Neural Networks

Cynthia Rudin

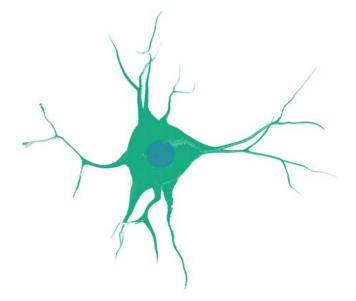
Duke Machine Learning

Neurons

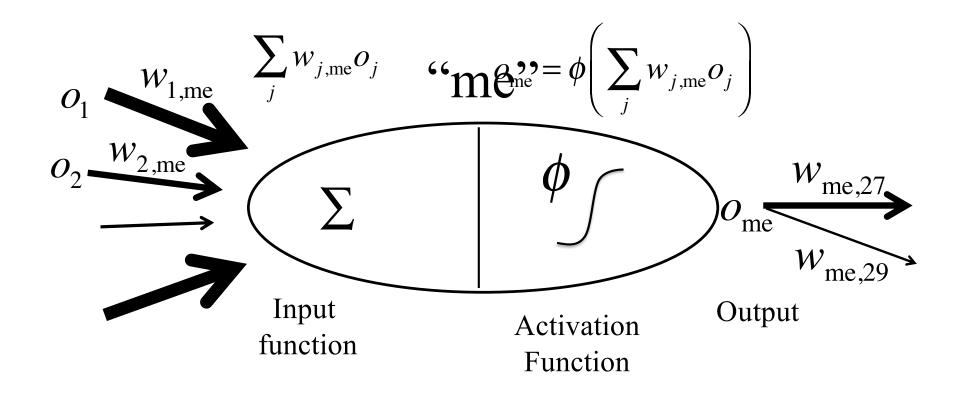
• 10¹¹ neurons in a brain, 10¹⁴ synapses (connections).

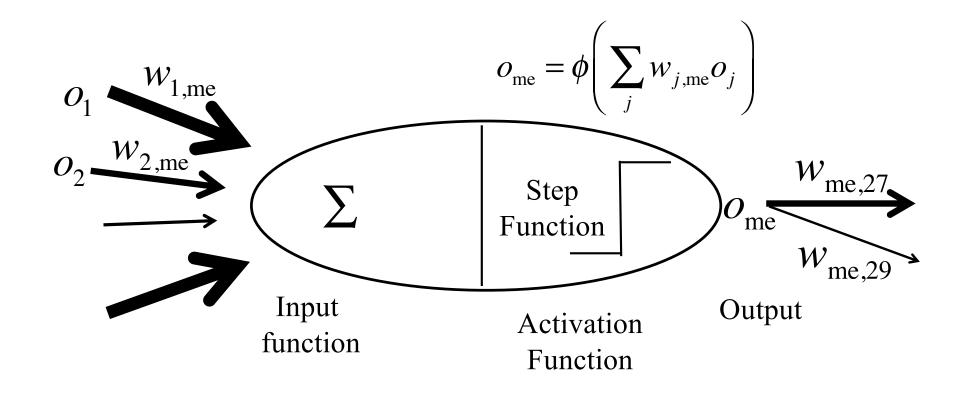
• Signals are electrical potential spikes that travel through the

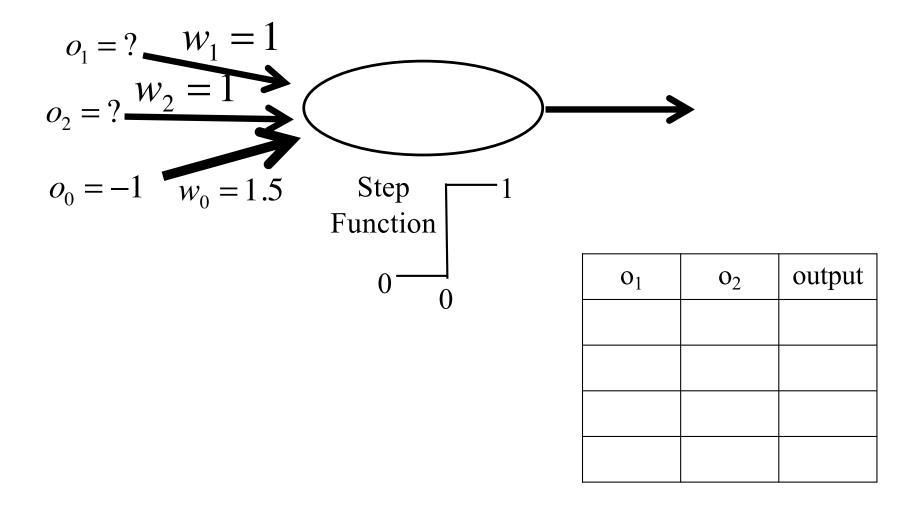
network.

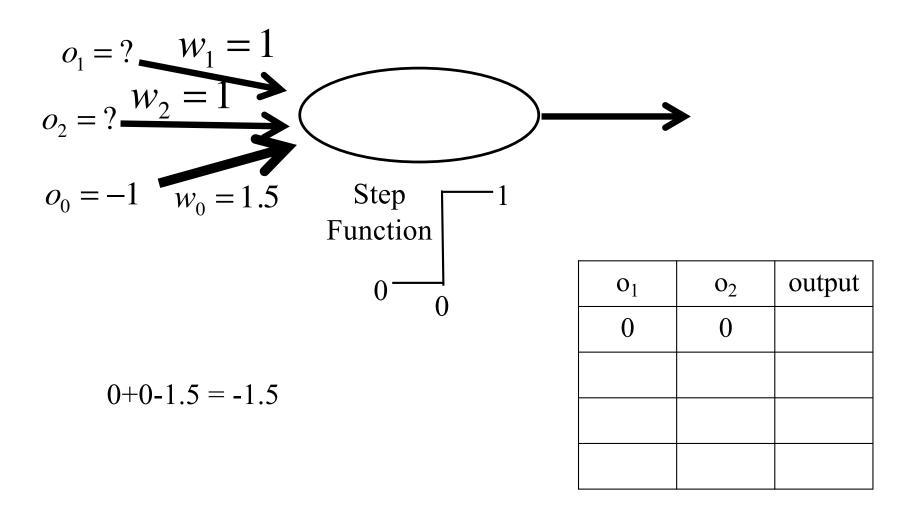


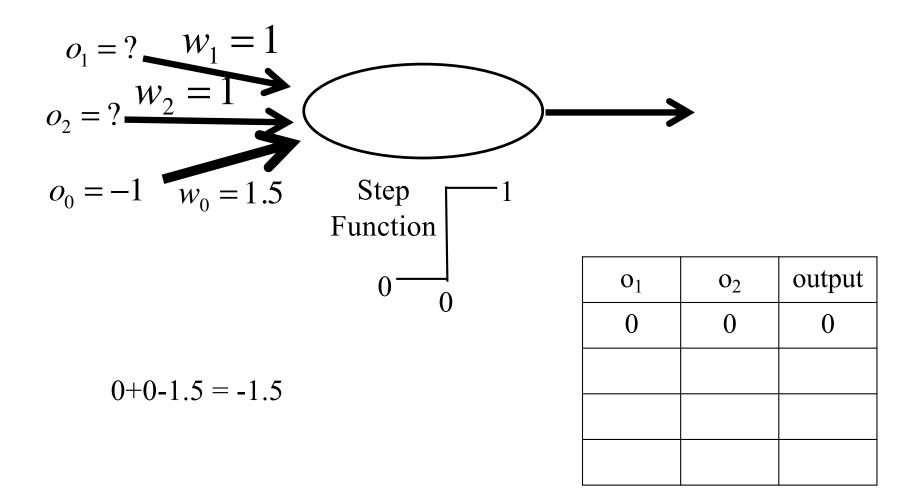
(Credit: Adapted from Russell and Norvig)

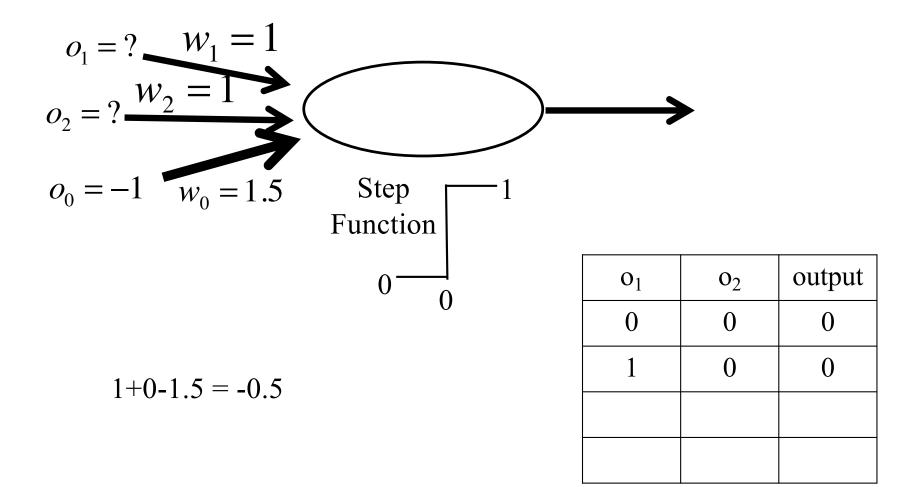


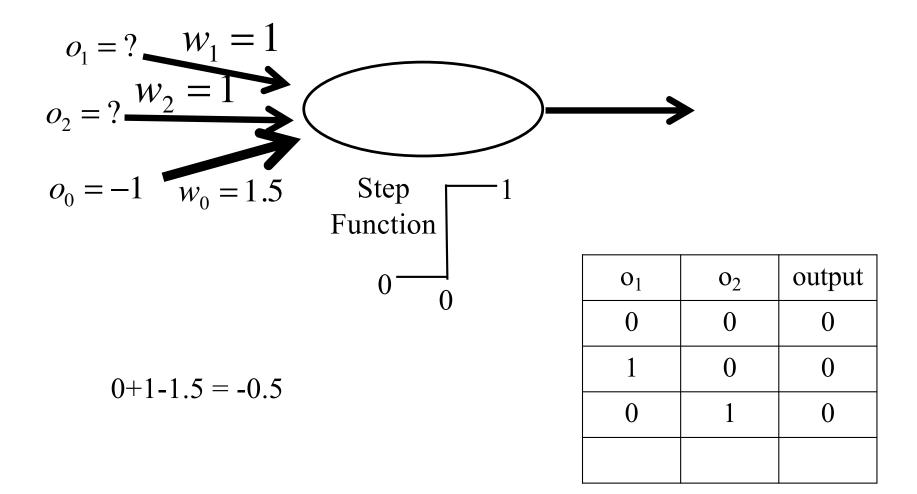


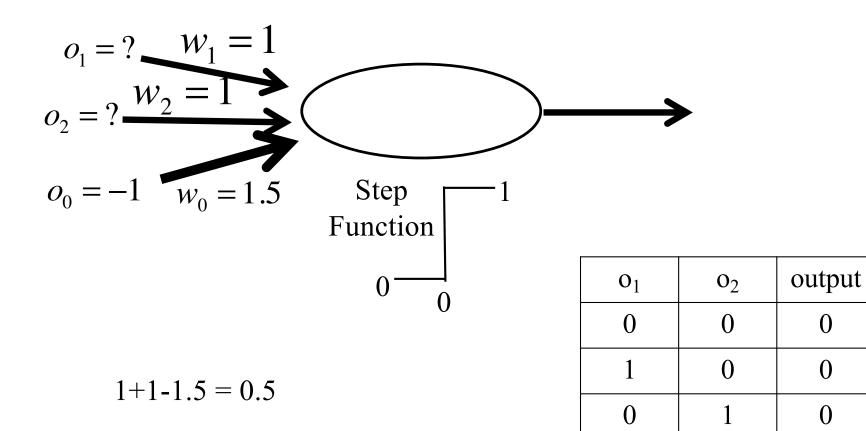


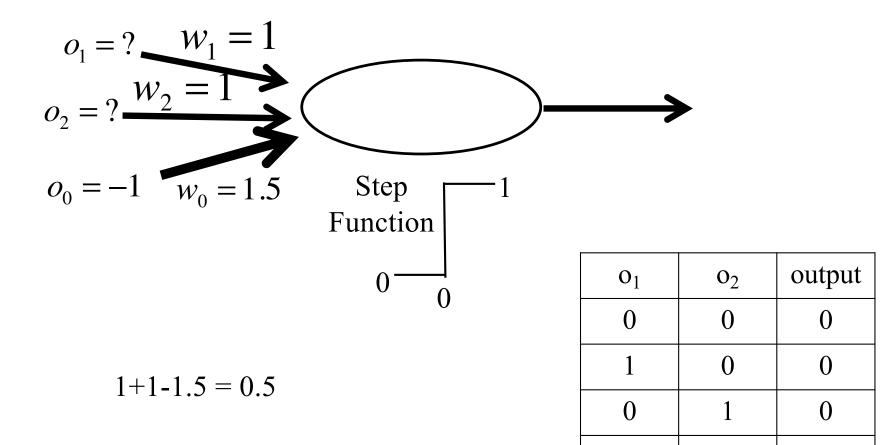


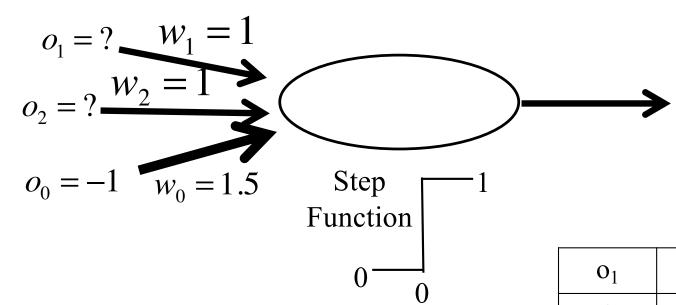












This neuron computes the function "and."

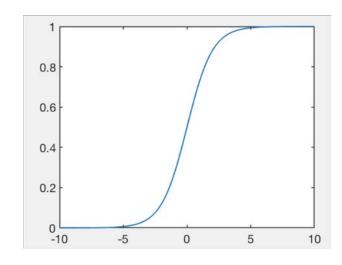
There are "or" and "not" neurons too.

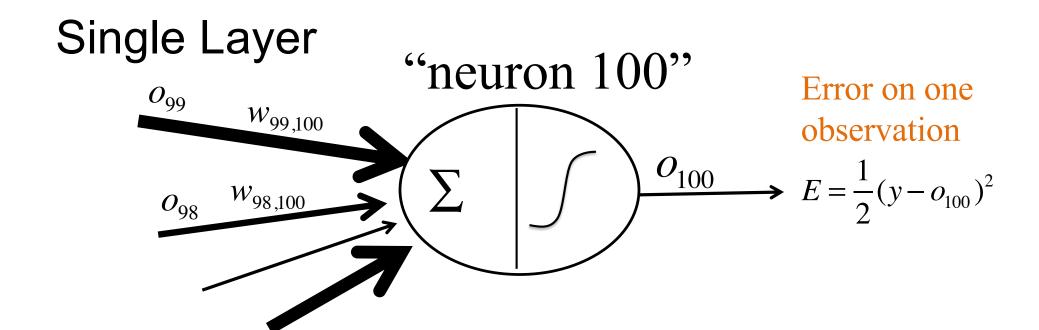
| 01 | 02 | output |
|----|----|--------|
| 0 | 0 | 0 |
| 1 | 0 | 0 |
| 0 | 1 | 0 |
| 1 | 1 | 1 |

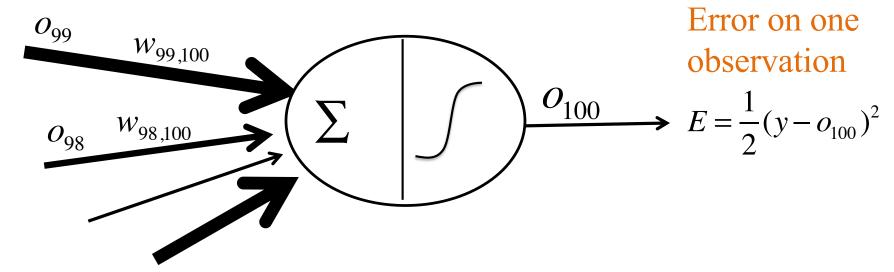
$$\phi\left(\sum_{j} w_{j,\text{me}} a_{j}\right) = 1/(1+e^{-x}) \quad \text{"Sigmoid"}$$



Activation Function



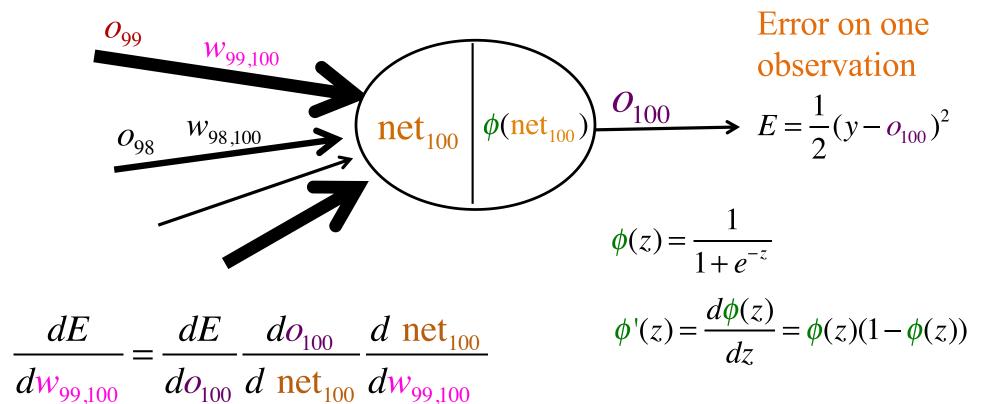


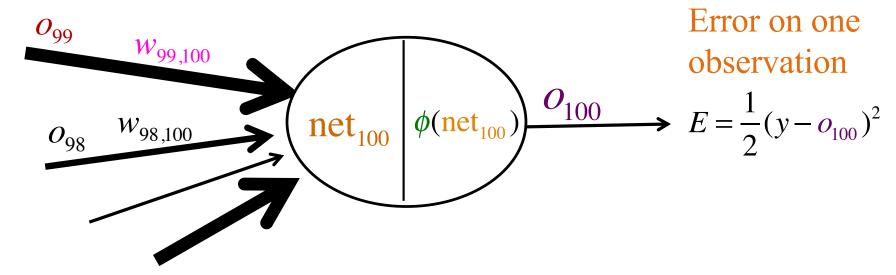


- In a brain, the synapses strengthen and weaken in order to learn.
- Say the same thing happens here.
- How should we set the weights in order to learn (reduce the error)?
- Minimize E with respect to the weights.

Backpropagation

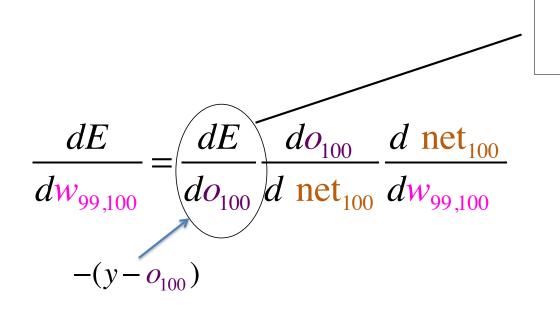
- An algorithm that trains the weights of a neural network
- Requires us to propagate information backwards through the network, then forwards, then backwards, then forwards, etc.
- Propagate backwards = chain rule from calculus.





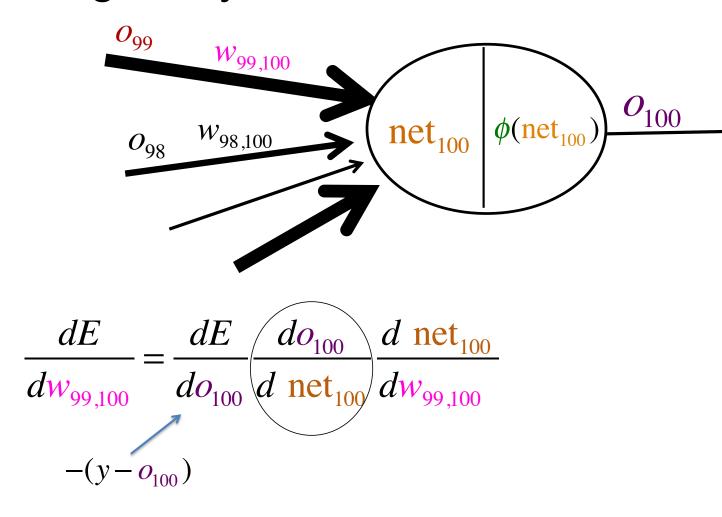
$$\frac{dE}{dw_{99,100}} = \frac{dE}{do_{100}} \frac{do_{100}}{d \cot_{100}} \frac{d \cot_{100}}{dw_{99,100}}$$

$$E = \frac{1}{2}(y - o_{100})^2$$



$$E = \frac{1}{2}(y - o_{100})^2$$

$$\frac{dE}{dw_{99,100}} = \frac{dE}{do_{100}} \frac{do_{100}}{d \text{ net}_{100}} \frac{d \text{ net}_{100}}{dw_{99,100}}$$
$$-(y - o_{100})$$



$$O_{100} \rightarrow E = \frac{1}{2} (y - o_{100})^2$$

$$\frac{do_{100}}{d \text{ net}_{100}} = \frac{d\phi(\text{net}_{100})}{d \text{ net}_{100}} = \phi'(\text{net}_{100}) = \phi(\text{net}_{100})(1 - \phi(\text{net}_{100})) = o_{100}(1 - o_{100})$$

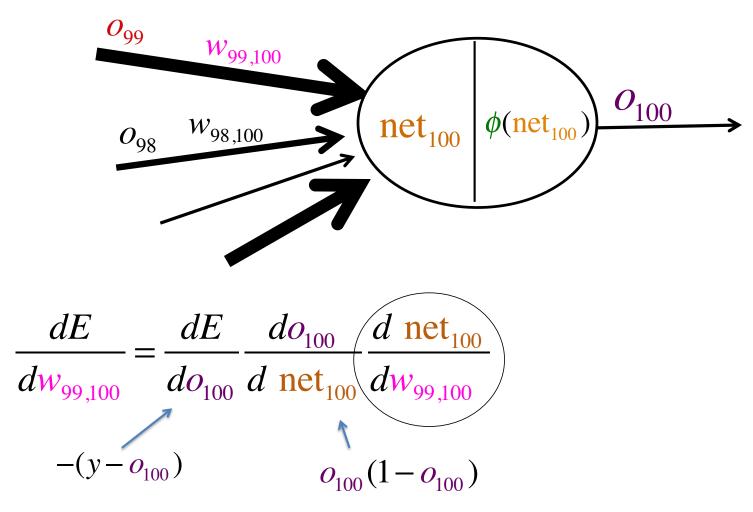
$$\frac{dE}{dw_{99,100}} = \frac{dE}{do_{100}} \underbrace{\frac{do_{100}}{d \text{ net}_{100}}}_{100} \underbrace{\frac{d \text{ net}_{100}}{dw_{99,100}}}_{-(y - o_{100})}$$

$$\frac{do_{100}}{d \operatorname{net}_{100}} = \frac{d\phi(\operatorname{net}_{100})}{d \operatorname{net}_{100}} = \phi'(\operatorname{net}_{100}) = \phi(\operatorname{net}_{100})(1 - \phi(\operatorname{net}_{100})) = o_{100}(1 - o_{100})$$

$$\frac{dE}{dw_{99,100}} = \frac{dE}{do_{100}} \underbrace{\frac{do_{100}}{d \operatorname{net}_{100}}}_{0100} \underbrace{\frac{d\operatorname{net}_{100}}{dw_{99,100}}}_{o_{100}(1 - o_{100})}$$

$$\frac{dE}{dw_{99,100}} = \frac{dE}{do_{100}} \frac{do_{100}}{d \cot_{100}} \frac{d \cot_{100}}{dw_{99,100}}$$

$$-(y - o_{100}) \qquad o_{100}(1 - o_{100})$$



$$O_{100} \rightarrow E = \frac{1}{2}(y - o_{100})^2$$

$$\frac{d \operatorname{net}_{100}}{dw_{99,100}} = \frac{d (w_{99,100}o_{99} + w_{98,100}o_{98} + w_{97,100}o_{97} + ...)}{dw_{99,100}} = o_{99}$$

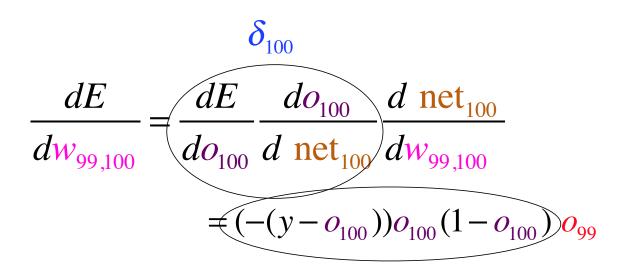
$$\frac{dE}{dw_{99,100}} = \frac{dE}{do_{100}} \frac{do_{100}}{d \operatorname{net}_{100}} \frac{d \operatorname{net}_{100}}{dw_{99,100}}$$

$$-(y - o_{100}) \qquad o_{100}(1 - o_{100})$$

$$\frac{dE}{dw_{99,100}} = \frac{dE}{do_{100}} \frac{do_{100}}{d \cot_{100}} \frac{d \cot_{100}}{dw_{99,100}}$$

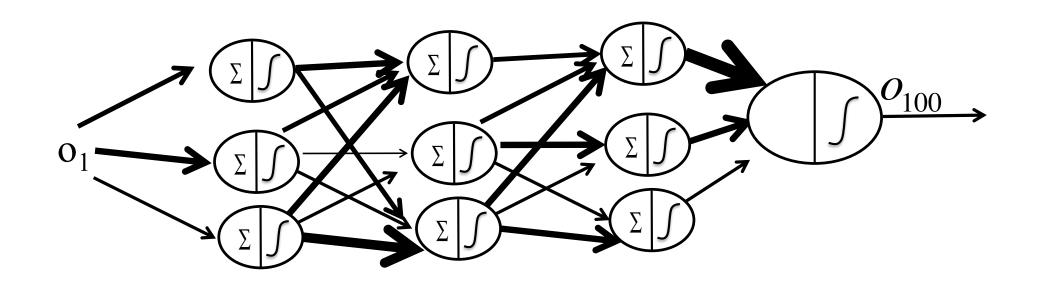
$$-(y - o_{100}) \qquad o_{100}(1 - o_{100})$$

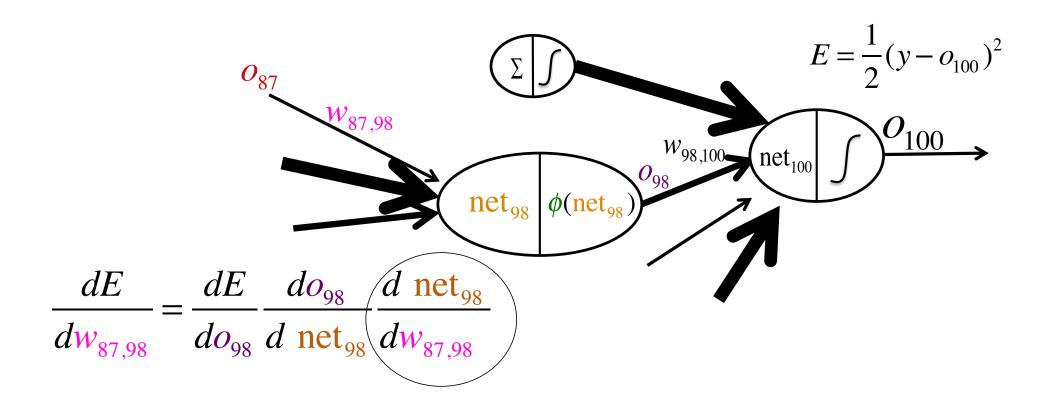
We will need this later – it depends only on node 100



Backpropagation

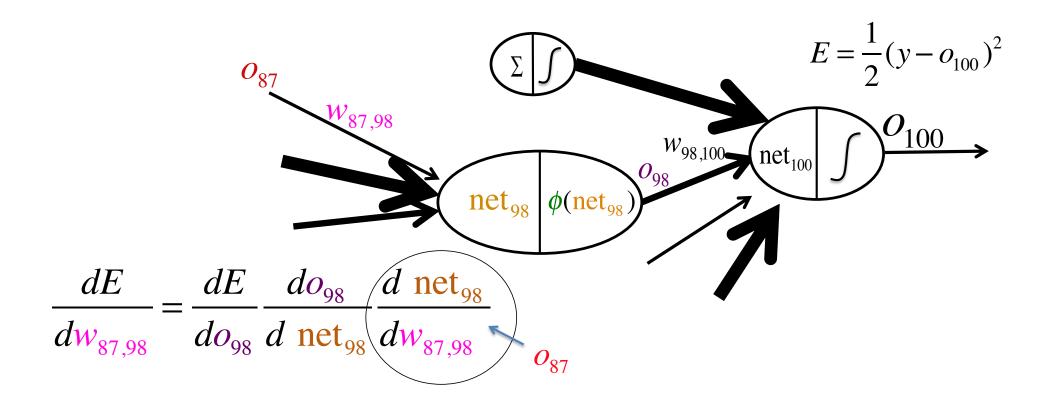
• Go one layer deeper.





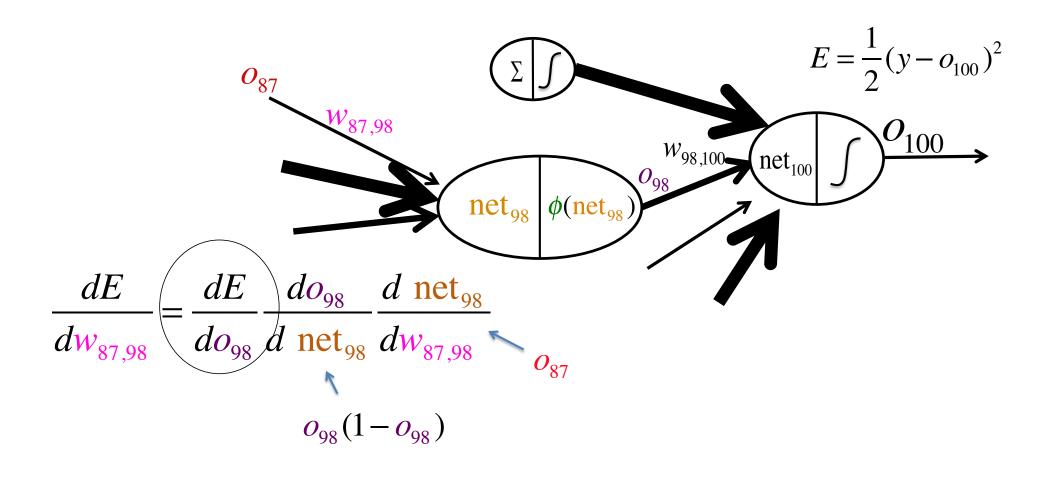
$$\frac{dE}{dw_{87,98}} = \frac{dE}{do_{98}} \frac{do_{98}}{d \text{ net}_{98}} \frac{d \text{ net}_{98}}{dw_{87,98}}$$

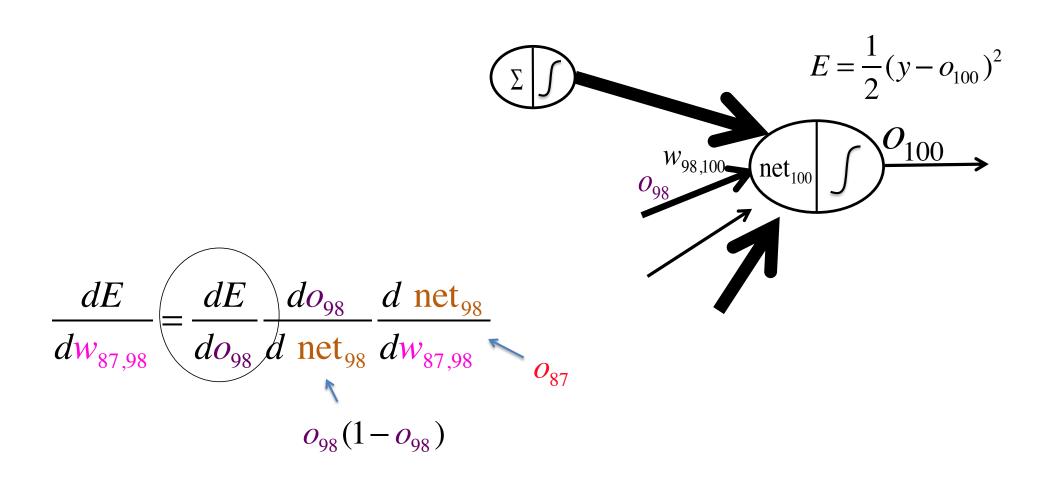
$$\frac{d \text{ net}_{98}}{dw_{87,98}} = \frac{d (w_{87,98}o_{87} + w_{86,98}o_{86} + w_{85,98}o_{85} + ...)}{dw_{87,98}} = o_{87}$$

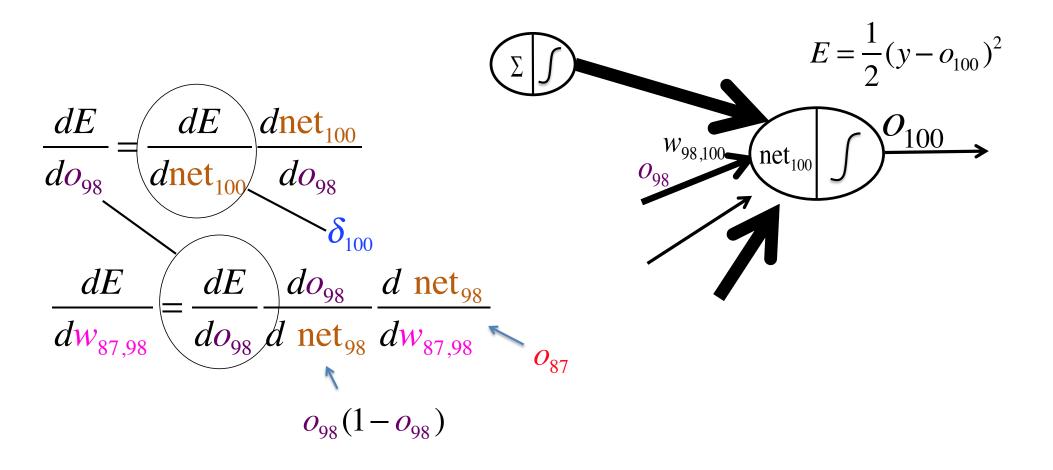


$$\frac{dE}{dw_{87,98}} = \frac{dE}{do_{98}} \frac{do_{98}}{d \text{ net}_{98}} \frac{d \text{ net}_{98}}{dw_{87,98}} o_{87}$$

$$\frac{do_{98}}{d \text{ net}_{98}} = \frac{d\phi(\text{net}_{98})}{d \text{ net}_{98}} = \phi'(\text{net}_{98}) = \phi(\text{net}_{98})(1 - \phi(\text{net}_{98})) = o_{98}(1 - o_{98})$$





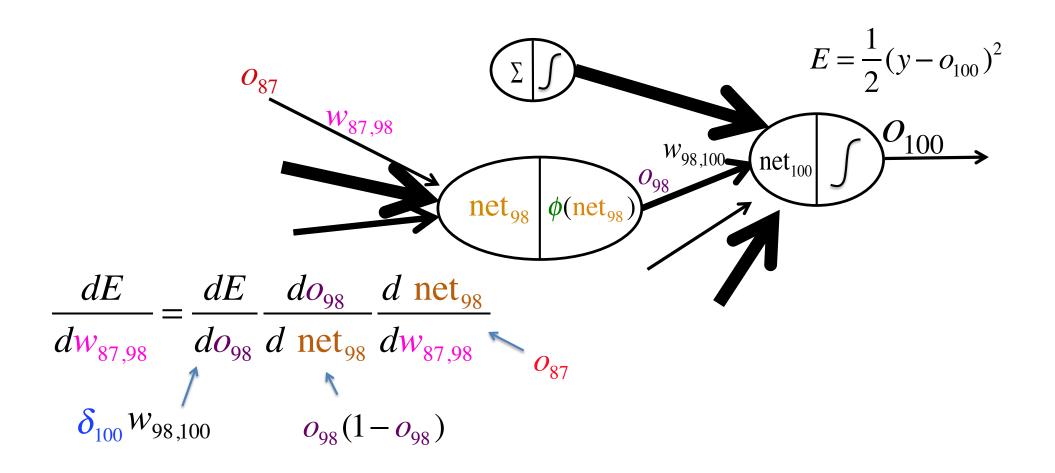


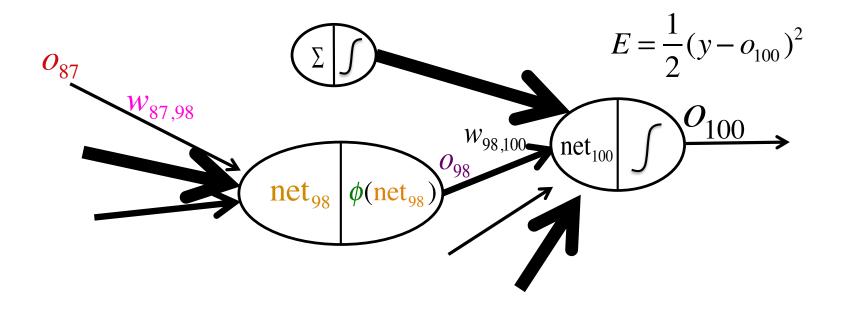
$$\frac{d\text{net}_{100}}{do_{98}} = \frac{d(w_{99,100}o_{99} + w_{98,100}o_{98} + ...)}{do_{98}} = w_{98,100}$$

$$\frac{dE}{do_{98}} = \frac{dE}{dnet_{100}} \frac{do_{98}}{do_{98}}$$

$$\frac{dE}{dw_{87,98}} = \frac{dE}{do_{98}} \frac{do_{98}}{dw_{87,98}} \frac{do_{98}}{dw_{87,98}}$$

$$o_{98}(1 - o_{98})$$

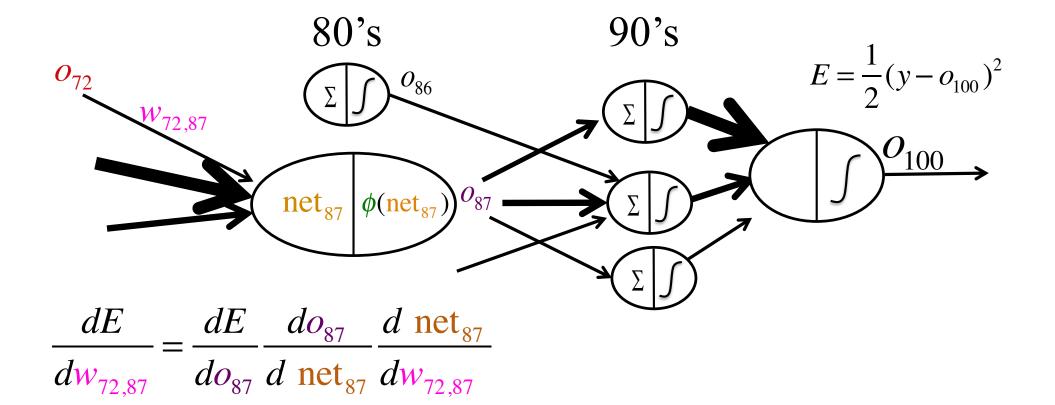


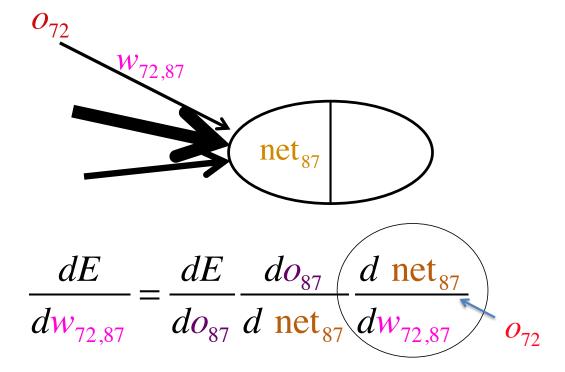


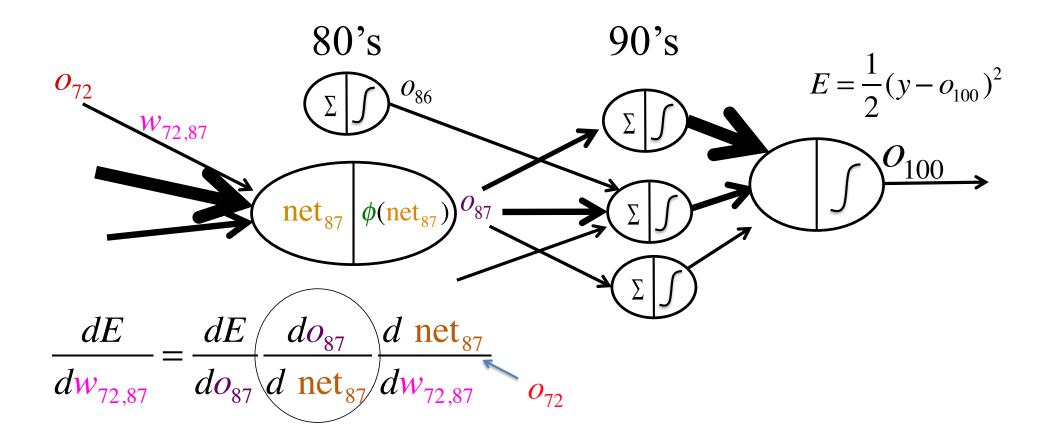
$$\frac{dE}{dw_{87,98}} = \delta_{100} w_{98,100} o_{98} (1 - o_{98}) o_{87}$$

Backpropagation

- Go even one layer deeper.
- Third time is a charm.

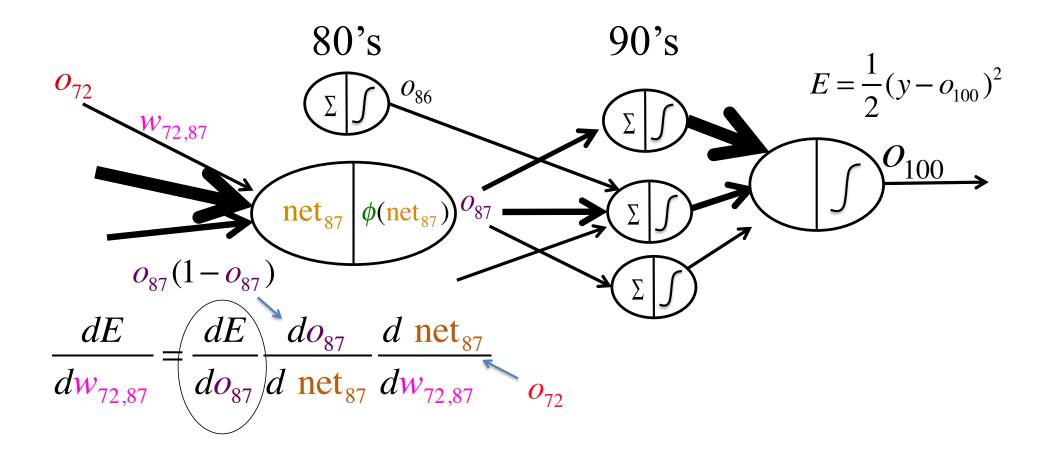


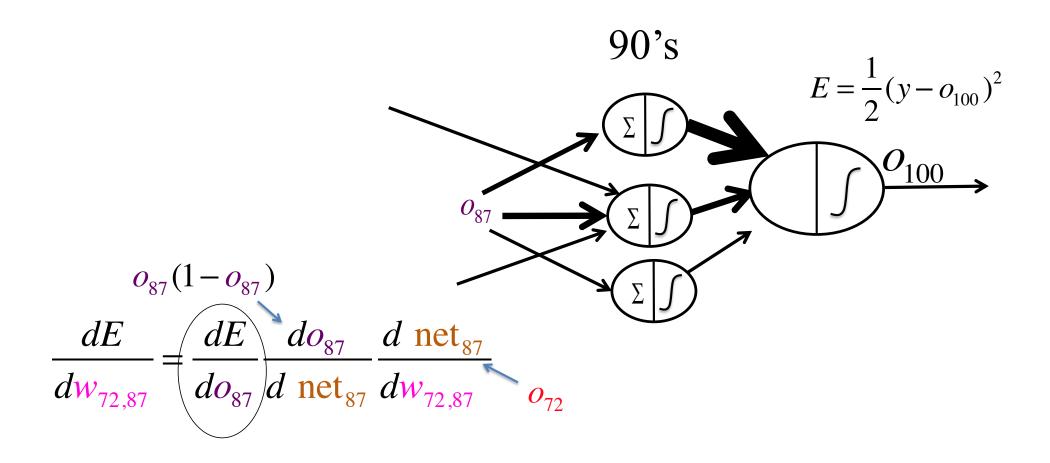


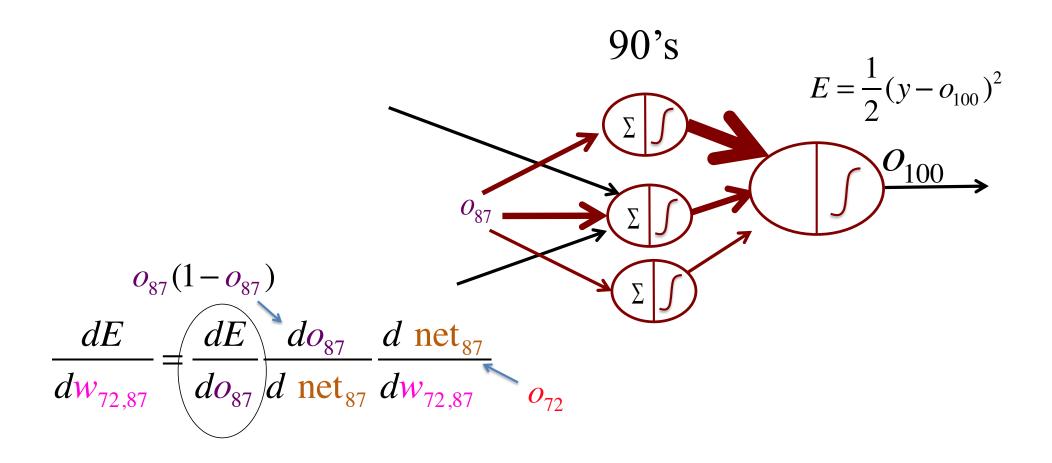


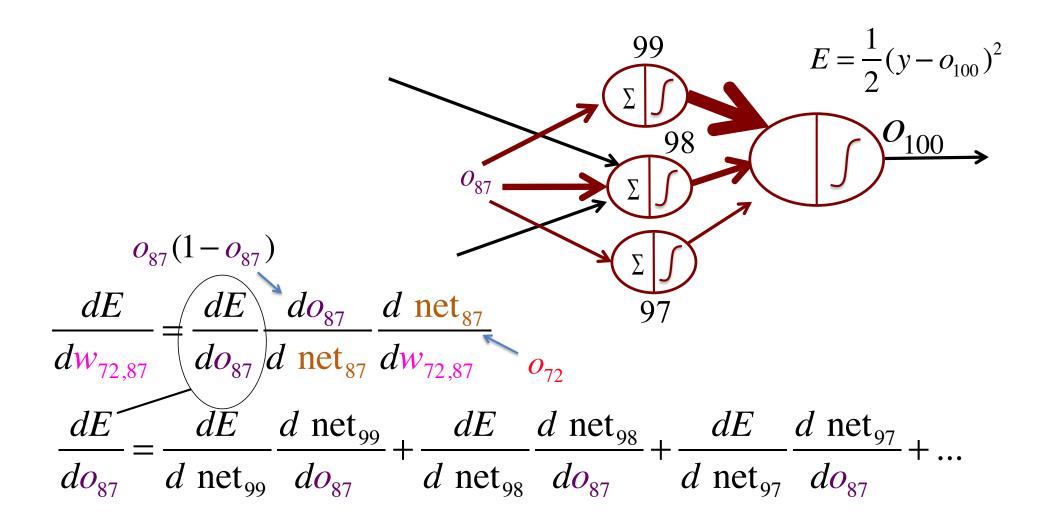
$$\frac{dE}{dw_{72,87}} = \frac{dE}{do_{87}} \frac{do_{87}}{d \text{ net}_{87}} \frac{d \text{ net}_{87}}{dw_{72,87}} o_{72}$$

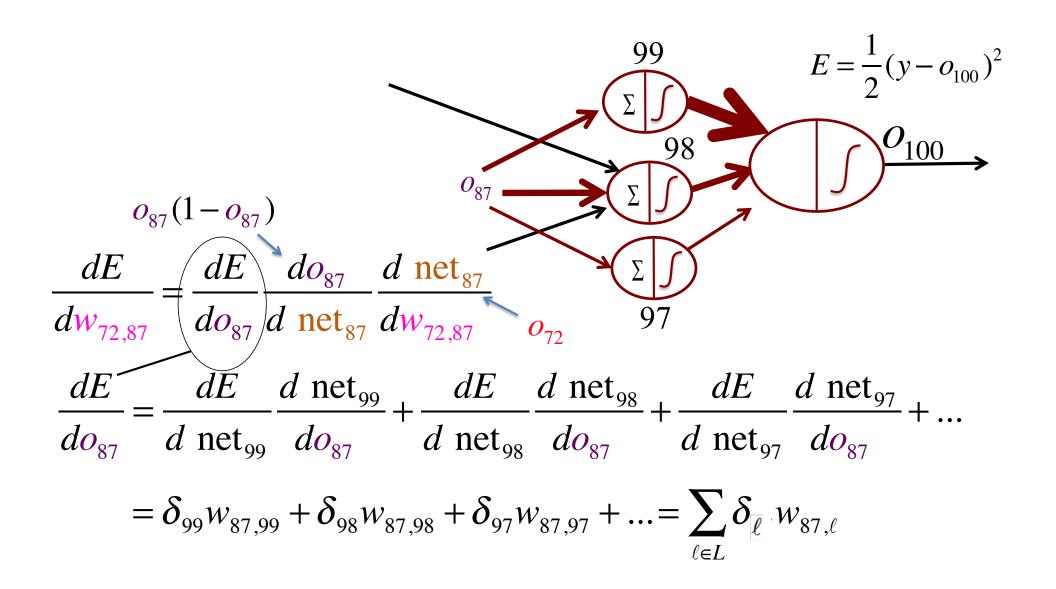
$$\frac{do_{87}}{d \text{ net}_{87}} = \frac{d\phi(\text{net}_{87})}{d \text{ net}_{87}} = \phi'(\text{net}_{87}) = \phi(\text{net}_{87})(1 - \phi(\text{net}_{87})) = o_{87}(1 - o_{87})$$





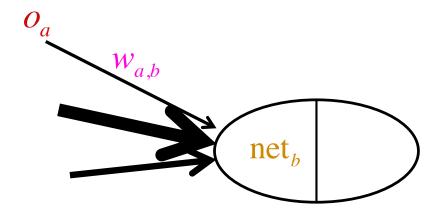






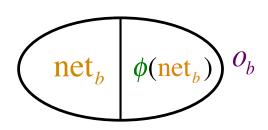
$$\frac{dE}{dw_{a,b}} = \frac{dE}{do_b} \frac{do_b}{d \text{ net}_b} \frac{d \text{ net}_b}{dw_{a,b}}$$

$$= \frac{dE}{do_b} \frac{do_b}{d \text{ net}_b} o_a$$



$$\frac{dE}{dw_{a,b}} = \frac{dE}{do_b} \frac{do_b}{d \text{ net}_b} \frac{d \text{ net}_b}{dw_{a,b}}$$

$$= \frac{dE}{do_b} o_b (1 - o_b) o_a$$

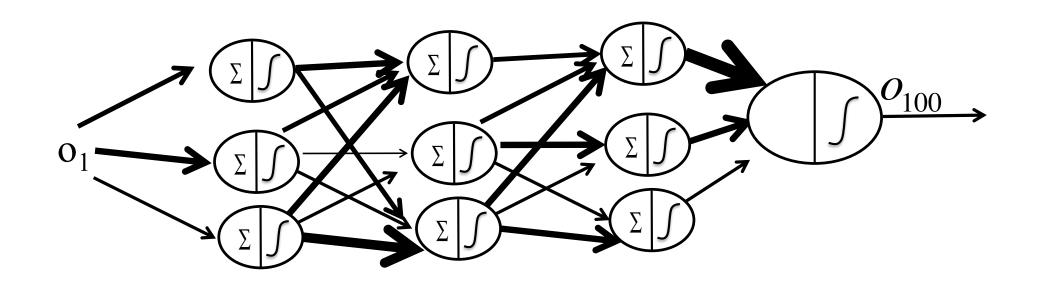


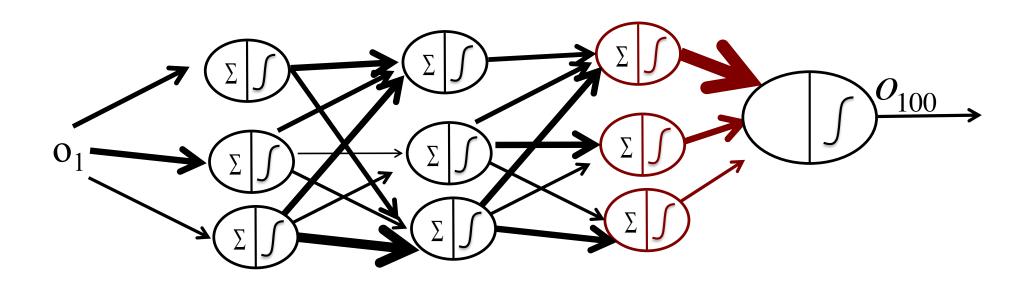
$$\frac{dE}{dw_{a,b}} = \frac{dE}{do_b} \frac{do_b}{d \text{ net}_b} \frac{d \text{ net}_b}{dw_{a,b}}$$

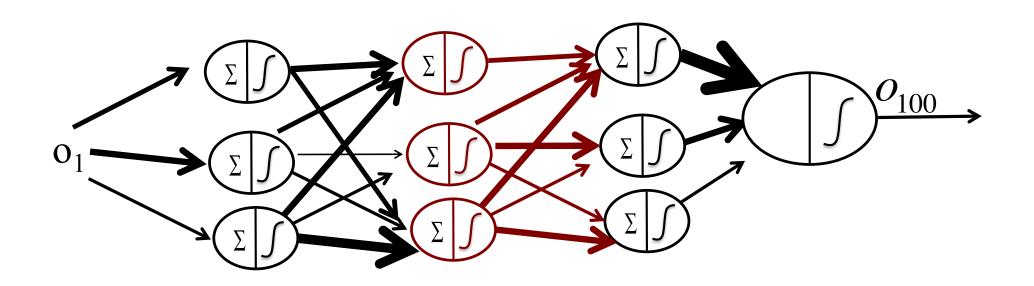
$$= \left(\sum_{\ell \in L} \delta_{\ell} w_{b,\ell}\right) o_b (1 - o_b) o_a$$

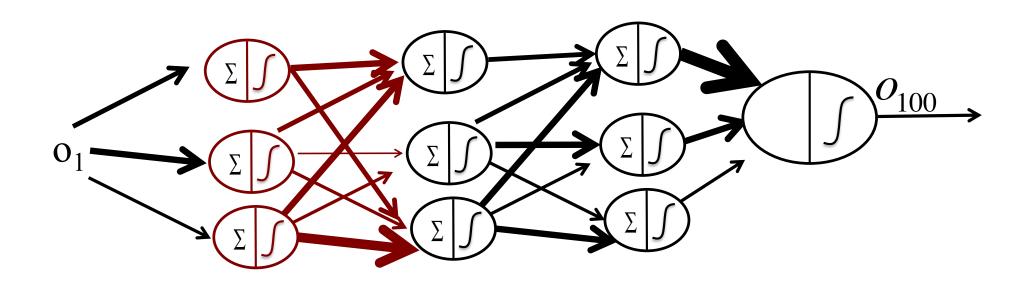
$$\sum_{\ell \in L} \delta_{\ell} w_{b,\ell} \int_{0}^{\infty} d \text{ net}_b \int_{0}^{\infty} d \text{ ne$$

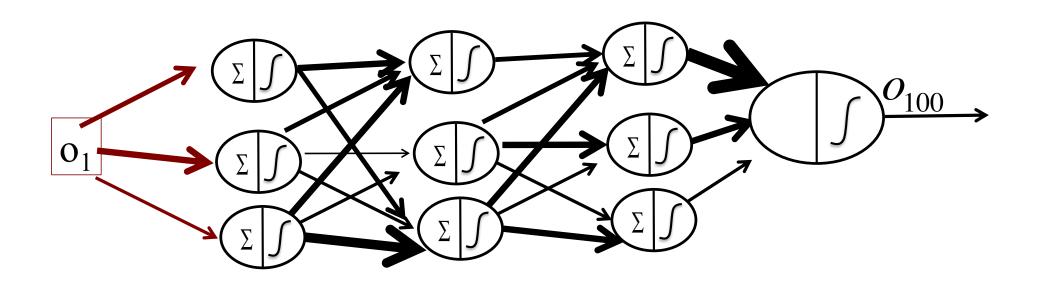
The ℓ 's are downstream. We must have already computed all the δ_{ℓ} 's ahead of us to compute this.

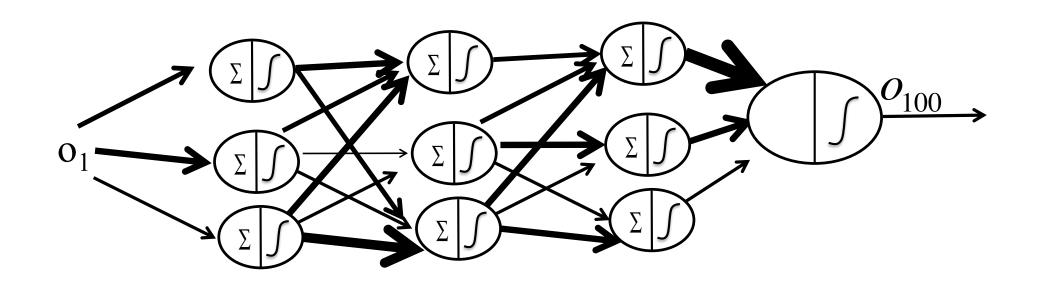










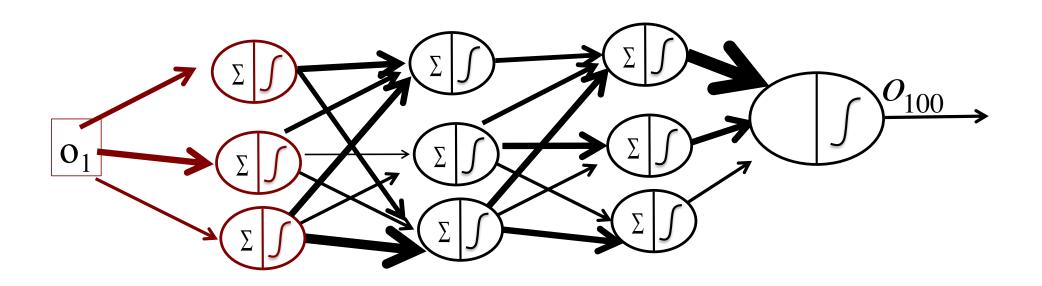


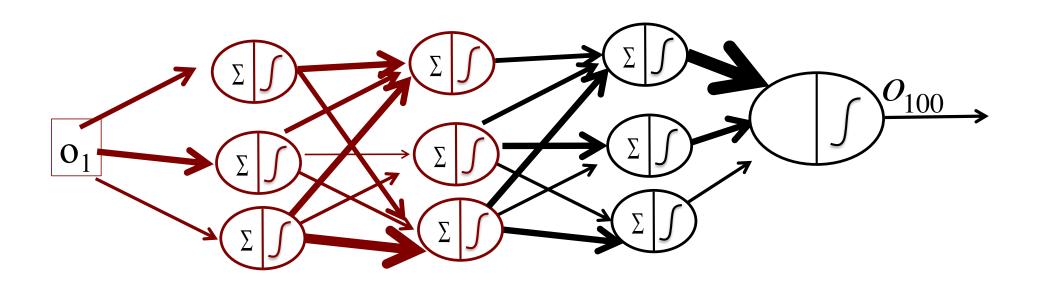
Backpropagation

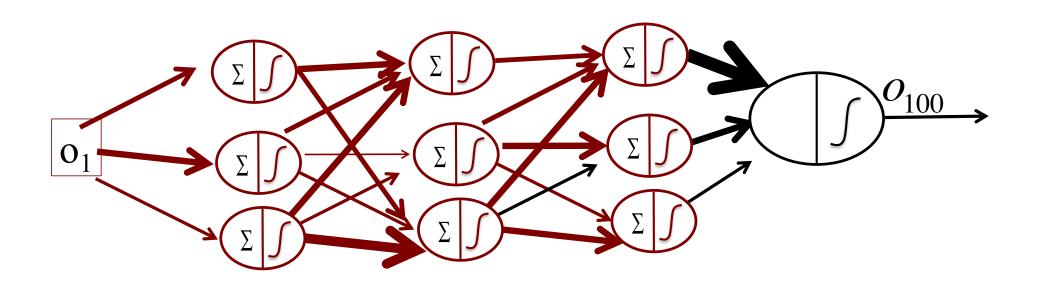
- Now we know how to compute $\frac{dE}{dw_{a,b}}$ for all of the $w_{a,b}$'s.
- Let's do gradient descent.

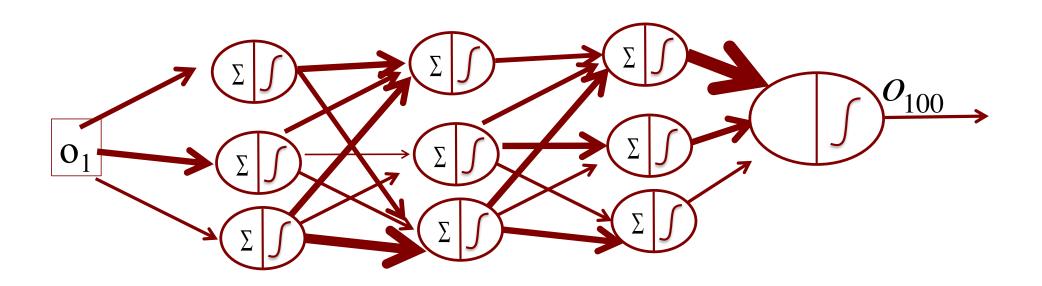
$$w_{a,b} \longleftarrow w_{a,b} - \alpha \frac{dE}{dw_{a,b}}$$

- α is between 0 and 1. Called the "learning rate".
- Now we know how to propagate errors back through the network.
- Remember how to go forward?





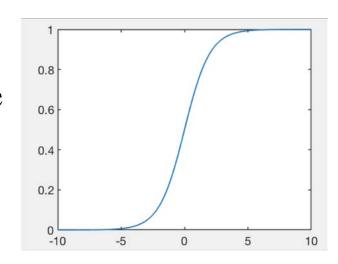




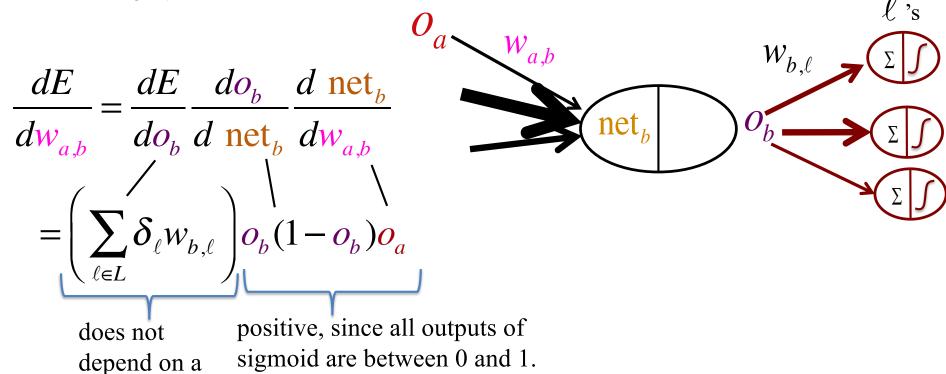
Backpropagation

• Repeat going backwards (to calculate the gradients), adjusting the weights, and going forwards (to calculate the errors) over and over in order to learn.

- NN's have problems with convergence due to vanishing/exploding gradients and saddle points.
- Vanishing gradients come from the flat part of the activation function.
- Exploding gradients happen when we realize that our gradient has vanished and so increase the learning rate and take huge step sizes to compensate (but then mess everything up!)
- Stick to 10⁻⁵ to 10⁻³ learning rate perhaps?



• With the sigmoid activation, the derivatives of the input weights for each node are always either all positive or all negative. This is a limitation.



• Bottom line – most people do not use sigmoid-like activation functions, even though this is more biologically relevant.

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

Hyperbolic tangent tanh(x)

Rectified Linear Unit (ReLU)

 $\max(0,x)$

Removes vanishing gradients when nodes are "activated," meaning x>0.

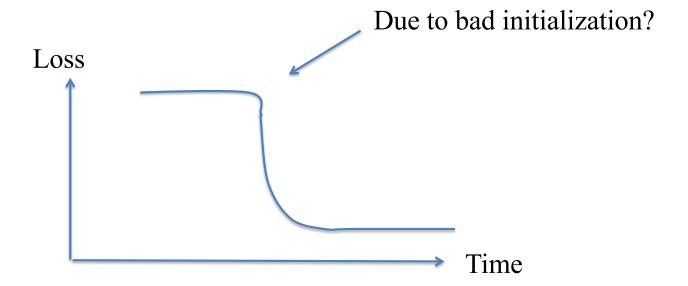
(Krizhevsky et al., 2012)

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

Removes vanishing gradients, but prefers that non-activated nodes be as "non-activated" as possible, which doesn't make much sense.

(Mass et al., 2013; He et al., 2015)

• Initialization of the networks weights is really important. I have no idea how to do it.



- Batch Normalization (Ioffe and Szegedy, 2015) is a step in a NN that:
 - Normalizes the outputs o_i of several nodes (a "mini-batch") in the same layer (as usual, subtract the mean of the o_i 's divide by their standard deviation).
 - Includes the mean and standard deviation as separate parameters to be learned.
 - Usually the normalization is before the nonlinear activation function.
 - This adds regularization and helps gradient flow in the network but sometimes it messes things up.

Data Augmentation



Chinese Lantern Festival, Cary NC, 2017

Data Augmentation

- include artificial data, such as horizontal flips, rotations, resized, cropped training images, change contrast and brightness, distortion, etc.









Chinese Lantern Festival, Cary NC, 2017

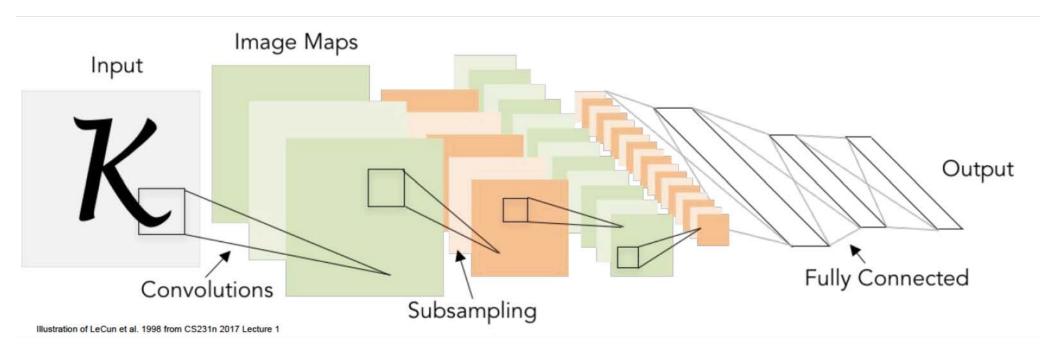
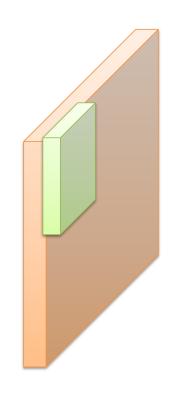


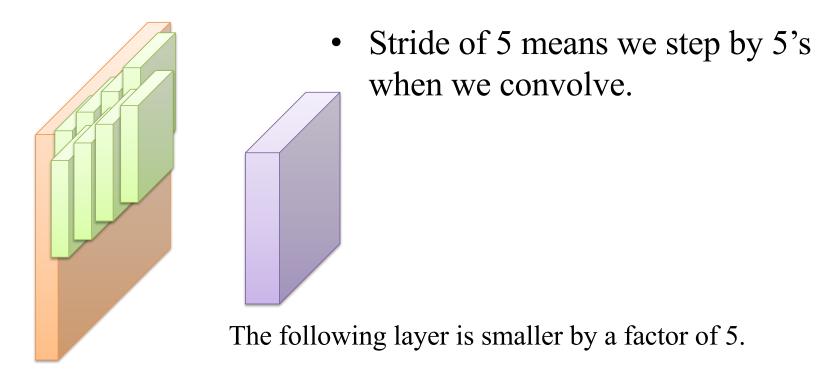
Image from LeCun et al 1998, reproduced also from Li, Johnson, Yeung, 2017

• Convolve means to slide the filter over all spatial locations, and sum up the filter weights times the input.



• An edge filter will detect edges.

• Convolve means to slide the filter over all spatial locations, and sum up the filter weights times the input.



- Max pooling means to convolve with a max function.
- Intuitively keeps track of whether an earlier filter has detected something.

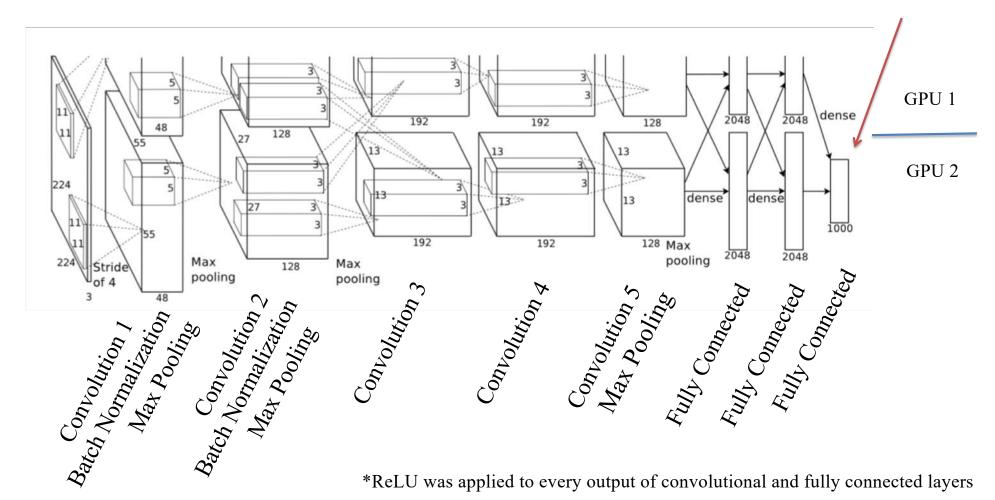
| 1 | 2 | 2 | 4 |
|---|---|---|---|
| 2 | 5 | 1 | 8 |
| 3 | 0 | 4 | 4 |
| 6 | 1 | 7 | 6 |

2 x 2 max pool filter and stride 2

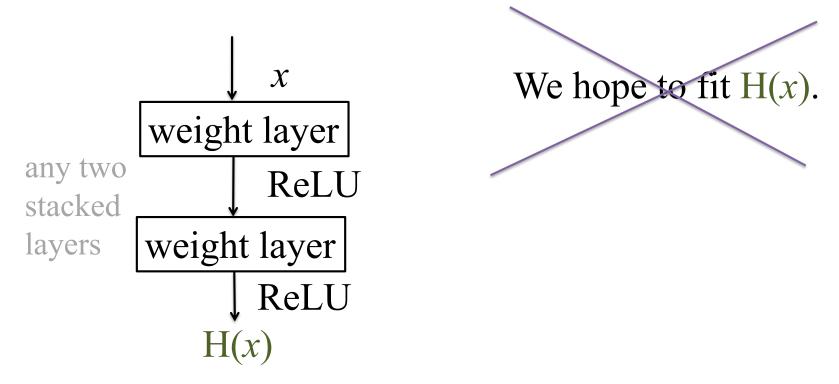
| 5 | 8 | |
|---|---|--|
| 6 | 7 | |

AlexNet (Krizhevsky et al. 2012)

softmax over 1000 classes

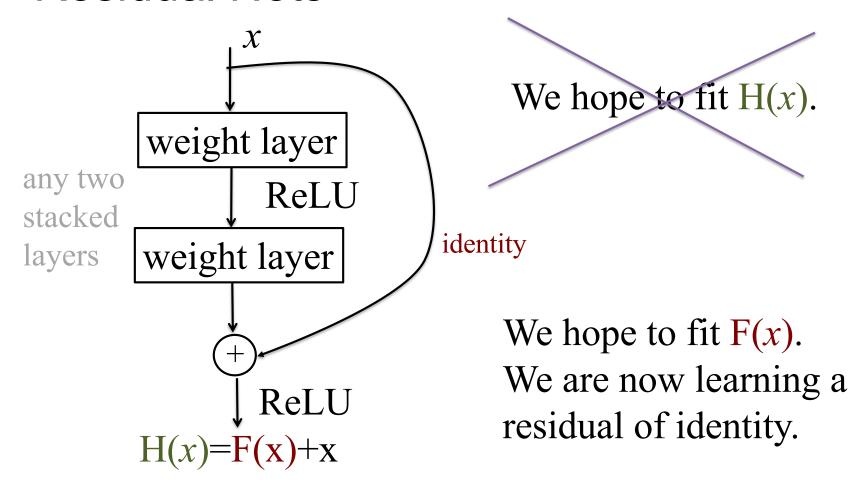


Residual Nets (He et al., 2016)



Slides recreated from Kaiming He's tutorial http://kaiminghe.com/icml16tutorial/icml2016_tutorial_deep_residual_networks_kaiminghe.pdf

Residual Nets



http://kaiminghe.com/icml16tutorial/icml2016_tutorial_deep_residual_networks_kaiminghe.pdf

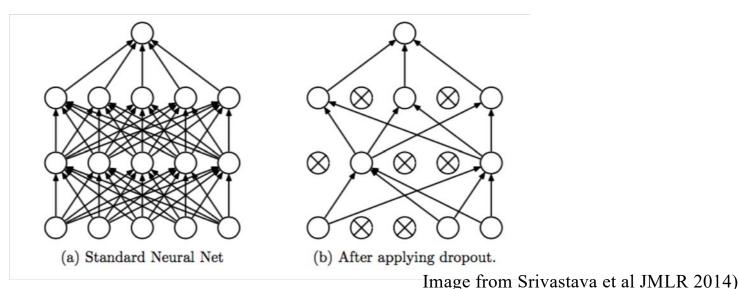
Residual Nets

- By adding x, the derivative of the error with respect to x increases by 1. Thus, less vanishing derivatives.
- Allowed networks to go much deeper than before. "From 10 to 1000 layers"

$$H(x)=F(x)+x$$

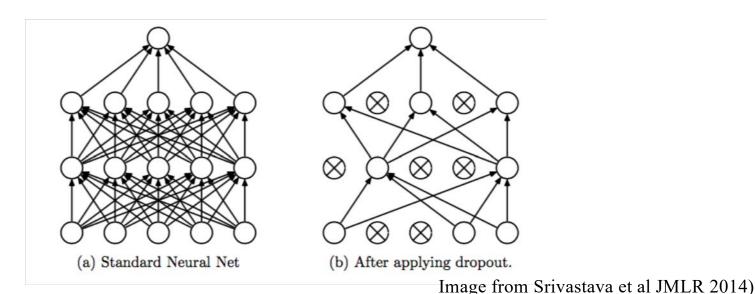
Dropout (Srivastava et al., JMLR 2014)

- In each forward pass, for each neuron, with probability p, set all of its output weights to 0.
- p is a hyperparameter, usually p = 0.5.
- During testing, use all nodes.



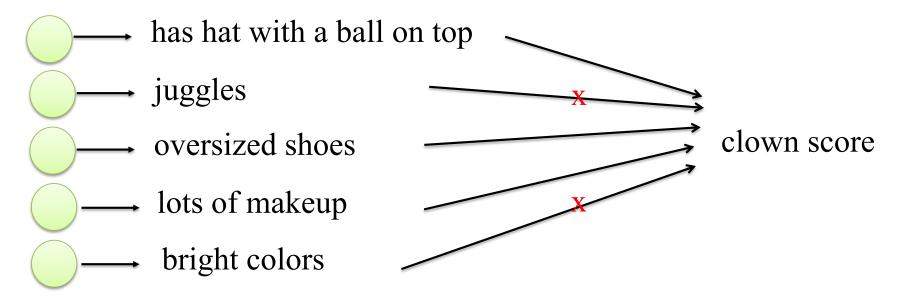
Dropout (Srivastava et al., JMLR 2014)

- As if we are training exponentially many "sub" models. Similar idea to bagging (averaging many separately trained models together).
- Creates a redundant encoding.



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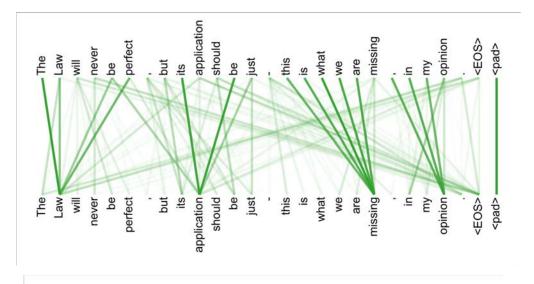


A Big Bag of Tricks

- Dropout
- Batch Normalization
- Data Augmentation
- Residual Networks
- Convolutional Networks
- Activation Functions (ReLU, Leaky ReLU)
- Initialization
- Max Pooling
- :

RNN's have recently been surpassed by Transformers

- RNN's used to be the standard for machine translation (sequence-to-sequence). These were useful because they kept a memory of longer-term relationships between words.
- The new standard is the transformer, which places several "multihead attention nodes" together. The transformer compares all words to all other words in the sentence. It is not recursive.



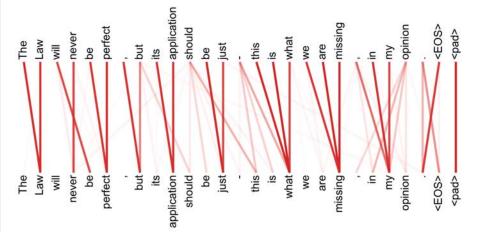


Figure 5: Many of the attention heads exhibit behaviour that seems related to the structure of the sentence. We give two such examples above, from two different heads from the encoder self-attention at layer 5 of 6. The heads clearly learned to perform different tasks.

"Attention is all you need" Vaswani et al 2017

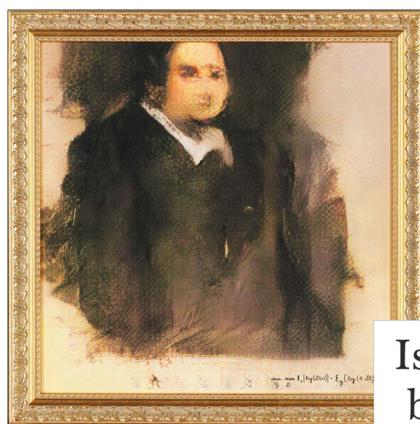
GANS – Generative Adversarial Networks

From Goodfellow et al 2014:

In other words, D and G play the following two-player minimax game with value function V(G, D):

$$\min_{G} \max_{D} V(D, G) = \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]. \tag{1}$$

- GANS are actor-critic models
- They produce realistic-looking images/data (some ethical/legal concerns)
- Used commonly for AI artwork



Is artificial intelligence set to become art's next medium?

Al artwork sells for \$432,500 — nearly 45 times its high estimate — as Christie's becomes the first auction house to offer a work of art created by an algorithm

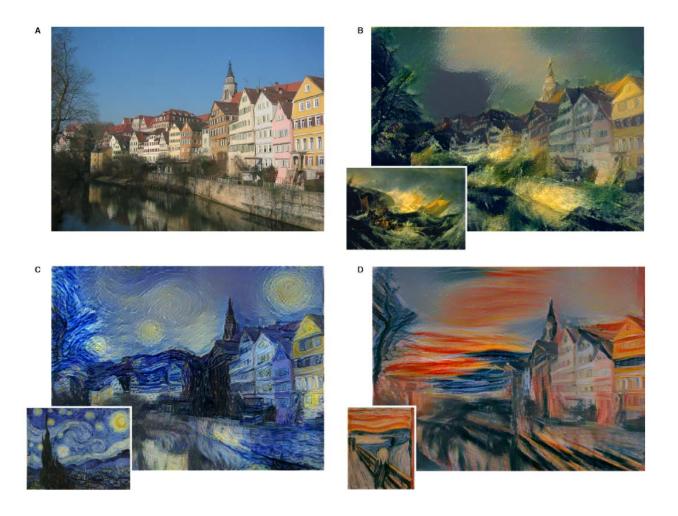


Figure adapted from L. Gatys et al. "A Neural Algorithm of Artistic Style" (2015) by Google AI Blog

Neural networks

- Advantages:
 - highly expressive nonlinear models
 - have advances in computer vision and speech that other methods have not achieved
 - can capture latent structure within the hidden layers
- Disadvantages
 - can get stuck in local optima, could produce bad solutions
 - black box
 - lots of tuning parameters (e.g., the structure of the network)
- There is a recent bag of tricks

Thanks