Lecture 4: Backpropagation and Neural Networks

Where we are...

input parameter

$$s = f(x; W) = Wx$$ output: score vector.

scores function

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

: total loss

SVM loss loss function

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

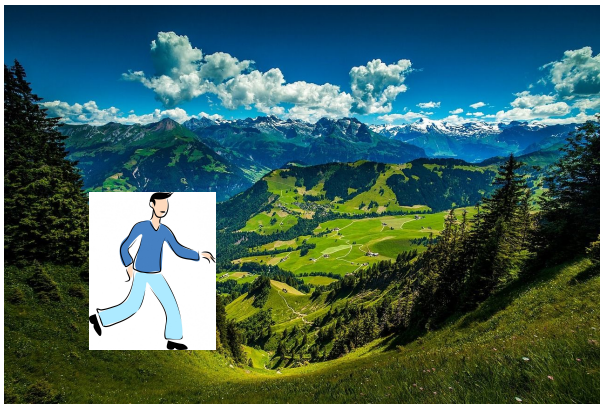
data loss + regularization

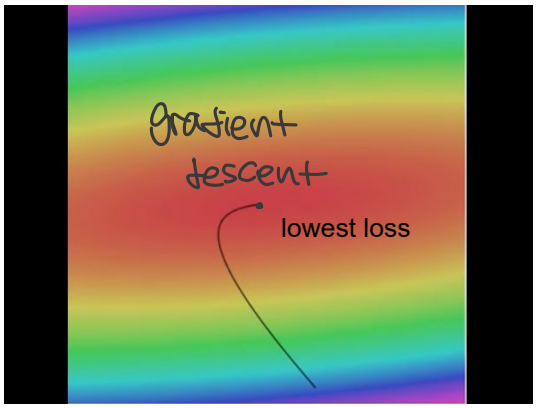
일반화 자연성 판단

want $\nabla_W L$

want to find parameter W: that minimize loss
-> find gradient about W

Optimization → we gradient 찾기






```
# Vanilla Gradient Descent

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


Gradient descent

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

finite difference approximation - slow, easy - can get gradient by this way any time

Numerical gradient: slow :(, approximate :(, easy to write :)

Analytic gradient: fast :), exact :), error-prone :(error ↑

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

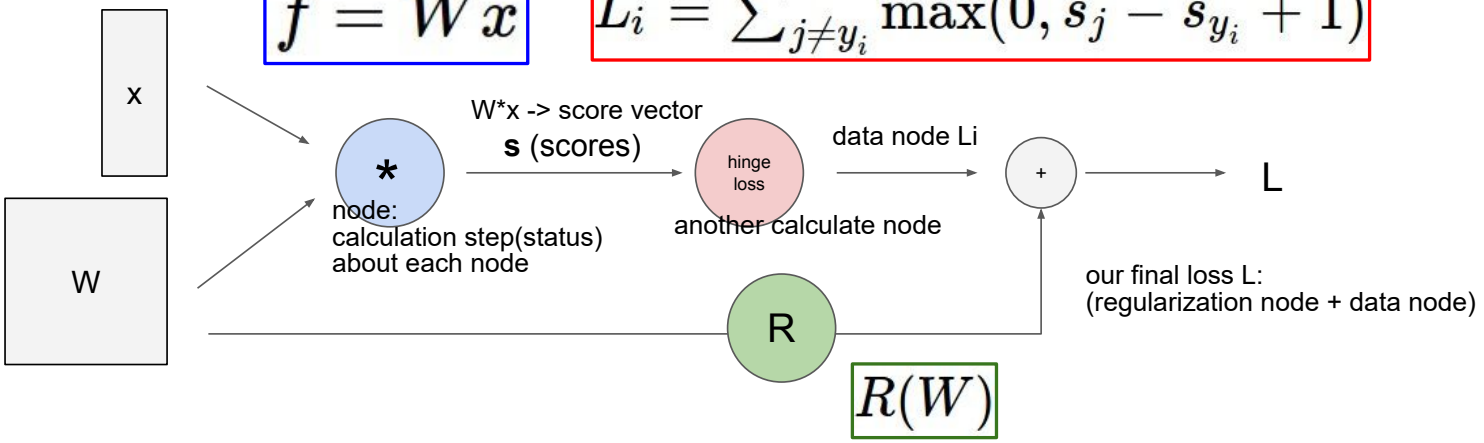
Computational graphs → 모든 function에 대해 적용 가능!

framework - can discribe any function by this type of graph

we can use back propagation by computational graphs

$$f = Wx$$

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



we have also Regularization node R to calculate data node L
- this node R: calculate Regularization node

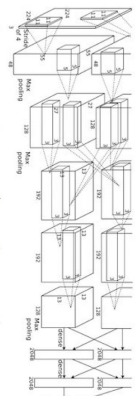
Convolutional network (AlexNet)

many layers

input image

weights

loss

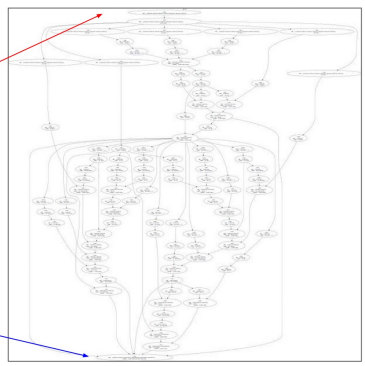


Neural Turing Machine

deep learning model

input image

loss



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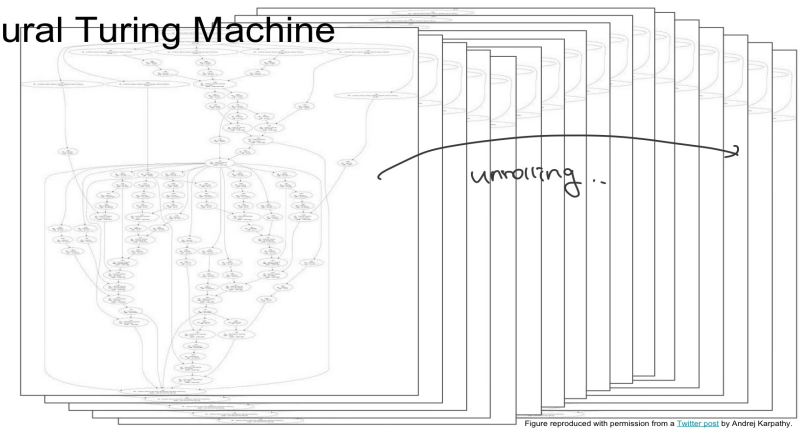
Neural Turing Machine



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Backpropagation: a simple example

we want to know some gradient about some variable about the output of function f

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

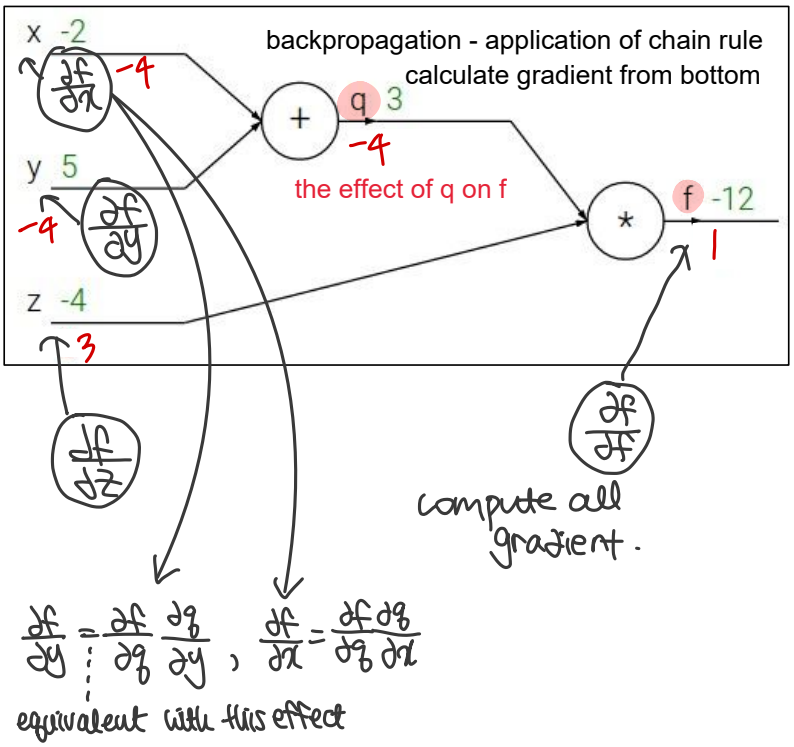
e.g. x = -2, y = 5, z = -4

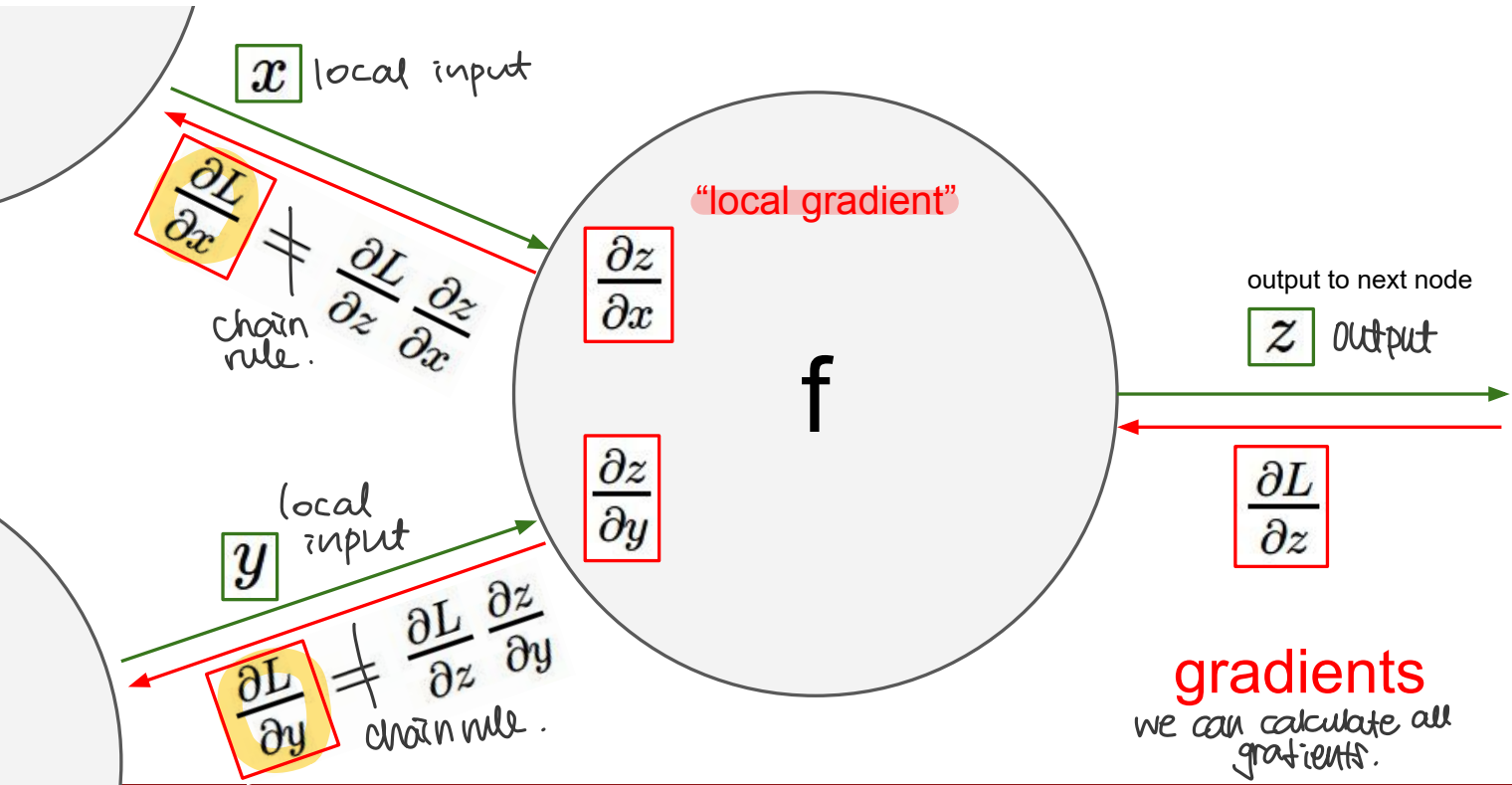
when we change y - q will change for the amout equals to the effect of y on q

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

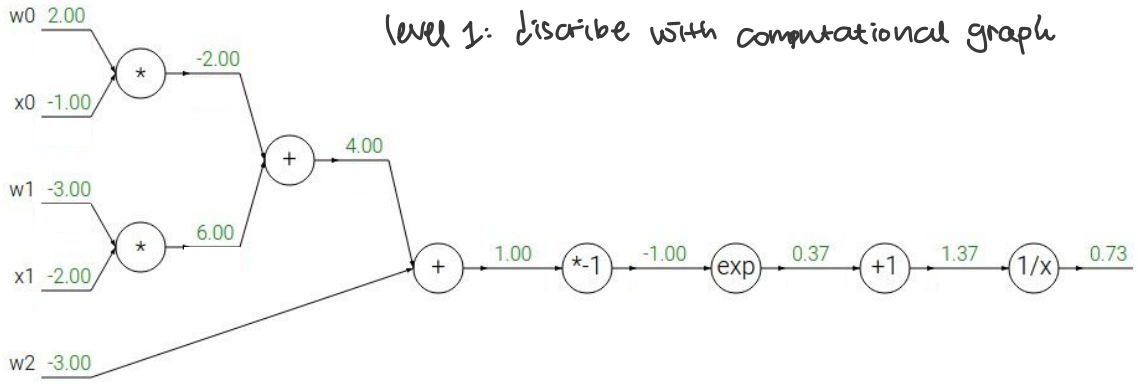
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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





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



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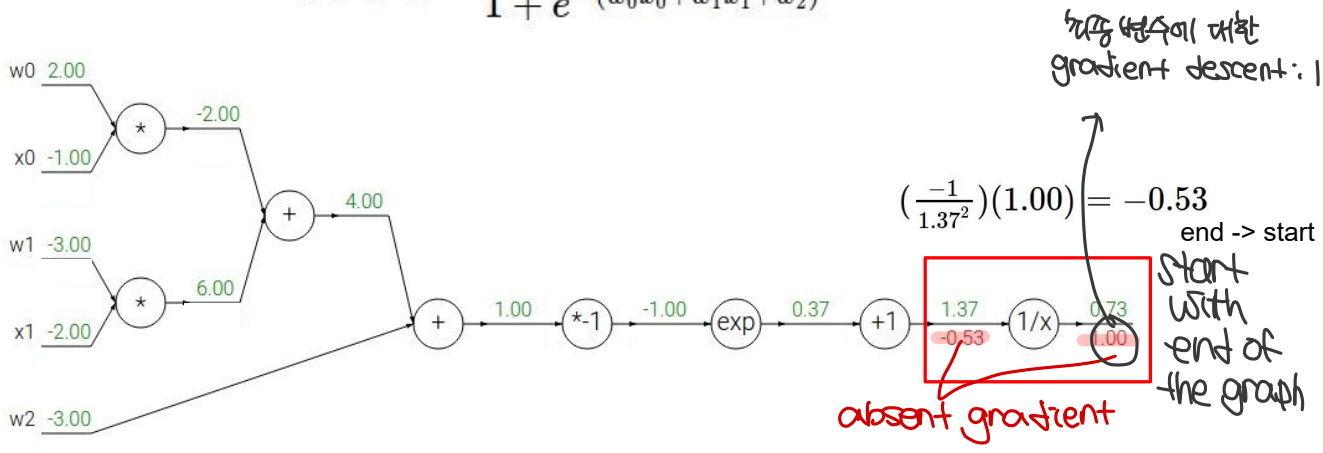
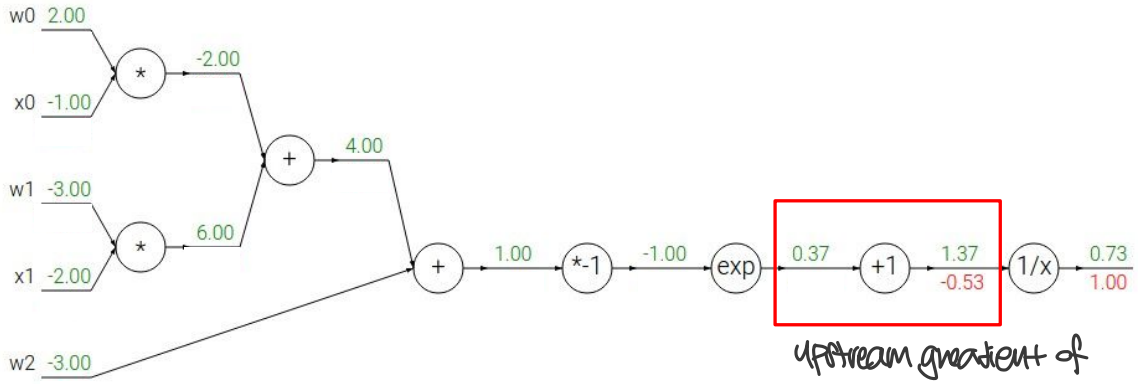


$(\frac{-1}{1.37^2})(1.00) = -0.53$

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

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



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

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

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

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

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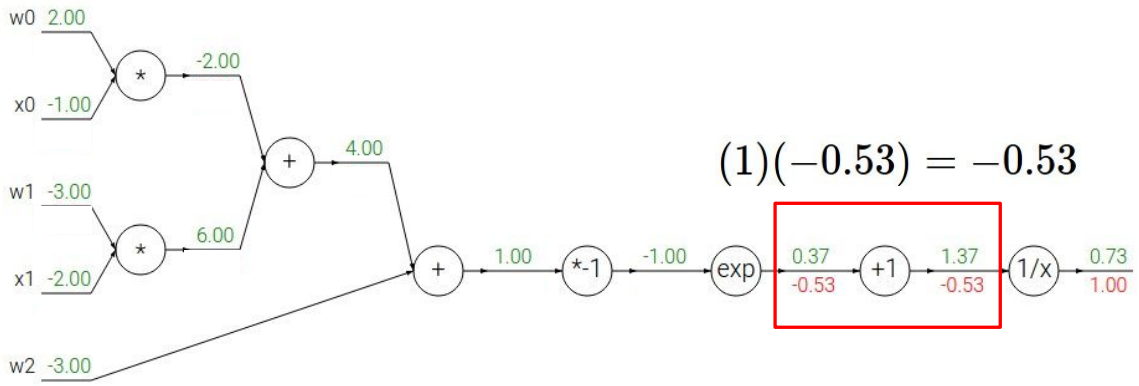

$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$

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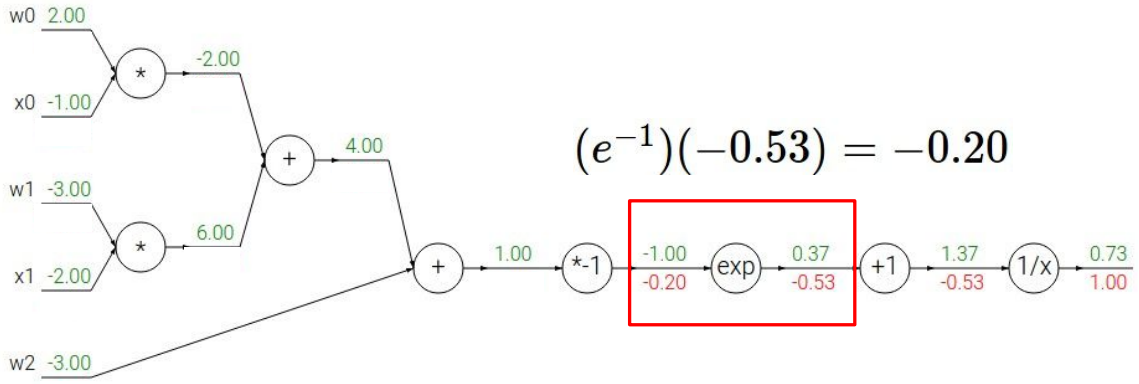

$(e^{-1})(-0.53) = -0.20$

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

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

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

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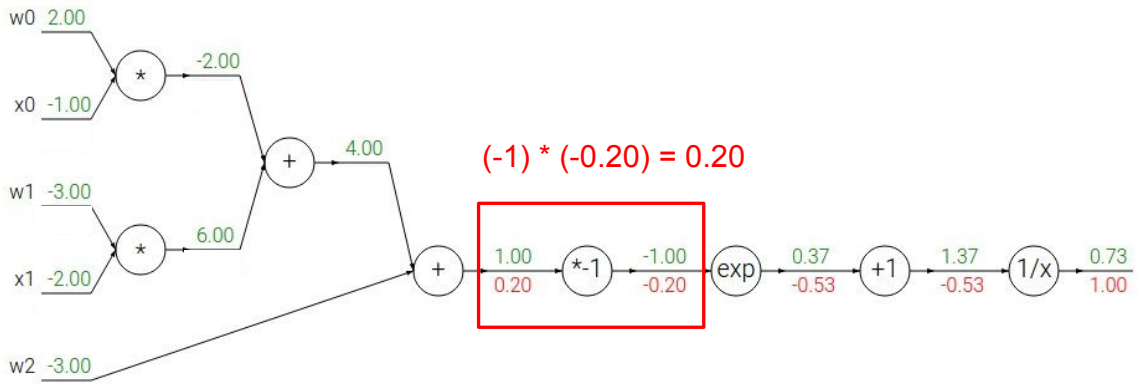

(-1) * (-0.20) = 0.20

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

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

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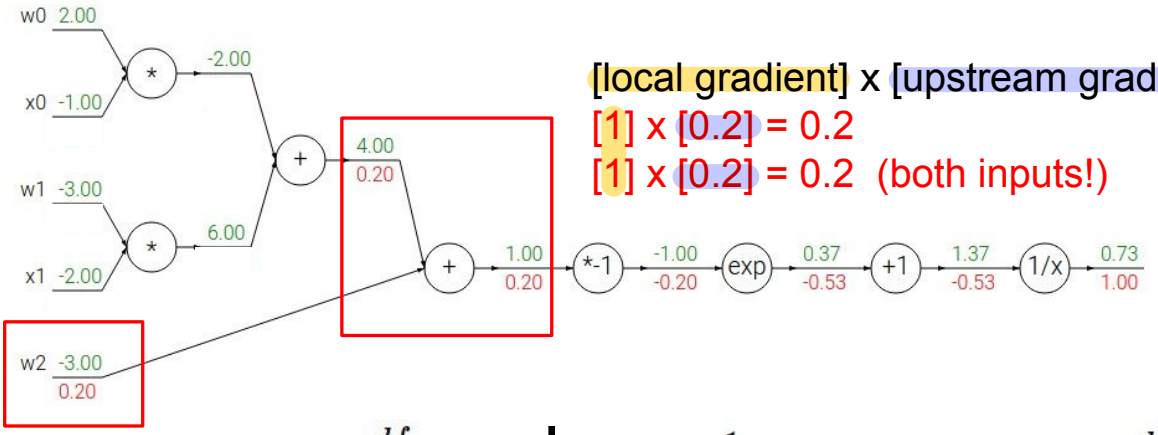


[local gradient] x [upstream gradient]
[1] x [0.2] = 0.2
[1] x [0.2] = 0.2 (both inputs!)

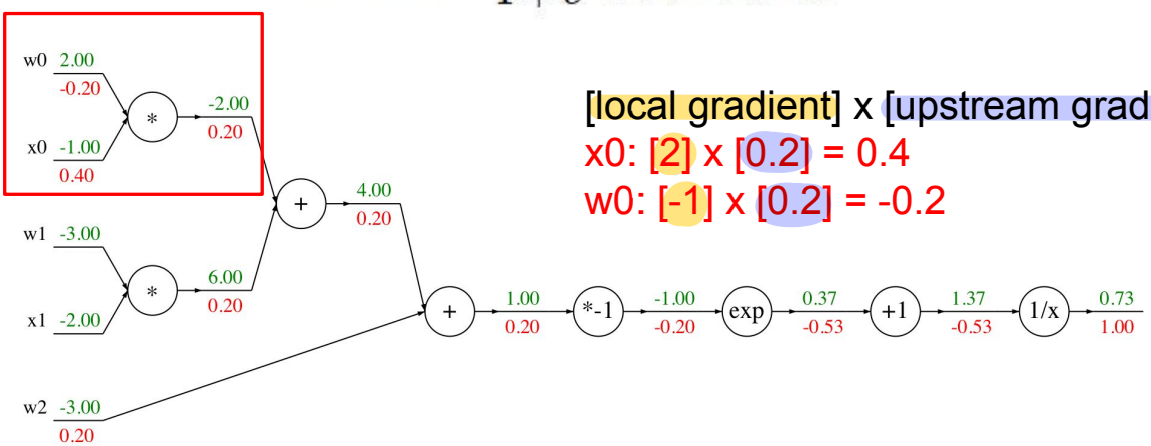
$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$

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

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

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

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



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

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

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

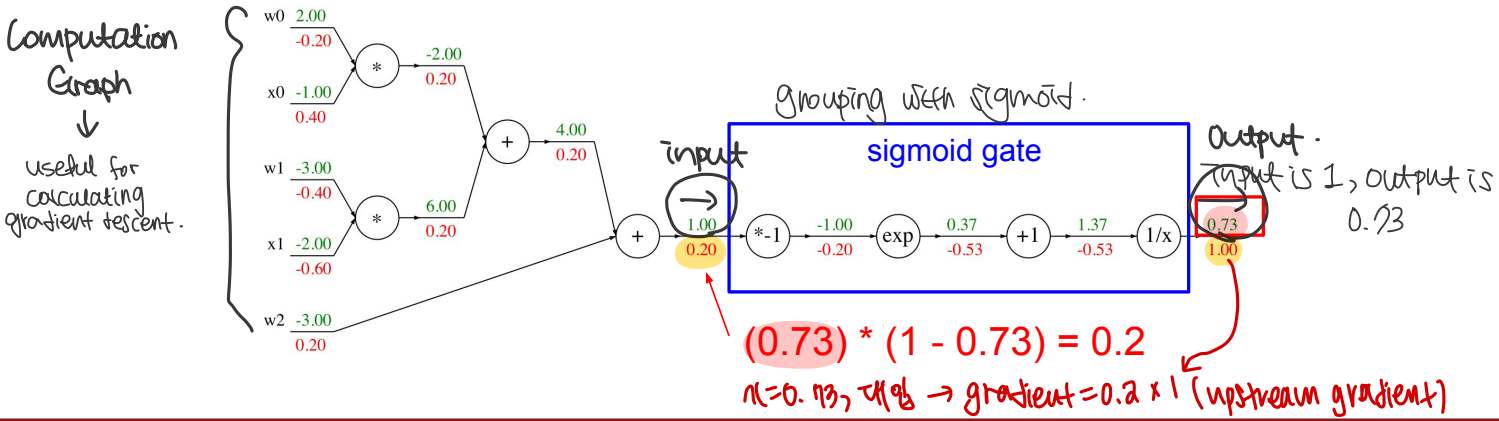
$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$

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

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

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

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



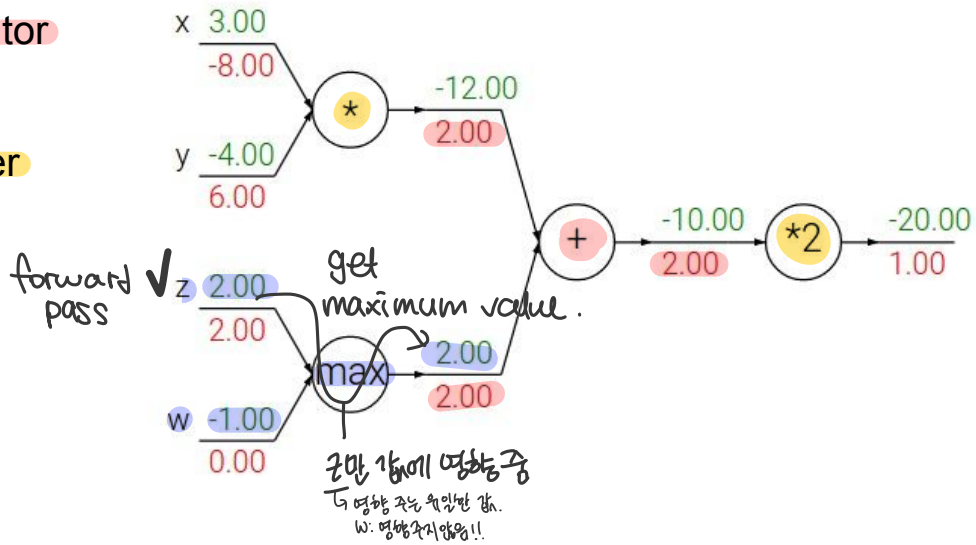
Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

mul gate: gradient switcher

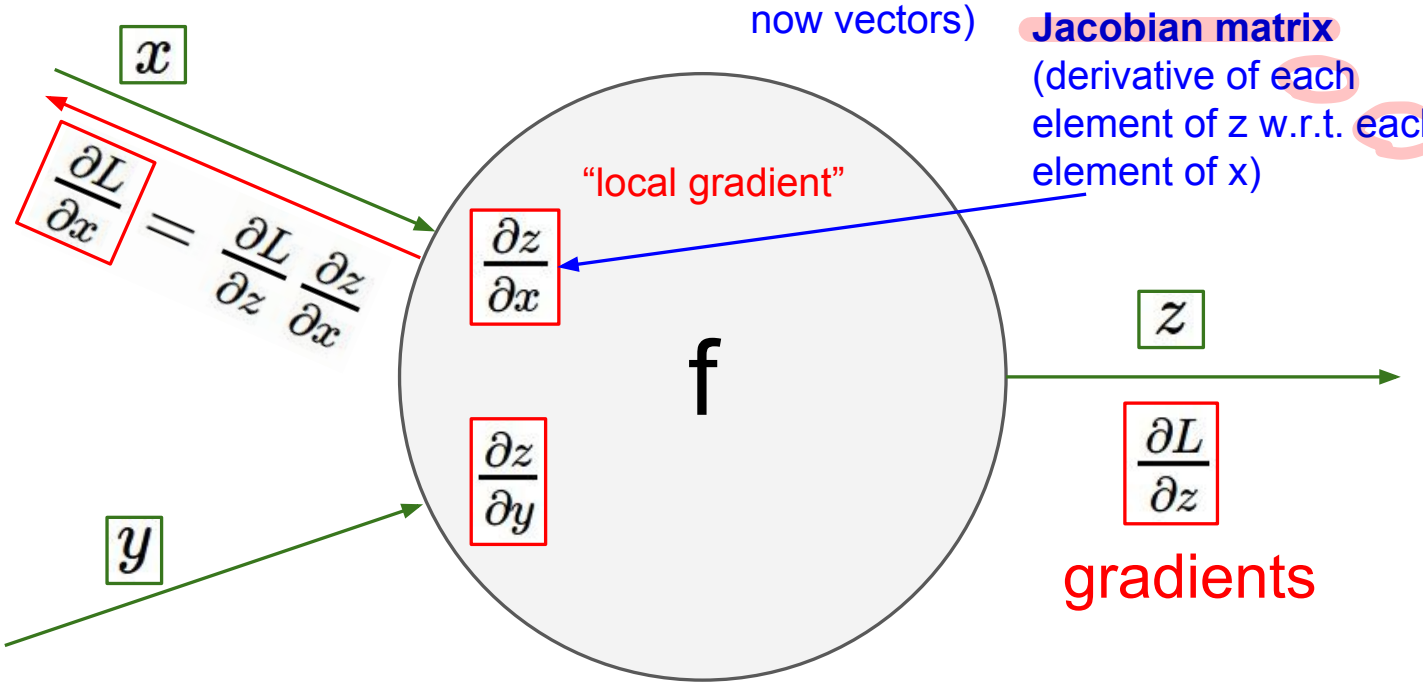
↳ scaler upstream gradient → scale 방식으로 Other branch's value.



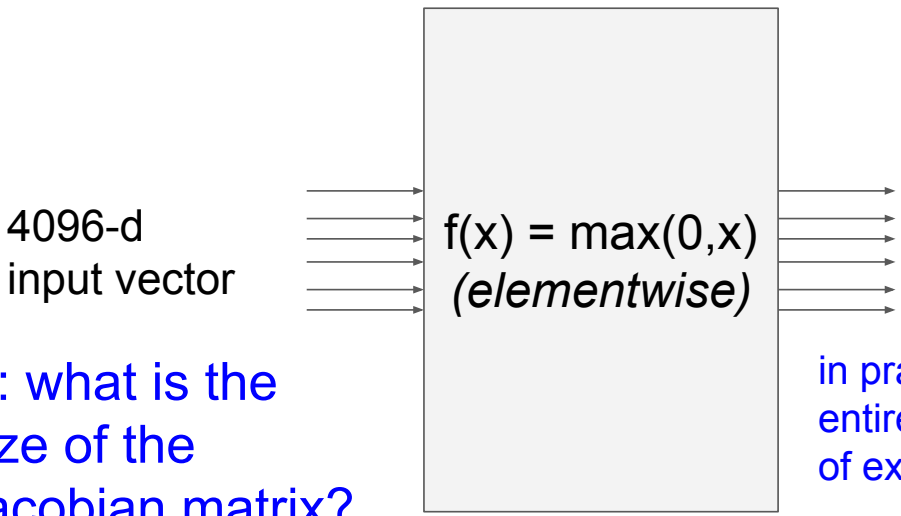
Gradients for vectorized code

(x,y,z are now vectors)

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



Vectorized operations



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

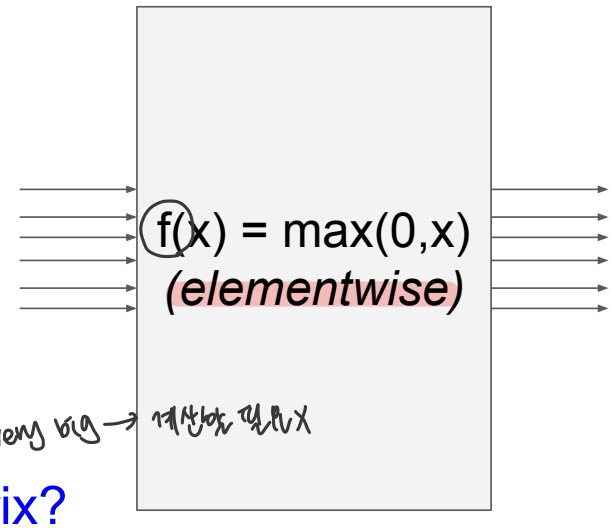
in practice we process an entire minibatch (e.g. 100) of examples at one time:

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

Vectorized operations

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

Jacobian matrix



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

very big → 계산하기 힘들다

Q2: what does it look like?

diagonal matrix

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

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

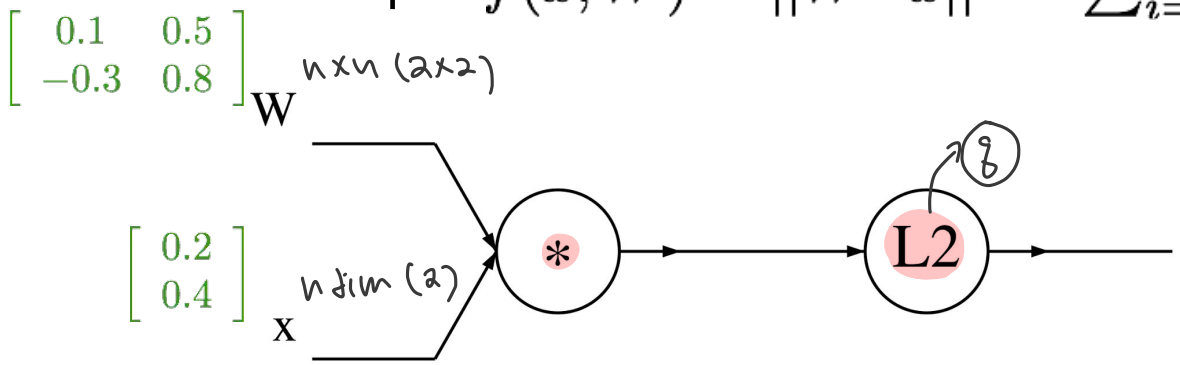
input dimension → out demension

each ~~~~ each (that)

the first dimension only effects that corresponding element in the output ∴ Jacobian → diagonal

- don't have to write the entire Jacobian, can just know the effect of x on the output.
→ can just use it.

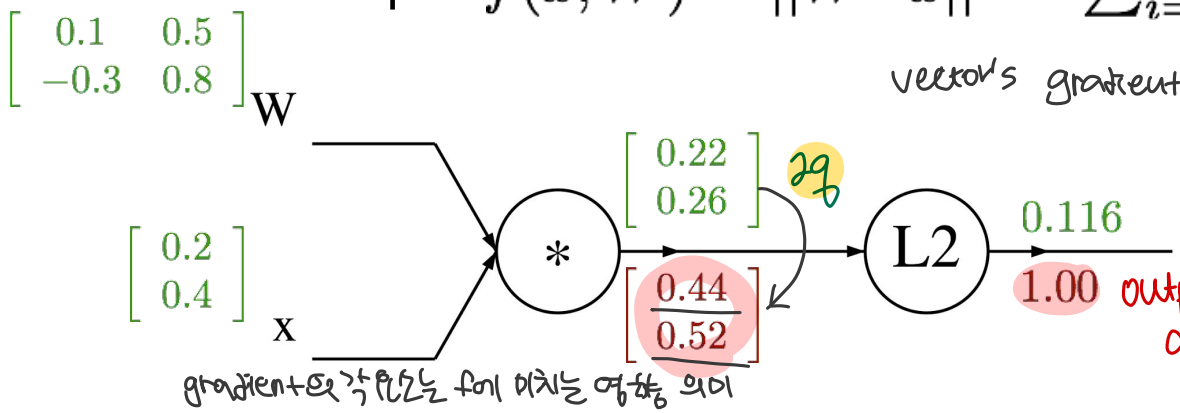
A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$



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

$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$ q_2: L2 norm of q. == $q_1^2 + q_2^2$

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



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

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

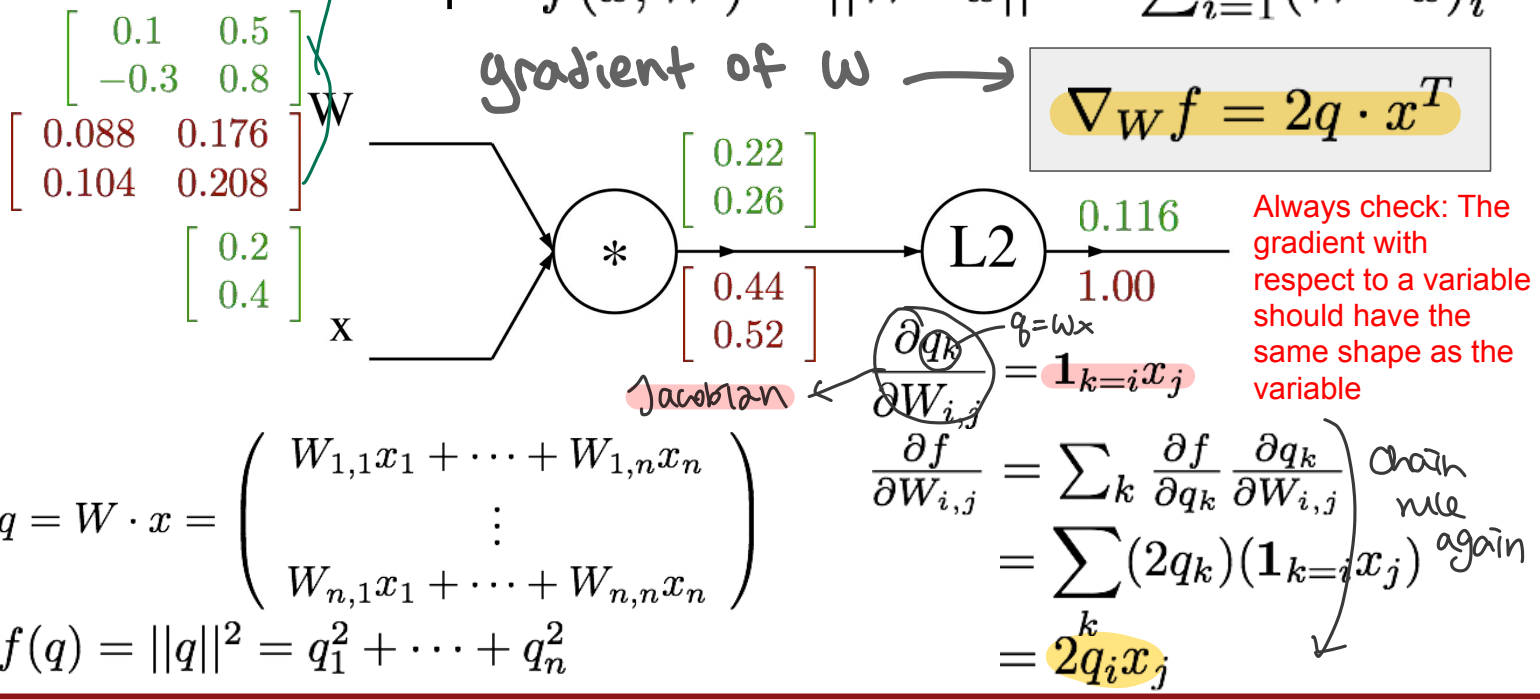
q: 2 dim vector we want to know what will effect what each qs to final value.

$\frac{\partial f}{\partial q_i} = 2q_i$ q_i에 대한 f의 gradient

$\nabla_q f = 2q$ gradient of q

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

gradient shape == variable shape (check!)



gradient of W → $\nabla_W f = 2q \cdot x^T$

Always check: The gradient with respect to a variable should have the same shape as the variable

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

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

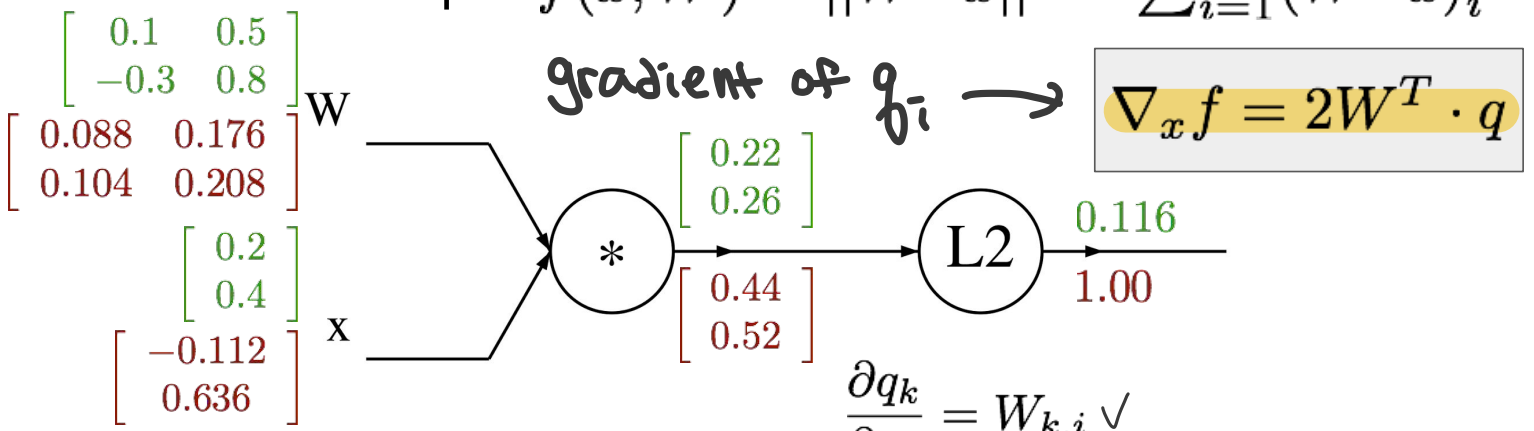
$q = Wx$

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

$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} = \sum_k (2q_k)(\mathbf{1}_{k=i} x_j) = 2q_i x_j$$

chain rule again

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



gradient of q_i → $\nabla_x f = 2W^T \cdot q$

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

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

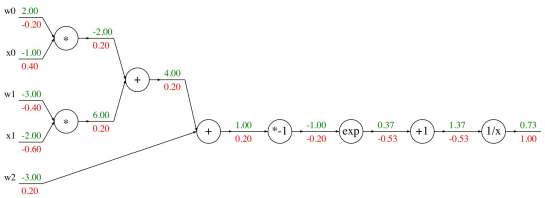
$$\frac{\partial q_k}{\partial x_i} = W_{k,i} \checkmark$$

$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i} = \sum_k 2q_k W_{k,i}$$

chain rule

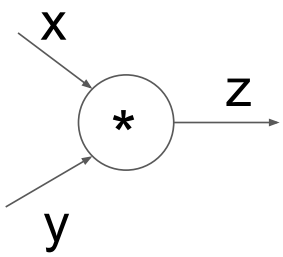
Modularized implementation: forward / backward API

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



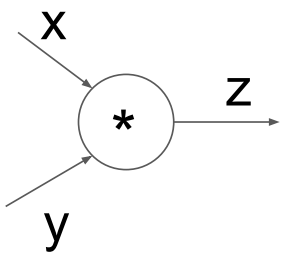
(x,y,z are "scalars")

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

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

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

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]
```

cache. ↓ use it at backward.

chain rule

Example: Caffe layers

framework → sigmoid, convolution, Avgmax..

Branch: master ▾ caffe / src / caffe / layers / Create new file Upload files Find file History

shelhamer committed on GitHub Merge pull request #4630 from BIGene/load_hdf5_fix ... Latest commit e687a71 21 days ago

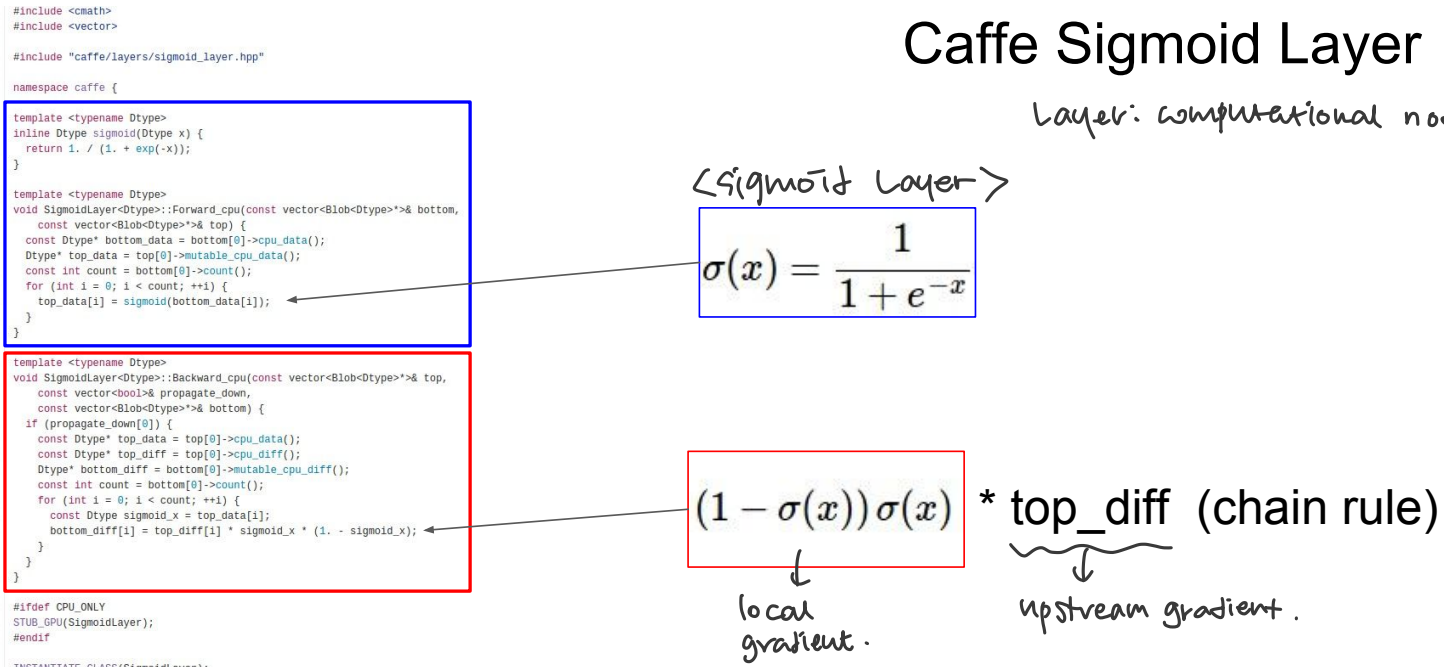
..

absval_layer.cpp	dismantle layer headers	a year ago
absval_layer.cu	dismantle layer headers	a year ago
accuracy_layer.cpp	dismantle layer headers	a year ago
argmax_layer.cpp	dismantle layer headers	a year ago
base_conv_layer.cpp	enable dilated deconvolution	a year ago
base_data_layer.cpp	Using default from proto for prefetch	3 months ago
base_data_layer.cu	Switched multi-GPU to NCCL	3 months ago
batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_layer.cpp	4 months ago
batch_norm_layer.cu	dismantle layer headers	a year ago
batch_reindex_layer.cpp	dismantle layer headers	a year ago
batch_reindex_layer.cu	dismantle layer headers	a year ago
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BiasLayer	a year ago
bias_layer.cu	Separation and generalization of ChannelwiseAffineLayer into BiasLayer	a year ago
bnll_layer.cpp	dismantle layer headers	a year ago
bnll_layer.cu	dismantle layer headers	a year ago
concat_layer.cpp	dismantle layer headers	a year ago
concat_layer.cu	dismantle layer headers	a year ago
contrastive_loss_layer.cpp	dismantle layer headers	a year ago
contrastive_loss_layer.cu	dismantle layer headers	a year ago
conv_layer.cpp	add support for 2D dilated convolution	a year ago
conv_layer.cu	dismantle layer headers	a year ago
crop_layer.cpp	remove redundant operations in Crop layer (#5138)	2 months ago
crop_layer.cu	remove redundant operations in Crop layer (#5138)	2 months ago
cudnn_conv_layer.cpp	dismantle layer headers	a year ago
cudnn_conv_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago

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_layer.cu	dismantle layer headers	a year ago

Caffe Sigmoid Layer

Layer: computational node.



```cpp
#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);
#endif

INSTANTIATE_CLASS(SigmoidLayer);


}  // namespace caffe
```


Summary so far...

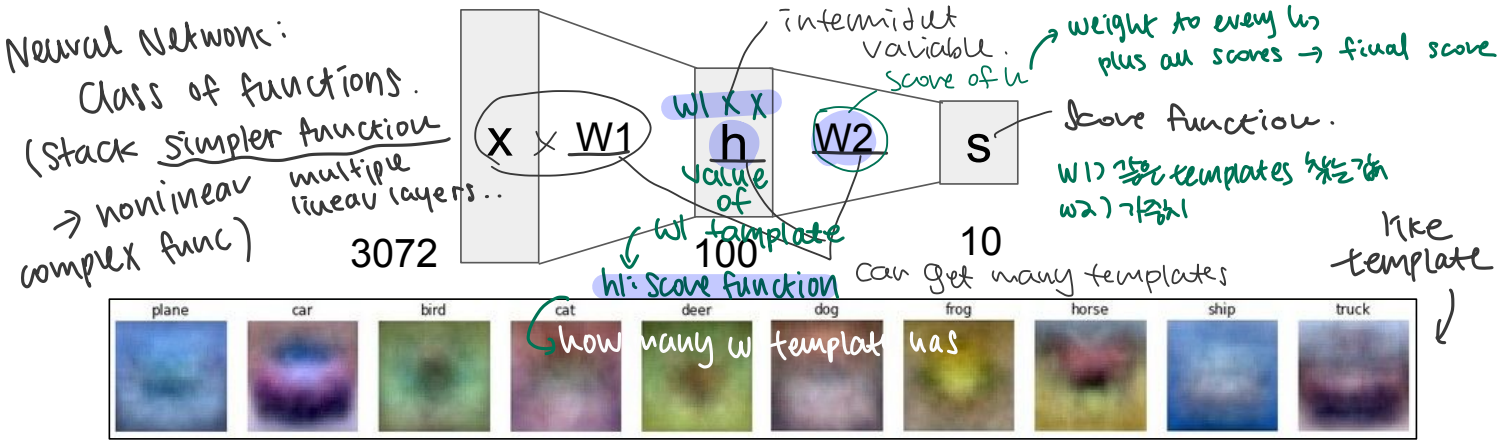
- neural nets will be very large: impractical to write down gradient formula by hand for all parameters
- **backpropagation** = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates
- implementations maintain a graph structure, 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

Neural networks: without the brain stuff

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

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



Neural networks: without the brain stuff

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

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

or 3-layer Neural Network

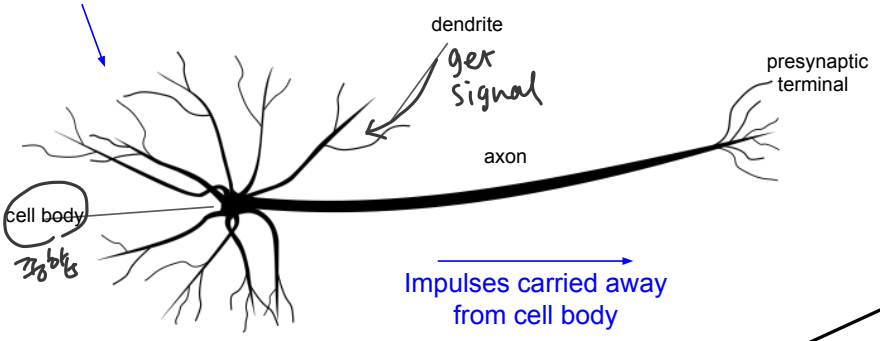
$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

many layer → complex network

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

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

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

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

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

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

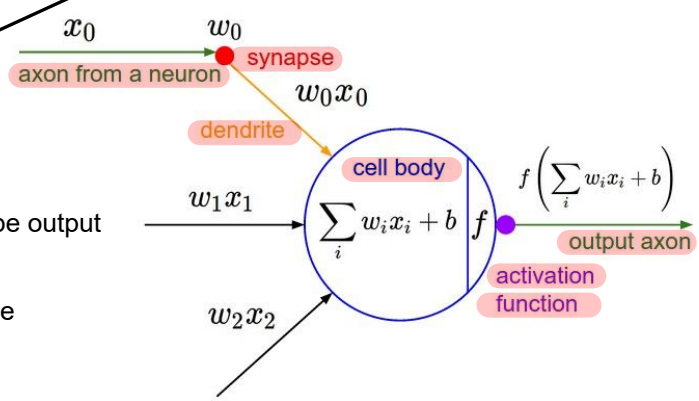
Impulses carried toward cell body

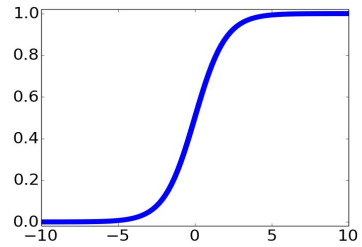


Impulses carried away from cell body

nodes are connected with computational graph
input: x
every x combined with W
everything - combined
get output and give it to connected neuron
- we can think it is very similar way..

work of computational node
- similar with that work





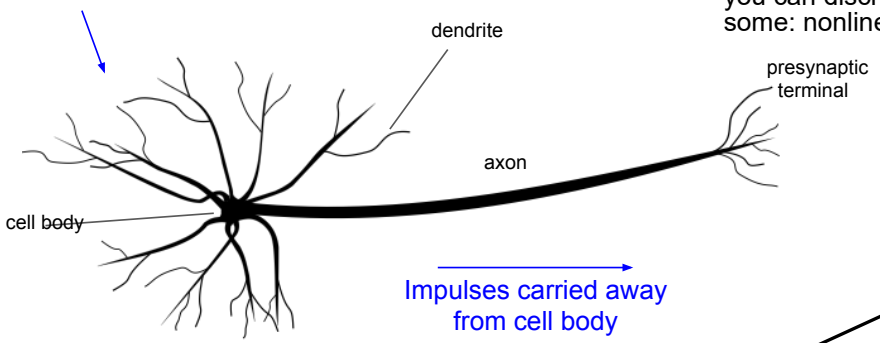
activation function - get input and
show the only one number that would be output

sigmoid activation function

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

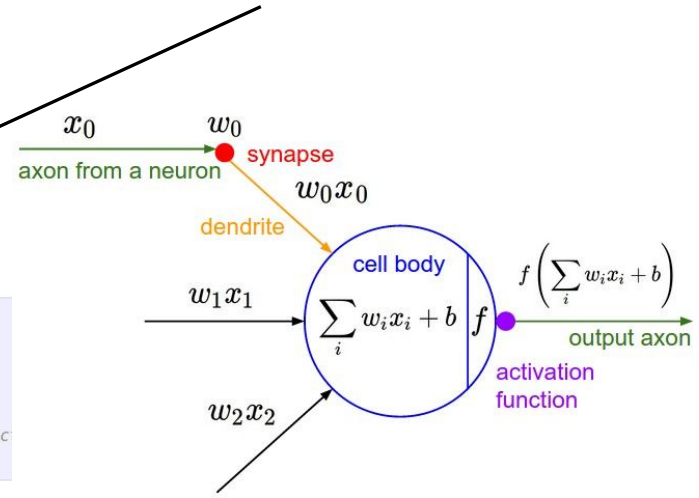
it is loooose one

Impulses carried toward cell body



Impulses carried away from cell body

you can discribe about firing.. spiking with nonlinear
some: nonlinear activation that similar with real way: ReLu (function)




```
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 func
    return firing_rate
```

Be very careful with your brain analogies!

it's similar with neuron, but biological neurons are more complex than this

Biological Neurons:

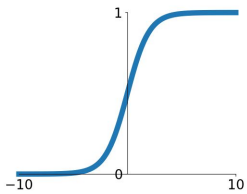
- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate

[Dendritic Computation. London and Hausser]

Activation functions

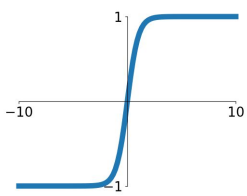
Sigmoid

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



tanh

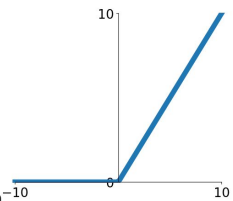
$$\tanh(x)$$



ReLU

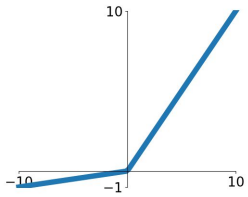
$$\max(0, x)$$

every minus value: 0
every plus value: linear function



Leaky ReLU

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

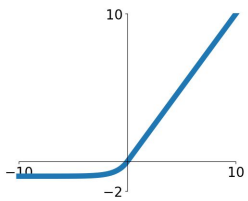


Maxout

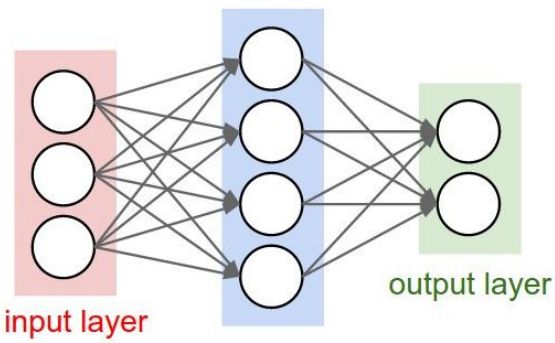
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

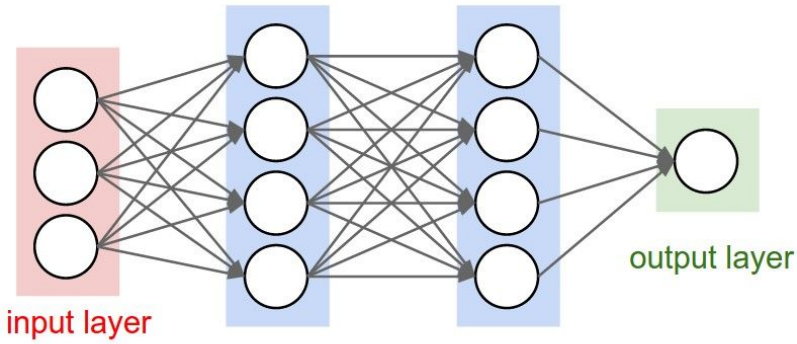
ELU

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



Neural networks: Architectures





"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

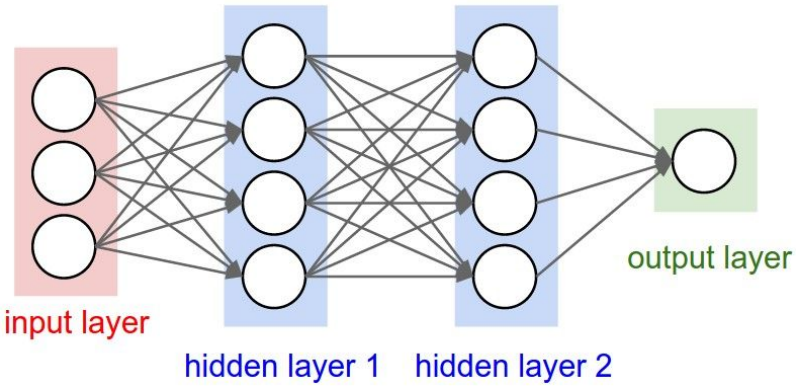
"Fully-connected" layers

Example feed-forward computation of a neural network

```
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




```
# 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