MA666: Neural Networks and Learning

Part 1
Backpropagation

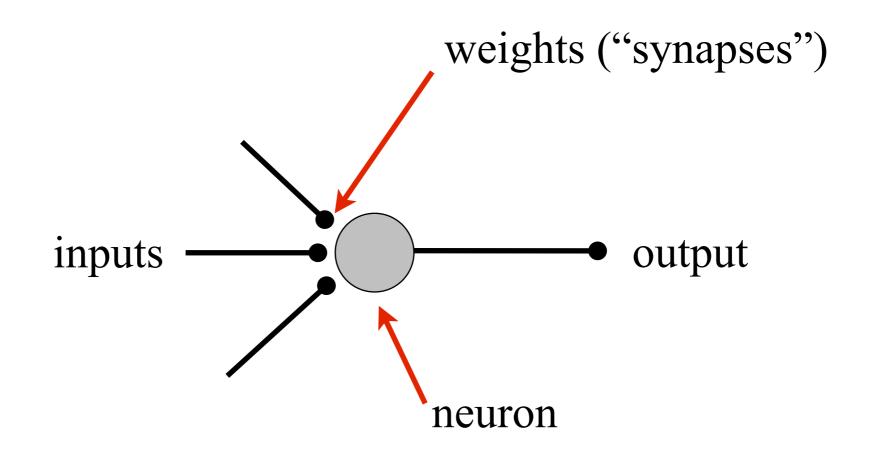
Today

We'll study learning in a "simple" neural network:

-Backpropagation

Remember, the Perceptron

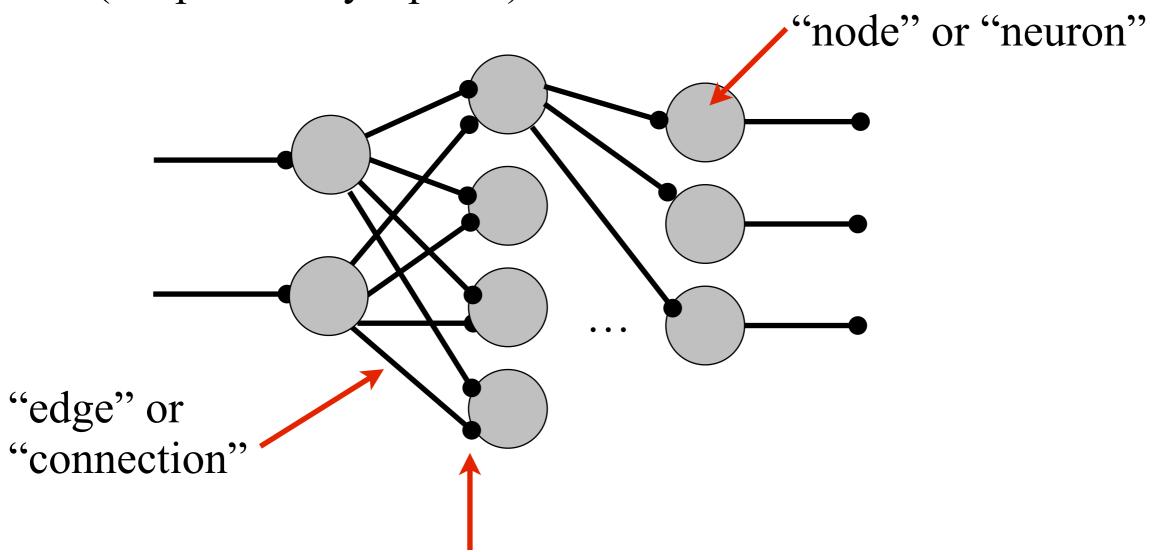
Cartoon & Cast of Characters



Note: there's only one neuron.

Today, a neural network

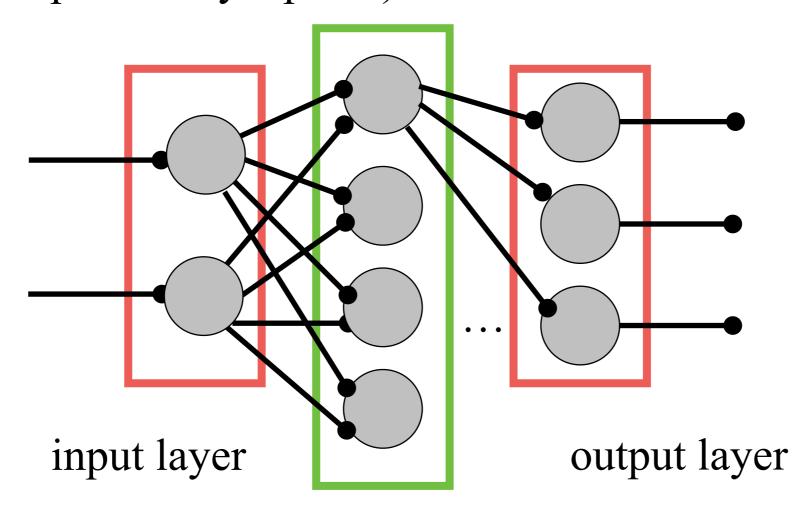
Today, **neural networks**: collections of abstracted neurons connected to each other through weighted connections (simplified "synapses").



weight controls signal between neurons

Today, a neural network

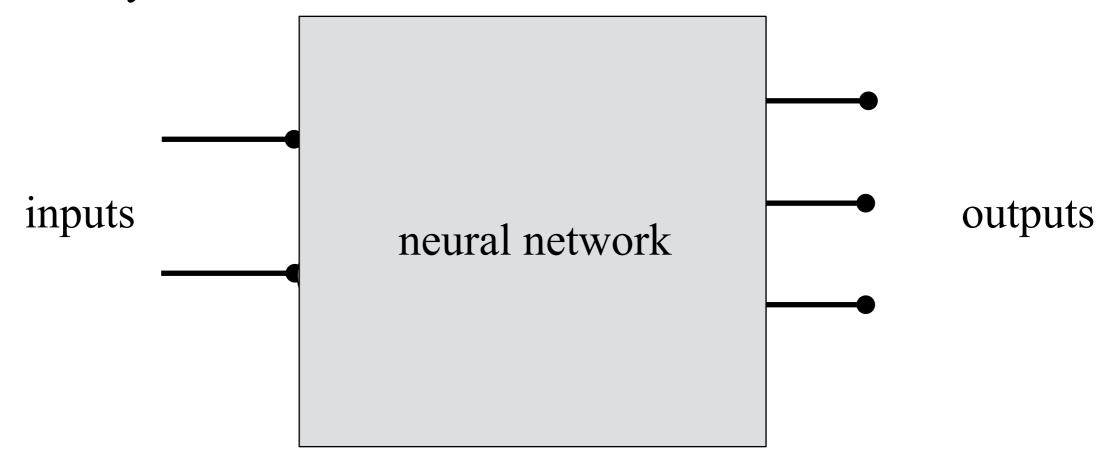
Today, **neural networks**: collections of abstracted neurons connected to each other through weighted connections (simplified "synapses").



hidden layer

Information processed through the network

Abstractly:



Neural networks can exhibit rich behavior.

Cool example: playground.tensorflow.org

Neural networks can learn

Neural networks are:

– adaptive

- internal structure changes based on information flowing through the network.
- -To do so, adjust weights.

-<u>Idea</u>:

- When network outputs are "good", preserve the weights.
- When network output are "bad", changes the weights.
 - When the network makes errors, adapt.

We trained a perceptron ...

Now, we'll train a neural network to do what we want ...

Neural networks can learn

Some terminology:

-"training a neural network" calibrate weights to get output we want.

-Forward propagation

For a set of weights & input, calculate output.

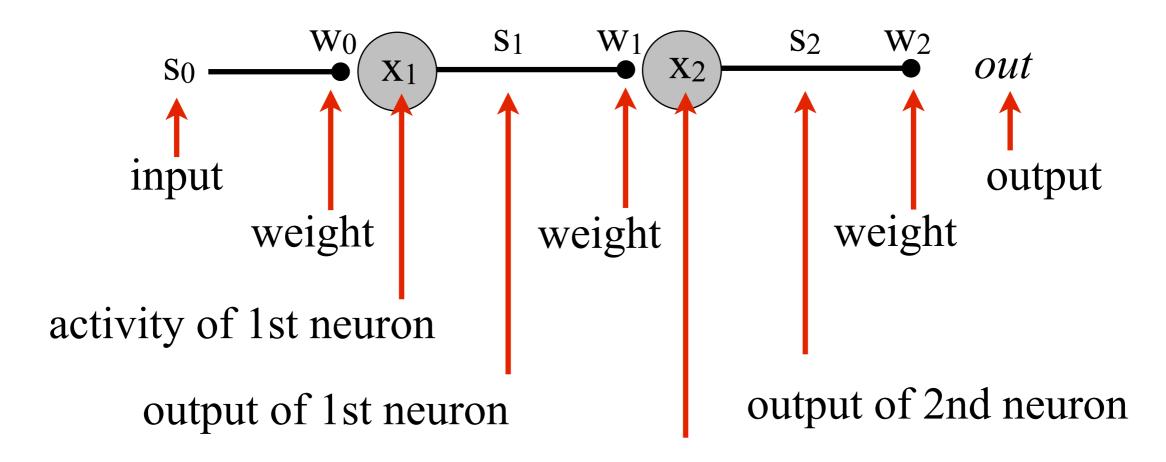
Backpropagation

Determine error in output, and adjust weights to decrease error.

Let's train a "simple" neural network to do our bidding ...

A "simple" neural network

Start with perceptron ... add a node ... and label everything.



activity of 2nd neuron

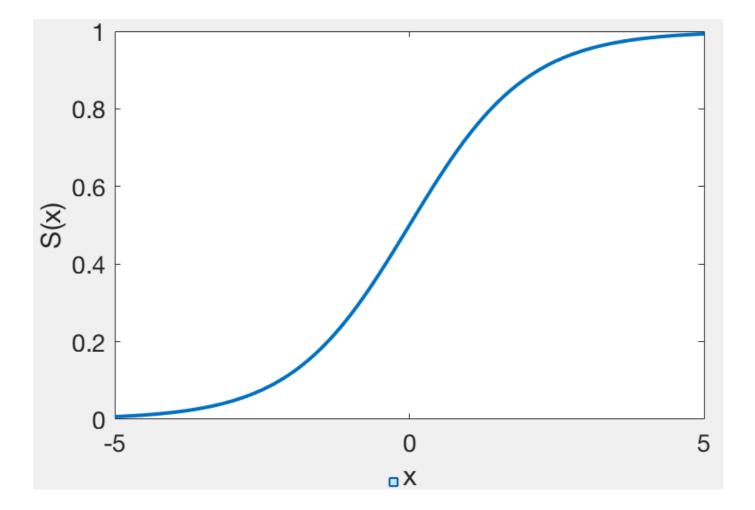
Activation function

Remember, the <u>activation function</u>:

$$x ext{ (activity)} ext{ activation function} ext{ output}$$

Here we'll use a **sigmoid** activation function:

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



NOTE: It's like a "smoothed" binary threshold.

The challenge

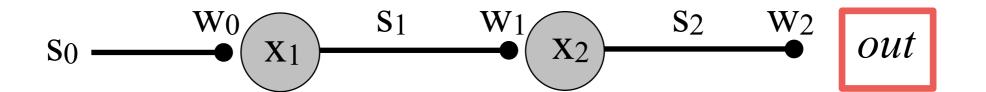
We're given a list of inputs (s_0) and outputs (out):

Q: What weights $(w_0 \ w_1 \ w_2)$ produced these data?

$$S_0 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow X_2 \longrightarrow Out$$

A "simple" neural network

We want our network to learn ...



so that when then input $s_0=2$,

the input *out*=0.7

Q: How do we do it?

A: We need to choose the right weights: $w_0 w_1 w_2$

So, how do we find the right weights?

What are the right model weights?

Let's guess:

$$\mathbf{w}_0 = \mathbf{w}_1 \quad \mathbf{w}_1 \quad \mathbf{w}_2 \quad \mathbf{w}_2 \quad \mathbf{w}_2 \quad \mathbf{w}_3 \quad \mathbf{w}_4 \quad \mathbf{w}_4 \quad \mathbf{w}_5 \quad \mathbf{w}_4 \quad \mathbf{w}_5 \quad \mathbf{w}_5 \quad \mathbf{w}_6 \quad \mathbf$$

Q: How did I choose these?

Q: Do they work?

A: Let's check ... forward propagation

Forward propagation

$$S_0 \longrightarrow X_1 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow X_2 \longrightarrow Out$$

$$s_0=2$$
 $w_0=2$

$$w_1 = 1$$

$$w_1 = 1$$
 $w_2 = 0.5$

target:

Let's do it.

$$x_1 = w_0 s_0 = 2 * 2 = 4$$

$$s_1 = S(x_1) = S(4) = 0.982$$

$$x_2 = w_1 s_1 = 1*0.982 = 0.982$$

$$s_2 = S(x_2) = S(0.982) = 0.7275$$

out =
$$w_2 s_2 = 0.5*0.7275 = 0.3638$$

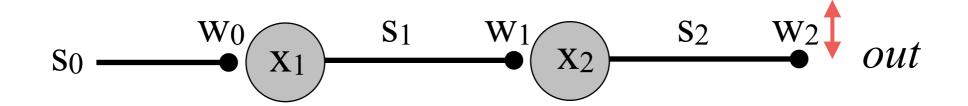
Match?

14

NO

Q: So now what?

(intermediate) Goal: get output (out) closer to target (0.7)



Q: How does a change in weight w₂ impact the output?

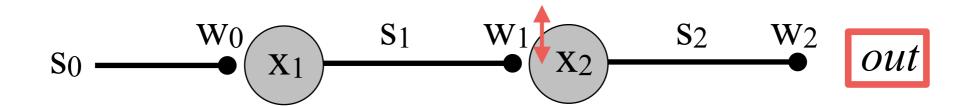
<u>Idea</u>: wiggle w_2 how does *out* change? $out = s_2 w_2$

$$out = s_2 w_2$$

Mathematically,

$$\frac{d out}{d w_2} = \frac{d (s_2 w_2)}{d w_2} = s_2$$

Let's keep going, working backwards.



Q: How does a change in weight w₁ impact the output?

<u>Idea</u>: wiggle w₁ how does *out* change?

Mathematically,
$$\frac{d out}{d w_1} = \text{Hmm} \dots$$

out does not depend directly on w₁

$$S_0 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow X_2 \longrightarrow X_2 \longrightarrow X_2 \longrightarrow X_2 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow X_2$$

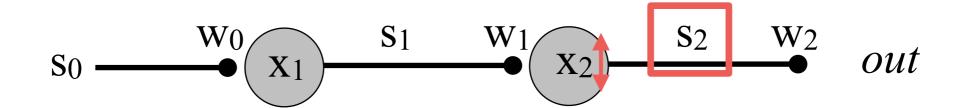
out does depend on s_2 and s_2 depend on s_2 and s_2 depend on s_2

Mathematically ... the chain rule

$$\frac{d out}{d w_1} = \begin{bmatrix} d out \\ d s_2 \end{bmatrix} \frac{d s_2}{d x_2} \frac{d x_2}{d w_1}$$

wiggle s_2 and *out* changes Remember: $out = s_2 w_2$

$$\frac{d out}{d s_2} = \frac{d (s_2 w_2)}{d s_2} = w_2$$



Continue the chain rule

$$\frac{d out}{d w_1} = \frac{d out}{d s_2} \frac{d s_2}{d x_2} \frac{d x_2}{d w_1}$$

wiggle x₂ and s₂ changes

so
$$\frac{d s_2}{d x_2} = \frac{d}{d x_2} \left(\frac{1}{1 + e^{-x_2}}\right)$$

We need to compute:

$$\frac{d}{dx_{2}} \left(\frac{1}{1 + e^{-x_{2}}} \right) = \text{Hmm ... Quotient Rule}$$

$$= \frac{(1 + e^{-x_{2}}) \frac{d(\mathbf{I})^{0}}{dx_{2}} - (1) \frac{d(1 + e^{-x_{2}})}{dx_{2}}}{(1 + e^{-x_{2}})^{2}}$$

$$\mathbf{Q}: \text{What is } \frac{d(1 + e^{-x_{2}})}{dx_{2}} ? = 1$$

$$= \frac{d(\mathbf{I})^{0}}{dx_{2}} + \frac{d(e^{-x_{2}})}{dx_{2}} = (e^{-x_{2}}) \frac{d(-x_{2})}{dx_{2}} = -e^{-x_{2}}$$

So,

$$\frac{d}{dx_2} \left(\frac{1}{1 + e^{-x_2}} \right) = \frac{0 - (1)(-e^{-x_2})}{(1 + e^{-x_2})^2}$$
$$= \frac{e^{-x_2}}{(1 + e^{-x_2})^2}$$

Q: Can we simplify this expression?

A: Yes, but requires faith ...

- Split up denominator: $\frac{e^{-x_2}}{(1+e^{-x_2})^2} = \left(\frac{1}{1+e^{-x_2}}\right) \left(\frac{e^{-x_2}}{1+e^{-x_2}}\right)$

- Add 0 to the second term:

 $= (s_2) (1 - s_2)$

Sum is 0

$$\left(\frac{1}{1+e^{-x_2}}\right)\left(\frac{e^{-x_2}}{1+e^{-x_2}}\right) = \left(\frac{1}{1+e^{-x_2}}\right)\left(\frac{1+e^{-x_2}-1}{1+e^{-x_2}}\right)$$

Q: Why?

A: Let's organize terms ...

$$= \left(\frac{1}{1+e^{-x_2}}\right) \left(\frac{1+e^{-x_2}}{1+e^{-x_2}} - \frac{1}{1+e^{-x_2}}\right)$$

$$= s_2$$

$$= 1$$
Remember:
$$s_2 = \left(\frac{1}{1+e^{-x_2}}\right)$$

$$s_2 = \left(\frac{1}{1+e^{-x_2}}\right)$$

Remember:

$$\mathbf{s}_2 = \left(\frac{1}{1 + e^{-x_2}}\right)$$

So, for our chain rule calculation:

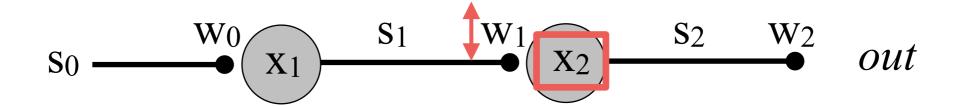
$$\frac{d out}{d w_1} = \frac{d out}{d s_2} = \frac{d s_2}{d x_2} = \frac{d x_2}{d w_1}$$

And we found:

$$\frac{d s_2}{d x_2} = \frac{d}{dx_2} \left(\frac{1}{1 + e^{-x_2}} \right) = \dots \text{ many steps } \dots = s_2 (1 - s_2)$$

$$= s_2$$

To complete the chain rule, one more derivative ...



Continue the chain rule:

$$\frac{d out}{d w_1} = \frac{d out}{d s_2} \frac{d s_2}{d x_2} \frac{d x_2}{d w_1}$$

wiggle w₁ and x₂ changes

Remember: $x_2 = s_1 w_1$

$$\frac{d x_2}{d w_1} = \frac{d (s_1 w_1)}{d w_1} = s_1$$

Back to our original question:

$$S_0 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow S_2 \longrightarrow Out$$

Q: How does a change in weight w₁ impact the output?

Mathematically ... the chain rule

$$\frac{d out}{d w_1} = \frac{d out}{d s_2} \qquad \frac{d s_2}{d w_2} \qquad \frac{d x_2}{d w_1}$$

$$\frac{d out}{d w_1} = w_2 \qquad s_2 (1 - s_2) \qquad s_1$$

Slide 16 Slide 21 Slide 22

We're almost there ...

$$s_0 \xrightarrow{\text{tw}_0} x_1 \xrightarrow{\text{s}_1} \text{tw}_1 \xrightarrow{\text{s}_2} \text{tw}_2 \quad out$$

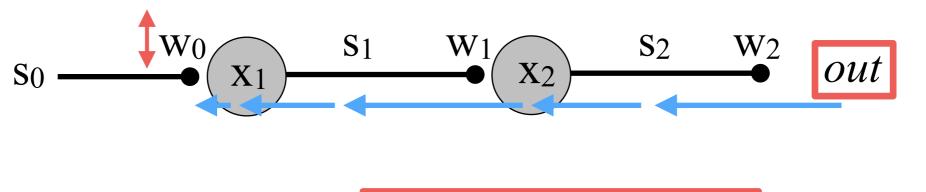
$$\frac{d \text{ out}}{d \text{ w}_2} = s_2$$

$$\frac{d \text{ out}}{d \text{ w}_1} = w_2 s_2 (1 - s_2) s_1$$

Q: How does a change in weight w_0 impact the output?

A: Chain rule ...

Q: How does a change in weight w_0 impact the output?



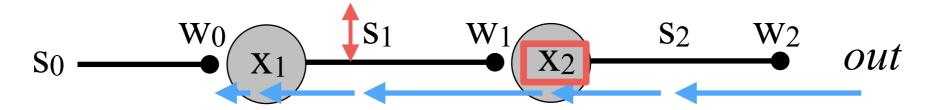
$$\frac{d out}{d w_0} = \frac{d out}{d s_2} \quad \frac{d s_2}{d x_2} \quad \frac{d x_2}{d s_1} \quad \frac{d s_1}{d x_1} \quad \frac{d x_1}{d w_0} \quad Ugh \dots$$

Luckily, we've already calculated two of these.

$$w_2 s_2 (1 - s_2)$$

Let's compute the last 3 terms ...

3rd term:

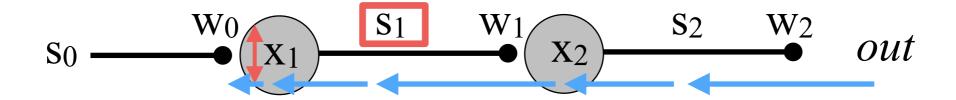


$$\frac{d out}{d w_0} = \frac{d out}{d s_2} \quad \frac{d s_2}{d x_2} \quad \frac{d x_2}{d s_1} \quad \frac{d s_1}{d x_1} \quad \frac{d x_1}{d w_0}$$

Remember: $x_2 = s_1 w_1$

$$\frac{d x_2}{d s_1} = \frac{d (s_1 w_1)}{d s_1} = w_1$$

4th term:



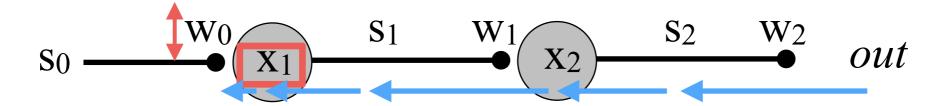
$$\frac{d \, out}{d \, w_0} = \frac{d \, out}{d \, s_2} \quad \frac{d \, s_2}{d \, x_2} \quad \frac{d \, x_2}{d \, s_1} \quad \frac{d \, s_1}{d \, x_1} \quad \frac{d \, x_1}{d \, w_0}$$

We found earlier that:

$$\frac{d s_2}{d x_2} = s_2 (1 - s_2) \qquad \dots so \dots \qquad \frac{d s_1}{d x_1} = s_1 (1 - s_1)$$

This involved many steps!

5th term:



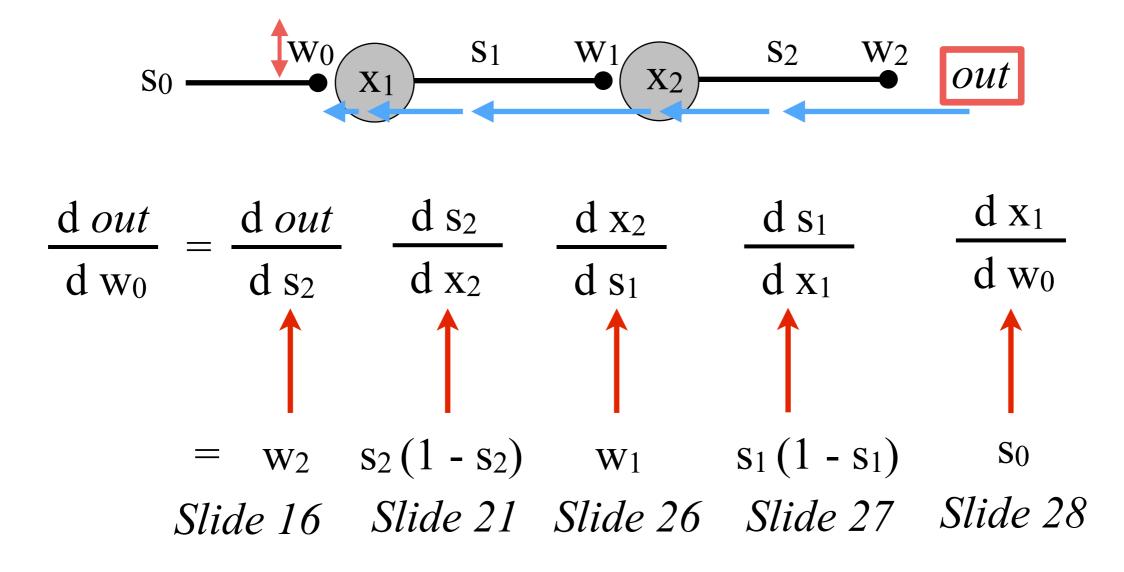
$$\frac{d \, out}{d \, w_0} = \frac{d \, out}{d \, s_2} \quad \frac{d \, s_2}{d \, x_2} \quad \frac{d \, x_2}{d \, s_1} \quad \frac{d \, s_1}{d \, x_1} \quad \frac{d \, x_1}{d \, w_0}$$

Remember: $x_1 = s_0 w_0$

$$\frac{d x_1}{d w_0} = \frac{d (s_0 w_0)}{d w_0} = s_0$$

We now have the pieces to answer:

Q: How does a change in weight w_0 impact the output?



To summarize:

- We've found how changes in model weights impact output.

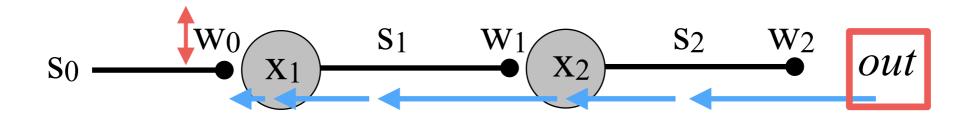
$$s_0 \xrightarrow{\text{v_0}} x_1 \xrightarrow{\text{v_1}} x_2 \xrightarrow{\text{v_2}} out$$

$$\frac{d out}{d w_2} = s_2$$

$$\frac{d out}{d w_1} = w_2 s_2 (1 - s_2) s_1$$

$$\frac{d out}{d w_0} = w_2 s_2 (1 - s_2) w_1 s_1 (1 - s_1) s_0$$

So, how does a change in weight impact output? backpropagation!



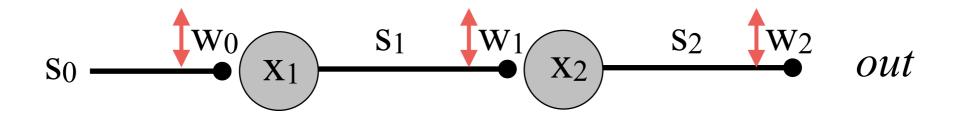
Backpropagation:

Work "backwards" from output to weight, computing derivatives along the way

Q: How do these derivatives help us update weights and obtain desired output?

Define our goal

We want:



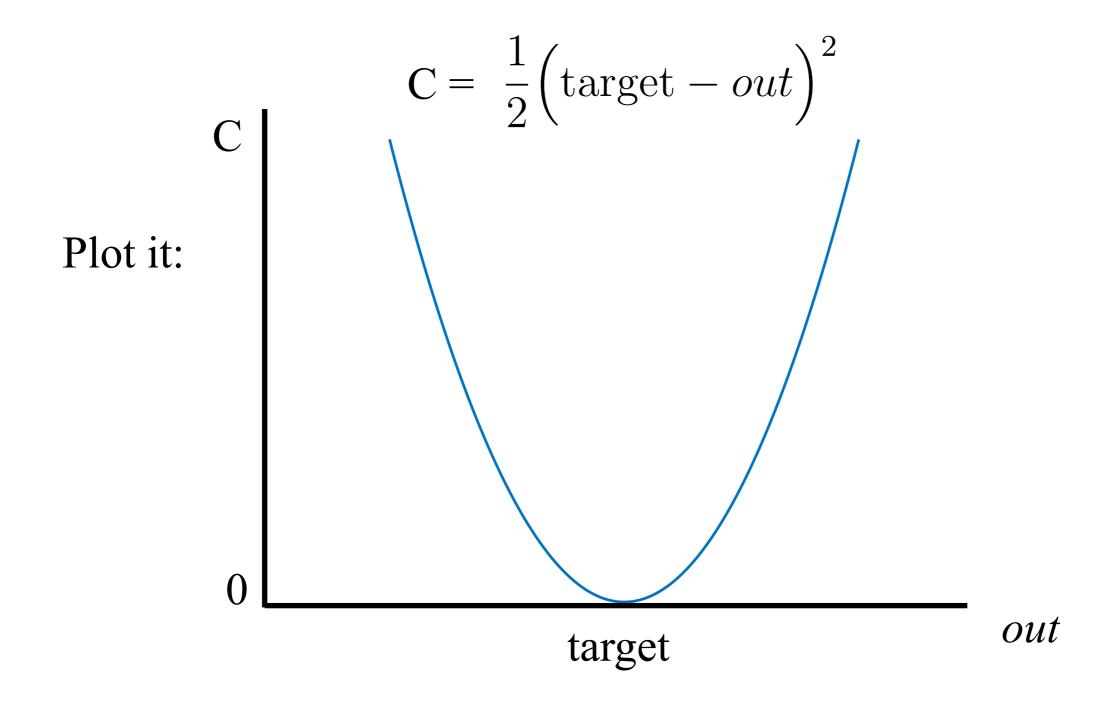
$$out = target$$

rearrange
$$out$$
 - target = 0 GOAL

Let's use this to define a **cost function** ...

Create a cost function

Define the cost function:



Q: Where is the cost zero?

A: When out = target.

Create a cost function

Q: Why this cost function?

$$C = \frac{1}{2} \left(\text{target} - out \right)^2$$

- Minimum (the "lowest cost") when out = target.
- It's convenient (a quadratic).
- It steadily increases as out deviates from target.
- It's "easy" to compute derivatives.

Create a cost function

Q: How does the cost function <u>change</u> due to changes in *out*?

A: We need to compute a derivative ...

$$\frac{dC}{dout} = \frac{d}{out} \left[\frac{1}{2} \left(\text{target} - out \right)^2 \right] = ?$$

Chain rule ...

$$\frac{dC}{dout} = 2\sqrt{\frac{1}{2}} \left(\text{target} - out \right)^{1} \left(\frac{d(-out)}{dout} \right)$$

$$\frac{dC}{dout} = -\left(\text{target} - out \right)$$

$$\frac{dC}{dout}$$

$$\frac{dC}{dout} = out - \text{target}$$

Q: Does this derivative make sense?

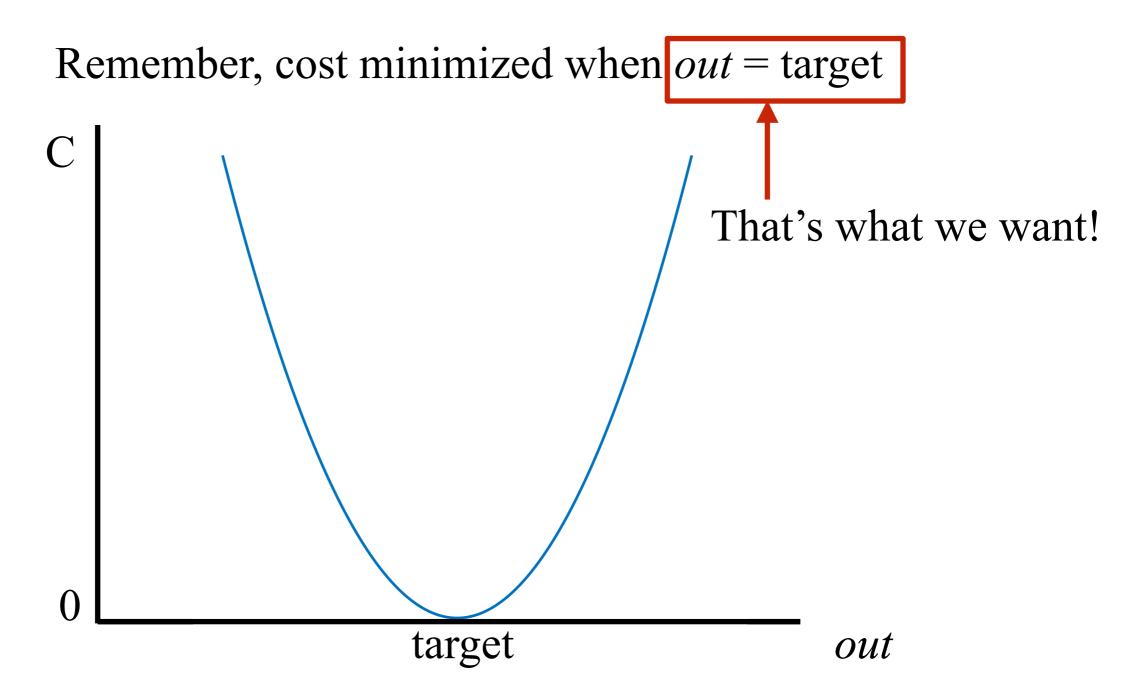
$$\frac{dC}{dout} = out - \text{target}$$

When out < target C $\frac{dC}{dout} < 0$ $\frac{dC}{dout} > 0$ $\frac{dC}{dout} > 0$ $\frac{dC}{dout} > 0$ $\frac{dC}{dout} > 0$

target

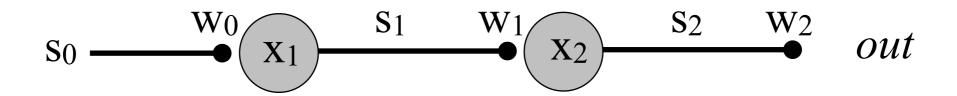
out

Now, our goal: Choose weights to minimize the cost function



Here, we plot C versus out. But out depends on weights ...

Q: How does *out* depend on weights?

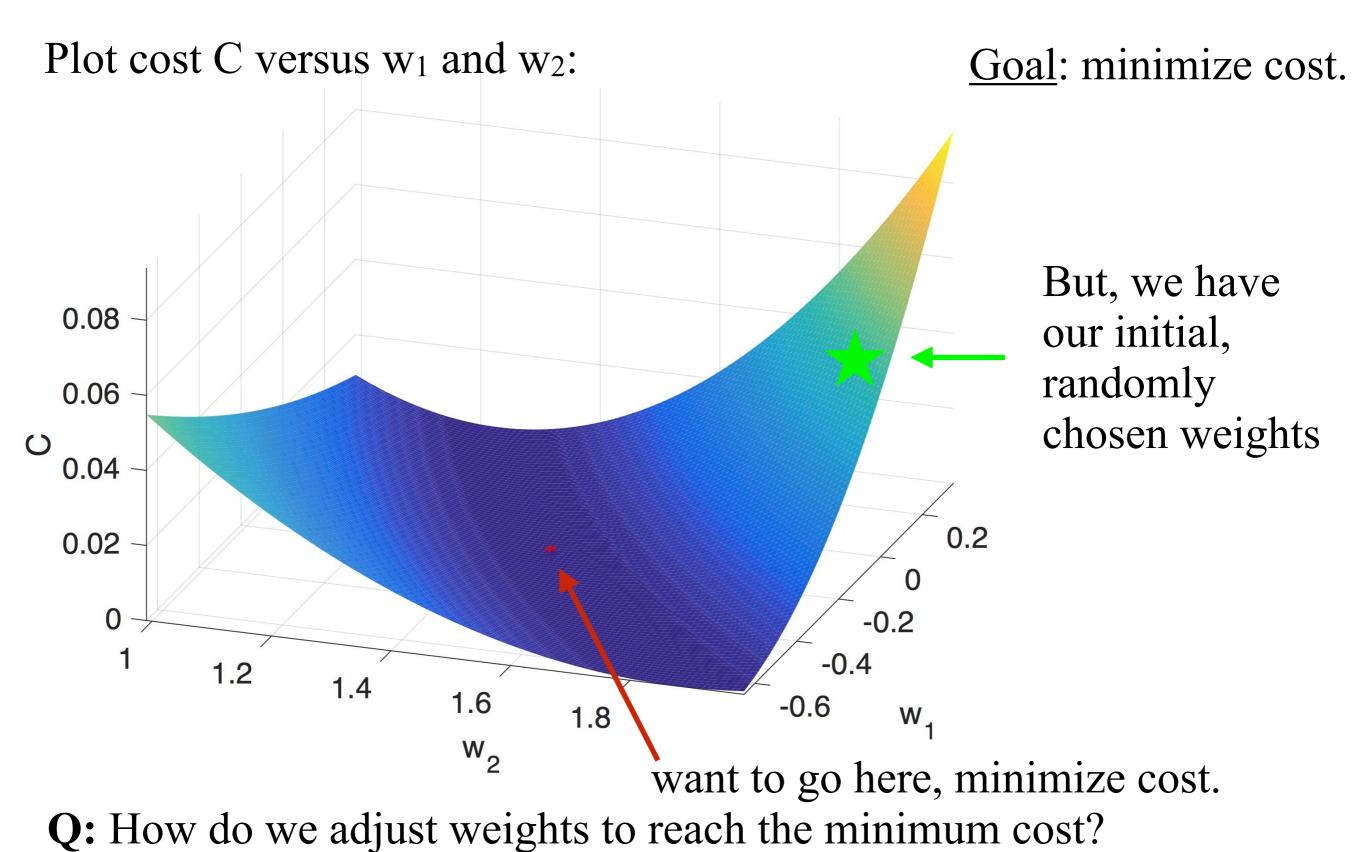


A: It's complicated.

Consider feedforward solution ...

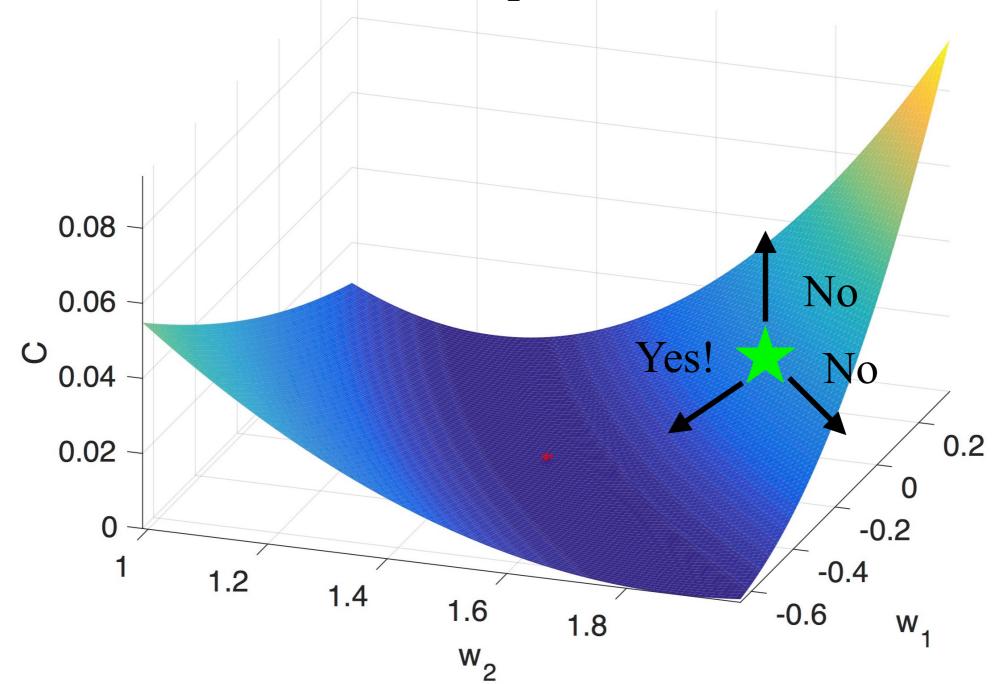
$$x_1 = s_0 w_0 \longrightarrow s_1 = S(x_1) \longrightarrow x_2 = s_1 w_1 \longrightarrow s_2 = S(x_2) \longrightarrow out = s_2 w_2$$

If out depends on weights, so does the cost ... $C(w_0, w_1, w_2) = ?$



A: Move "downhill" ...

<u>Intuition</u>: move down the **steepest direction** of cost function



Imagine placing a marble ... where does it roll? To the minimum.

Q: How do we find the steepest direction? **A:** Compute the gradient

Gradient of the cost function.

How C changes due to small changes in w₀, w₁, w₂.

We need to compute:

$$\frac{dC}{dw_0}$$

$$\frac{dC}{dw_1}$$

$$\frac{dC}{dw_2}$$

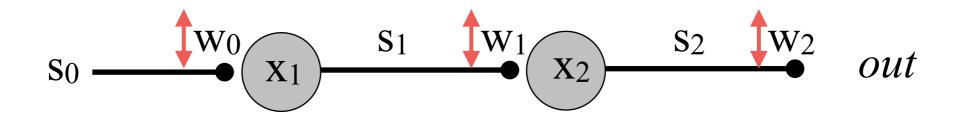
Then, update the weights in steps proportional to the negative gradient.

$$w_0 \leftarrow w_0 - \alpha \frac{d\,C}{d\,w_0} \qquad w_1 \leftarrow w_1 - \alpha \frac{d\,C}{d\,w_1} \qquad w_2 \leftarrow w_2 - \alpha \frac{d\,C}{d\,w_2}$$
 "new" weight "original" weight (negative) steepest direction of C

Procedure: gradient descent

 α = learning rate

Q: How does the cost function change due to changes in weights?



Consider:
$$\frac{dC}{dw_2} = ???$$

We know how C depends on *out*:
$$C = \frac{1}{2} \left(\text{target} - out \right)^2$$

And we know how *out* depends on w_2 : $out = s_2 w_2$

To compute the derivative, use the **chain rule** ...

Our goal:

$$\frac{dC}{dw_2} = ???$$

We know C depends on out, and out depends on w2 ...

$$\frac{dC}{dw_2} = \frac{dC}{dout} \frac{dout}{dw_2}$$

We've already solved the first derivative!

$$\frac{dC}{dout} = out - \text{target} \qquad Slide 35$$

Let's compute the next derivative ...

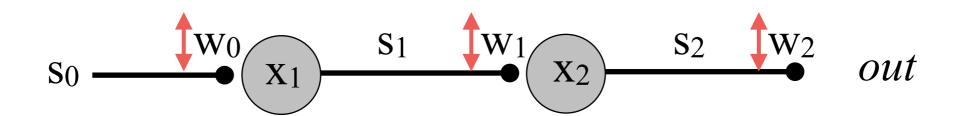
$$\frac{d out}{d w_2} = ??? We know: out = s_2 w_2$$

So,
$$\frac{dout}{dw_2} = \frac{d(s_2w_2)}{dw_2} = s_2 \frac{dw_2}{dw_2} = s_2$$

Then,
$$\frac{dC}{dw_2} = \frac{dC}{dout} \frac{dout}{dw_2}$$

$$\frac{dC}{dw_2} = (out - target) \quad s_2$$

Q: How does the cost function change due to changes in weights?

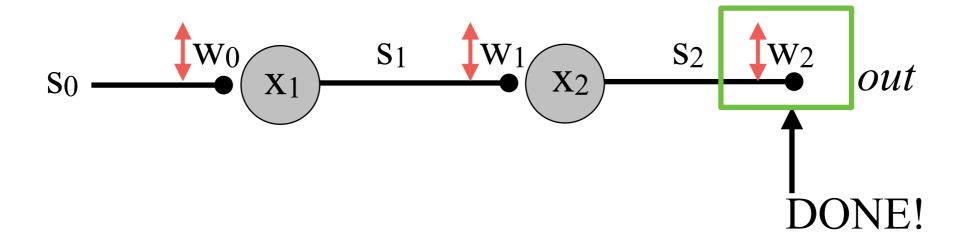


We found,
$$\frac{dC}{dw_2} = \begin{bmatrix} out - target \\ & & \\$$

Update the weight w₂:

$$w_2 \leftarrow w_2 - \alpha \frac{dC}{dw_2}$$
 becomes $w_2 \leftarrow w_2 - \alpha (out - target)s_2$

So, we've now found an equation to update one of the weights w₂ that acts to minimize the cost function.



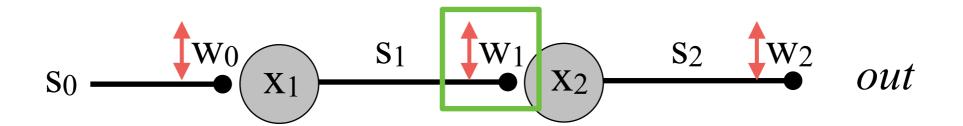
$$w_2$$
 update: $w_2 \leftarrow w_2 - \alpha(out - target)s_2$

Q: Can we find equations to update w_1 and w_0 ?

A: Yes we can.

It'll seem difficult, but we've already done the hard work ...

Q: How does the cost function change due to change in w_1 ?



$$\frac{dC}{dw_1} = ???$$

 $\frac{dC}{dw_1} = ???$ We don't know this ... but can write it using things we do know things we do know.

We need the **chain rule**:

$$\frac{dC}{dw_1} = \frac{dC}{dout} \frac{dout}{dw_1}$$

Q: How does the cost function change due to change in w_1 ?

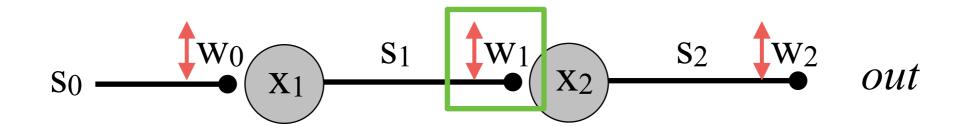
$$\frac{dC}{dw_1} = \frac{dC}{dout} \frac{dout}{dw_1}$$

We already found:

$$\frac{dC}{dout} = out - \text{target} \qquad (Slide 35)$$

$$\frac{d out}{d w_1} = w_2 s_2 (1 - s_2) s_1$$
 (Slide 23)

Q: How does the cost function change due to change in w_1 ?



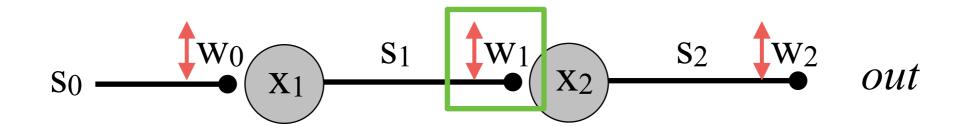
We conclude:

$$\frac{dC}{dw_1} = \frac{dC}{dout} \frac{dout}{dw_1}$$

$$\frac{dC}{dw_1} = \underbrace{ (out - \text{target})}_{\text{How bad we're doing.}} w_2 \, s_2 \, (1 - s_2) \, s_1$$

complicated expression of outputs and weight

Q: How does the cost function change due to change in w_1 ?



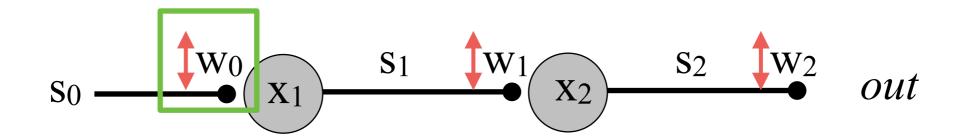
Update the weight w₁:

becomes
$$w_1 \leftarrow w_1 - \alpha \frac{d\,C}{d\,w_1} \text{ substitute in for this!}$$

$$w_1 \leftarrow w_1 - \alpha (out - \text{target}) w_2 s_2 (1 - s_2) s_1$$

Q: What happens when out = target?

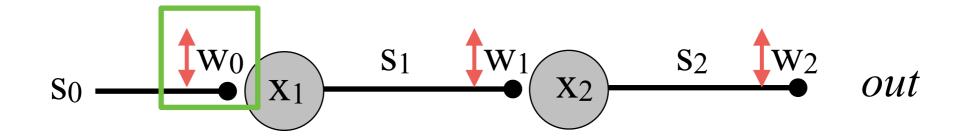
Q: How does the cost function change due to change in w_0 ?



$$\frac{dC}{dw_0} = ???$$

Try it ...

Q: How does the cost function change due to change in w_0 ?



We conclude:

$$\frac{dC}{dw_0} = (out - target) w_2 s_2(1 - s_2) w_1 s_1(1 - s_1) s_0$$

and

$$w_0 \leftarrow w_0 - \alpha(out - target)w_2s_2(1 - s_2)w_1s_1(1 - s_1)s_0$$

Impressive expression!

Put it all together

<u>Prescription</u> to find the weights that minimize cost function (so that *out* is near target).

1. Choose random initial weights.

$$w_0 = 2$$
 $w_1 = 1$ $w_2 = 0.5$

2. Fix input at desire value, and calculate *out*.

$$S_0$$
 forward propagation $\rightarrow out$

Put it all together

Prescription (continued)

3. Update the weights

$$w_2 \leftarrow w_2 - \alpha(out - target)s_2$$

$$w_1 \leftarrow w_1 - \alpha(out - target)w_2s_2(1 - s_2)s_1$$

$$w_0 \leftarrow w_0 - \alpha(out - target)w_2s_2(1 - s_2)w_1s_1(1 - s_1)s_0$$

Note: We know all of the values required

 α = learning rate, we choose this.

 s_0, s_1, s_2 = calculated during forward propagation

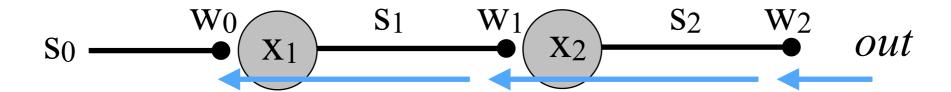
Put it all together

Prescription (continued)

4. Repeat Steps 2 & 3 until error is small enough.

or *out* is close enough to target.

This procedure is called backpropagation

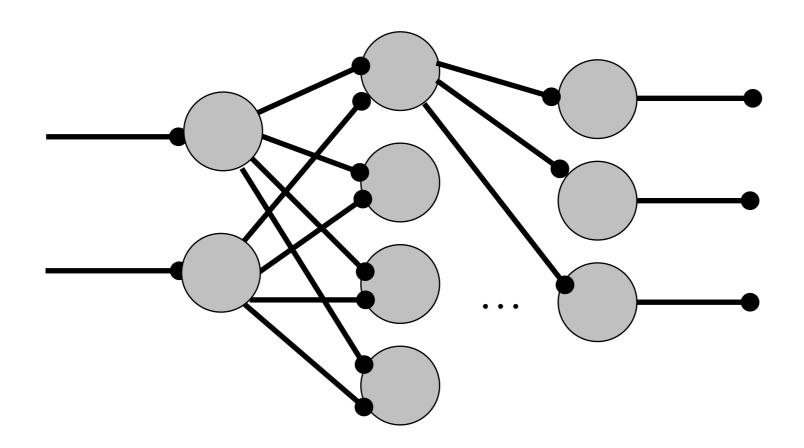


we work "backwards" through our neural network

from out to changes in w₂ to changes in w₁ to changes in w₀

Backpropagation

Can evaluate more complicated neural networks



Same ideas apply, but algebra is intense.

Cool example: playground.tensorflow.org

Next ...

Implement backpropagation in Python

Q: What weights $(w_0 \ w_1 \ w_2)$ produced these data?

$$S_0 \longrightarrow X_1 \longrightarrow X_1 \longrightarrow X_2 \longrightarrow X_2 \longrightarrow Out$$