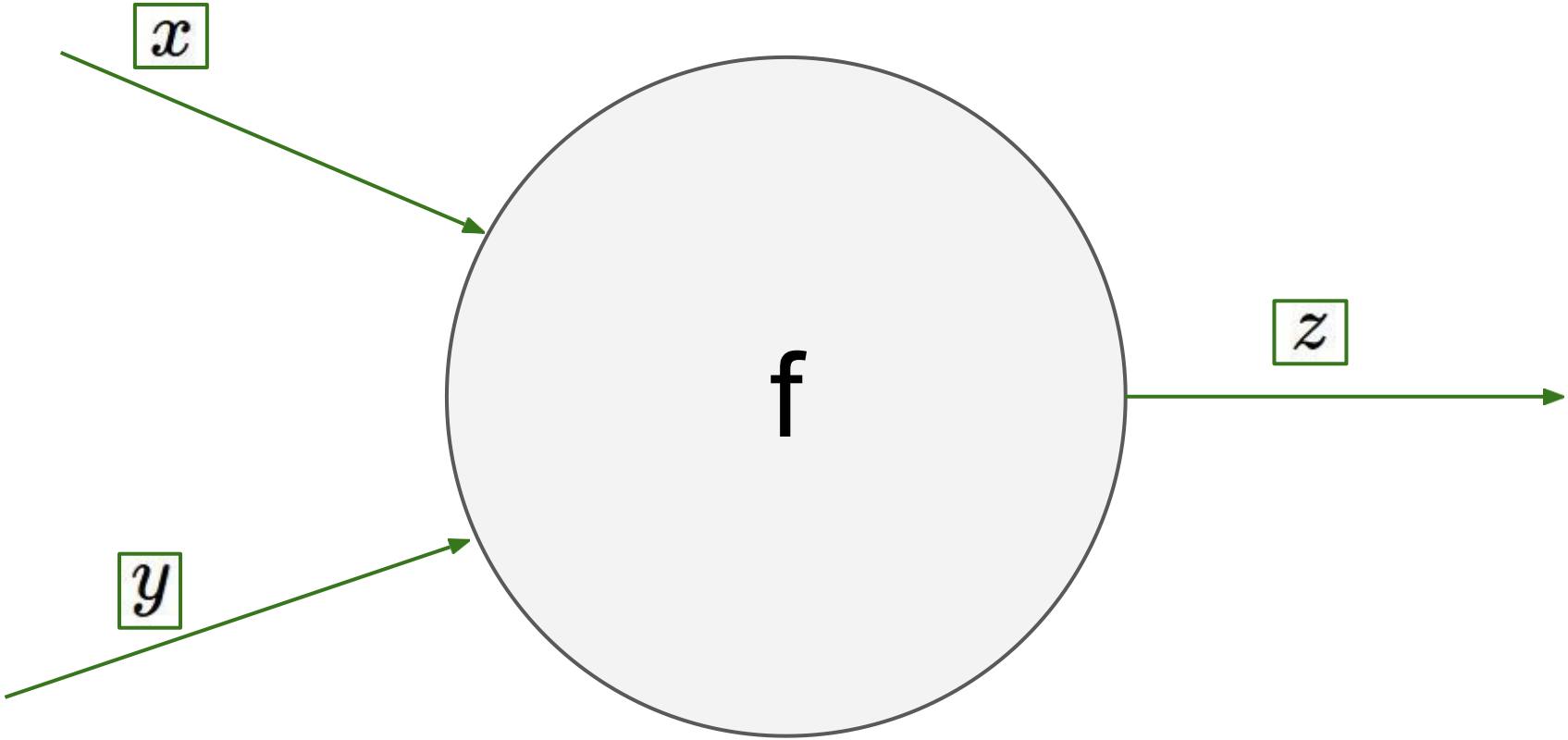


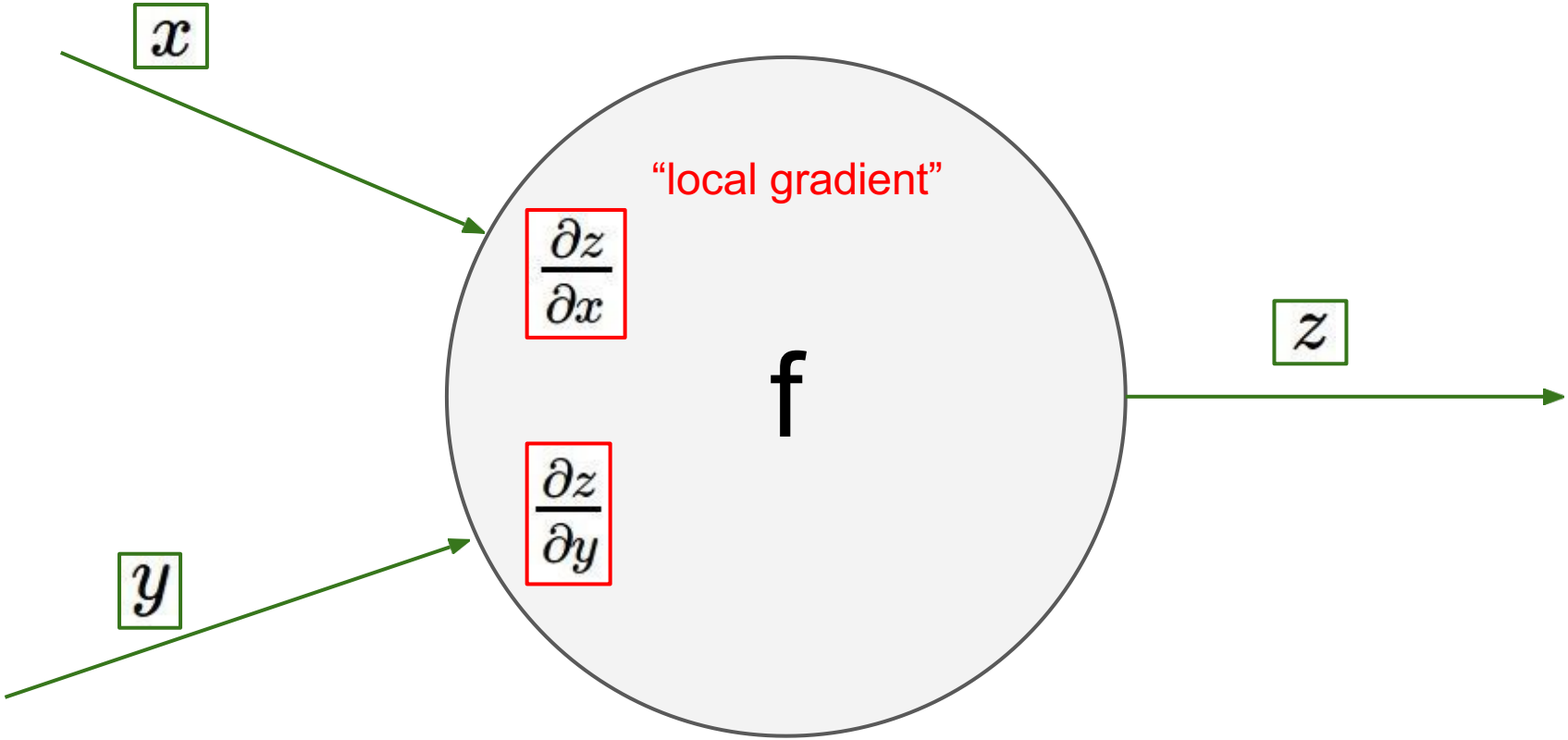
Chain rule:

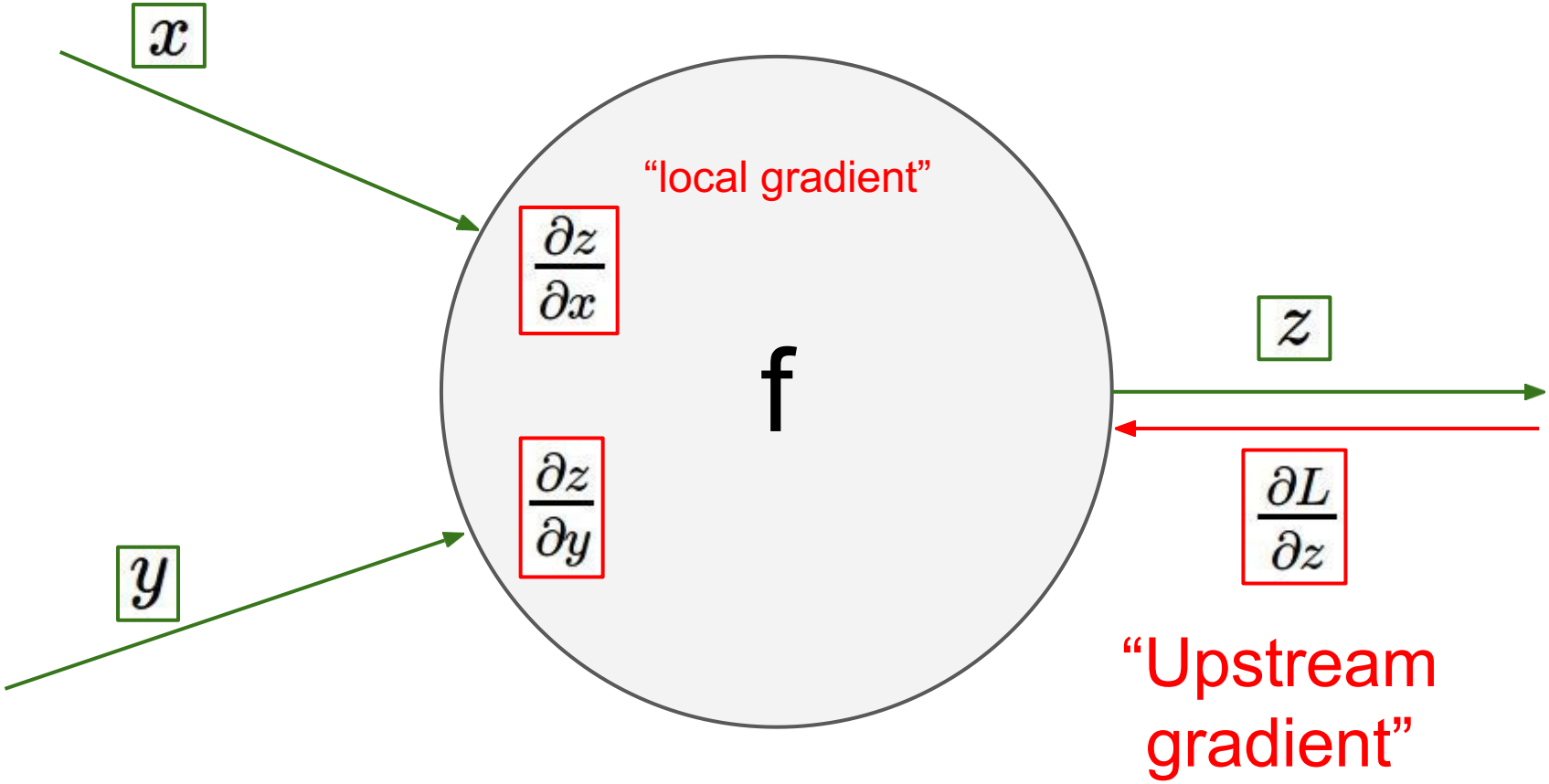
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x}$$

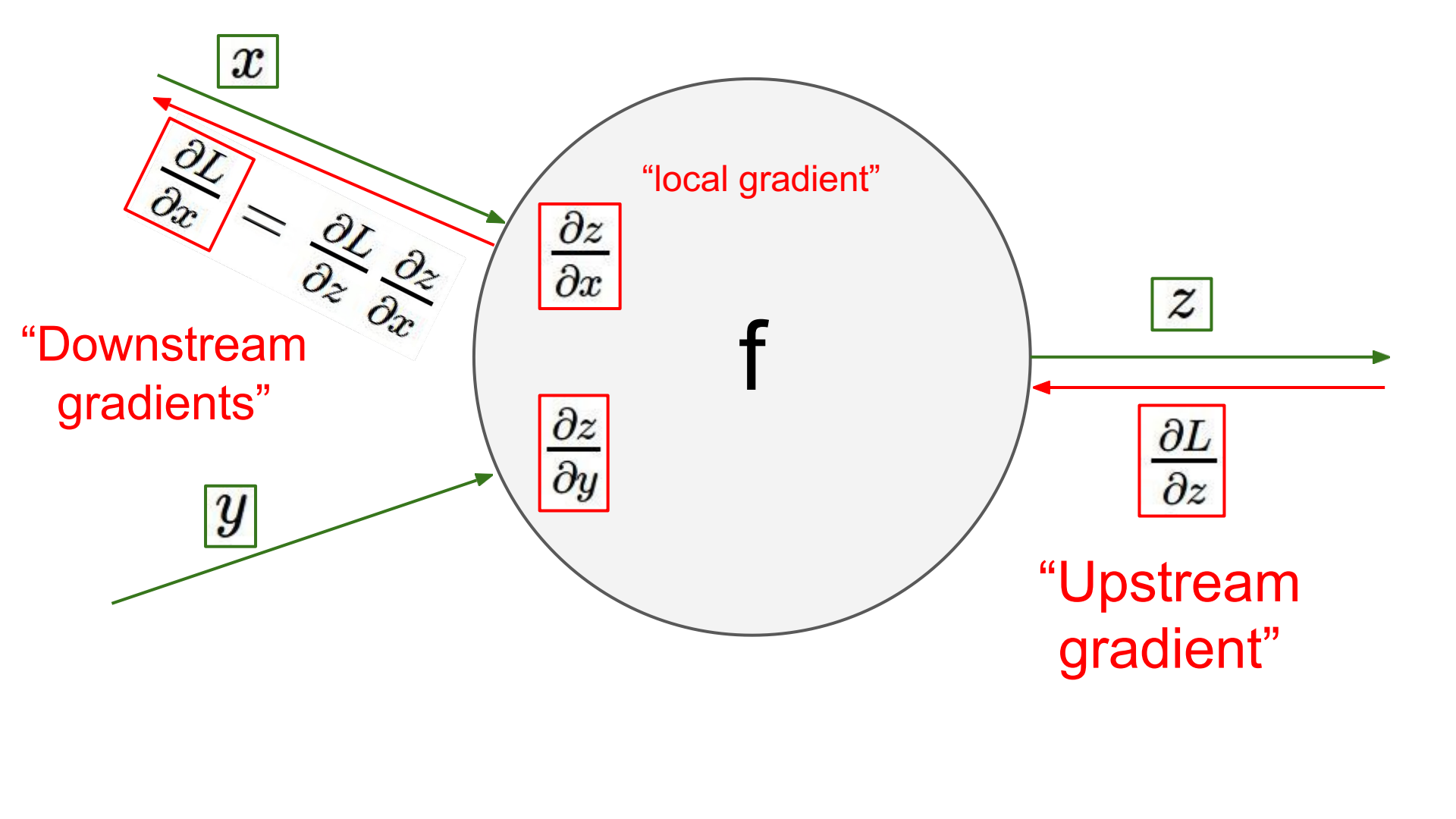
Upstream gradient

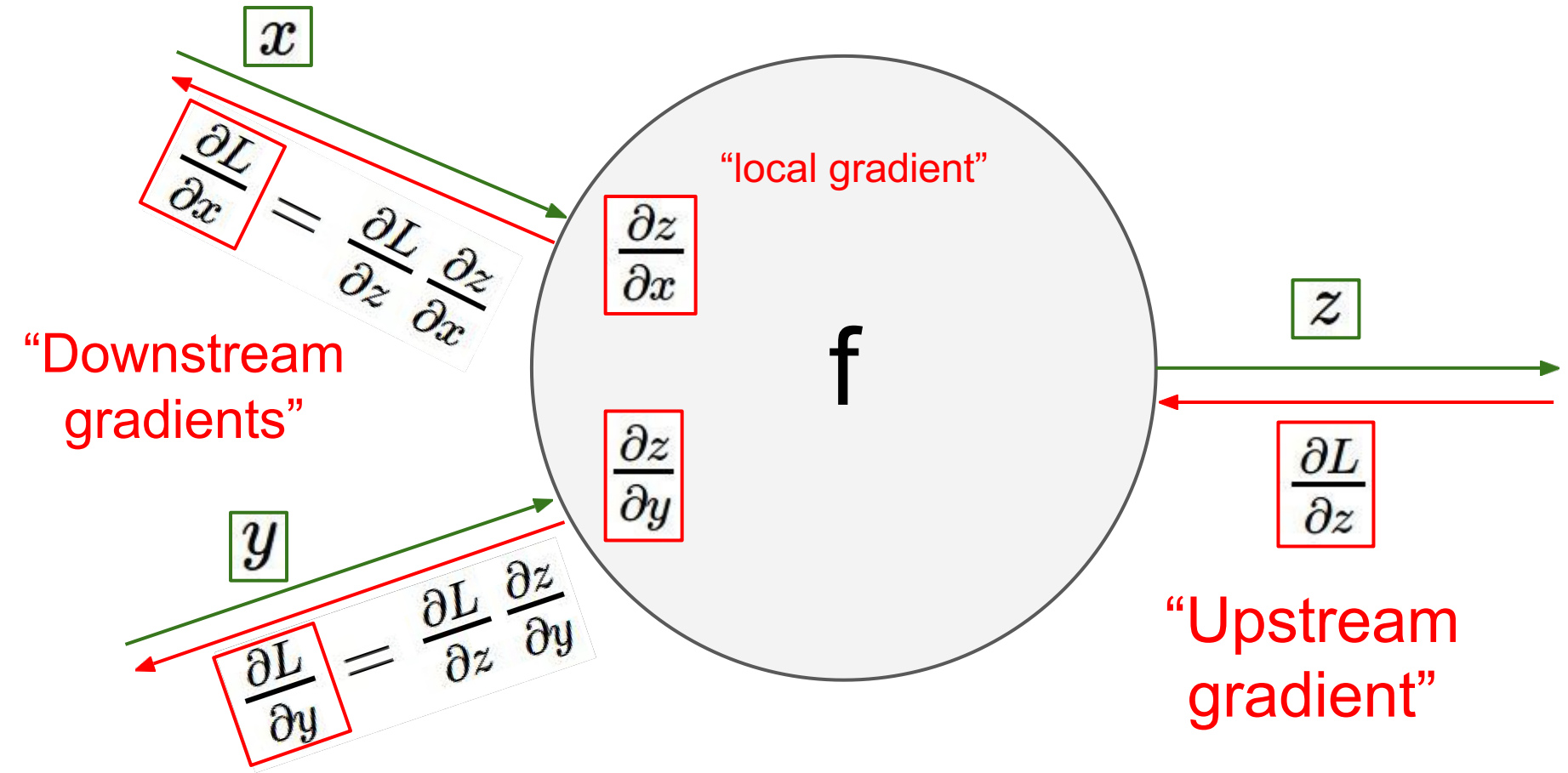
Local gradient

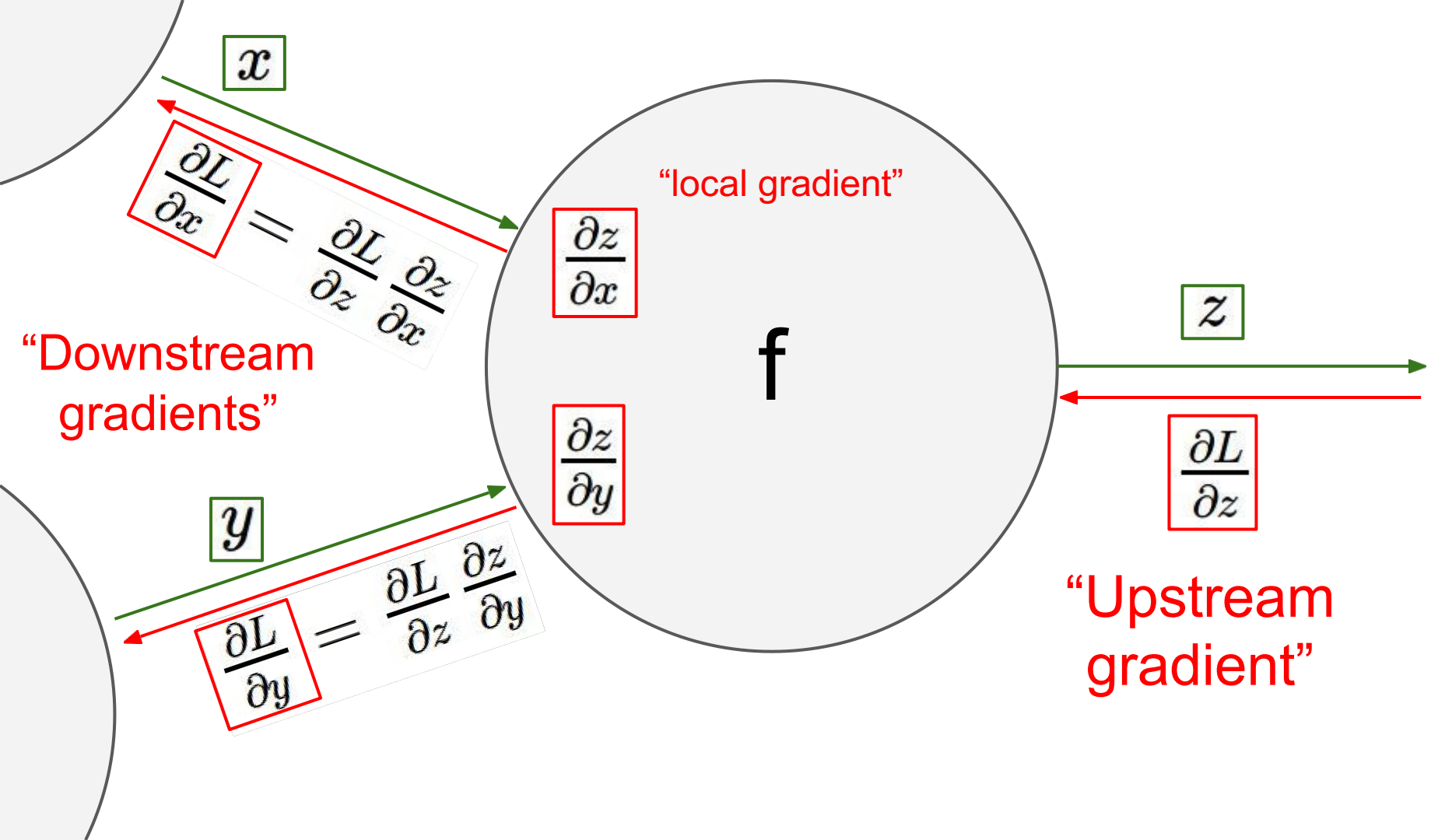

x
y
f
z


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

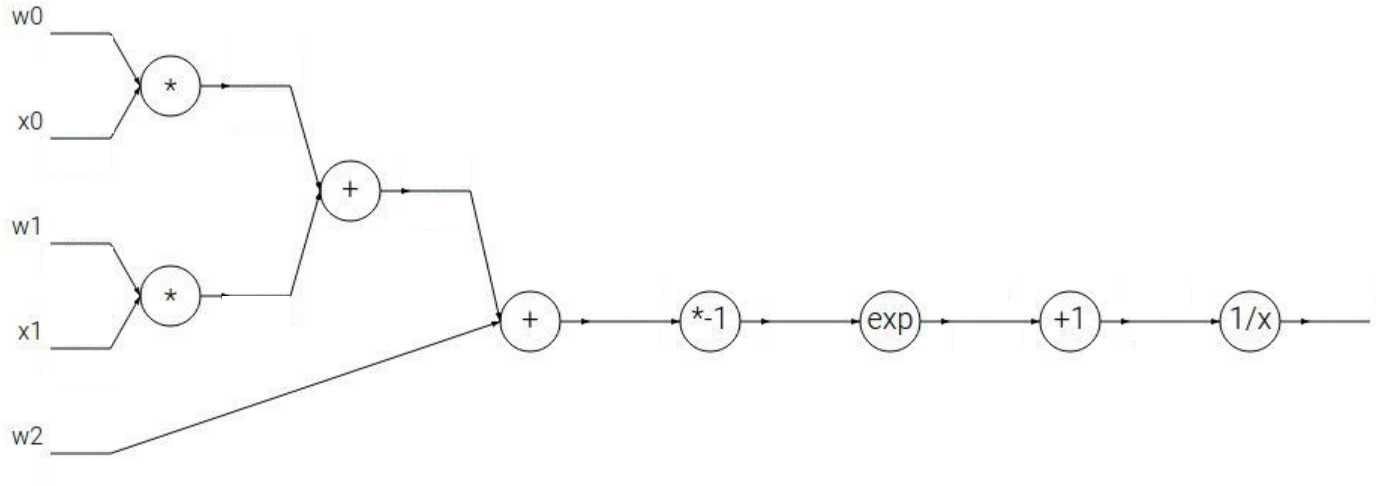

x
y
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
"local gradient"
"Upstream gradient"


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

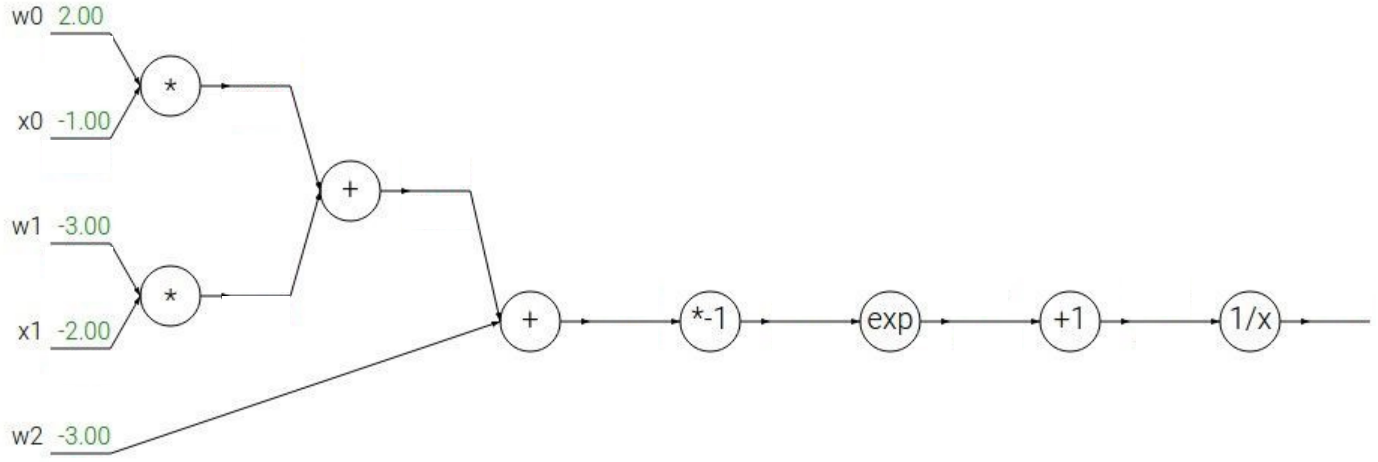

x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
"local gradient"
$\frac{\partial z}{\partial x}$
f
$\frac{\partial z}{\partial y}$
z
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial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


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

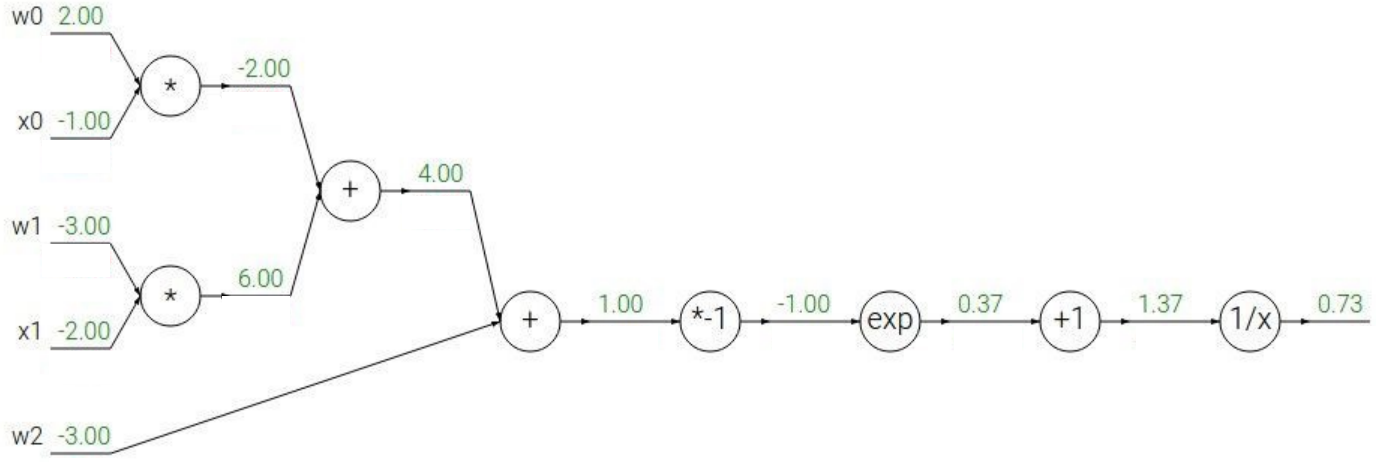
Another example: $$f(w,x) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$



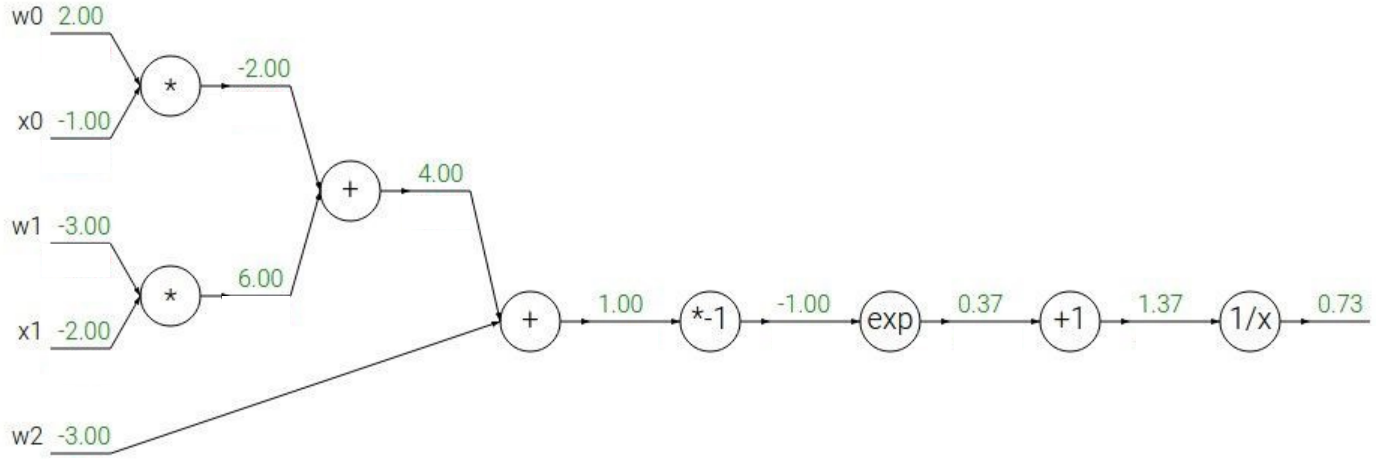
Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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



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



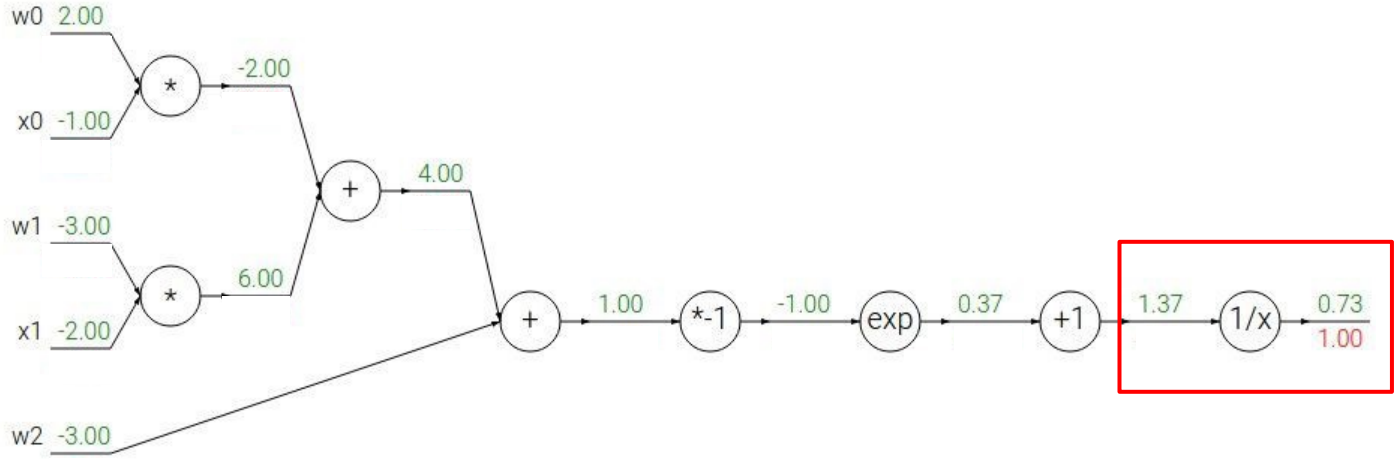
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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

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

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

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



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

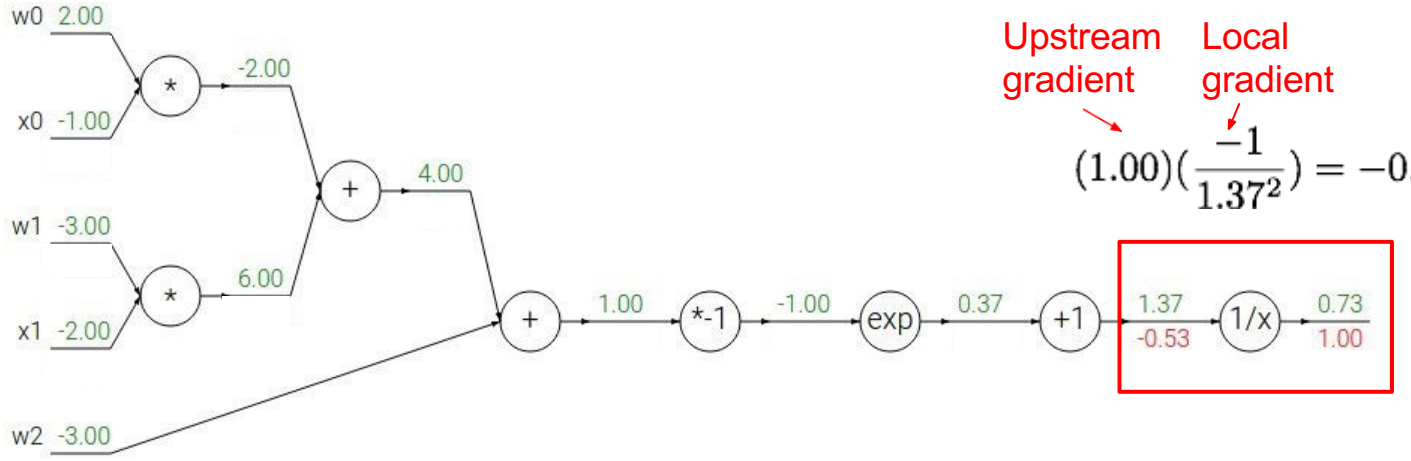
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



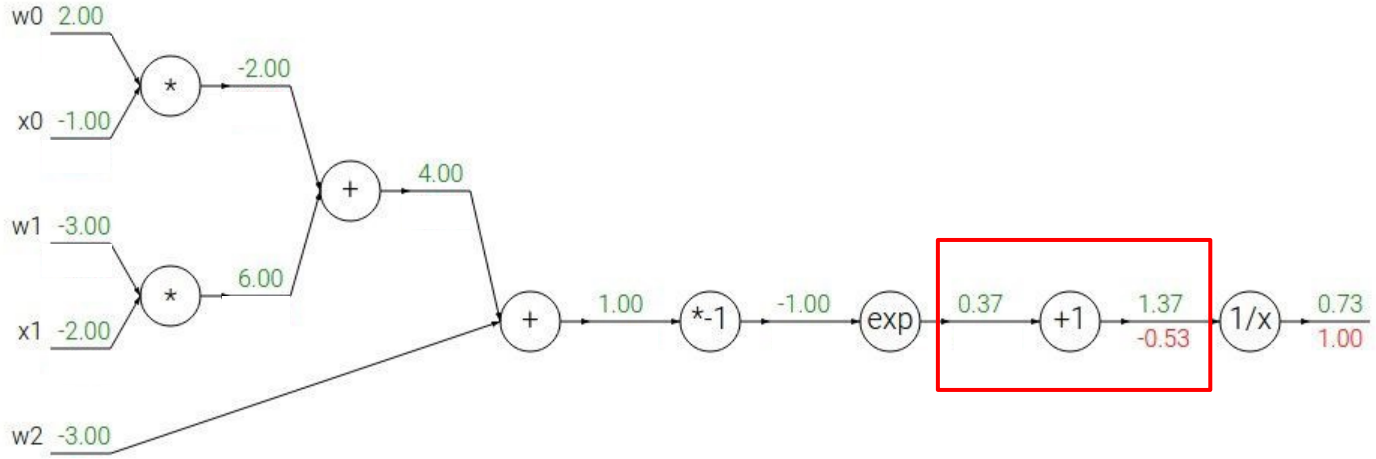
$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$

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

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

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

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



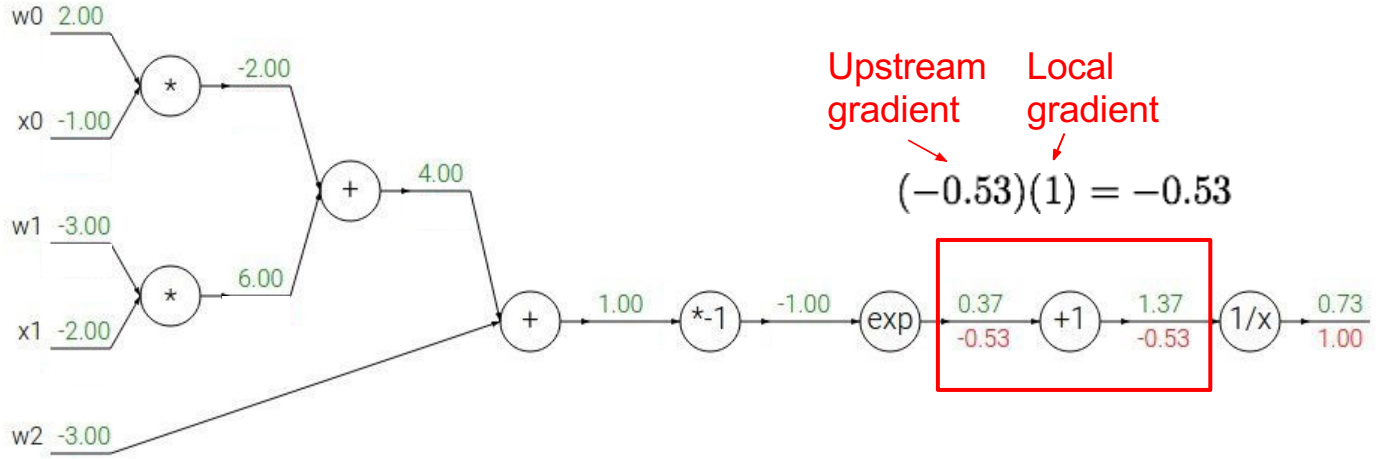
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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

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

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

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



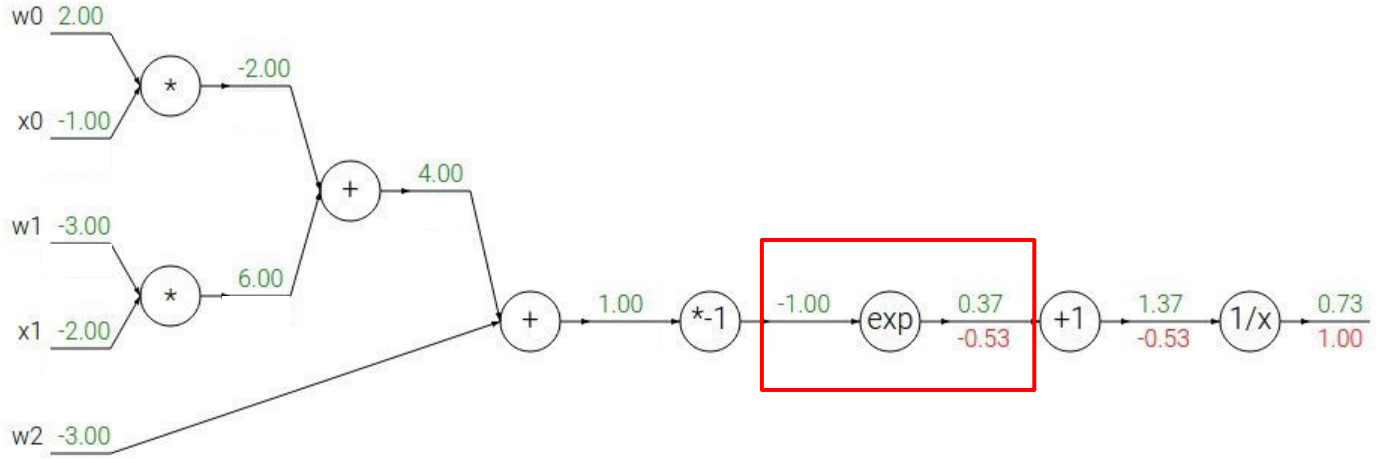
$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$

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

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

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

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



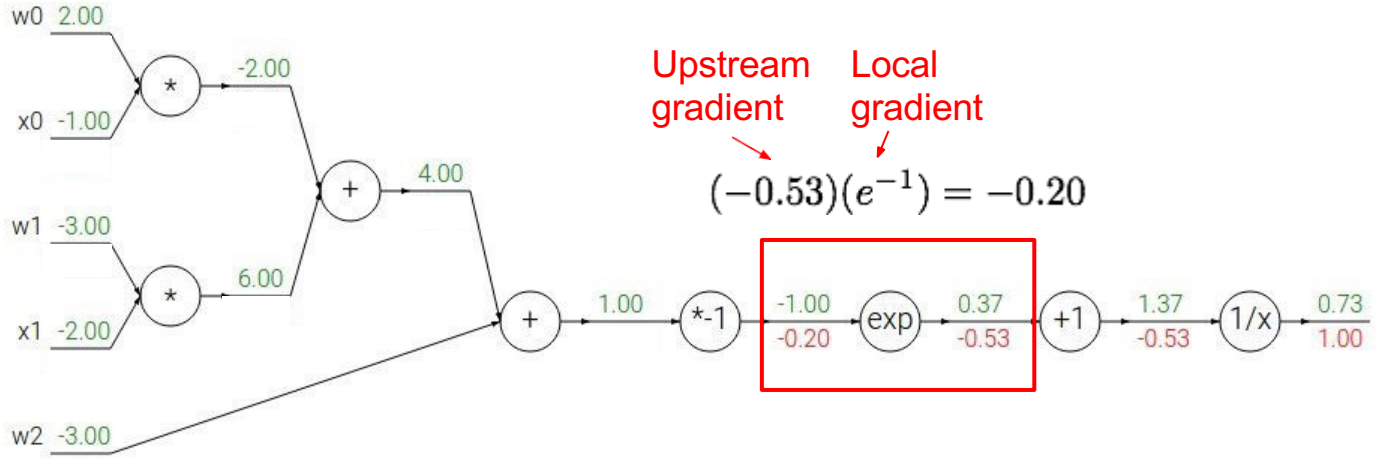
$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$

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

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

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

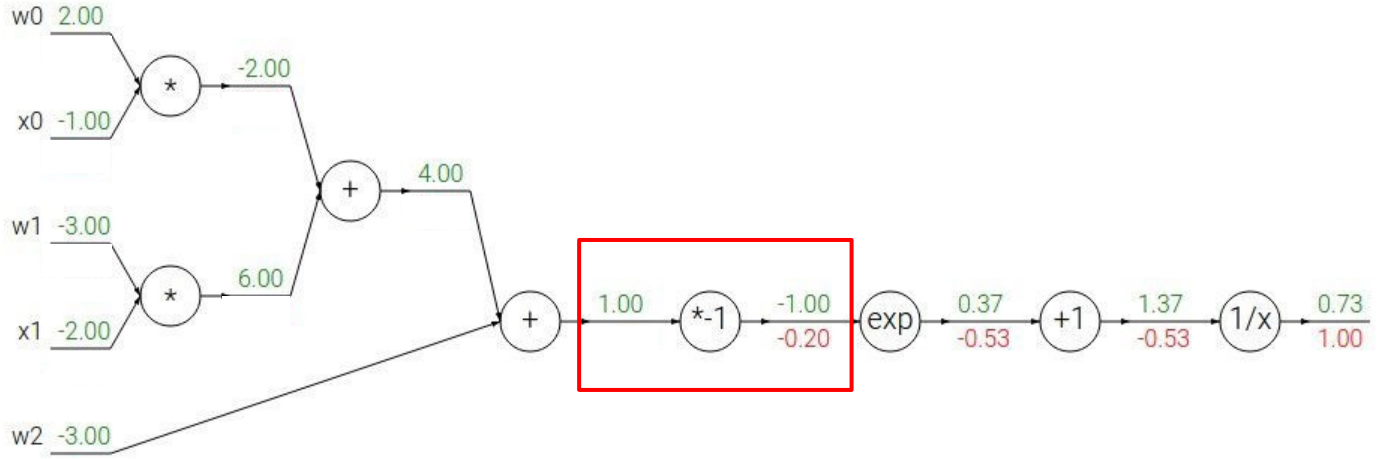
Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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

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

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



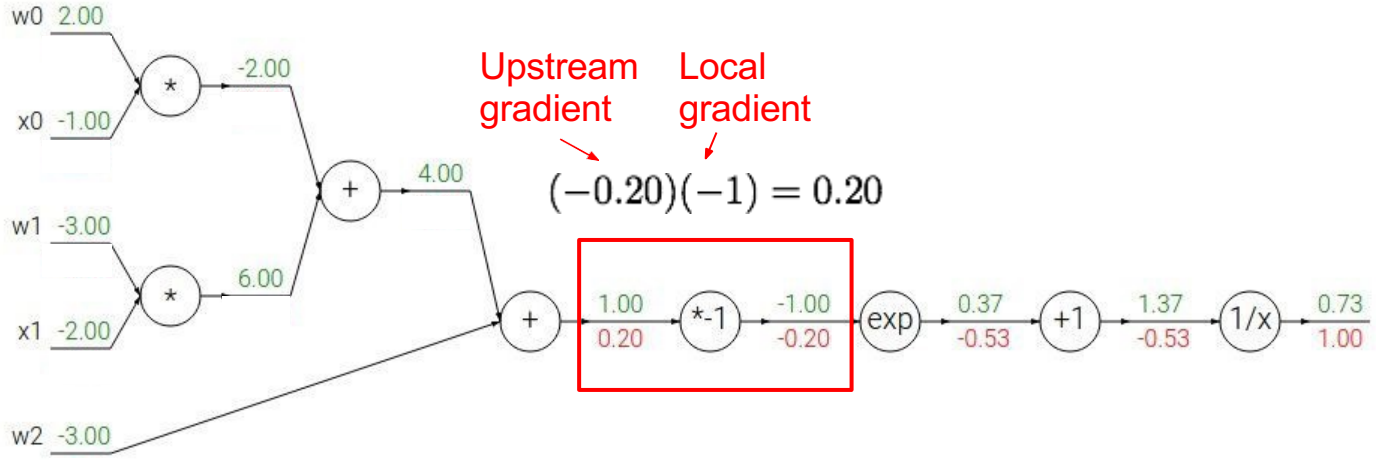
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



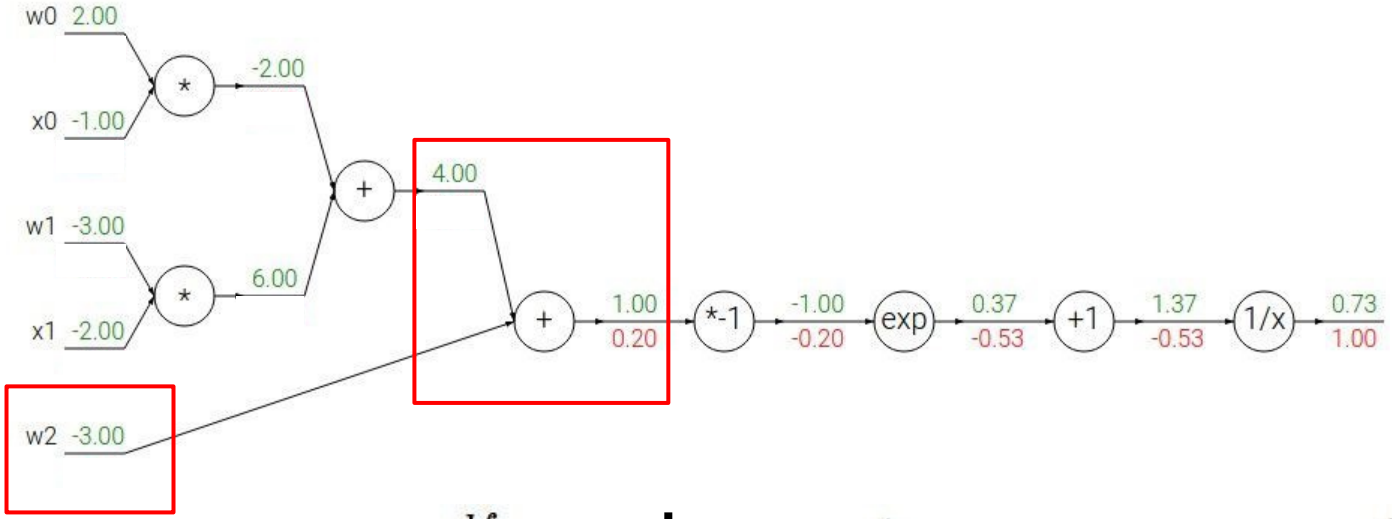
$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$

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

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

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

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



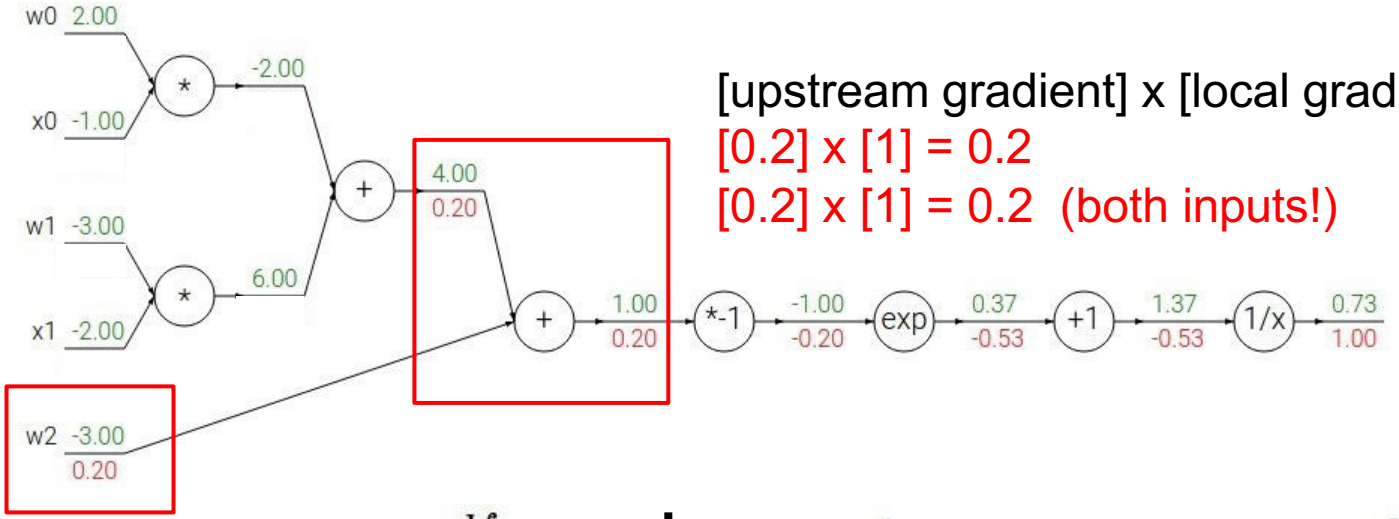
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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

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

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

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



[upstream gradient] x [local gradient]

[0.2] x [1] = 0.2

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

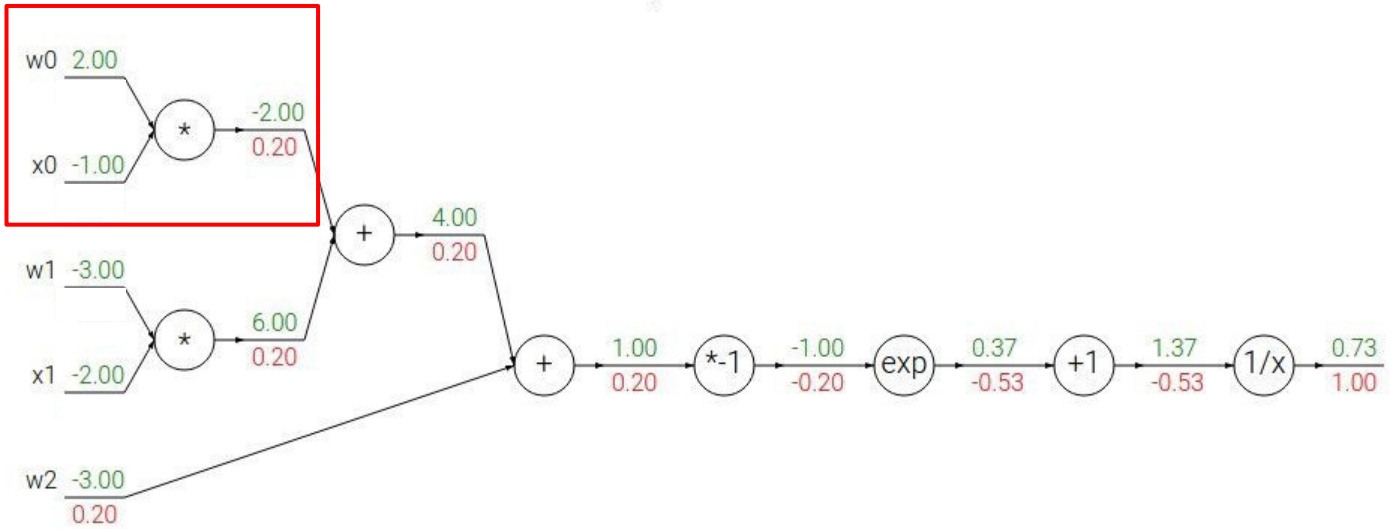
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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

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

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

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



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

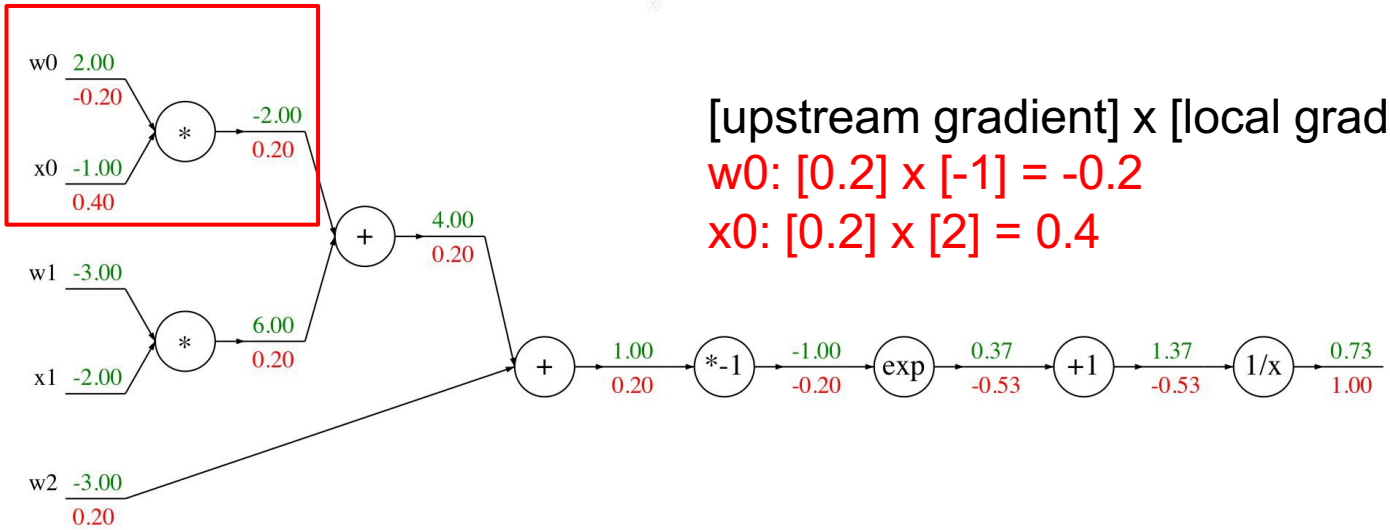
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



[upstream gradient] x [local gradient]

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

x0: [0.2] x [2] = 0.4

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

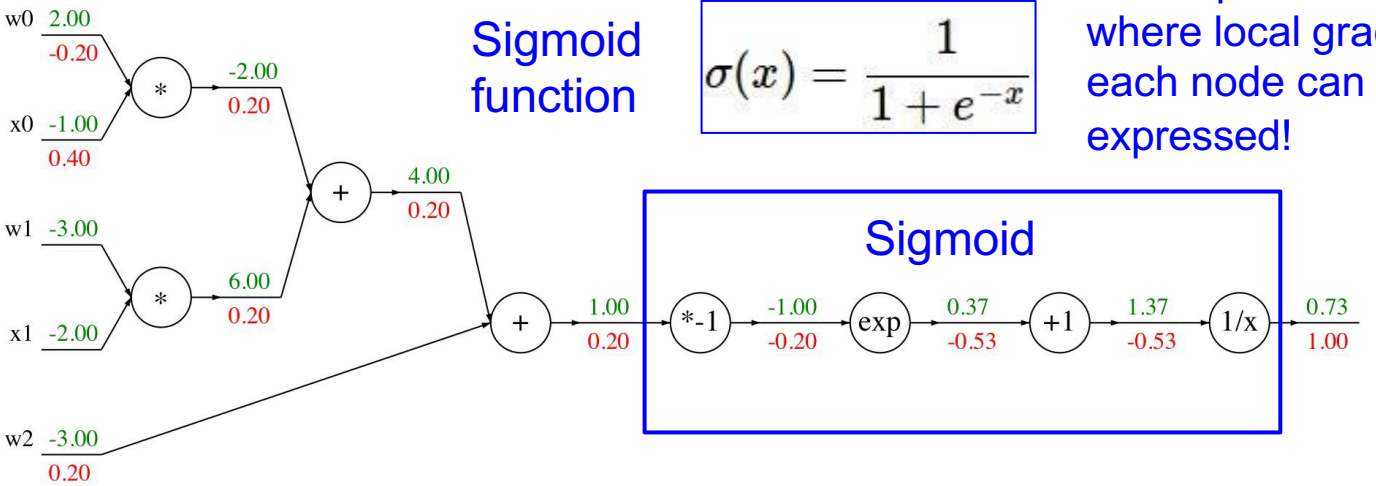
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



Sigmoid function

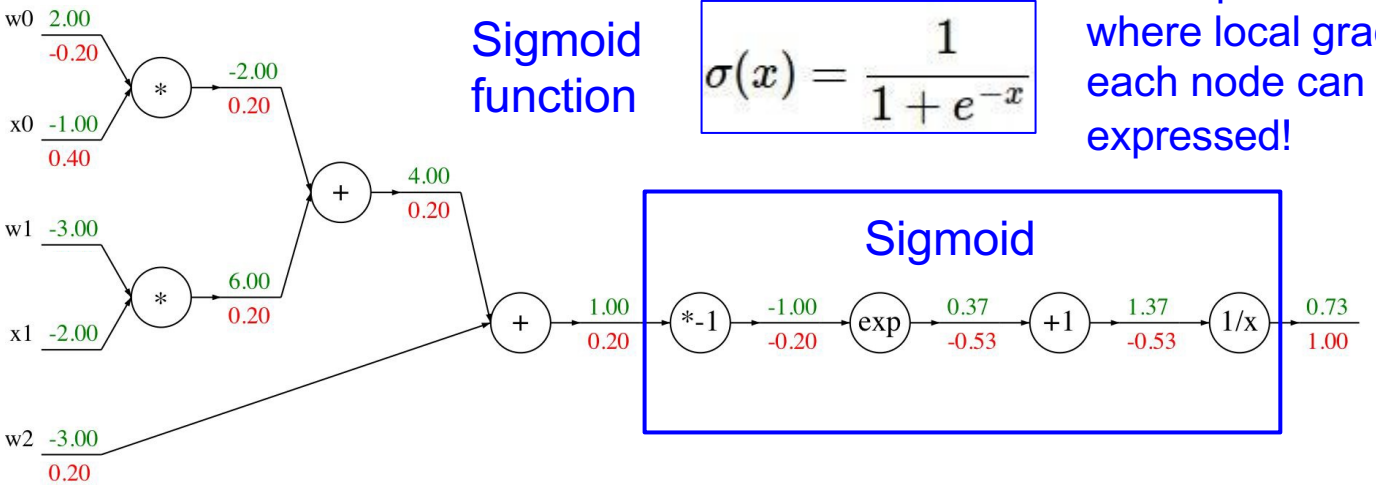
$$\sigma(x) = \frac{1}{1+e^{-x}}$$

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

Another example:

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

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



Sigmoid function

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

Sigmoid local gradient:

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

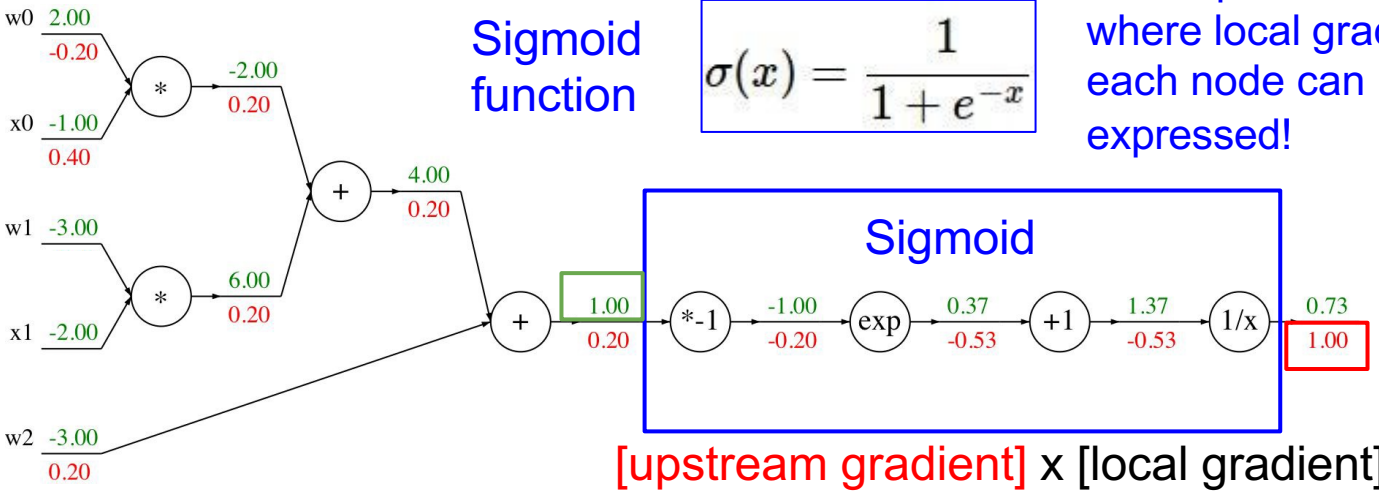
Another example:

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

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

Sigmoid function

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



[upstream gradient] x [local gradient]

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

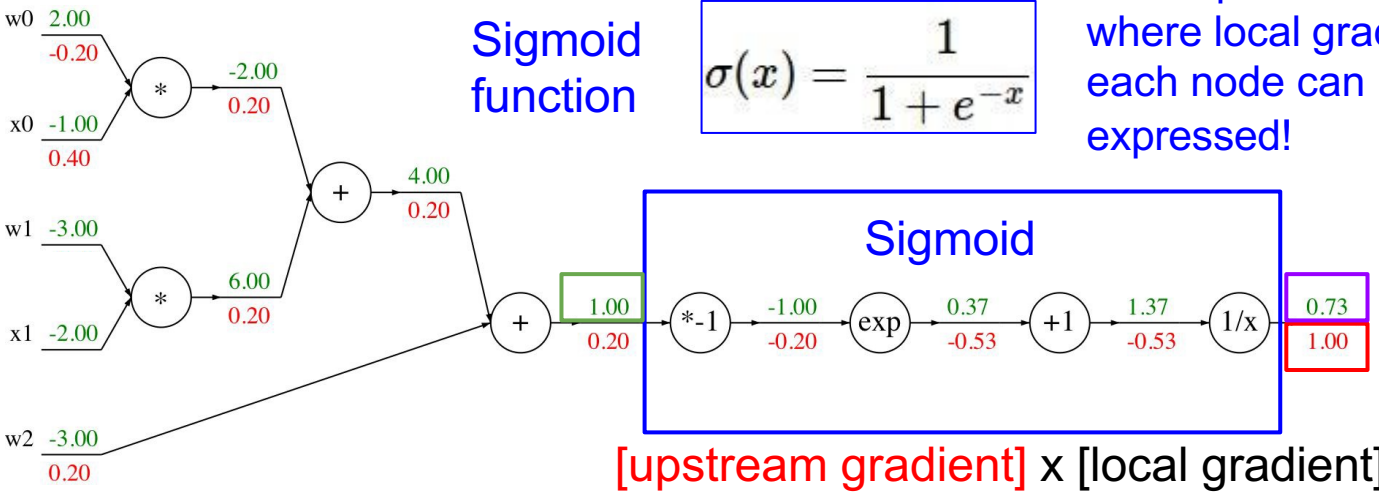
Sigmoid local gradient:

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

Another example:

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

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



Sigmoid function

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

[upstream gradient] x [local gradient]

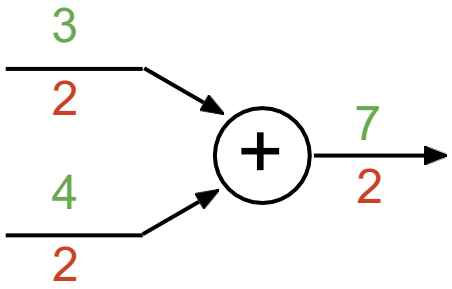
[1.00] x [(1 - 0.73) (0.73)] = 0.2

Sigmoid local gradient:

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

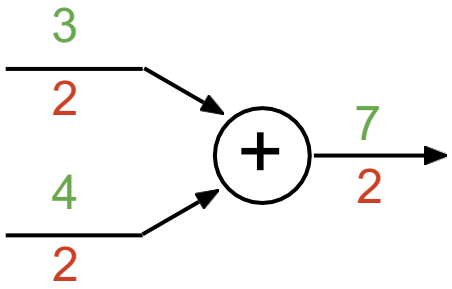
Patterns in gradient flow

add gate: gradient distributor

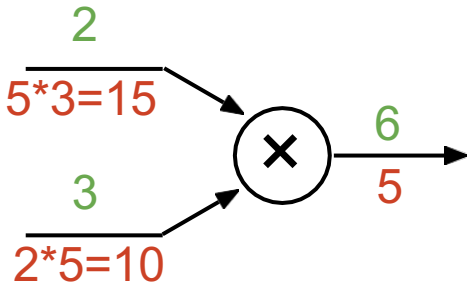


Patterns in gradient flow

add gate: gradient distributor

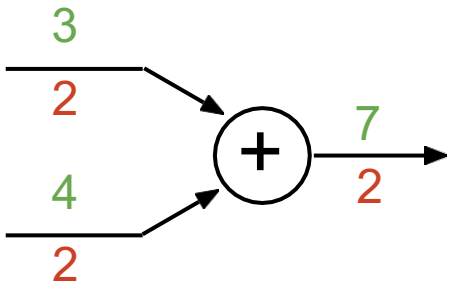


mul gate: “swap multiplier”

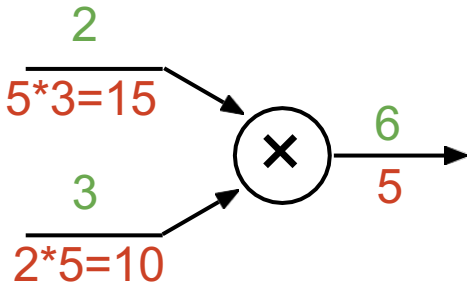


Patterns in gradient flow

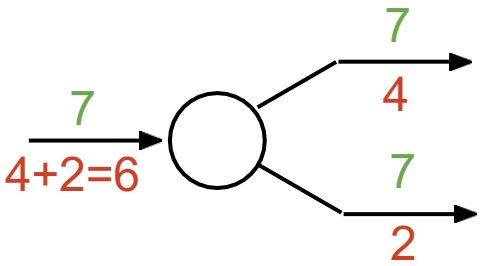
add gate: gradient distributor



mul gate: “swap multiplier”

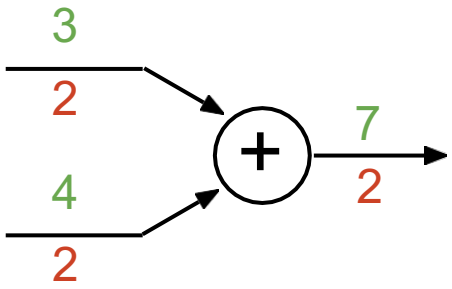


copy gate: gradient adder

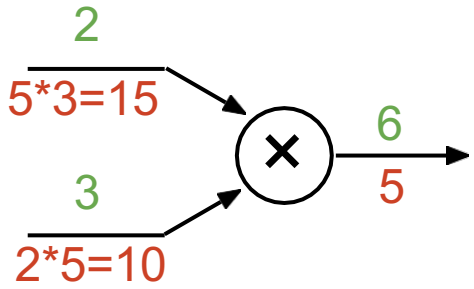


Patterns in gradient flow

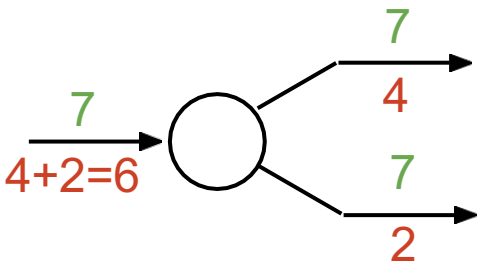
add gate: gradient distributor



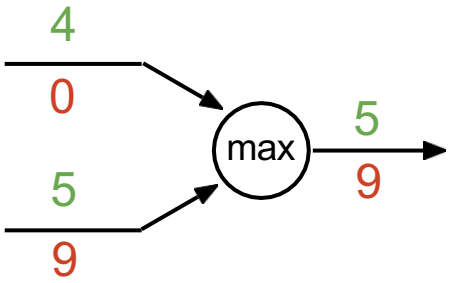
mul gate: “swap multiplier”



copy gate: gradient adder



max gate: gradient router



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

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?

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?

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?

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?

Vector to Vector

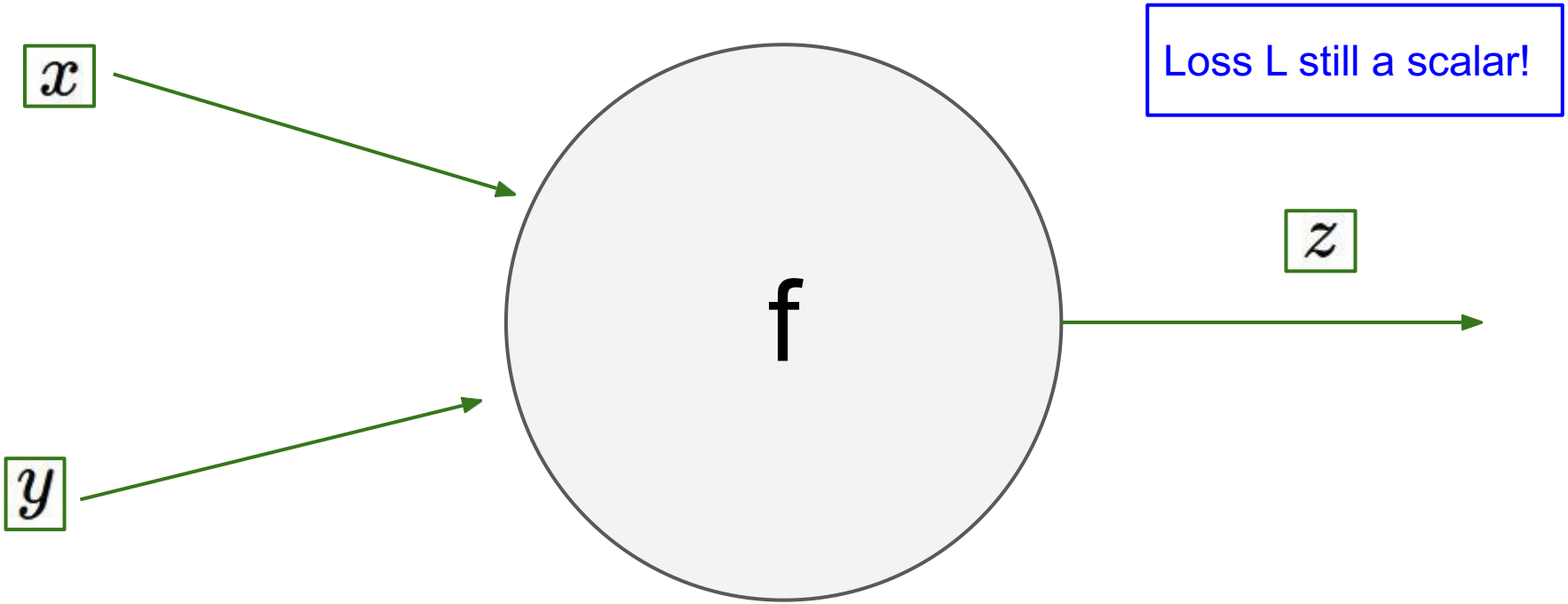
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

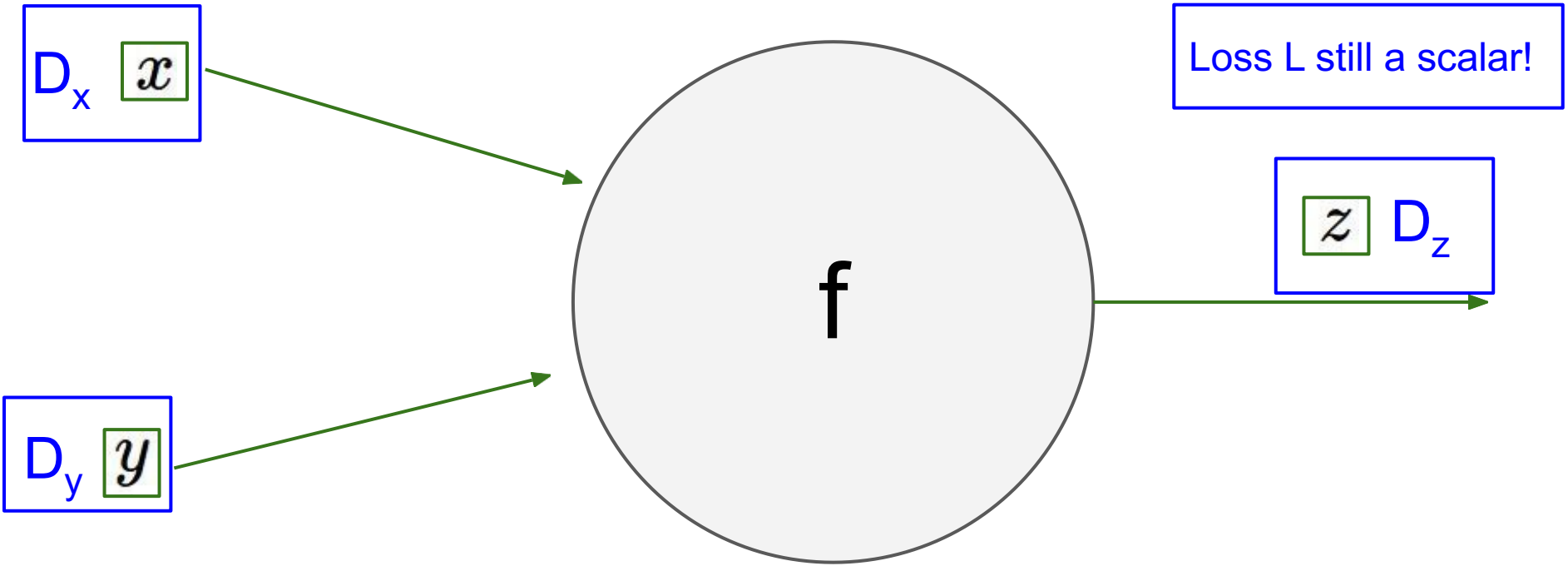
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

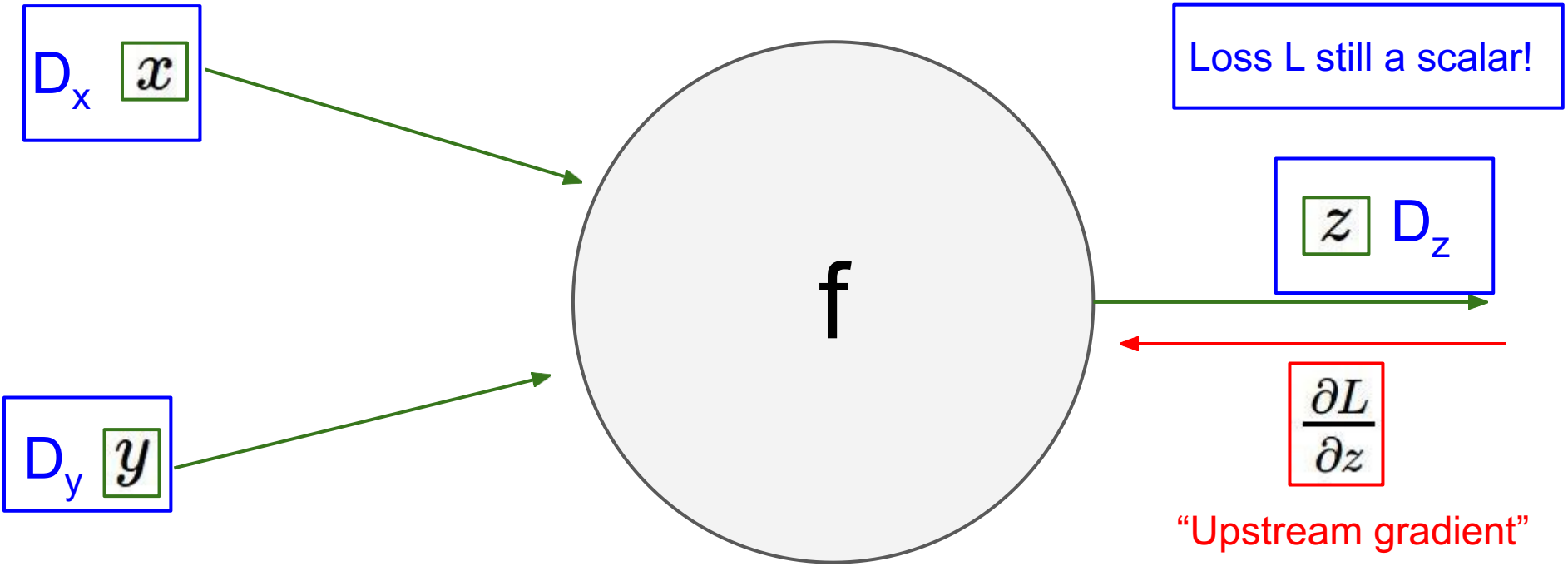
Backprop with Vectors



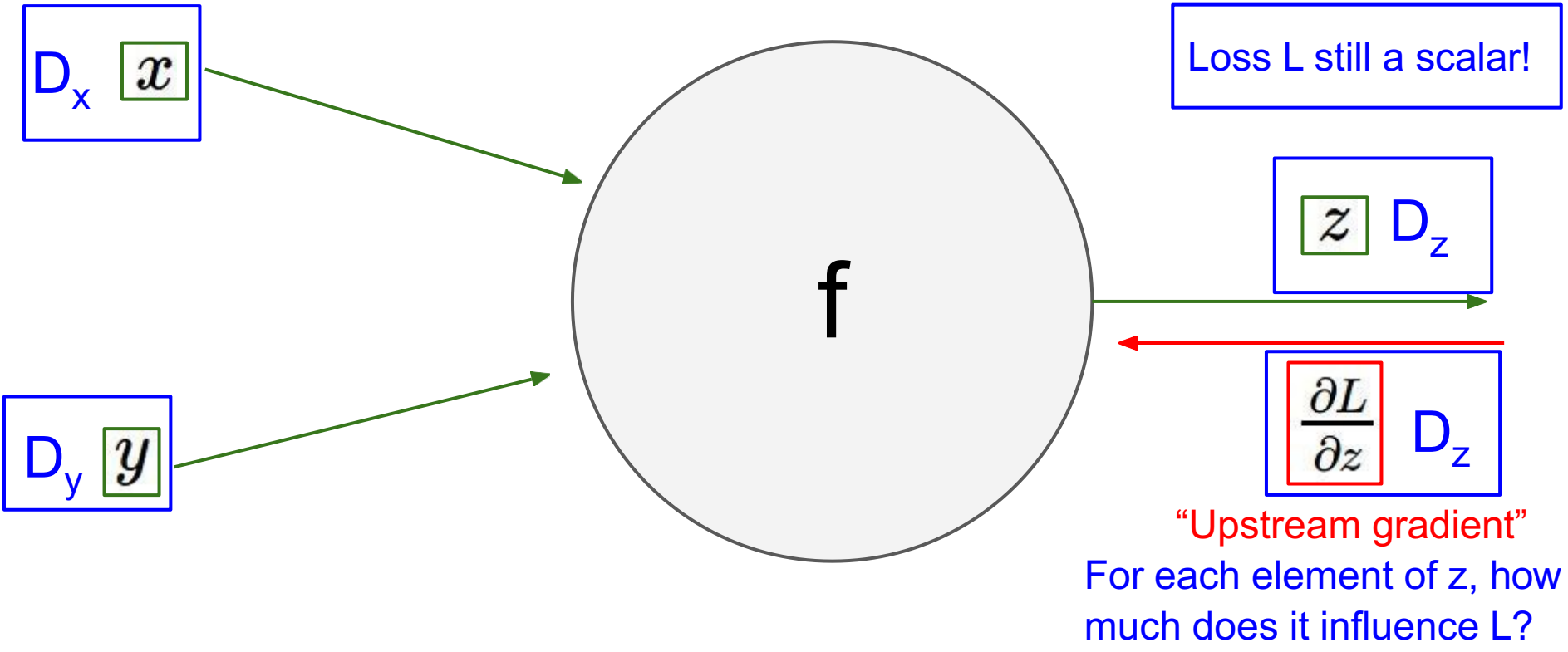
Backprop with Vectors



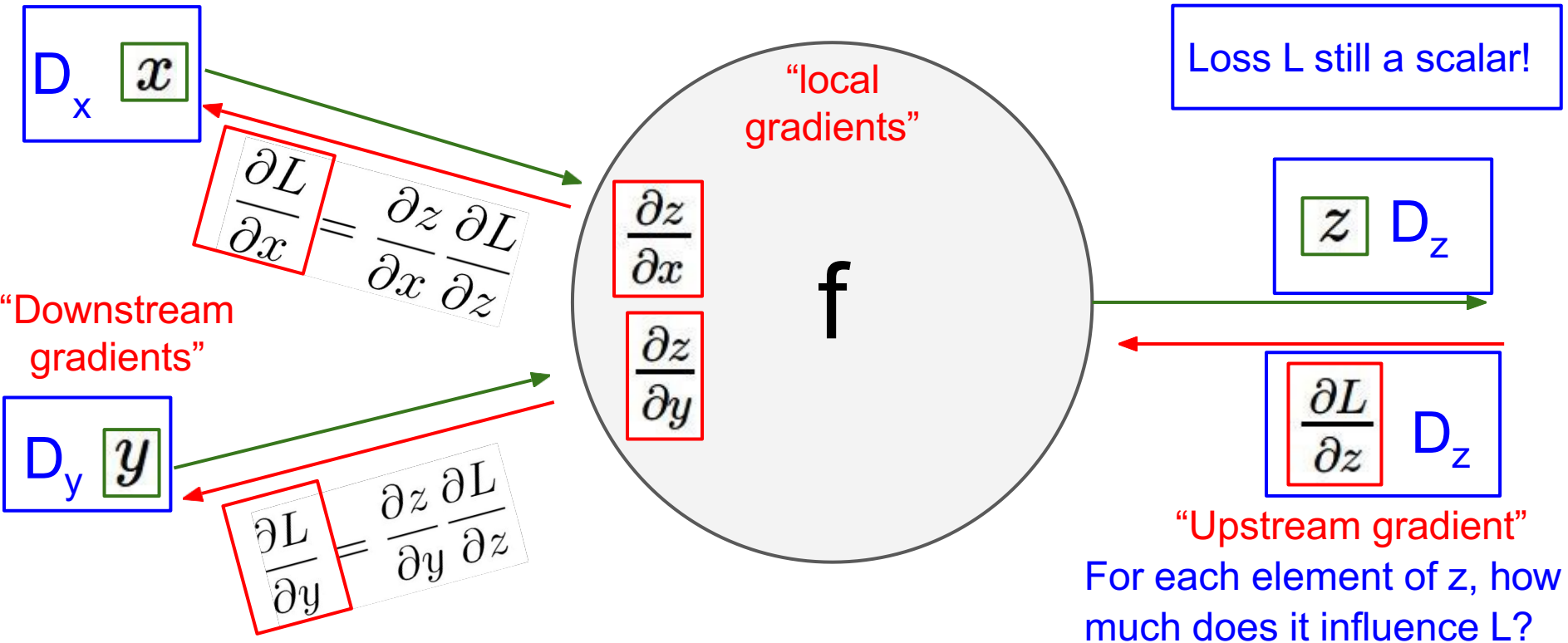
Backprop with Vectors



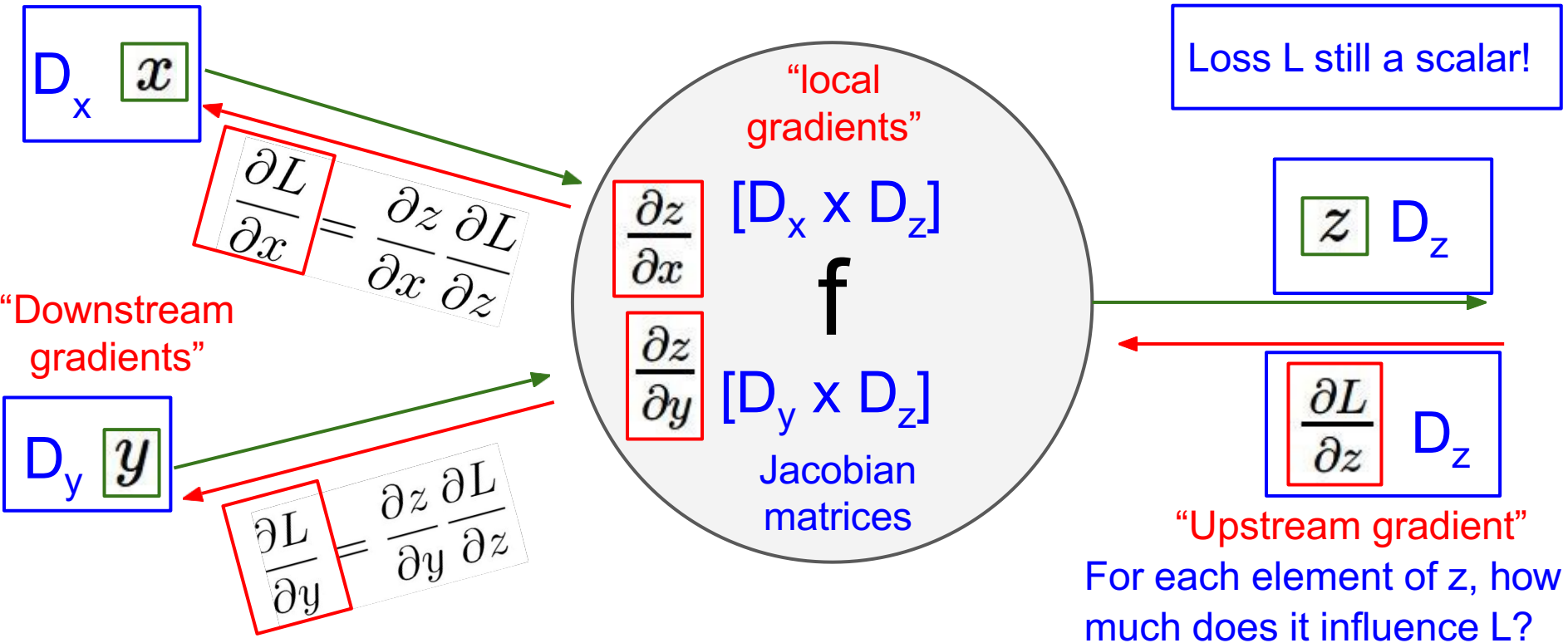
Backprop with Vectors



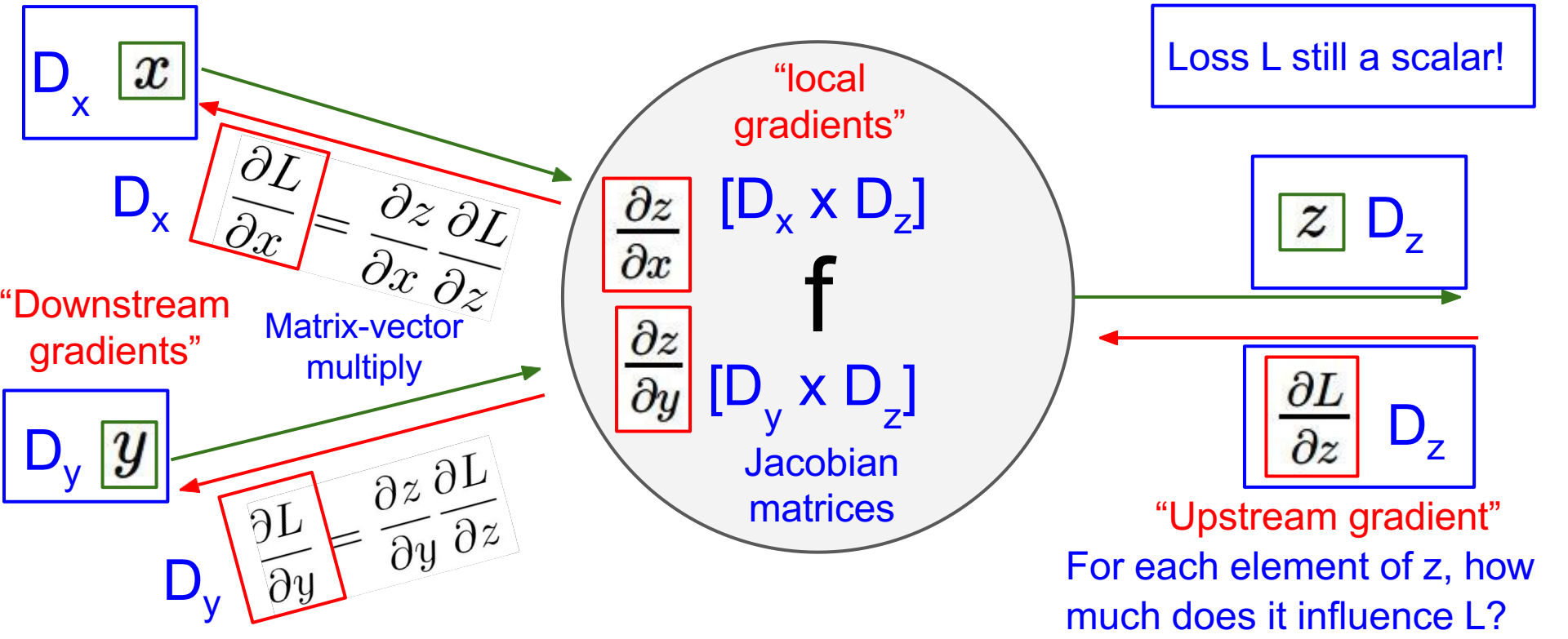
Backprop with Vectors



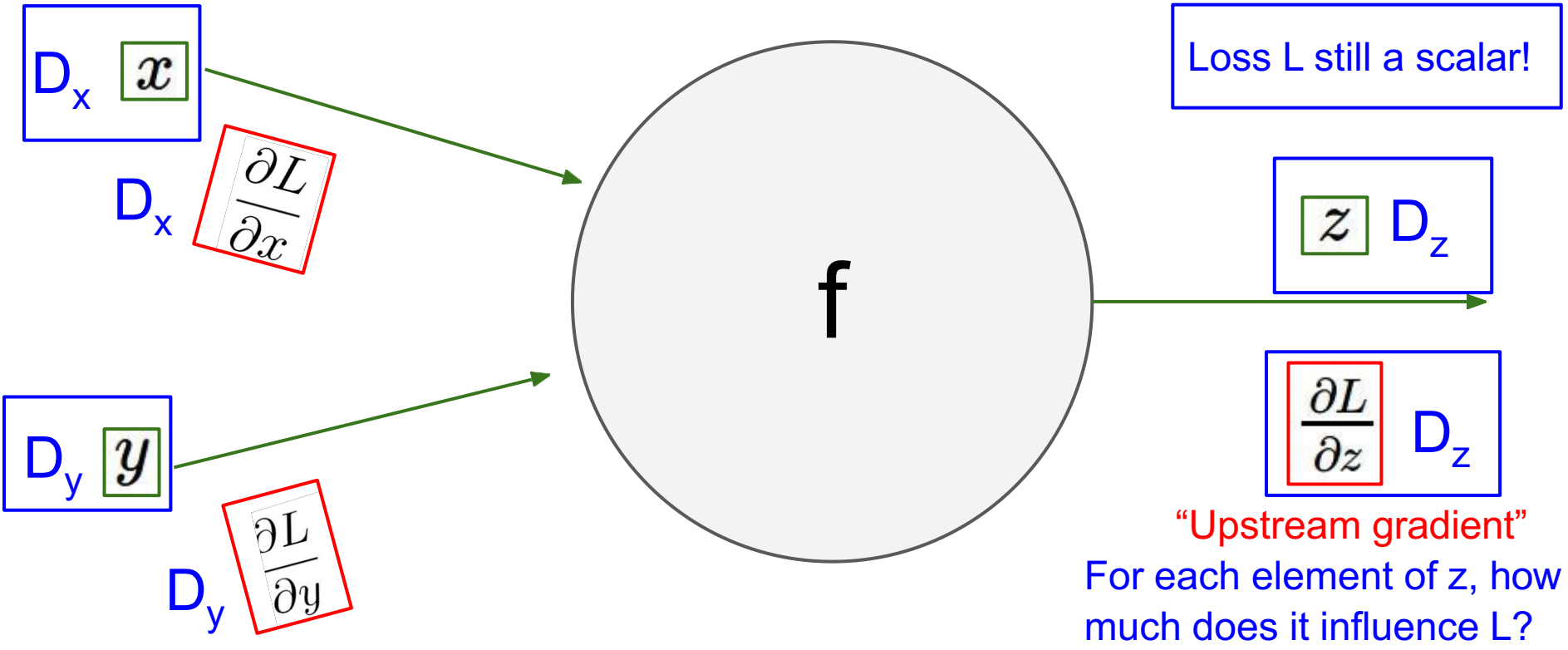
Backprop with Vectors



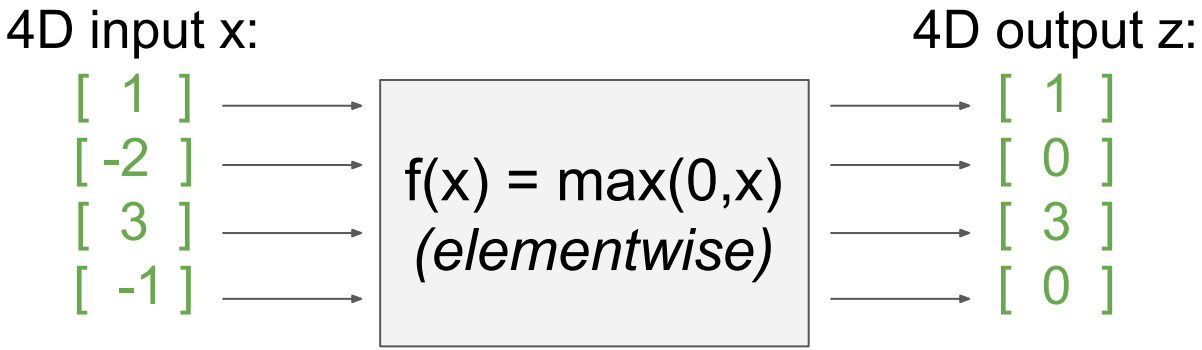
Backprop with Vectors



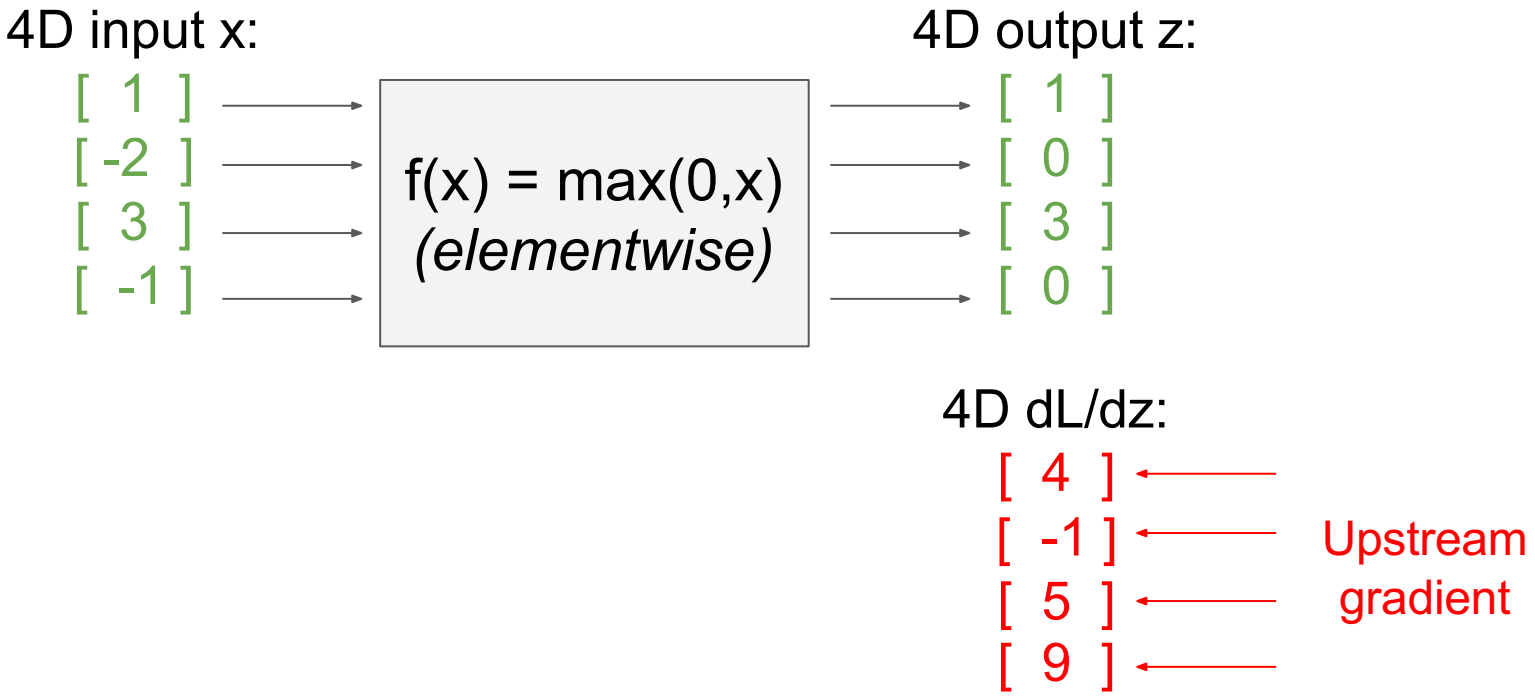
Gradients of variables wrt loss have same dims as the original variable



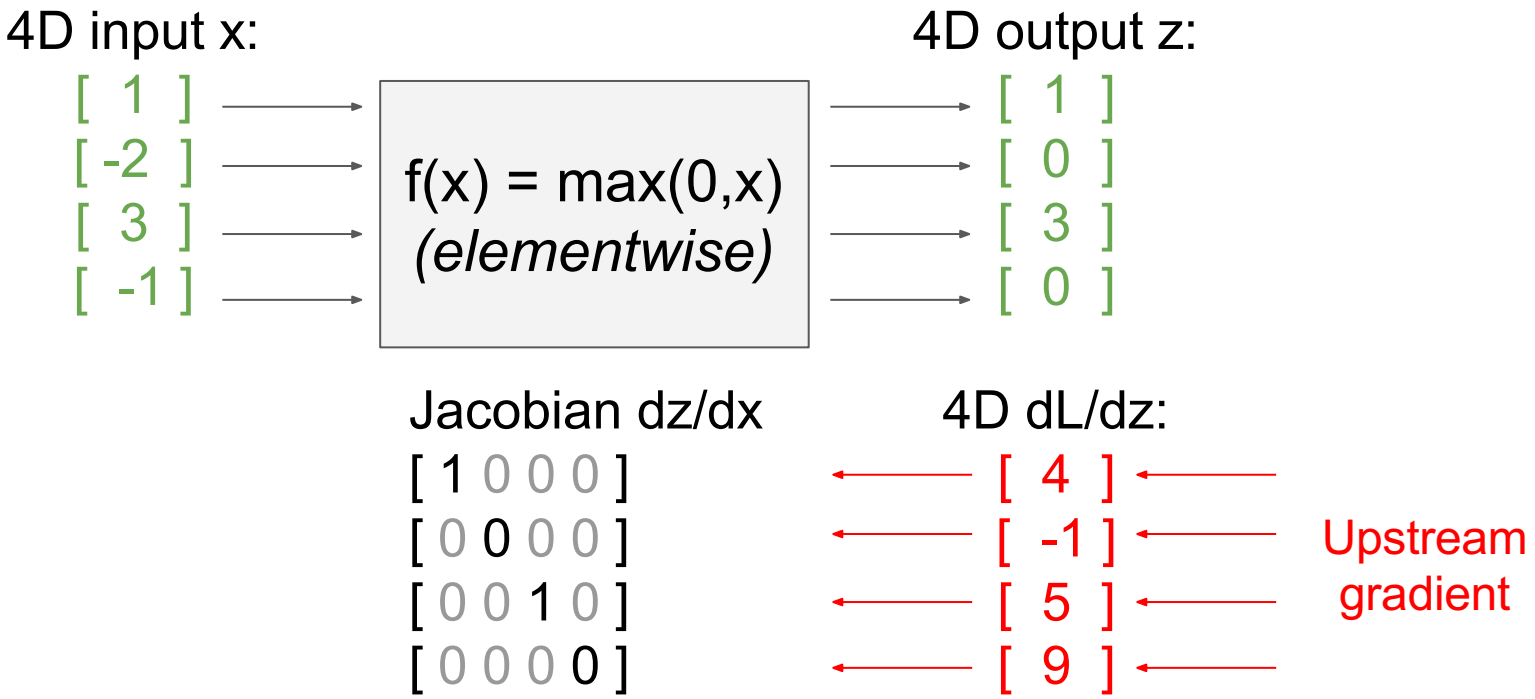
Backprop with Vectors



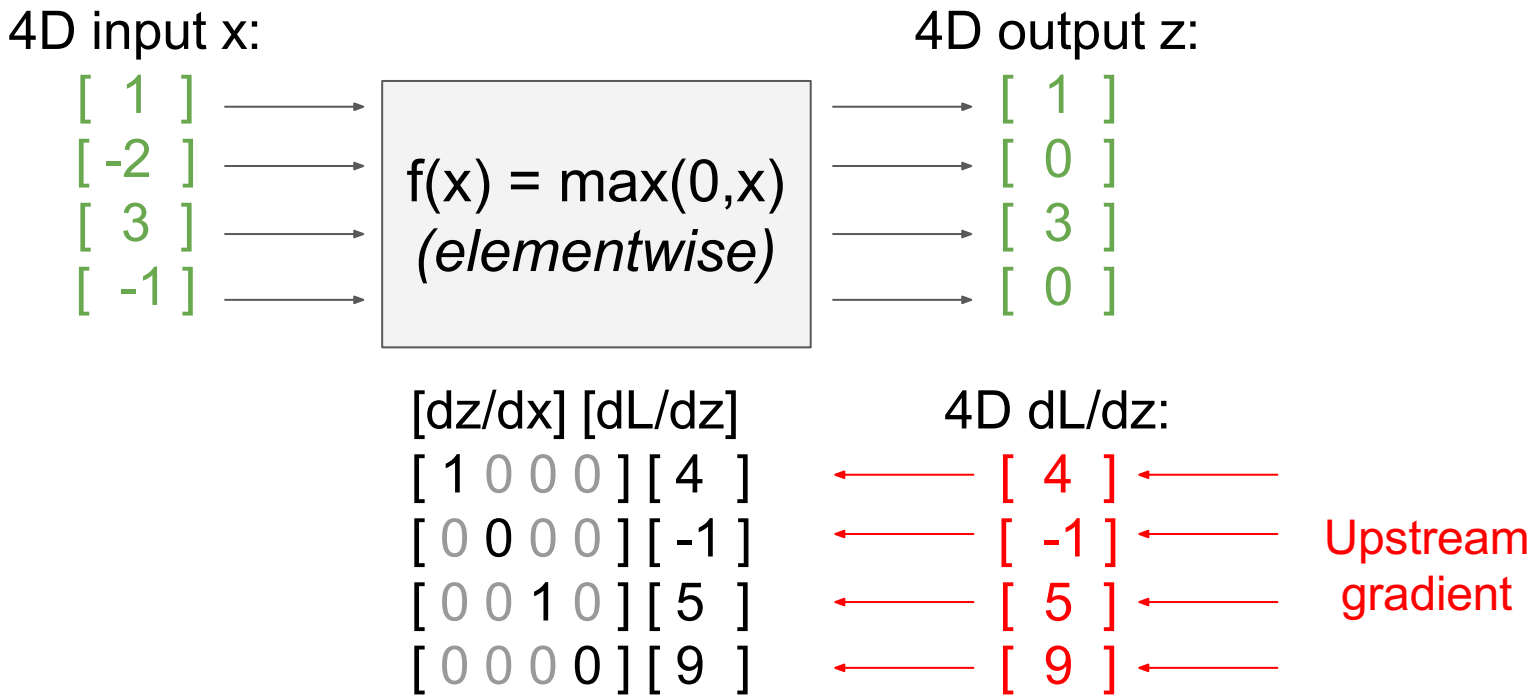
Backprop with Vectors



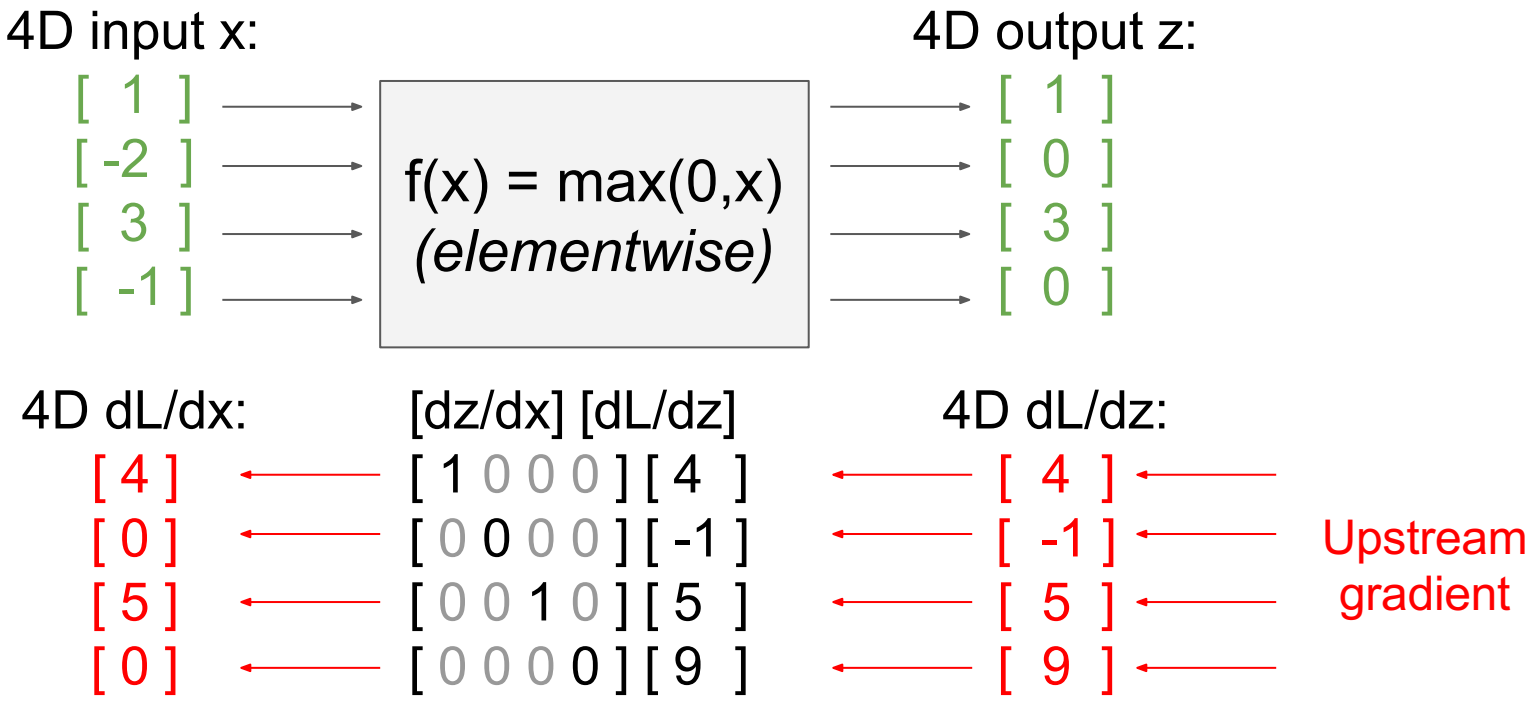
Backprop with Vectors



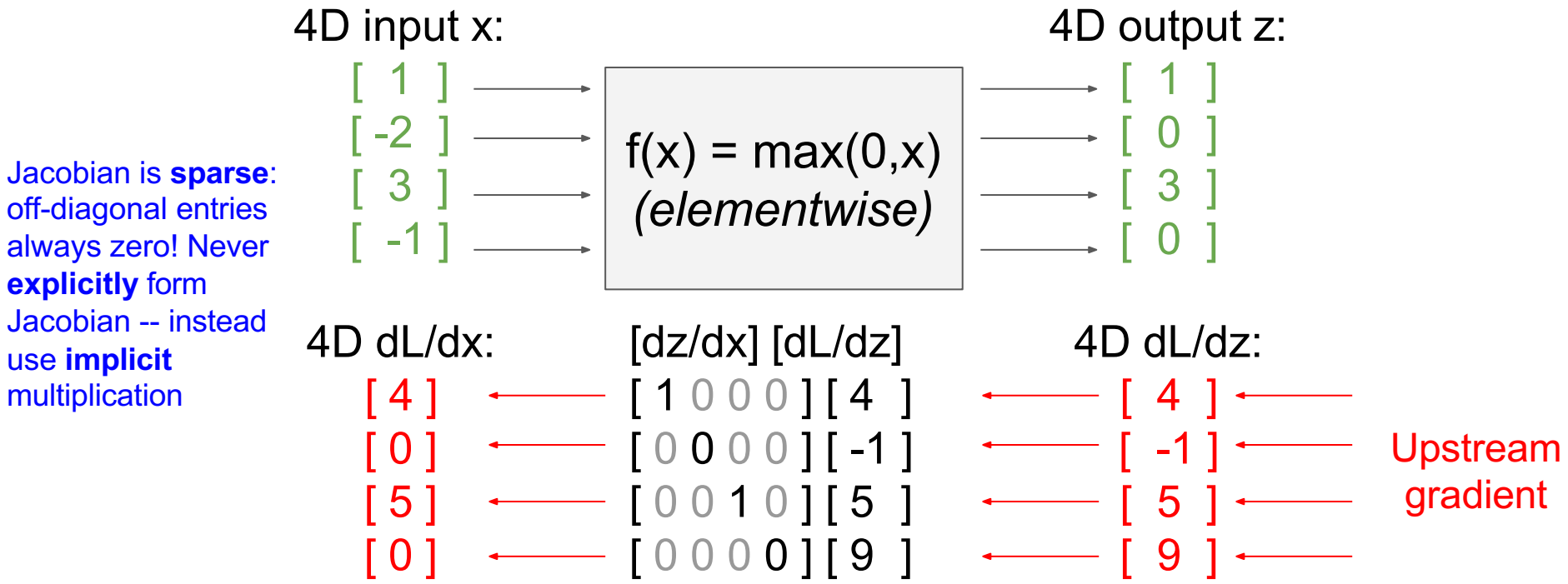
Backprop with Vectors



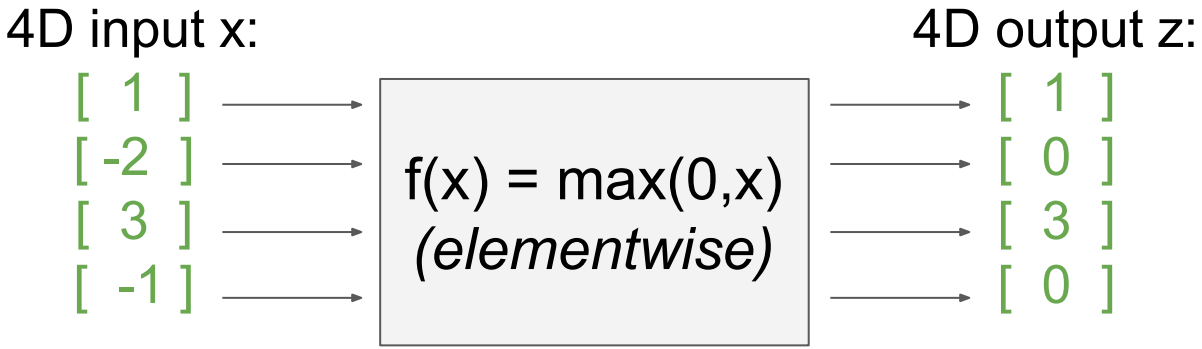
Backprop with Vectors



Backprop with Vectors



Backprop with Vectors



Jacobian is **sparse**: off-diagonal entries always zero! Never **explicitly** form Jacobian -- instead use **implicit** multiplication

4D dL/dx:

[4]
[0]
[5]
[0]

[dz/dx] [dL/dz]

$$\left(\frac{\partial L}{\partial x}\right)_i = \begin{cases} \left(\frac{\partial L}{\partial z}\right)_i & \text{if } x_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

4D dL/dz:

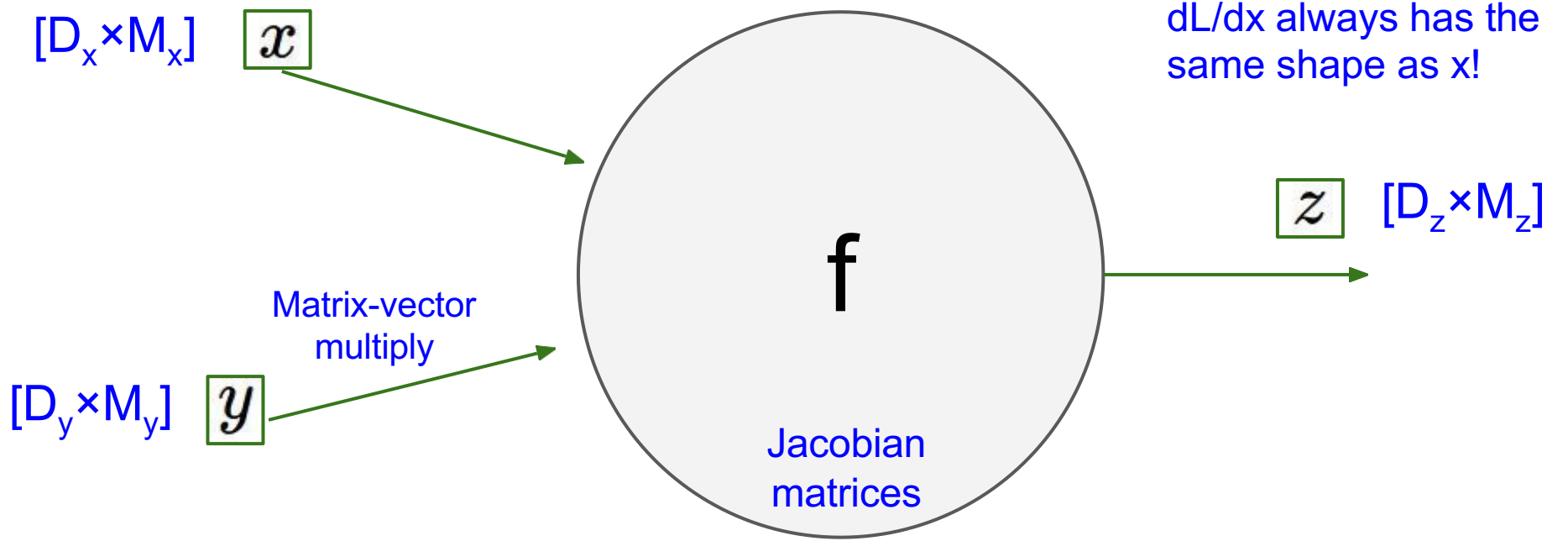
[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Matrices (or Tensors)

Loss L still a scalar!

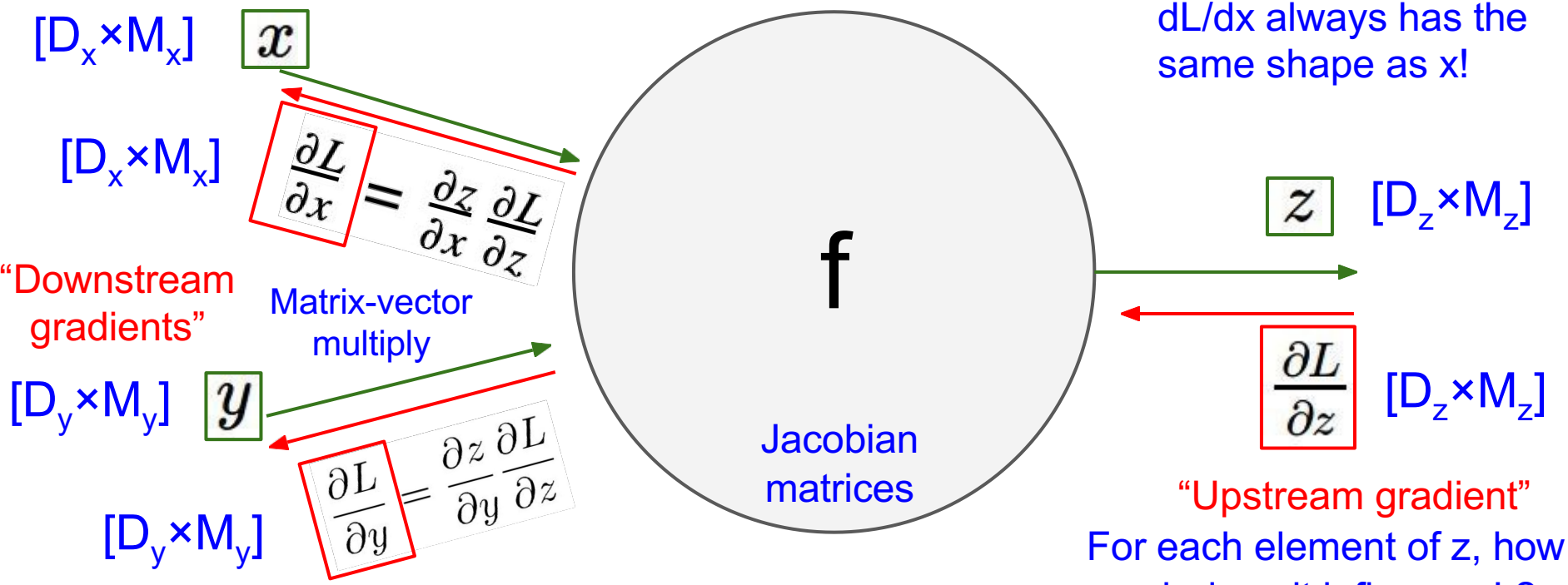
dL/dx always has the same shape as x!



Backprop with Matrices (or Tensors)

Loss L still a scalar!

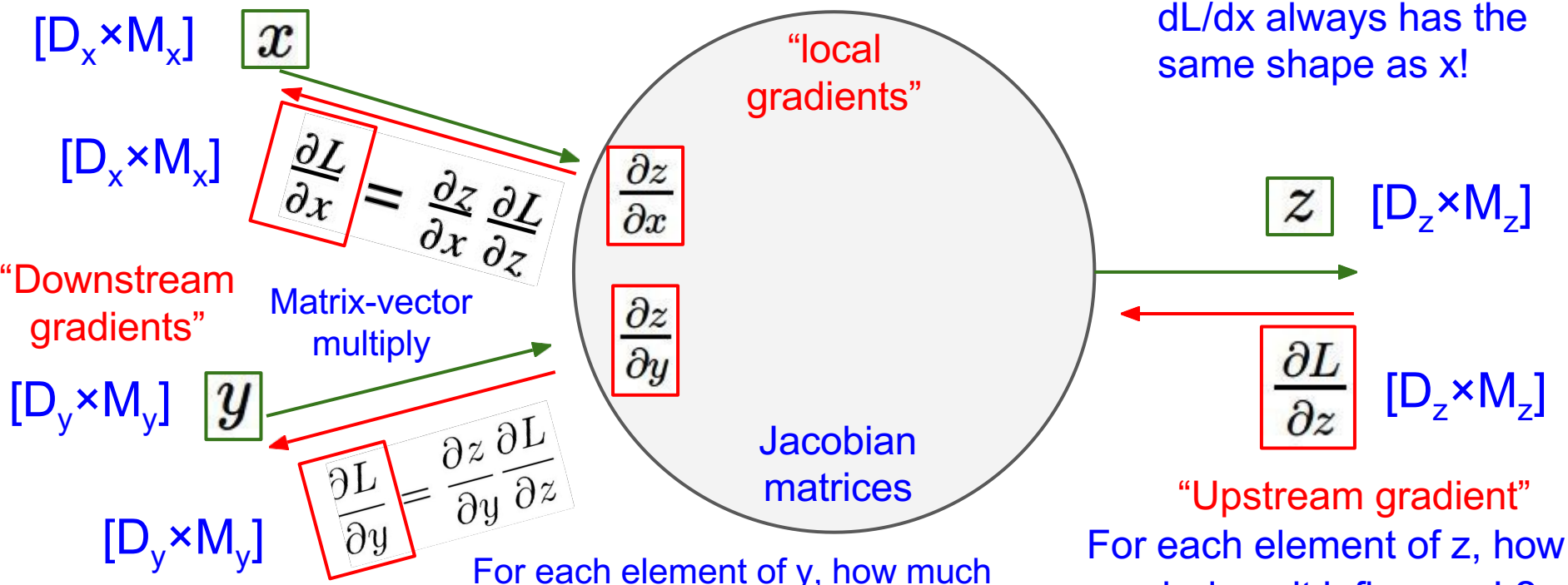
dL/dx always has the same shape as x!



Backprop with Matrices (or Tensors)

Loss L still a scalar!

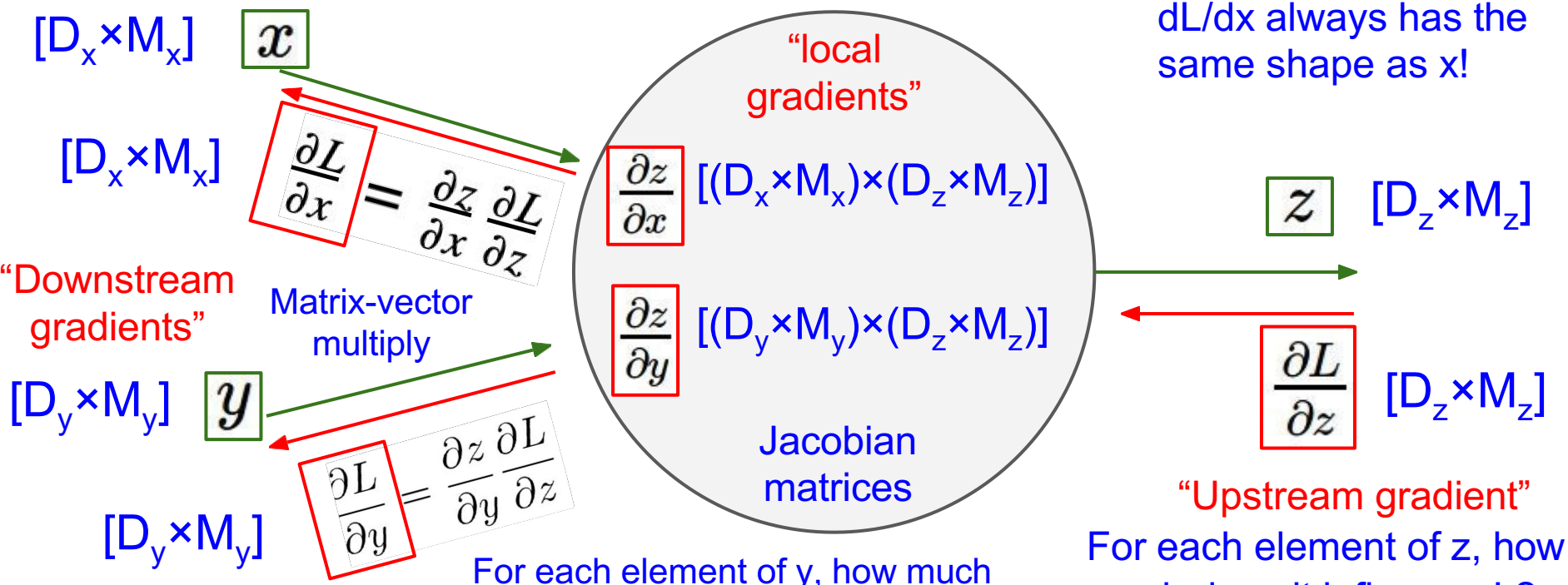
dL/dx always has the same shape as x!



Backprop with Matrices (or Tensors)

Loss L still a scalar!

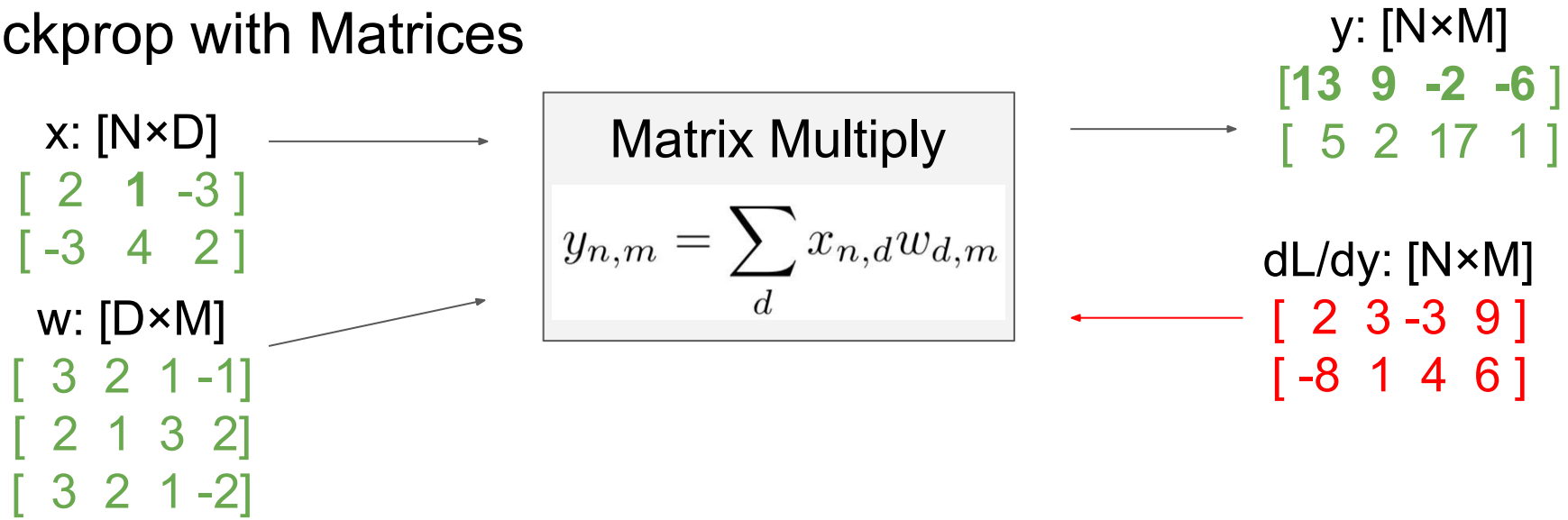
dL/dx always has the same shape as x!



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



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]

[**13 9 -2 -6**]
[5 2 17 1]

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

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]

[**13 9 -2 -6**]
[5 2 17 1]

dL/dy: [N×M]

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

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

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]

[13 9 -2 -6]
[5 2 17 1]

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]
[3 2 1 -2]

Matrix Multiply

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

y: [N×M]

[13 9 -2 -6]
[5 2 17 1]

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 $y_{n,}$.

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]
[3 2 1 -2]

Matrix Multiply

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

y: [N×M]

[13 9 -2 -6]
[5 2 17 1]

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 $y_{n,.}$

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

[13 9 -2 -6]
[5 2 17 1]

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 $y_{n,.}$

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

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]

[13 9 -2 -6]
[5 2 17 1]

dL/dy: [N×M]

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

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!

Autoencoders and self-supervision

Autoencoding: the basic idea

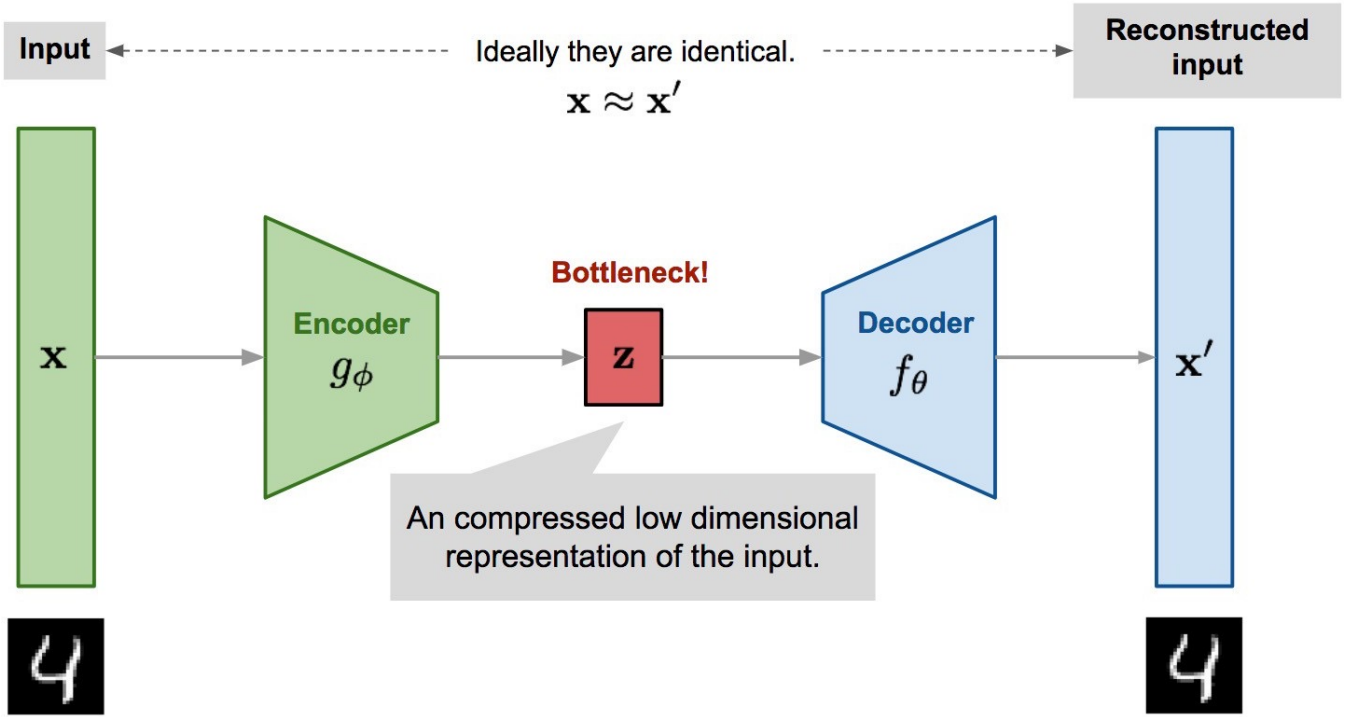


Image credit: https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Learning an autoencoder function

- Goal: Learn a compressed representation of the input data.
- We have two functions (usually neural networks):
  - Encoder:

$$\mathbf{z} = g_\phi(\mathbf{x})$$

  - Decoder:

$$\hat{\mathbf{x}} = f_\theta(\mathbf{z})$$

Learning an autoencoder function

- Goal: Learn a compressed representation of the input data.
- We have two functions (usually neural networks):
  - Encoder:

$$\mathbf{z} = g_\phi(\mathbf{x})$$

  - Decoder:

$$\hat{\mathbf{x}} = f_\theta(\mathbf{z})$$

- Train using a reconstruction loss:

$$\begin{aligned} J(\mathbf{x}, \hat{\mathbf{x}}) &= \|\mathbf{x} - \hat{\mathbf{x}}\|^2 \\ &= \|\mathbf{x} - f_\theta(g_\phi(\mathbf{x}))\|^2 \end{aligned}$$

Learning an autoencoder function

- Goal: Learn a compressed representation of the input data.
- We have two functions (usually neural networks):
  - Encoder:

$$\mathbf{z} = g_\phi(\mathbf{x})$$

  - Decoder:

$$\hat{\mathbf{x}} = f_\theta(\mathbf{z})$$

Only interesting when $\mathbf{z}$ has much smaller dimension than $\mathbf{x}$!

- Train using a reconstruction loss:

$$\begin{aligned} J(\mathbf{x}, \hat{\mathbf{x}}) &= \|\mathbf{x} - \hat{\mathbf{x}}\|^2 \\ &= \|\mathbf{x} - f_\theta(g_\phi(\mathbf{x}))\|^2 \end{aligned}$$

Autoencoding

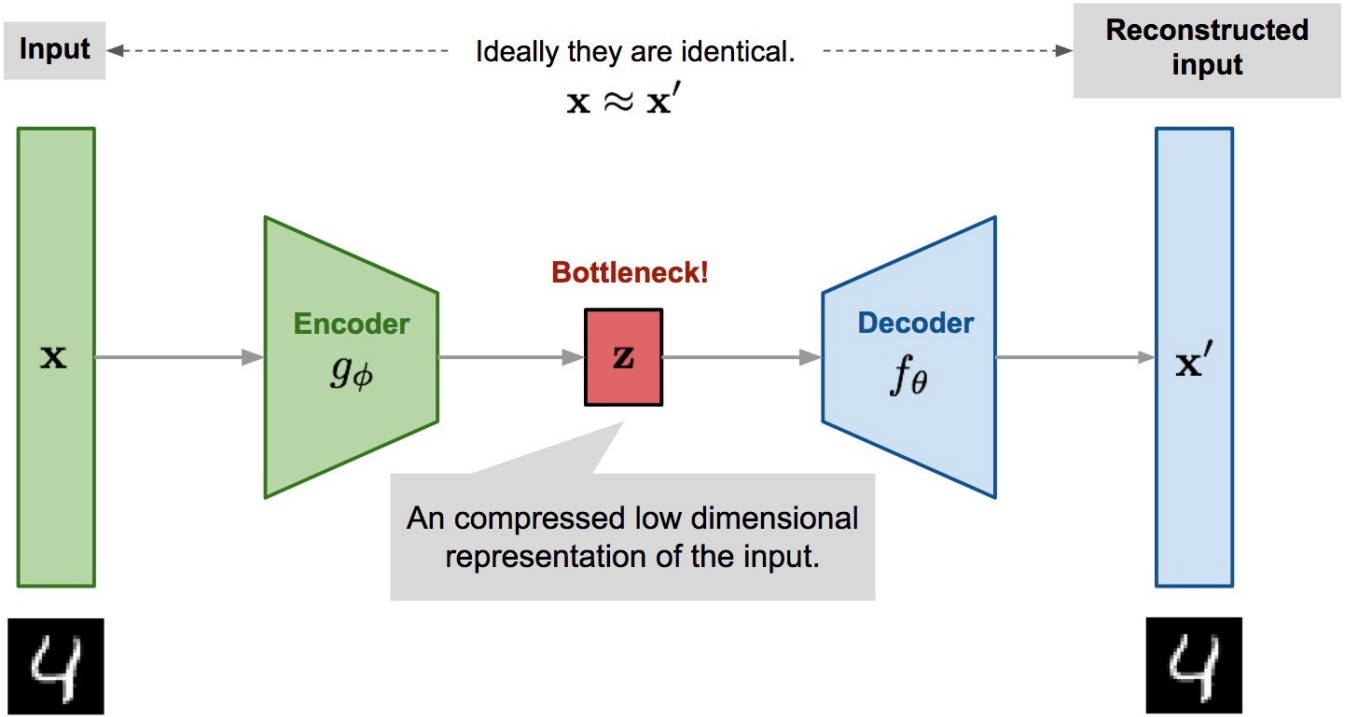


Image credit: https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Recall: Principal Component Analysis (PCA)

- Idea: Project data into a lower-dimensional sub-space, $R^m \dashrightarrow R^{m'}$, where $m' < m$.

Recall: Principal Component Analysis (PCA)

- Idea: Project data into a lower-dimensional sub-space, $R^m \dashrightarrow R^{m'}$, where $m' < m$.

- Consider a linear mapping, $x_i \dashrightarrow W^T x_i$
  - W is the compression matrix with dimension $R^{mxm'}$.
  - Assume there is a decompression matrix $U^{m'xm}$.

Recall: Principal Component Analysis (PCA)

- Idea: Project data into a lower-dimensional sub-space, $R^m \dashrightarrow R^{m'}$, where $m' < m$.

- Consider a linear mapping, $x_i \dashrightarrow W^T x_i$
  - W is the compression matrix with dimension $R^{m \times m'}$.
  - Assume there is a decompression matrix $U^{m' \times m}$.

- Solve the following problem: $\text{argmin}_{W,U} \Sigma_{i=1:n} || x_i - UW^T x_i ||^2$

Recall: Principal Component Analysis (PCA)

- Solve the following problem: $\text{argmin}_{W,U} \Sigma_{i=1:n} || x_i - UW^T x_i ||^2$
- Equivalently: $\text{argmin}_{W,U} || X - XWU^T ||^2$

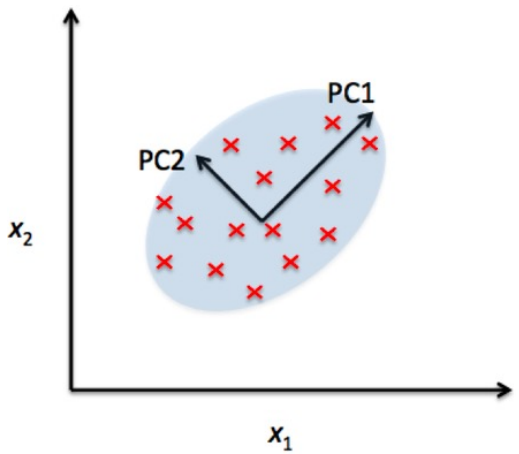
- Solution is given by eigen-decomposition of X^TX.
  - W is mxm' matrix corresponding to the first m' eigenvectors of X^TX (sorted in descending order by the magnitude of the eigenvalue).
  - Equivalently: W is mxm' matrix containing the first m' left singular vectors of X
  - Note: The columns of W are orthogonal!

PCA vs autoencoders

In the case of a linear encoders and decoders:

$$f_W(x) = Wx \qquad g_{\hat{W}}(h) = W'h \,,$$

with squared-error reconstruction loss we can show that the minimum error solution W yields the same subspace as PCA.



More advanced encoders and decoders

- What to use as encoders and decoders?

- Most data (e.g., arbitrary real-valued or categorical features).
  - Encoder and decoder are feed-forward neural networks.

- Sequence data
  - Encoder and decoder are RNNs.

- Image data
  - Encoder is a CNN; decoder is a deconvolutional network.

Regularization of autoencoders

- How can we generate sparse autoencoders? (And also, why?)

Regularization of autoencoders

- How can we generate sparse autoencoders? (And also, why?)

- Weight tying of the encoder and decoder weights ($\theta = \phi$) to explicitly constrain (regularize) the learned function.

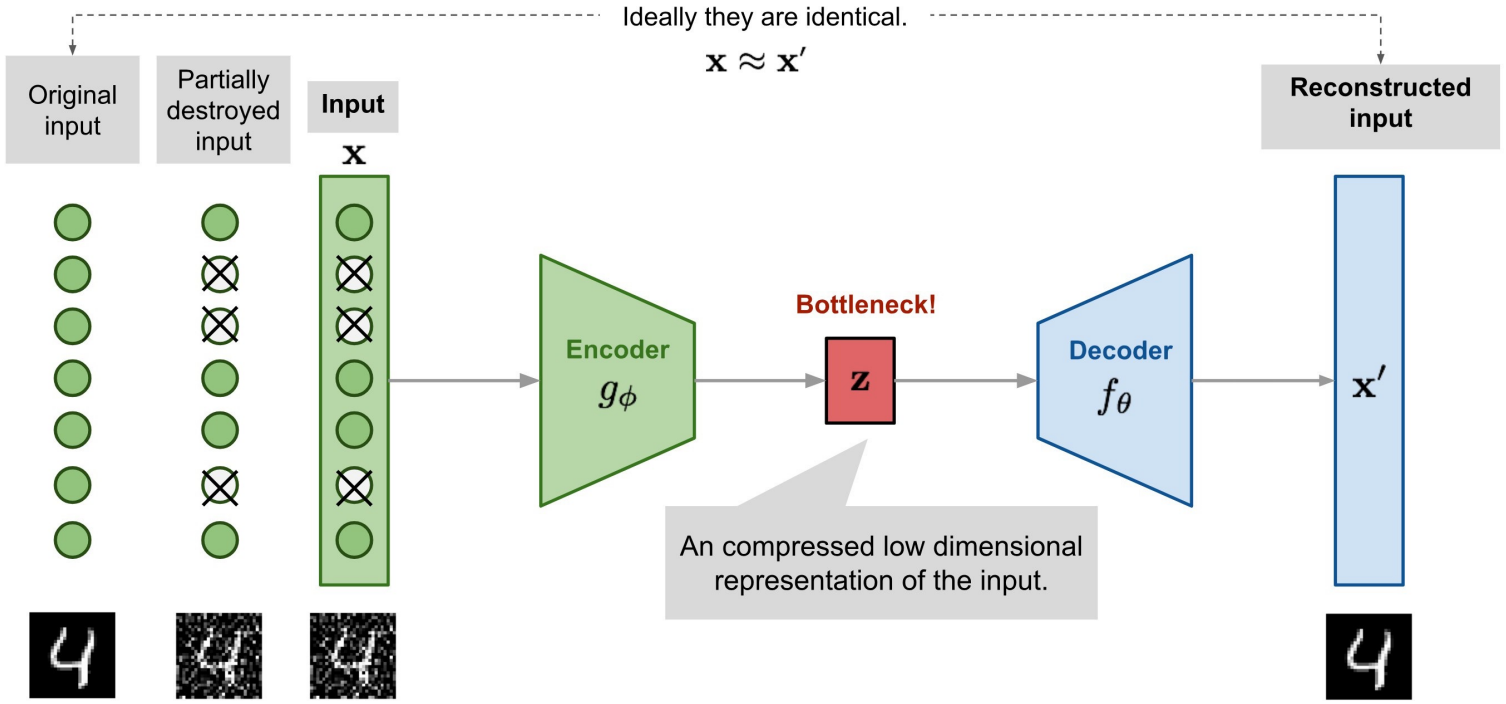
Regularization of autoencoders

- How can we generate sparse autoencoders? (And also, why?)
- Weight tying of the encoder and decoder weights ($\theta = \phi$) to explicitly constrain (regularize) the learned function.
- Directly penalize the output of the hidden units (e.g. with L1 penalty) to introduce sparsity in the weights.

Regularization of autoencoders

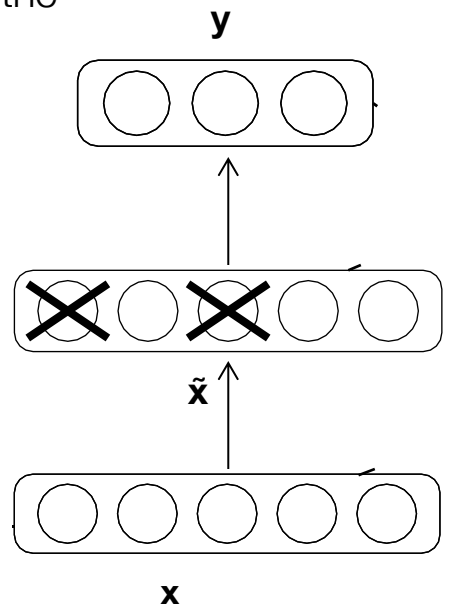
- How can we generate sparse autoencoders? (And also, why?)
- Weight tying of the encoder and decoder weights ($\theta = \phi$) to explicitly constrain (regularize) the learned function.
- Directly penalize the output of the hidden units (e.g. with L1 penalty) to introduce sparsity in the weights.
- Penalize the average output (over a batch of data) to encourage it to approach a fixed target.

Denoising autoencoders



Denoising autoencoders

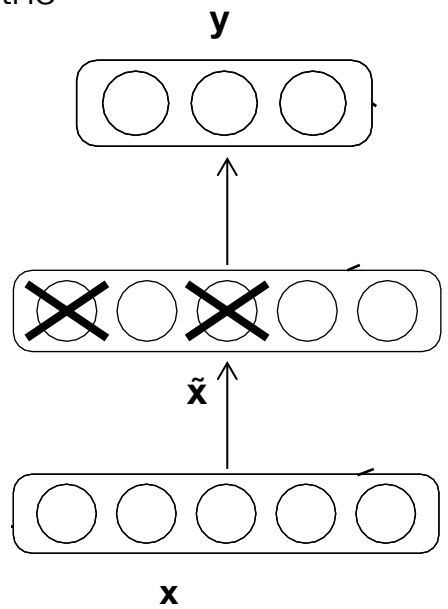
- Idea: To force the hidden layer to discover more robust features, train the autoencoder with a corrupted version of the input.



Denoising autoencoders

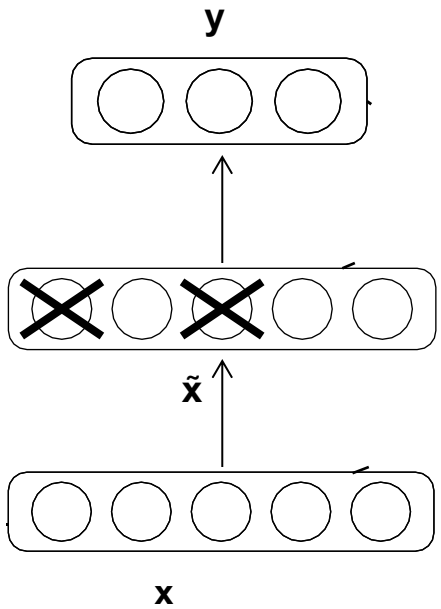
- Idea: To force the hidden layer to discover more robust features, train the autoencoder with a corrupted version of the input.

- Corruption processes:
  - Additive Gaussian noise
  - Randomly set some input features to zero.
  - *More noise models in the literature*.



Denoising autoencoders

- Idea: To force the hidden layer to discover more robust features, train the autoencoder with a corrupted version of the input.



- Corruption processes:
  - Additive Gaussian noise
  - Randomly set some input features to zero.
  - *More noise models in the literature*.

- Training criterion:

$$Err = \sum_{i=1:n} E_{q(x_i'|x_i)} L[\, x_i, f_{w'}(g_w(x_i')) \,]$$

where L is some reconstruction loss x is the original input, x' is the corrupted input, and $q()$ is the corruption process.

Contractive autoencoders

- Goal: Learn a representation that is robust to noise and perturbations of the input data, by regularizing the latent space (represented by L2 norm of the Jacobian of the encoded input.)

- Contractive autoencoder training criterion:

$$\mathrm{Err}(W,W') = \sum_{i=1:n} L\left[\, x_i, f_{W'}(g_W(x_i)) \,\right] + \lambda ||J(x_i)||_F^2$$

where L is some reconstruction loss, $J(x_i)=\partial f_W(x_i)/\partial x_i$ is a Jacobian matrix of the encoder evaluated at x_i, F is the Frobenius norm, and λ controls the strength of the regularization.

Many more similar ideas in the literature…

Autoencoding: The key idea

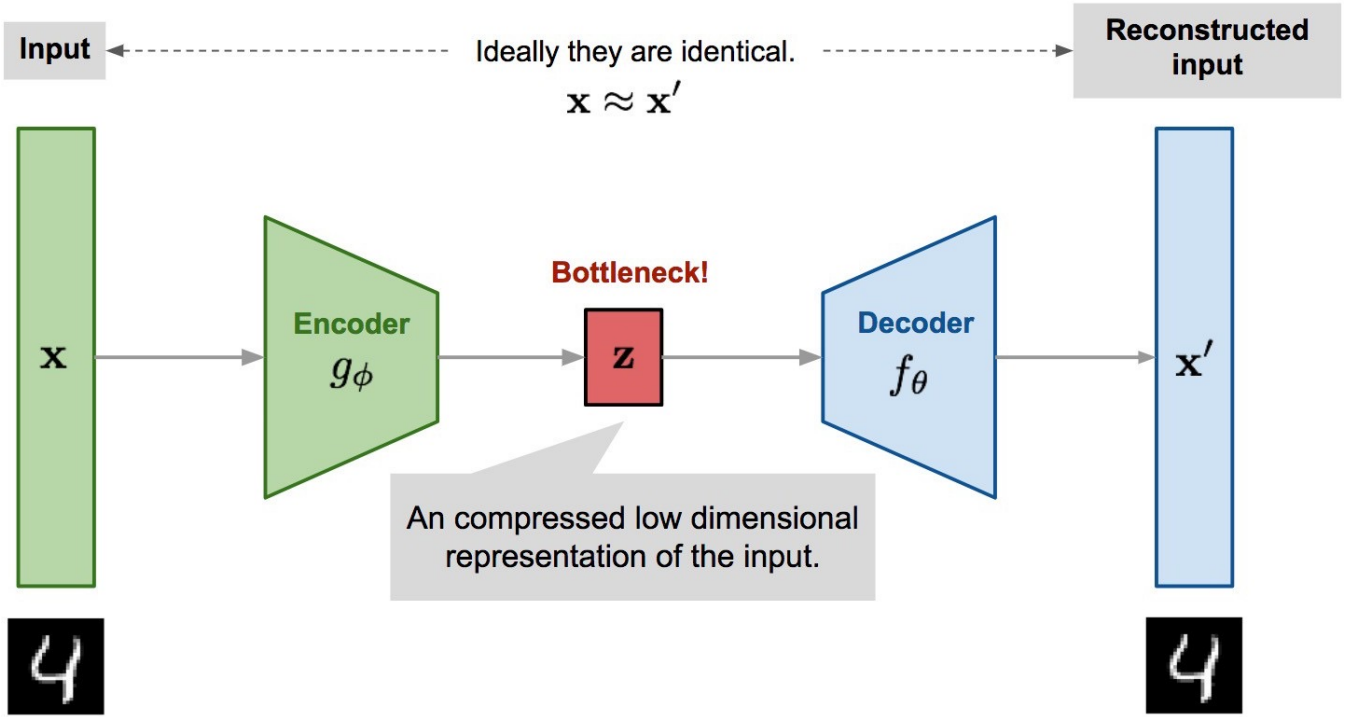
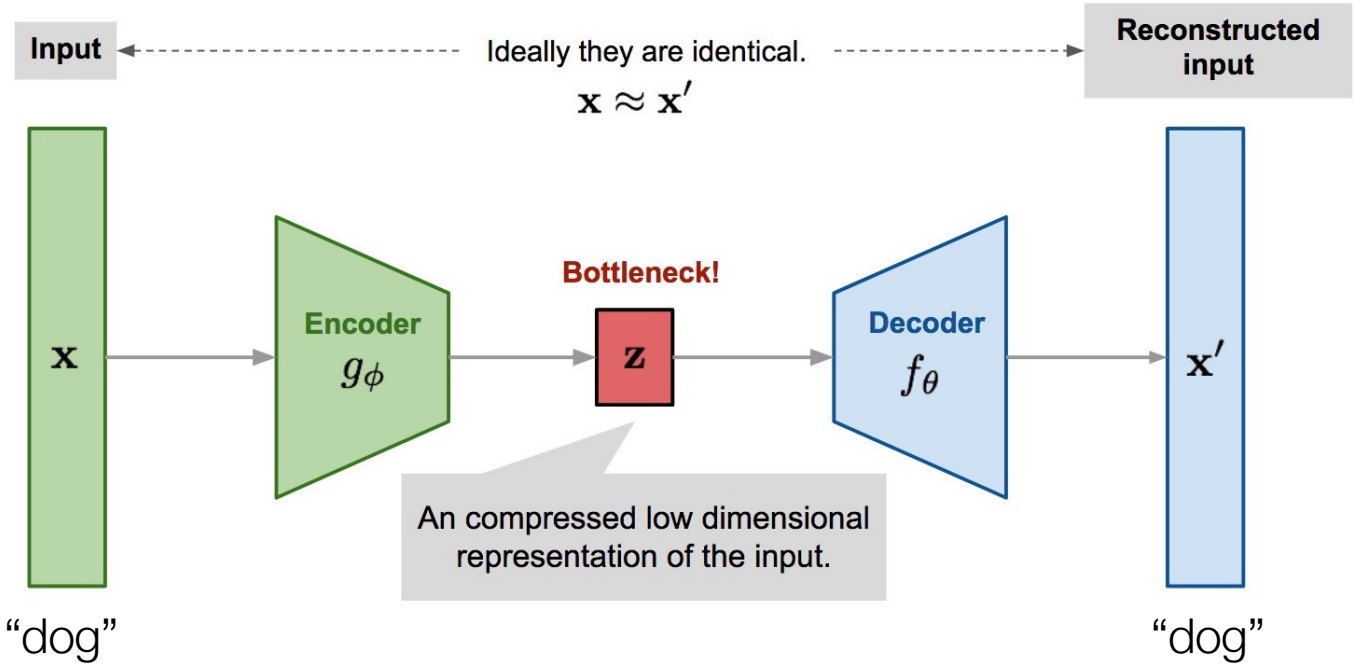


Image credit: https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Autoencoding language?



Autoencoding language

- Autoencoding can generate high-quality low-dimensional features.
- Works well when the original space x is rich and high-dimensional.
  - Images
  - MRI data
  - Speech data
  - Video
- But what if we don't have a good feature space to start with? E.g., for representing words?

Autoencoders and self-supervision

- Two approaches to dimensionality reduction using deep learning.
  - This is a rough categorization and not a strict division!!

- Autoencoders:
  - Optimize a “reconstruction loss.”
  - Encoder maps input to a low-dimensional space and decoder tries to recover the original data from the low-dimensional space.

- “Self-supervision”:
  - Try to predict some parts of the input from other parts of the input.
  - I.e., make up labels from $\mathbf{x}$.

Words embeddings / self-supervision

- What is the input space for words/language?
- In the unsupervised case, generally all we have is a text corpus (i.e., a set of documents).
- How can we learn representations from this data?

Words embeddings / self-supervision

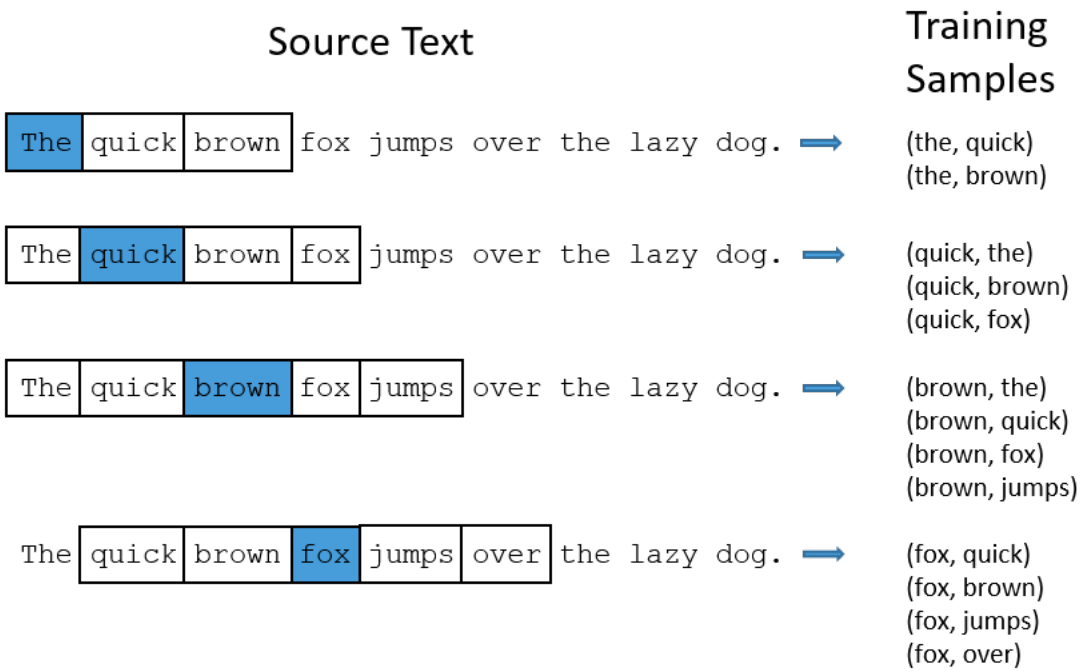
- Idea: Make up a supervised learning task in order to learn representations for words!

- Co-occurrence information tells us a lot about word meaning.
  - For example, “dog” and “pitbull” occur in many of the same contexts.
  - For example, “loved” and “appreciated” occur in many of the same contexts.

- Let’s learn features/representations for words that are good for predicting their context!

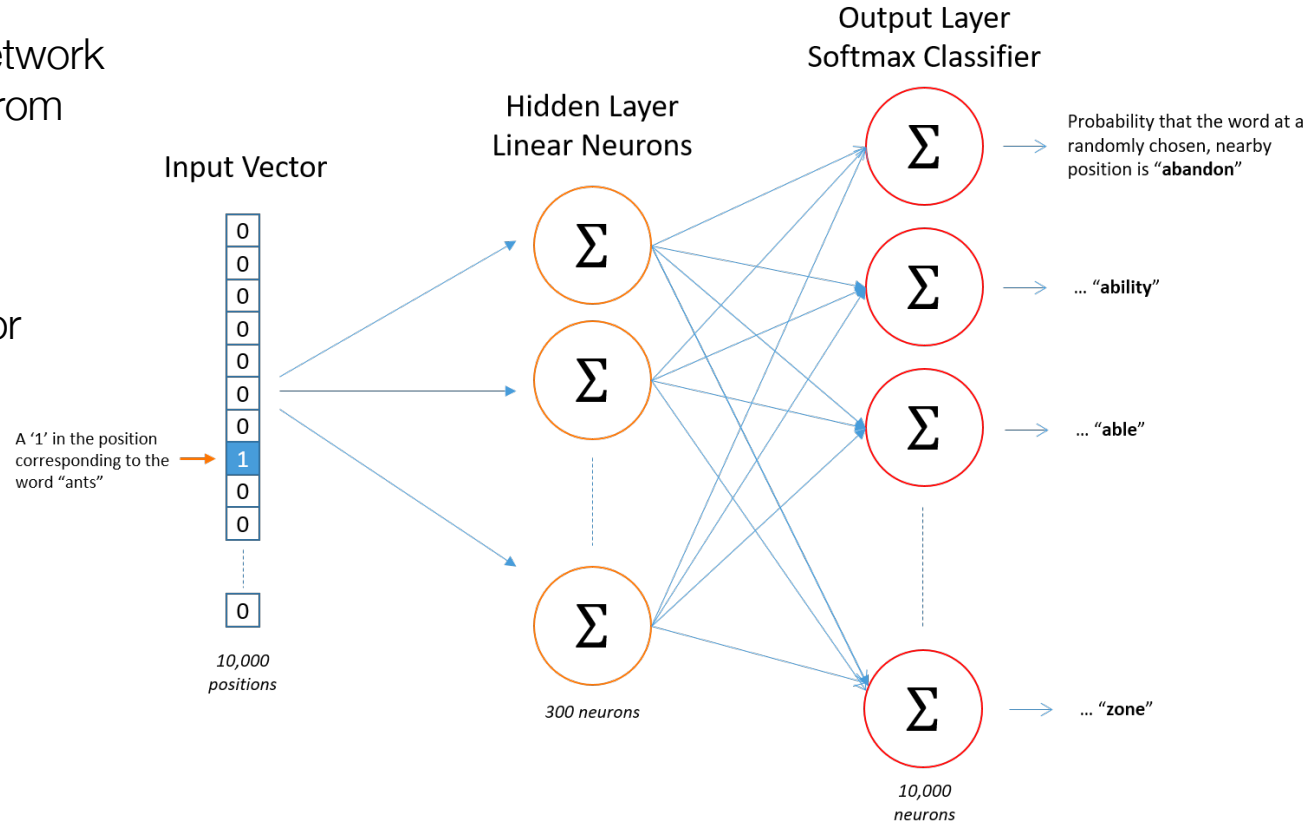
Words embeddings / self-supervision

- Create a training set by applying a “sliding window” over the corpus.
- I.e., given a word, we try to predict what words are likely to occur around it.



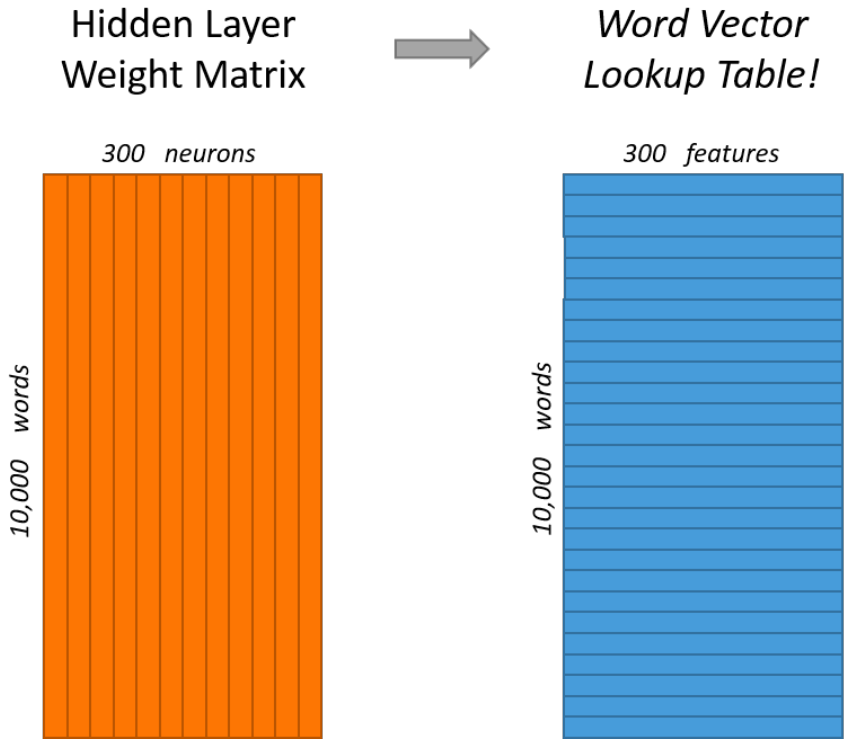
Word2Vec / SkipGram Model

- Key idea: Train a neural network to predict context words from input word.
- Hidden layer learns representations/features for words!



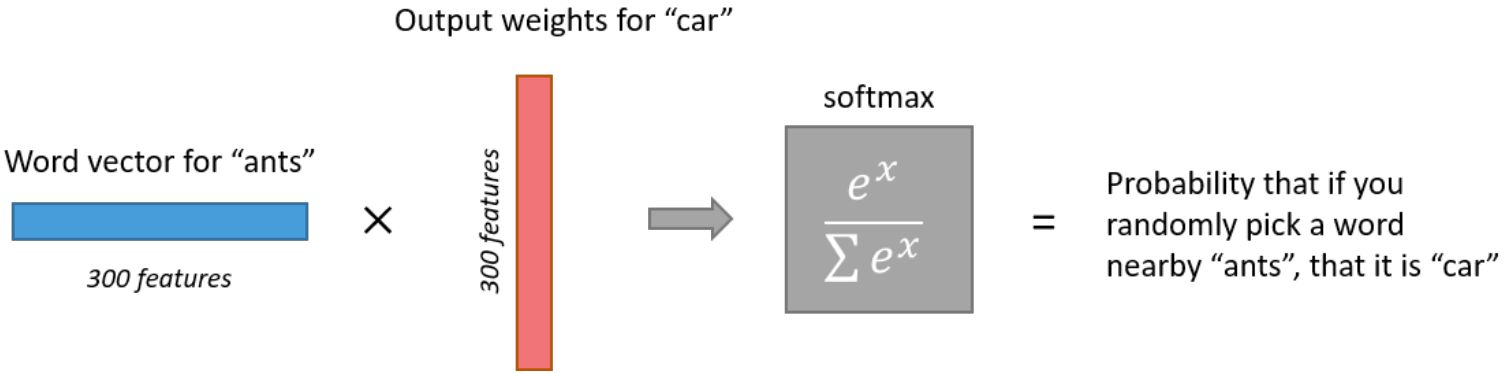
Word2Vec / SkipGram Model

- Key idea: Train a neural network to predict context words from input word.
- Hidden layer learns representations/features for words!



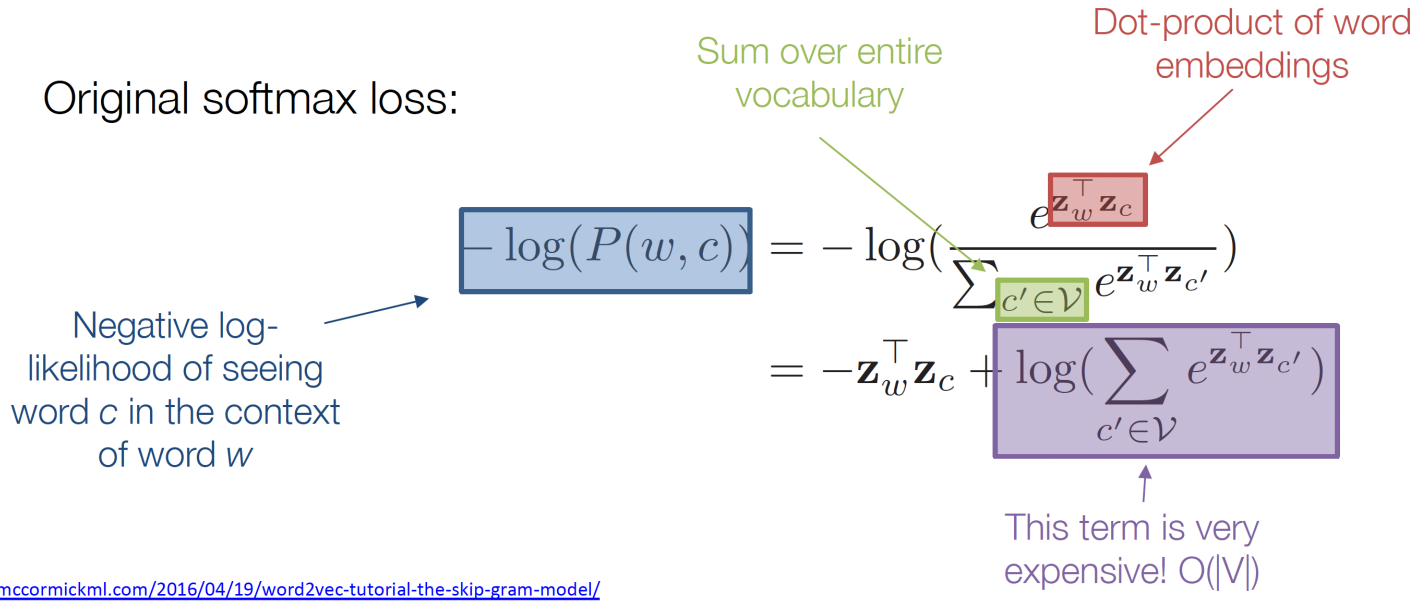
Word2Vec / SkipGram Model

- Intuition: dot-product between word representations is proportional to the probability that they co-occur in the corpus!
- One issue is that the output layer is very big!
  - We need to do a softmax over the entire vocabulary!



Negative sampling

- Instead of using a softmax, we approximate it!
- Original softmax loss:



http://mccormickml.com/2016/04/19/word2vec-tutorial-the-skip-gram-model/

Negative sampling

- Instead of using a softmax, we approximate it!
- Negative sampling loss:

Instead of summing over entire vocabulary. We just sample N "negative example" words.

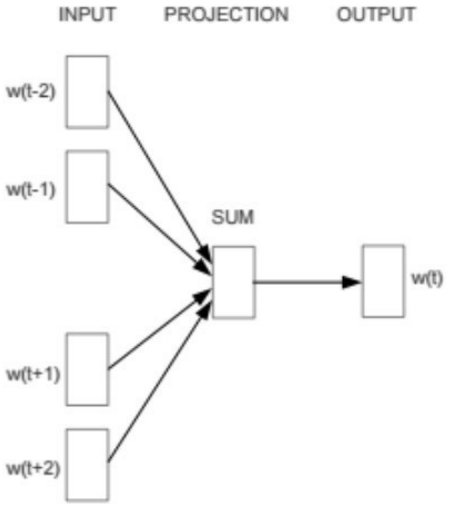
$$-\log(P(w,c)) \approx -\log(\sigma(\mathbf{z}_w^\top \mathbf{z}_c)) - \sum_{j=1}^{N} \log(\sigma(-\mathbf{z}_w^\top \mathbf{z}_{c'_j}))$$

Probability that w and c co-occur approximated with sigmoid.

Key idea: Dot-product for co-occurring pairs should be higher than random pairs!.

Variants of word2vec

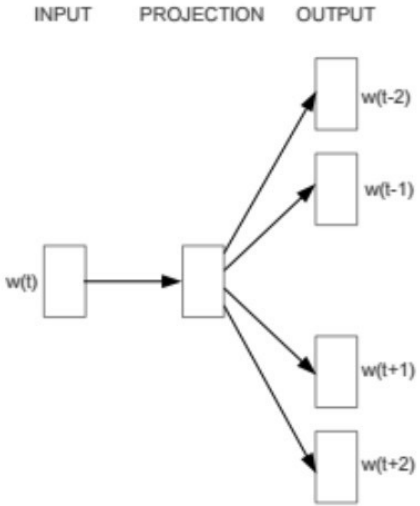
Given a set of (neighboring) words, **guess single words** that potentially occur along with this set of words.



CBOW

(Continuous Bag Of Words)

or

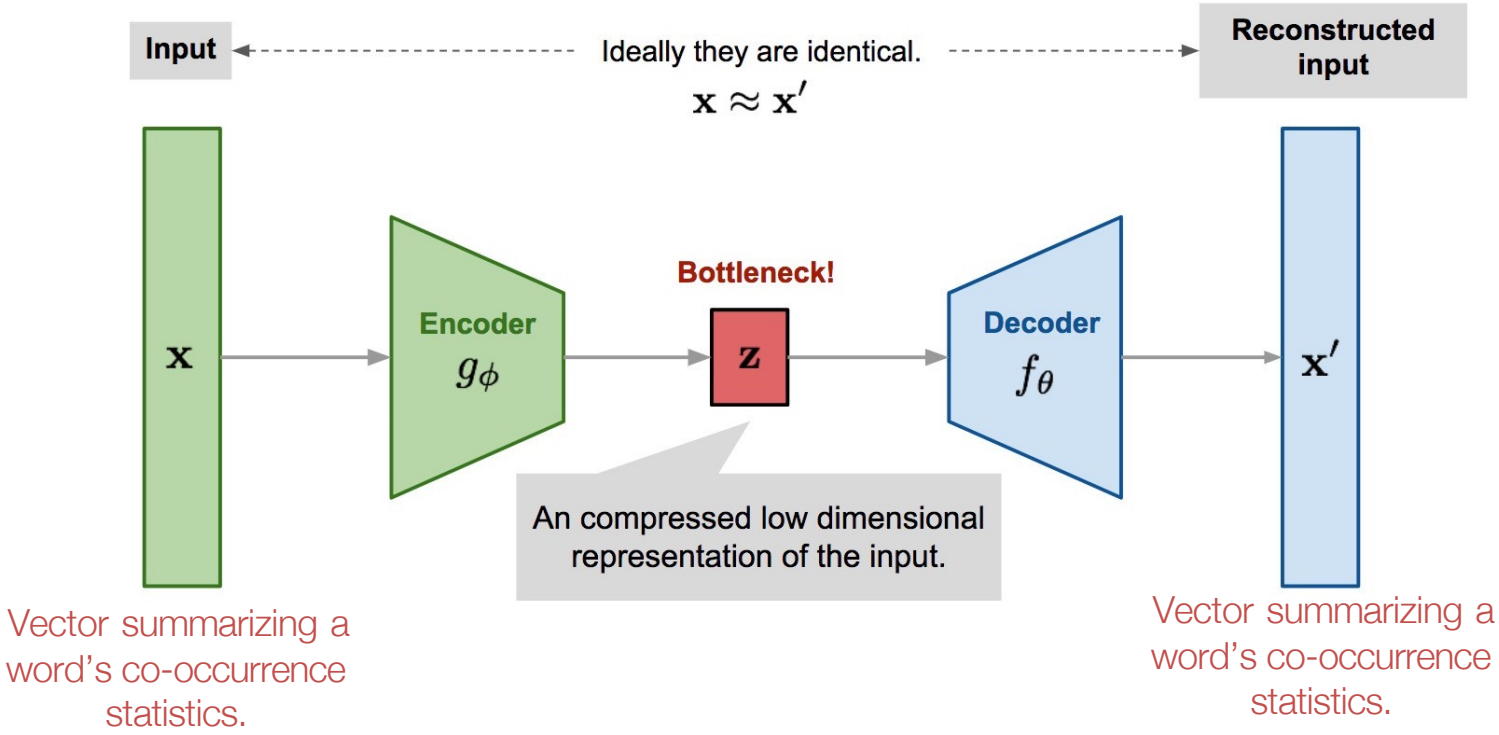


Skip-gram

Guess potential neighboring words based on the single word being analyzed.

https://towardsdatascience.com/an-implementation-guide-to-word2vec-using-numpy-and-google-sheets-13445eebd281

Word2Vec and autoencoders



"Self-supervised learning" more generally

- Key idea: Create supervised data from unsupervised data by predicting some parts of the input from other parts of the input.
- A relatively new/recent idea.
- Has led to new state-of-the-art in language and vision tasks.
- E.g., BERT and ELMO in NLP.