

Chemical Engineering 4H03

Artificial Neural Networks (ANNs) Deep Learning

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Where are We?

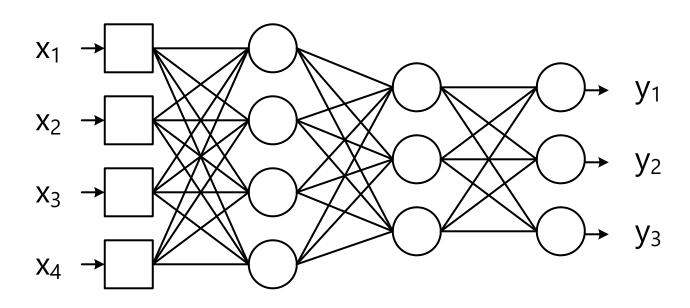
 We have looked at "simple" single-layer ANNs with several input nodes and a single output node

- Where to now?
 - Multiple input AND output nodes
 - Addition of more hidden layers
 - Underlying math and analysis
 - Coded examples
- Where will we end up?
 - Discussion on more advanced deep networks
 - Applications of deep networks (image/speech recognition)



Deep Learning

- Deep Learning is the phrase coined for having multiple hidden layers in an ANN
 - The hidden layers can have any number of nodes
 - Each node in every hidden layer has an activation function



INPUT HIDDEN HIDDEN OUTPUT



Quantifying Activations

 Recall that each layer's output corresponds to the input of the subsequent layer:

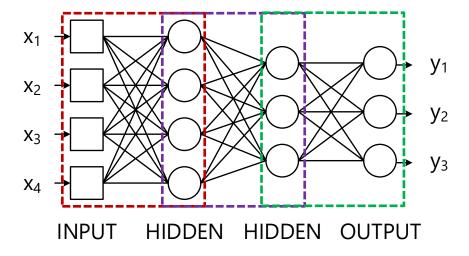
$$\mathbf{y}^{(1)} = \varphi \left(W^{(1)} \mathbf{y}^{(0)} + \mathbf{b}^{(1)} \right)$$

$$\mathbf{y}^{(2)} = \varphi (W^{(2)} \mathbf{y}^{(1)} + \mathbf{b}^{(2)})$$

$$\mathbf{y}^{(3)} = \varphi(W^{(3)}\mathbf{y}^{(2)} + \mathbf{b}^{(3)})$$

Note that $y^{(0)}$ is the OUTPUT of the input layer (layer 0)

Note that $b^{(l)}$ is the BIAS of layer l





Quantifying The First Layer

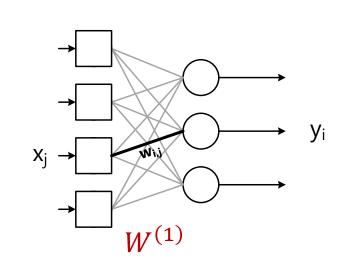
 Recall that each layer's output corresponds to the input of the subsequent layer:

$$\mathbf{y^{(1)}} = \varphi\{\mathbf{v^{(1)}}\}$$
 $\mathbf{v^{(1)}} = W^{(1)}\mathbf{x^{(1)}} + \mathbf{b^{(1)}}$

Note here that each activation function can be applied to each row (or all be the same)

$$\begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \\ y_3^{(1)} \end{bmatrix} = \varphi \left\{ \begin{bmatrix} w_{11}^{(1)} & w_{12}^{(1)} & w_{13}^{(1)} & w_{14}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} & w_{23}^{(1)} & w_{24}^{(1)} \\ w_{31}^{(1)} & w_{32}^{(1)} & w_{33}^{(1)} & w_{34}^{(1)} \end{bmatrix} \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \\ x_3^{(1)} \\ x_4^{(1)} \end{bmatrix} + \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ b_3^{(1)} \end{bmatrix} \right\}$$

$$\begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \\ y_3^{(1)} \end{bmatrix} = \varphi \left\{ \begin{bmatrix} w_{11}^{(1)} & w_{12}^{(1)} & w_{13}^{(1)} & w_{14}^{(1)} \\ w_{21}^{(1)} & w_{22}^{(1)} & w_{23}^{(1)} & w_{24}^{(1)} \\ w_{31}^{(1)} & w_{32}^{(1)} & w_{33}^{(1)} & w_{34}^{(1)} \end{bmatrix} \begin{bmatrix} y_1^{(0)} \\ y_2^{(0)} \\ y_3^{(0)} \\ y_4^{(0)} \end{bmatrix} + \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ b_3^{(1)} \end{bmatrix} \right\}$$





$$\mathbf{y}^{(1)} = \varphi (W^{(1)} \mathbf{y}^{(0)} + \mathbf{b}^{(1)})$$

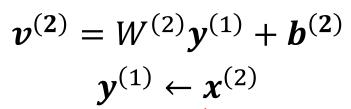
Quantifying The Second Layer

 Recall that each layer's output corresponds to the input of the subsequent layer:

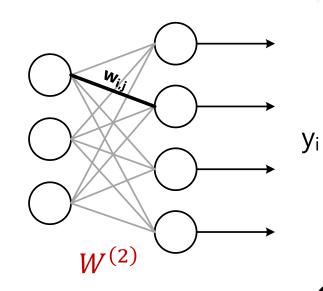
$$\boldsymbol{y^{(2)}} = \boldsymbol{\varphi} \{ \boldsymbol{v}^{(2)} \}$$

$$\begin{bmatrix} y_1^{(2)} \\ y_2^{(2)} \\ y_3^{(2)} \end{bmatrix} = \varphi \left\{ \begin{bmatrix} w_{11}^{(2)} & w_{12}^{(2)} & w_{13}^{(2)} \\ w_{21}^{(2)} & w_{22}^{(2)} & w_{23}^{(2)} \\ w_{31}^{(2)} & w_{32}^{(2)} & w_{33}^{(2)} \\ \dots^{(2)} & \dots^{(2)} & \dots^{(2)} \end{bmatrix} \begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \\ x_3^{(2)} \end{bmatrix} + \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \\ b_3^{(2)} \\ b_3^{(2)} \end{bmatrix} \right\}$$

$$\begin{bmatrix} y_1^{(2)} \\ y_2^{(2)} \\ y_3^{(2)} \end{bmatrix} = \varphi \left\{ \begin{bmatrix} w_{11}^{(2)} & w_{12}^{(2)} & w_{13}^{(2)} \\ w_{21}^{(2)} & w_{22}^{(2)} & w_{23}^{(2)} \\ w_{31}^{(2)} & w_{32}^{(2)} & w_{33}^{(2)} \\ w_{41}^{(2)} & w_{42}^{(2)} & w_{43}^{(2)} \end{bmatrix} \begin{bmatrix} y_1^{(1)} \\ y_2^{(1)} \\ y_3^{(1)} \end{bmatrix} + \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \\ b_3^{(2)} \\ b_4^{(2)} \end{bmatrix} \right\}$$



Just consider the output from layer 1 as the input to layer 2!





$$\mathbf{y}^{(2)} = \varphi(W^{(2)}\mathbf{y}^{(1)} + \mathbf{b}^{(2)})$$

Quantifying The _____ Layer

- And so on
- SO our method of training each layer using the delta rule can be applied to all layers of the network sequentially!
 - One question though... We only have the error ϵ for the output layer, so how do we relate that to the hidden layers?
 - We **KNOW** that the inputs to layer l can be influenced by weights in layer (l-1), but what "should" those weights be?
 - We don't know if we don't know the desired inputs!
- Our strategy is actually quite simple we will treat the outputs of each layer as the inputs to the next!



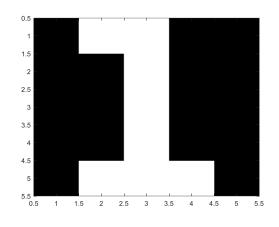


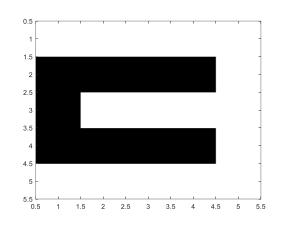
Training Deep Networks

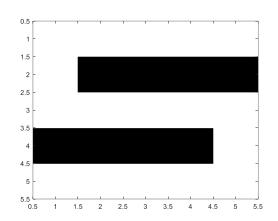
Here's Hoping you can FATHOM it

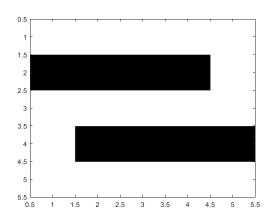
A MOTIVATING EXAMPLE

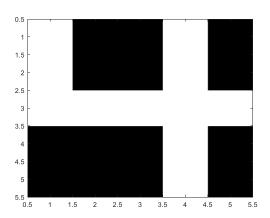
• Consider the following five digital digits (1...5)













A MOTIVATING EXAMPLE

• As matrices, they are 5×5 matrices of 0 or 1:

0	1	1	0	0
0	0	1	0	0
0	0	1	0	0
0	0	1	0	0
0	1	1	1	0

1	1	1	1	1
0	0	0	0	1
0	1	1	1	1
0	0	0	0	1
1	1	1	1	1

1	1	1	1	1
1	0	0	0	0
1	1	1	1	1
0	0	0	0	1
1	1	1	1	1

1	1	1	1	1
0	0	0	0	1
1	1	1	1	1
1	0	0	0	0
1	1	1	1	1

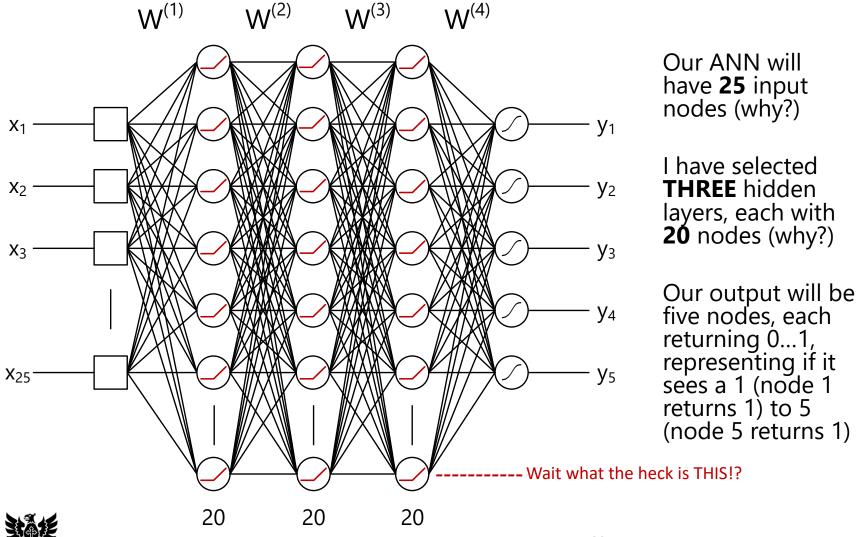
1	0	0	1	0
1	0	0	1	0
1	1	1	1	1
0	0	0	1	0
0	0	0	1	0



4HU3_ANN_INTro

A MOTIVATING EXAMPLE

We desire to train a deep ANN that recognizes these digits



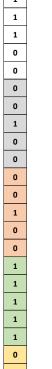
We'll need some tools...

- All ANNs require a "vector" of inputs x
 - Our 25-pixel image is not going to work
 - However, we can **unpack** the image into one vector!

"1"

0	1	1	0	0
0	0	1	0	0
0	0	1	0	0
0	0	1	0	0
0	1	1	1	0

U	
0	
0	
0	
0	
1	
0	
0	
0	
1	
1	
1	
1	
1	
1	
0	
0	
0	
0	
1	
0	
0	
0	
0	



11	4	<i> </i>

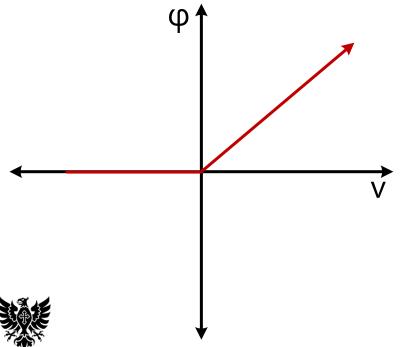
1	0	0	1	0
1	0	0	1	0
1	1	1	1	1
0	0	0	1	0
0	0	0	1	0



4H03 ANN Intro

We'll need some tools...

- We have a new activation function
 - Deep networks tend to behave nicely with the ReLU function
 - ReLU is for "Rectified Linear Unit"
 - ReLU has been shown to aid in passing errors backwards through the ANN
 - Sigmoids (for example) "diminish" the effects of hidden layers, thus preventing the ANN from exploiting the full value of hidden layers



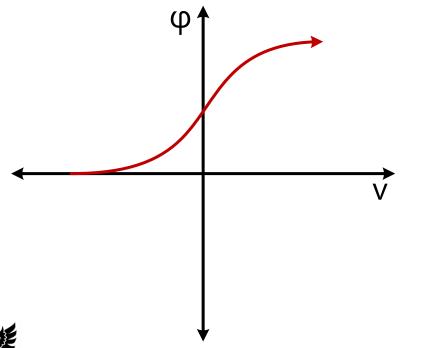
$$\varphi(v) = \begin{cases} 0; & v \le 0 \\ v; & v > 0 \end{cases}$$

$$\varphi'(v) = \begin{cases} 0; & v \le 0 \\ 1; & v > 0 \end{cases}$$



We'll need some tools...

- We have a new output activation function
 - Classification networks (such as this one) tend to use the softmax function
 - Softmax is a logistical function similar to sigmoid
 - Weights probabilities so that the total probability is 1.0



Here, ${m v}$ needs to be a vector, as opposed to the sigmoid which has its own value

$$\varphi(v_i) = \frac{e^{v_i}}{\sum_k e^{v_k}}$$



Back Propagation Procedure

- Back propagation begins with computing the OUTPUT of the ANN given initial guesses for weights $W^{(1)} \dots W^{(L)}$
 - Note that I am assuming we have L layers here (including the output)
 - In our example, we have L=4 layers
- 1. Initialize the weights $W^{(1)} \dots W^{(L)}$
- 2. In a loop, until convergence
 - 1. FOR all data points x
 - 1. Compute the ANN output \hat{y} through all layers
 - 2. FOR each layer $L \dots l \dots 1$ in the ANN (working **backwards**)
 - 1. Compute the error $\epsilon^{(l)}$
 - 2. Compute $\boldsymbol{\delta}^{(l)}$
 - 3. Propagate error backwards to $\epsilon^{(l-1)}$
 - 3. Adjust all weights
 - 2. Check for convergence of $W^{(1)} \dots W^{(L)}$
 - 3. Return to (2.1)



Back-Propagation Algorithm

- 1. Initialize the weights
 - Most people use a normally distributed random number between 0 and 1



Back-Propagation Algorithm

- In a loop (for each epoch):
 - 1. In a loop (for each point):
 - 1. In a loop (for each layer l from $1 \dots L$)

There's the input to each layer from the ANN

2. In a loop (for each layer l from $L \dots 1$)

- IF
$$l=L$$

» $\boldsymbol{\epsilon}^{(L)}=\mathbf{y}-\mathbf{y}^{(L)}$
» $\boldsymbol{\delta}^{(L)}=\varphi'(\boldsymbol{v}(L))\boldsymbol{\epsilon}^{(L)}$

ELSE

»
$$\boldsymbol{\epsilon}^{(l)} = \left(W^{(l+1)}\right)^T \boldsymbol{\delta}^{(l+1)}$$
 ----- BACK PROPAGATION » $\boldsymbol{\delta}^{(l)} = \varphi'(v(l))\boldsymbol{\epsilon}^{(l)}$

3. Update $W^{(l)} \leftarrow W^{(l)} + \alpha \delta^{(l)} (y^{(l-1)})^T$ ----- UPDATE

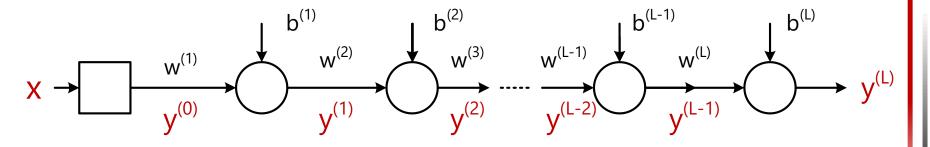




Derivation of Back Propagation

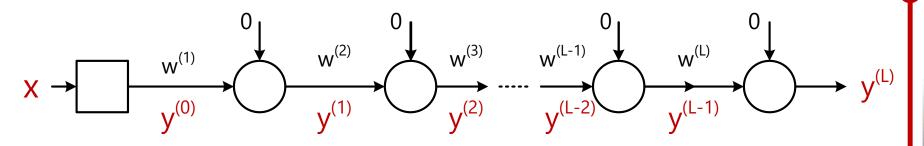
Episode VI: Return of the Chain Rule

To see how back-propagation works, consider this ANN



- We are going to make a couple of assumptions...
 - The biases for each node exist for now (removed later)
 - Each layer only has one node (relaxed later)
- What is our objective?
 - To minimize the error between $y^{(L)}$ and y





- Let's assign an error function that accepts an input
 - For the sake of argument, let's consider the SSE

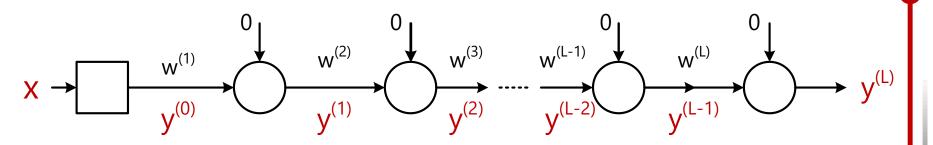
$$\mathcal{E} = \frac{1}{2} \left(y^{(L)} - y \right)^2$$

• We know that $v^{(L)}$ and $y^{(L)}$ are:

$$v^{(L)} = w^{(L)}y^{(L-1)} + b^{(L)}$$

$$y^{(L)} = \varphi(v^{(L)})$$





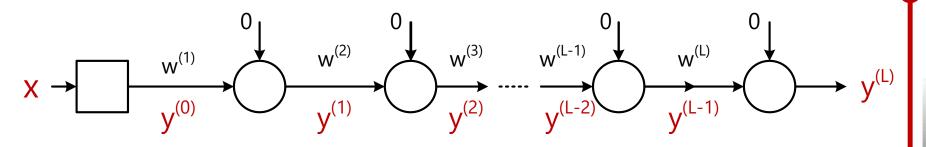
- We want to ask ourselves, what is the derivative of \mathcal{E} with respect to our decision variables?
- Recall these decisions are $w^{(L)}$, $b^{(L)}$ and $y^{(L-1)}$

$$\frac{\partial \mathcal{E}}{\partial w^{(L)}} = \frac{\partial \mathcal{E}}{\partial y^{(L)}} \cdot \frac{\partial y^{(L)}}{\partial v^{(L)}} \cdot \frac{\partial v^{(L)}}{\partial w^{(L)}}$$

For those of us that might not remember, this is the fundamental application of the chain rule

So, now we just need to figure out each piece!





•
$$\frac{\partial \mathcal{E}}{\partial y^{(L)}} = \frac{\partial}{\partial y^{(L)}} \left\{ \frac{1}{2} \left(y^{(L)} - y \right)^2 \right\} = \left(y^{(L)} - y \right)$$

•
$$\frac{\partial y^{(L)}}{\partial v^{(L)}} = \frac{\partial}{\partial v^{(L)}} \{ \varphi(v^{(L)}) \}$$
 $= \varphi'(v^{(L)})$

•
$$\frac{\partial v^{(L)}}{\partial w^{(L)}} = \frac{\partial}{\partial w^{(L)}} \{ w^{(L)} y^{(L-1)} + b^{(L)} \} = y^{(L-1)}$$

$$\frac{\partial \mathcal{E}}{\partial w^{(L)}} = (y^{(L)} - y) \cdot \varphi'(v^{(L)}) \cdot y^{(L-1)}$$



• Moreover, we can do the same thing wrt $b^{(L)}$

$$\frac{\partial \mathcal{E}}{\partial b^{(L)}} = \frac{\partial \mathcal{E}}{\partial y^{(L)}} \cdot \frac{\partial y^{(L)}}{\partial v^{(L)}} \cdot \frac{\partial v^{(L)}}{\partial b^{(L)}}$$

$$\frac{\partial \mathcal{E}}{\partial h^{(L)}} = (y^{(L)} - y) \cdot \varphi'(v^{(L)}) \cdot \mathbf{1}$$



• One more time, we can do the same thing wrt $y^{(L-1)}$

$$\frac{\partial \mathcal{E}}{\partial b^{(L)}} = \frac{\partial \mathcal{E}}{\partial y^{(L)}} \cdot \frac{\partial y^{(L)}}{\partial v^{(L)}} \cdot \frac{\partial v^{(L)}}{\partial y^{(L-1)}}$$

•
$$\frac{\partial \mathcal{E}}{\partial y^{(L)}} = \frac{\partial}{\partial y^{(L)}} \left\{ \frac{1}{2} \left(y^{(L)} - y \right)^2 \right\} = \left(y^{(L)} - y \right)$$

•
$$\frac{\partial y^{(L)}}{\partial v^{(L)}} = \frac{\partial}{\partial v^{(L)}} \{ \varphi(v^{(L)}) \}$$
 $= \varphi'(v^{(L)})$

•
$$\frac{\partial v^{(L)}}{\partial v^{(L-1)}} = \frac{\partial}{\partial v^{(L-1)}} \{ w^{(L)} y^{(L-1)} + b^{(L)} \} = w^{(L)}$$

$$\frac{\partial \mathcal{E}}{\partial v^{(L-1)}} = (y^{(L)} - y) \cdot \varphi'(v^{(L)}) \cdot \mathbf{w}^{(L)}$$



Some Remarks

Our three derivatives should make a great deal of sense

$$-\frac{\partial \mathcal{E}}{\partial w^{(L)}} = (y^{(L)} - y) \cdot \varphi'(v^{(L)}) \cdot y^{(L-1)}$$

• The rate of change of the error *wrt* each weight is proportional to the input to layer *L*

$$-\frac{\partial \mathcal{E}}{\partial h^{(L)}} = (y^{(L)} - y) \cdot \varphi'(v^{(L)}) \cdot \mathbf{1}$$

• The rate of change of the error is unit-proportional to the bias in layer *L*. In other words, it only depends on how the activation function changes *w.r.t*. the input

$$- \frac{\partial \mathcal{E}}{\partial y^{(L-1)}} = (y^{(L)} - y) \cdot \varphi'(v^{(L)}) \cdot \mathbf{w}^{(L)}$$

• The rate of change of the error wrt the input to the layer is proportional to weights in layer L. This means that inputs connected to nodes with higher weights will impact $\mathcal E$ more. This is the fundamental relationship for back propagation.



Let's Generalize

- First of all, let's note that what we just did was for a **single output instance**, whereas there could be many!
 - We just have to express $\mathcal E$ as the sum of those errors:

$$\mathcal{E} = \sum_{i=1}^{I} \frac{1}{2} \left(y_i^{(L)} - y_i \right)^2$$

- Next, let's recognize that the bias term can also be treated as the output of an activation node with an output of $\varphi(\cdot) = 1$
 - Thus, the biases will get their own weight w

$$\frac{\partial \mathcal{E}}{\partial h^{(L)}} = (y^{(L)} - y) \cdot \varphi'(v^{(L)}) \cdot \mathbf{0} = 0$$



Let's Generalize

• Next, recognize that if you have multiple inputs to a given node, you need to take the derivative wrt each of the weights $w_{i,j}$

$$\frac{\partial \mathcal{E}}{\partial w_{i,j}^{(L)}} = \frac{\partial \mathcal{E}}{\partial y_i^{(L)}} \cdot \frac{\partial y_i^{(L)}}{\partial v_i^{(L)}} \cdot \frac{\partial v_i^{(L)}}{\partial w_{i,j}^{(L)}}$$

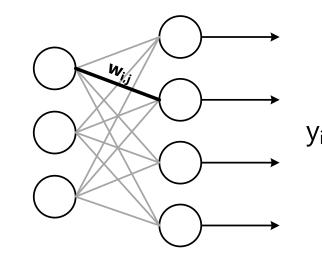
I'll remind you that $\frac{\partial y_i^{(L)}}{\partial v_i^{(L)}} = \varphi'(v_i)$

- Finally, let's make a sneaky notation change and use $\delta_i^{(L)} \triangleq \frac{\partial \mathcal{E}}{\partial v_i^{(L)}} = \frac{\partial \mathcal{E}}{\partial y_i^{(L)}} \cdot \frac{\partial y_i^{(L)}}{\partial v_i^{(L)}}$
- So NOWWWW I can write

$$\frac{\partial \mathcal{E}}{\partial w_{i,j}^{(L)}} = \delta_i^{(L)} \cdot y_j^{(L-1)}$$

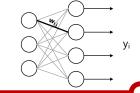
• That's for the FINAL layer, to let's make one more jump and refer to layer $\it l$ instead

$$\frac{\partial \mathcal{E}}{\partial w_{i,j}^{(l)}} = \delta_i^{(l)} \cdot y_j^{(l-1)}$$





Now Apply It to Layer L



WHEW. OK. That was fun! Let's see it work...

• Recall
$$\mathcal{E} = \sum_{i=1}^{I} \frac{1}{2} \left(y_i^{(L)} - y_i \right)^2$$

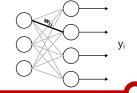
•
$$\delta_i^{(L)} \triangleq \frac{\partial \mathcal{E}}{\partial v_i^{(L)}} = \frac{\partial \mathcal{E}}{\partial y_i^{(L)}} \cdot \frac{\partial y_i^{(L)}}{\partial v_i^{(L)}} = \left(y_i^{(L)} - y_i\right) \cdot \varphi'\left(v_i^{(L)}\right)$$

•
$$\frac{\partial \mathcal{E}}{\partial w_{i,i}^{(L)}} = \delta_i^{(L)} \cdot y_j^{(L-1)}$$

... Not so bad.



Now Apply It to Layer L-1



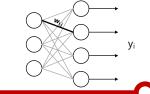
- Easy enough for the first layer since $\frac{\partial \mathcal{E}}{\partial y_i^{(L)}}$ is easy. But what about δ_i^{L-1} ?
 - Note this is a bit annoying but the indices of the input/output nodes are swapped here to represent i as the "current" layer. This makes way more sense in vector form. We'll get there in a second

•
$$\delta_i^{(L-1)} \triangleq \frac{\partial \mathcal{E}}{\partial v_i^{(L-1)}} = \frac{\partial y_i^{(L-1)}}{\partial v_i^{(L-1)}} \cdot \frac{\partial \mathcal{E}}{\partial y_i^{(L-1)}} = \varphi'\left(v_i^{(L-1)}\right) \cdot \sum_j w_{j,i}^{(L)} \delta_j^{(L)}$$

•
$$\frac{\partial \mathcal{E}}{\partial w_{i,j}^{(L-1)}} = \delta_i^{(L-1)} \cdot y_j^{(L-2)}$$



And in General...



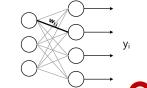
• In general, we can compute $\frac{\partial \mathcal{E}}{\partial y_i^{(l)}}$ as:

•
$$\delta_i^{(l)} \triangleq \frac{\partial \mathcal{E}}{\partial v_i^{(l)}} = \frac{\partial y_i^{(l)}}{\partial v_i^{(l)}} \cdot \frac{\partial \mathcal{E}}{\partial y_i^{(l)}} = \varphi'\left(v_i^{(l)}\right) \cdot \sum_j w_{j,i}^{(l+1)} \delta_j^{(l+1)}$$

$$\bullet \ \frac{\partial \mathcal{E}}{\partial w_{i,i}^{(l)}} = \delta_i^{(l)} \cdot y_j^{(l-1)}$$



As Vectors...



 IMO it is WAY easier to think of this using vectors and weight matrices for each layer:

•
$$\boldsymbol{\delta}^{(l)} \triangleq \nabla \mathcal{E}_{\boldsymbol{v}^{(l)}} = \nabla y_{\boldsymbol{v}^{(l)}}^{(l)} \cdot \nabla \mathcal{E}_{\boldsymbol{v}^{(l)}}^{(l)}$$

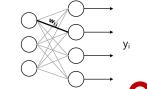
•
$$\boldsymbol{\delta}^{(l)} = \varphi'(\boldsymbol{v}^{(l)}) \cdot (W^{(l+1)})^T \delta^{(l+1)}$$

•
$$\frac{\partial \mathcal{E}}{\partial w^{(l)}} = \boldsymbol{\delta}^{(l)} \cdot \left(\boldsymbol{y}^{(l-1)} \right)^T$$

- And THIS is the equation we use in our algorithm!
 - It will always work since we always have $\boldsymbol{\delta}^{(l+1)}$ \odot



Annnnd Done!



Now you just have to do that for all points!

- Once you are finished calculating $\frac{\partial \mathcal{E}}{\partial W^{(l)}}$, you can assume you are using a straight-up gradient search and consider this $\Delta W^{(l)}$ and update the weights
 - Note that you can update W every point (SGF) or take batches
 - ALSO note that this is why the training regimen is known as a modification of the *gradient search*. Each expression for $\frac{\partial \mathcal{E}}{\partial W^{(l)}}$ is in fact the gradient of the ERROR *wrt* every entry in $W^{(l)}$
 - We can use other optimization methods now, too! Since we know how to compute the gradient



Back Propagation Algorithm Again

- 2. In a loop (for each epoch):
 - 1. In a loop (for each point):
 - 1. In a loop (for each layer l from $1 \dots L$)

$$- v^{(l)} = W^{(l)}y^{(l-1)} + b^{(l)}$$

$$- \qquad \mathbf{y}^{(l)} = \varphi\{\mathbf{v}^{(l)}\}$$

2. In a loop (for each layer l from $L \dots 1$)

- IF
$$l = L$$

$$\epsilon^{(L)} = \mathbf{y} - \mathbf{y}^{(L)}$$

»
$$\boldsymbol{\delta}^{(L)} = \varphi'(\boldsymbol{v}^{(L)})\boldsymbol{\epsilon}^{(L)} = \varphi'(\boldsymbol{v}^{(L)})(\boldsymbol{y} - \boldsymbol{y}^{(L)})$$

ELSE

$$\boldsymbol{\epsilon}^{(l)} = \left(W^{(l+1)}\right)^T \boldsymbol{\delta}^{(l+1)}$$

»
$$\boldsymbol{\delta}^{(l)} = \varphi'(\boldsymbol{v}^{(l)})\boldsymbol{\epsilon}^{(l)} = \varphi'(\boldsymbol{v}^{(l)})(W^{(l+1)})^T\boldsymbol{\delta}^{(l+1)}$$

3. Update
$$W^{(l)} \leftarrow W^{(l)} + \alpha \delta^{(l)} (y^{(l-1)})^T$$

Now we can fundamentally see how this works!



Final Remarks

- And that, friends, is how you train your deep ANN!
- Key takeaways
 - Calculus can be used to relate changing inner weights to the objective function through chain rule
 - Only has to be done one layer at a time
 - First layer can be calculated directly
 - Vector/Matrix math should always be used for simplicity
- Motivating example
 - Completed in MATLAB!!

