

Image Classification

A Core Task in Computer Vision

Today:

- The image classification task
- Two basic data-driven approaches to image classification
 - K-nearest neighbor and linear classifier

Image Classification: A core task in Computer Vision



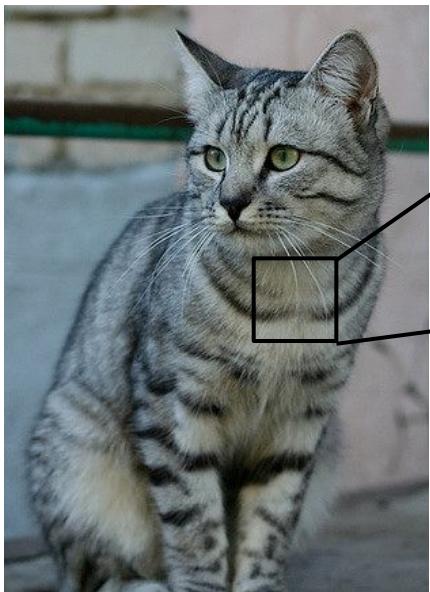
(assume given a set of possible labels)
{dog, cat, truck, plane, ...}



cat

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The Problem: Semantic Gap



[105 112 108 111 104 99 106 99 96 103 112 119 104 97 93 87]
[91 98 102 106 104 79 98 103 99 105 123 136 110 105 94 85]
[76 85 90 105 128 105 87 96 95 99 115 112 106 103 99 85]
[99 81 93 120 131 127 100 95 98 102 99 96 93 101 94]
[106 91 61 64 69 91 88 85 101 107 109 98 75 84 96 95]
[114 108 85 55 55 69 64 54 64 87 112 129 98 74 84 91]
[133 137 147 103 65 81 80 65 52 54 74 84 102 93 85 82]
[128 137 144 140 109 95 86 70 62 65 63 63 60 73 86 101]
[125 133 148 137 119 121 117 94 65 79 80 65 54 64 72 98]
[127 125 131 147 133 127 126 131 111 96 89 75 61 64 72 84]
[115 114 109 123 150 148 131 118 113 109 100 92 74 65 72 78]
[89 93 90 97 108 147 131 118 113 114 113 109 106 95 77 80]
[63 77 86 81 77 79 102 123 117 115 117 125 125 130 115 87]
[62 65 82 89 78 71 80 101 124 126 119 101 107 114 131 119]
[63 65 75 88 89 71 62 81 128 138 135 105 81 98 110 118]
[87 65 71 87 106 95 69 45 76 130 126 107 92 94 105 112]
[118 97 82 86 117 123 116 66 41 51 95 93 89 95 102 107]
[164 146 112 88 82 120 124 104 76 48 45 66 88 101 102 109]
[157 170 157 128 93 86 114 132 112 97 69 55 70 82 99 94]
[130 128 134 161 139 100 109 118 121 134 114 87 65 53 69 86]
[128 112 96 117 150 144 128 115 104 107 102 93 87 81 72 79]
[123 107 96 86 83 112 153 149 122 109 104 75 80 107 112 99]
[122 121 102 88 82 86 94 117 145 148 153 102 58 78 92 107]
[122 164 148 103 71 56 78 83 93 103 119 139 102 61 69 84]]

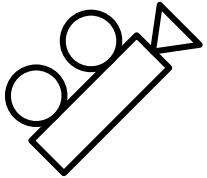
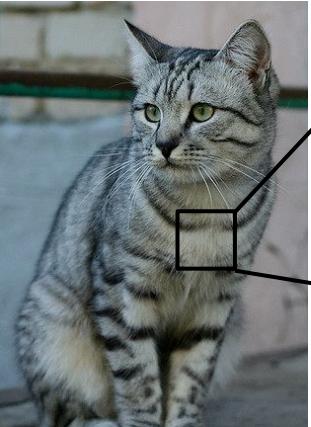
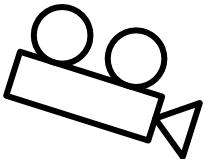
What the computer sees

An image is a tensor of integers between [0, 255]:

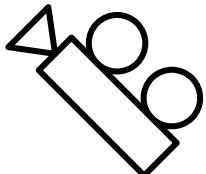
e.g. 800 x 600 x 3
(3 channels RGB)

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Challenges: Viewpoint variation



```
[1185 112 188 111 184 99 186 99 96 183 112 119 184 97 93 87]  
[ 91 98 182 106 184 79 98 183 99 185 123 136 118 185 94 85]  
[ 76 85 98 185 128 105 87 96 95 99 115 112 106 183 99 85]  
[ 99 80 81 100 128 103 127 98 98 101 108 109 98 75 84 94]  
[104 91 86 84 60 91 68 85 101 108 109 98 75 84 94 95]  
[114 108 85 55 55 69 64 54 64 87 112 129 98 74 84 94 91]  
[133 137 147 183 65 81 80 65 52 54 74 84 102 93 85 82]  
[128 137 144 148 105 95 86 78 62 65 63 68 68 73 86 101]  
[102 125 131 147 133 127 116 131 111 98 89 75 61 64 72 80]  
[127 125 131 147 133 127 116 131 111 98 89 75 61 64 72 84]  
[115 115 189 123 150 148 131 118 113 109 108 92 74 65 72 78]  
[ 89 93 98 97 108 147 131 118 113 114 113 108 106 95 77 80]  
[ 63 77 86 81 77 79 182 123 137 115 111 125 125 130 115 87]  
[ 62 85 88 89 73 62 81 128 138 135 105 81 98 118 118]  
[ 63 65 75 88 89 73 62 81 128 138 135 105 81 98 118 118]  
[ 87 65 71 87 100 95 69 45 76 126 126 107 92 94 105 112]  
[118 97 82 86 117 123 116 66 41 51 95 93 89 89 95 102 107]  
[164 147 112 88 100 128 126 184 78 48 66 70 101 102 108]  
[157 98 100 118 103 92 86 104 105 108 109 95 70 84 85 94]  
[138 128 134 161 139 180 109 118 121 134 114 87 65 53 69 86]  
[128 112 96 117 150 144 120 115 104 107 102 93 87 81 72 79]  
[123 107 96 86 83 112 153 149 122 189 184 75 88 107 112 99]  
[122 121 102 88 82 86 94 117 145 148 153 105 58 78 92 107]  
[122 164 148 103 71 56 78 83 93 103 119 139 102 61 69 84]
```



All pixels change when
the camera moves!

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Challenges: Illumination



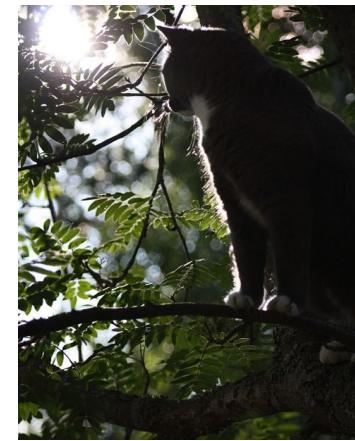
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Challenges: Background Clutter



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Challenges: Occlusion



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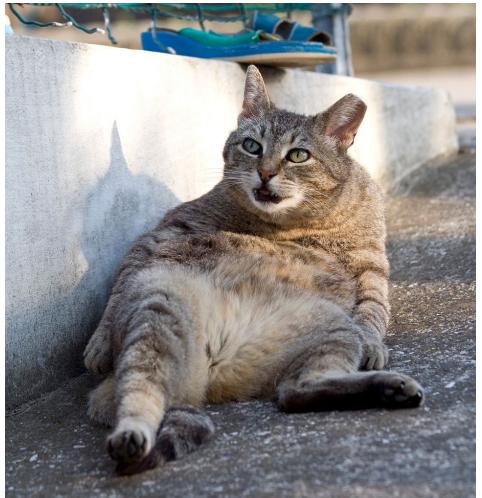


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Challenges: Deformation



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Challenges: Intraclass variation



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Challenges: Context

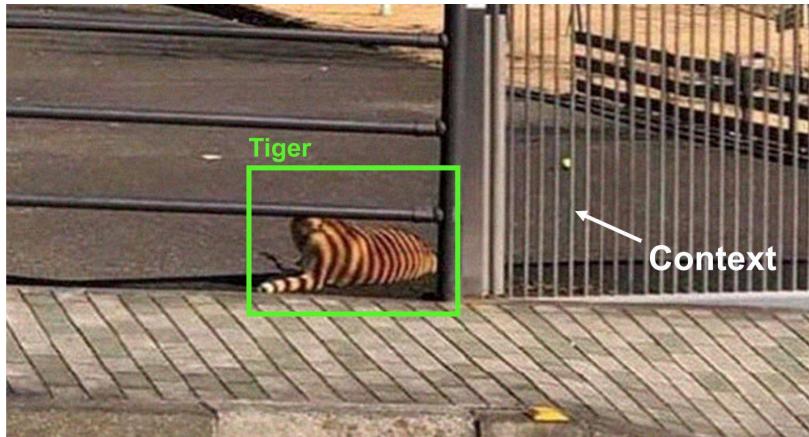
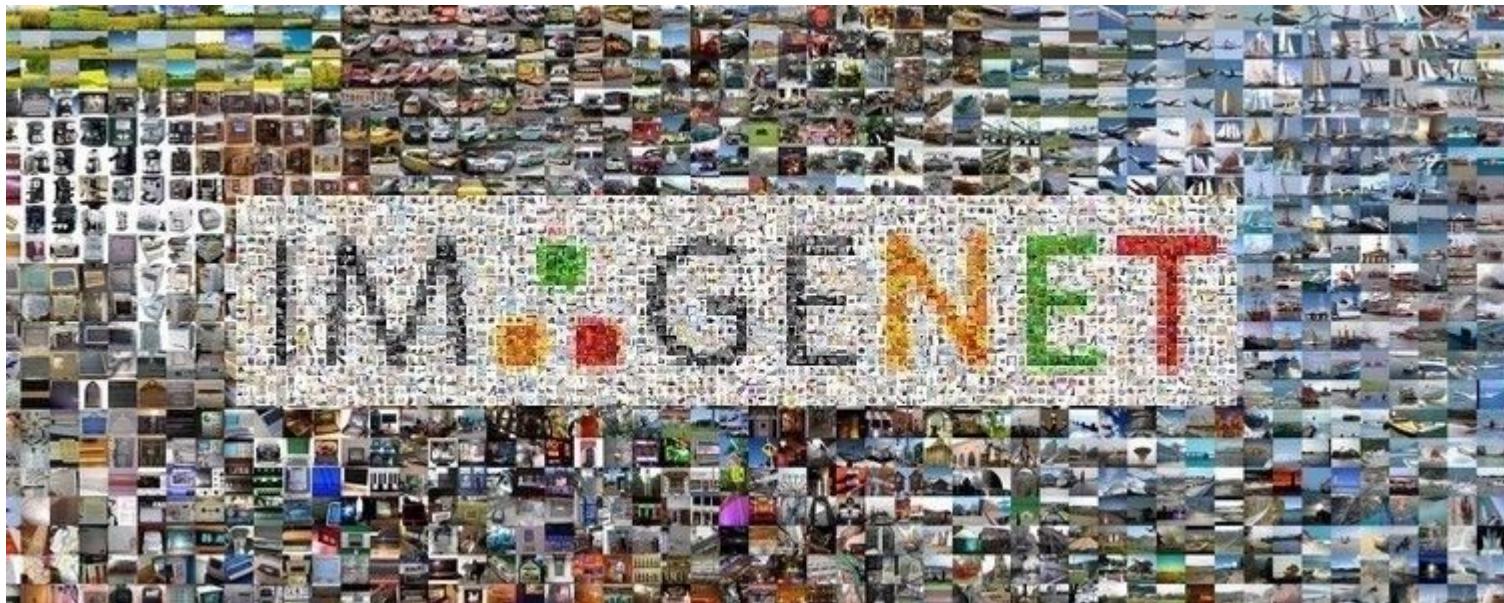


Image source:

https://www.linkedin.com/posts/ralph-aboujaoude-diaz-40838313_technology-artificialintelligence-computervision-activity-6912446088364875776-h-lq/?utm_source=linkedin_share&utm_medium=member_desktop_web

Modern computer vision algorithms



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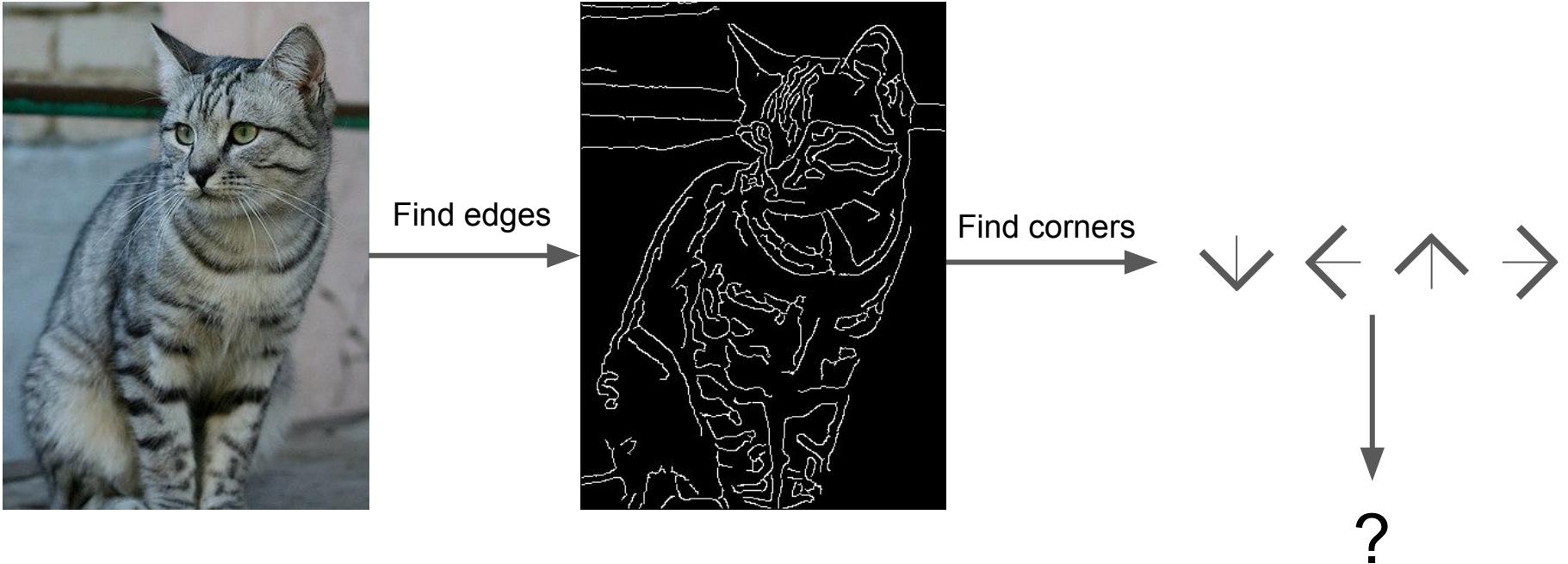
An image classifier

```
def classify_image(image):  
    # Some magic here?  
    return class_label
```

Unlike e.g. sorting a list of numbers,

no obvious way to hard-code the algorithm for
recognizing a cat, or other classes.

Attempts have been made



John Canny, "A Computational Approach to Edge Detection", IEEE TPAMI 1986

Machine Learning: Data-Driven Approach

1. Collect a dataset of images and labels
2. Use Machine Learning algorithms to train a classifier
3. Evaluate the classifier on new images

Example training set

```
def train(images, labels):  
    # Machine learning!  
    return model
```

```
def predict(model, test_images):  
    # Use model to predict labels  
    return test_labels
```

airplane



automobile



bird



cat



deer



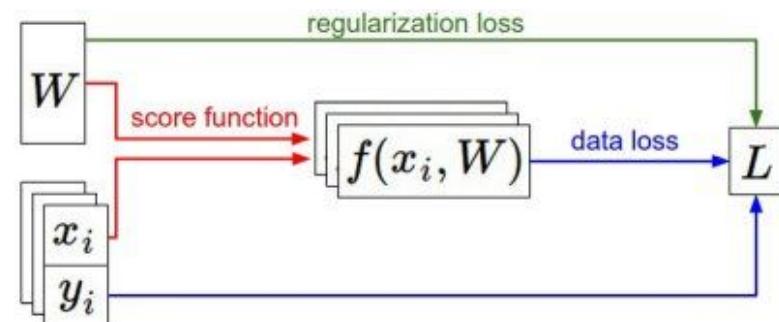
Recap

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

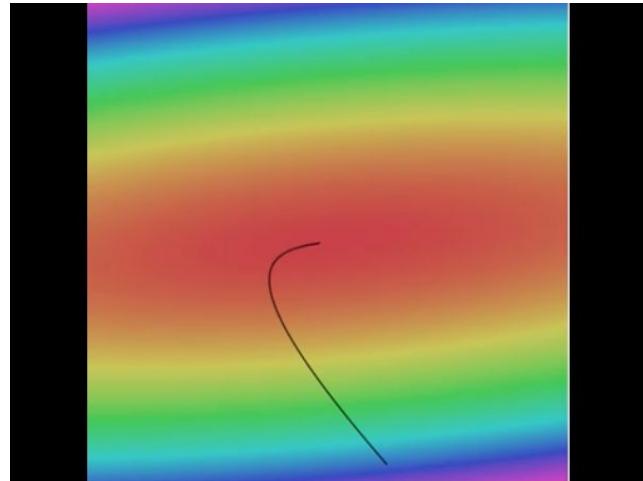
$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{sj}}\right) \text{ Softmax}$$

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

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



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
```

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Walking man image is [CC0 1.0](#) public domain

Gradient descent

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

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)

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

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

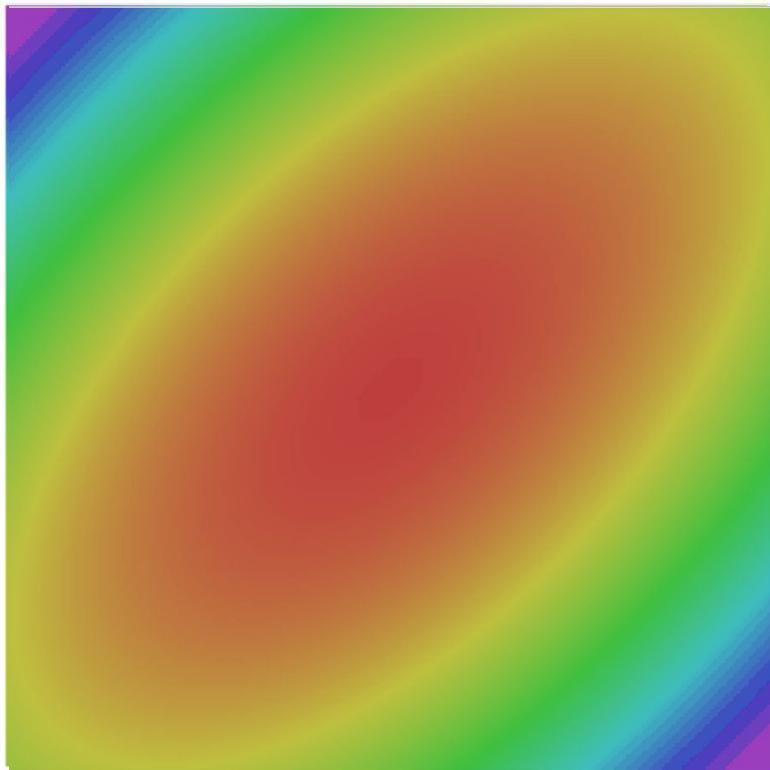
Full sum expensive
when N is large!

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

```
# Vanilla Minibatch Gradient Descent
```

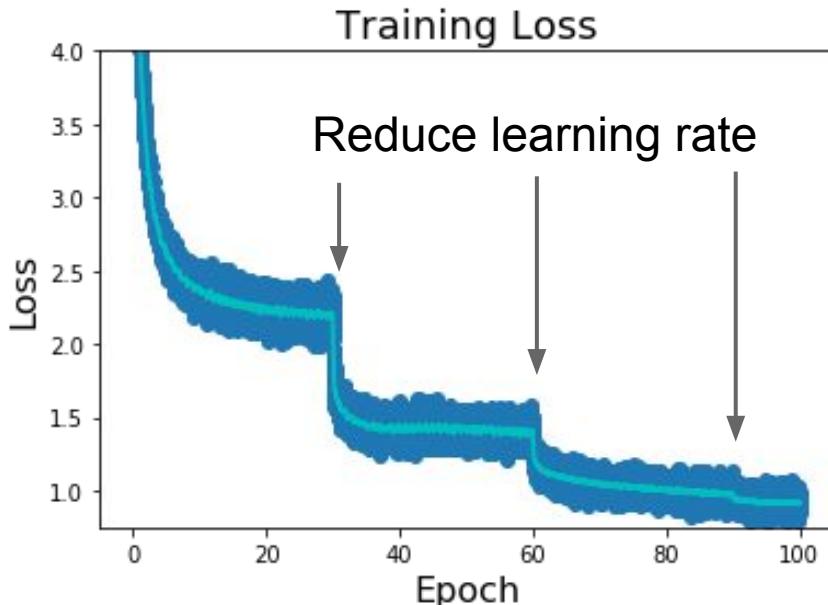
```
while True:  
    data_batch = sample_training_data(data, 256) # sample 256 examples  
    weights_grad = evaluate_gradient(loss_fun, data_batch, weights)  
    weights += - step_size * weights_grad # perform parameter update
```

Last time: fancy optimizers



- SGD
- SGD+Momentum
- RMSProp
- Adam

Last time: learning rate scheduling



Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

Cosine: $\alpha_t = \frac{1}{2}\alpha_0 (1 + \cos(t\pi/T))$

Linear: $\alpha_t = \alpha_0(1 - t/T)$

Inverse sqrt: $\alpha_t = \alpha_0/\sqrt{t}$

α_0 : Initial learning rate

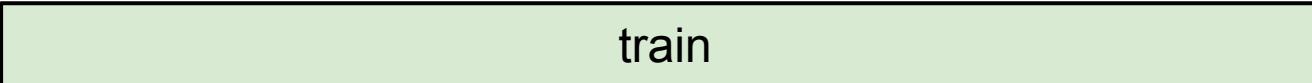
α_t : Learning rate at epoch t

T : Total number of epochs

Setting Hyperparameters

Idea #1: Choose hyperparameters that work best on the **training data**

BAD: $K = 1$ always works perfectly on training data



train

Idea #2: choose hyperparameters that work best on **test data**

BAD: No idea how algorithm will perform on new data



train

test

Idea #3: Split data into **train**, **val**; choose hyperparameters on val and evaluate on test

Better!



train

validation

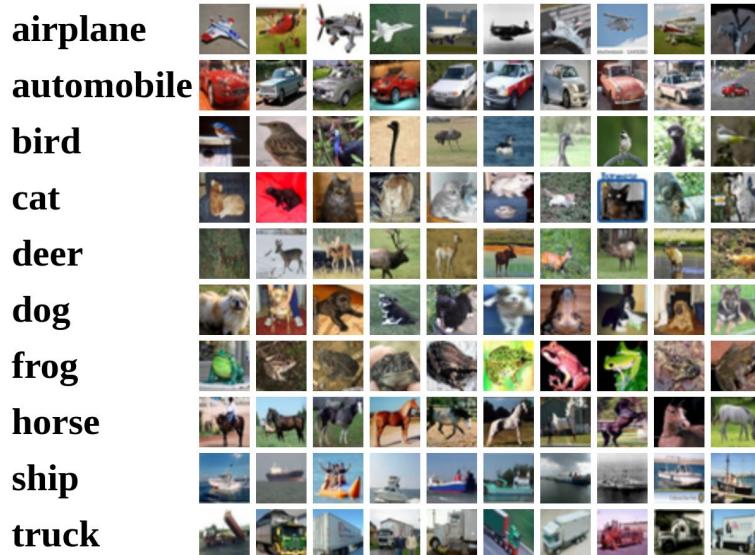
test

Example Dataset: CIFAR10

10 classes

50,000 training images

10,000 testing images



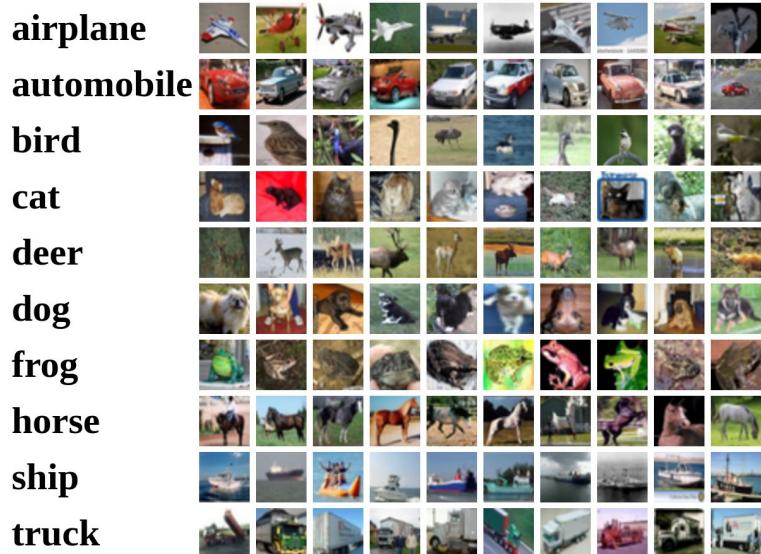
Alex Krizhevsky, "Learning Multiple Layers of Features from Tiny Images", Technical Report, 2009.

Example Dataset: CIFAR10

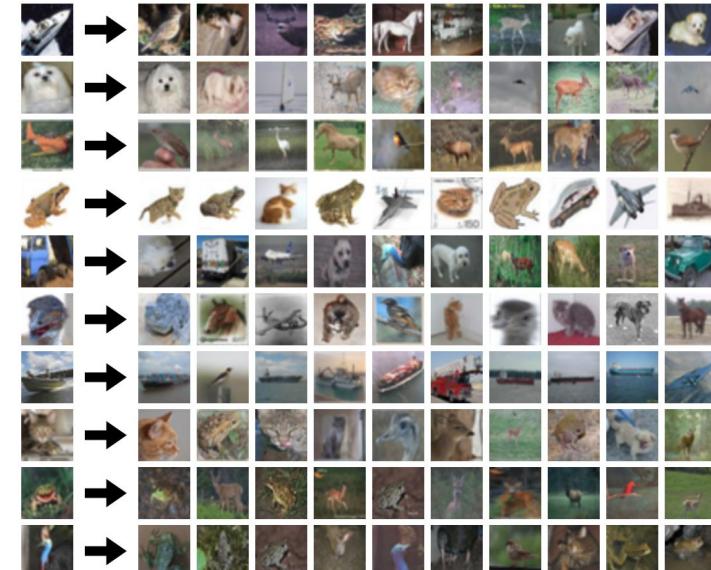
10 classes

50,000 training images

10,000 testing images



Test images and nearest neighbors



Alex Krizhevsky, "Learning Multiple Layers of Features from Tiny Images", Technical Report, 2009.

What does this look like?



What does this look like?



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

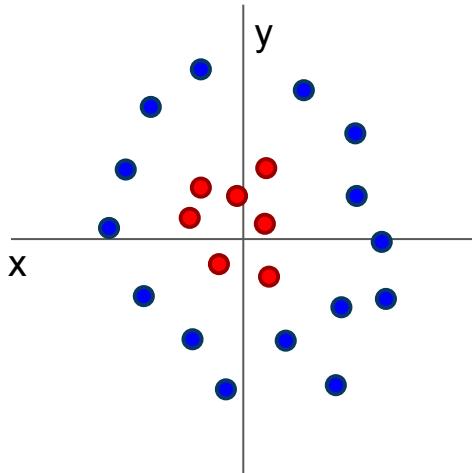
(Before) Linear score function: $f = Wx$

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

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

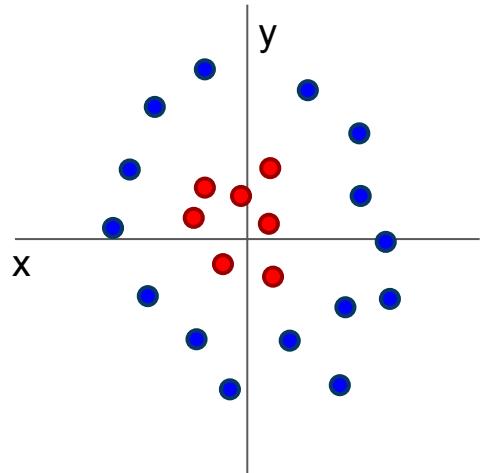
(In practice we will usually add a learnable bias at each layer as well)

Why do we want non-linearity?



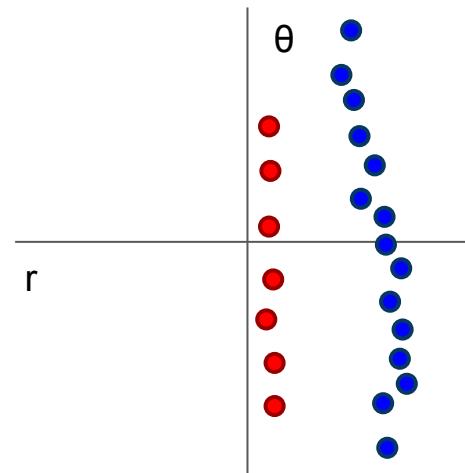
Cannot separate red
and blue points with
linear classifier

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

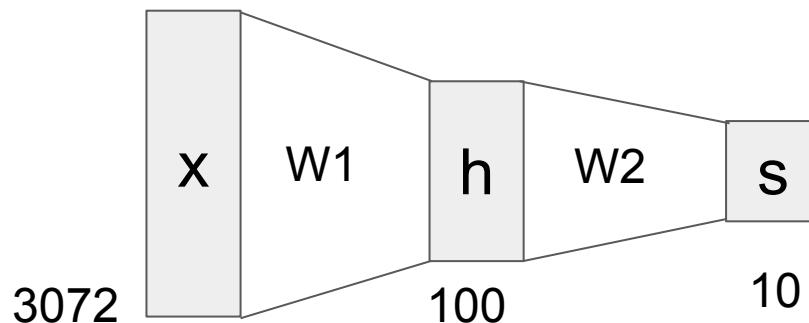
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

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

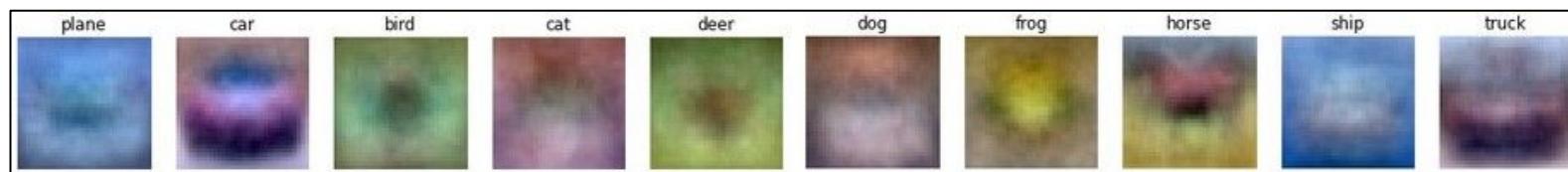
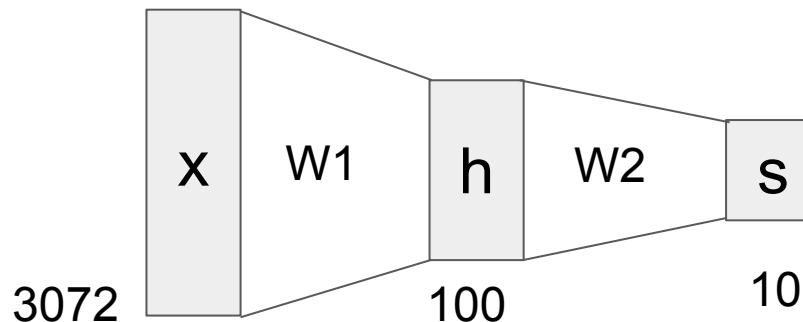


$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

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?

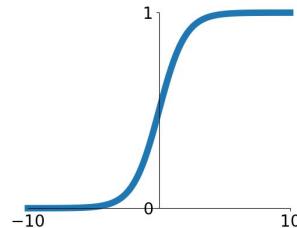
$$f = W_2 W_1 x \quad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

A: We end up with a linear classifier again!

Activation functions

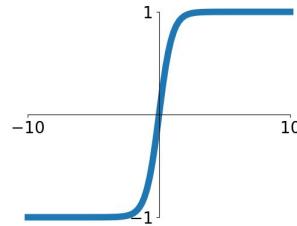
Sigmoid

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



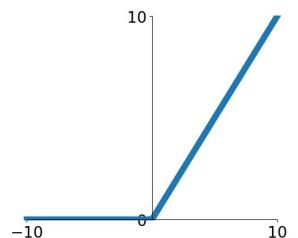
tanh

$$\tanh(x)$$



ReLU

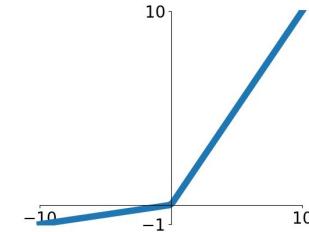
$$\max(0, x)$$



ReLU is a good default choice for most problems

Leaky ReLU

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

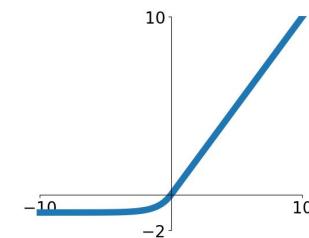


Maxout

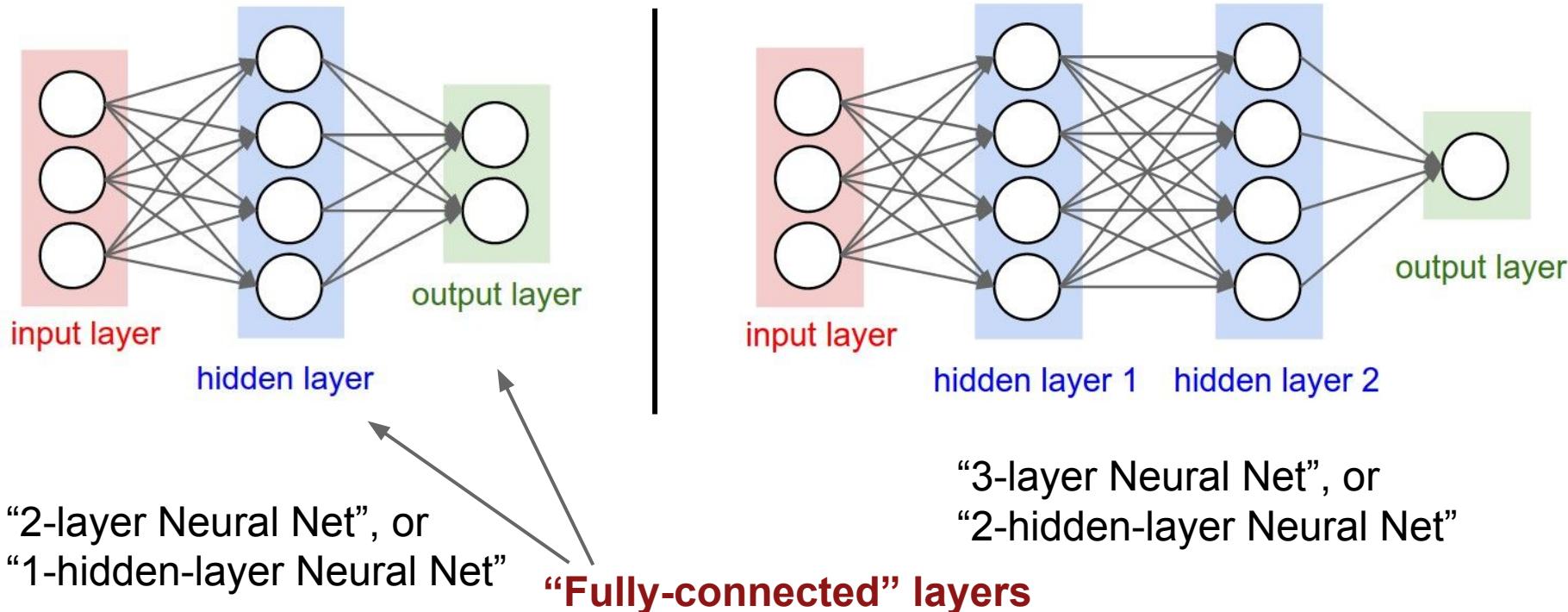
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

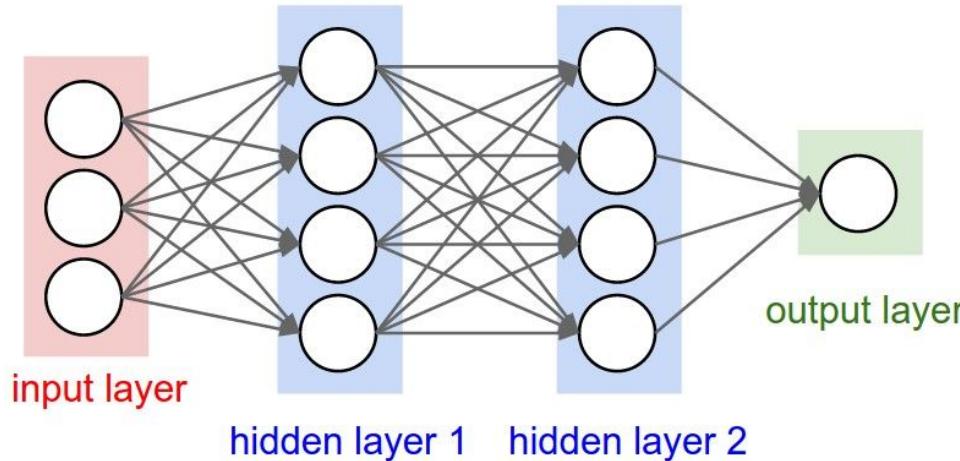
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Neural networks: Architectures



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:

```
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
```

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Define the network

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

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20    w2 -= 1e-4 * grad_w2
```

Define the network

Forward pass

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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
```

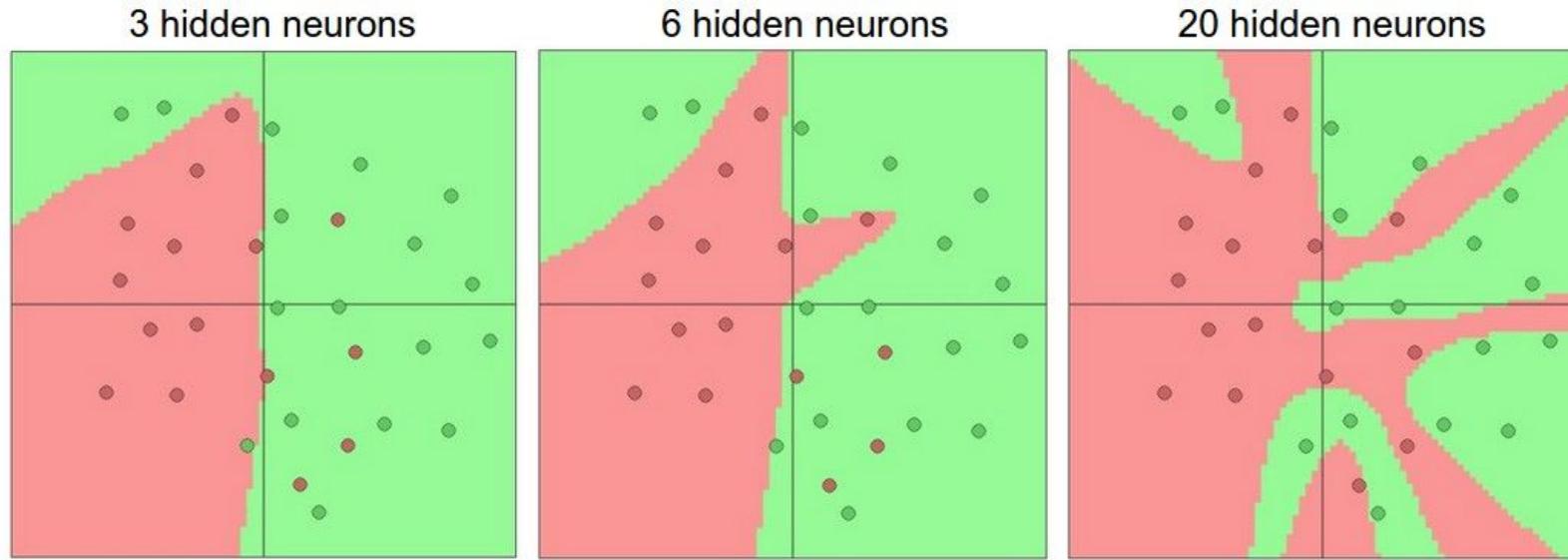
Define the network

Forward pass

Calculate the analytical gradients

Gradient descent

Setting the number of layers and their sizes



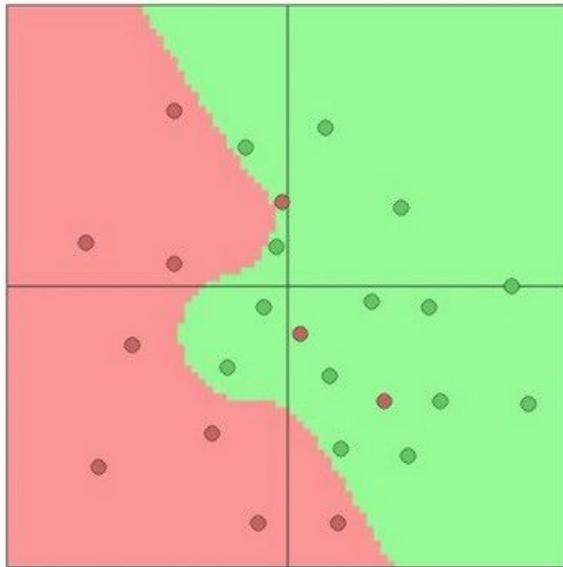
more neurons = more capacity

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

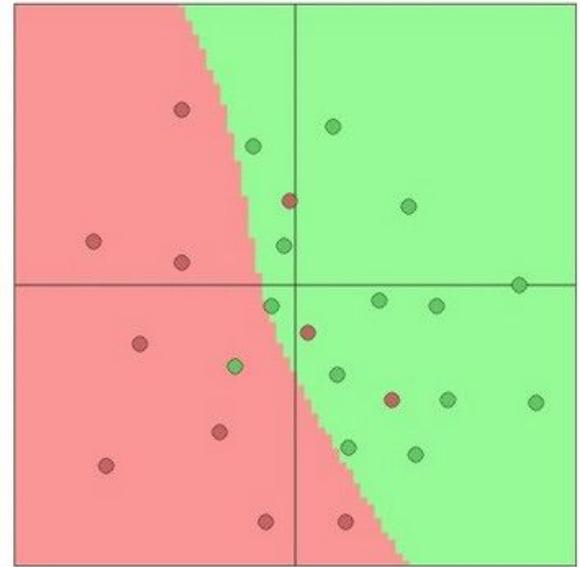
$\lambda = 0.001$



$\lambda = 0.01$



$\lambda = 0.1$



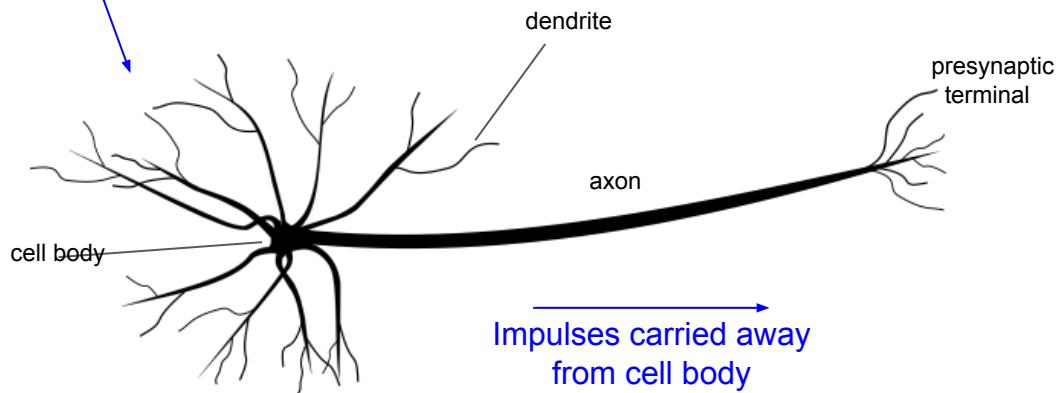
(Web demo with ConvNetJS:
[http://cs.stanford.edu/people/karpathy/convnetjs/demo
/classify2d.html](http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html))

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



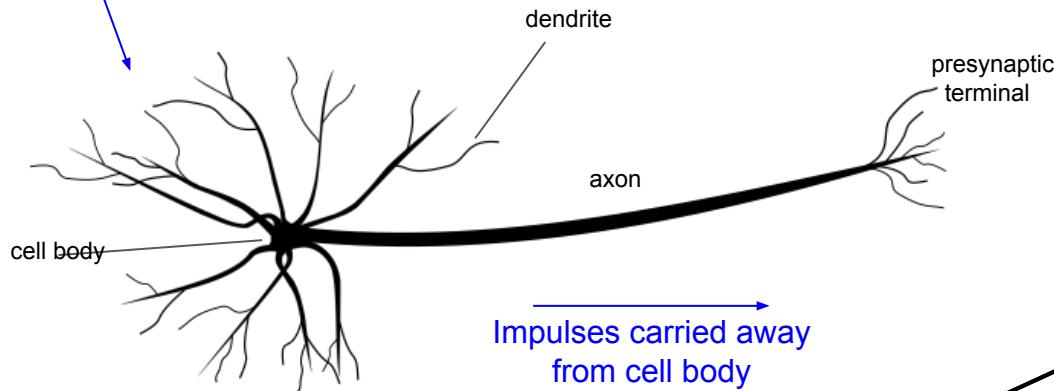
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Impulses carried toward cell body



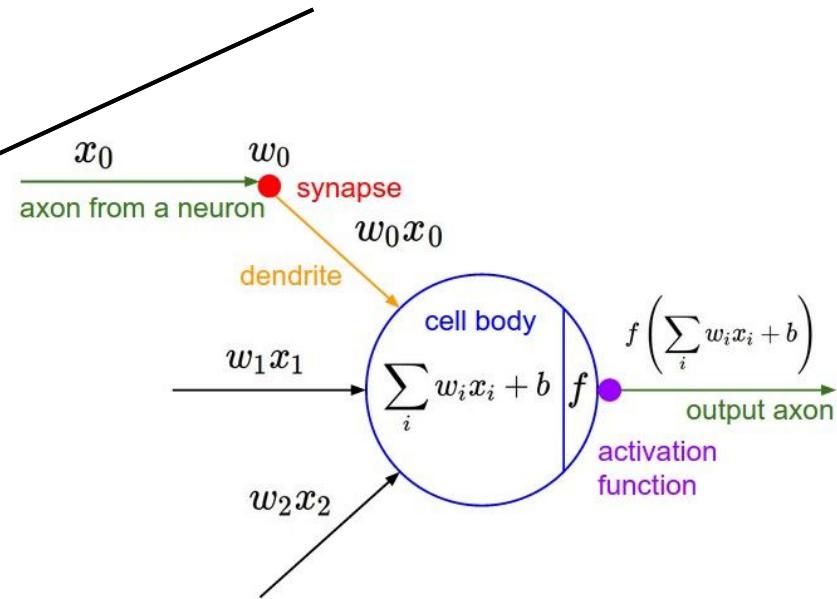
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Impulses carried toward cell body

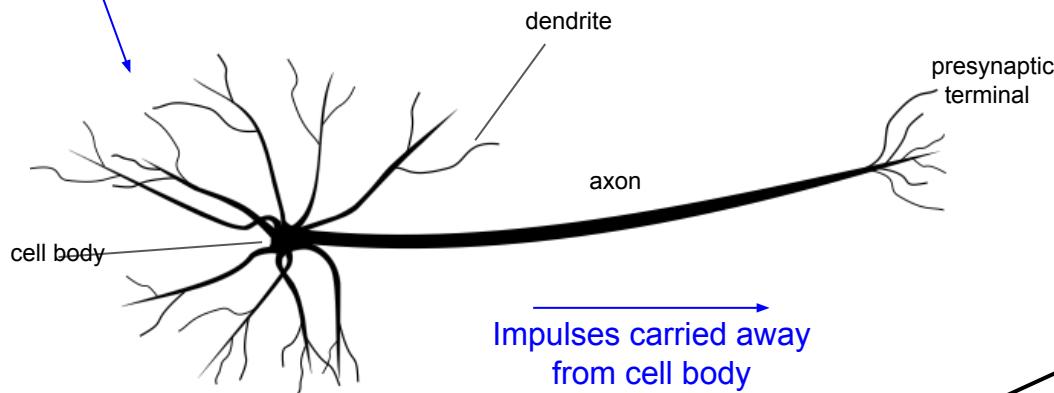


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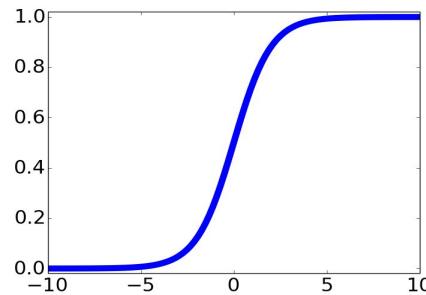
Impulses carried away
from cell body



Impulses carried toward cell body



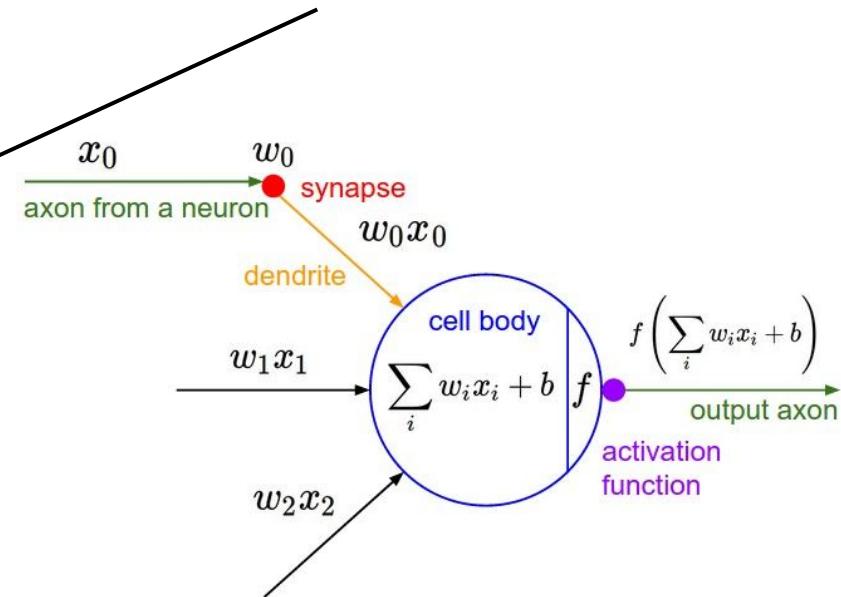
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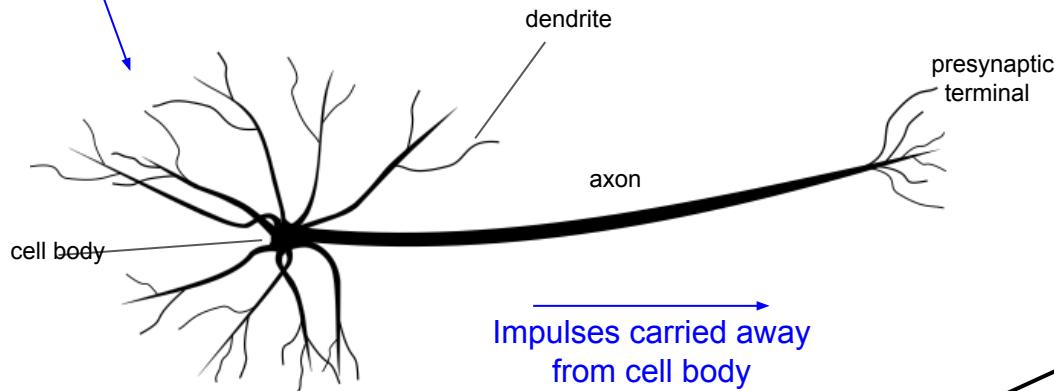
sigmoid activation function

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

Impulses carried away from cell body

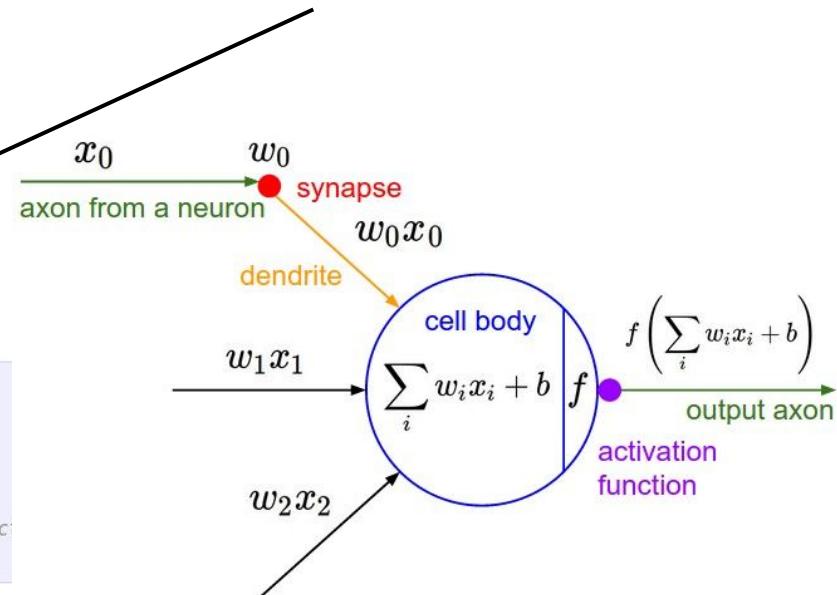


Impulses carried toward cell body

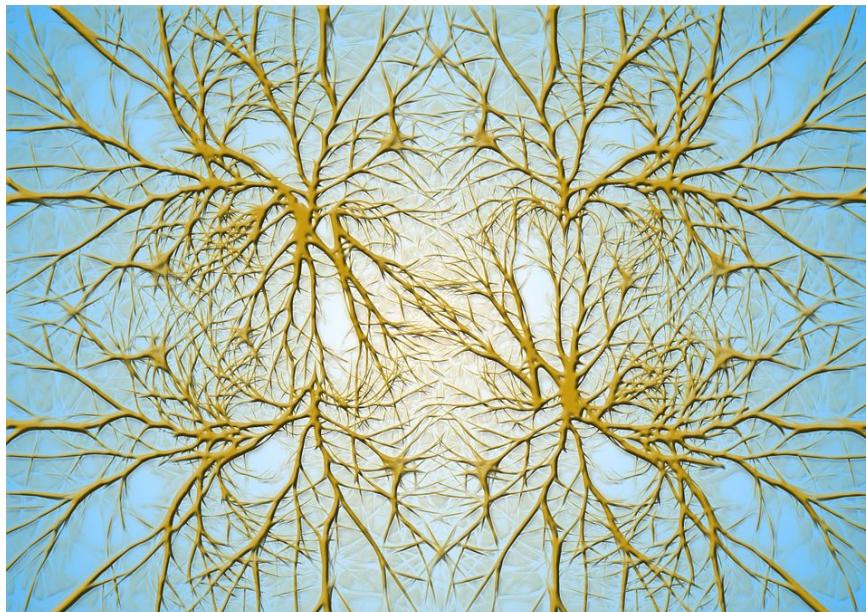


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is licensed under CC-BY 3.0

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

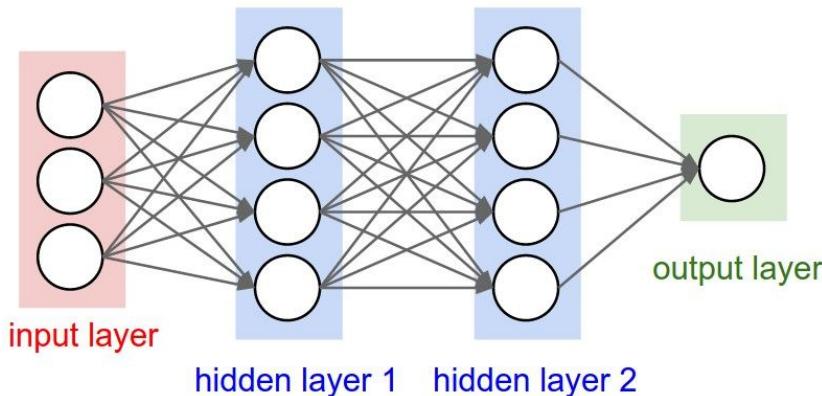


Biological Neurons: Complex connectivity patterns

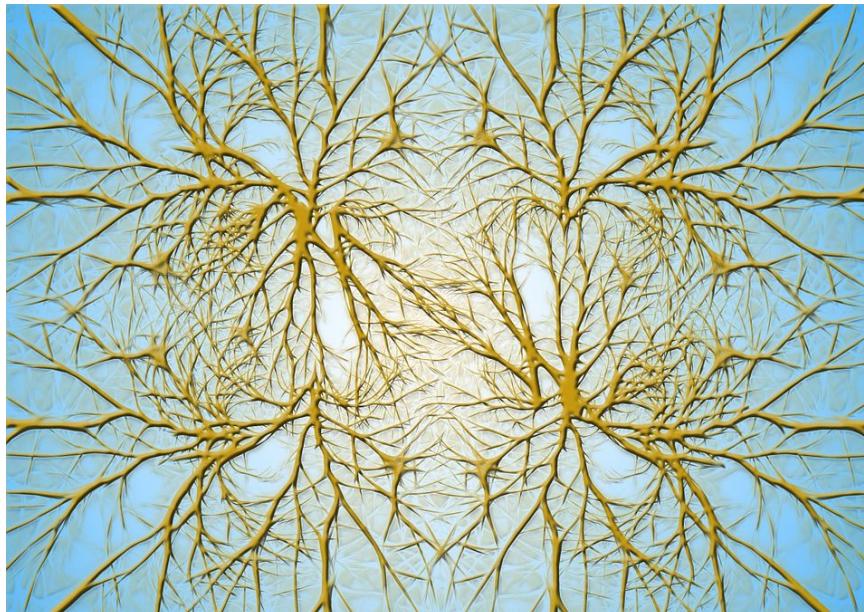


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Neurons in a neural network:
Organized into regular layers for
computational efficiency

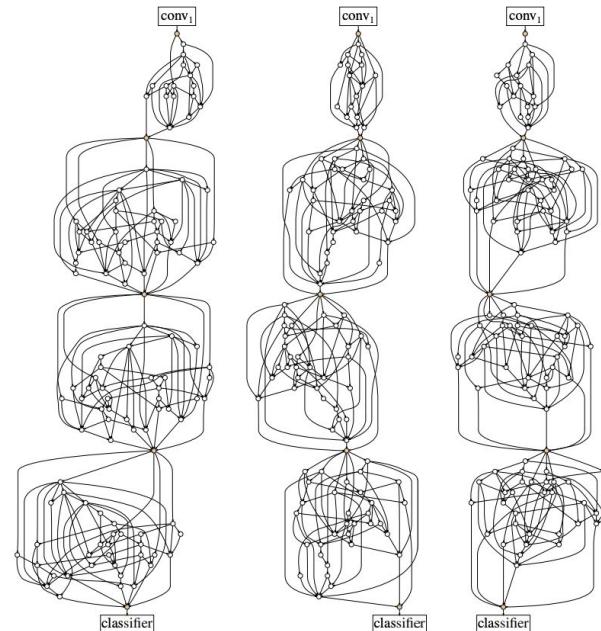


Biological Neurons: Complex connectivity patterns



[This image is CC0 Public Domain](#)

But neural networks with random connections can work too!



Xie et al, "Exploring Randomly Wired Neural Networks for Image Recognition", arXiv 2019

Be very careful with your brain analogies!

Biological Neurons:

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

[Dendritic Computation. London and Häusser]

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?

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

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

$$R(W) = \sum_k W_k^2 \quad \text{Regularization}$$

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

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

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

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

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

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

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

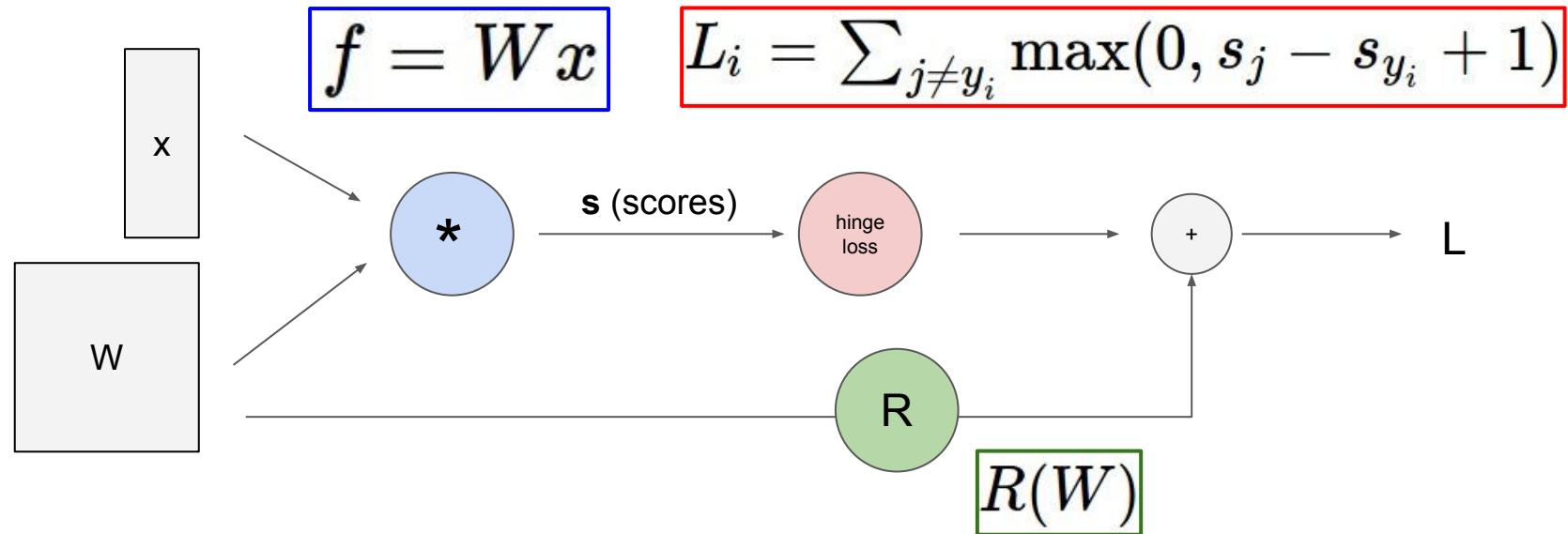
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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

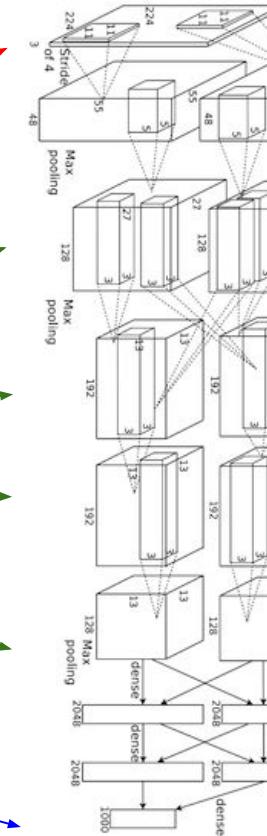


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Really complex neural networks!!

input image

loss

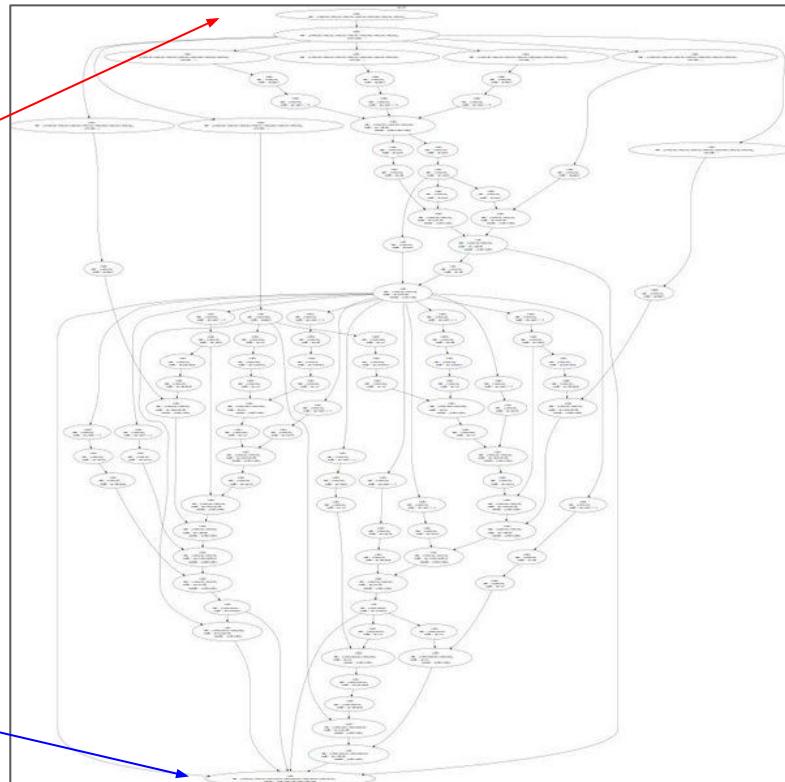


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

Neural Turing Machine

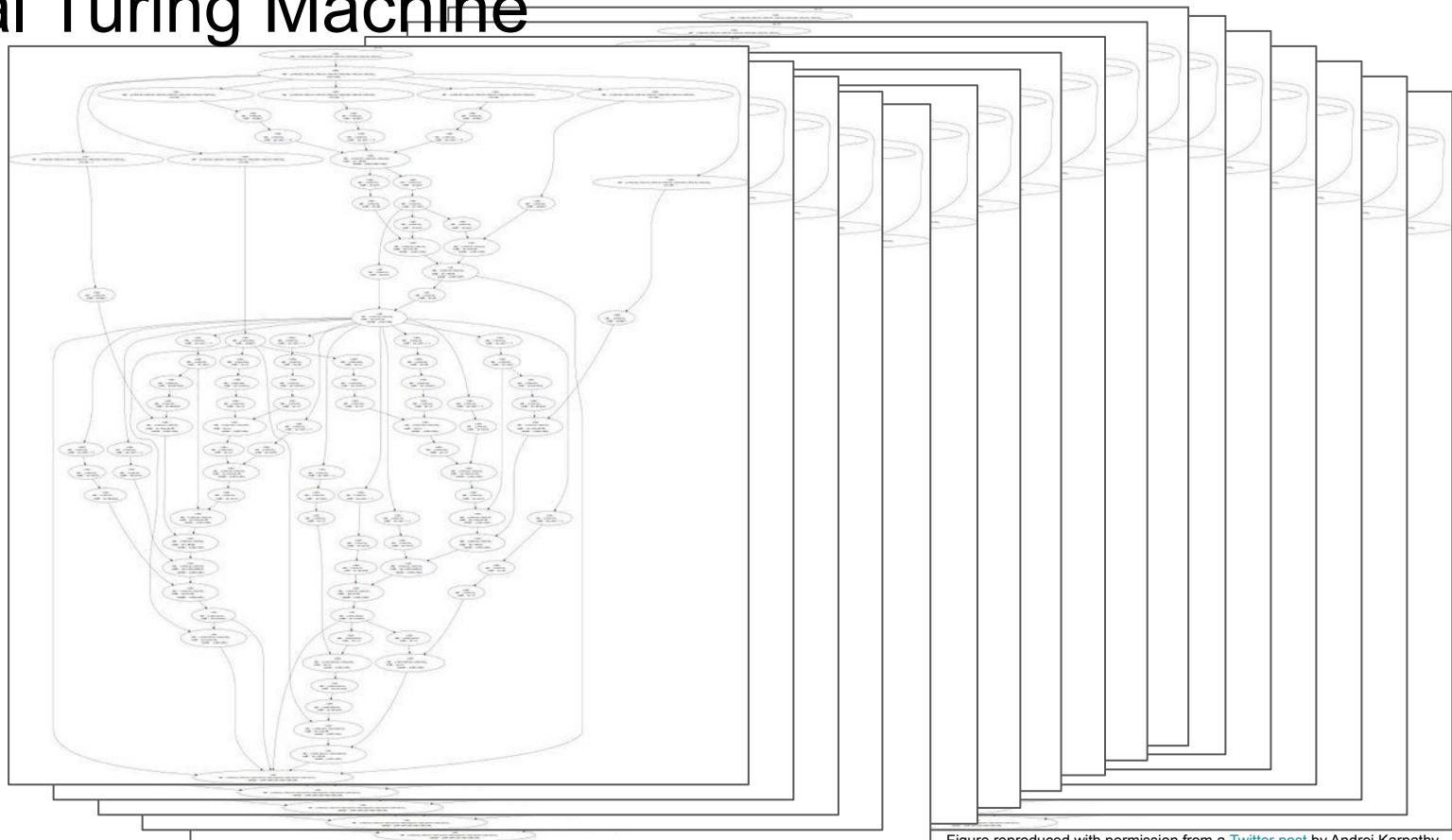


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

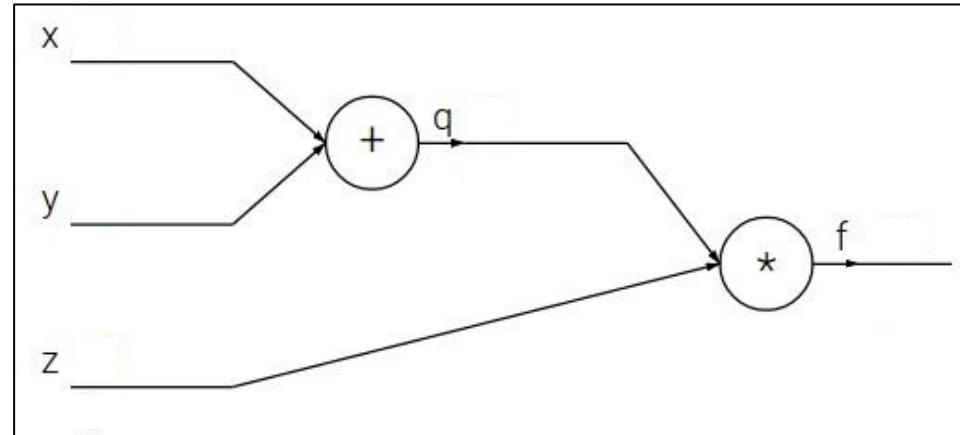
Solution: Backpropagation

Backpropagation: a simple example

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

Backpropagation: a simple example

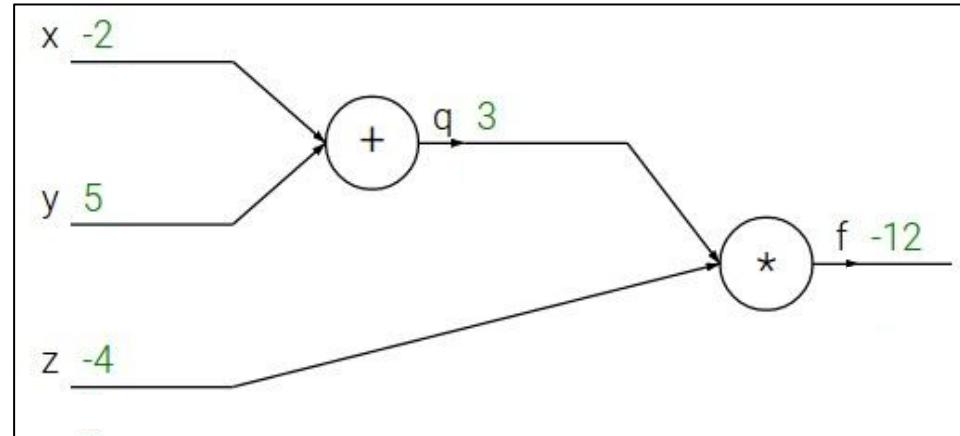
$$f(x, y, z) = (x + y)z$$



Backpropagation: a simple example

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

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

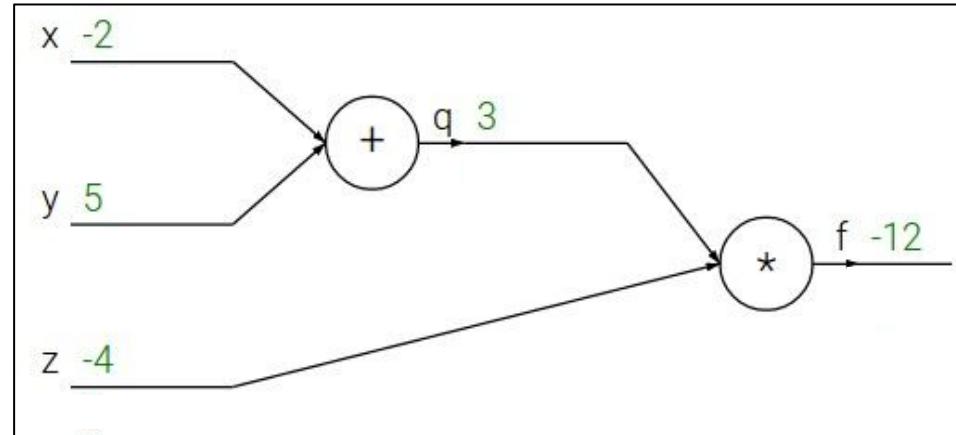


Backpropagation: a simple example

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

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

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



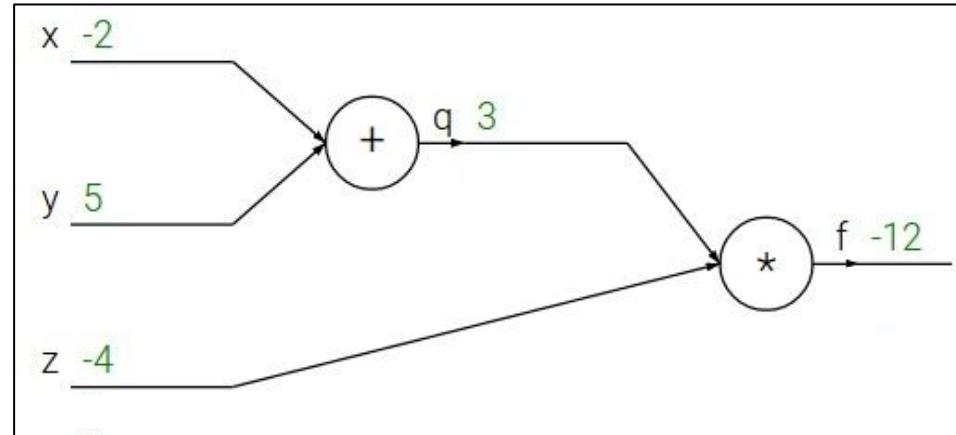
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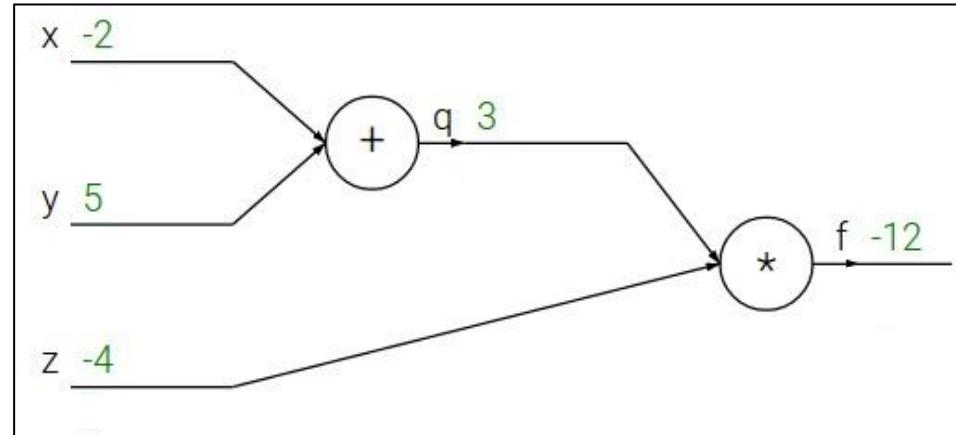
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Backpropagation: a simple example

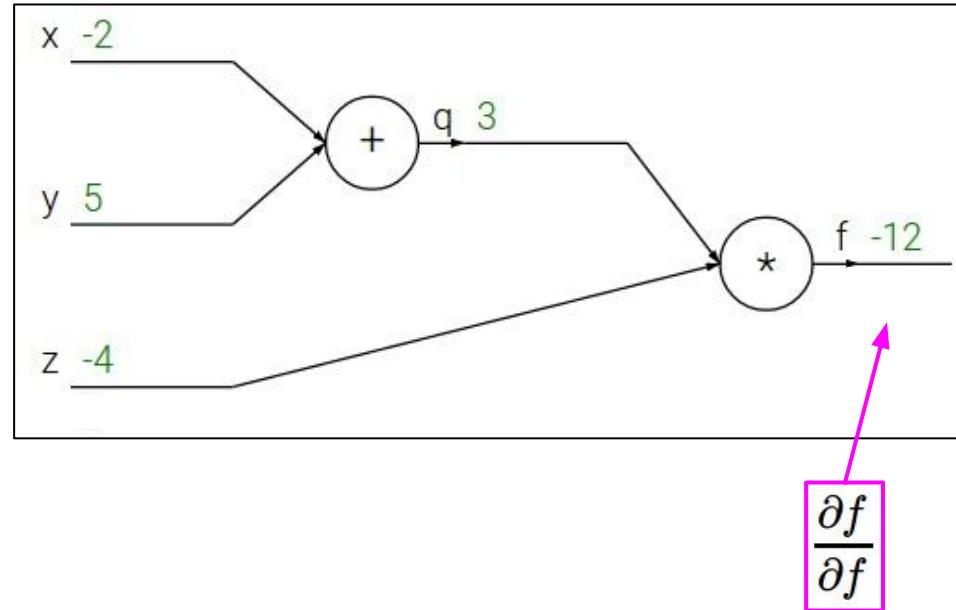
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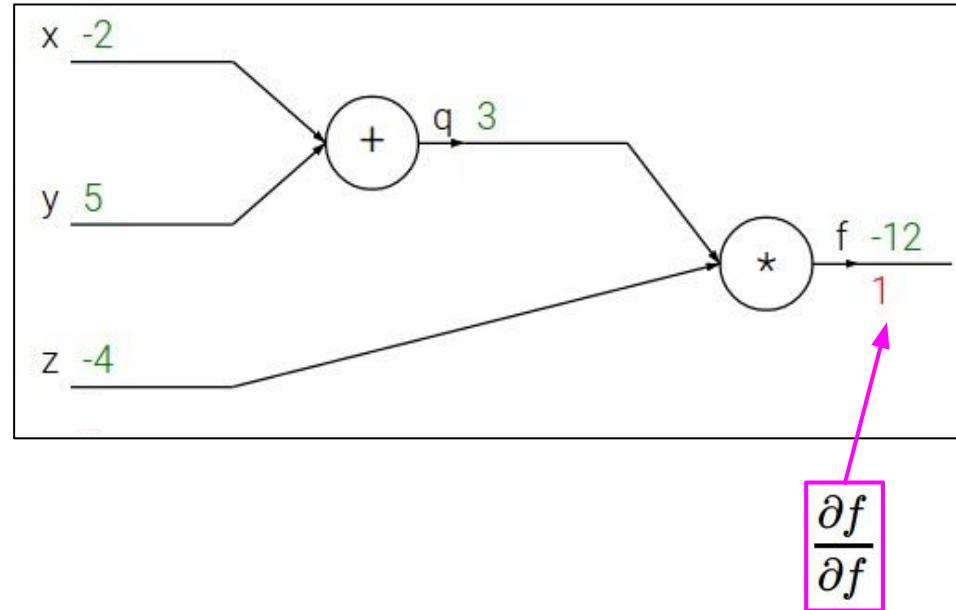
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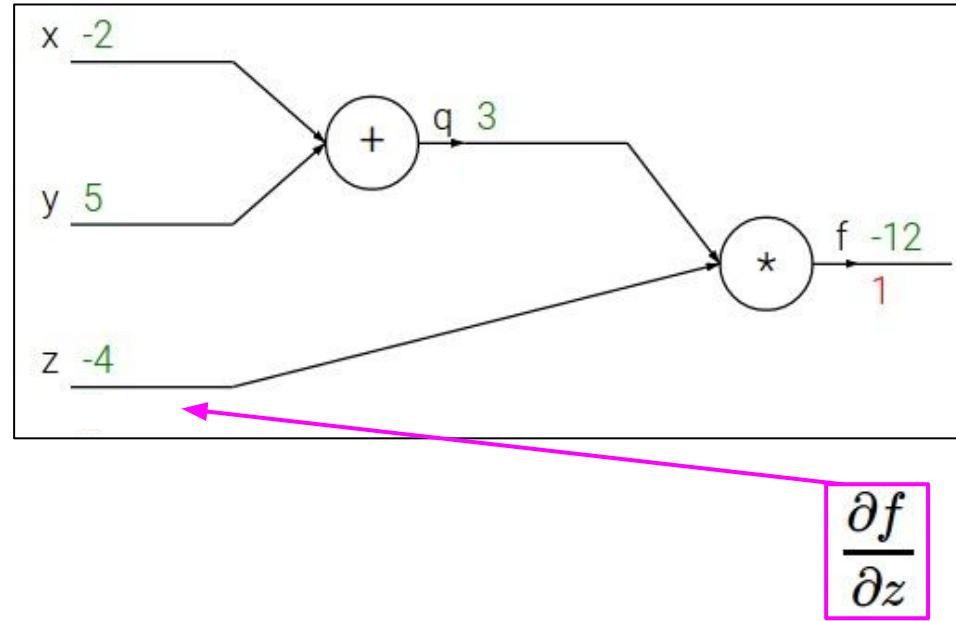
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$$\frac{\partial f}{\partial z}$$

Backpropagation: a simple example

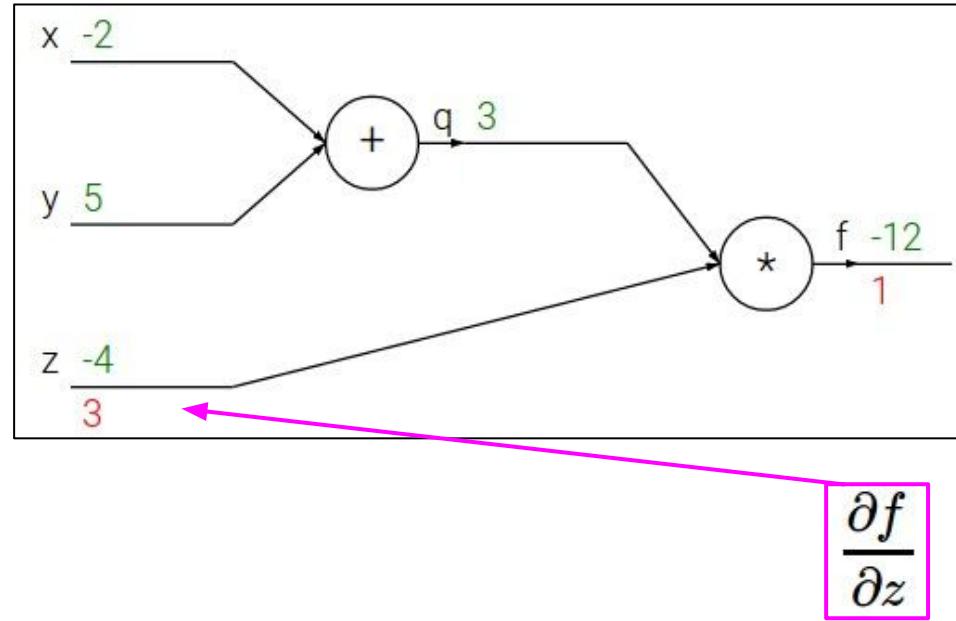
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$$\frac{\partial f}{\partial z}$$

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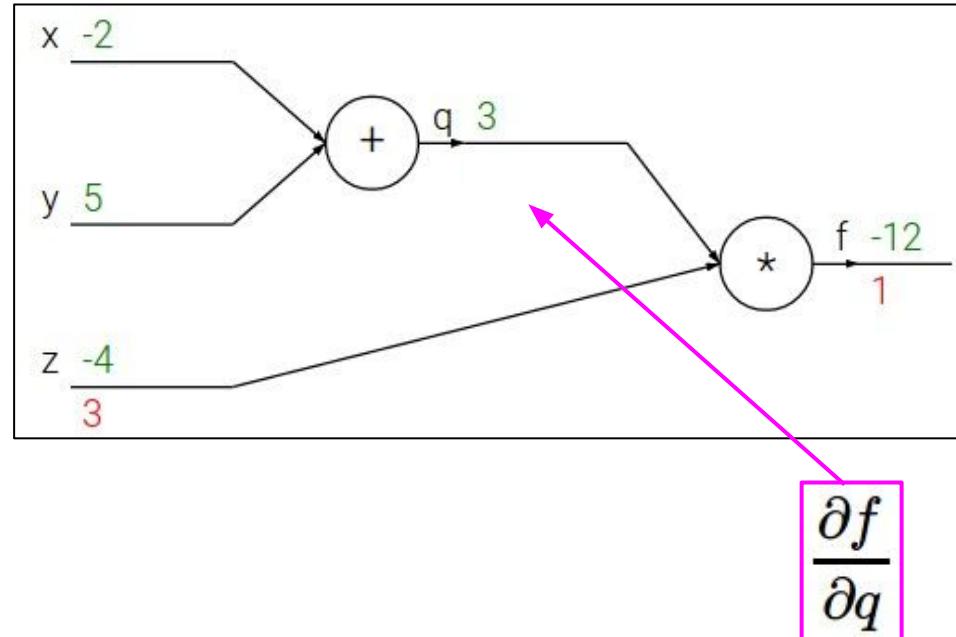
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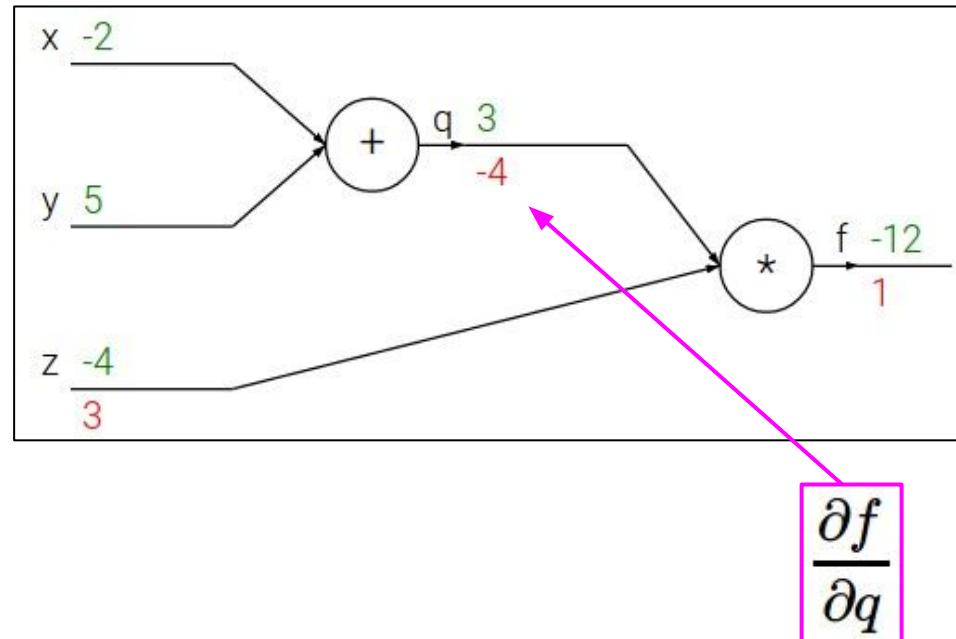
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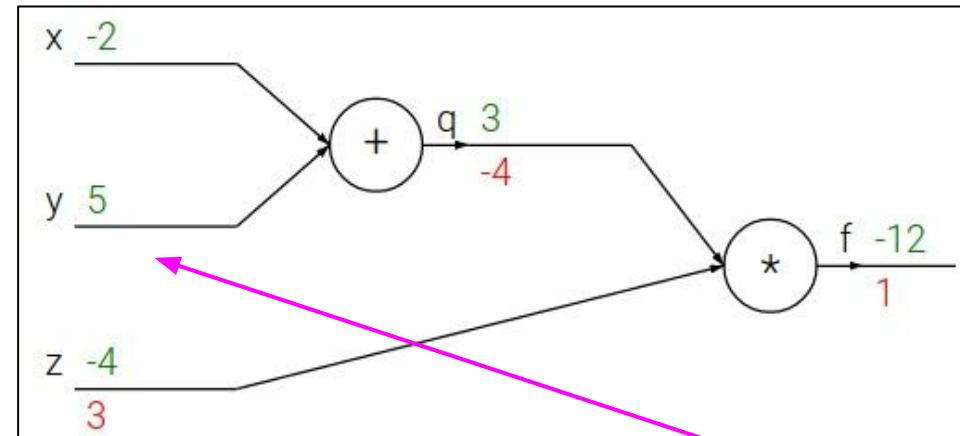
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Chain rule:

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

Upstream
gradient

Local
gradient

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

Backpropagation: a simple example

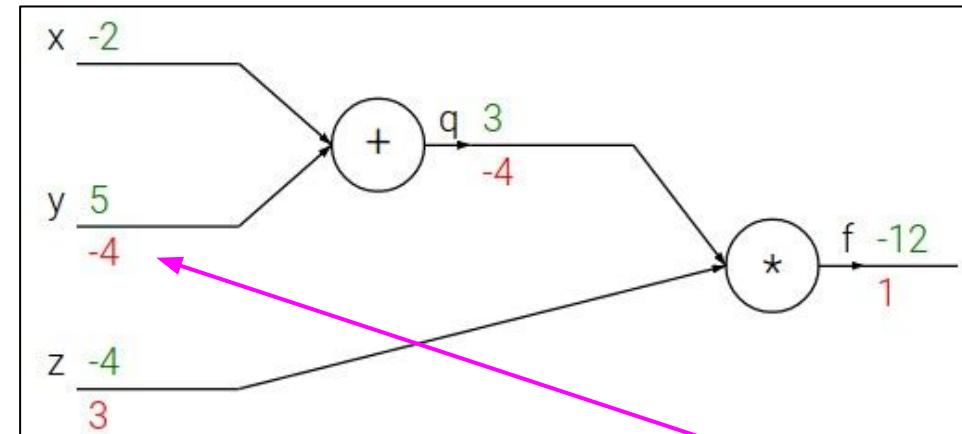
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gradient

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Backpropagation: a simple example

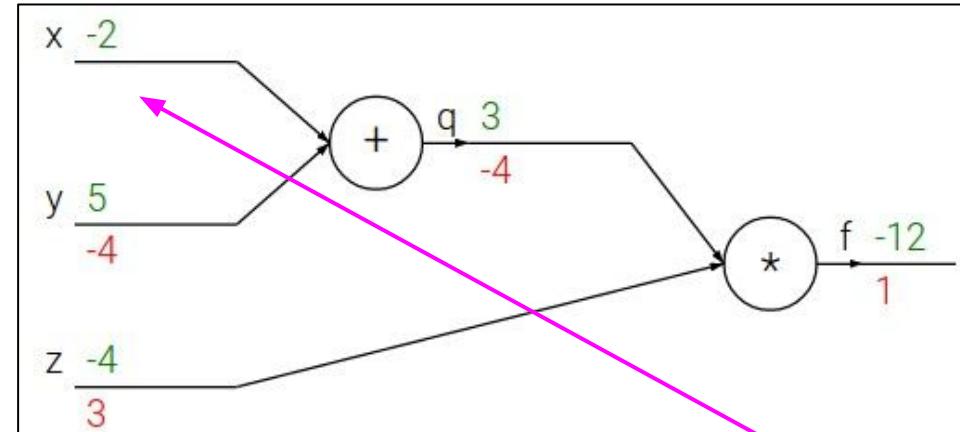
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Local
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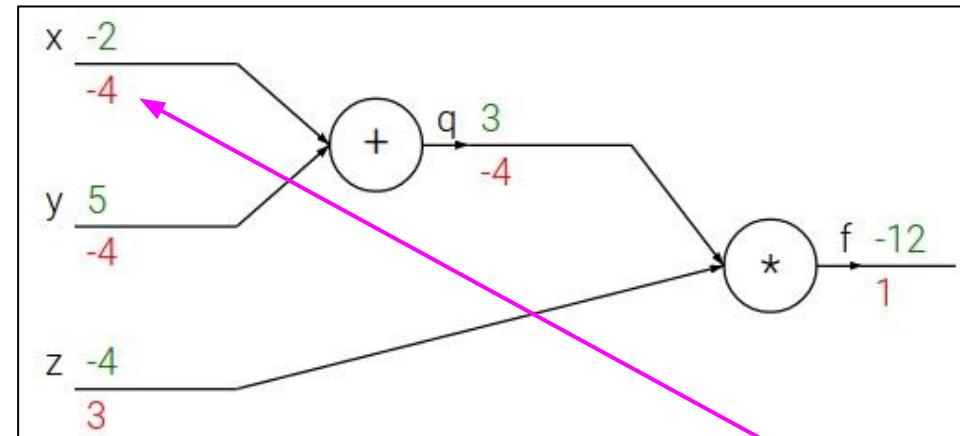
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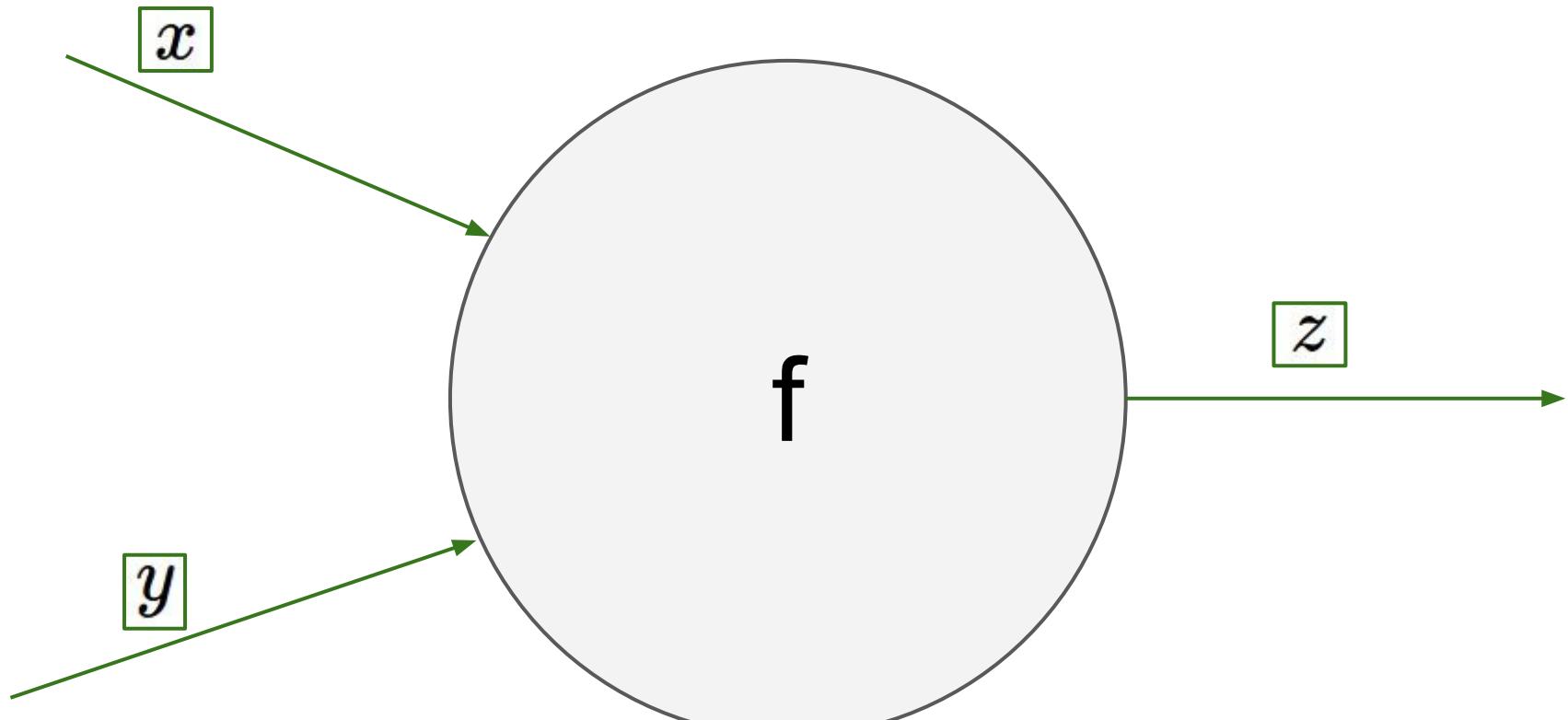


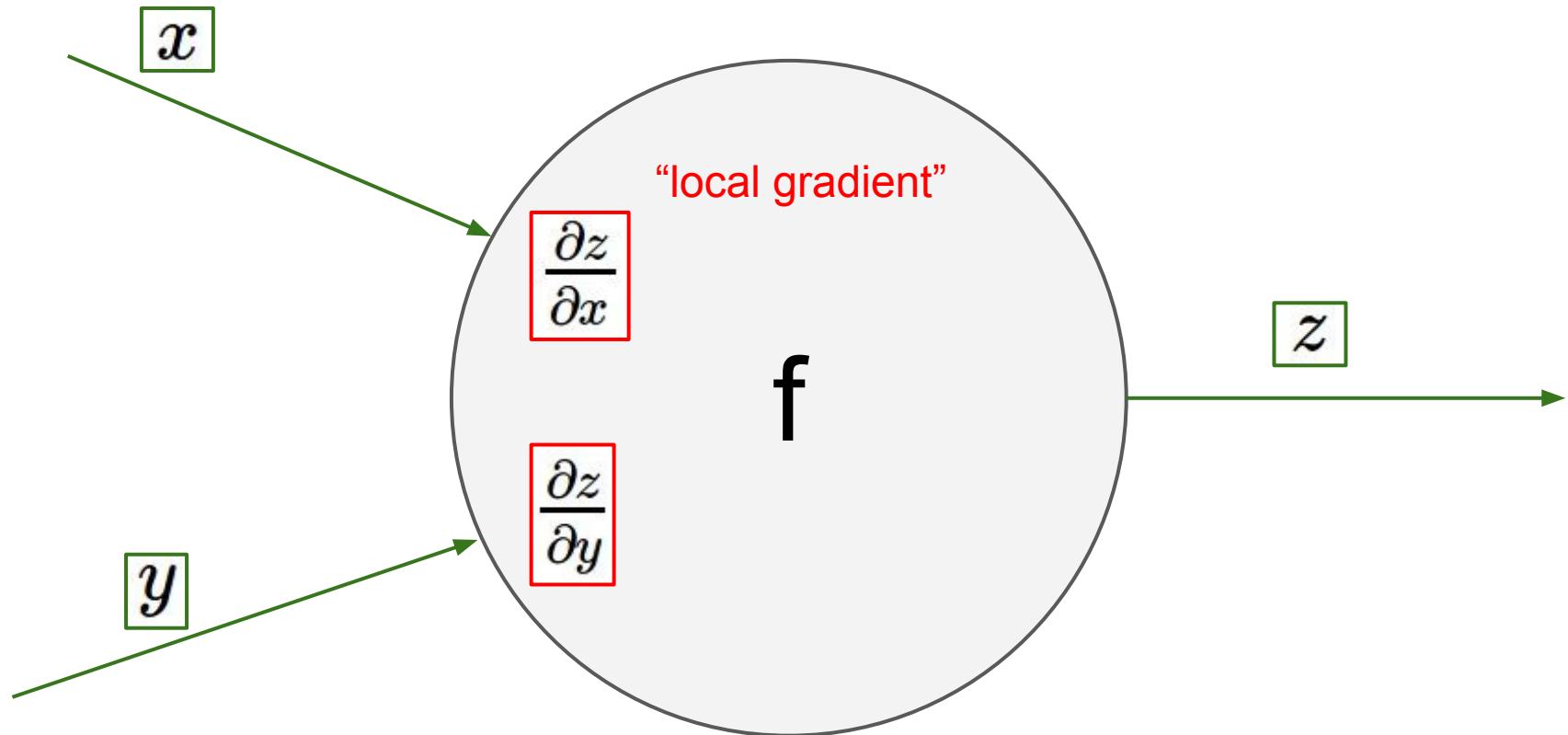
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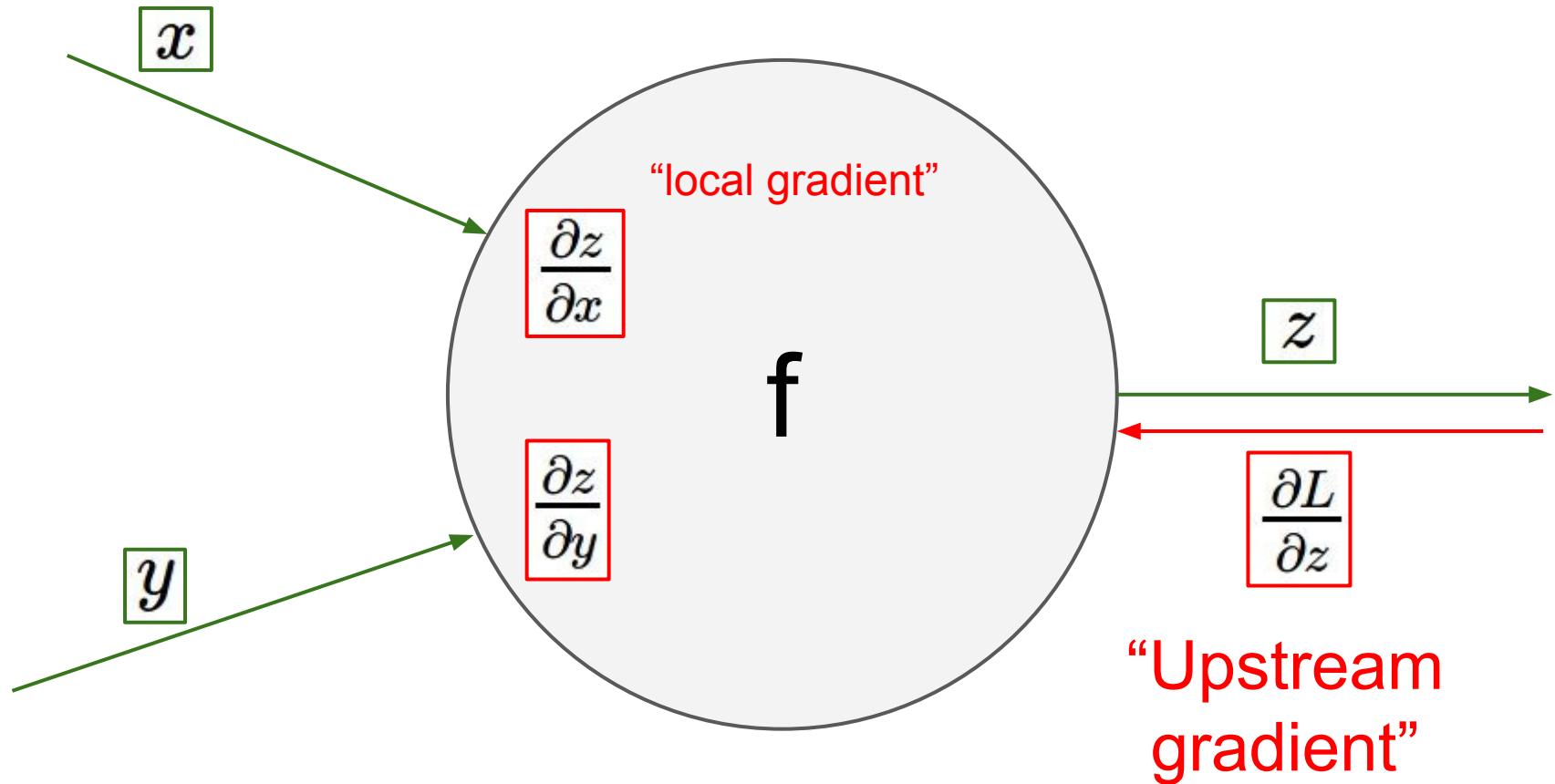
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

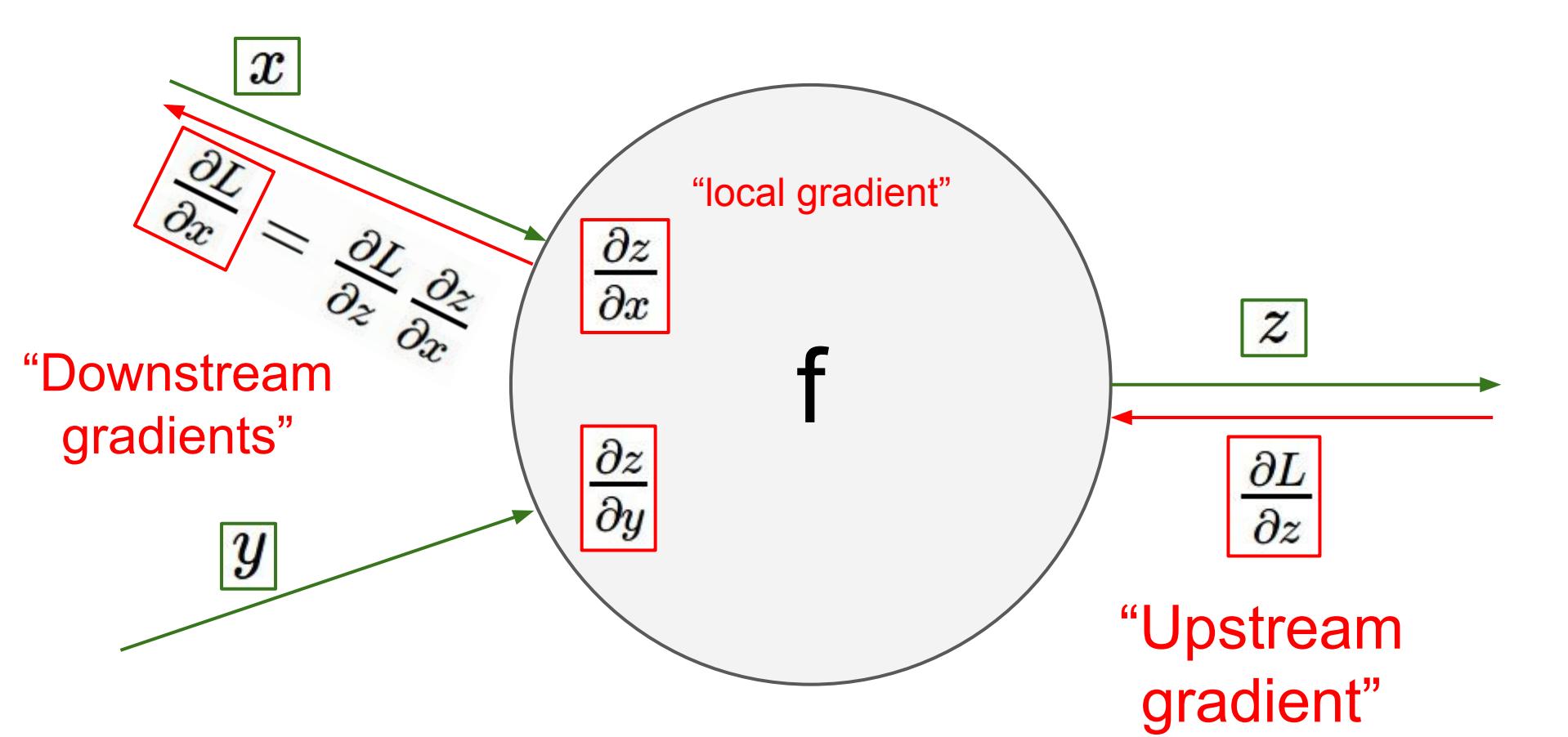
Upstream
gradient

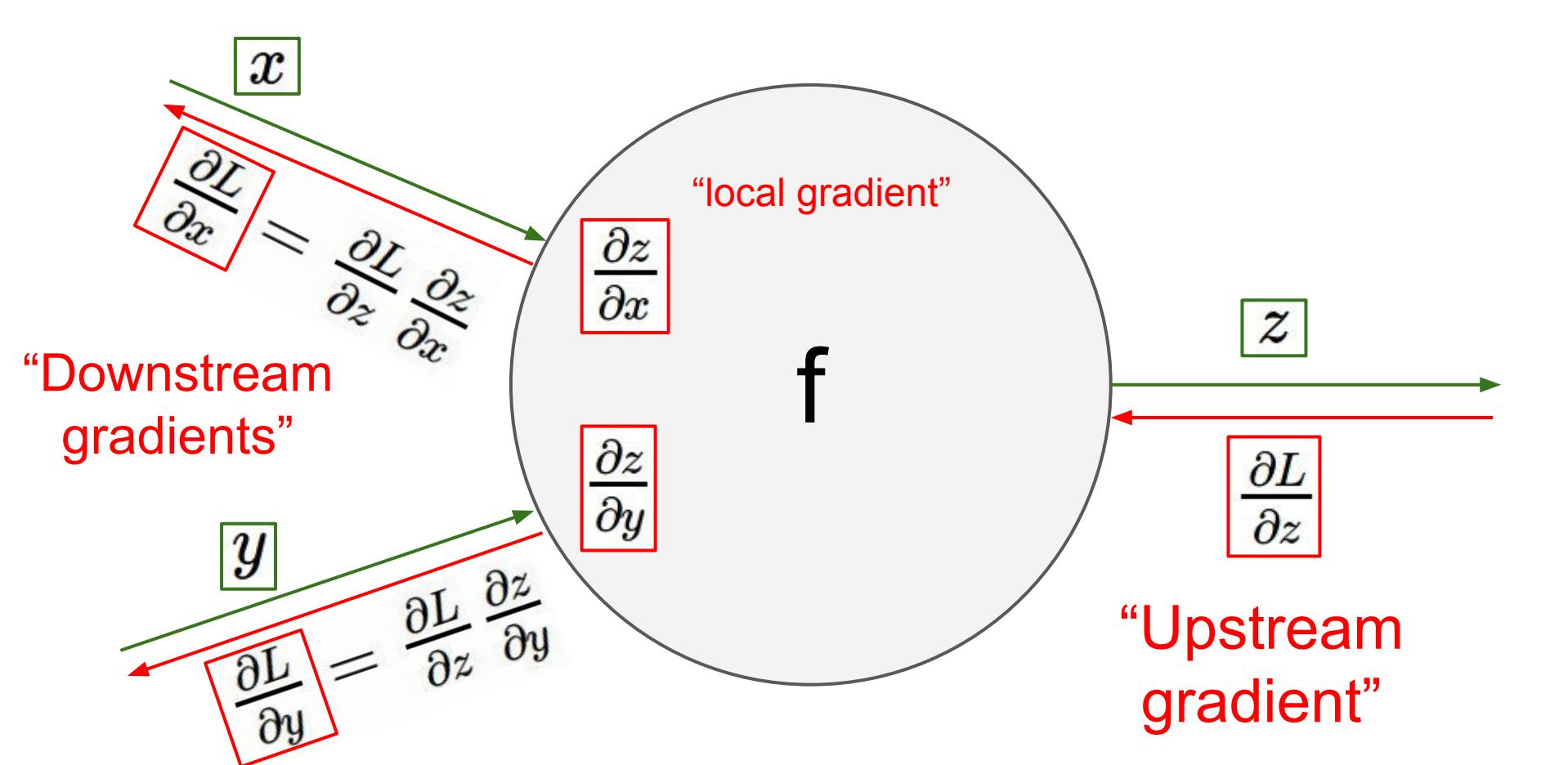
Local
gradient

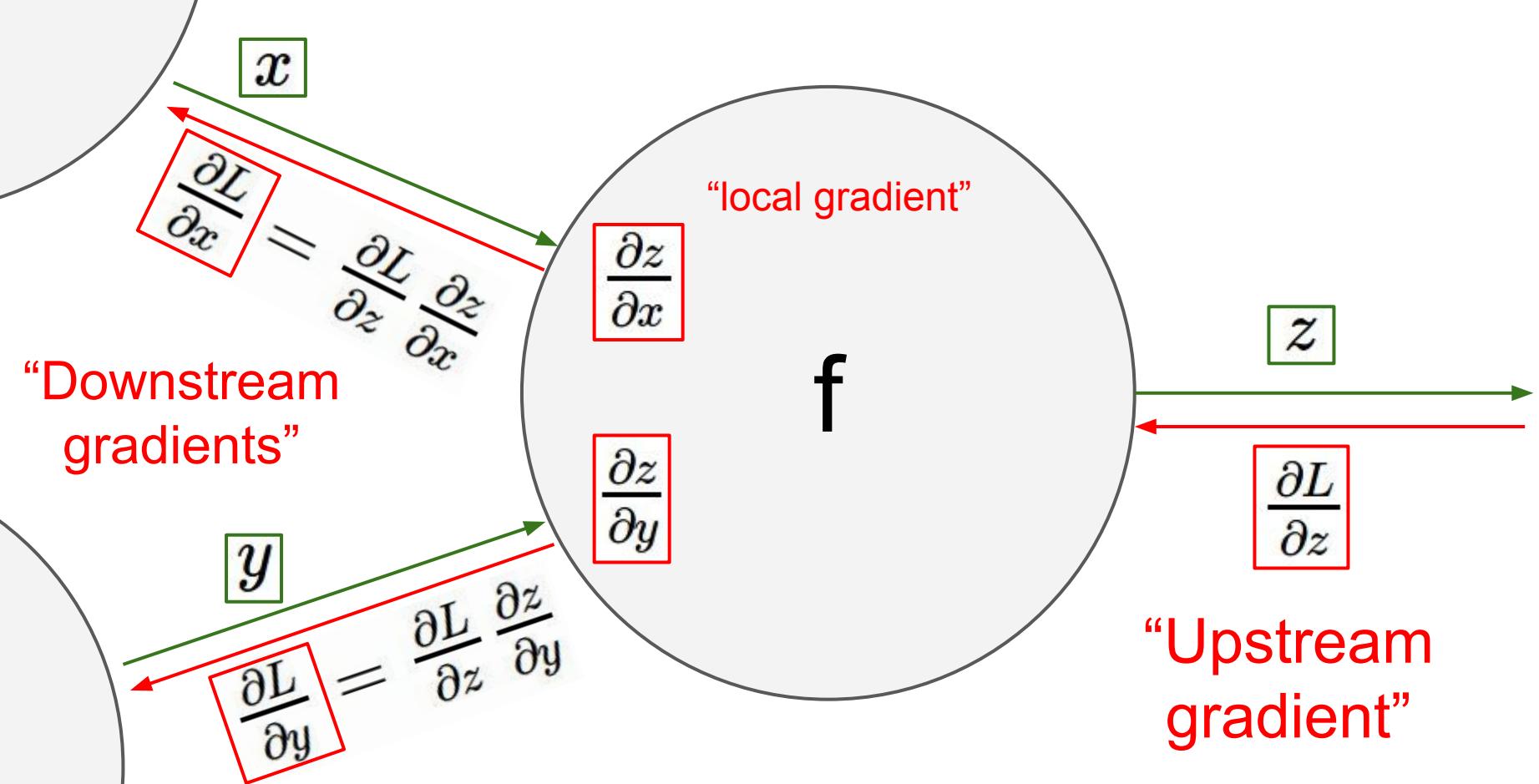






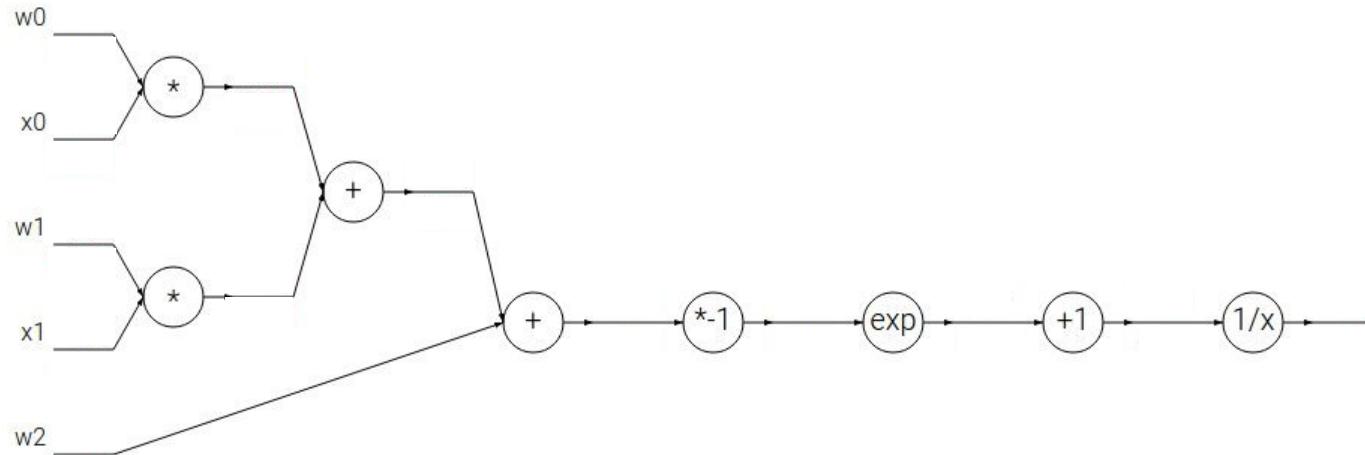






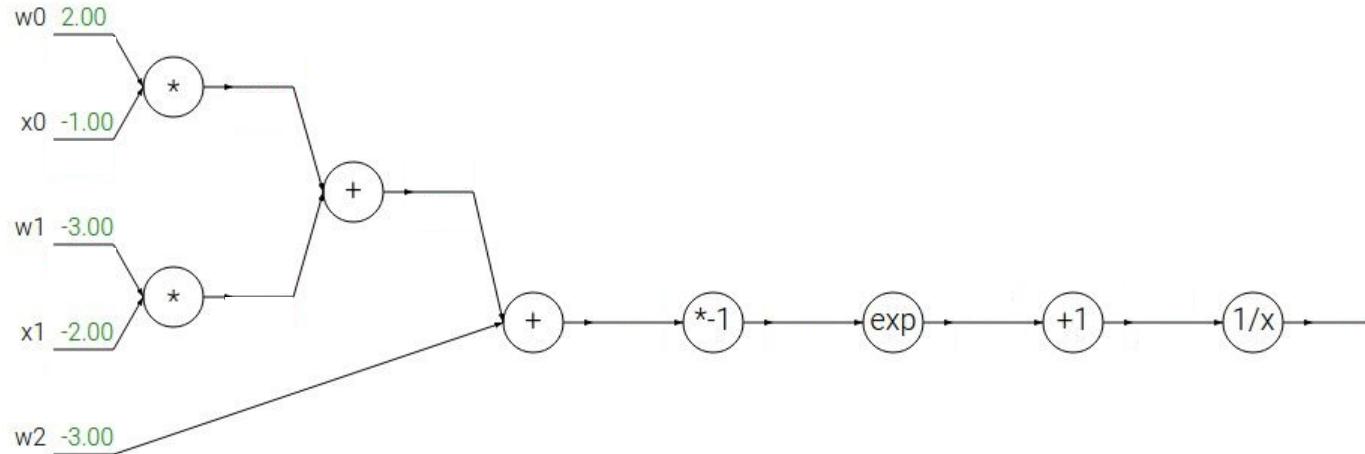
Another example:

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



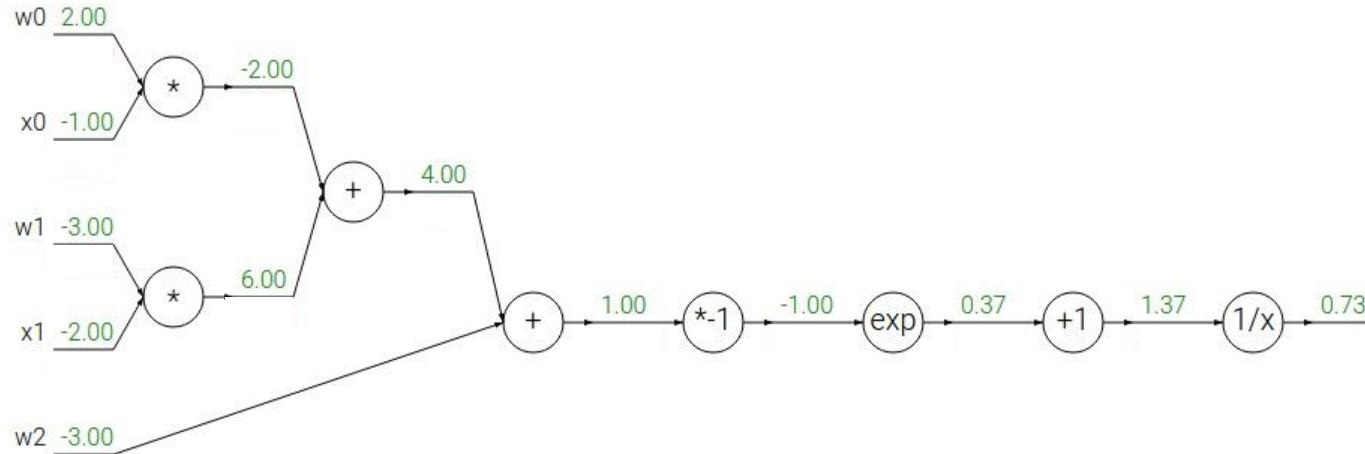
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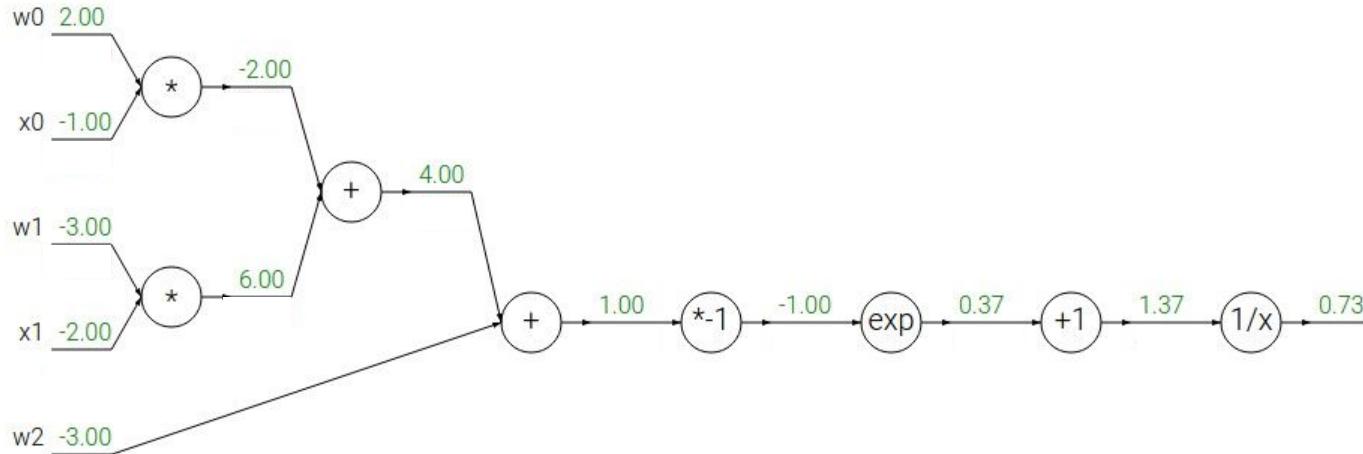
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Another example:

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



$$f(x) = e^x$$

\rightarrow

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

\rightarrow

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

\rightarrow

$$\frac{df}{dx} = -1/x^2$$

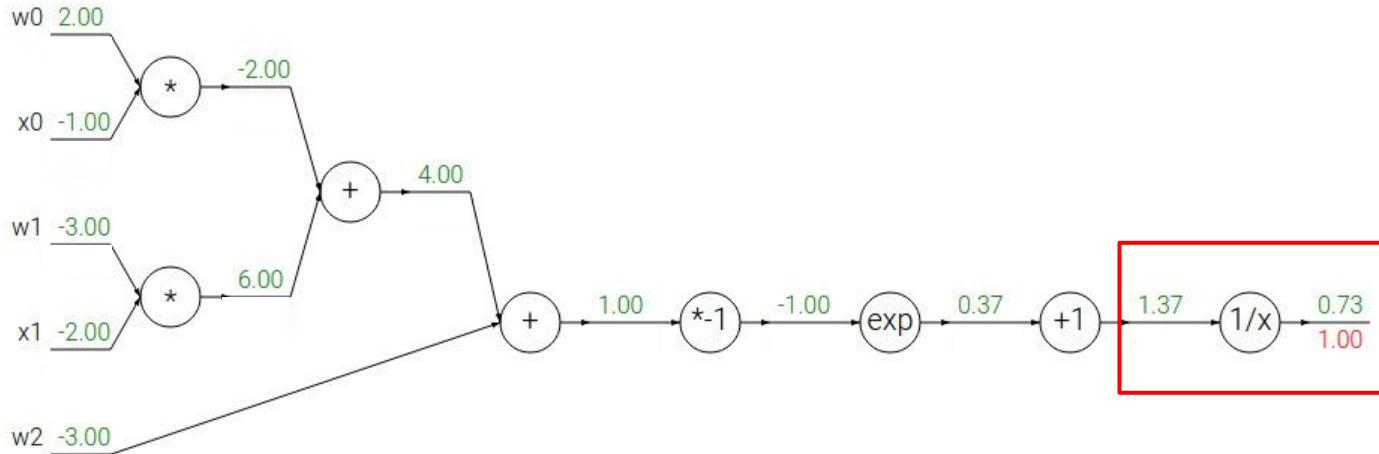
$$f_c(x) = c + x$$

\rightarrow

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

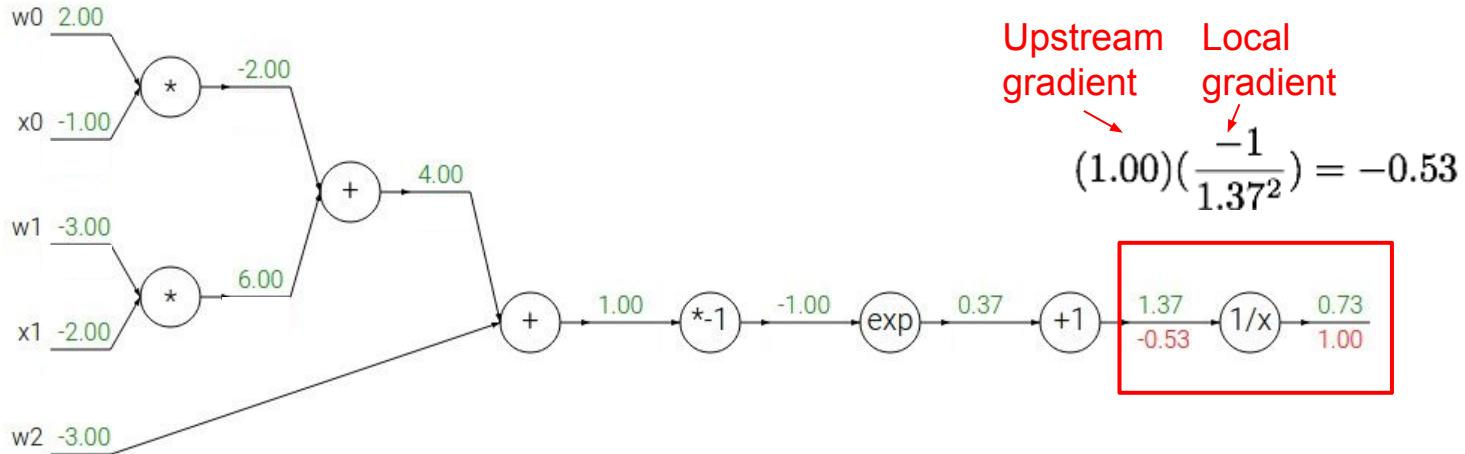
$$f_c(x) = c + x$$

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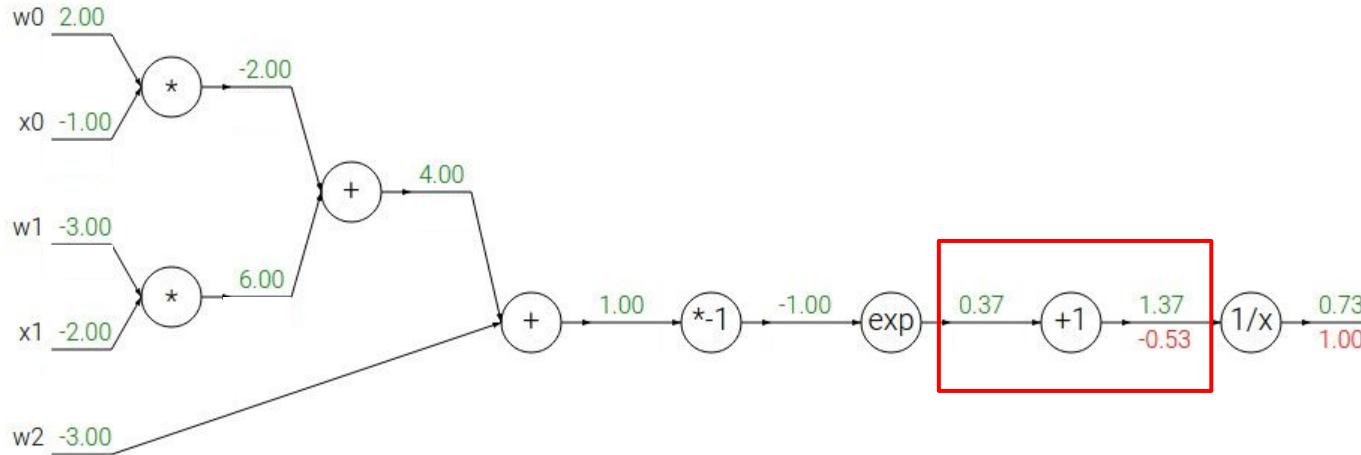
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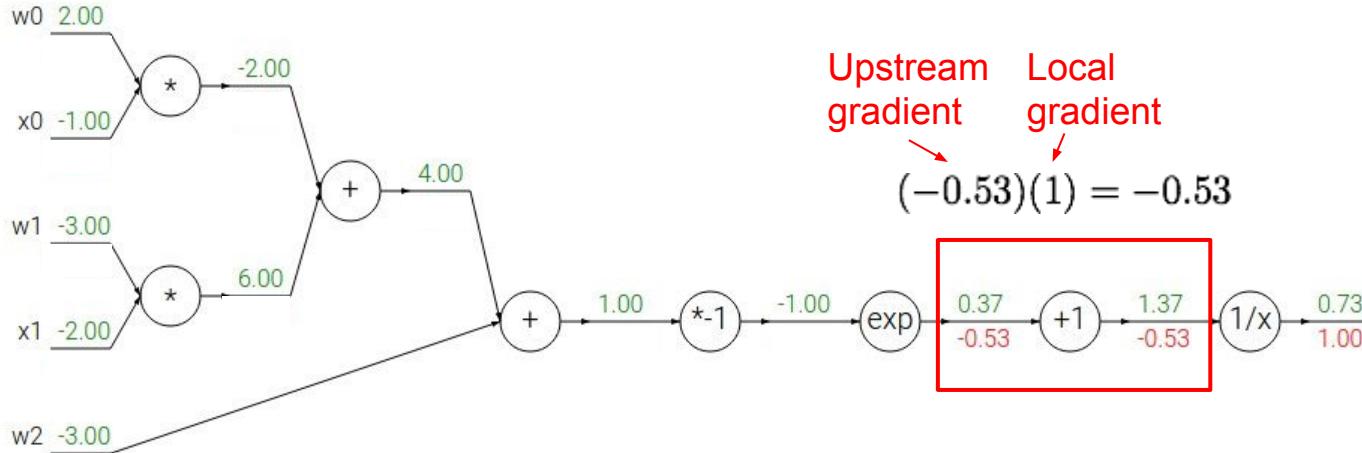
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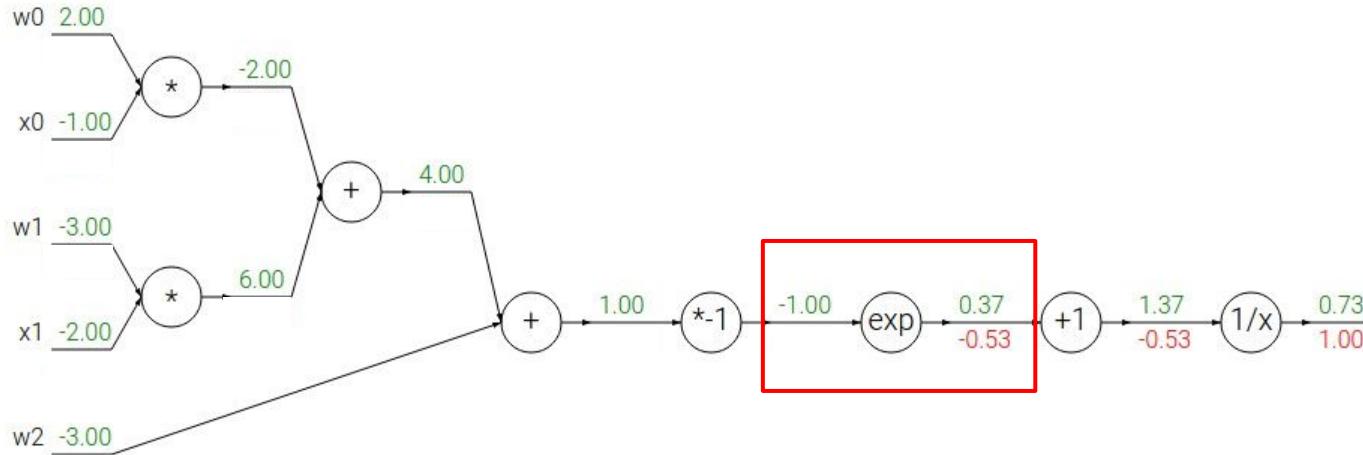
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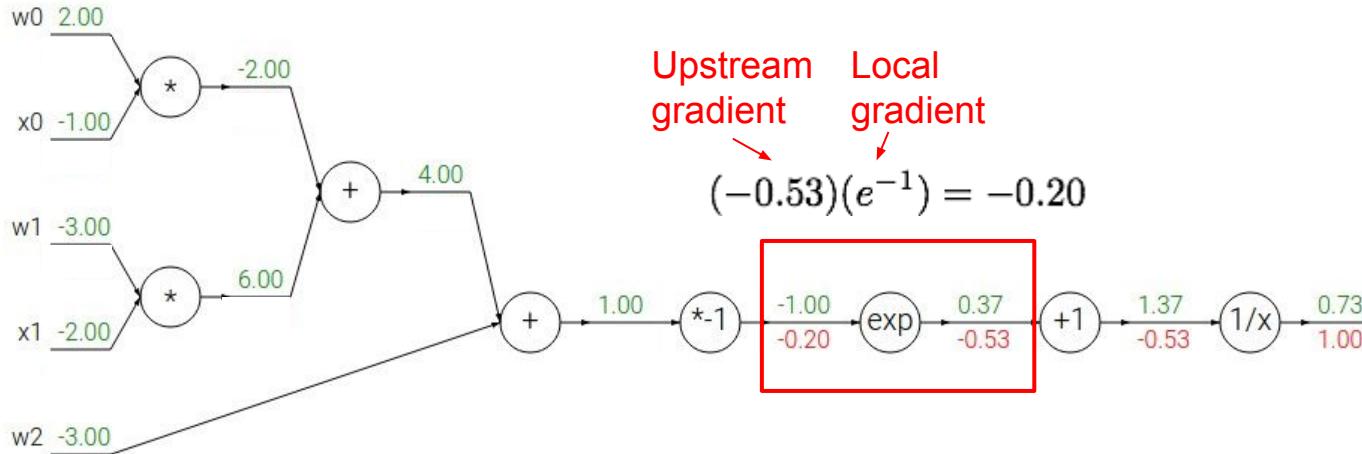
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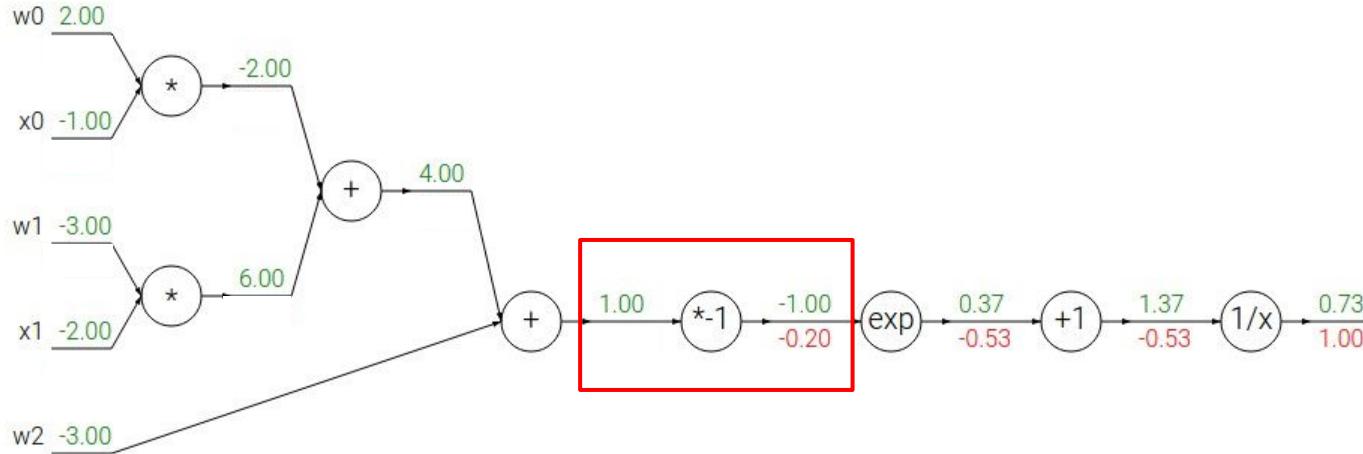
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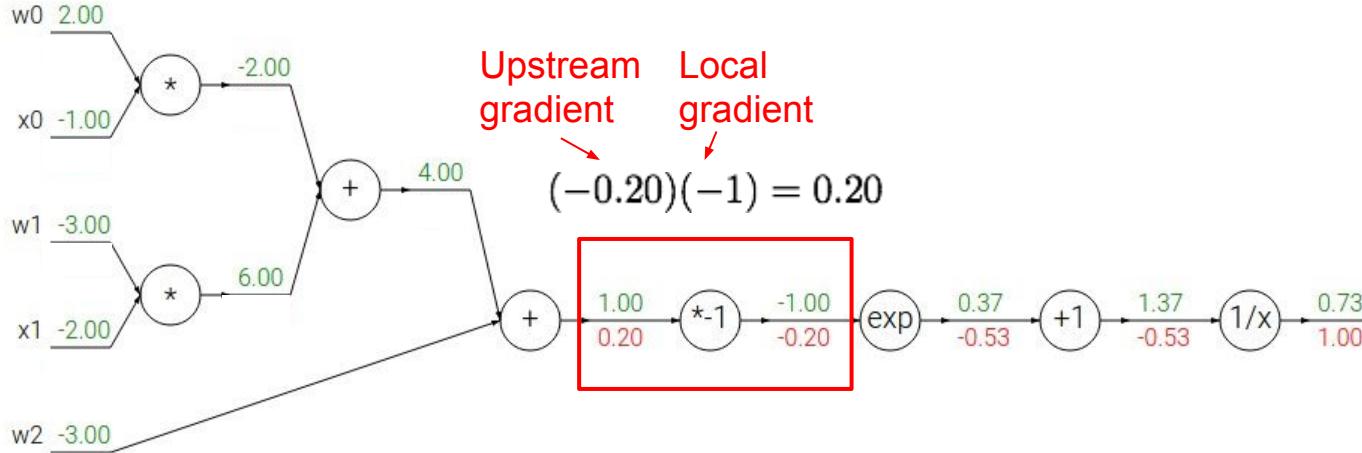
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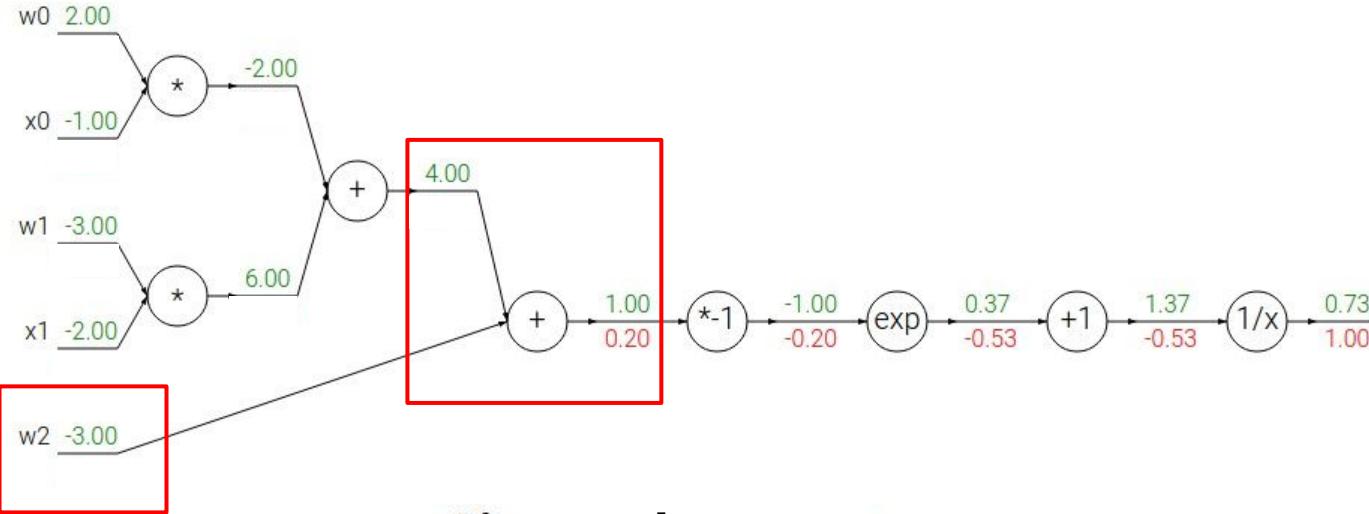
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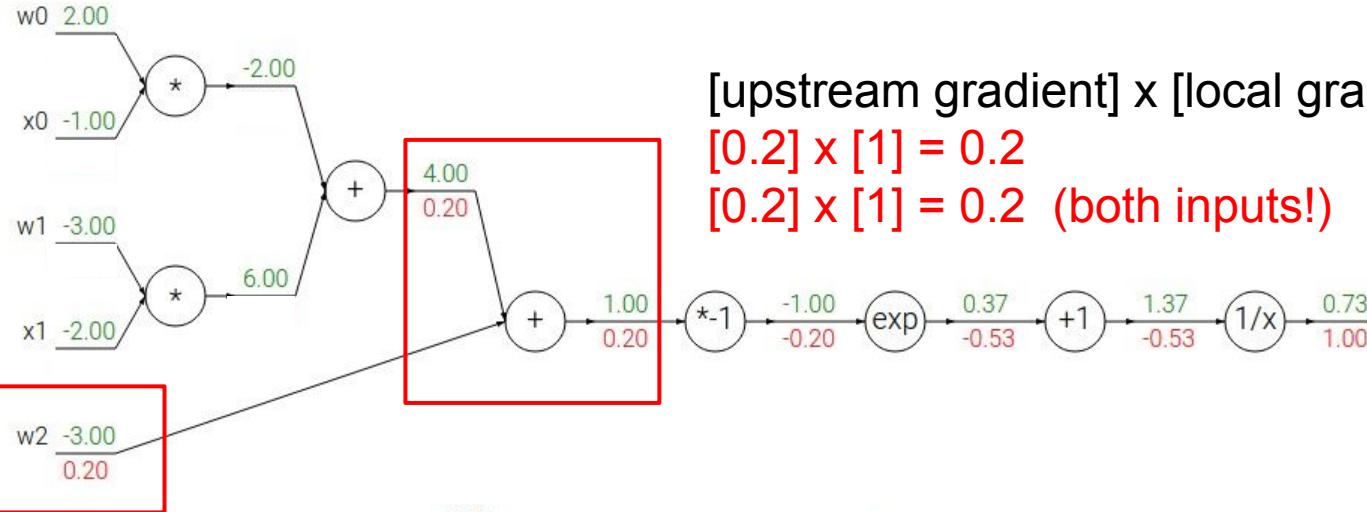
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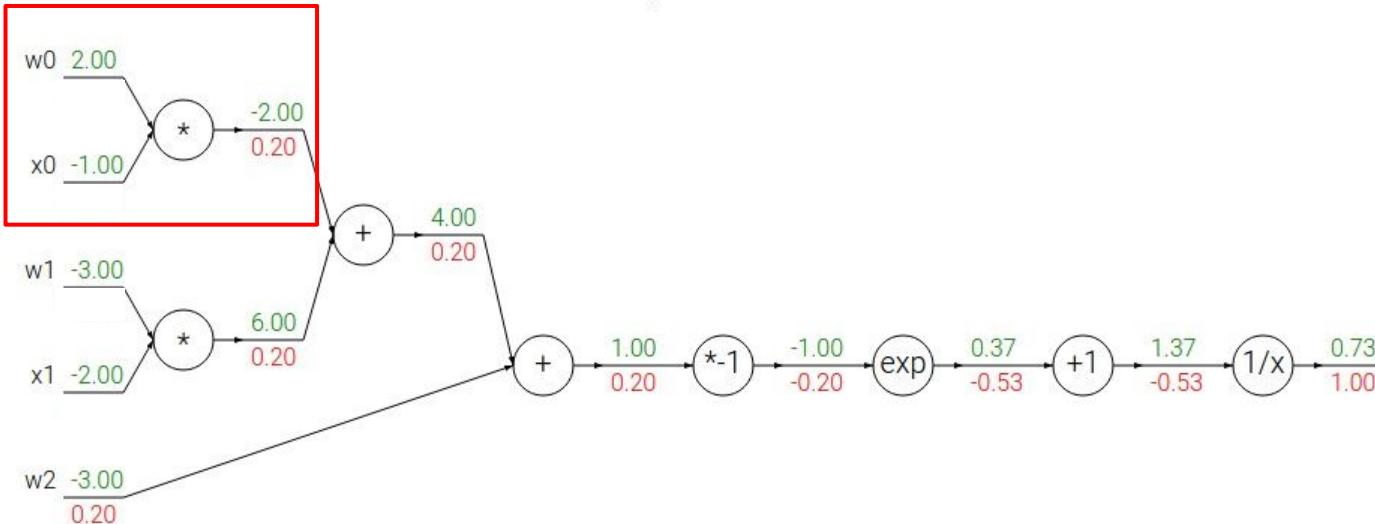
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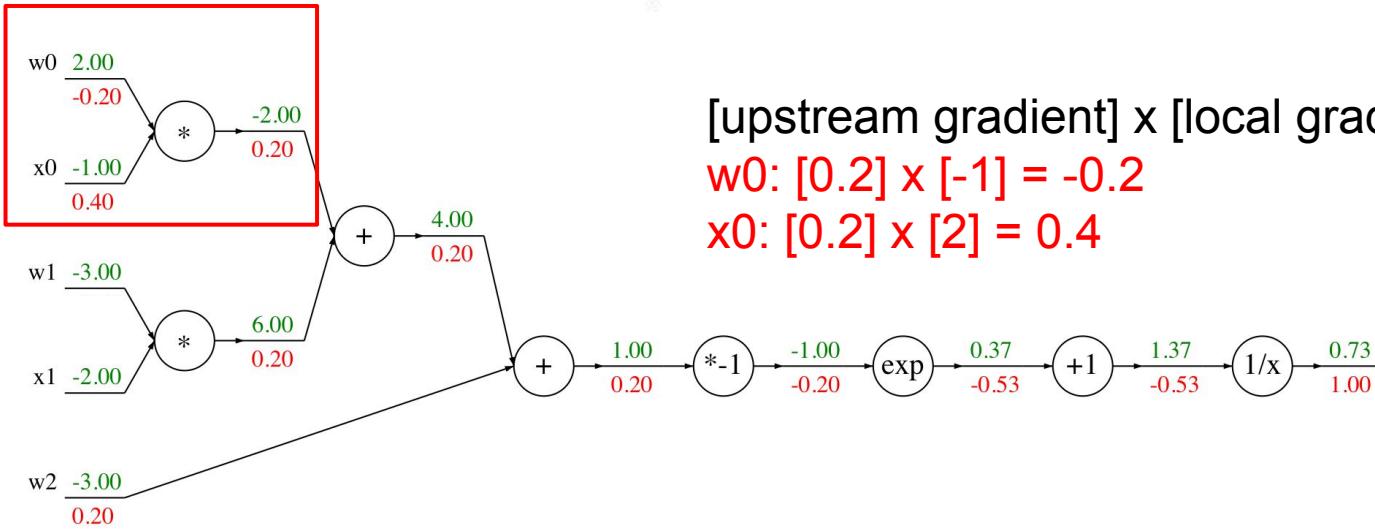
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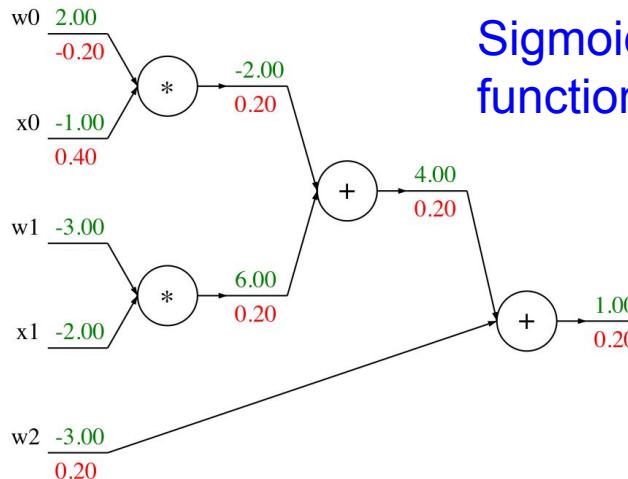
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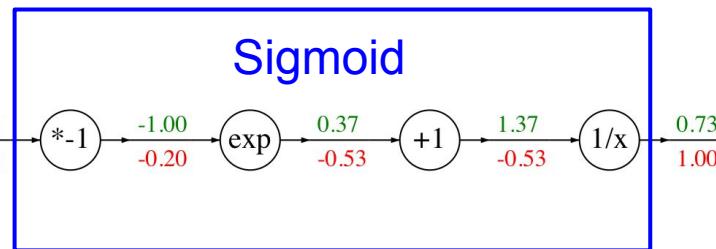
Another example:

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



Sigmoid
function

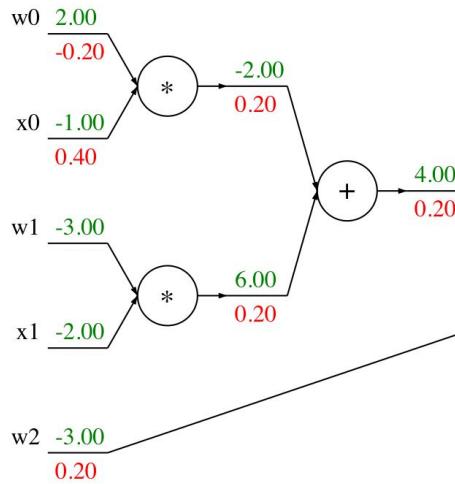
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



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

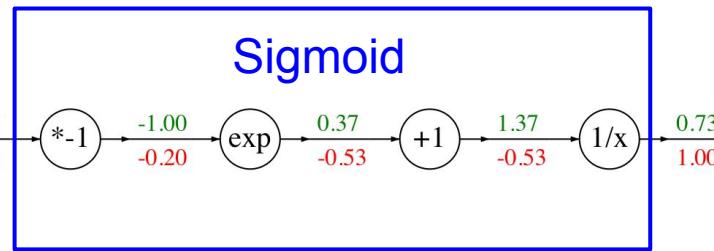
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Sigmoid
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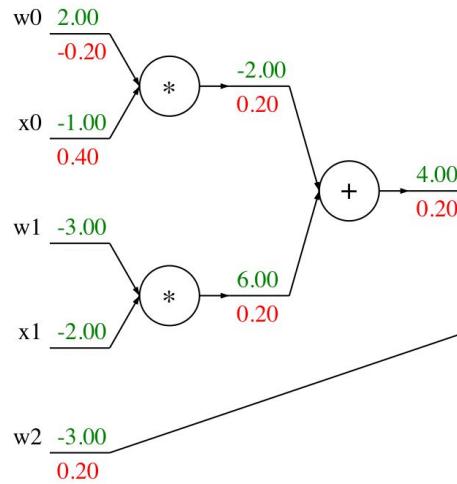
Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

Sigmoid local gradient:

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

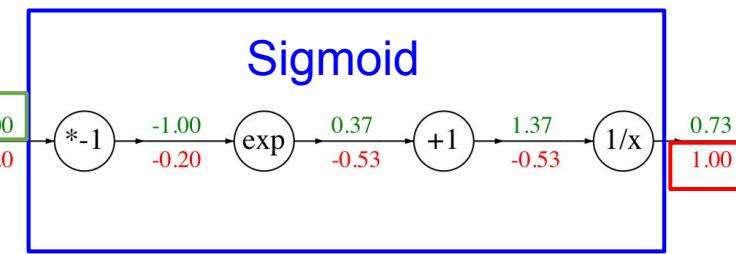
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Sigmoid
function

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



$$\begin{aligned} &[\text{upstream gradient}] \times [\text{local gradient}] \\ &[1.00] \times [(1 - 1/(1+e^{-1})) (1/(1+e^{-1}))] = 0.2 \end{aligned}$$

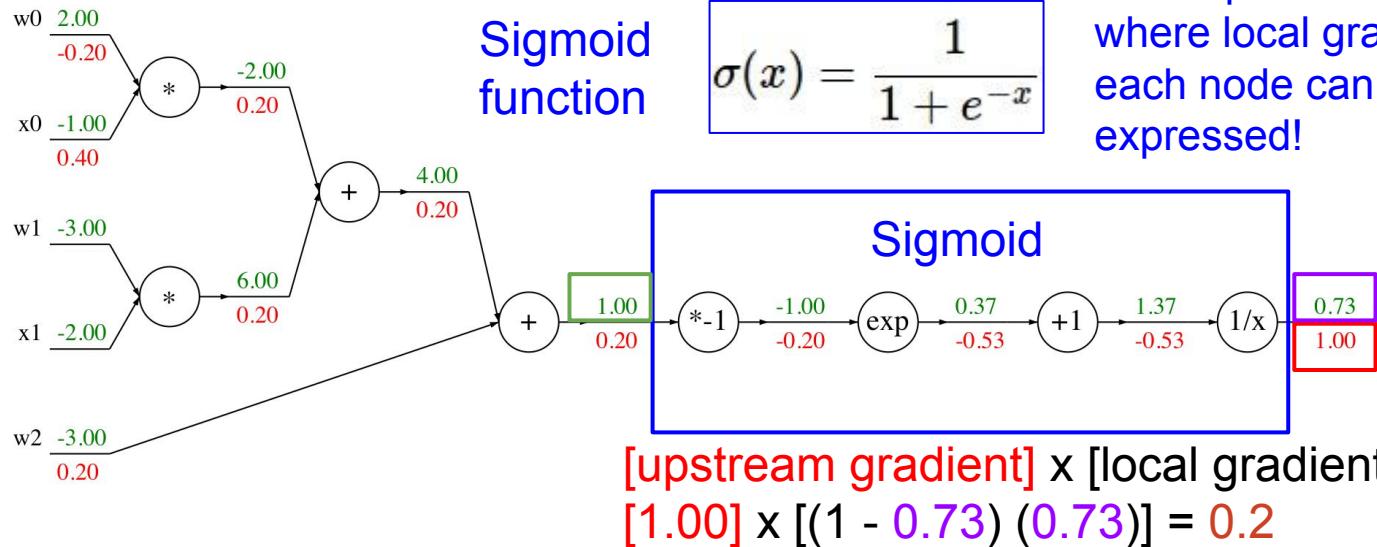
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Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

Another example:

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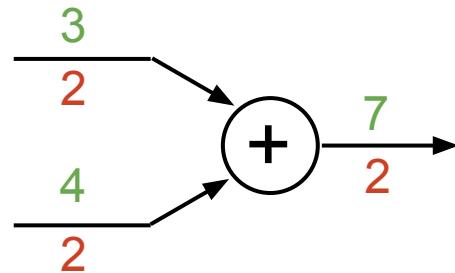
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Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

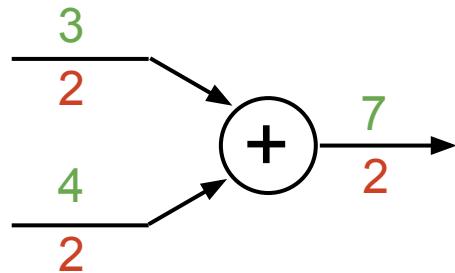
Patterns in gradient flow

add gate: gradient distributor

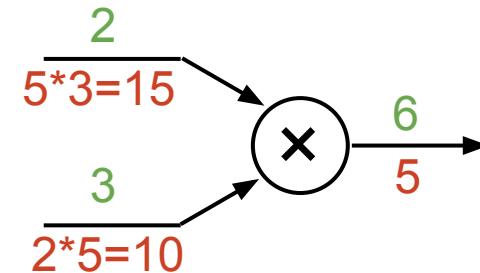


Patterns in gradient flow

add gate: gradient distributor

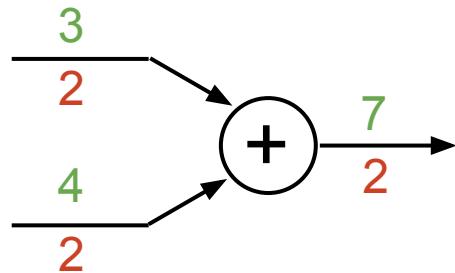


mul gate: “swap multiplier”

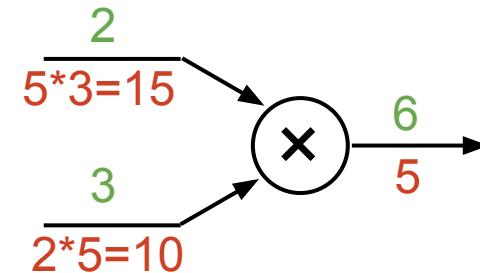


Patterns in gradient flow

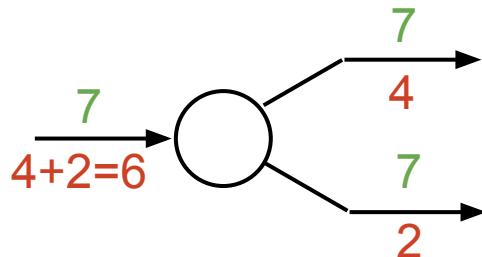
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mul gate: “swap multiplier”

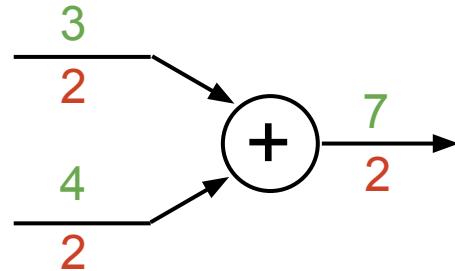


copy gate: gradient adder

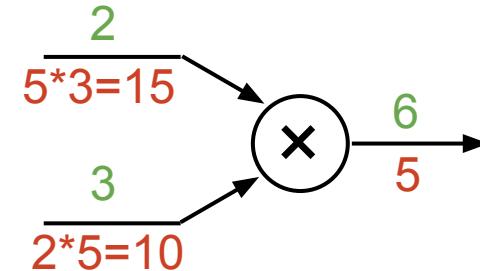


Patterns in gradient flow

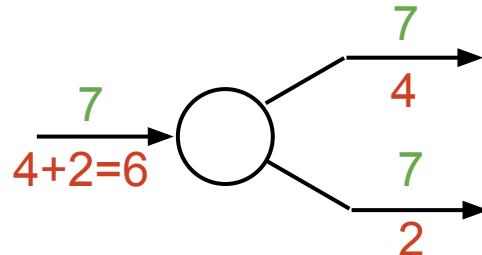
add gate: gradient distributor



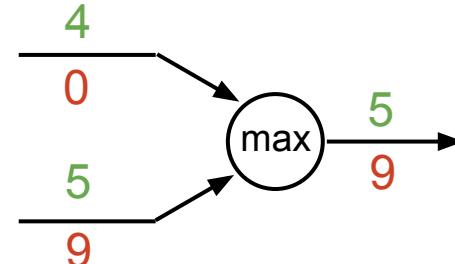
mul gate: “swap multiplier”



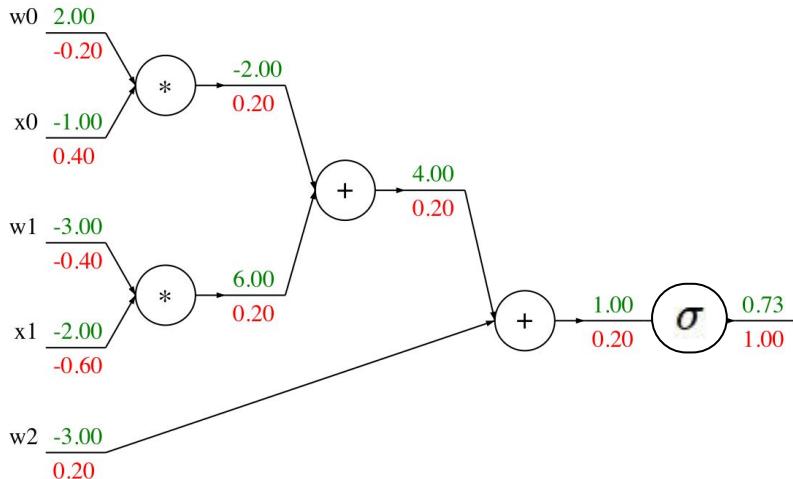
copy gate: gradient adder



max gate: gradient router



Backprop Implementation: “Flat” code



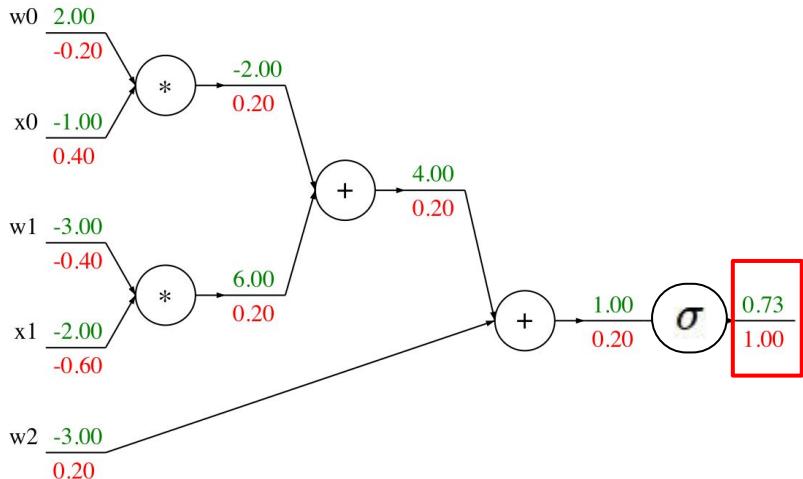
Forward pass:
Compute output

```
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

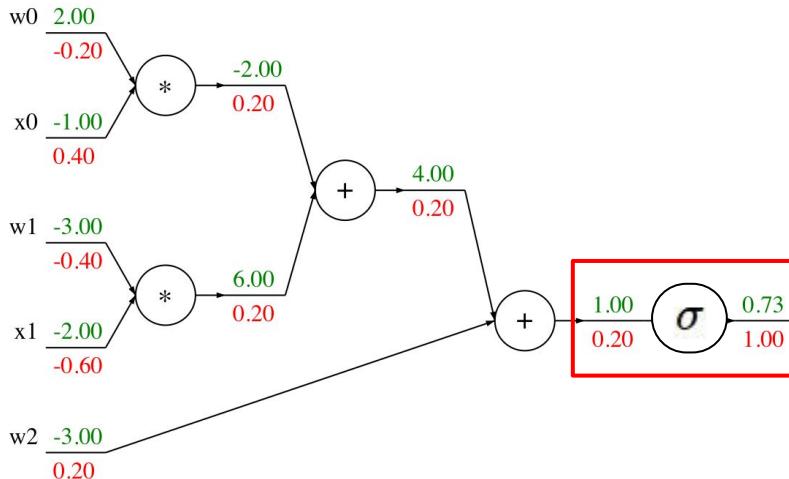
```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

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



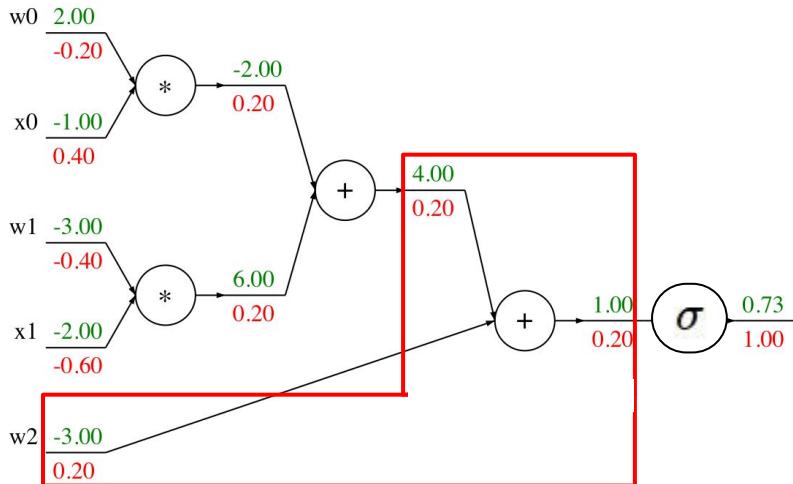
Forward pass:
Compute output

Sigmoid

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

```
grad_L = 1.0  
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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



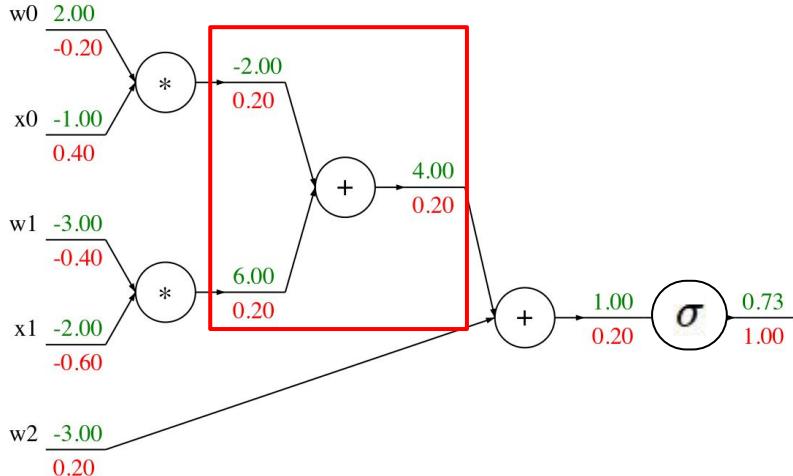
Forward pass:
Compute output

Add gate

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

Backprop Implementation: “Flat” code



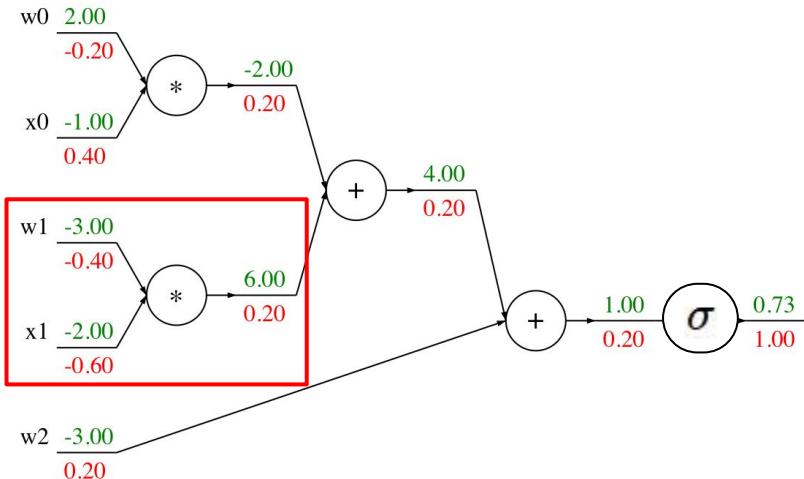
Forward pass:
Compute output

Add gate

```
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    s0 = w0 * x0  
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```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
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grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Backprop Implementation: “Flat” code



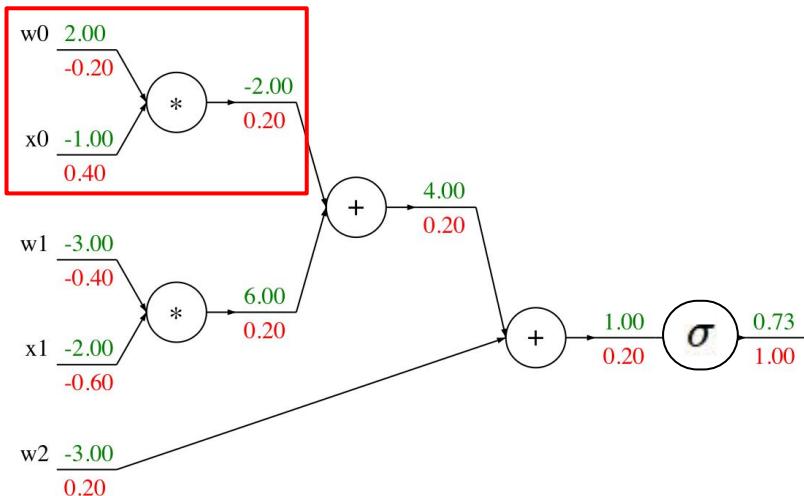
Forward pass:
Compute output

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

```
grad_L = 1.0  
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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)
```

```
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
```

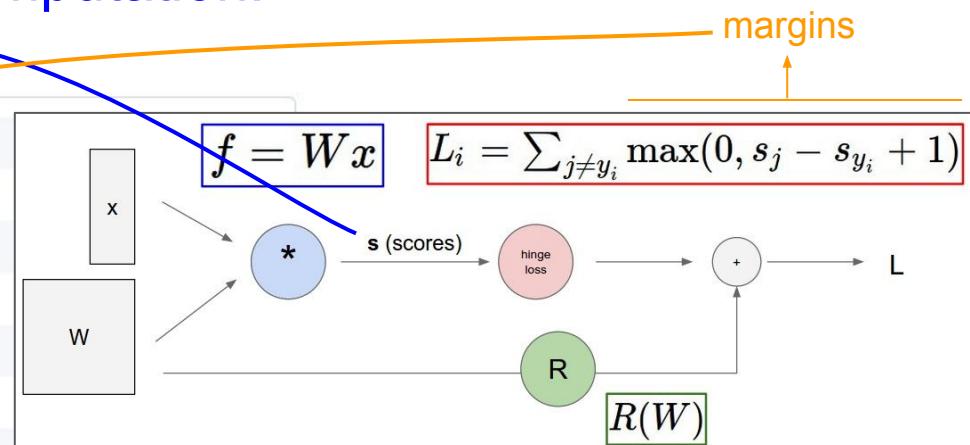
Multiply gate

“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 = #...
```



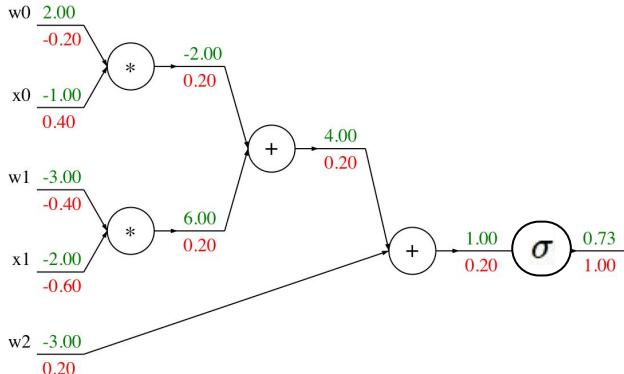
“Flat” Backprop: Do this for assignment 1!

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

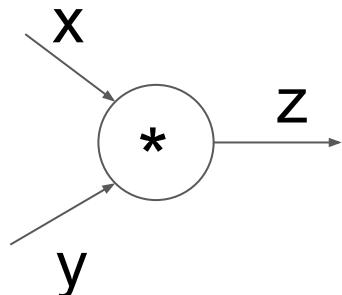
Graph (or Net) object (*rough pseudo code*)



```
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

pytorch / pytorch		
Code	Issues 2,286	Pull requests 561
Tree: 517c7c9861 → pytorch / aten / src / THNN / generic /	Create new file	Upload files
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
Col2im.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ELU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
FeatureLPPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
GatedLinearUnit.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
HardTanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Im2Col.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
IndexLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LeakyReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LogSigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MSECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiLabelMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
RReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Sigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SmoothL1Criterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftPlus.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftShrink.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SparseLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAdaptiveAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialDilatedMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialFractionalMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialUpSamplingBilinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
THNN.h	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Tanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalRowConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalUpSamplingLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAdaptiveAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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VolumetricFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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

```
1 #ifndef TH_GENERIC_FILE
2 #define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
3 #else
4
5 void THNN_(Sigmoid_updateOutput)(
6     THNNState *state,
7     THTensor *input,
8     THTensor *output)
9 {
10    THTensor_(sigmoid)(output, input);
11 }
12
13 void THNN_(Sigmoid_updateGradInput)(
14     THNNState *state,
15     THTensor *gradOutput,
16     THTensor *gradInput,
17     THTensor *output)
18 {
19     THNN_CHECK_NELEMENT(output, gradOutput);
20     THTensor_(resizeAs)(gradInput, output);
21     TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
22         scalar_t z = *output_data;
23         *gradInput_data = *gradOutput_data * (1. - z) * z;
24     );
25 }
26
27 #endif
```

Forward

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

[Source](#)

PyTorch sigmoid layer

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22         scalar_t z = *output_data;
23         *gradInput_data = *gradOutput_data * (1. - z) * z;
24     );
25 }
26
27 #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

```
1 #ifndef TH_GENERIC_FILE
2 #define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
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5 void THNN_(Sigmoid_updateOutput)(
6     THNNState *state,
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16     THTensor *gradInput,
17     THTensor *output)
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20     THTensor_(resizeAs)(gradInput, output);
21     TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
22         scalar_t z = *output_data;
23         *gradInput_data = *gradOutput_data * (1. - z) * z;
24     );
25 }
26
27 #endif
```

Forward

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

```
static void sigmoid_kernel(TensorIterator& iter) {
    AT_DISPATCH_FLOATING_TYPES(iter.dtype(), "sigmoid_cpu", [&]() {
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            [=](scalar_t a) { 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...

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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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

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Vector to Vector

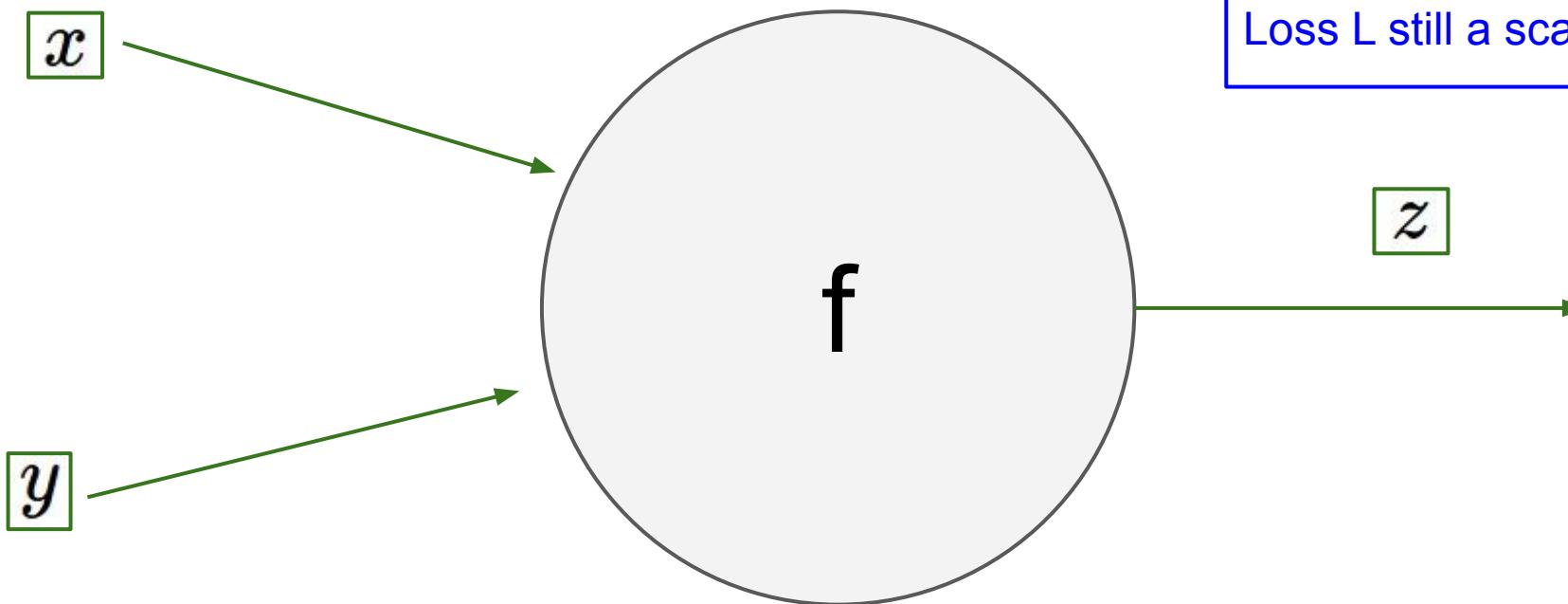
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

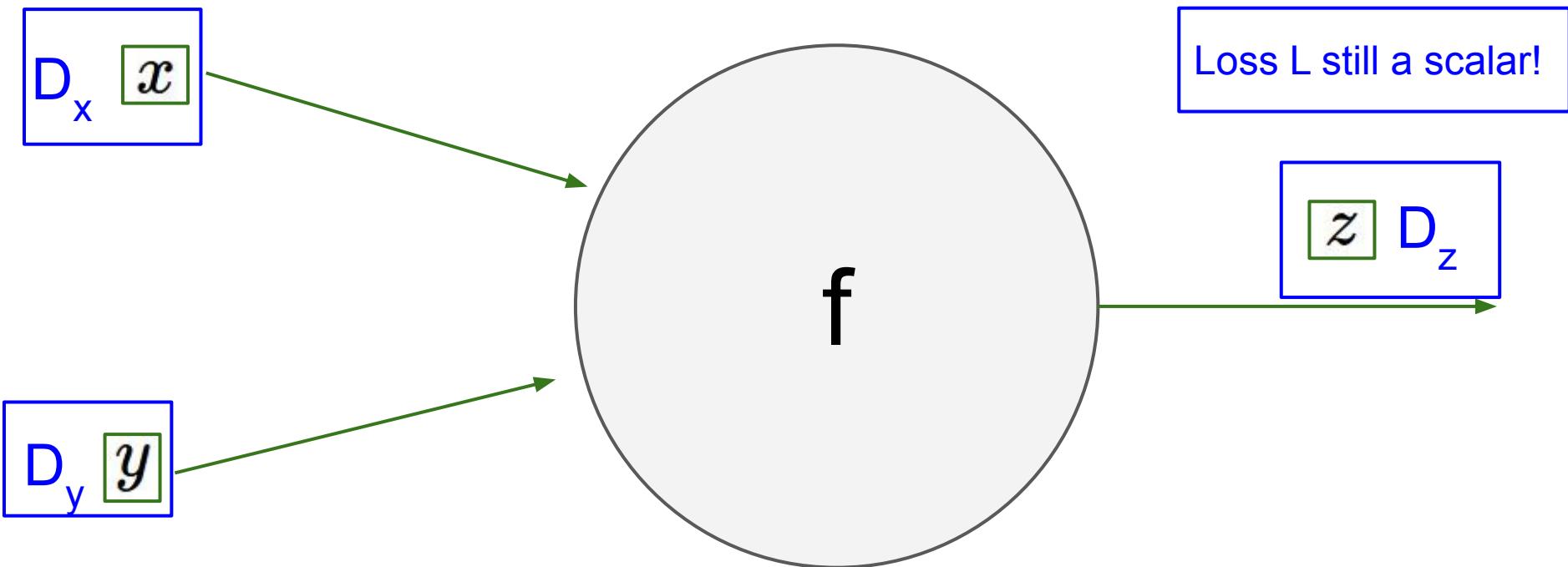
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x} \right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

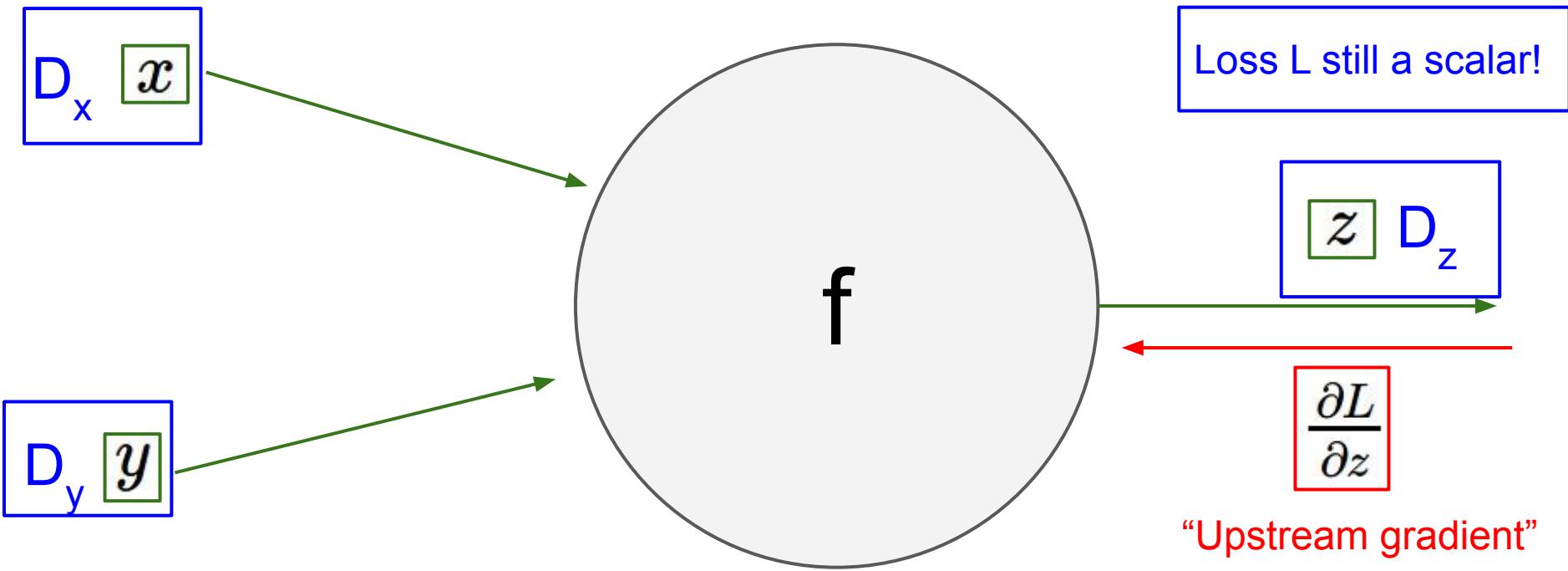
Backprop with Vectors



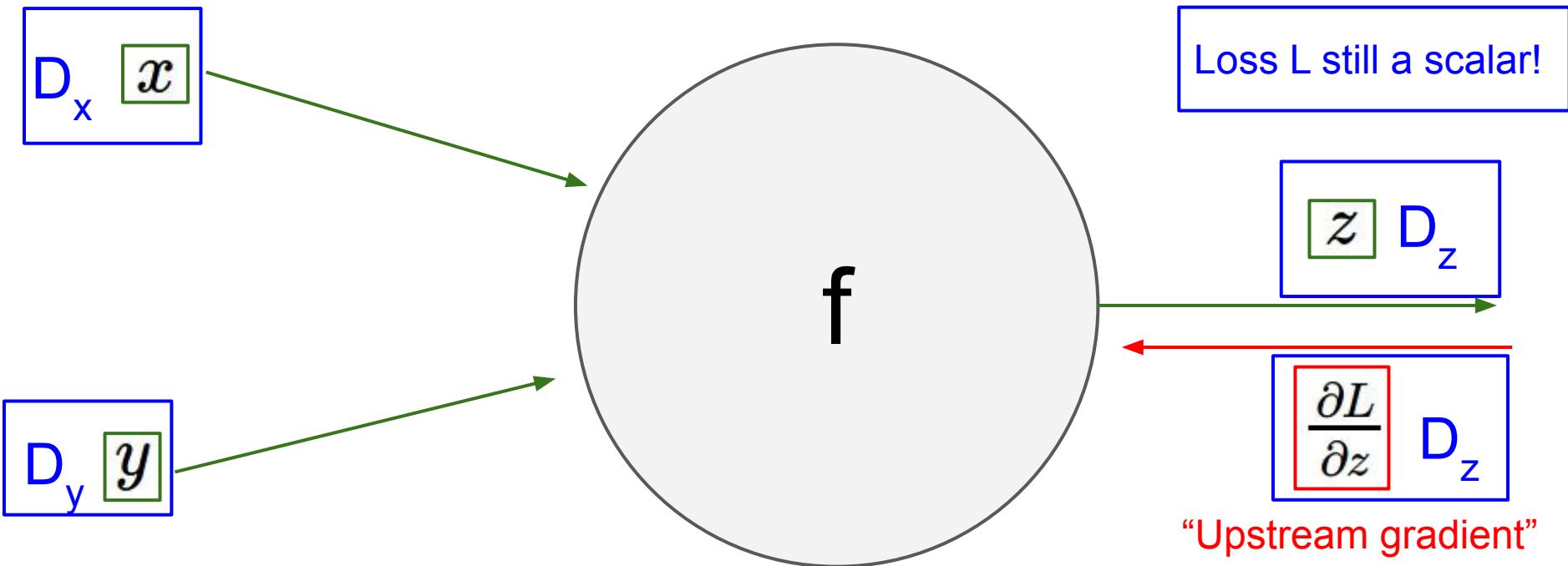
Backprop with Vectors



Backprop with Vectors



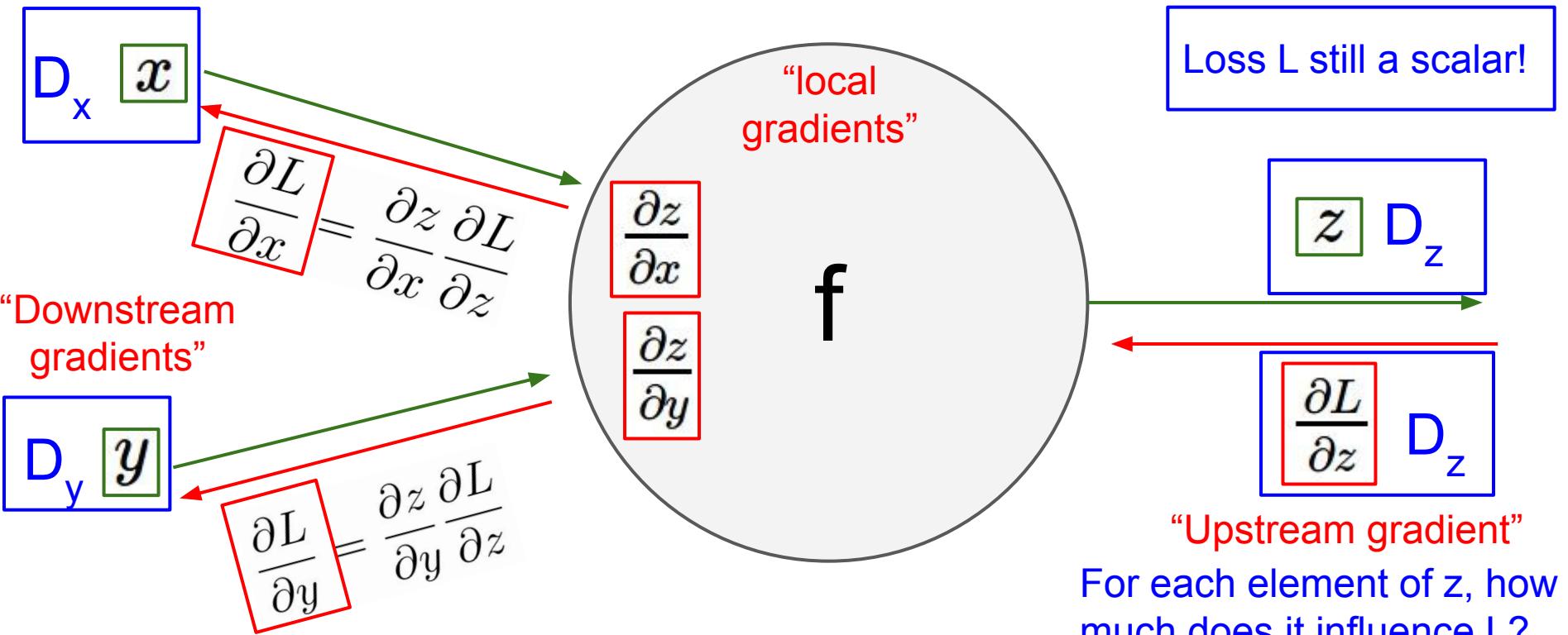
Backprop with Vectors



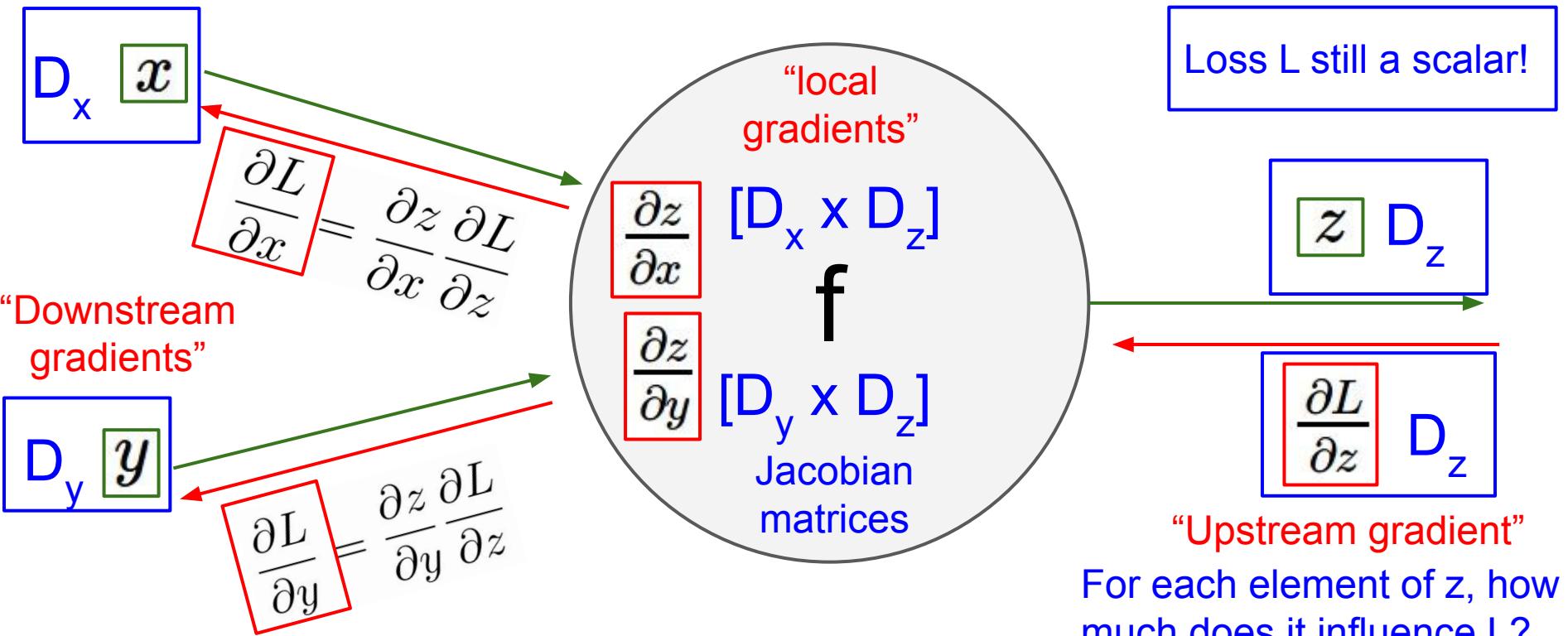
Loss L still a scalar!

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

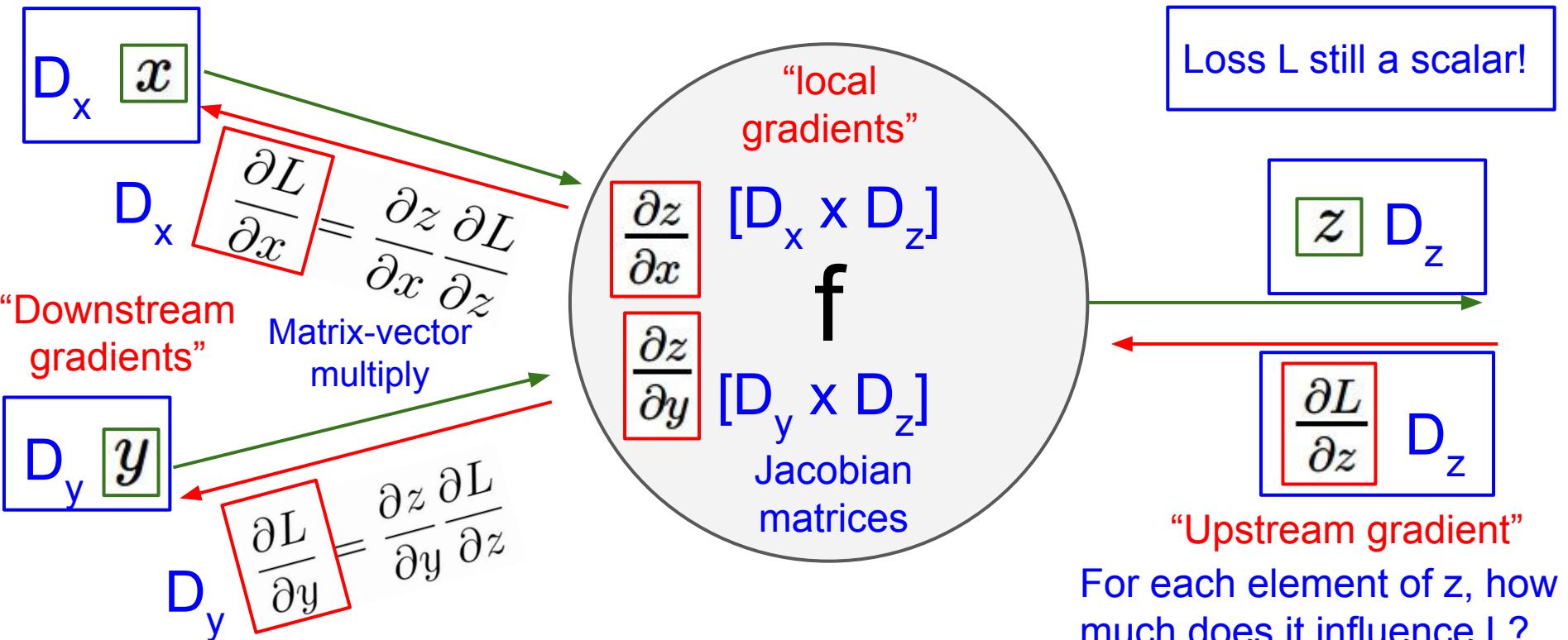
Backprop with Vectors



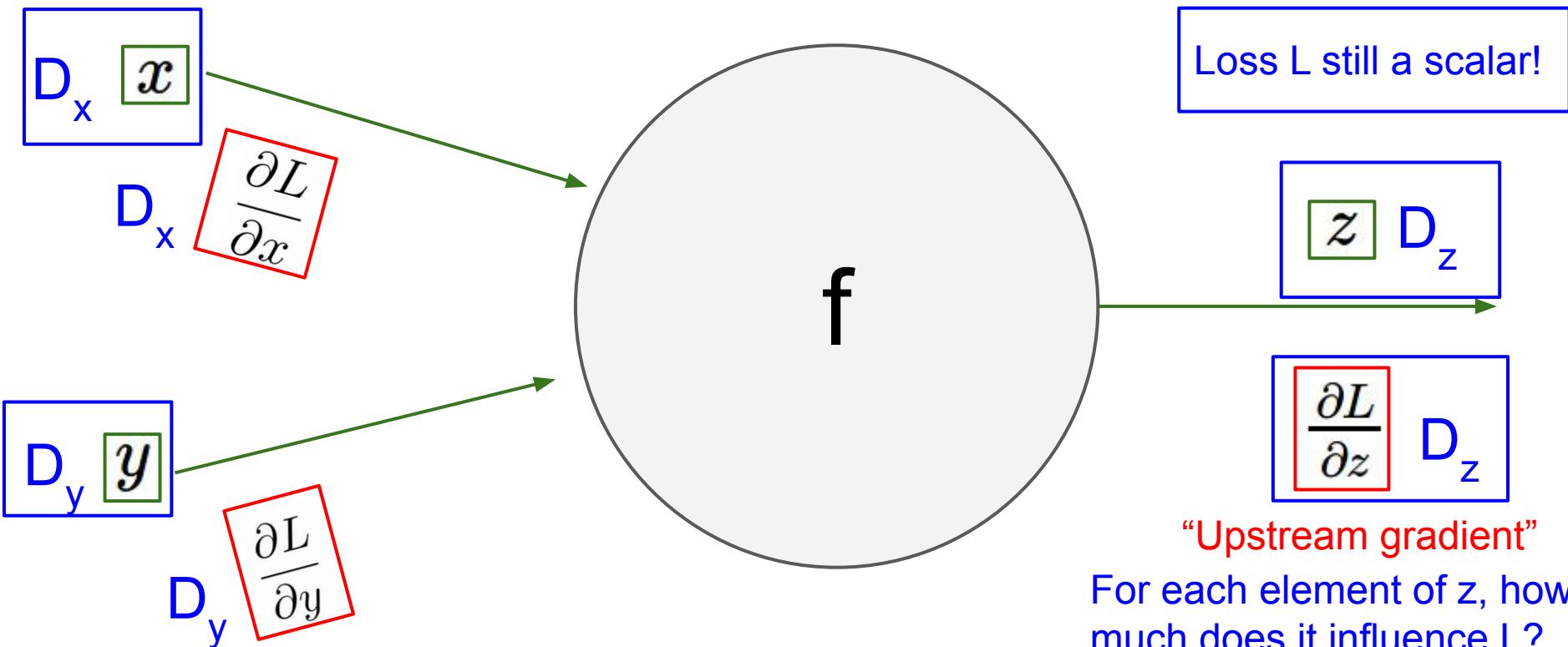
Backprop with Vectors



Backprop with Vectors



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



Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\hspace{1cm}} \begin{array}{c} \text{f}(x) = \max(0, x) \\ (\text{elementwise}) \end{array}$$

4D output z :

$$\begin{array}{l} \xrightarrow{\hspace{1cm}} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix} \\ \xrightarrow{\hspace{1cm}} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 3 \end{bmatrix} \\ \xrightarrow{\hspace{1cm}} \begin{bmatrix} 3 \\ 0 \\ 0 \\ 1 \end{bmatrix} \\ \xrightarrow{\hspace{1cm}} \begin{bmatrix} 0 \\ 3 \\ 1 \\ 0 \end{bmatrix} \end{array}$$

Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\hspace{1cm}} \begin{array}{c} f(x) = \max(0, x) \\ (\text{elementwise}) \end{array}$$

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4D dL/dz :

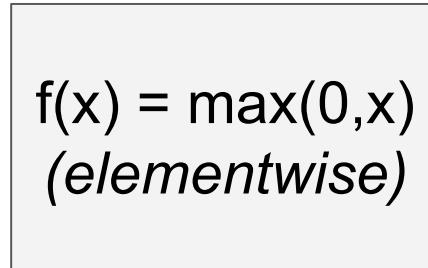
$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

Upstream
gradient

Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\quad}$$



4D output z :

$$\xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

Jacobian $\frac{\partial z}{\partial x}$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

4D $\frac{\partial L}{\partial z}$:

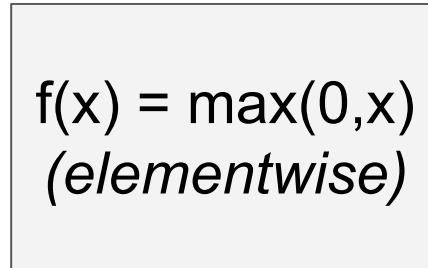
$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \xleftarrow{\quad}$$

Upstream
gradient

Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\quad}$$



4D output z :

$$\xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

$[dz/dx]$ $[dL/dz]$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} [4]$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \end{bmatrix} [-1]$$

$$\begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix} [5]$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \end{bmatrix} [9]$$

4D dL/dz :

$$\leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

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$$\leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

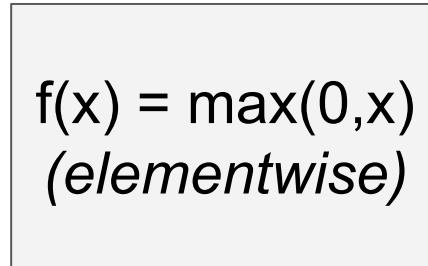
$$\leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

Upstream
gradient

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4D input x :

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4D output z :

$$\xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D dL/dx :

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \xleftarrow{\quad}$$

$[dz/dx] [dL/dz]$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

4D dL/dz :

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \xleftarrow{\quad}$$

Upstream
gradient

Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\quad} \begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$$

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

4D output z :

$$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix} \xleftarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

$$f(x) = \max(0, x)$$

(elementwise)

4D dL/dx :

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \xleftarrow{\quad} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

4D dL/dz :

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \xleftarrow{\quad} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

Upstream
gradient

Backprop with Vectors

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4D output z :

$$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix} \xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

$$f(x) = \max(0, x) \quad (\text{elementwise})$$

4D dL/dx :

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \leftarrow$$

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

$[dz/dx]$ $[dL/dz]$

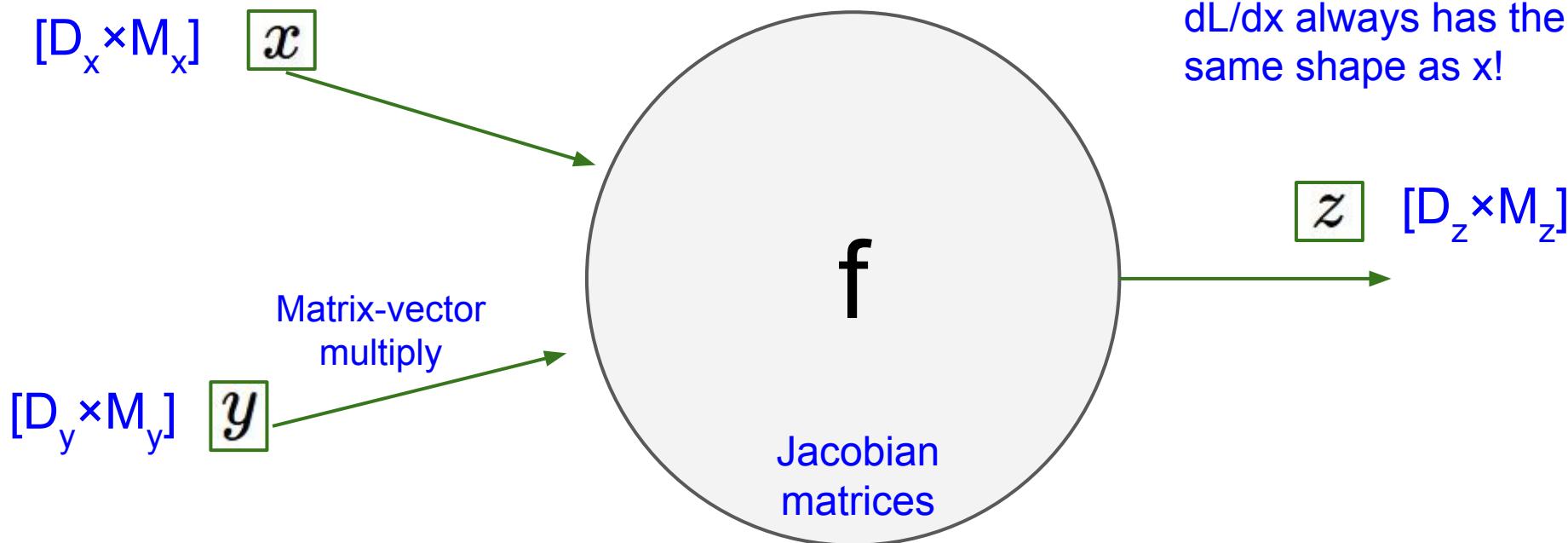
4D dL/dz :

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

Upstream
gradient

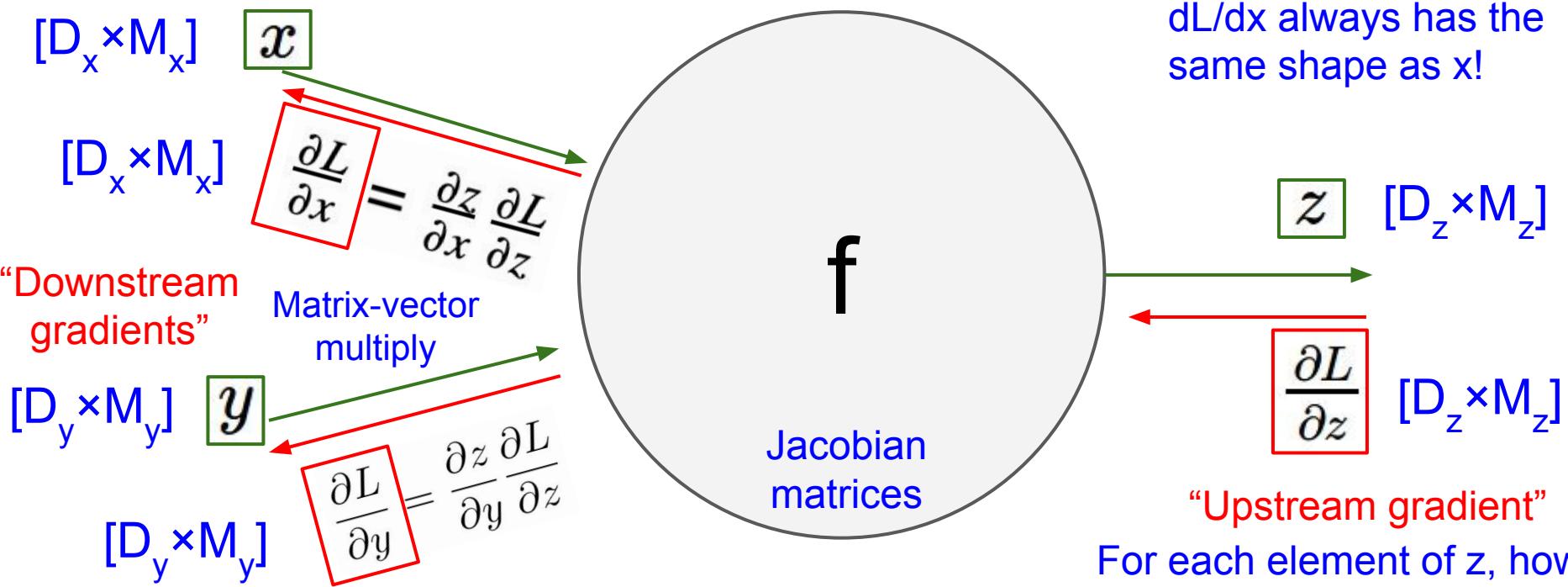
Backprop with Matrices (or Tensors)

Loss L still a scalar!



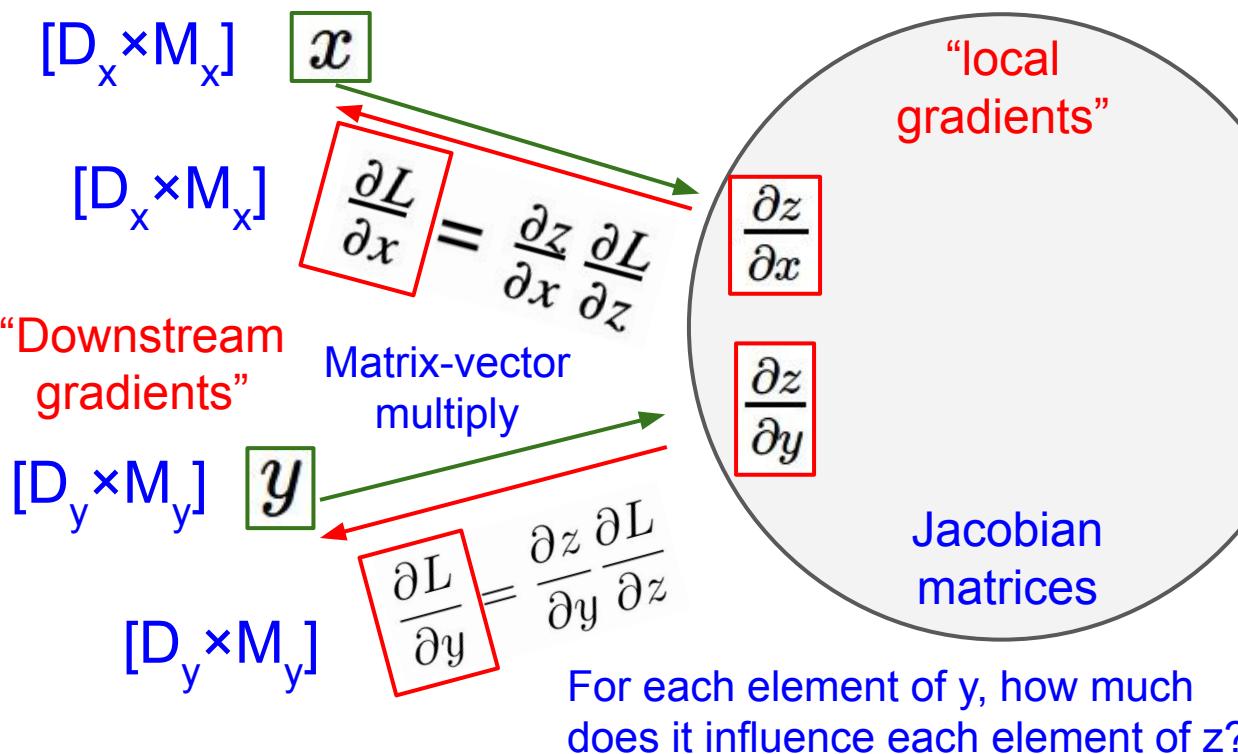
Backprop with Matrices (or Tensors)

Loss L still a scalar!



Backprop with Matrices (or Tensors)

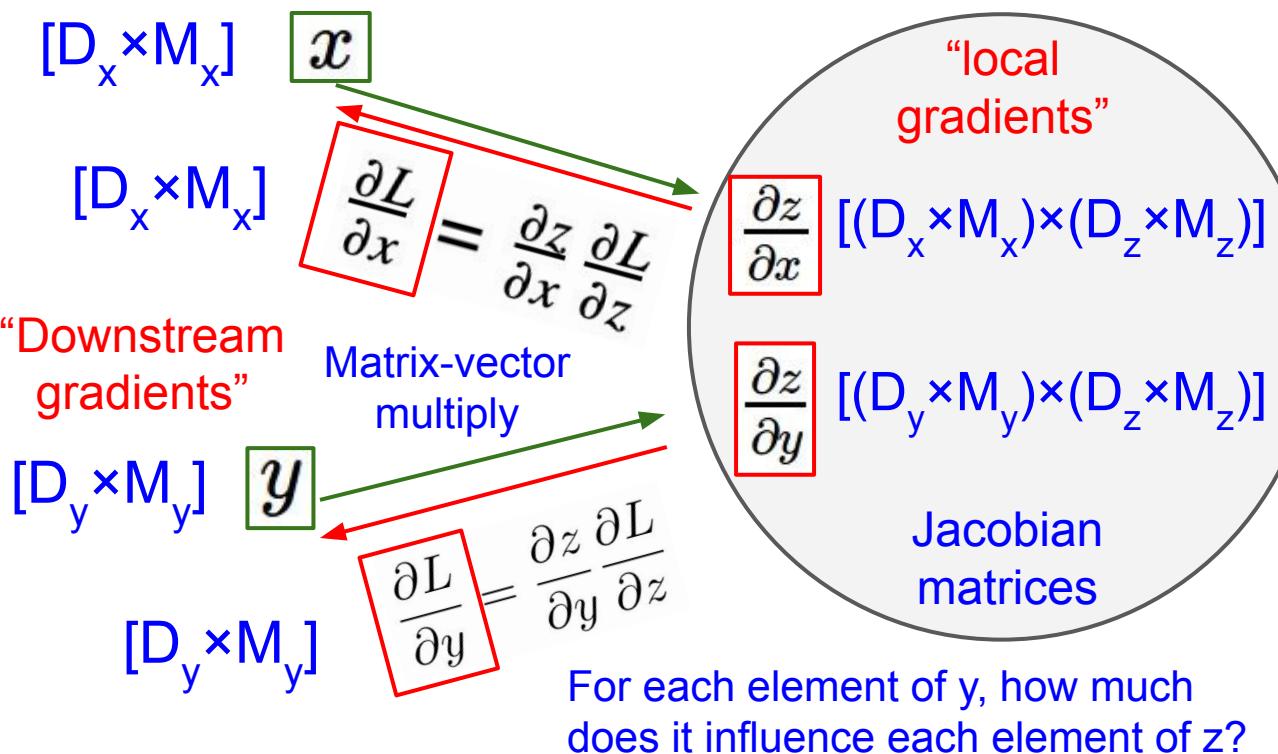
Loss L still a scalar!



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

x: [N×D]

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

w: [D×M]

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply

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

y: [N×M]

$$\begin{bmatrix} 13 & 9 & -2 & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

dL/dy: [N×M]

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Also see derivation in the course notes:

<http://cs231n.stanford.edu/handouts/linear-backprop.pdf>

Backprop with Matrices

$x: [N \times D]$

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

$w: [D \times M]$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply

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

Jacobians:

$$\begin{aligned} dy/dx: [(N \times D) \times (N \times M)] \\ dy/dw: [(D \times M) \times (N \times M)] \end{aligned}$$

$y: [N \times M]$

$$\begin{bmatrix} 13 & 9 & -2 & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

$dL/dy: [N \times M]$

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

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]

$$\begin{bmatrix} 2 & \boxed{1} & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

w: [D×M]

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply

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

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

y: [N×M]

$$\begin{bmatrix} 13 & 9 & -2 & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

dL/dy: [N×M]

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Backprop with Matrices

$x: [N \times D]$

[2 **1** -3]

[-3 4 2]

$w: [D \times M]$

[3 2 1 -1]

[2 1 3 2]

[3 2 1 -2]

Matrix Multiply

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

$y: [N \times M]$

[13 9 -2 -6]

[5 2 17 1]

$dL/dy: [N \times M]$

[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

$x: [N \times D]$

[2 **1** -3]

[-3 4 2]

$w: [D \times M]$

[3 2 1 -1]

[2 1 3 2]

[3 2 1 -2]

Matrix Multiply

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

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

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

$y: [N \times M]$

[13 9 **-2** -6]

[5 2 17 1]

$dL/dy: [N \times M]$

[2 3 -3 9]

[-8 1 4 6]

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

$x: [N \times D]$

[2 **1** -3]

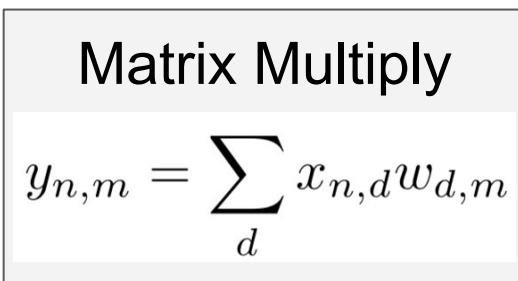
[-3 4 2]

$w: [D \times M]$

[3 2 1 -1]

[2 1 **3** 2]

[3 2 1 -2]



$y: [N \times M]$

13	9	-2	-6
5	2	17	1

$dL/dy: [N \times M]$

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

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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]

$$\begin{bmatrix} 2 & \boxed{1} & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

w: [D×M]

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & \boxed{3} & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

[N×D] [N×M] [M×D]

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

Matrix Multiply

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

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: $w_{d,m}$

y: [N×M]

$$\begin{bmatrix} 13 & 9 & \boxed{-2} & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

dL/dy: [N×M]

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Backprop with Matrices

$x: [N \times D]$

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

$w: [D \times M]$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply

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

$y: [N \times M]$

$$\begin{bmatrix} 13 & 9 & -2 & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

$dL/dy: [N \times M]$

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

By similar logic:

$[N \times D] \quad [N \times M] \quad [M \times D]$

$[D \times M] \quad [D \times N] \quad [N \times M]$

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

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

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

Softmax classifier

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



cat	3.2
car	5.1
frog	-1.7

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



$$s = f(x_i; W)$$

$$P(Y = k | X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax
Function

cat	3.2
car	5.1
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Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



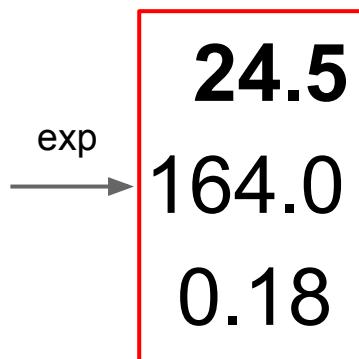
$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax
Function

Probabilities
must be ≥ 0

cat	3.2
car	5.1
frog	-1.7



unnormalized
probabilities

Softmax Classifier (Multinomial Logistic Regression)

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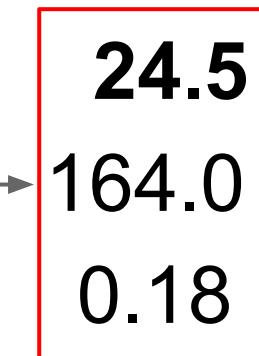
Probabilities
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Softmax
Function

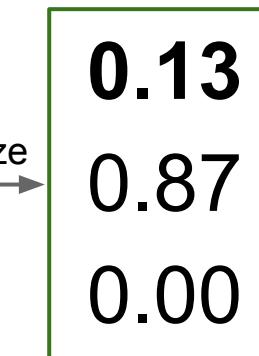
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car	5.1
frog	-1.7

exp



unnormalized
probabilities

normalize



probabilities

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax Function

Probabilities
must be ≥ 0

Probabilities
must sum to 1

cat
car
frog

3.2
5.1
-1.7

Unnormalized
log-probabilities / logits

exp

24.5
164.0
0.18

unnormalized
probabilities

normalize

0.13
0.87
0.00

probabilities

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax Function

Probabilities
must be ≥ 0

Probabilities
must sum to 1

$$L_i = -\log P(Y = y_i|X = x_i)$$

cat
car
frog

3.2
5.1
-1.7

Unnormalized
log-probabilities / logits

exp

24.5
164.0
0.18

unnormalized
probabilities

normalize

0.13
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probabilities

$$\rightarrow L_i = -\log(0.13) \\ = 2.04$$

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax Function

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Unnormalized
log-probabilities / logits

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$$L_i = -\log P(Y = y_i|X = x_i)$$

$$\rightarrow L_i = -\log(0.13) \\ = 2.04$$

Maximum Likelihood Estimation
Choose weights to maximize the likelihood of the observed data
(See CS 229 for details)

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



$$s = f(x_i; W)$$

Probabilities
must be ≥ 0

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax
Function

cat
car
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Unnormalized
log-probabilities / logits

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unnormalized
probabilities

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0.13
0.87
0.00

probabilities

compare

1.00
0.00
0.00

Correct
probs

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



$$s = f(x_i; W)$$

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Softmax Function

cat
car
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Unnormalized
log-probabilities / logits

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unnormalized
probabilities

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0.87
0.00

probabilities

compare

1.00

0.00

0.00

$$L_i = -\log P(Y = y_i|X = x_i)$$

Kullback–Leibler divergence

$$D_{KL}(P||Q) = \sum_y P(y) \log \frac{P(y)}{Q(y)}$$

Correct
probs

Softmax Classifier (Multinomial Logistic Regression)



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Probabilities
must be ≥ 0

cat
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$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax
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Probabilities
must sum to 1

0.13
0.87
0.00

probabilities

$$L_i = -\log P(Y = y_i|X = x_i)$$

compare

1.00

0.00

0.00

Cross Entropy

$$H(P, Q) = H(p) + D_{KL}(P||Q)$$

Correct
probs

Softmax Classifier (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**



$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax
Function

Maximize probability of correct class

cat	3.2
car	5.1
frog	-1.7

Putting it all together:

$$L_i = -\log P(Y = y_i|X = x_i)$$

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

Softmax Classifier (Multinomial Logistic Regression)



Want to interpret raw classifier scores as **probabilities**

$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

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cat	3.2
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Q1: What is the min/max possible softmax loss L_i ?

Q2: At initialization all s_j will be approximately equal;
what is the softmax loss L_i , assuming C classes?

Softmax Classifier (Multinomial Logistic Regression)



Want to interpret raw classifier scores as **probabilities**

$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax Function

Maximize probability of correct class

Putting it all together:

$$L_i = -\log P(Y = y_i|X = x_i)$$

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

cat	3.2
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frog	-1.7

Q2: At initialization all s will be approximately equal; what is the loss?
A: $-\log(1/C) = \log(C)$,
If $C = 10$, then $L_i = \log(10) \approx 2.3$

Next Time: Convolutional Neural Networks!

