MA666: Neural Networks and Learning

Part 1
Backpropagation

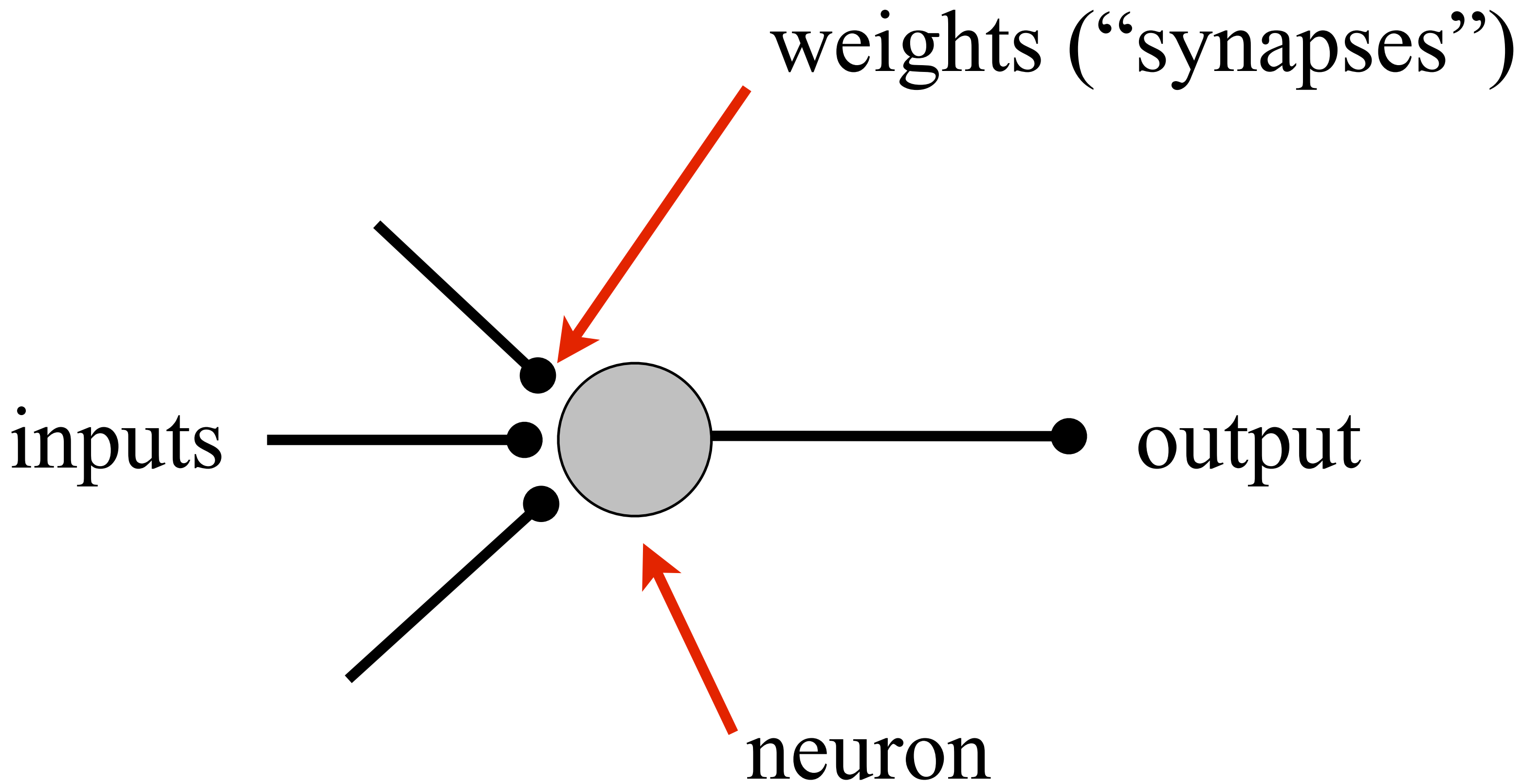
Today

This week we'll study learning in a "simple" neural network:

– Backpropagation

Remember, the Perceptron

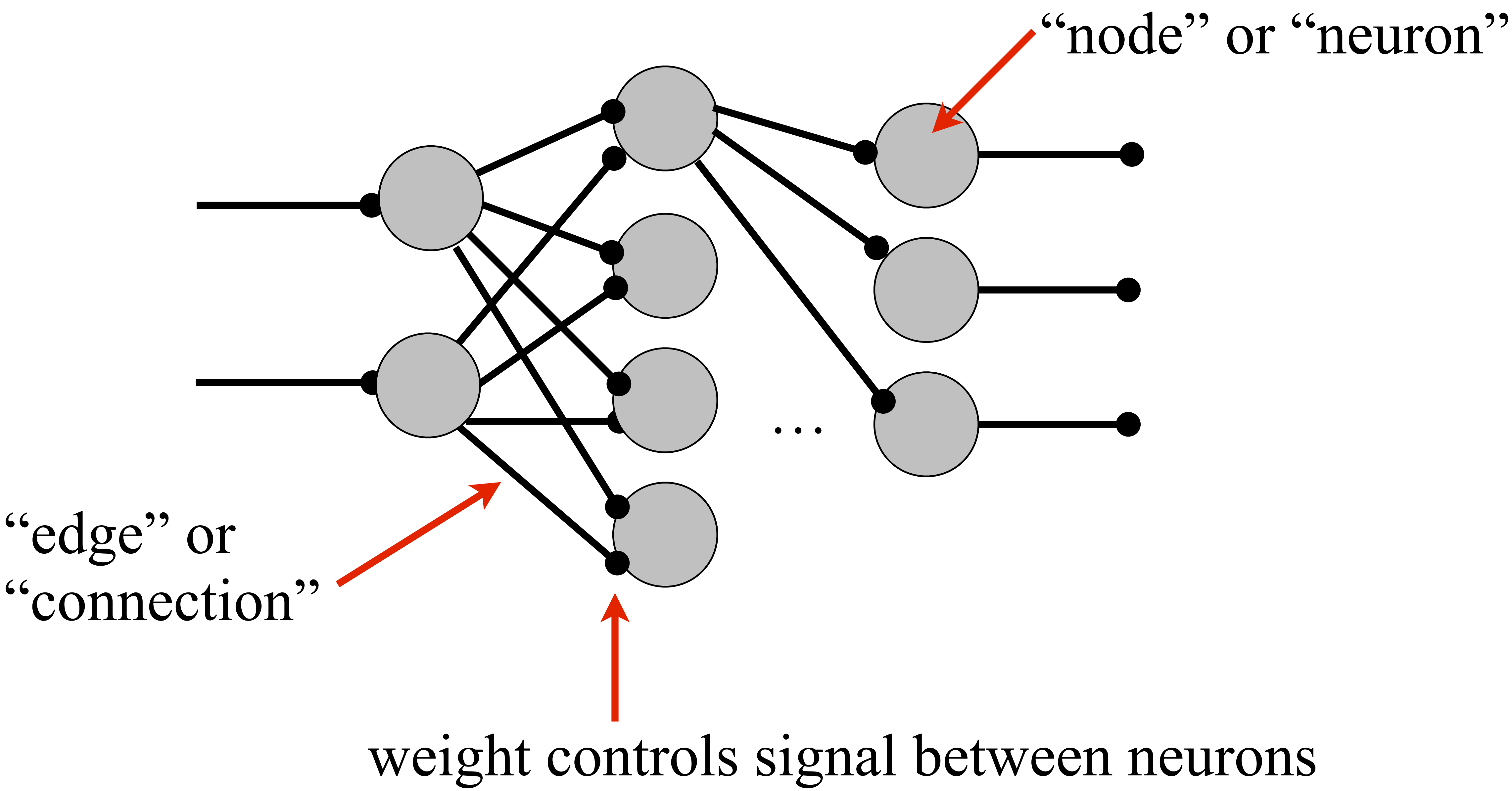
<u>Cartoon & Cast of Characters</u>



<u>Note</u>: there's only one neuron.

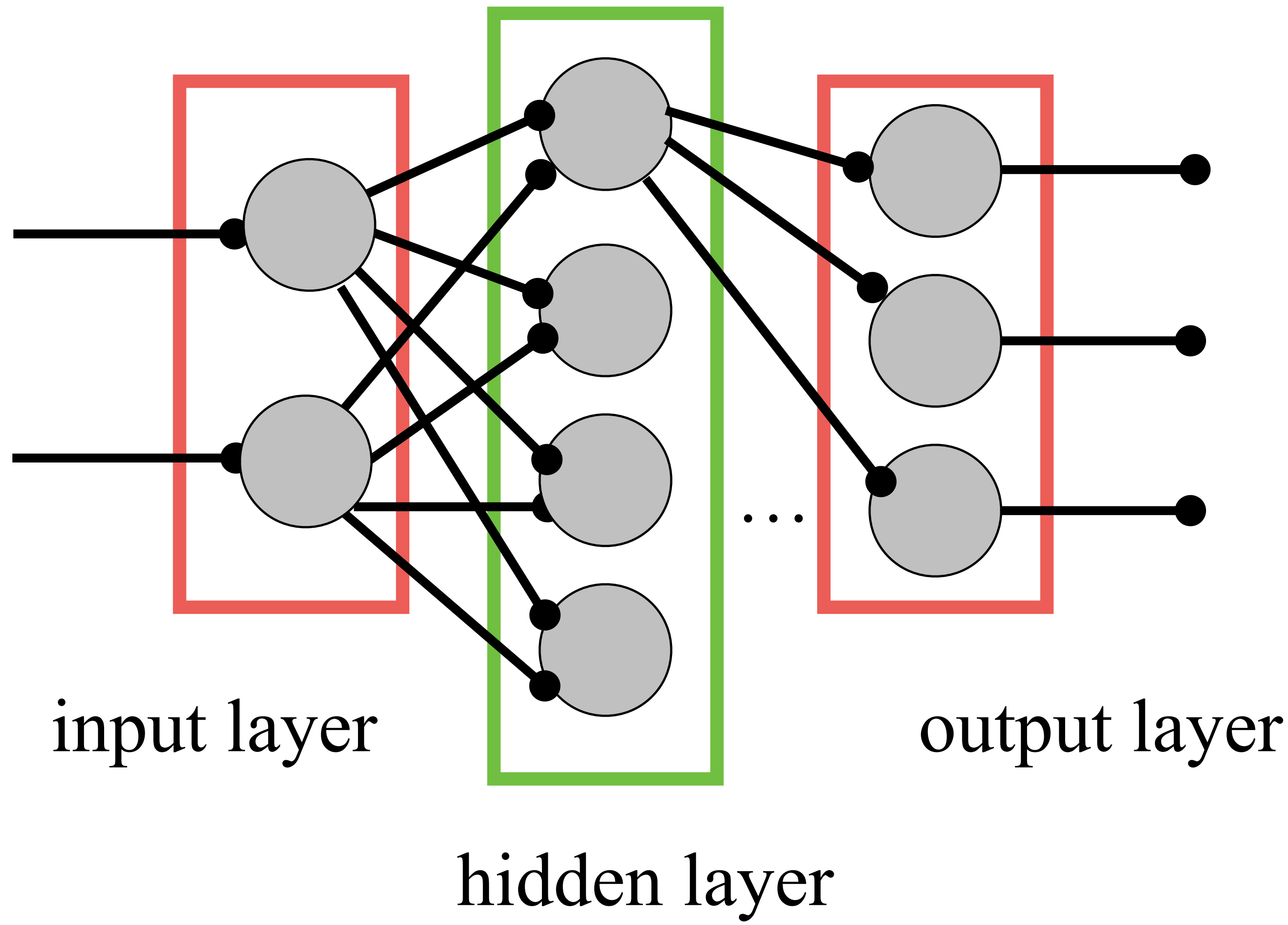
Today, a neural network

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



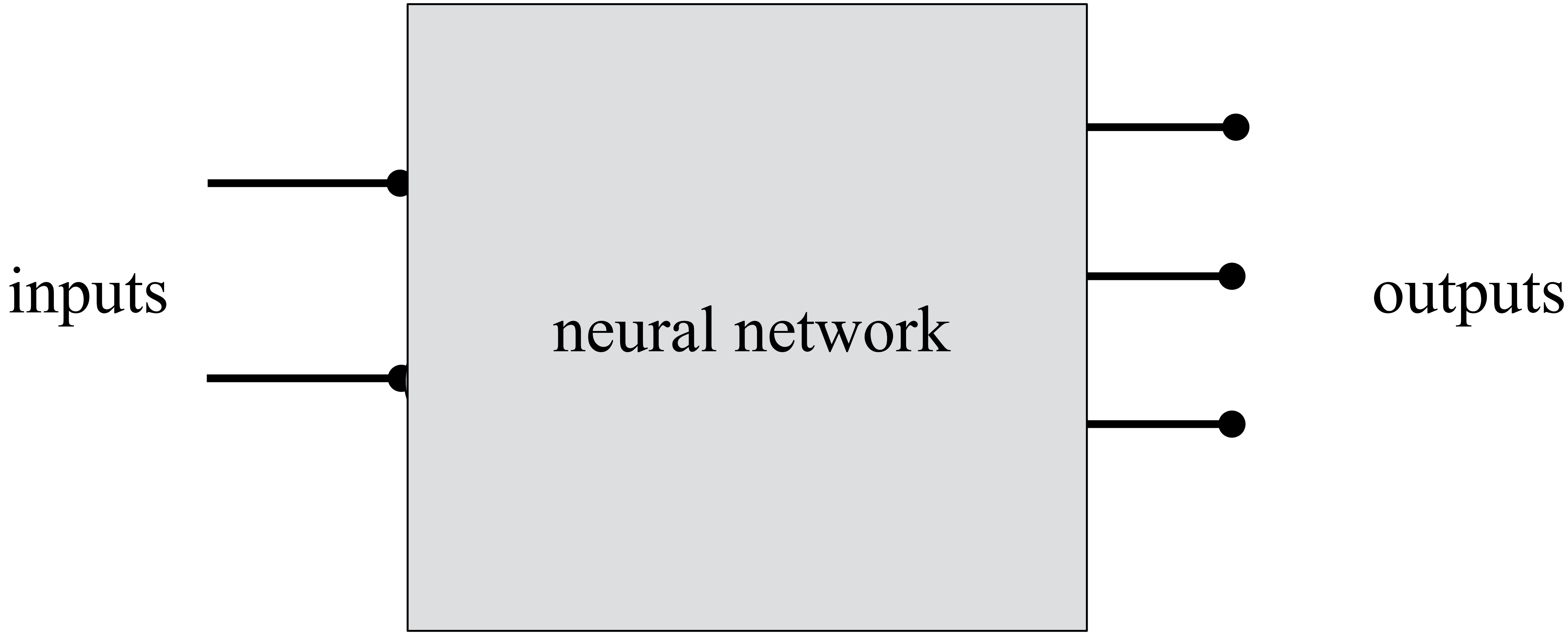
Today, a neural network

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



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**.
- Idea:
  - 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.

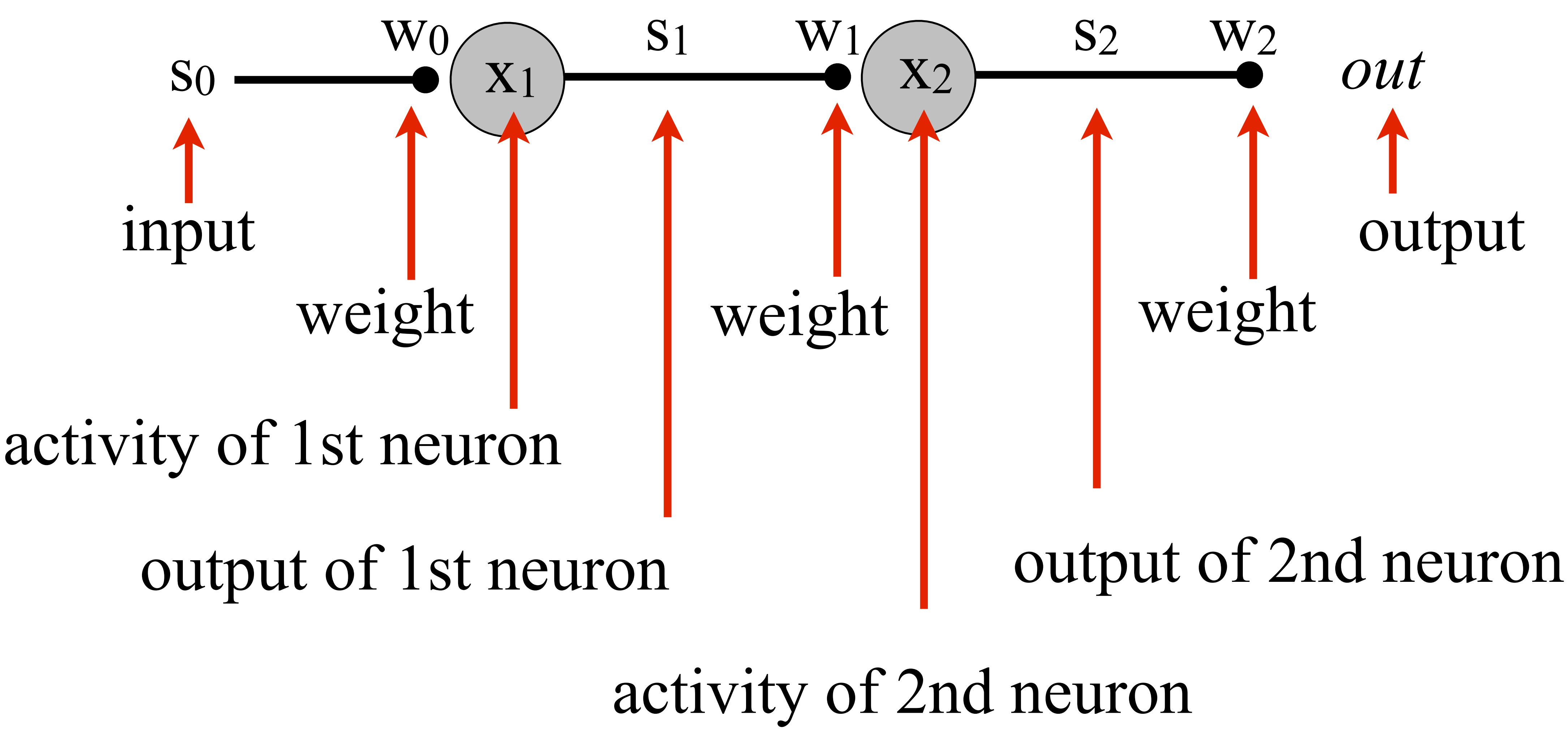
- **Forward propagation**
  For a set of weights & input, calculate output.

- **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.



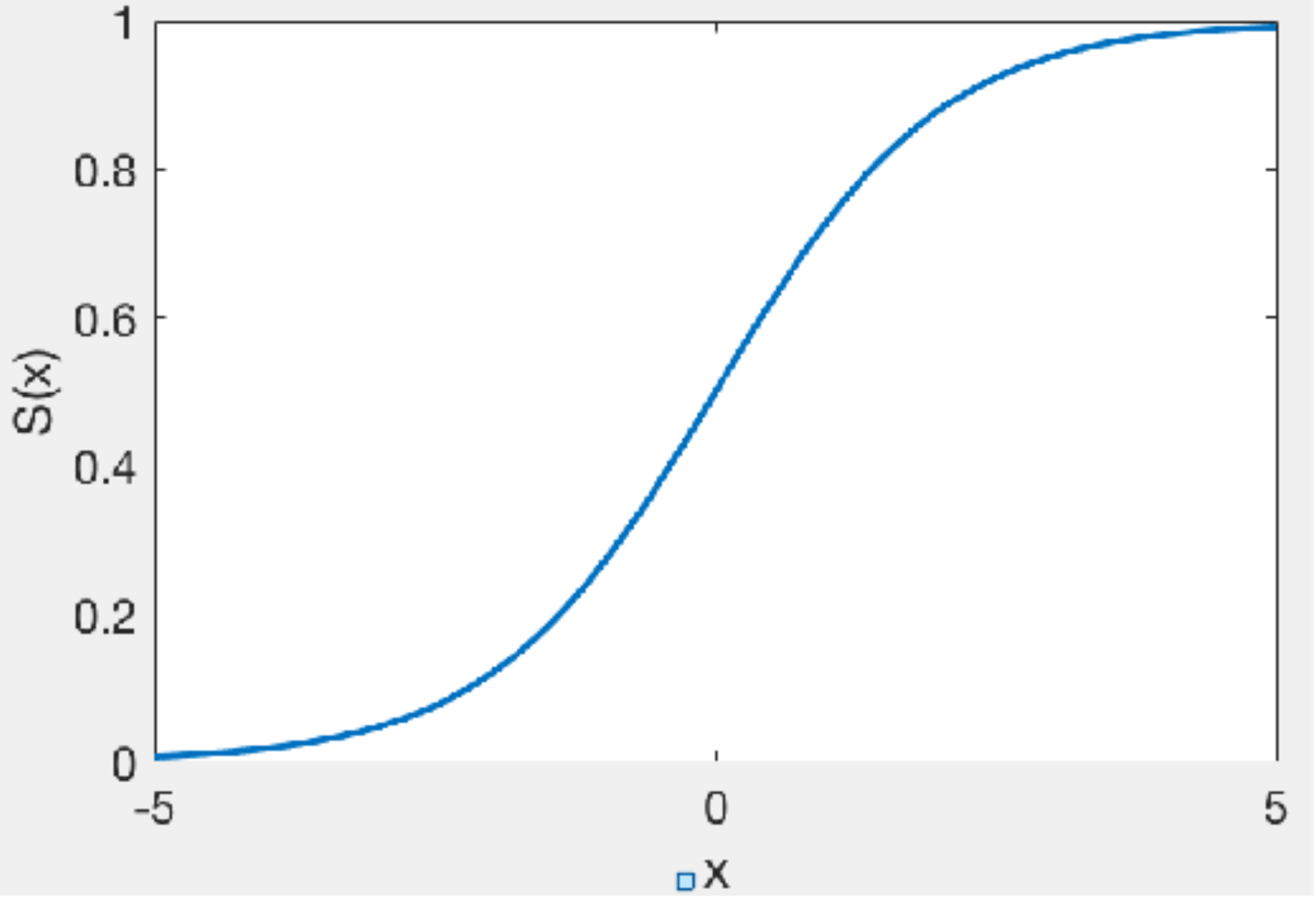
Activation function

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

$$x \text{ (activity)} \xrightarrow{\text{activation function}} \text{output}$$

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

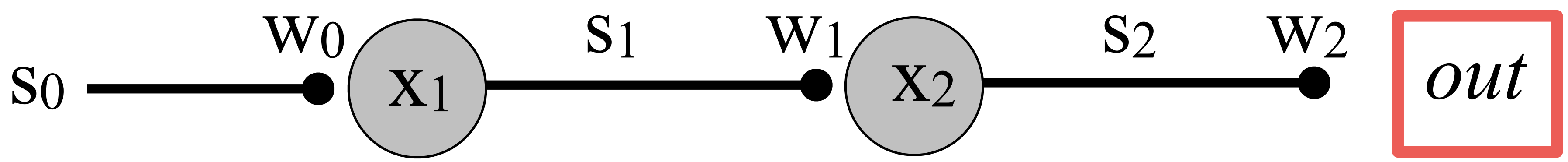
$$S(x) = 1 / (1 + e^{-x})$$



<u>NOTE</u>: It's like a "smoothed" binary threshold.

A “simple” neural network

We want our network to **learn** …



so that when then input s_0=2, the input *out*=0.7

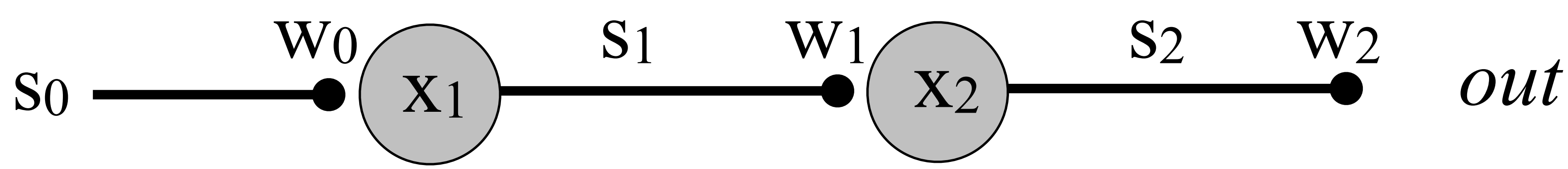
Q: How do we do it?

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:



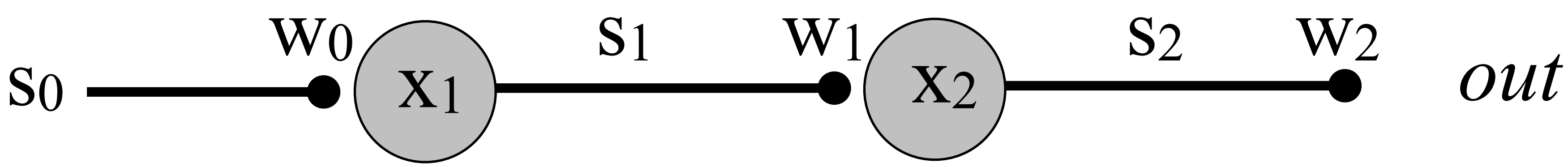
$w_0 = 2$ $\quad$ $w_1 = 1$ $\quad$ $w_2 = 0.5$

Q: How did I choose these?

Q: Do they work?

A: Let’s check … **forward propagation**

Forward propagation



$s_0 = 2$ $\quad w_0 = 2$ $\quad w_1 = 1$ $\quad w_2 = 0.5$

target:
$out = 0.7$

Let's do it.

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

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

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

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

$$out = w_2\, s_2 = 0.5 * 0.7275 = \boxed{0.3638}$$

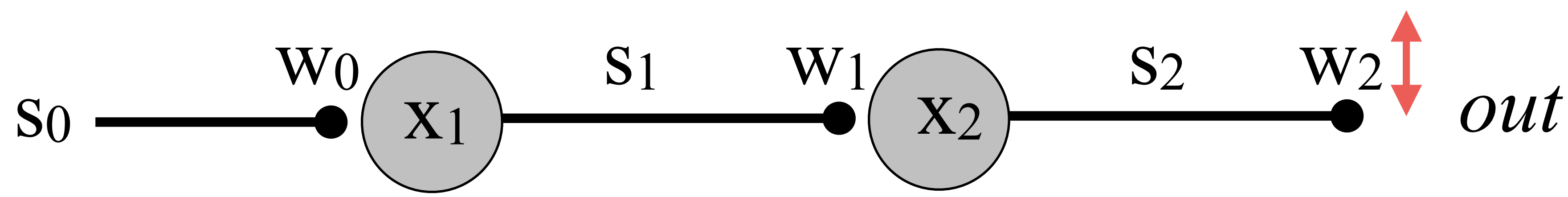
Match?

NO

How does a change in weight w_2 impact output?

Q: So now what?

<u>(intermediate) Goal</u>: get output (*out*) closer to target (0.7)



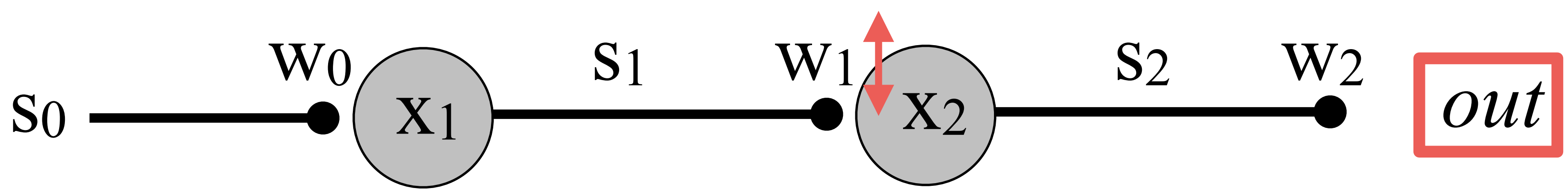
Q: How does a change in weight w_2 impact the output?

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

Mathematically, $\dfrac{d\,out}{d\,w_2} = \dfrac{d\,(s_2 w_2)}{d\,w_2} = s_2$

How does a change in weight w_1 impact output?

Let's keep going, working backwards.



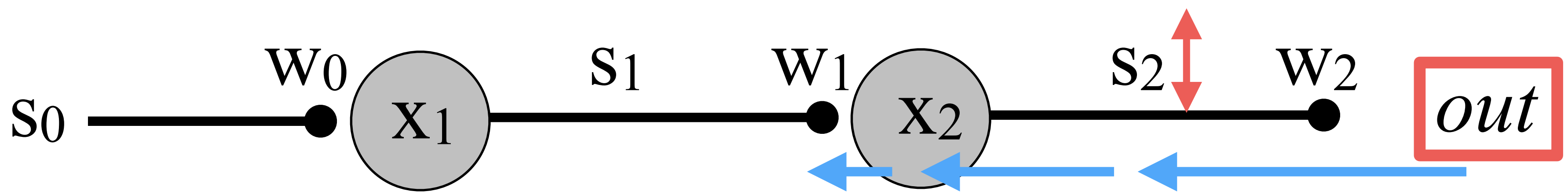
Q: How does a change in weight w_1 impact the output?

<u>Idea</u>: wiggle w_1 how does *out* change?

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

out does <u>not</u> depend directly on w_1

How does a change in weight w_1 impact output?



out does depend on s_2 and s_2 depend on x_2 and x_2 depend on w_1

Mathematically … the **chain rule**

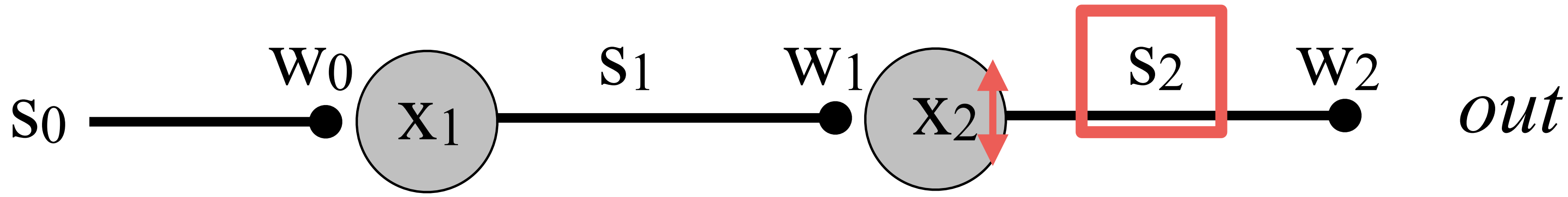
$$\frac{d\,out}{d\,w_1} = \boxed{\frac{d\,out}{d\,s_2}} \frac{d\,s_2}{d\,x_2} \frac{d\,x_2}{d\,w_1}$$

wiggle s_2 and *out* changes

Remember: $out = s_2 w_2$

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

How does a change in weight w_1 impact output?



Continue the **chain rule**

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

wiggle x_2 and s_2 changes

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

so $$\frac{d\ s_2}{d\ x_2} = \frac{d}{dx_2}\left(\frac{1}{1+e^{-x_2}}\right)$$

A complicated derivative

We need to compute:

$$\frac{d}{dx_2}\left(\frac{1}{1+e^{-x_2}}\right) = \text{Hmm} \ldots \ \textbf{Quotient Rule}$$

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

Q: What is $\frac{d(1+e^{-x_2})}{dx_2}$?

$$= \cancel{\frac{d(1)}{dx_2}}^{0} + \frac{d(e^{-x_2})}{dx_2} = (e^{-x_2})\underbrace{\boxed{\frac{d(-x_2)}{dx_2}}}_{} = \boxed{-e^{-x_2}}$$

$= - 1$

A complicated derivative

So,

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

$$= \frac{e^{-x_2}}{(1+e^{-x_2})^2}$$

Q: Can we simplify this expression?

A: Yes, but requires faith …

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

A complicated derivative

- Add 0 to the second term:

Sum is 0

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

Q: WHY?????? **A:** Let's organize terms …

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

Remember:

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

$= (s_2)\ (1 - s_2)$

A complicated derivative

So, for our chain rule calculation:

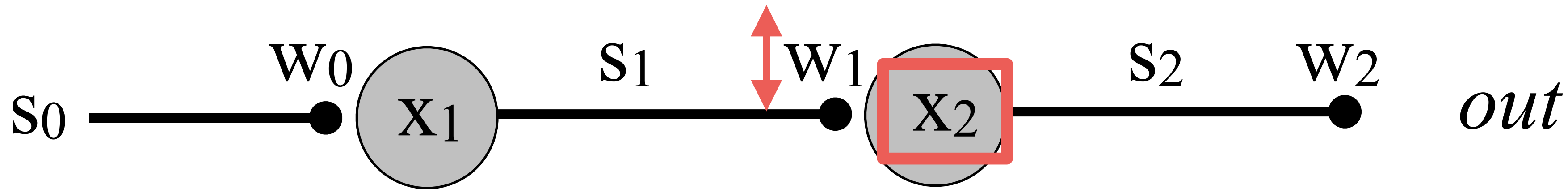
$$\frac{d\,out}{d\,w_1} = \frac{d\,out}{d\,s_2} \boxed{\frac{d\,s_2}{d\,x_2}} \frac{d\,x_2}{d\,w_1}$$

And we found:

$$\frac{d\,s_2}{d\,x_2} = \frac{d}{dx_2}\Bigg(\underbrace{\boxed{\frac{1}{1+e^{-x_2}}}}_{= s_2}\Bigg) = \text{… many steps …} \boxed{= s_2\,(1 - s_2)}$$

To complete the chain rule, one more derivative …

How does a change in weight w_1 impact output?



Continue the **chain rule**:

$$\frac{d\,out}{d\,w_1} = \frac{d\,out}{d\,s_2}\;\frac{d\,s_2}{d\,x_2}\;\boxed{\frac{d\,x_2}{d\,w_1}}$$

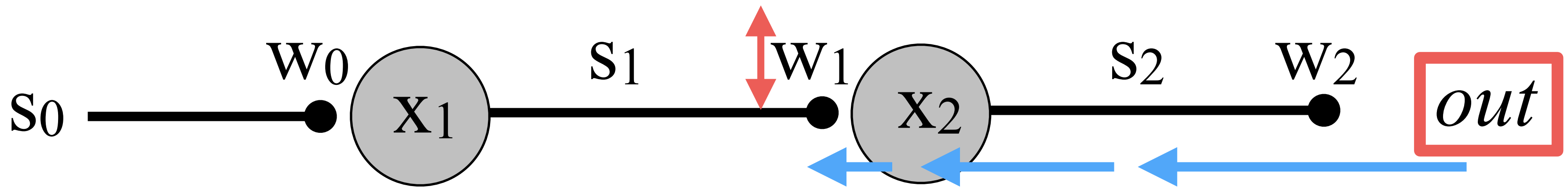
wiggle w_1 and x_2 changes

Remember: $x_2 = s_1\,w_1$

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

How does a change in weight w_1 impact output?

Back to our original question:



Q: How does a change in weight w_1 impact the output?

Mathematically … the **chain rule**

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

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

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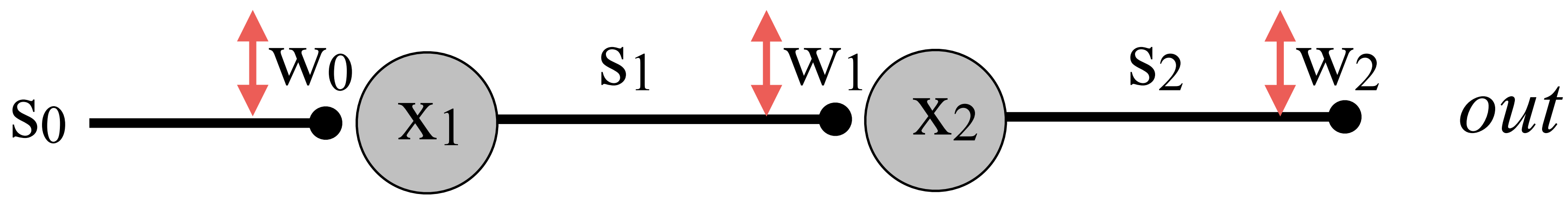
How does a change in weight w_0 impact output?

We're almost there …



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

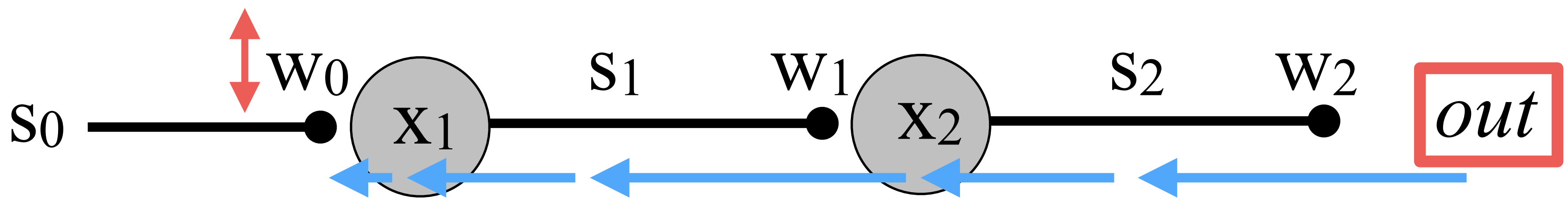
$$\frac{d\,out}{d\,w_1} = w_2\, s_2\, (1 - s_2)\, s_1$$

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

A: Chain rule …

How does a change in weight w_0 impact output?

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



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

Ugh …

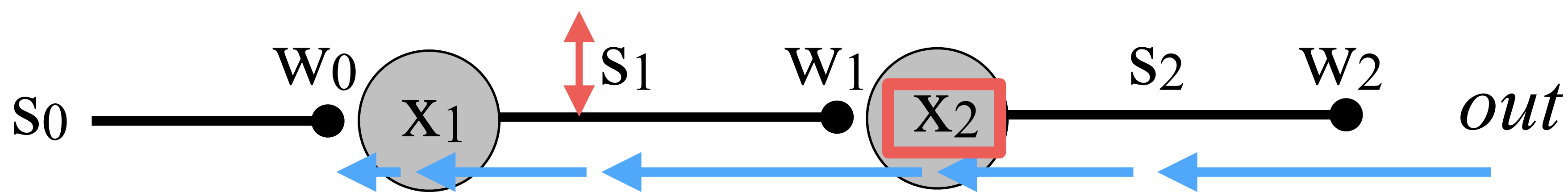
Luckily, we've already calculated two of these.

w_2 $\quad$ $s_2\,(1 - s_2)$

Let's compute the last 3 terms …

How does a change in weight w_0 impact output?

3rd term:



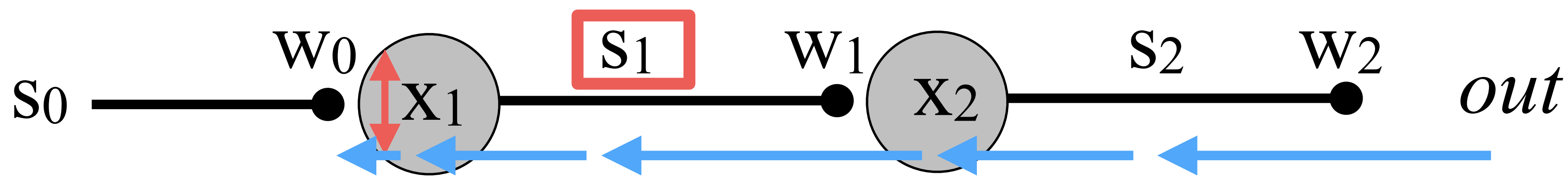
$$\frac{d\,out}{d\,w_0} = \frac{d\,out}{d\,s_2} \frac{d\,s_2}{d\,x_2} \boxed{\frac{d\,x_2}{d\,s_1}} \frac{d\,s_1}{d\,x_1} \frac{d\,x_1}{d\,w_0}$$

Remember: $x_2 = s_1 w_1$

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

How does a change in weight w_0 impact output?

4th term:



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

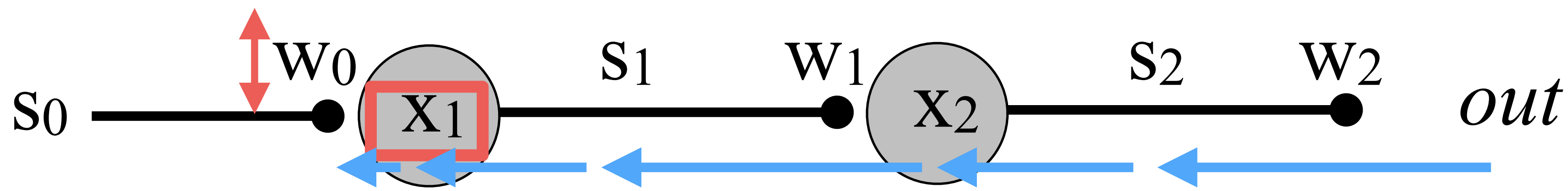
We found earlier that:

$$\frac{d\,s_2}{d\,x_2} = s_2\,(1 - s_2) \qquad \ldots \text{ so } \ldots \qquad \frac{d\,s_1}{d\,x_1} = \boxed{s_1\,(1 - s_1)}$$

This involved many steps!

How does a change in weight w_0 impact output?

5th term:



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

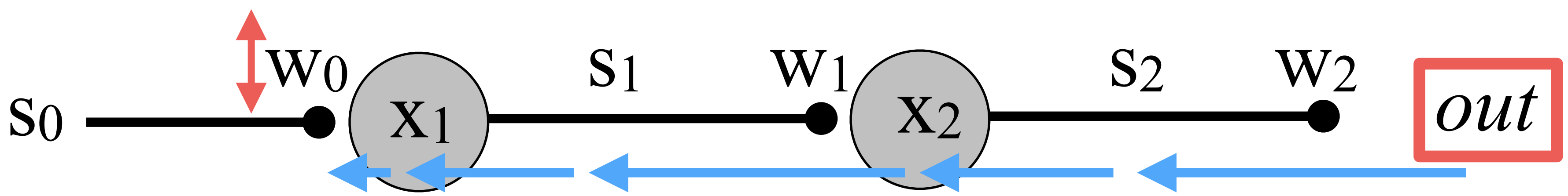
Remember: $x_1 = s_0\,w_0$

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

How does a change in weight w_0 impact output?

We now have the pieces to answer:

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



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

$$= \quad w_2 \quad s_2\,(1 - s_2) \quad w_1 \quad s_1\,(1 - s_1) \quad s_0$$

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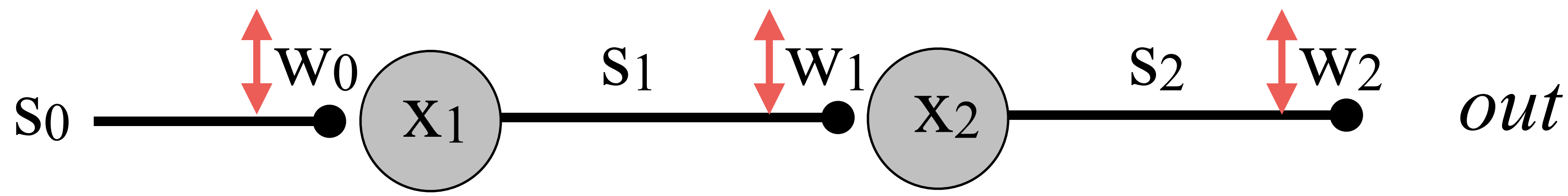
How does a change in weight impact output?

To summarize:

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



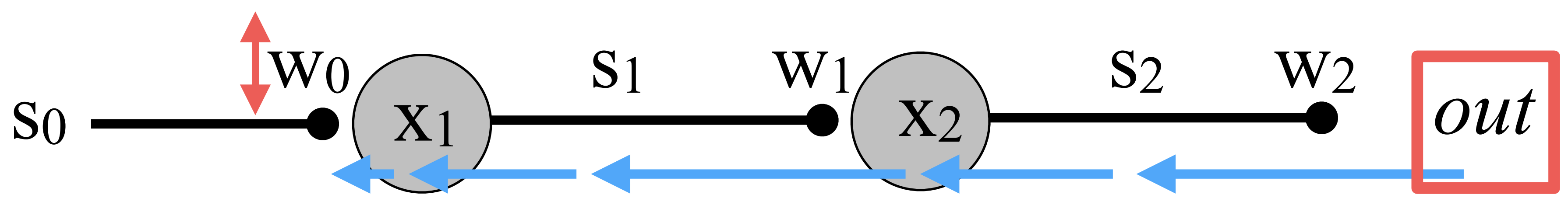
$$\frac{d\,out}{d\,w_2} = s_2$$

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

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

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

How does a change in weight impact output?



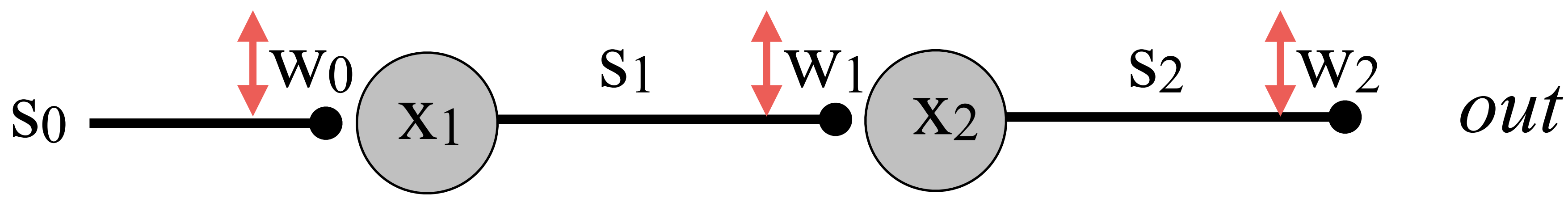
Backpropagation:

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:



$$out = \text{target}$$

rearrange $\quad out - \text{target} = 0 \quad$ **GOAL**

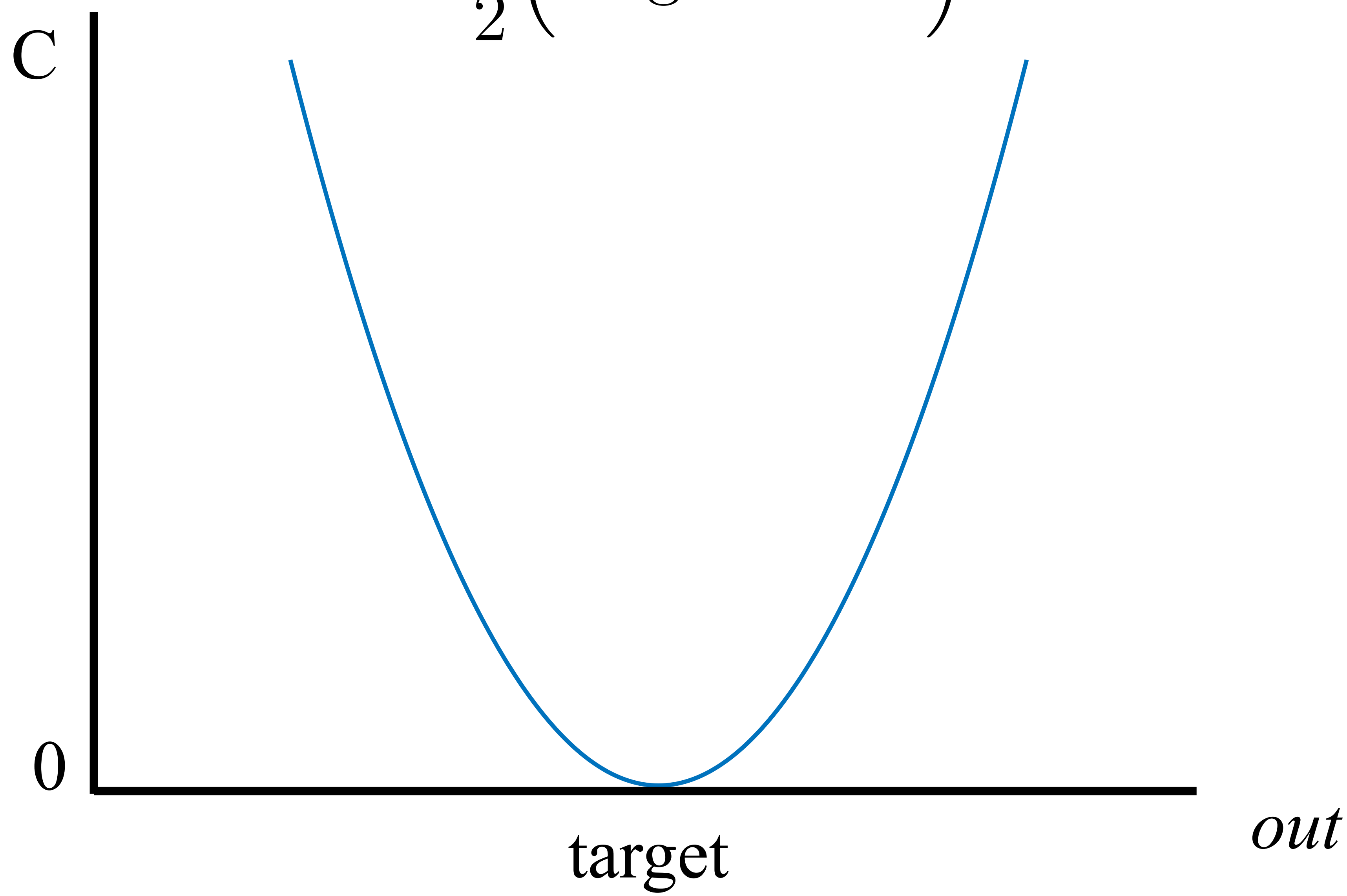
Let's use this to define a **cost function** …

Create a cost function

Define the cost function:

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

Plot it:



Q: Where is the cost zero?

A: When *out* = target.

Create a cost function

Q: Why this cost function?

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

- 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 …

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

Chain rule …

$$\frac{dC}{dout} = \underbrace{2\frac{1}{2}}_{1}\Big(\text{target} - out\Big)^1 \underbrace{\boxed{\left(\frac{d\,(-out)}{d\,out}\right)}}_{-1}$$

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

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

Create a cost function

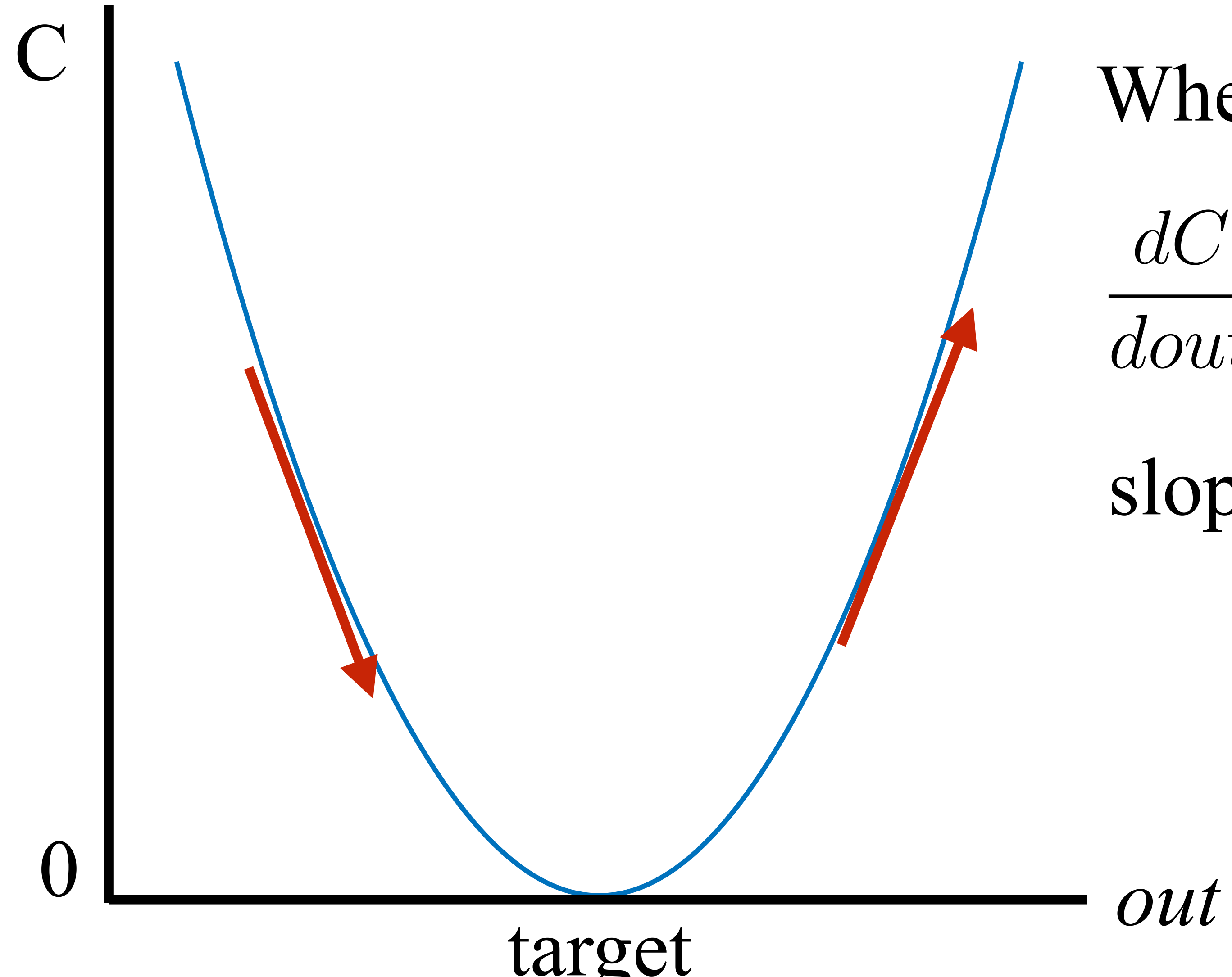
Q: Does this derivative make sense?

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

When *out* < target

$$\frac{dC}{dout} < 0$$

slope < 0



When *out* > target

$$\frac{dC}{dout} > 0$$

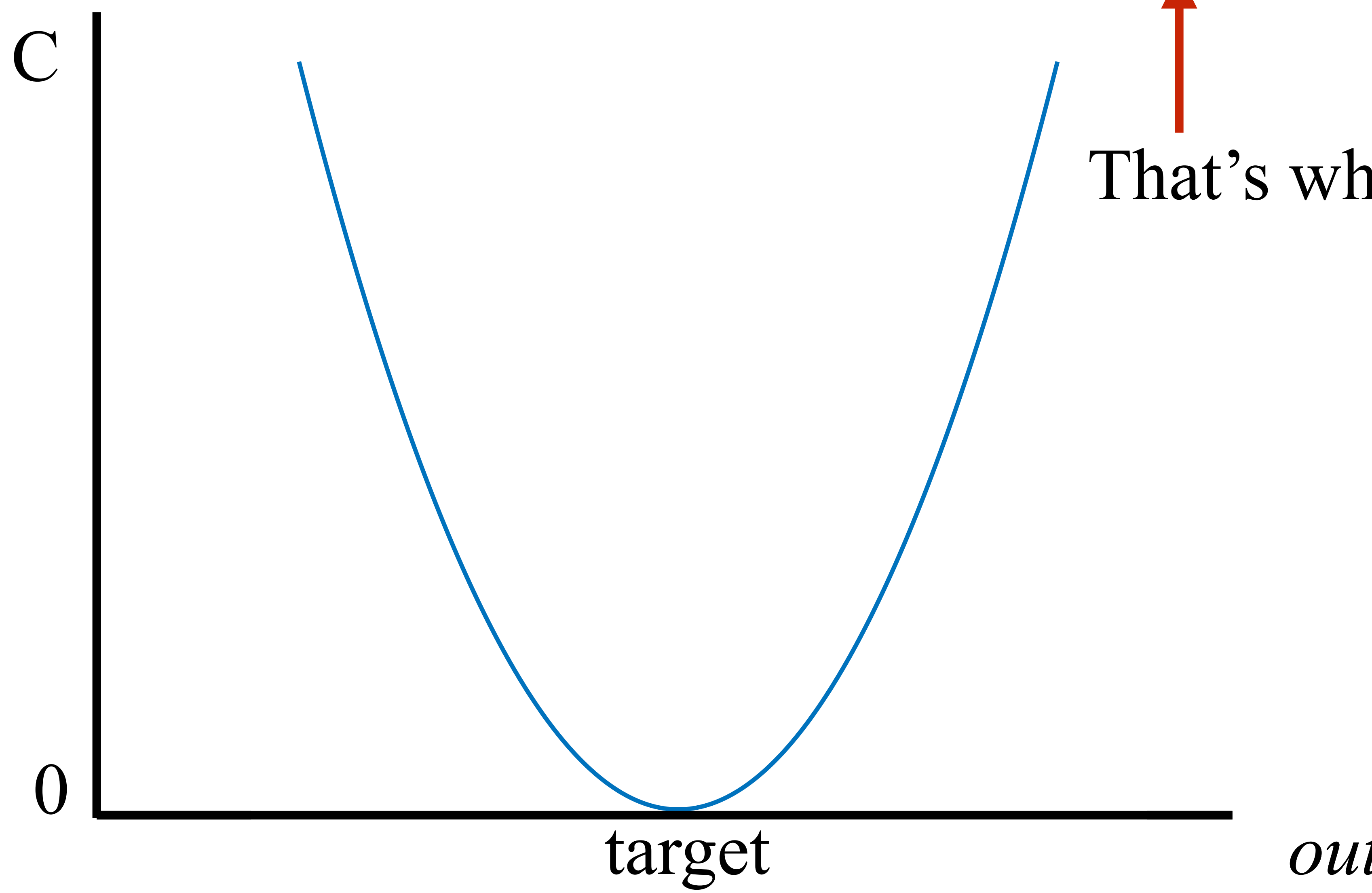
slope > 0

Create a cost function

Now, our goal: Choose weights to <u>minimize</u> the cost function

Remember, cost minimized when $\boxed{out = \text{target}}$

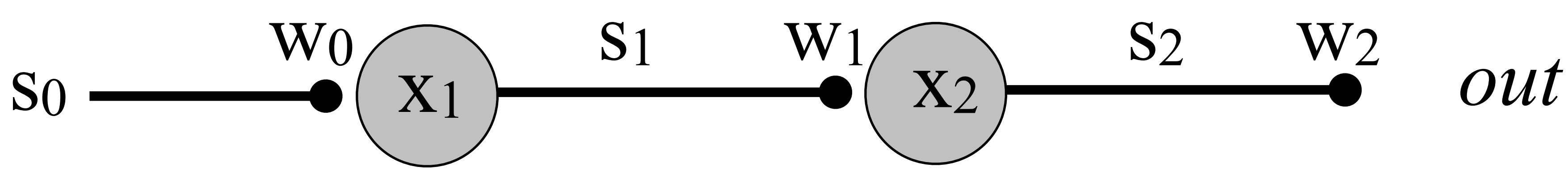
That's what we want!



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

Create a cost function

Q: How does *out* depend on weights?



A: It's complicated.

So, if *out* depends on weights, so does the cost … $C(w_0, w_1, w_2) = ?$

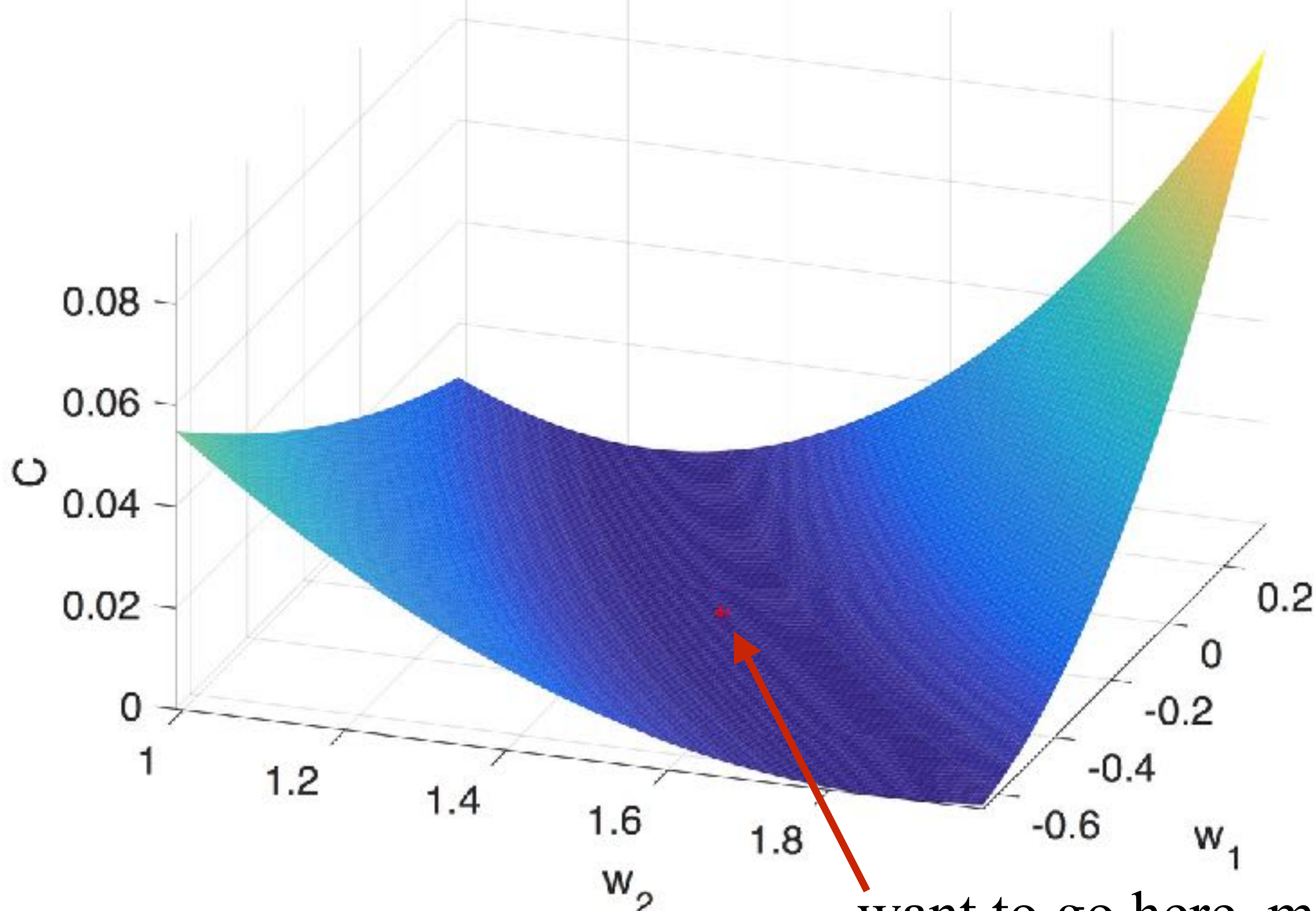
Consider feedforward solution …

$$x_1 = s_0\, w_0 \rightarrow s_1 = S(x_1) \rightarrow x_2 = s_1\, w_1 \rightarrow s_2 = S(x_2) \rightarrow \boxed{out} = s_2\, w_2$$

Create a cost function

Plot cost C versus w_1 and w_2:

<u>Goal</u>: minimize cost.



want to go here, minimize cost.

Imagine a “top-down” view …

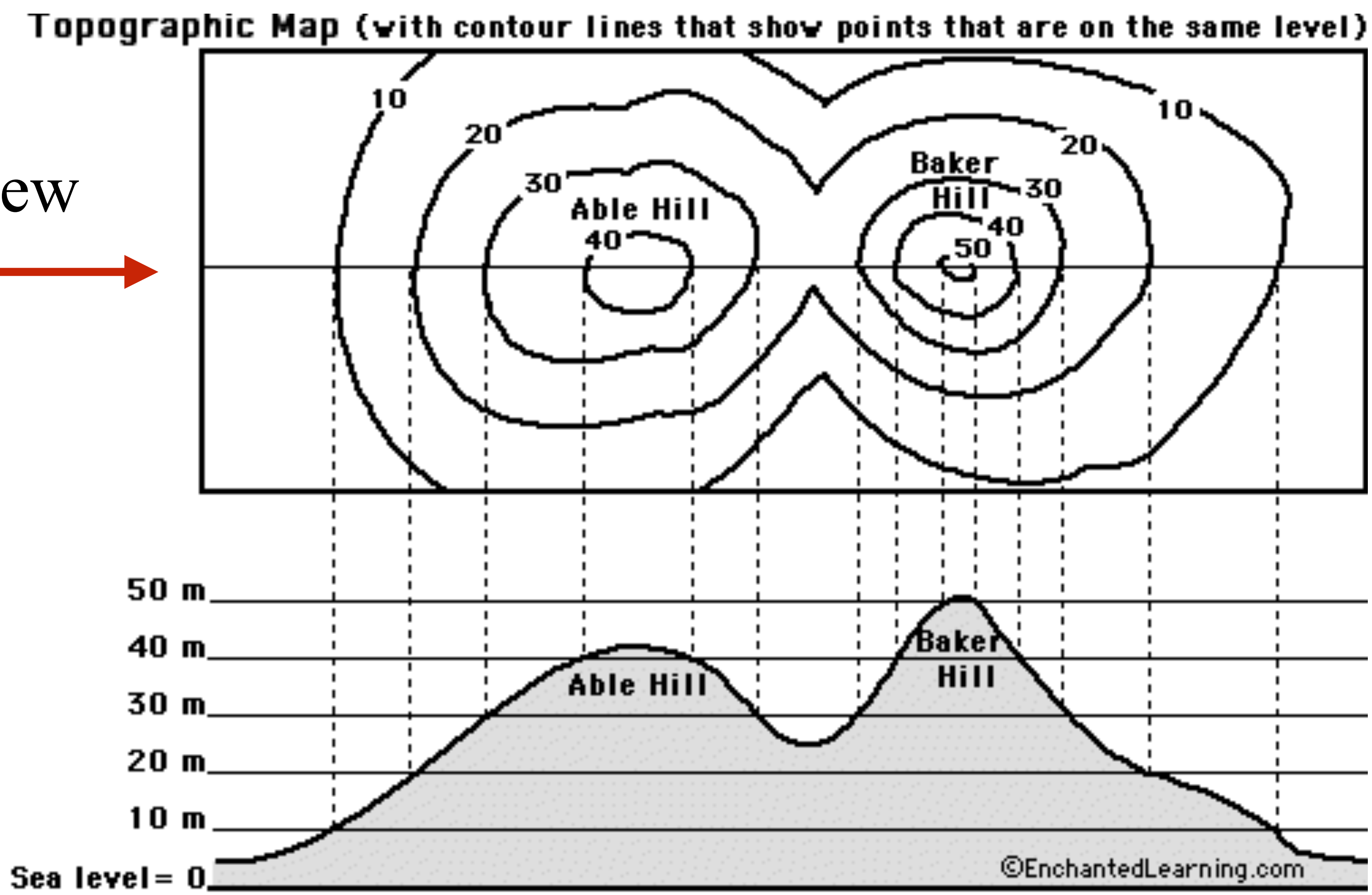
Create a cost function

<u>Contour map</u> or topographic map of cost function:

Related example:

top-down view

hills

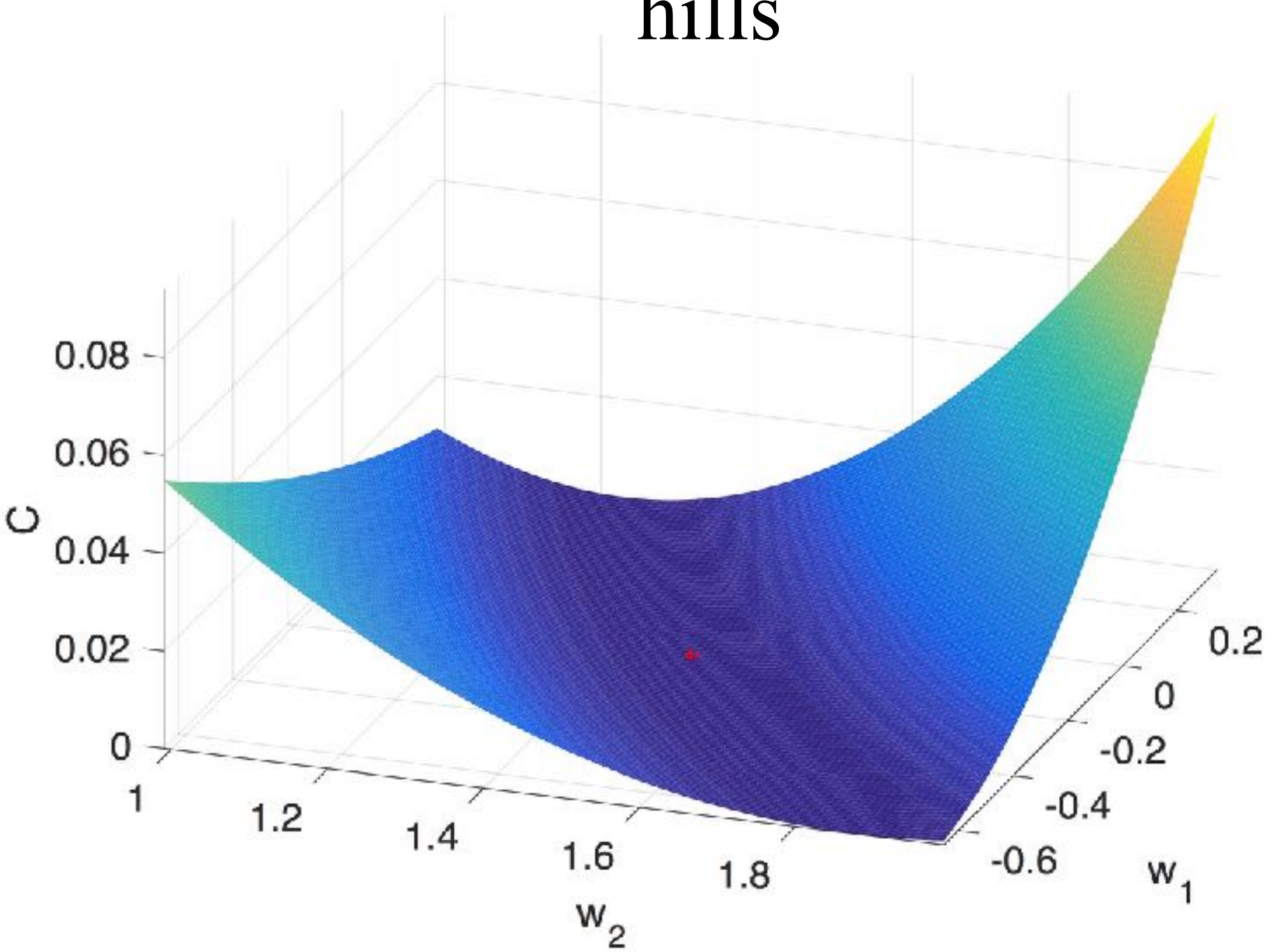


The two hills seen from the side, with elevations marked and dotted lines pointing to the corresponding contour lines.

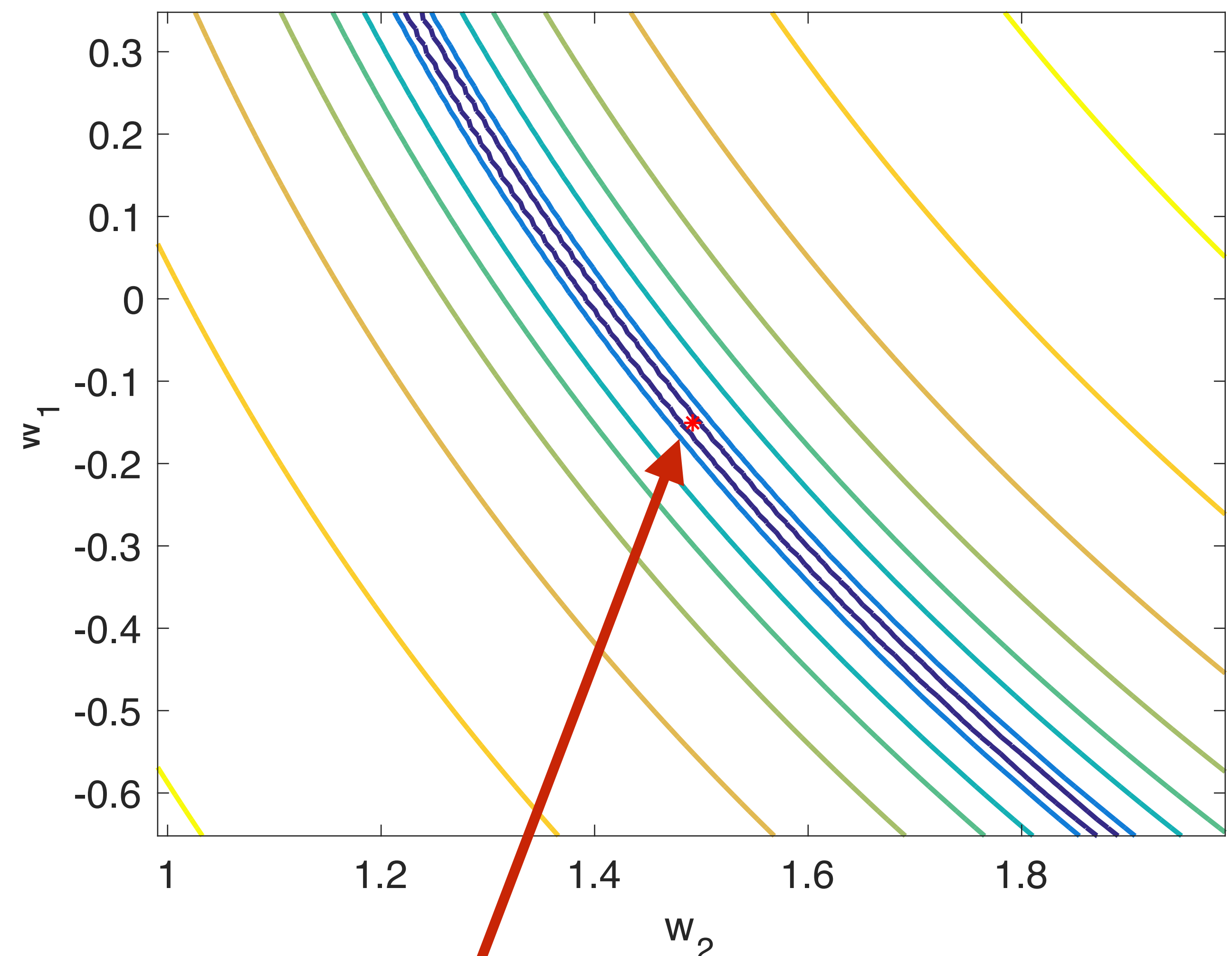
Create a cost function

<u>Contour map</u> of cost function:

hills



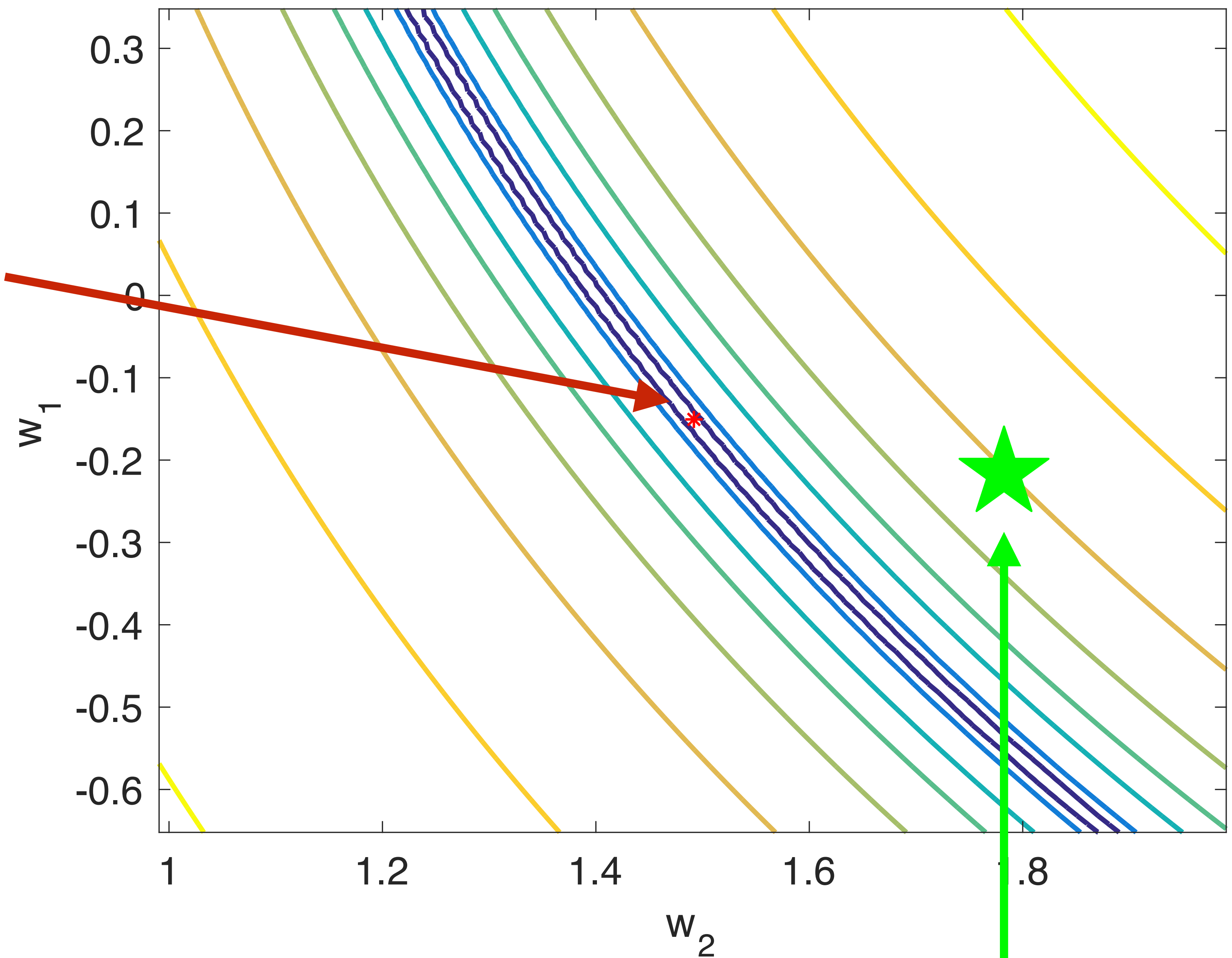
top-down view



minimum cost

Follow the cost function

We want the weights here
at the minimum cost



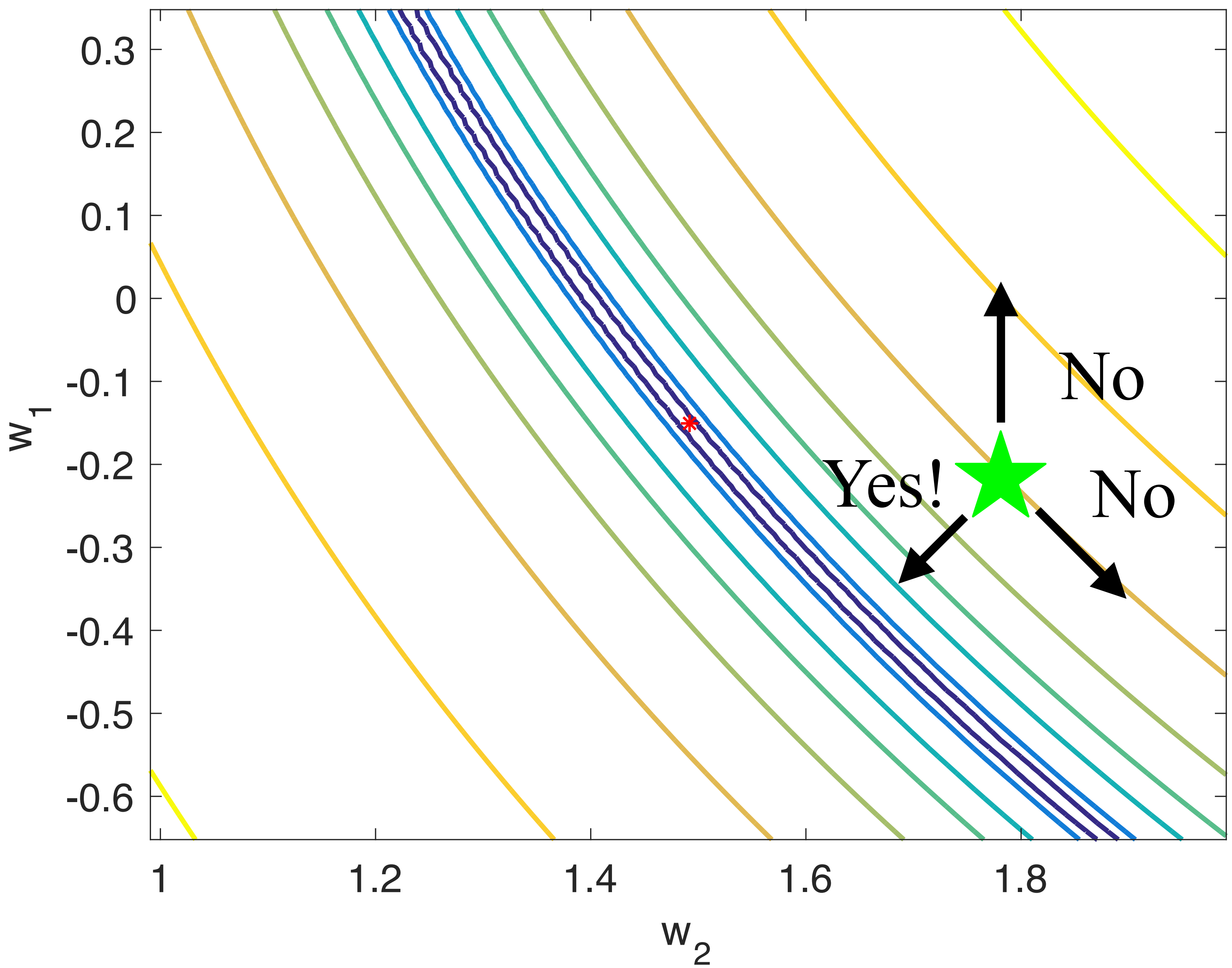
But, we have our initial,
randomly chosen weights

Q: How do we adjust weights to go from to minimum cost?

A: Move "downhill" …

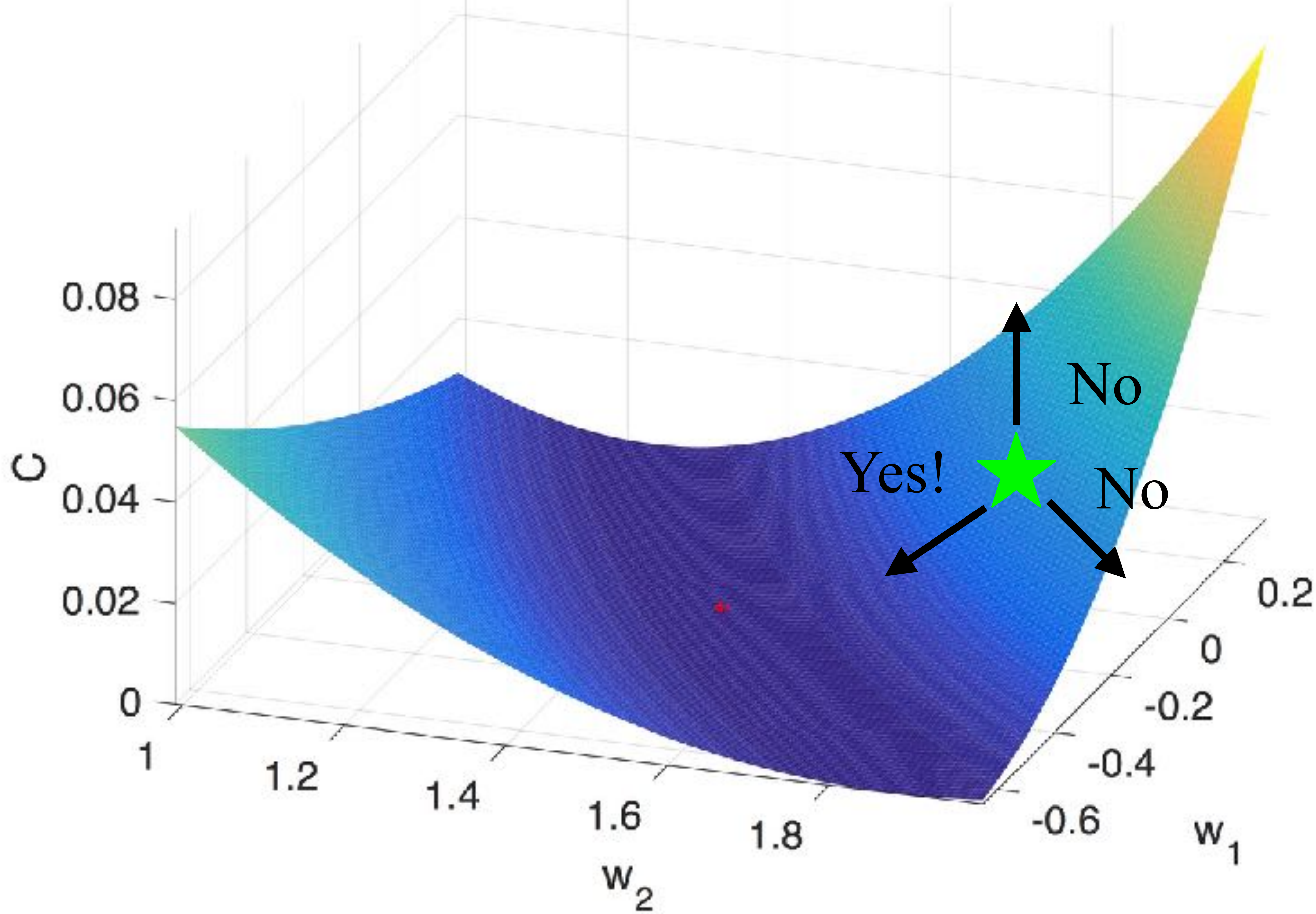
Follow the cost function

Intuition: move down the **steepest direction** of cost function



Follow the cost function

Intuition: 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

Follow the cost function

Gradient of the cost function.

- How C changes due to small changes in w_0, w_1, w_2 .

We need to compute: $$\frac{d\,C}{d\,w_0} \qquad \frac{d\,C}{d\,w_1} \qquad \frac{d\,C}{d\,w_2}$$

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

$$w_0 \leftarrow w_0 - \alpha\frac{d\,C}{d\,w_0} \qquad \underbrace{w_1}_{\text{“new” weight}} \leftarrow \underbrace{w_1}_{\text{“original” weight}} \underbrace{\boxed{- \alpha\frac{d\,C}{d\,w_1}}}_{\text{update}} \qquad w_2 \leftarrow w_2 - \alpha\frac{d\,C}{d\,w_2}$$

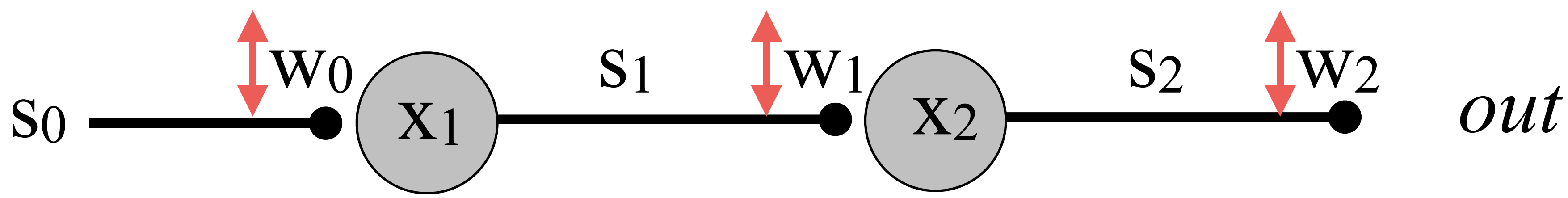
steepest direction of C

Procedure: gradient descent

α = learning rate

Follow the cost function

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



Consider: $$\frac{d\,C}{d\,w_2} = ???$$

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** …

Follow the cost function

Our goal:

$$\frac{d\,C}{d\,w_2} = ???$$

We know C depends on *out*, and *out* depends on w_2 …

$$\frac{d\,C}{d\,w_2} = \frac{d\,C}{d\,\boxed{out}}\,\frac{d\,\boxed{out}}{d\,w_2}$$

We've already solved the first derivative!

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

Slide 8

Let's compute the next derivative …

Follow the cost function

$$\frac{d\,out}{d\,w_2} = ???$$

We know: $out = s_2\, w_2$

So,

$$\frac{d\,out}{d\,w_2} = \frac{d\,(s_2 w_2)}{dw_2} = s_2 \frac{d\,w_2}{dw_2} = \boxed{s_2}$$

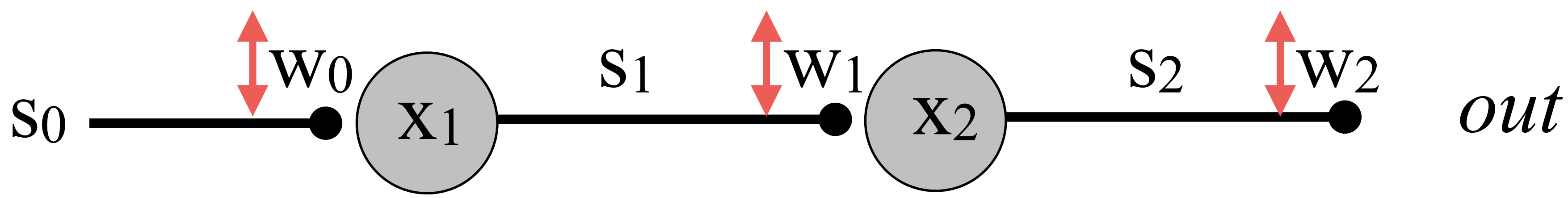
Then,

$$\frac{d\,C}{d\,w_2} = \frac{d\,C}{d\,out} \quad \frac{d\,out}{d\,w_2}$$

$$\boxed{\frac{d\,C}{d\,w_2} = (out - \text{target}) \quad s_2}$$

Follow the cost function

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



We found,

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

How bad we're doing.

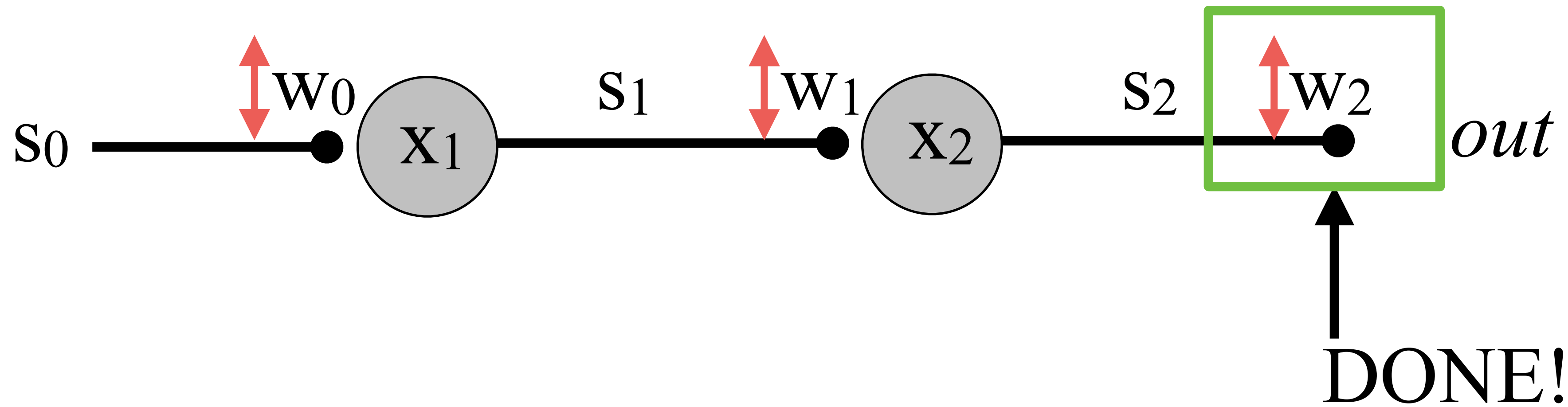
output from x_2

Update the weight w_2:

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

Follow the cost function

So, we've now found an equation to update one of the weights w_2 that acts to minimize the cost function.



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

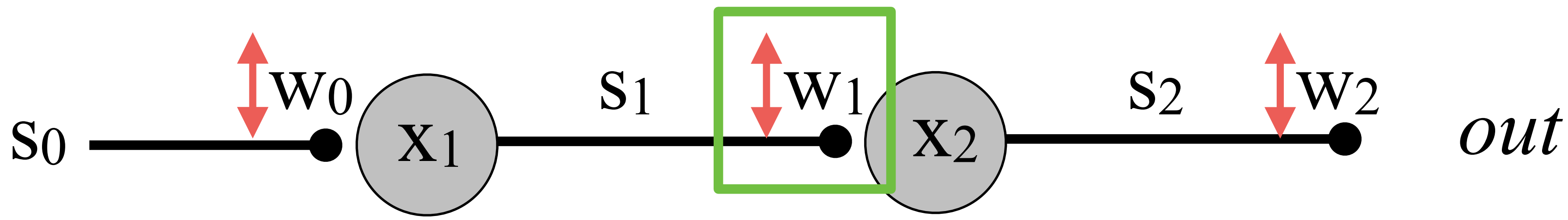
Q: Can we find equations to update w_1 and w_0 ?

A: Yes we can.

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

Follow the cost function

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



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

We don't know this … but can write it using things we do know.

We need the **chain rule**:

$$\frac{dC}{dw_1} = \frac{dC}{d\,out}\frac{d\,out}{dw_1}$$

Follow the cost function

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

$$\frac{d\,C}{d\,w_1} = \frac{d\,C}{d\,out}\,\frac{d\,out}{d\,w_1}$$

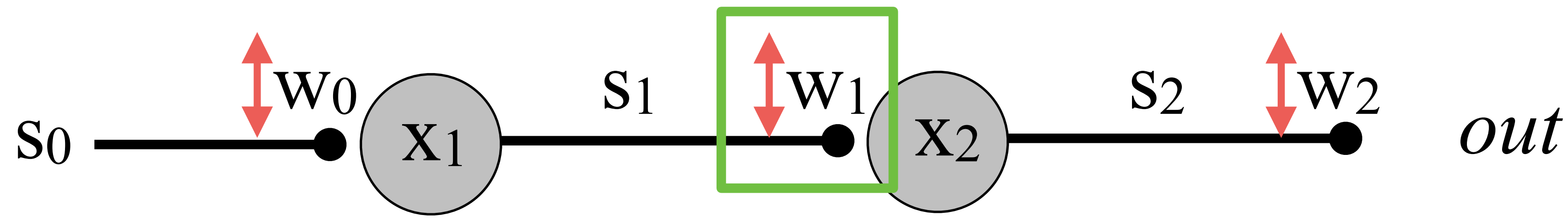
We already found:

$$\frac{dC}{dout} = out - \text{target} \qquad (\textit{Slide 8})$$

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

Follow the cost function

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



We conclude:

$$\frac{dC}{dw_1} = \frac{dC}{d\,out}\,\frac{d\,out}{dw_1}$$

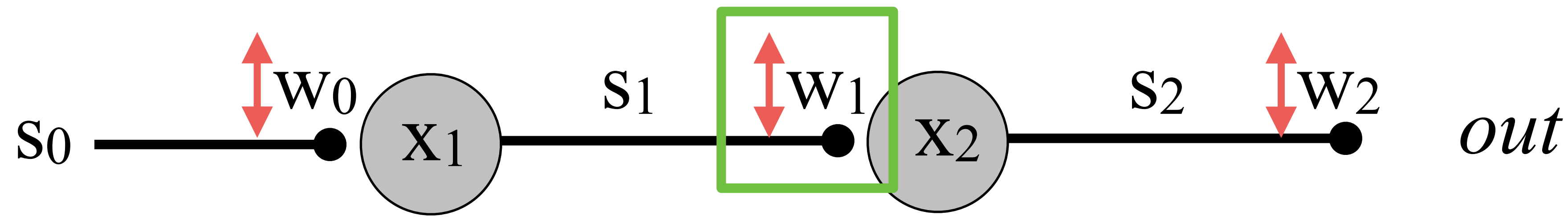
$$\frac{dC}{dw_1} = \boxed{(out - \text{target})}\; w_2\, s_2\, (1 - s_2)\, s_1$$

How bad we're doing.

complicated expression of outputs and weight

Follow the cost function

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



Update the weight w_1:

$$w_1 \leftarrow w_1 - \alpha \boxed{\frac{dC}{dw_1}}$$ substitute in for this!

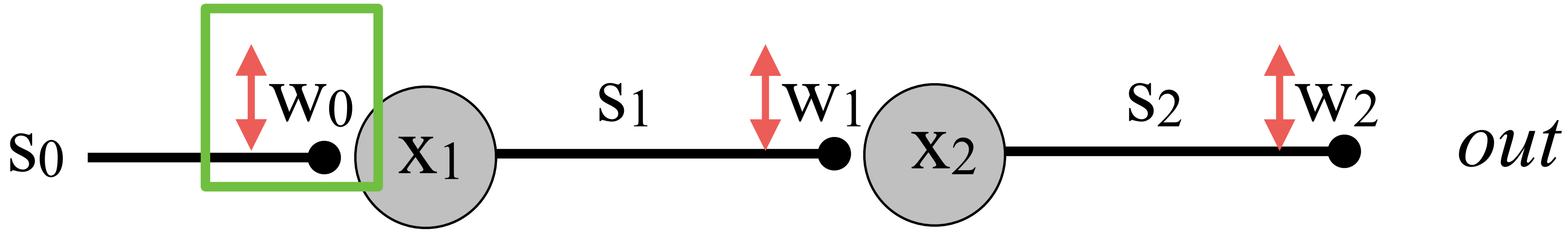
becomes

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

Q: What happens when *out* = target?

Follow the cost function

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

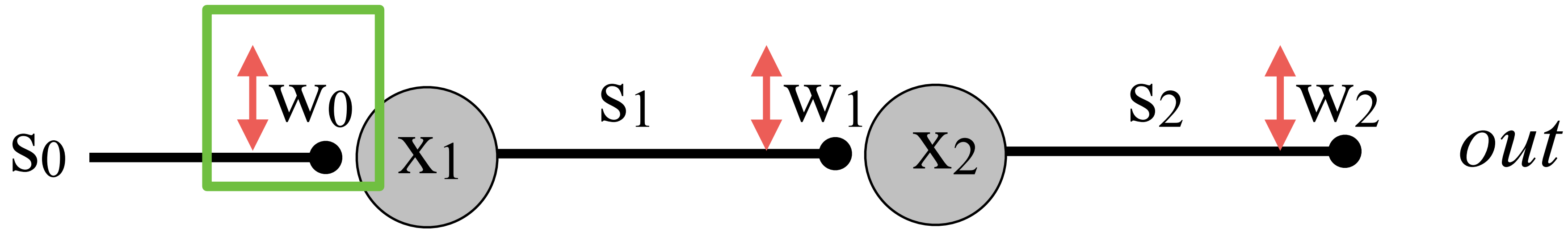


$$\frac{d\,C}{d\,w_0} = \quad ???$$

Try it …

Follow the cost function

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



We conclude:

$$\frac{d\,C}{d\,w_0} = \quad ???$$

and

$$w_0 \leftarrow w_0 - \alpha \frac{d\,C}{d\,w_0}$$ where we need to replace last term …

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.

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

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

$$s_0 \xrightarrow{\textbf{forward propagation}} out$$

Put it all together

Prescription (continued)

3. Update the weights

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

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

$$w_0 \leftarrow w_0 - \alpha(out - \text{target})w_2 s_2(1 - s_2)w_1 s_1(1 - s_1)s_0$$

Note: We know all of the values required

α = learning rate, we choose this.

s_0, s_1, s_2 = calculated during forward propagation

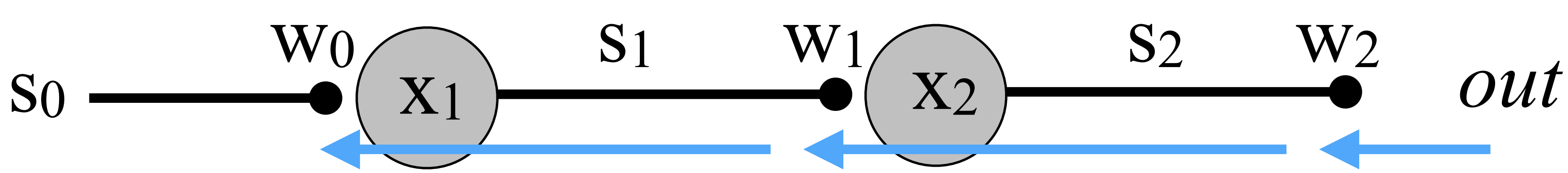
Put it all together

<u>Prescription</u> (continued)

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

or *out* is close enough to target.

This procedure is called **backpropagation**

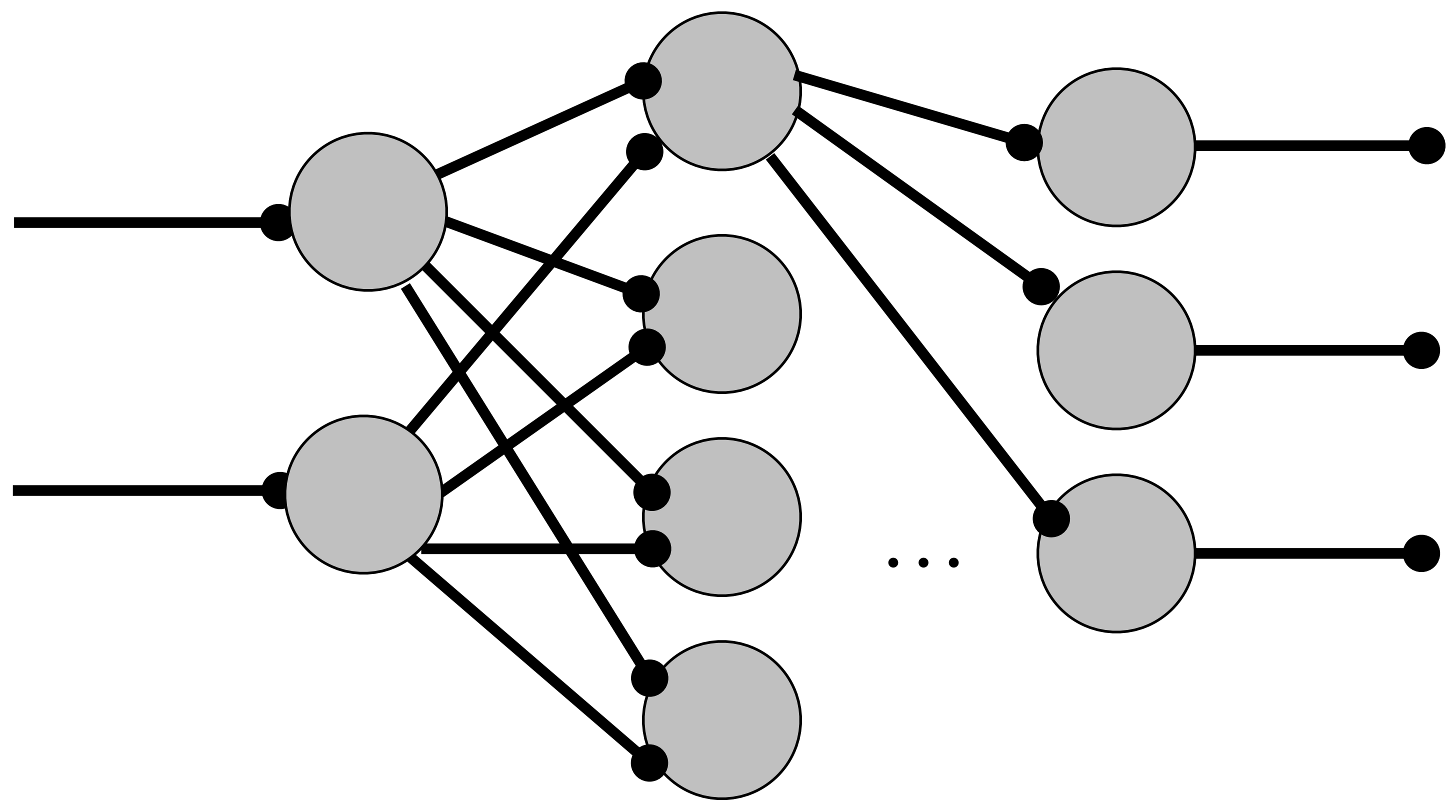


we work "backwards" through our neural network

from *out* to changes in w_2 to changes in w_1 to changes in w_0

Backpropagation

Can evaluate more complicated neural networks



Same ideas apply, but algebra is intense.

Cool example: playground.tensorflow.org

Next time

Implement backpropagation in Python