Lecture#7

Artificial Neural Networks

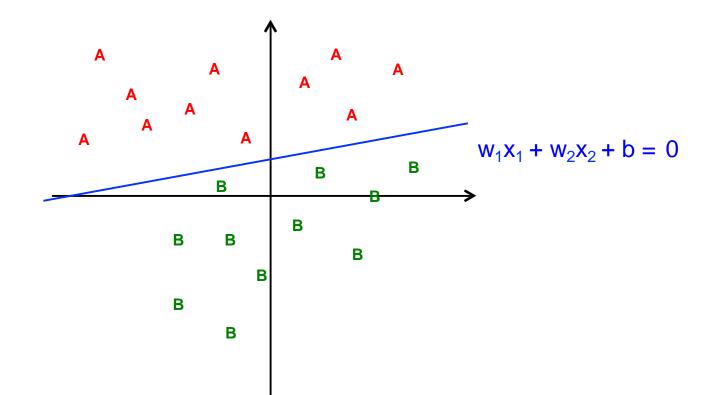
Linear Classifier

- We will begin by implementing a linear classifier
- It will have two major components:
- A score function that maps the data to categories
- A loss function that calculates the difference between predicted categories and actual categories in the dataset
- The loss function will be used for training the classifier

• We have a linear function:

 $w_1x_1 + w_2x_2 + \ldots + w_nx_n + b = 0$

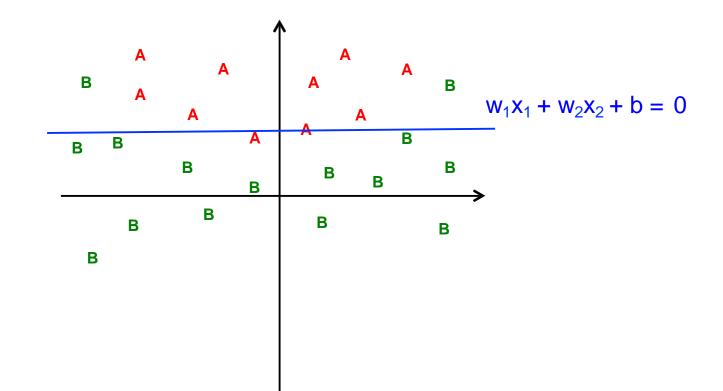
- X is the input data, with one value x_i for each attribute
- Each attribute is multiplied by a weight wi
- And finally a bias **b** is added
 - So the linear function doesn't have to cross the origin
- The linear function is used to separate categories:



Linear Separation

- As the name implies, the linear classificer can only separate linearly separable categories
- It will never be 100% accurate if we have a dataset that looks like this:

Linear Separation



• If we calculate the score function:

 $w_1 x_1 + w_2 x_2 + \ldots + w_n x_n + b = 0$

- ... for an instance we see the confidence that the example belongs to the category
 - Higher values = more confidence
- This is our score function!
- What if we have more than one category?

Mutiple Categories

 If we have two or more categories, we need one linear function for each category:

```
w_{11}x_{11} + w_{12}x_{12} + \ldots + w_{1n}x_{1n} + b_1 = 0

w_{21}x_{21} + w_{22}x_{22} + \ldots + w_{2n}x_{2n} + b_2 = 0

\ldots

w_{k1}x_{k1} + w_{k2}x_{k2} + \ldots + w_{kn}x_{kn} + b_k = 0
```

• The most efficient way to calculate the score function is to use matrix/vector operations:

• The weights can be seen as a matrix:

$$oldsymbol{W} = egin{bmatrix} w_{11} & w_{12} & w_{13} & \dots & w_{1n} \ w_{21} & w_{22} & w_{23} & \dots & w_{2n} \ \dots & & & & \ \dots & & & & \ w_{k1} & w_{k2} & w_{k3} & \dots & w_{kn} \end{bmatrix}$$

• ... and the bias and example as column vectors:

$$oldsymbol{b} = egin{bmatrix} b_1 \ b_2 \ \dots \ b_k \end{bmatrix} \qquad oldsymbol{x_i} = egin{bmatrix} x_1 \ x_2 \ \dots \ x_n \end{bmatrix}$$

• Calculating the score function is then a matrix-vector multiplication plus addition:

 $f(\boldsymbol{x_i}, \boldsymbol{W}, \boldsymbol{b}) = \boldsymbol{W} \boldsymbol{x_i} + \boldsymbol{b}$

- This produces a vector with one confidence value for each category
- The example is classified as the category with the highest confidence:

 $y_{pred} = argmax(scores)$

How it works

• Assume we have two categories and three inputs:

$$oldsymbol{W} oldsymbol{x}_{oldsymbol{i}} = egin{bmatrix} w_{11} & w_{12} & w_{13} \ w_{21} & w_{22} & w_{23} \end{bmatrix} egin{bmatrix} x_1 \ x_2 \ x_3 \end{bmatrix} = egin{bmatrix} w_{11} x_1 + w_{12} x_2 + w_{13} x_3 \ w_{21} x_1 + w_{22} x_2 + w_{23} x_3 \end{bmatrix}$$

• ... and with the bias vector:

$$oldsymbol{W}oldsymbol{x_i} + oldsymbol{b} = egin{bmatrix} w_{11}x_1 + w_{12}x_2 + w_{13}x_3 \ w_{21}x_1 + w_{22}x_2 + w_{23}x_3 \end{bmatrix} + egin{bmatrix} b_1 \ b_2 \end{bmatrix} = egin{bmatrix} w_{11}x_1 + w_{12}x_2 + w_{13}x_3 + b_1 \ w_{21}x_1 + w_{22}x_2 + w_{23}x_3 + b_2 \end{bmatrix}$$

- This is actually the dot-product of \mathbf{x}_i with each row in \mathbf{W}
- Number of columns in \boldsymbol{W} must be equal to the number of components in \boldsymbol{x}_i

How it works

- We don't even need to split the input data X into columns
- When calculating a product between matrices **W** and **X**, we can see **X** as a bunch of lined up column vectors:

$$oldsymbol{WX} = egin{bmatrix} w_{11} & w_{12} & w_{13} \ w_{21} & w_{22} & w_{23} \end{bmatrix} egin{bmatrix} x_{11} \ x_{12} \ x_{13} \end{bmatrix} egin{bmatrix} x_{21} \ x_{22} \ x_{23} \end{bmatrix}$$

• This results in a new matrix:

$$oldsymbol{WX} = egin{bmatrix} w_{11}x_{11}+w_{12}x_{12}+w_{13}x_{13} & w_{11}x_{21}+w_{12}x_{22}+w_{13}x_{23} \ w_{21}x_{11}+w_{22}x_{12}+w_{23}x_{13} & w_{21}x_{21}+w_{22}x_{22}+w_{23}x_{23} \end{bmatrix}$$

How it works

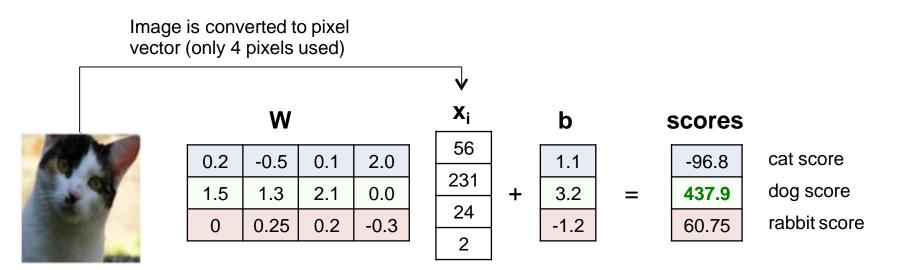
• The bias vector **b** is then added to each column:

 $oldsymbol{WX} + oldsymbol{b} = egin{bmatrix} w_{11}x_{11} + w_{12}x_{12} + w_{13}x_{13} + b_1 & w_{11}x_{21} + w_{12}x_{22} + w_{13}x_{23} + b_1 \ w_{21}x_{11} + w_{22}x_{12} + w_{23}x_{13} + b_2 & w_{21}x_{21} + w_{22}x_{22} + w_{23}x_{23} + b_2 \end{bmatrix}$

- Now we have a matrix where each column is a score vector for an example x_i in X
- Taking *argmax* for each column produces a row vector with the predicted category for each example:

 $Y_{pred} = \begin{bmatrix} argmax(scores_1) & argmax(scores_2) \end{bmatrix}$

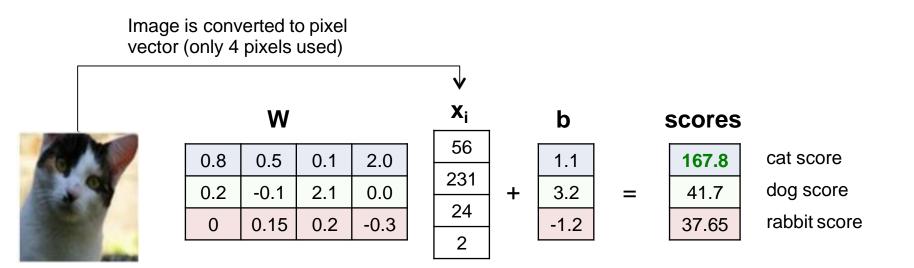
Simple example



This is clearly a dog...

The weights need to be modified (learned) to produce correct output!

Simple example



Now we get correct output!

How can we automatically learn weights from training data?

Loss Function

Loss Function

- First, we need to define a loss function
 - Sometimes called cost function or objective
- The loss function measures how happy we are with the result
- The first set of weights gave a poor prediction we are not happy
- The second set of weights gave a good prediction we are happy!
- The loss will be high for bad predictions, and low for good predictions
- There are many loss functions, but we will focus on Softmax

Softmax

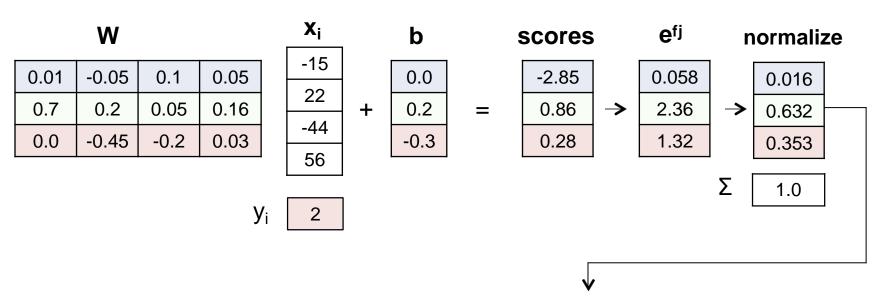
- Softmax calculates the normalized probabilities for belonging to each category
- This is then combined to a single loss value: crossentropy loss

Softmax

• The loss L_i is calculated as:

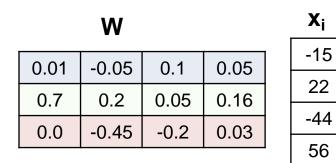
$$L_i = -log\left(rac{e^{f_{yi}}}{\sum_j e^{f_j}}
ight)$$

- We calculate the log probability for the correct category e^{fyi} and normalize by dividing with the sum of log probabilities for all categories
- Finally we calculate the negative natural logarithm of the normalized log probability for the correct class



loss = -log(0.353) = 1.04

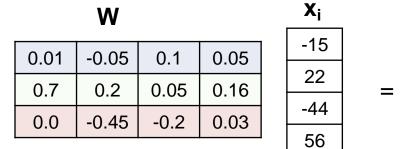
Matrix Multiplication



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	_	-

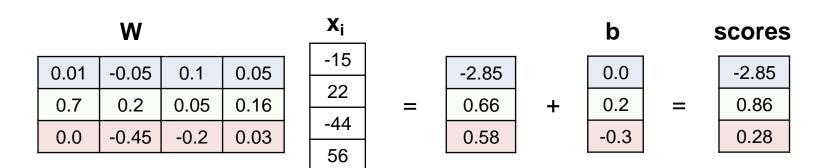
= dot-product of row 1 in W and column X_i
= dot-product of row 2 in W and column X_i
= dot-product of row 3 in W and column X_i

Matrix Multiplication



= 0.01 * -15 - 0.05 * 22 + 0.1 * -44 + 0.05 * 56 = -2.85
= 0.7 * -15 + 0.2 * 22 + 0.05 * -44 + 0.16 * 56 = 0.66
= 0 * -15 - 0.45 * 22 - 0.2 * -44 + 0.03 * 56 = 0.58

Matrix Addition



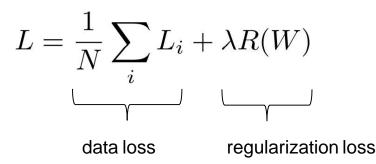
Simply add each element of vector **b**

Numerical Stability

- If we have very high scores, calculating e^{fj} and then sum all the values can lead to numerical problems
- The sum can blowup, i.e. we get outside the range of *double*
- This can be solved by shifting all scores so that the highest score is 0:
 - Find max(scores)
 - Subtract max(scores) for each score

Regularization

- Suppose we have a perfect set of weights: loss = 0.0
- The problem is that this set might not be unique!
- There can be multiple sets of weights that give the same loss
- To distinct between two such sets, we extend the loss function with a regularization penalty:



Regularization

- The most common one is the L2 norm, which penalizes large weights
 - Large weights can lead to numerical overflow...
 - Small weights improve generalization and reduces overflow
- The L2 norm is calculated as the squared sum of all weights:

$$R(W) = \sum_k \sum_l w_{k,l}^2$$

• The lambda parameter is called the regularization strength, and is typically set to a low value such as 0.01

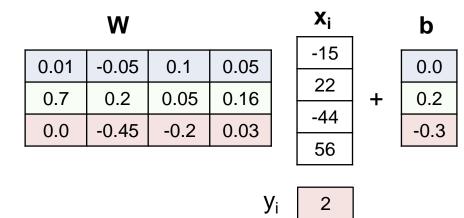


Squared W

0.01	-0.05	0.1	0.05	
0.7	0.2	0.05	0.16	→
0.0	-0.45	-0.2	0.03	

0.0001	0.0025	0.01	0.0025	
0.49	0.04	0.0025	0.0256	
0.0	0.2025	0.04	0.0009	

L2 norm = sum of all squared W = 0.8166

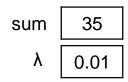


Loss = Data loss + regularization loss = 1.04 + 0.01 * 0.8166 = 1.048

W		b
1.00	2.00	0.00
2.00	-4.00	0.50
3.00	-1.00	-0.50

Squared W

1.0	4.0
4.0	16.0
9.0	1.0



Χ		
0.50	0.40	
0.80	0.30	
0.30	0.80	
-0.40	0.30	
-0.30	0.70	
-0.70	0.20	
0.70	-0.40	
0.50	-0.60	
-0.40	-0.50	

У	score	es
0	1.30	-
0	1.40	
0	1.90	-
1	0.20	-
1	1.10	-
1	-0.30	-
2	-0.10	
2	-0.70	
2	-1.40	

1.30	-0.10	0.60
1.40	0.90	1.60
1.90	-2.10	-0.40
0.20	-1.50	-2.00
1.10	-2.90	-2.10
-0.30	-1.70	-2.80
-0.10	3.50	2.00
-0.70	3.90	1.60
-1.40	1.70	-1.20

L

0.56
1.04
0.11
1.96
4.06
1.68
1.72
2.40
3.00

Data loss:	1.84
Regularization loss:	0.35
Total loss:	2.19

1.84 mean

Optimization

Optimization

- The loss function quantifies the quality of a set of weights
- The goal of optimization, or learning, is to find a set of weights that minimizes the loss function
- This can of course be done with random search or hill climbing, but it will most likely take ages to find a good set of weights
- Instead we can compute the best direction using the gradient of the loss function!

Gradient

- The task is to computer the best direction in which we should change the weights
- This direction turns out to be related to the gradient of the loss function
- The gradient is a vector of slopes (derivatives) for each dimension in the input space
- Mathematically, the derivative of a 1-D function with respect to its (single) input is:

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

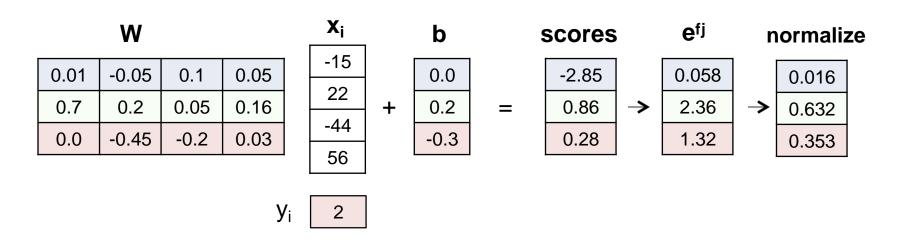
Gradient

- If we have a function that takes a vector of numbers instead of a single number, the derivatives are called partial derivatives
- The gradient is simply the vector of partial derivatives in each input dimension
- We can do this in two ways:
 - Numerical gradient: slow and approximate
 - Analytic gradient: fast and exact but error-prone
- Since speed is important, we will focus on the analytic gradient

Analytic Gradient

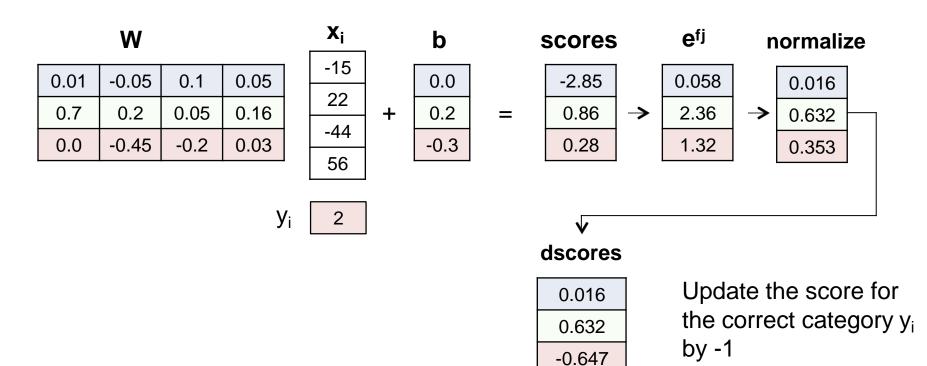
- To find the analytic gradient, we need to derive a formula for the gradient using our math skills
- Luckily, the loss functions we use are well known and we don't have to find the formula on our own
- Depending on the loss function, the formula can be quite complex to implement
- How can we implement the gradients formula for Softmax?

Softmax Gradients

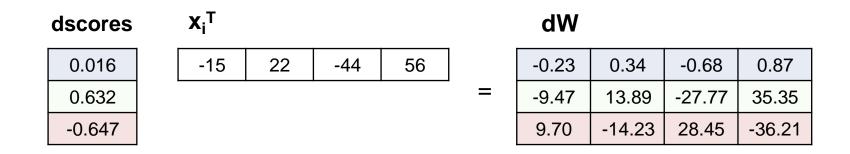


This is what we have already done when calculating loss

Softmax Gradients



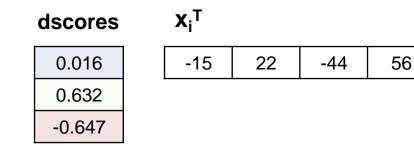
Softmax Gradients



Multiply **dscores** with the transpose of \mathbf{x}_i

Multiply column and row vector

=



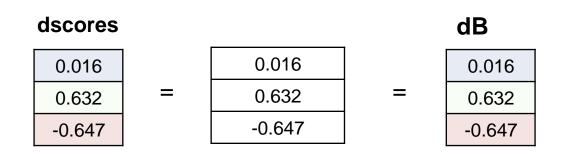
= 0.016 * -15	= 0.016 * 22	= 0.016 * -44	= 0.016 * 56
= -0.23	= 0.34	= -0.68	= 0.87
= 0.632 * -15	= 0.632 * 22	= 0.632 * -44	= 0.632 * 56
= -9.47	= 13.89	= -27.77	= 35.35
= -0.647 *	= -0.647 * 22	= -0.647 *	= -0.647 * 56
-15 = 9.70	= -14.23	-44 = 28.45	= -36.21

$$M_{0,0} = dscores_0 * X_{i 0}^{T}$$

$$M_{0,1} = dscores_0 * X_{i 1}^{T}$$

...

Softmax Gradients



Sum the values of all rows in **dscores** into a new vector

Softmax Gradients



dB

-0.23	0.34	-0.68	0.87	0.016
-9.47	13.89	-27.77	35.35	0.632
9.70	-14.23	28.45	-36.21	-0.647

Now we have the gradients!

What if we have multiple input examples?

	W		
0.01	-0.05	0.1	0.05
0.7	0.2	0.05	0.16
0.0	-0.45	-0.2	0.03

Xi	
-15	8
22	-12
-44	14
56	-5

	b	
	0.0	
+	0.2	
	-0.3	

=

ç	scores		
	-2.85	1.83	
	0.86	3.30	
	0.28	2.15	

e^{fj}

 \checkmark

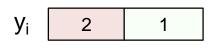
normalize

0.058	6.23	
2.36	27.11	→
1.32	8.59	

0.016	0.149
0.632	0.647
0.353	0.205

dscores

0.016	0.149
0.632	-0.353
-0.647	0.205

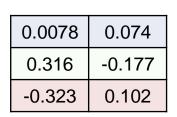


Update the score for the correct categories y_i by -1

dscores

0.0078	0.074
0.316	-0.177
-0.323	0.102

Divide by number of training examples (2 in this case)



dscores



-15	22	-44	56
8	-12	14	-5

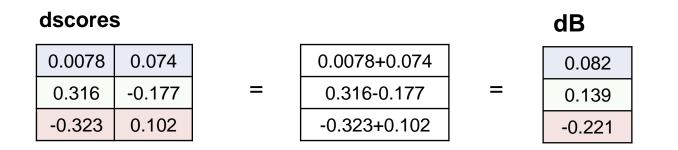
dW

=

0.479	-0.722	0.701	0.061
-6.147	9.063	-16.359	18.556
5.669	-8.341	15.659	-18.617

Multiply **dscores** with the transpose of \mathbf{x}_i

Softmax Gradients



Sum the values of all rows in **dscores** into a new vector

Regularization

- We also need to add a regularization factor to the weight gradients dW
- This is done by adding the weight matrix W scaled by lambda/2 to dW
- Let's go back to our first example with a single training example:

Regularization Factor

+

dW

-0.23	0.34	-0.68	0.87
-9.47	13.89	-27.77	35.35
9.70	-14.23	28.45	-36.21

W

0.01	-0.05	0.1	0.05
0.7	0.2	0.05	0.16
0.0	-0.45	-0.2	0.03

5 6 * λ * 0.5 =

dW + W * λ * 0.5

-0.2317	0.3396	-0.6793	0.8654
-9.4639	13.8866	-27.7709	35.3459
9.6992	-14.2277	28.4500	-36.2102

dB is not changed

=

Weights Upgrades

- The weights are upgraded by subtracting dW multiplied by a learning rate
- The learning rate is typically set to a low value such as 0.1 or 0.05
- The best learning rate for each dataset has to be discovered by trial and error...

Weights Upgrades

W

=

-

0.01	-0.05	0.1	0.05
0.7	0.2	0.05	0.16
0.0	-0.45	-0.2	0.03

-0.2317	0.3396	-0.6793	0.8654
-9.4639	13.8866	-27.7709	35.3459
9.6992	-14.2277	28.4500	-36.2102

* 0.1 =

newW

0.033	-0.084	0.168	-0.037
1.646	-1.189	2.827	-3.375
-0.970	0.973	-3.045	3.651

Bias Upgrades



If we calculate the loss, it has decreased from **1.04** to **0.48**

Back to our previous example

1.00	2.00	0.00
2.00	-4.00	0.50
3.00	-1.00	-0.50

b

	_	У
0.40		0
0.30		0
0.80		0
0.30		1
0.70		1
0.20		1
-0.40		2
-0.60		2
-0.50		2
	0.30 0.80 0.30 0.70 0.20 -0.40 -0.60	0.30 0.80 0.30 0.70 0.20 -0.40 -0.60

1.30	-0.10	0.60
1.40	0.90	1.60
1.90	-2.10	-0.40
0.20	-1.50	-2.00
1.10	-2.90	-2.10
-0.30	-1.70	-2.80
-0.10	3.50	2.00
-0.70	3.90	1.60
-1.40	1.70	-1.20

scores

0.56 1.04 0.11 1.96 4.06 1.68 1.72 2.40 3.00

L

Let's calculate the gradients!

Data loss:	1.84
Regularization loss:	0.35
Total loss:	2.19

mean | 1.84

Example - iteration 0

У

0

0

0

1

1

1

2

2

2

W		b
1.00 -0.20	2.00 0.07	0
2.00 0.24	-4.00 -0.27	0
3.00 -0.01	-1.00 <mark>0.19</mark>	-(-(

	b
)	0.00 0.15
0 7	0.50 0.04
0	-0.50 -0.19

Χ		
0.50	0.40	
0.80	0.30	
0.30	0.80	
-0.40	0.30	
-0.30	0.70	
-0.70	0.20	
0.70	-0.40	
0.50	-0.60	
-0.40	-0.50	

Score	5	_
1.30	-0.10	0.60
1.40	0.90	1.60
1.90	-2.10	-0.40
0.20	-1.50	-2.00
1.10	-2.90	-2.10
-0.30	-1.70	-2.80
-0.10	3.50	2.00
-0.70	3.90	1.60
-1.40	1.70	-1.20

COLOC

0.56
1.04
0.11
1.96
4.06
1.68
1.72
2.40
3.00

Data loss:	1.84
Regularization loss:	0.35
Total loss:	2.19

1.84 mean

Example - iteration 1

W		b
1.02	1.99	-C
-0.20	<mark>0.07</mark>	0
1.98 0.24	-3.97 -0.27	0
3.00	-1.02	-0
-0.01	<mark>0.19</mark>	-0

b	
-0.02 0.15	
0.50 0.04	
-0.48 -0.18	

Χ		
0.50	0.40	
0.80	0.30	
0.30	0.80	
0.40	0.30	
0.30	0.70	
0.70	0.20	
0.70	-0.40	
0.50	-0.60	
0.40	-0.50	

-

У	score	S
0	1.29	-
0	1.40	
0	1.89	-
1	0.17	-
1	1.07	-
1	-0.33	-
2	-0.10	
2	-0.70	
2	-1.42	

1.29	-0.10	0.61
1.40	0.89	1.61
1.89	-2.09	-0.40
0.17	-1.49	-1.99
1.07	-2.88	-2.09
-0.33	-1.68	-2.79
-0.10	3.47	2.03
-0.70	3.87	1.63
-1.42	1.69	-1.17

L

0.56
1.04
0.11
1.93
4.01
1.65
1.68
2.35
1.96

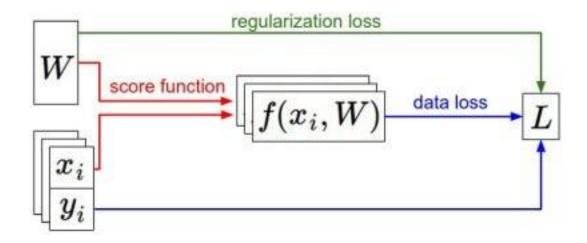
Data loss:	1.81
Regularization loss:	0.35
Total loss:	2.16

mean | 1.81

Gradient Descent

- The procedure of repeatedly evaluating the gradients and perform weights updates is call Gradient Descent
- It is the most common way of optimizing/training linear classifiers, and also Neural Networks which we will look into shortly
- We can also train on batches of the training examples instead of all examples
 - Mini-batch Gradient Descent
- Or we can train on one example at a time
 - Stochastic Gradient Descent

Overview of information flow



Linear Softmax classifier

- Now we have a complete linear Softmax classifier
- Let's see how well it works on the example data:

X		У
0.50	0.40	0
0.80	0.30	0
0.30	0.80	0
-0.40	0.30	1
-0.30	0.70	1
-0.70	0.20	1
0.70	-0.40	2
0.50	-0.60	2
-0.40	-0.50	2

- -

Linear Softmax classifier

λ: 0.01 Lrate: 1.0

Iteration	Loss	Accuracy	
0	2.19	2/9	22.2%
1	1.91	2/9	22.2%
2	1.67	2/9	22.2%
3	1.49	3/9	33.3%
4	1.34	4/9	44.4%
5	1.22	5/9	55.6%
6	1.11	6/9	66.7%
7	1.03	6/9	66.7%
8	0.96	7/9	77.8%
9	0.90	7/9	77.8%
10	0.85	7/9	77.8%
11	0.81	7/9	77.8%
12	0.77	7/9	77.8%
13	0.74	7/9	77.8%
14	0.71	7/9	77.8%
15	0.69	7/9	77.8%
16	0.67	7/9	77.8%
17	0.66	8/9	88.9%
18	0.64	8/9	88.9%
19	0.63	9/9	100%

Iris dataset

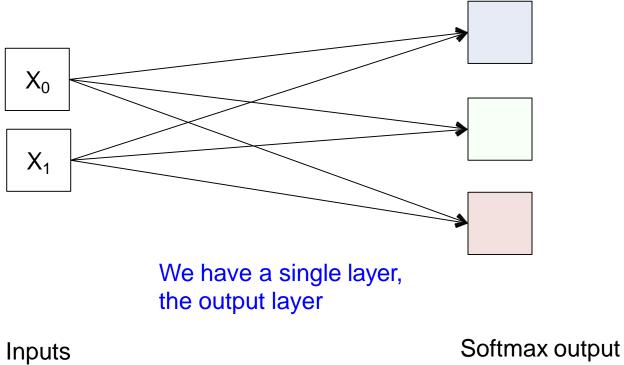
Iteration	Loss
0	1.0711
40	0.6935
80	0.5791
120	0.4842
160	0.4052
200	0.3655
240	0.3603
280	0.3591
300	0.3592

Final Result		
Loss:	0.3591	
Accuracy	147/150	98%

λ: 0.01 Lrate: 0.1 Iterations: 300

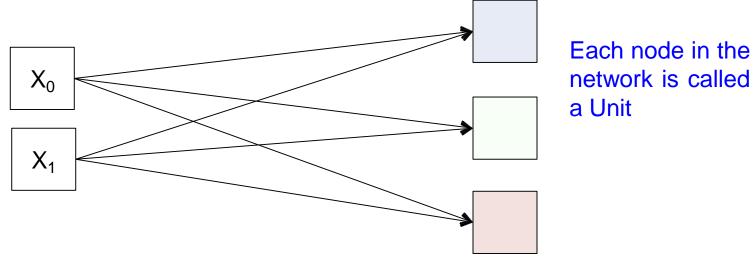
How can we expand this into a Neural Network?

Current network layout



layer

Current network layout

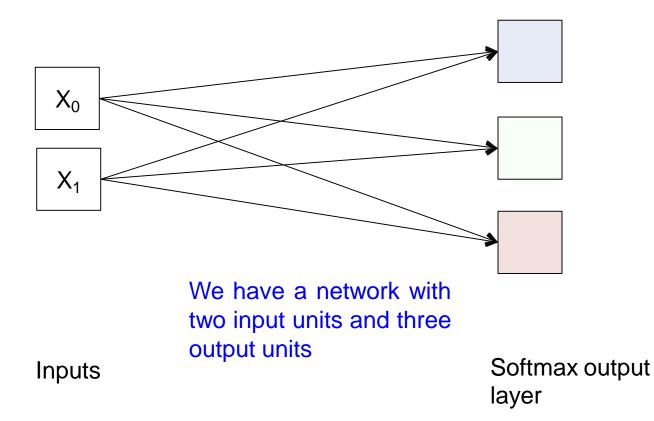


network is called

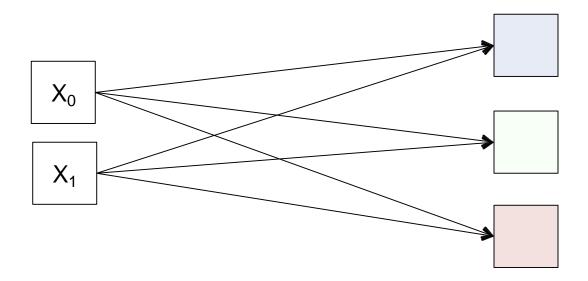
Inputs

Softmax output layer

Current network layout

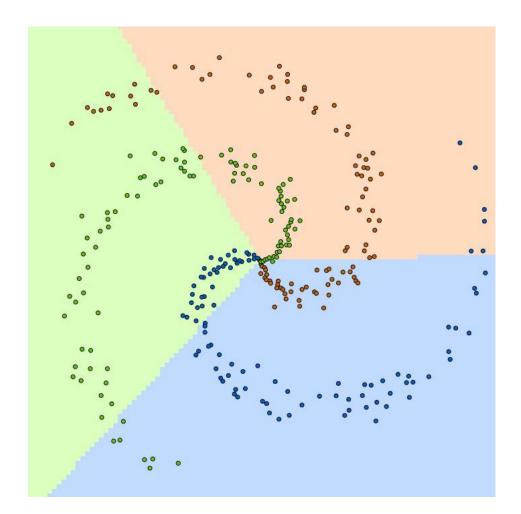


Limitations

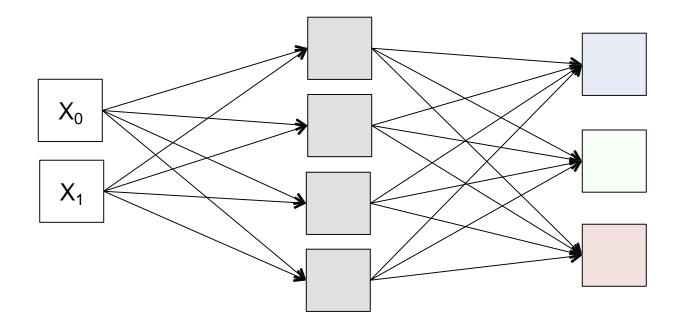


Even if this is a quite powerful classifier, it can only handle categories that are linearly separable!

Limitations



Layered network

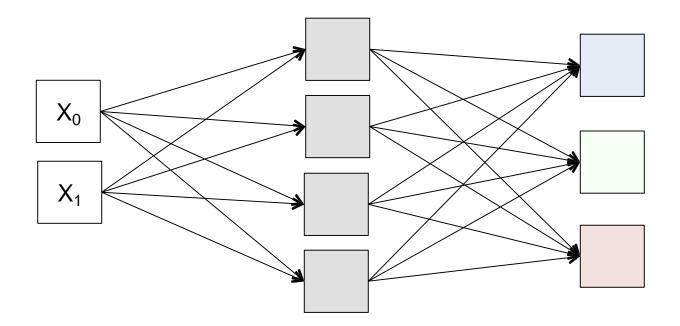


Inputs

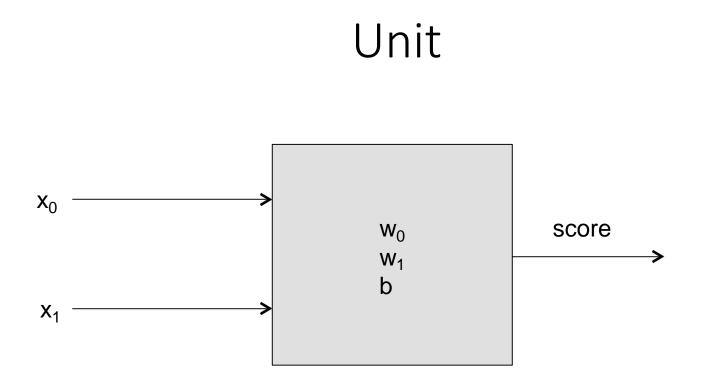
Expand with a layer of hidden nodes

Softmax output layer

Layered network



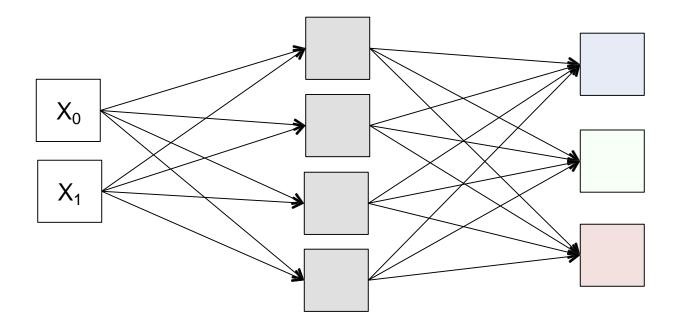
The layered (neural) network can learn categories that are not linearly separable!



Each unit has its own set of inputs, a weight for each input and a bias.

The output (score) can act as input to units in another layer.

Score Function



The input data x is the input to the hidden layer

The scores of the hidden layer is input to the output layer

Hidden Layer Units

- In the output layer we used the Softmax function
- In the hidden layer we need a slightly different type of activation function
- There is a wide range we can choose from:
 - Sigmoid
 - Tanh
 - ReLU
 - ...
- Here, we will use the ReLU function

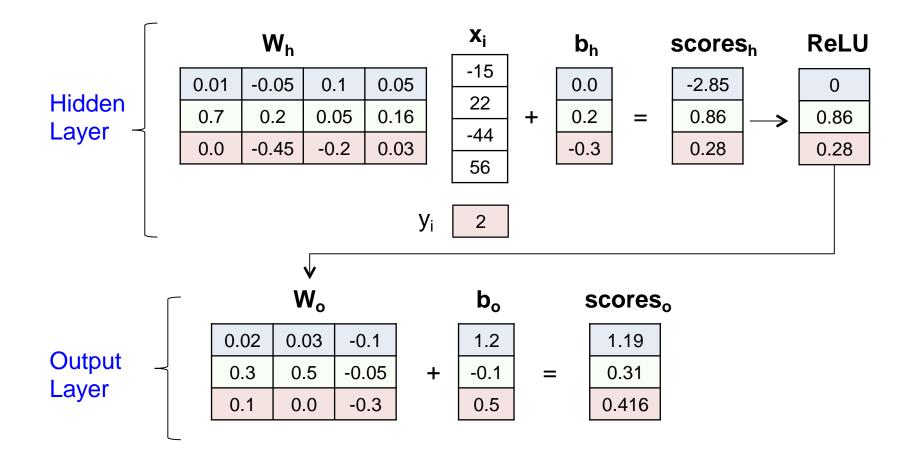
ReLU

• The ReLU (Rectified Linear Unit) calculates the function:

f(x) = max(0, x)

- First, the weighted sum of the inputs plus the bias is calculated (as we've done before)
- Then, the activation function is applied on the result

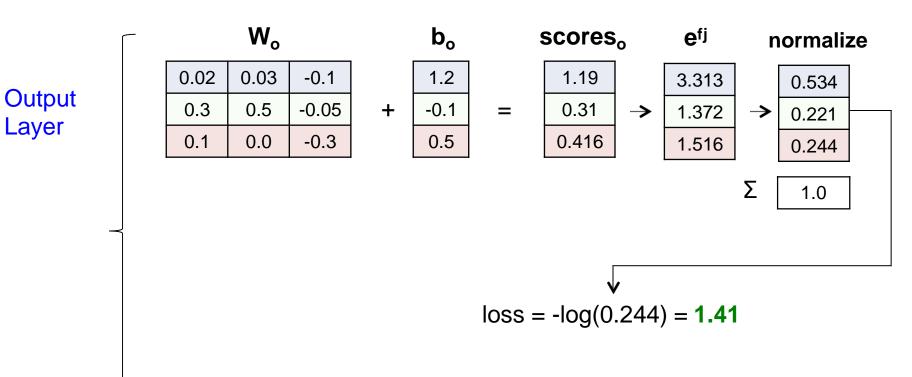
Score Function

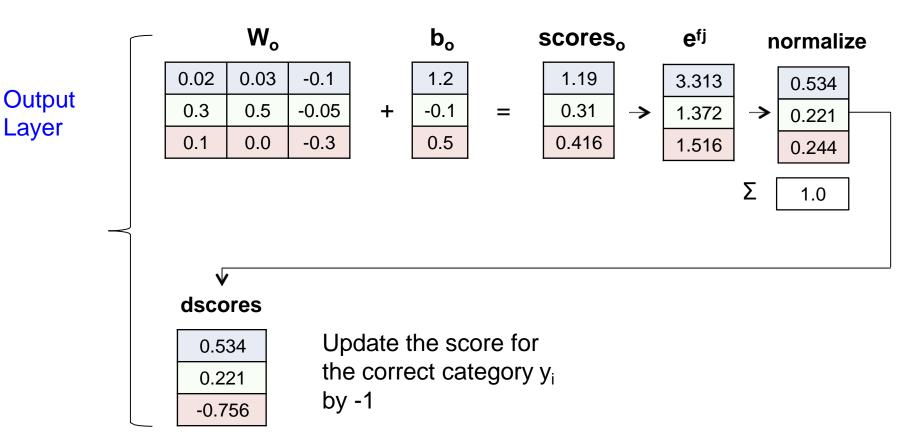


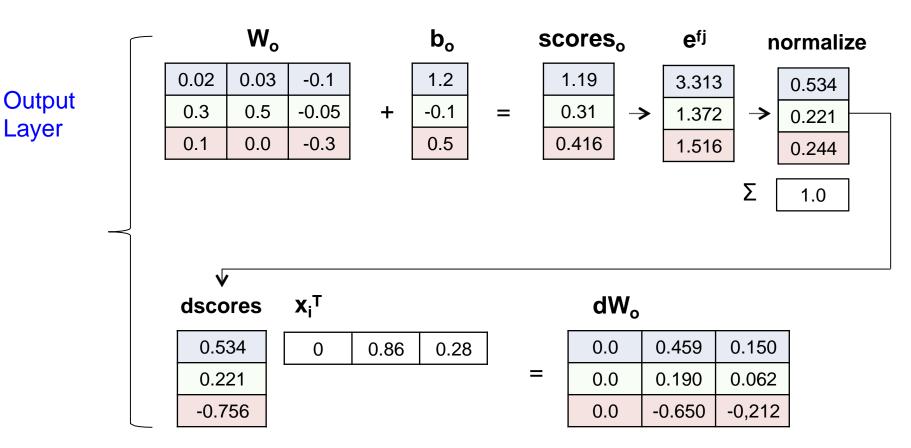
Loss Function

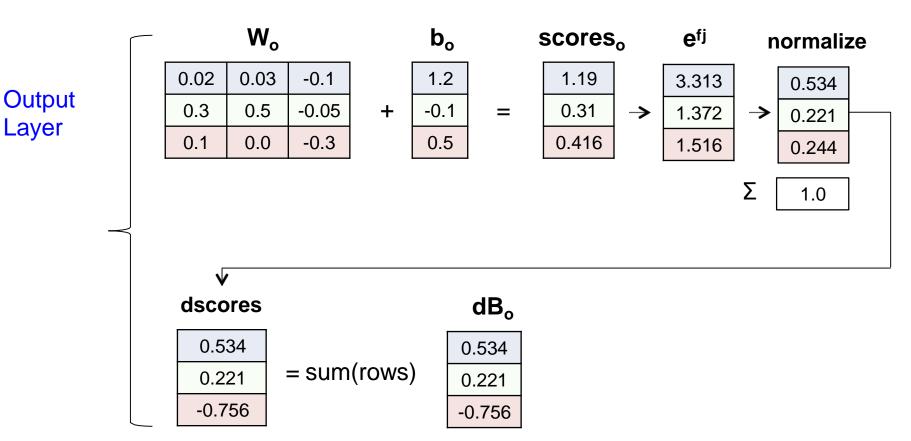
- The loss function/gradients are slightly more complex
- We need to calculate the loss and gradients for the output layer first (in the same way as we did before)
- The gradients are then backpropagated into the hidden layer
- The loss for both layers are summed

Loss Function

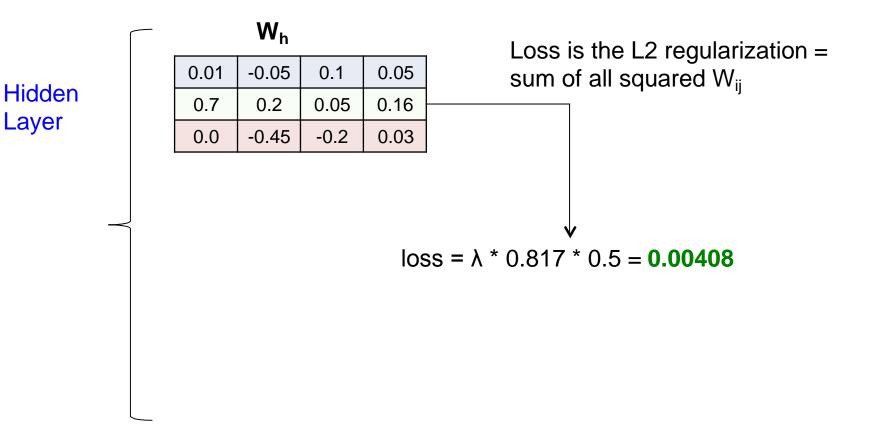


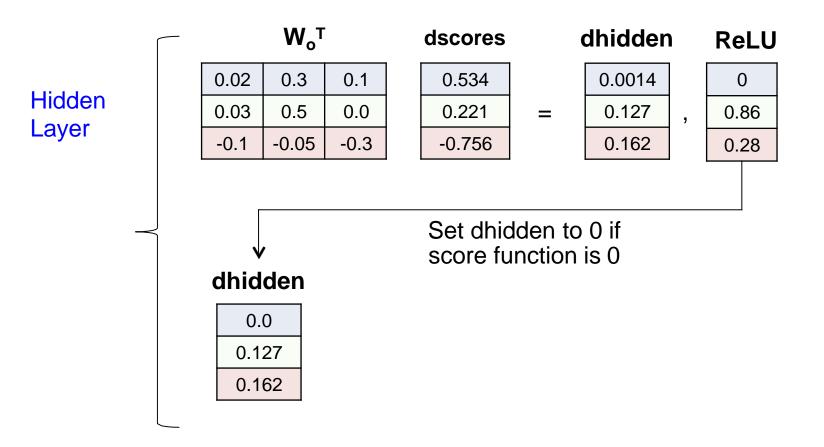


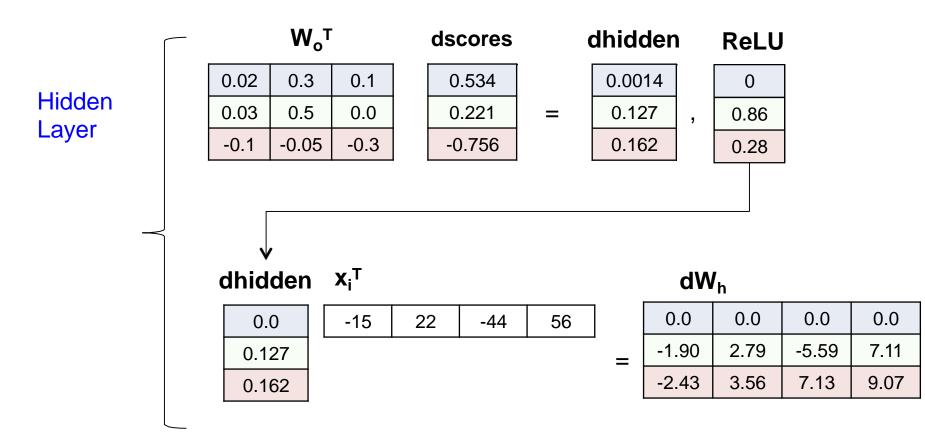


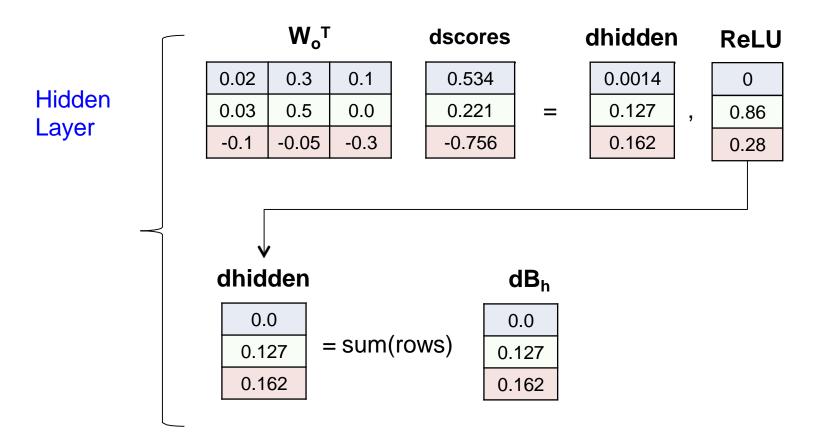


Loss Function









Regularization

- Regularization is added to loss and gradients in the output and hidden layer as before
- The total loss is the loss for the output plus the loss for the hidden layer

Weights Upgrades

-



0.01	-0.05	0.1	0.05
0.7	0.2	0.05	0.16
0.0	-0.45	-0.2	0.03

 $\mathbf{dW}_{\mathbf{h}}$

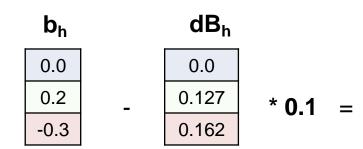
0.0	0.0	0.0	0.0
-1.90	2.79	-5.59	7.11
-2.43	3.56	7.13	9.07

* 0.1 =

newW_h

0.01	-0.05	0.10	0.05
0.89	-0.08	0.61	-0.55
0.24	-0.81	0.51	-0.88

Bias Upgrades



r	newB _h	
	0.0	
	0.19	
	-0.32	

=

Summary

- The linear classifier has now been extended to contain a hidden layer with ReLU nodes
- The hidden layer enables the classifier to learn categories that are not linearly separable

Non-linearly separable categories

