Backpropagation and Neural Networks

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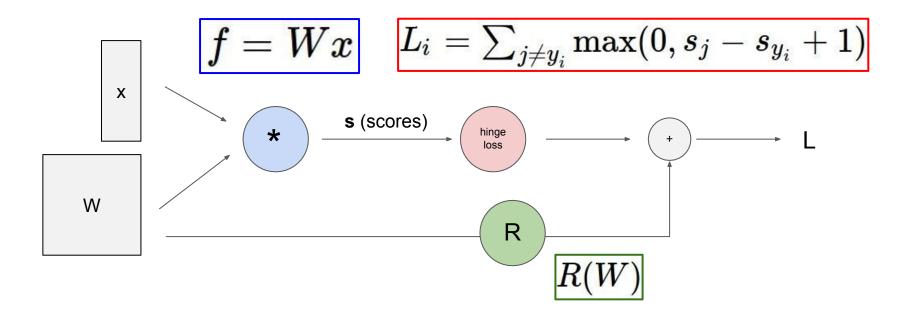
Gradient descent

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

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

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

Computational graphs



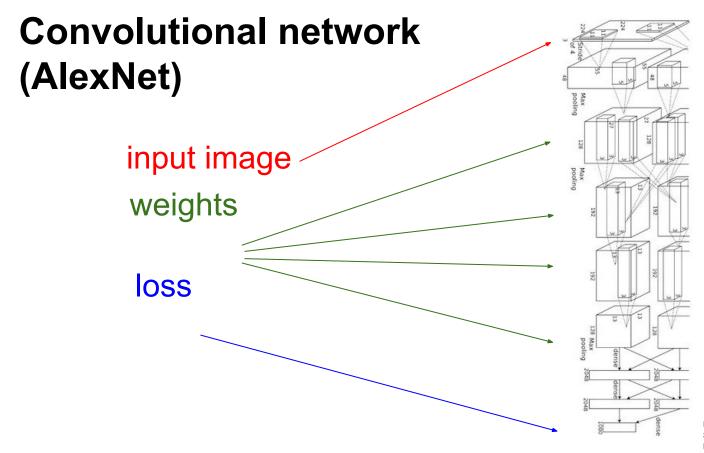
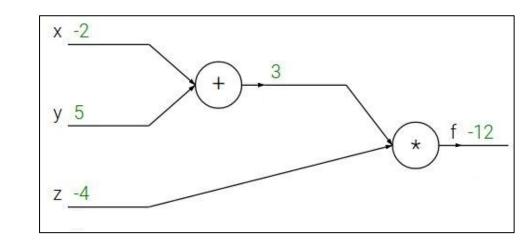


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$$f(x,y,z)=(x+y)z$$

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



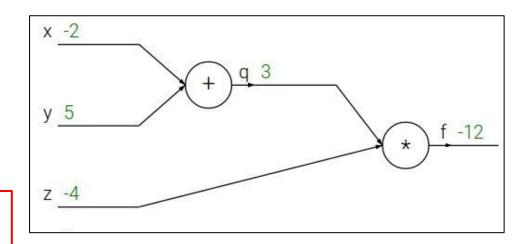
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$$f=qz$$
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



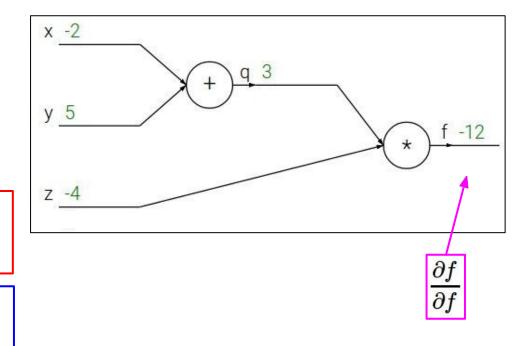
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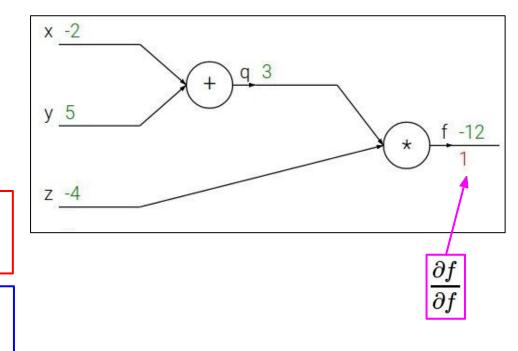
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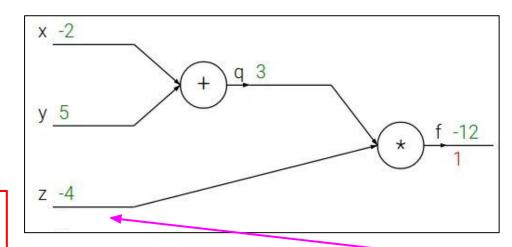
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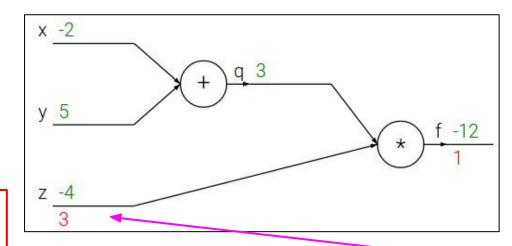
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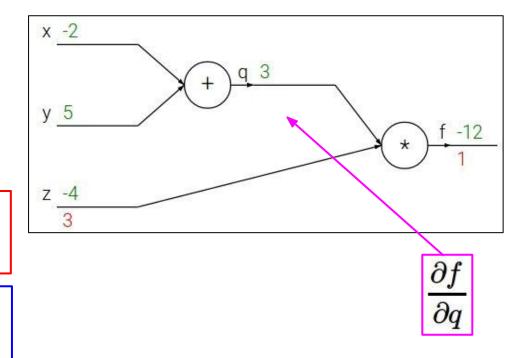
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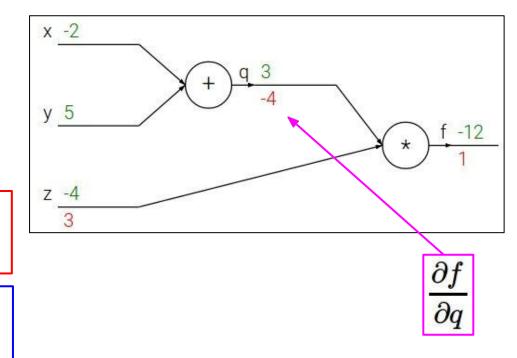
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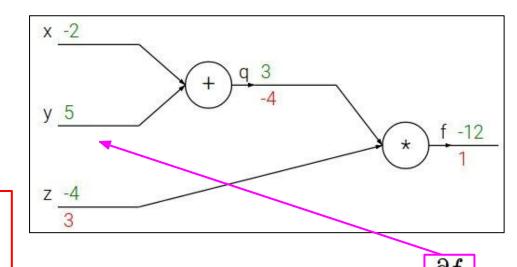
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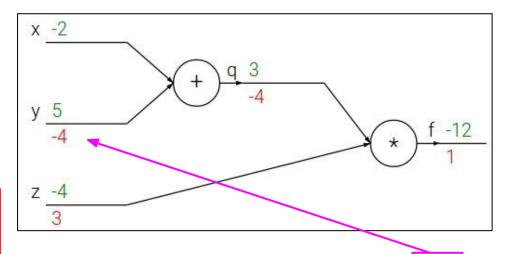
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Chain rule:

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

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

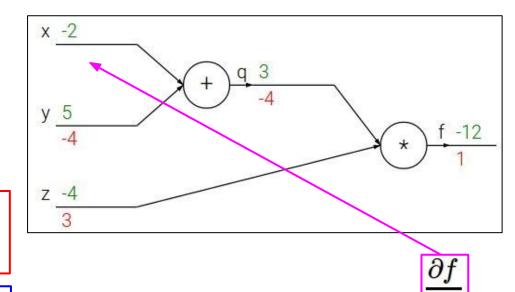
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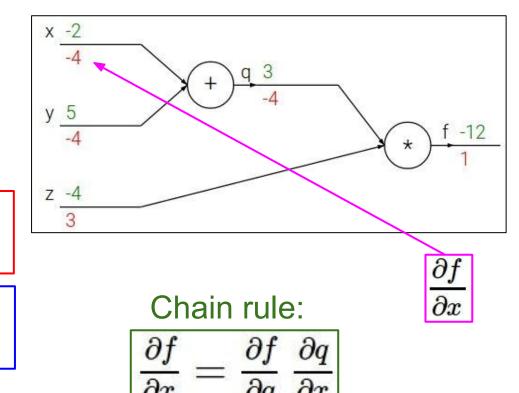
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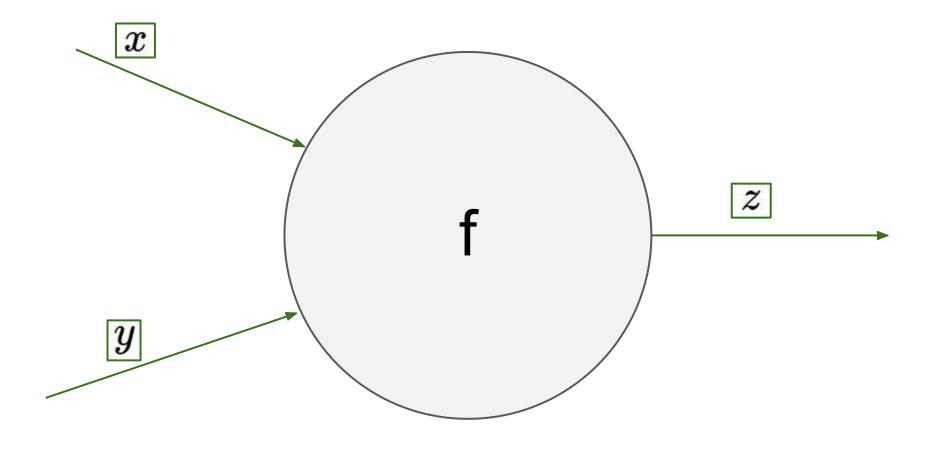
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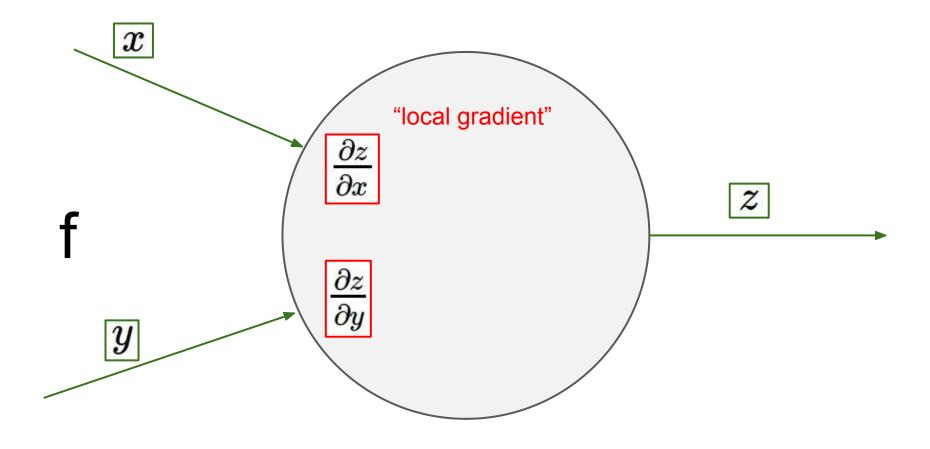
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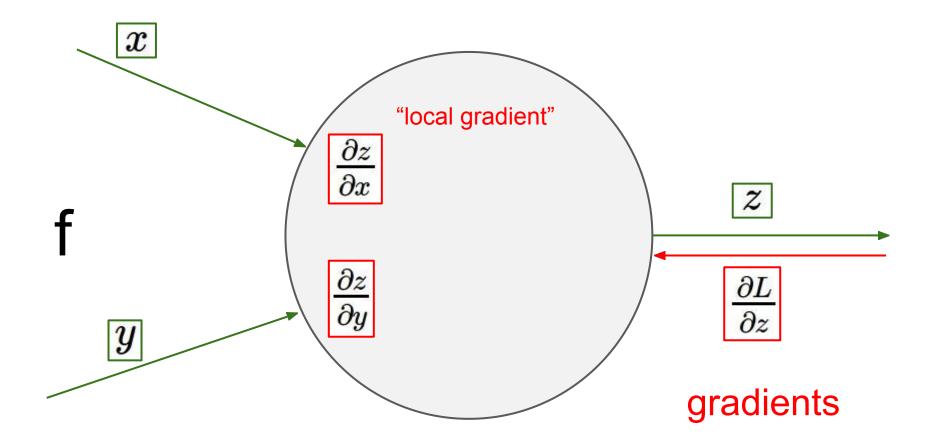
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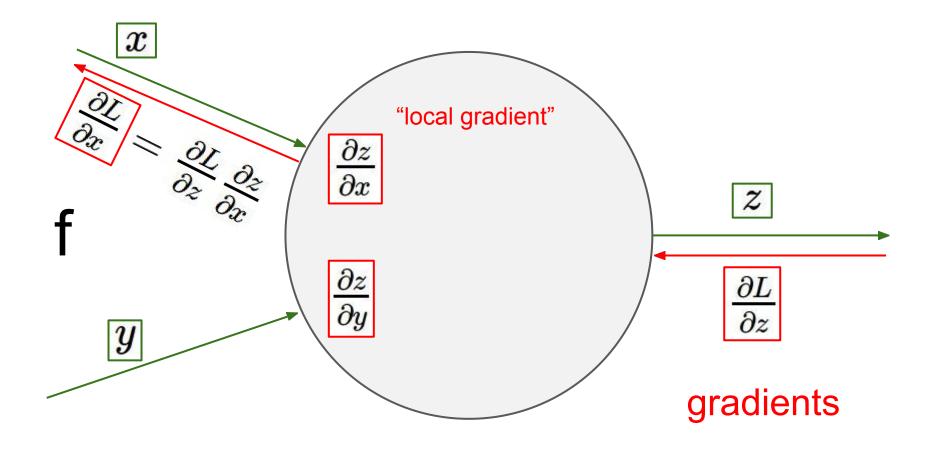
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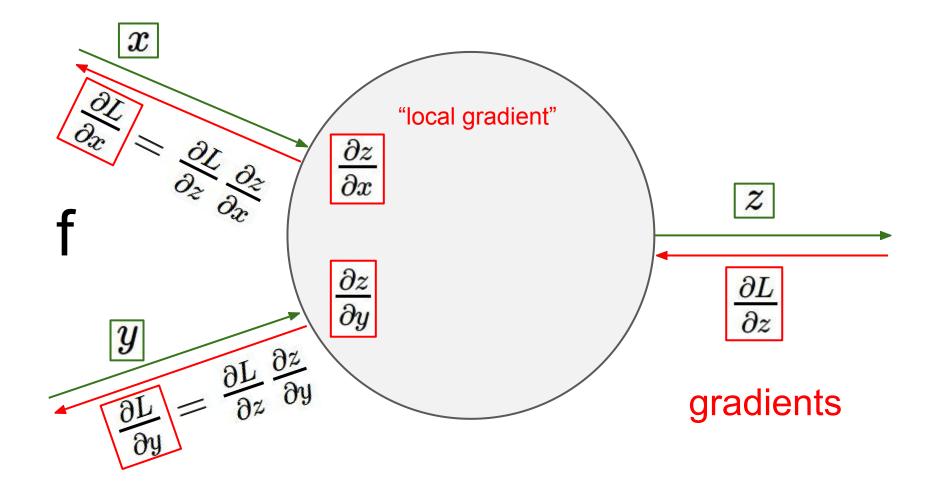


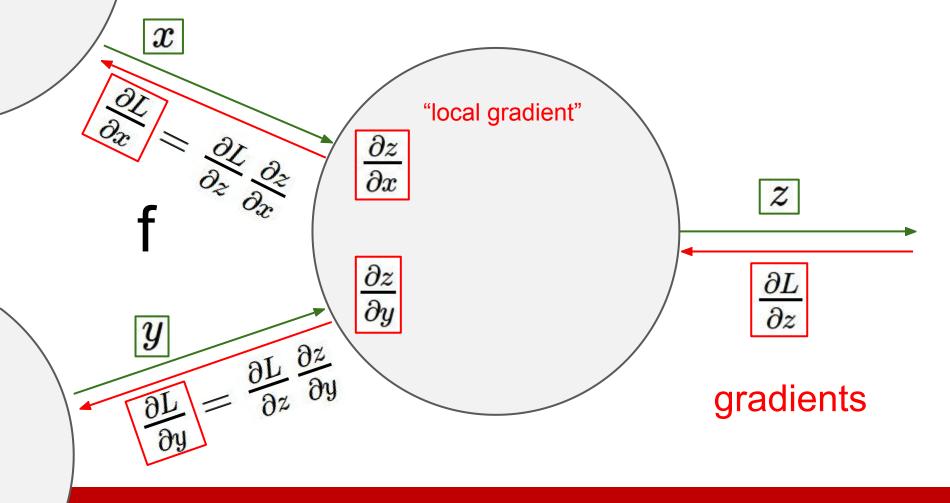






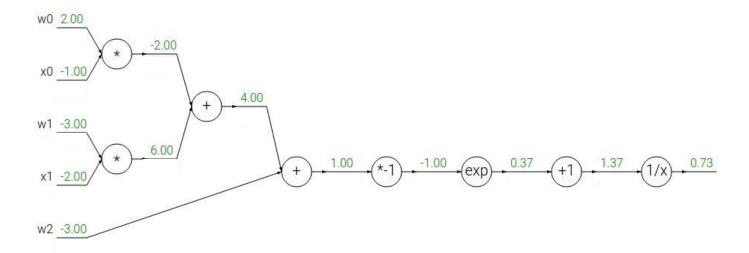




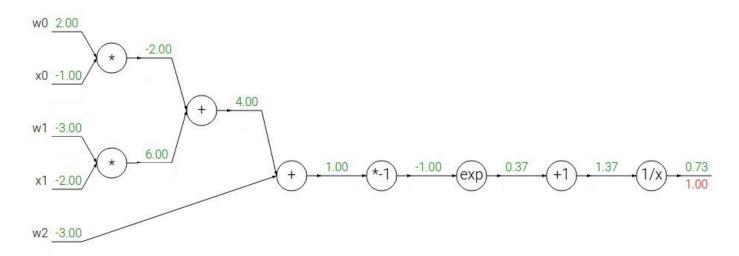


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Another example:
$$f(w,x) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$

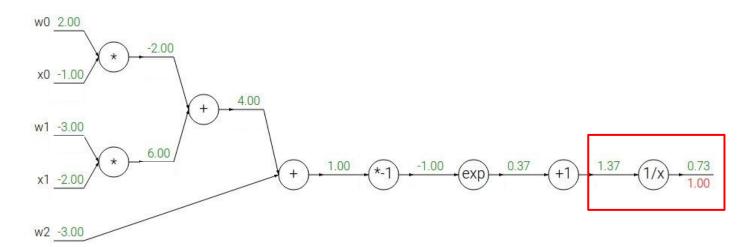


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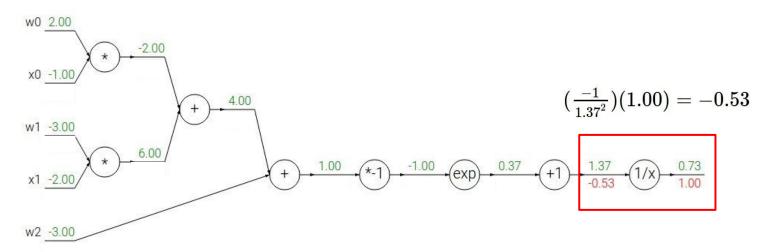
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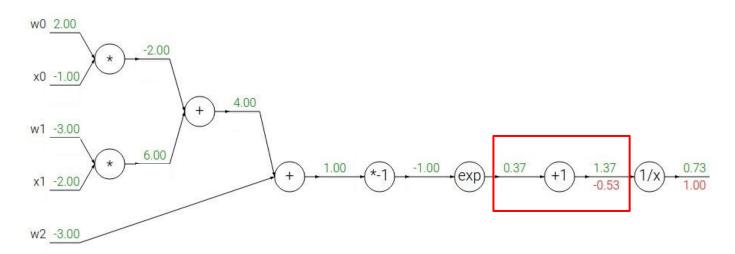
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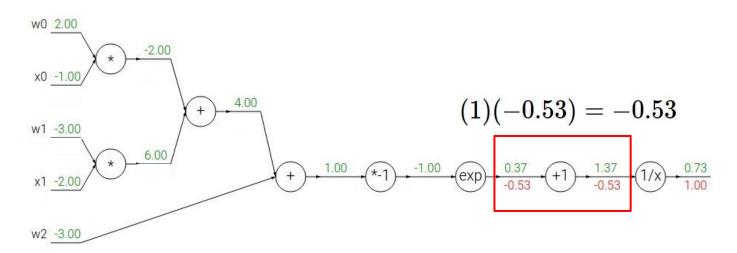
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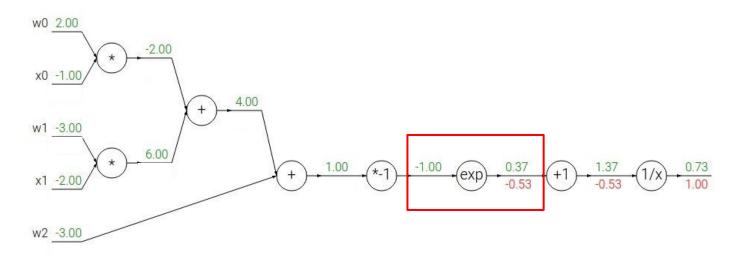
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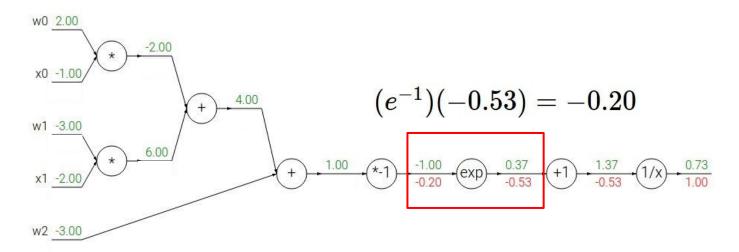
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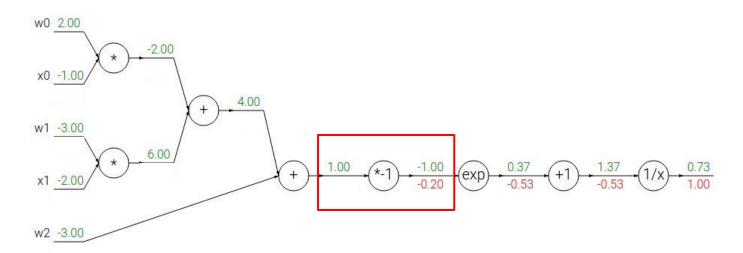
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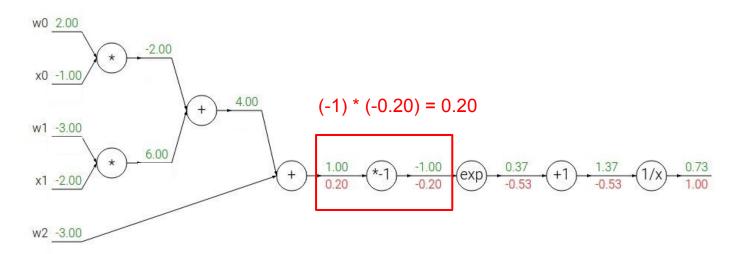
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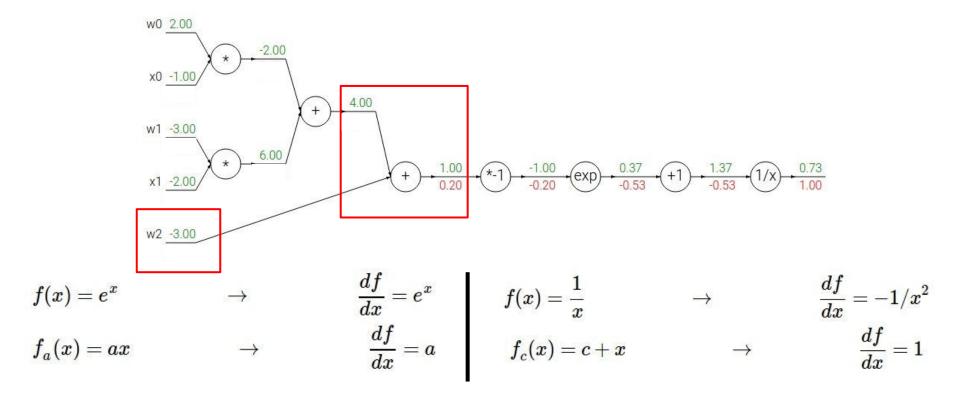
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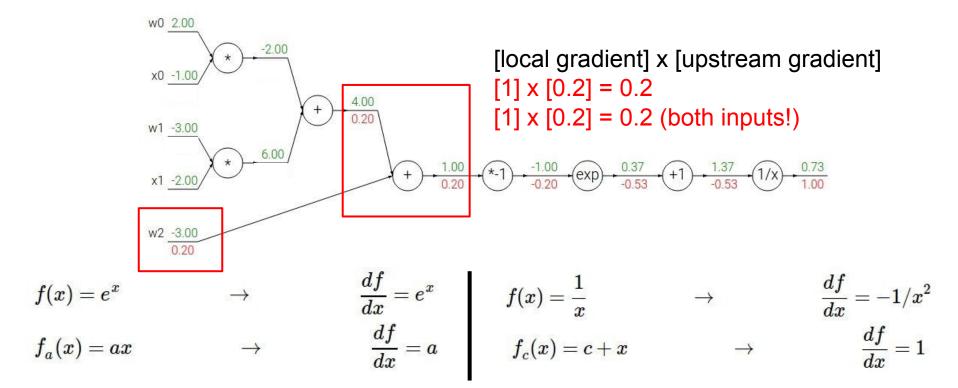
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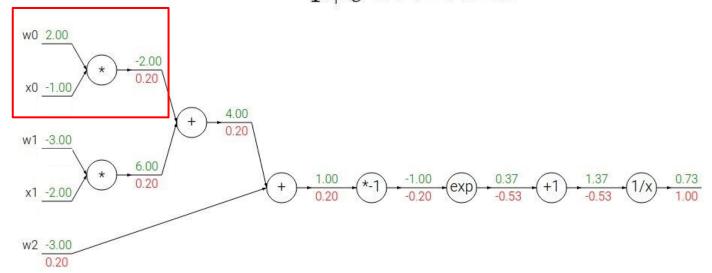
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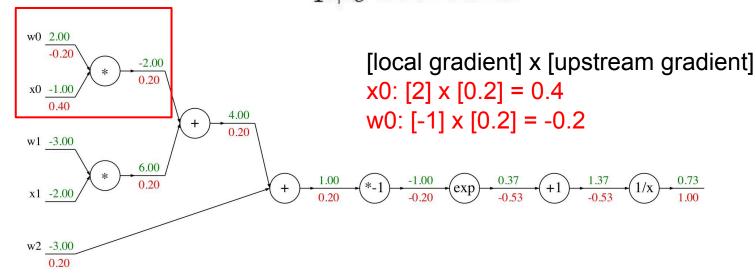
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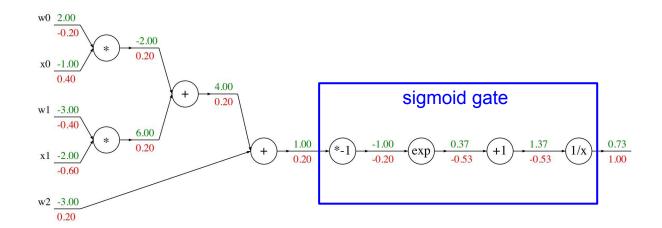
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$$f(w,x)=rac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

sigmoid function

$$rac{d\sigma(x)}{dx} = rac{e^{-x}}{(1+e^{-x})^2} = \left(rac{1+e^{-x}-1}{1+e^{-x}}
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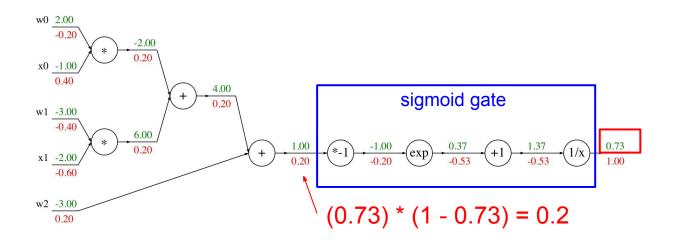
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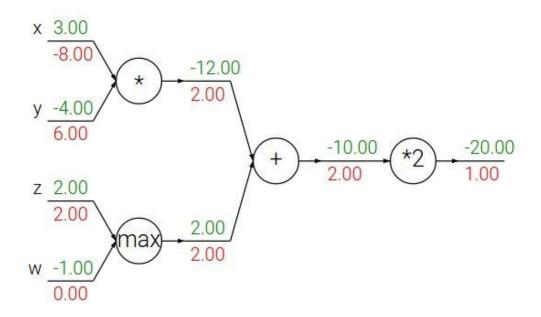
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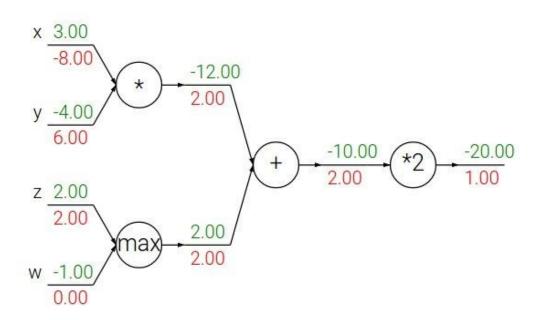
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add gate: gradient distributor



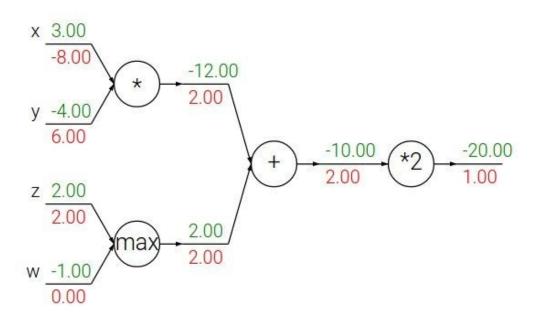
add gate: gradient distributor

Q: What is a **max** gate?



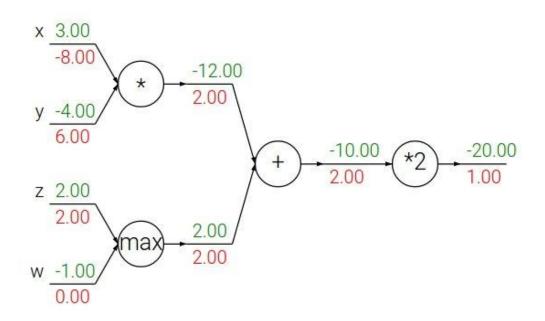
add gate: gradient distributor

max gate: gradient router



add gate: gradient distributor
max gate: gradient router

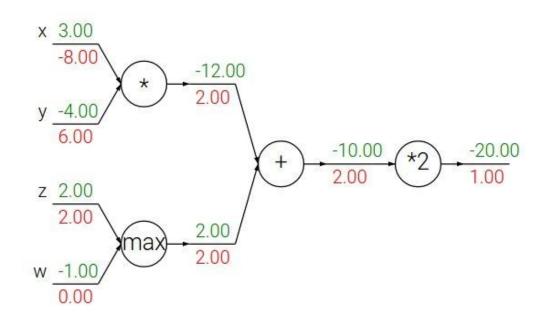
Q: What is a **mul** gate?



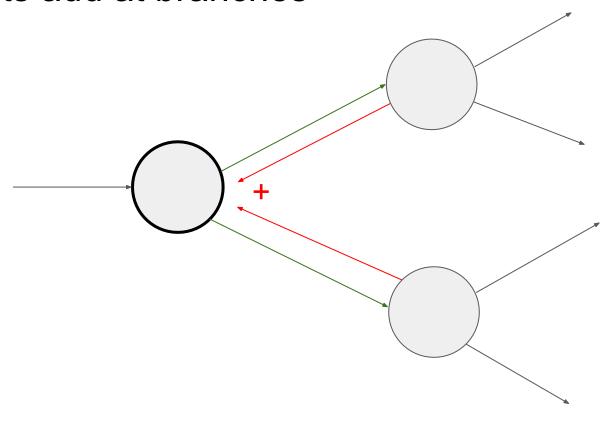
add gate: gradient distributor

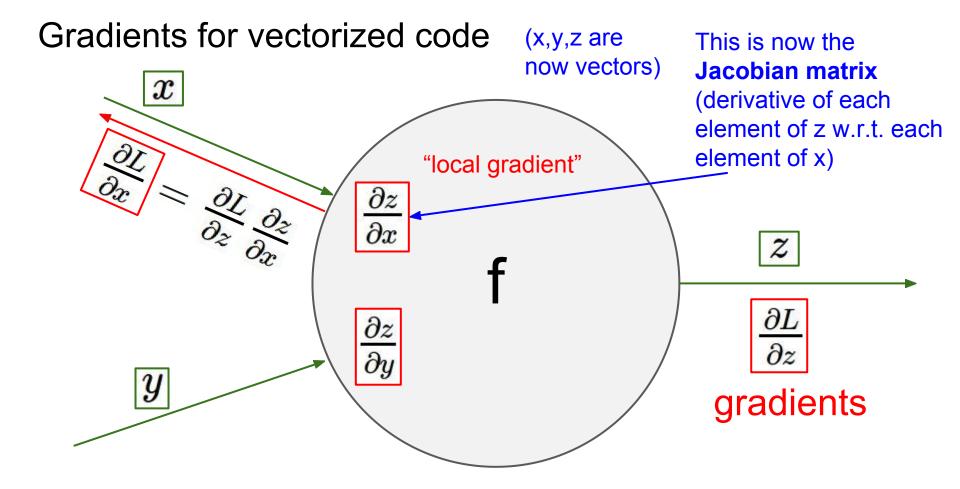
max gate: gradient router

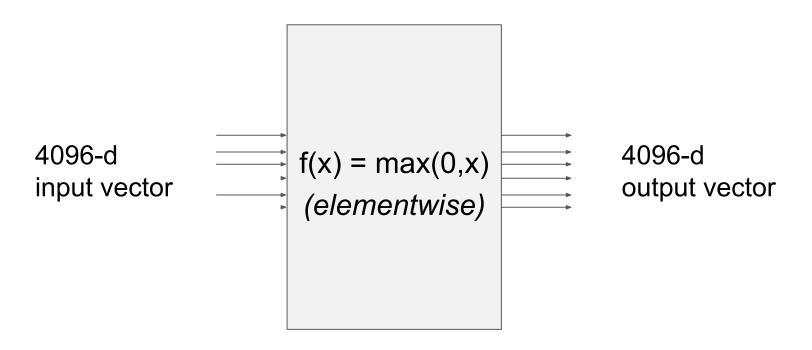
mul gate: gradient switcher

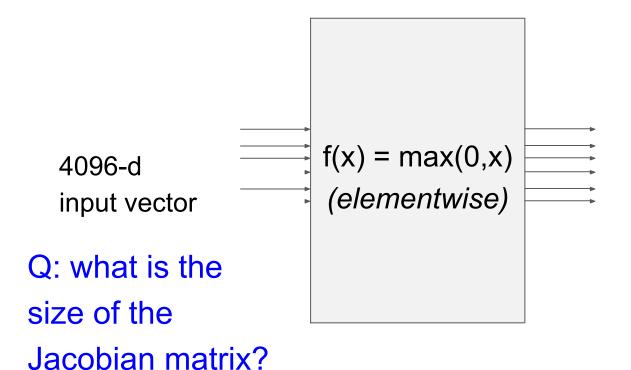


Gradients add at branches





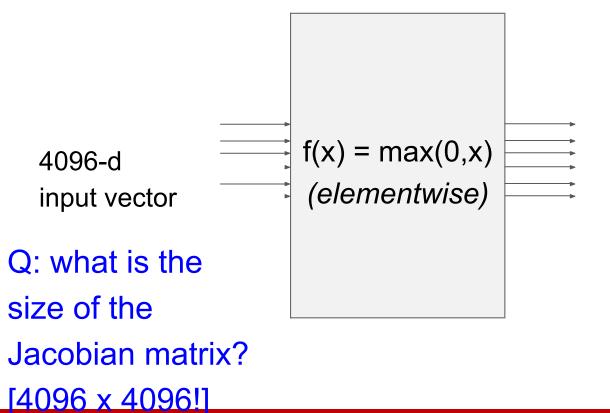




$$\frac{\partial L}{\partial x} = \frac{\partial f}{\partial x} \frac{\partial L}{\partial f}$$

Jacobian matrix

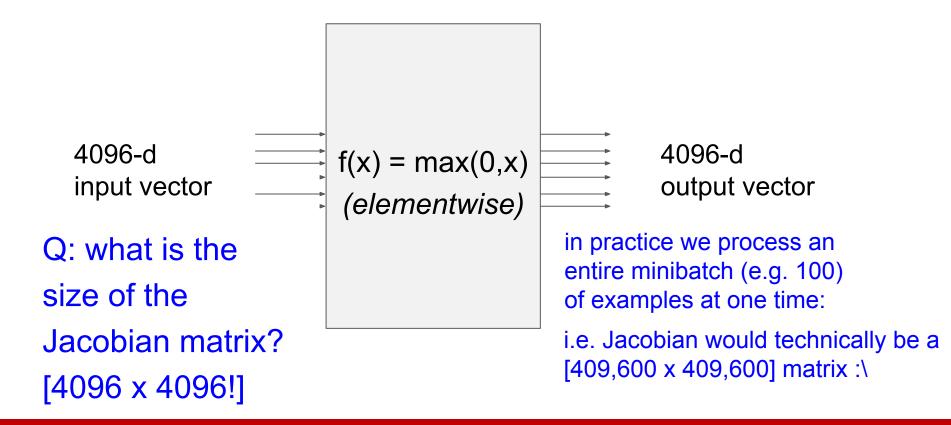
4096-d output vector



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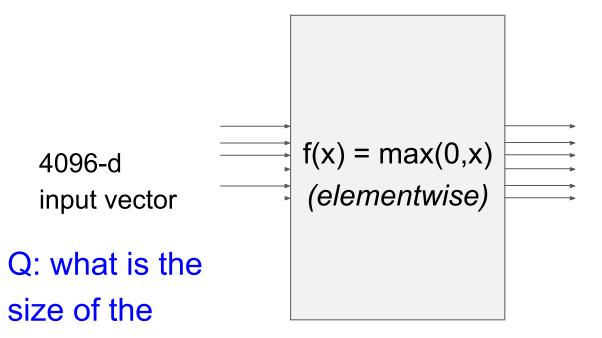
Jacobian matrix

4096-d output vector



Jacobian matrix?

[4096 x 4096!]



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

Jacobian matrix

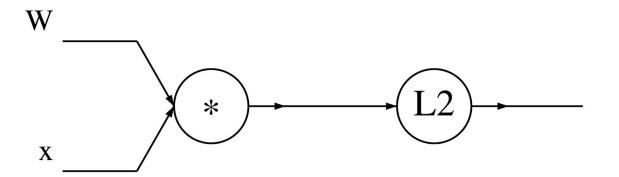
4096-d output vector

Q2: what does it look like?

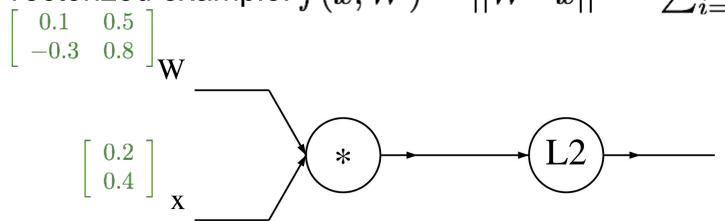
A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$

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 $\in \mathbb{R}^n \in \mathbb{R}^{n \times n}$

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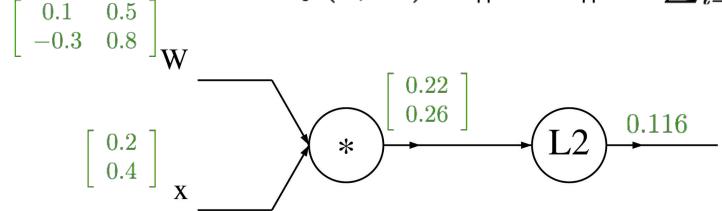


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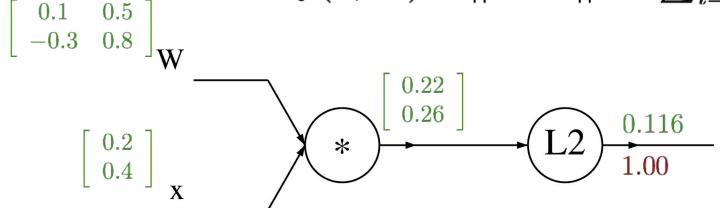
$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$
$$f(q) = ||q||^2 = q_1^2 + \dots + q_n^2$$

A vectorized example: $f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$



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A vectorized example:
$$f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix}_{\mathbf{W}}$$

$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix}_{\mathbf{X}}$$

$$*$$

$$\begin{bmatrix} 0.22 \\ 0.26 \end{bmatrix}$$

$$\mathbf{L2}$$

$$\boxed{1.00}$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$
$$f(q) = ||q||^2 = q_1^2 + \dots + q_n^2$$

$$rac{\partial f}{\partial q_i} = 2q_i$$
 $\nabla_q f = 2q_i$

A vectorized example:
$$f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix}_{\mathbf{W}}$$

$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix}_{\mathbf{X}}$$

$$\begin{bmatrix} 0.22 \\ 0.26 \end{bmatrix}$$

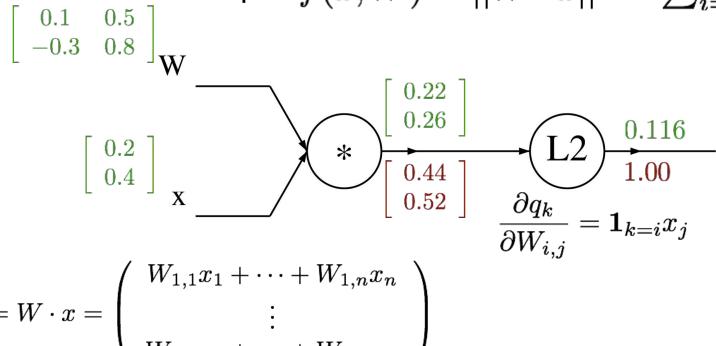
$$\begin{bmatrix} 0.44 \\ 0.52 \end{bmatrix}$$

$$\begin{bmatrix} 0.44 \\ 0.52 \end{bmatrix}$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$
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$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = ||q||^2 = q_1^2 + \dots + q_n^2$$

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A vectorized example:
$$f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix}_{\mathbf{W}}$$

$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix}_{\mathbf{X}}$$

$$\begin{bmatrix} 0.22 \\ 0.26 \end{bmatrix}$$

$$\begin{bmatrix} 0.44 \\ 0.52 \end{bmatrix}$$

$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i}x_j$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = ||q||^2 = q_1^2 + \dots + q_n^2$$

$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}}$$

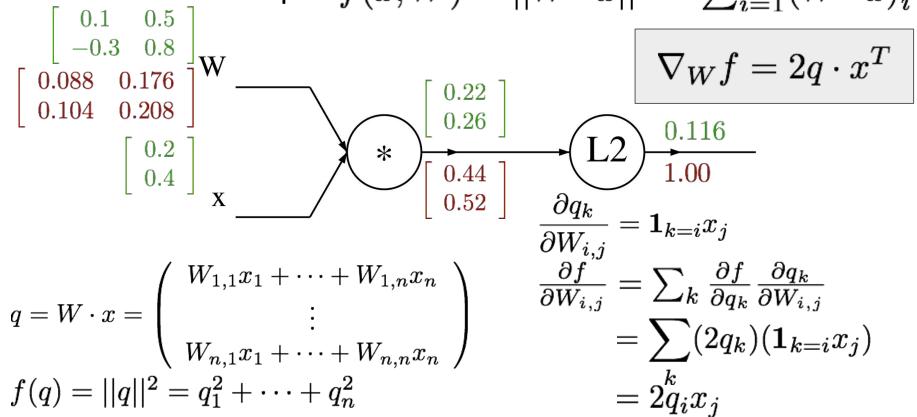
$$= \sum_k (2q_k)(\mathbf{1}_{k=i}x_j)$$

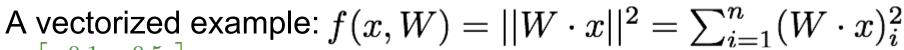
$$= 2q_ix_j$$

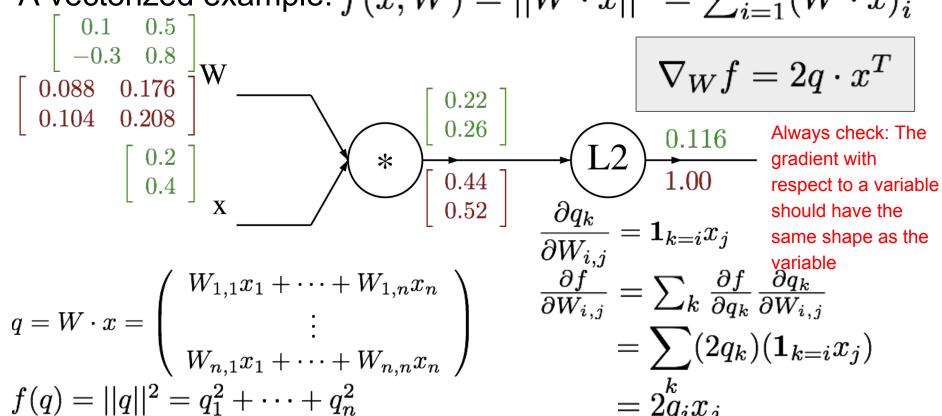
A vectorized example:
$$f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W \begin{bmatrix} 0.088 & 0.176 \\ 0.104 & 0.208 \end{bmatrix} W \begin{bmatrix} 0.22 \\ 0.4 \end{bmatrix} X \begin{bmatrix} 0.44 \\ 0.52 \end{bmatrix} \underbrace{\begin{pmatrix} 0.44 \\ 0.52 \end{pmatrix}} \underbrace{\begin{pmatrix} 0.116 \\ 1.00 \end{pmatrix}} \underbrace{\begin{pmatrix} 0.116 \\ 0.00 \\ 0.00 \\ 0.00 \end{pmatrix}} \underbrace{\begin{pmatrix} 0.116 \\ 0.00 \\ 0.00 \\ 0.00 \end{pmatrix}} \underbrace{\begin{pmatrix} 0.116 \\ 0.00 \\$$

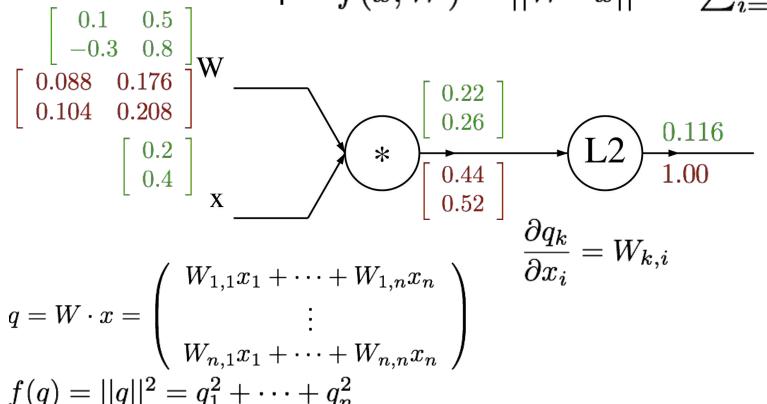
A vectorized example:
$$f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$$



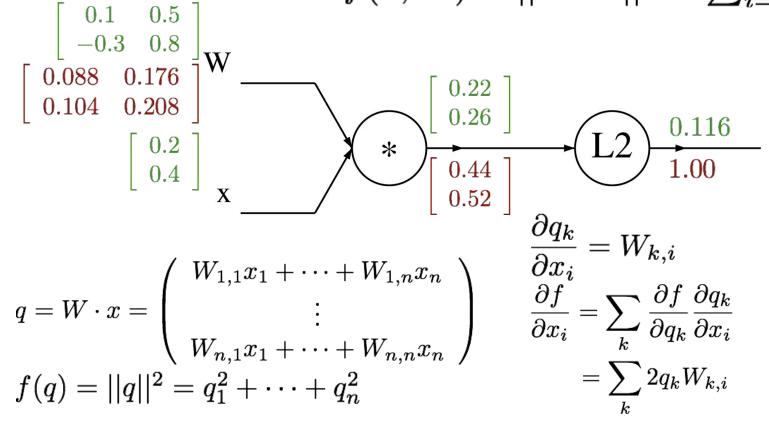


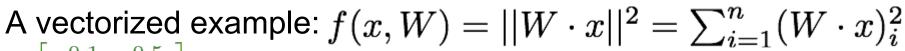


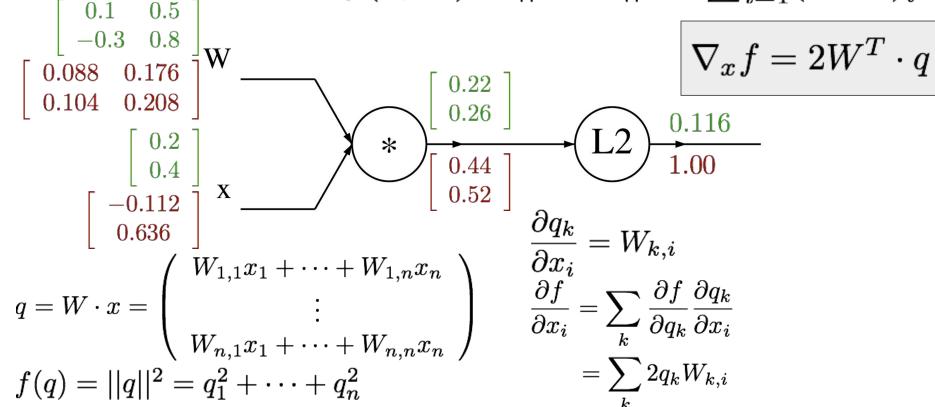
A vectorized example:
$$f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$$



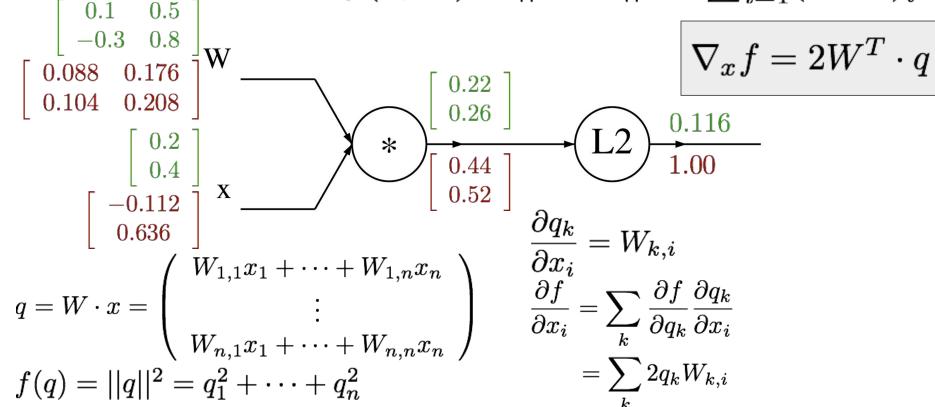
A vectorized example: $f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$



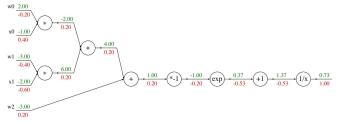




A vectorized example:
$$f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$$



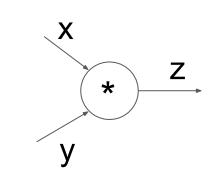
Modularized implementation: forward / backward API



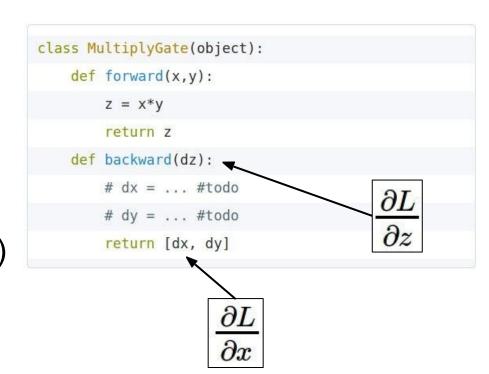
Graph (or Net) object (rough psuedo code)

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

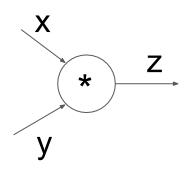
Modularized implementation: forward / backward API



(x,y,z are scalars)



Modularized implementation: forward / backward API



(x,y,z are scalars)

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

Example: Caffe layers

Branch: master v caffe / src / c	affe / layers /	le Upload files	Find file	Histor
shelhamer committed on GitHub Merge pull request #4630 from BlGene/load_hdf5_fix Latest commit e687a71 21 days ag				
absval_layer.cpp	dismantle layer headers		a	year ag
absval_layer.cu	dismantle layer headers		a	year ag
accuracy_layer.cpp	dismantle layer headers		a	year ag
argmax_layer.cpp	dismantle layer headers		a	year ag
base_conv_layer.cpp	enable dilated deconvolution		a	year ag
base_data_layer.cpp	Using default from proto for prefetch		3 moi	nths ag
base_data_layer.cu	Switched multi-GPU to NCCL		3 moi	nths ag
a batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_layer.cpp		4 moi	nths ag
abatch_norm_layer.cu	dismantle layer headers		a	year ag
abatch_reindex_layer.cpp	dismantle layer headers		a	year ag
abatch_reindex_layer.cu	dismantle layer headers		a	year ag
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BiasLayer		a	year ag
bias_layer.cu	Separation and generalization of ChannelwiseAffineLayer into BiasLay	er	a	year ag
bnll_layer.cpp	dismantle layer headers		a	year ag
bnll_layer.cu	dismantle layer headers		a	year ag
concat_layer.cpp	dismantle layer headers		a	year ag
concat_layer.cu	dismantle layer headers		a	year ag
contrastive_loss_layer.cpp	dismantle layer headers		a	year ag
contrastive_loss_layer.cu	dismantle layer headers		a	year ag
conv_layer.cpp	add support for 2D dilated convolution		a	year ag
conv_layer.cu	dismantle layer headers		a	year ag
crop_layer.cpp	remove redundant operations in Crop layer (#5138)		2 moi	nths ag
crop_layer.cu	remove redundant operations in Crop layer (#5138)		2 moi	nths ag
cudnn_conv_layer.cpp	dismantle layer headers		a	year ag
cudnn_conv_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support		11 moi	nths ag

cudnn_lcn_layer.cpp	dismantle layer headers	a year ago
cudnn_lcn_layer.cu	dismantle layer headers	a year ago
cudnn_lrn_layer.cpp	dismantle layer headers	a year ago
cudnn_lrn_layer.cu	dismantle layer headers	a year ago
cudnn_pooling_layer.cpp	dismantle layer headers	a year ago
cudnn_pooling_layer.cu	dismantle layer headers	a year ago
cudnn_relu_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_relu_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_softmax_layer.cpp	dismantle layer headers	a year ago
cudnn_softmax_layer.cu	dismantle layer headers	a year ago
cudnn_tanh_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_tanh_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
data_layer.cpp	Switched multi-GPU to NCCL	3 months ago
deconv_layer.cpp	enable dilated deconvolution	a year ago
deconv_layer.cu	dismantle layer headers	a year ago
dropout_layer.cpp	supporting N-D Blobs in Dropout layer Reshape	a year ago
dropout_layer.cu	dismantle layer headers	a year ago
dummy_data_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cu	dismantle layer headers	a year ago
elu_layer.cpp	ELU layer with basic tests	a year ago
elu_layer.cu	ELU layer with basic tests	a year ago
embed_layer.cpp	dismantle layer headers	a year ago
embed_layer.cu	dismantle layer headers	a year ago
euclidean_loss_layer.cpp	dismantle layer headers	a year ago
euclidean_loss_layer.cu	dismantle layer headers	a year ago
exp_layer.cpp	Solving issue with exp layer with base e	a year ago
exp laver.cu	dismantle laver headers	a year ago

Caffe is licensed under BSD 2-Clause

```
#include <cmath>
     #include <vector>
     #include "caffe/layers/sigmoid_layer.hpp"
    namespace caffe {
     template <typename Dtype>
     inline Dtype sigmoid(Dtype x) {
      return 1. / (1. + exp(-x));
     template <typename Dtype>
     void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
        const vector<Blob<Dtype>*>& top) {
       const Dtype* bottom_data = bottom[0]->cpu_data();
      Dtype* top_data = top[0]->mutable_cpu_data();
       const int count = bottom[0]->count();
       for (int i = 0; i < count; ++i) {
        top_data[i] = sigmoid(bottom_data[i]);
     template <typename Dtype>
     void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
         const vector<bool>& propagate_down,
         const vector<Blob<Dtype>*>& bottom) {
       if (propagate_down[0]) {
        const Dtype* top_data = top[0]->cpu_data();
        const Dtype* top_diff = top[0]->cpu_diff();
        Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
         const int count = bottom[0]->count();
         for (int i = 0; i < count; ++i) {
          const Dtype sigmoid_x = top_data[i];
          bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x); ◆
     #ifdef CPU ONLY
    STUB_GPU(SigmoidLayer);
     INSTANTIATE_CLASS(SigmoidLayer);
47 } // namespace caffe
```

Caffe Sigmoid Layer

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

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

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

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In Assignment 1: Writing SVM /

Saftmax forward/backward computation!

```
margins
E.g. for the SVM:
 # receive W (weights), X (data)
                                                                                   L_i = \sum_{j 
eq y_i} \max(0, s_j - s_{y_i} + 1)
                                                                        =Wx
 # forward pass (we have 8 lines)
 scores = #...
                                                                                s (scores)
 margins = #...
                                                            W
 data loss = #...
 reg loss = #...
 loss = data loss + reg loss
 # backward pass (we have 5 lines)
 dmargins = # ... (optionally, we go direct to dscores)
 dscores = #...
 dW = #...
```

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Summary so far...

- neural nets will be very large: impractical to write down gradient formula by hand for all parameters
- backpropagation = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates
- implementations maintain a graph structure, where the nodes implement the forward() / backward() API
- forward: compute result of an operation and save any intermediates needed for gradient computation in memory
- backward: apply the chain rule to compute the gradient of the loss function with respect to the inputs

Next: Neural Networks

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

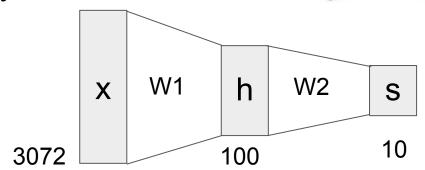
(Before) Linear score function:

(Now) 2-layer Neural Network

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

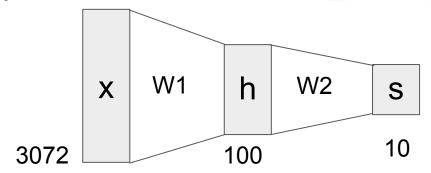
(**Before**) Linear score function:

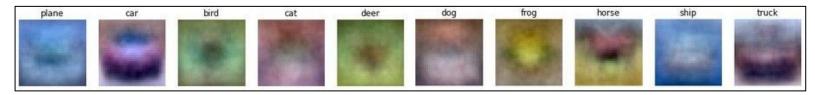
(Now) 2-layer Neural Network
$$f = W_2 \max(0, W_1 x)$$



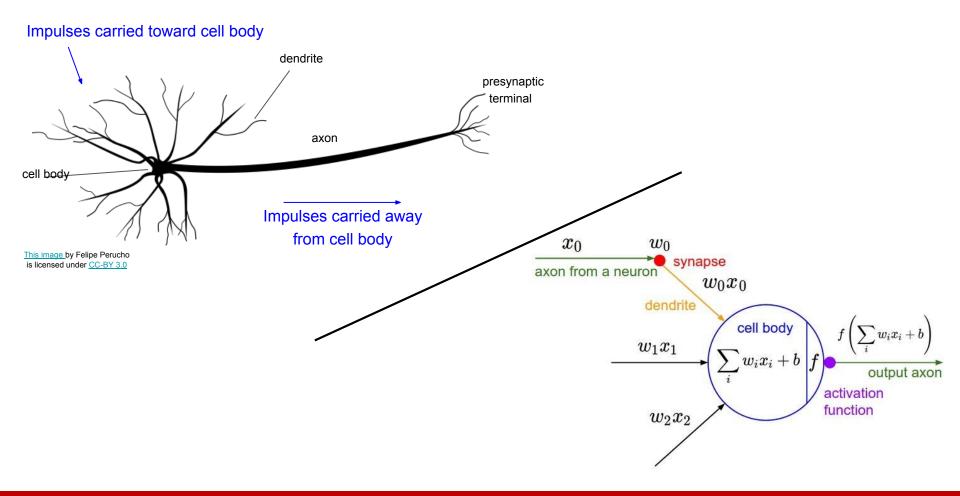
(**Before**) Linear score function:

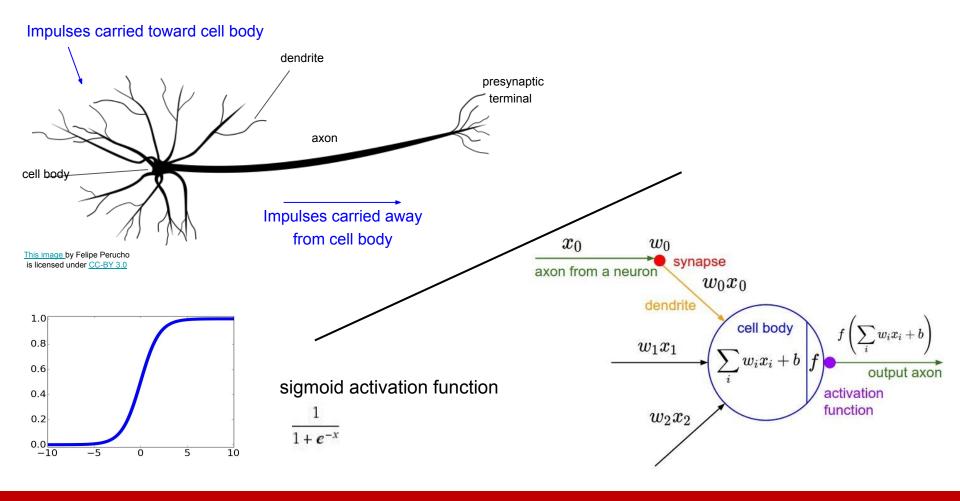
(Now) 2-layer Neural Network
$$f = W_2 \max(0, W_1 x)$$





(Now) 2-layer Neural Network f=Wx or 3-layer Neural Network $f=W_2\max(0,W_1x)$ $f=W_3\max(0,W_1x)$





Be very careful with your brain analogies!

Biological Neurons:

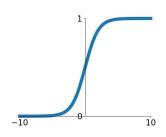
- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate

[Dendritic Computation. London and Hausser]

Activation functions

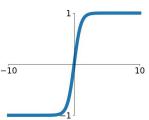
Sigmoid

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



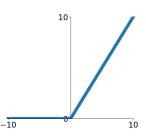
tanh

tanh(x)



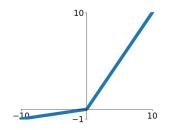
ReLU

 $\max(0, x)$



Leaky ReLU

 $\max(0.1x, x)$

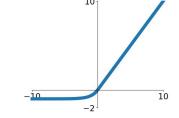


Maxout

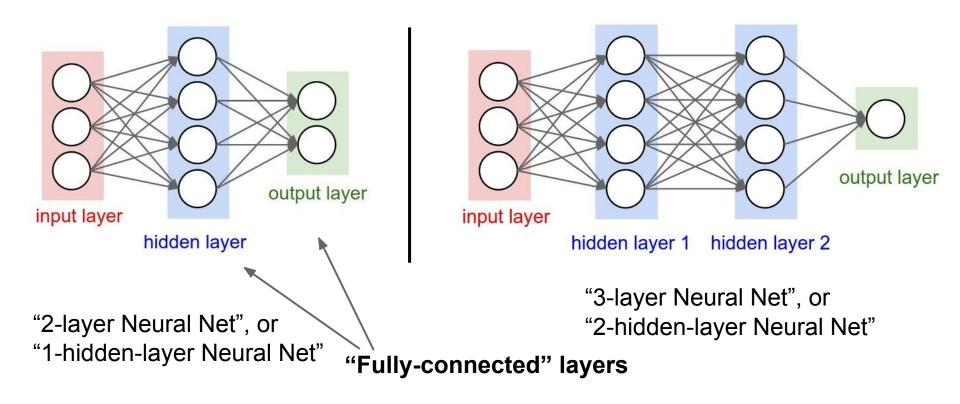
 $\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

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



Neural networks: Architectures

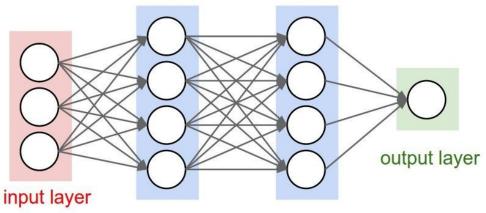


Example feed-forward computation of a neural network

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

We can efficiently evaluate an entire layer of neurons.

Example feed-forward computation of a neural network



hidden layer 1 hidden layer 2

```
# 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)
```

Summary

- We arrange neurons into fully-connected layers
- The abstraction of a **layer** has the nice property that it allows us to use efficient vectorized code (e.g. matrix multiplies)
- Neural networks are not really neural
- Next time: Convolutional Neural Networks