Lecture 4:

Backpropagation and Neural Networks part 1

Where we are...

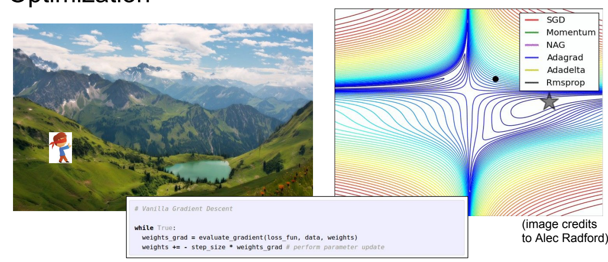
$s = f(x; W) = Wx$ scores function

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

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

want $\boxed{\nabla_W L}$

Optimization



(image credits to Alec Radford)

Gradient Descent

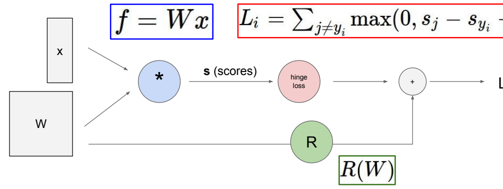
$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

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

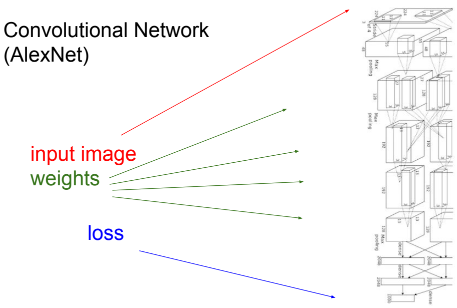
In practice: Derive analytic gradient, check your implementation with numerical gradient

Computational Graph

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

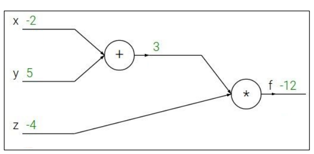


Convolutional Network (AlexNet)



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

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



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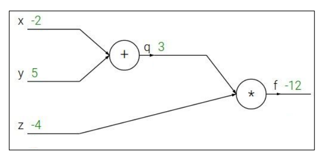

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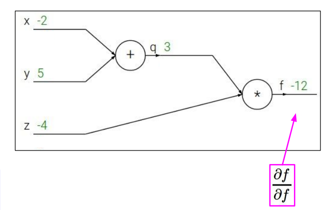

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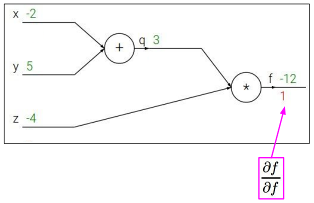

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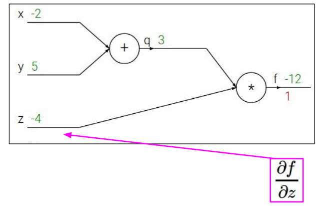

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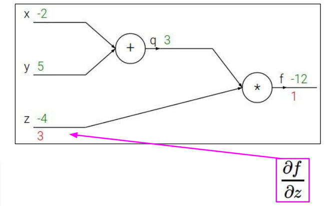

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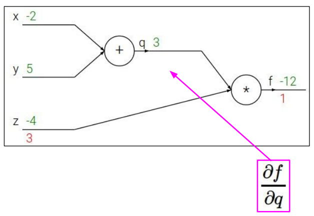

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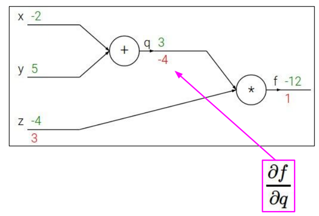

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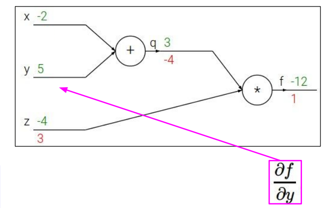

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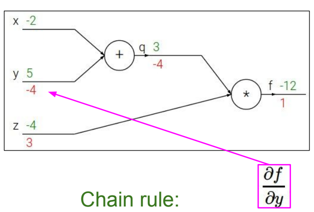

Chain rule:

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

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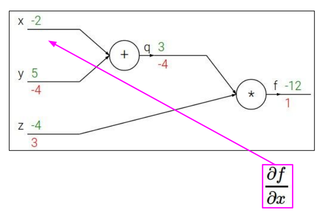

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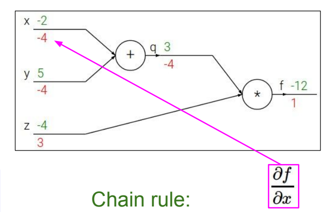

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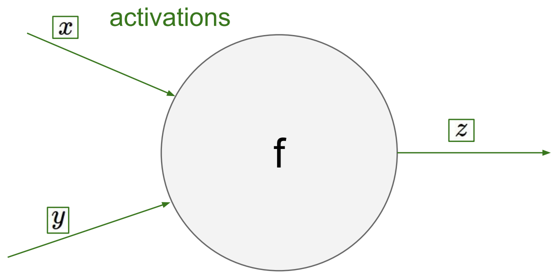
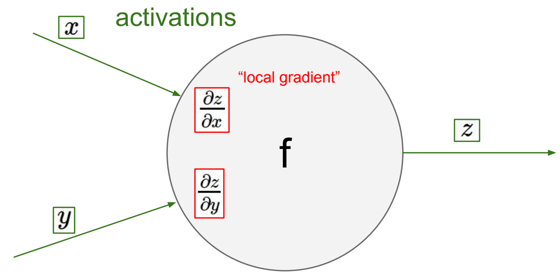
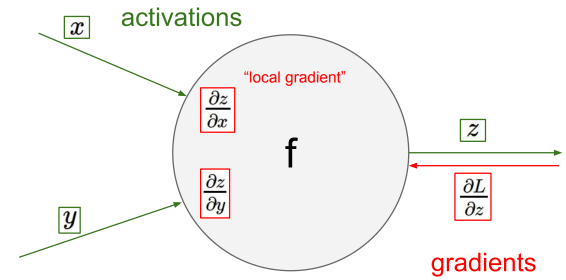
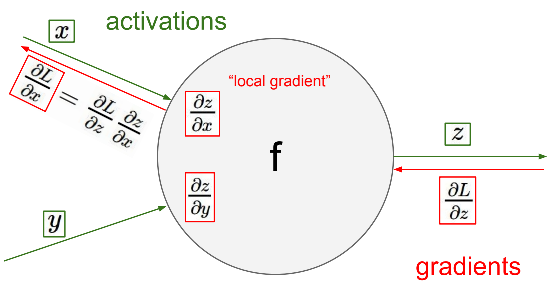
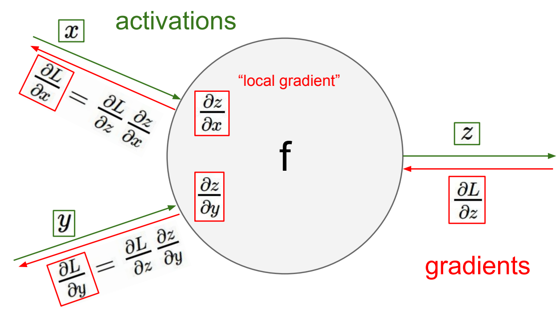
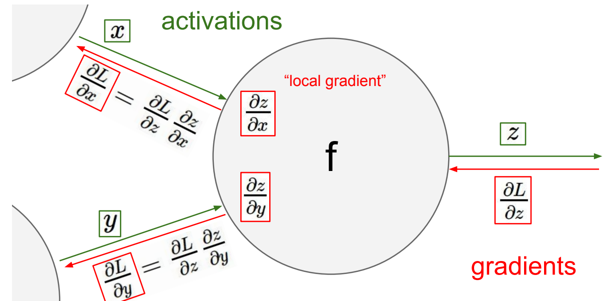




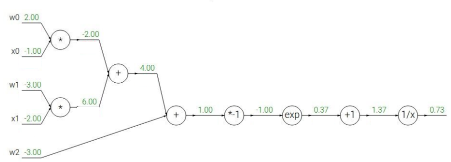








Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



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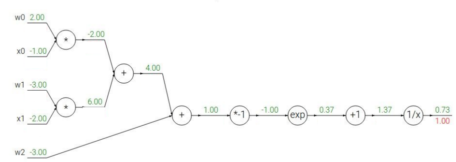

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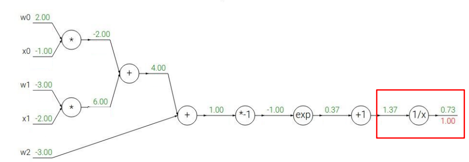

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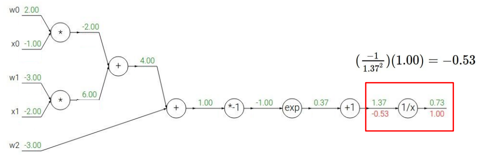

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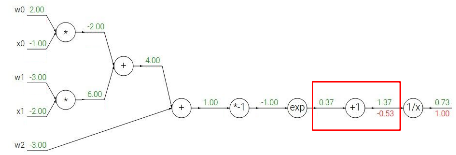

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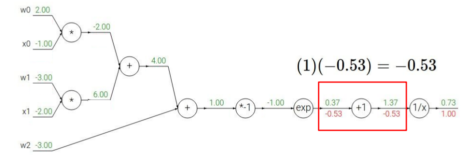

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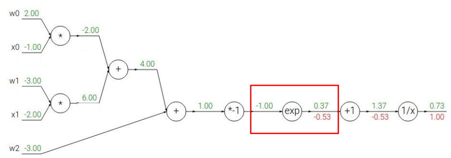

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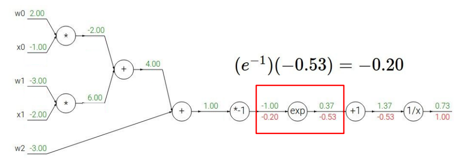

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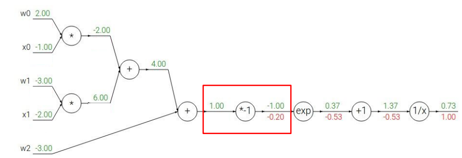

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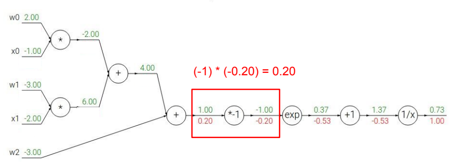

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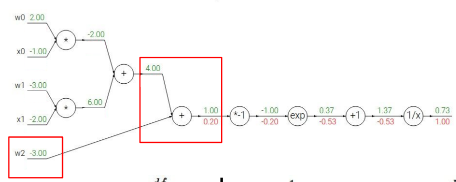

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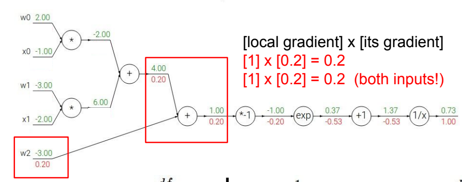

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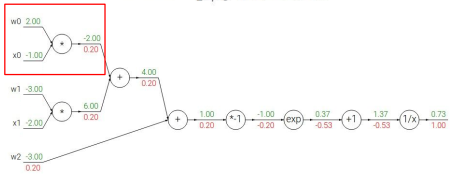

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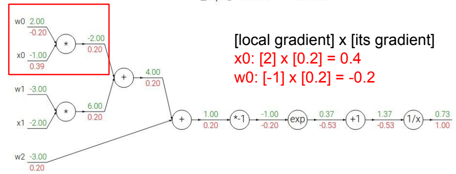

[local gradient] x [its gradient]
x0: [2] x [0.2] = 0.4
w0: [-1] x [0.2] = -0.2

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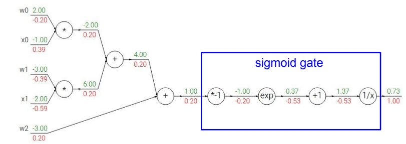
$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}} \qquad \boxed{\sigma(x) = \frac{1}{1+e^{-x}}} \quad \text{sigmoid function}$$

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



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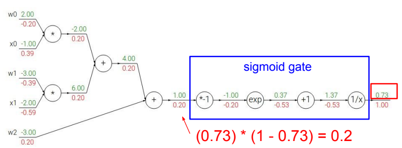
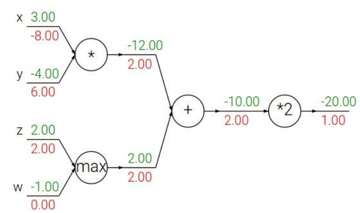
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$



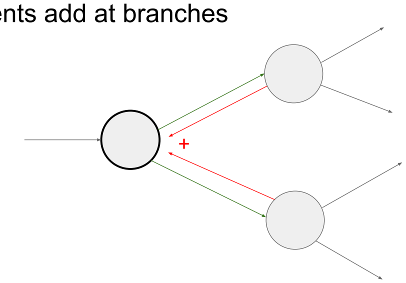
(0.73) * (1 - 0.73) = 0.2

Patterns in backward flow

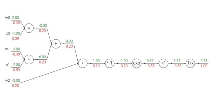
add gate: gradient distributor
max gate: gradient router
mul gate: gradient… "switcher"?



Gradients add at branches



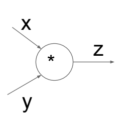
Implementation: forward/backward API



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
```


Implementation: forward/backward API



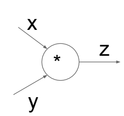
(x,y,z are scalars)

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

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

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

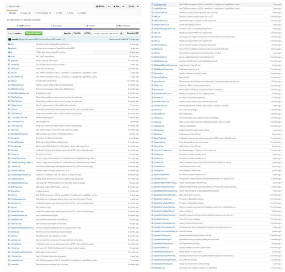
Implementation: forward/backward API



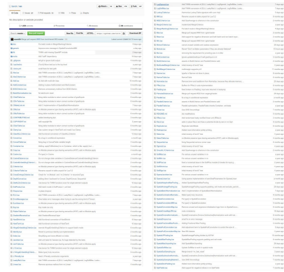
(x,y,z are scalars)

```
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]
```

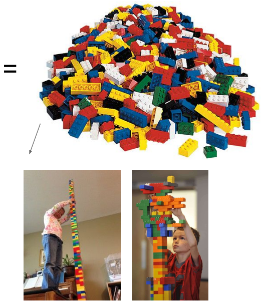
Example: Torch Layers



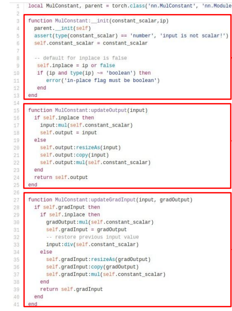
Example: Torch Layers



=



Example: Torch MulConstant



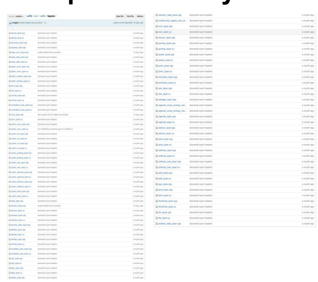
$$f(X) = aX$$

initialization

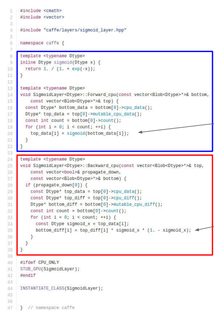
forward()

backward()

Example: Caffe Layers



Caffe Sigmoid Layer

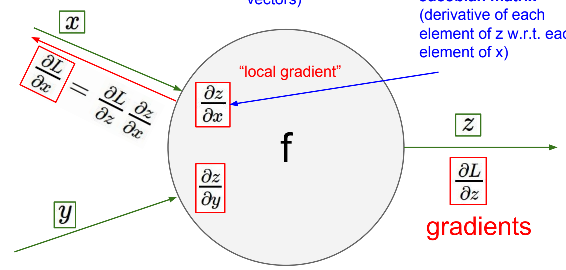


$$\sigma(x) = \frac{1}{1+e^{-x}}$$

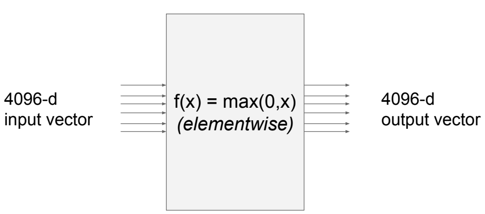
$(1-\sigma(x))\sigma(x)$ *top_diff (chain rule)

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)



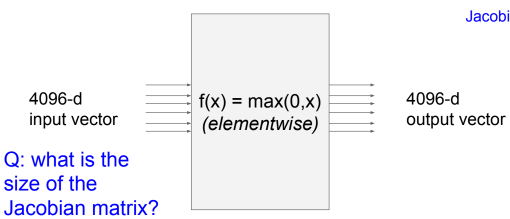
Vectorized operations



Vectorized operations

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

Jacobian matrix

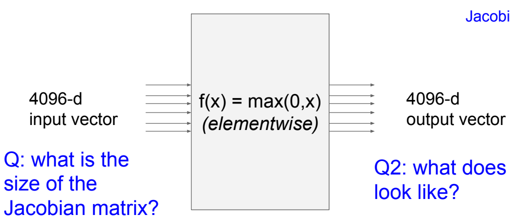


Q: what is the size of the Jacobian matrix?

Vectorized operations

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

Jacobian matrix

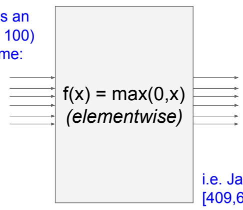


Q: what is the size of the Jacobian matrix? [4096 x 4096!]

Q2: what does it look like?

Vectorized operations

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



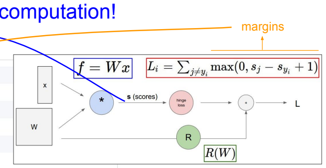
i.e. Jacobian would technically be a [409,600 x 409,600] matrix :\

Assignment: Writing SVM/Softmax

Stage your forward/backward computation!

E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 8 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 = #...
```



Summary so far

- neural nets will be very large: no hope of writing 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.

Neural Network: without the brain stuff

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

Neural Network: without the brain stuff

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

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

Neural Network: without the brain stuff

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

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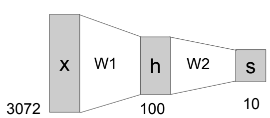
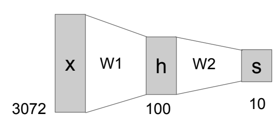


Neural Network: without the brain stuff

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

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



Neural Network: 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

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

Full implementation of training a 2-layer Neural Network needs ~11 lines:

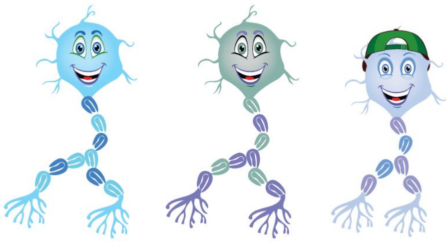
```
X = np.array([ [0,0,1],[0,1,1],[1,0,1],[1,1,1] ])
y = np.array([[0,1,1,0]]).T
syn0 = 2*np.random.random((3,4)) - 1
syn1 = 2*np.random.random((4,1)) - 1
for j in xrange(60000):
    l1 = 1/(1+np.exp(-(np.dot(X,syn0))))
    l2 = 1/(1+np.exp(-(np.dot(l1,syn1))))
    l2_delta = (y - l2)*(l2*(1-l2))
    l1_delta = l2_delta.dot(syn1.T) * (l1 * (1-l1))
    syn1 += l1.T.dot(l2_delta)
    syn0 += X.T.dot(l1_delta)
```

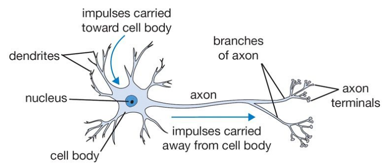
from @iamtrask, http://iamtrask.github.io/2015/07/12/basic-python-network/

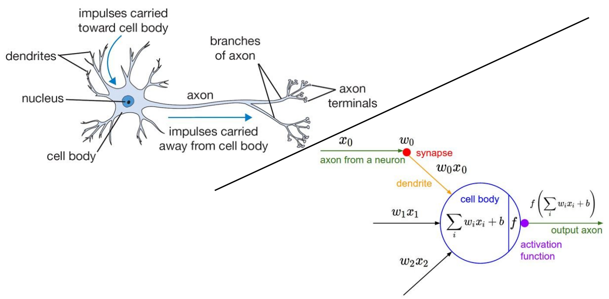
Assignment: Writing 2layer Net

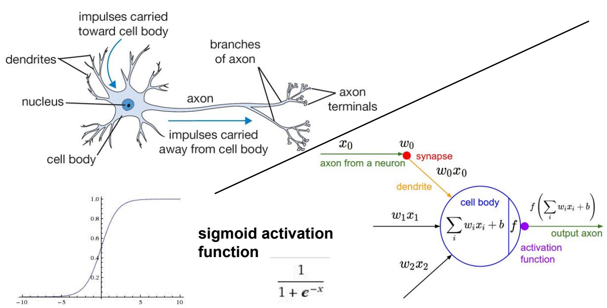
Stage your forward/backward computation!

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

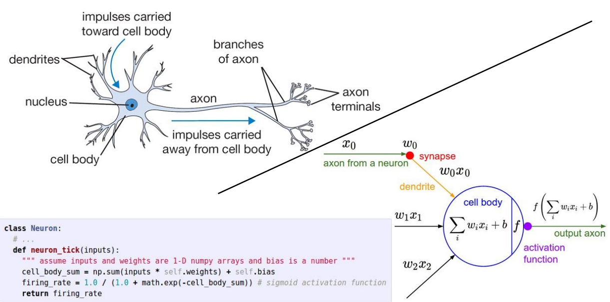






sigmoid activation function

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

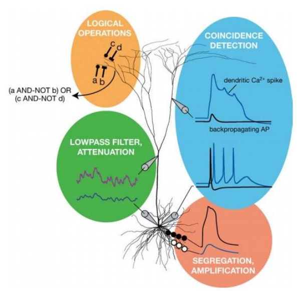



```
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation function
    return firing_rate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


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

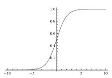


[Dendritic Computation. London and Hausser]

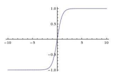
Activation Functions

Sigmoid

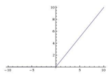
$\sigma(x) = 1/(1+e^{-x})$



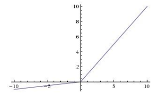
tanh tanh(x)



ReLU max(0,x)

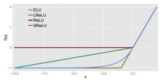


Leaky ReLU
max(0.1x, x)

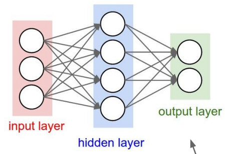


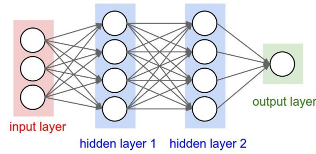
Maxout $\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU $f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \le 0 \end{cases}$



Neural Networks: Architectures





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

"Fully-connected" layers

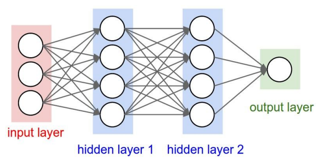
"3-layer Neural Net", or
"2-hidden-layer Neural Net"

Example Feed-forward computation of a Neural Network

```python
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
```

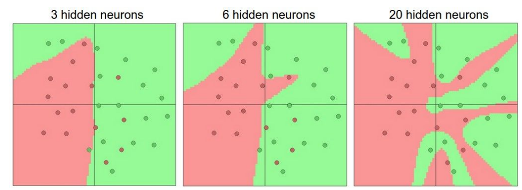
We can efficiently evaluate an entire layer of neurons.

Example Feed-forward computation of a Neural Network



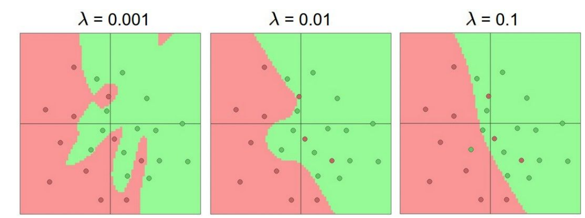

```python
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```


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:



(you can play with this demo over at ConvNetJS: http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html)

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*
- neural networks: bigger = better (but might have to regularize more strongly)