Machine Learning: Neural Networks

ROB 102: Introduction to AI & Programming

Lecture 13

2021/12/01

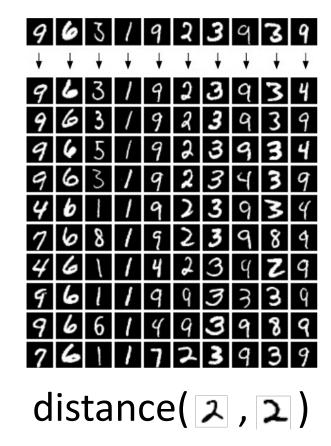
Project 4: Machine Learning

Implement three machine learning algorithms to classify images from the MNIST dataset.

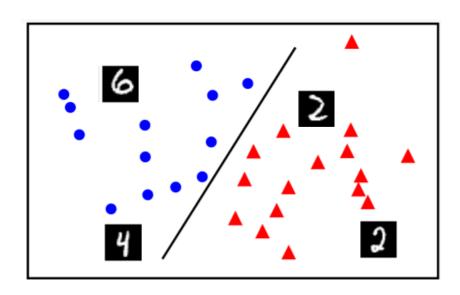
- 1. Nearest neighbors
- 2. Linear Classifier
- 3. Neural Network

Where we are

✓ P4.1: Nearest Neighbors



√ P4.2: Linear Classifier



$$f(X) = W \times X + b$$

Where we are

- ✓ P4.1: Nearest Neighbors
- + Straight-forward to implement
- + No training necessary
- Requires a lot of memory
- Expensive at computation time
- Distance isn't always a good indicator of class similarity

- √ P4.2: Linear Classifier
- + Only one matrix to learn
- + Fast at test time
- Can only represent linearly separable data

Can we do better than a linear model?

Project 4: Machine Learning

Implement three machine learning algorithms to classify images from the MNIST dataset.

- 1. Nearest neighbors
- 2. Linear Classifier
- 3. Neural Network (Today!)

Where we are

We'll use the same algorithm for training a neural network!

Training algorithm:

For linear classifier, this is just the weight matrix and the bias

Initialize the parameters randomly

For *N* iterations, do:

Mini-batch sampling

1. Sample a batch of training images

We used the SVM classification loss with regularization

- 2. Evaluate the loss and gradients for the batch using current parameters
- 3. Update the parameters using the gradients

Gradient Descent! The learning rate controls how fast we learn

Parameters to learn: W, b

Hyperparameters to tune:

learning rate, reg. coefficient

Where we are

We'll use the same algorithm for evaluating a neural network!

Prediction algorithm (test time):

Given a test image & parameters from the training stage:

- 1. Calculate class scores
- 2. Assign label of class with the highest score.

```
y pred = argmax(scores)
```

This time...

- The neural network model
 Training a neural network
- Briefly:

 - Backpropagation
 Convolutional Neural Networks

 Not needed for P4.3!

This time: Neural Networks

Linear classifier:

$$f(X) = W \times X + b$$

Q: How can we represent a more complex, non-linear function?

This time: Neural Networks

Linear classifier:

$$f(X) = W \times X + b$$

Neural network (2-layers):

$$f(X) = W_2 \times \max(W_1 \times X + b_1, 0) + b_2$$

A neural network can approximate any* function!

(*with some caveats)

A good visual explanation: (link)

This time: Neural Networks

Linear classifier:

$$f(X) = W \times X + b$$

Neural network (2-layers):

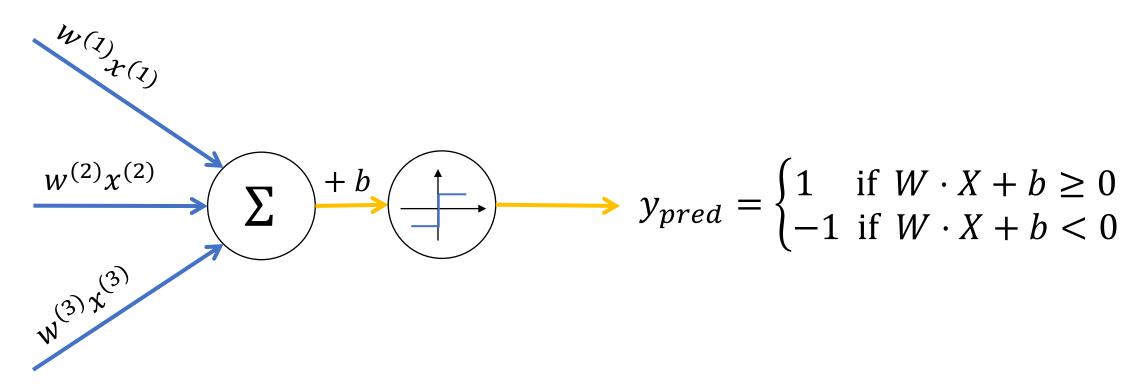
$$f(X) = W_2 \times \max(W_1 \times X + b_1, 0) + b_2$$

Neural network (3-layers):

$$f(X) = W_3 \times \max(W_2 \times \max(W_1 \times X + b_1) + b_2) + b_3$$

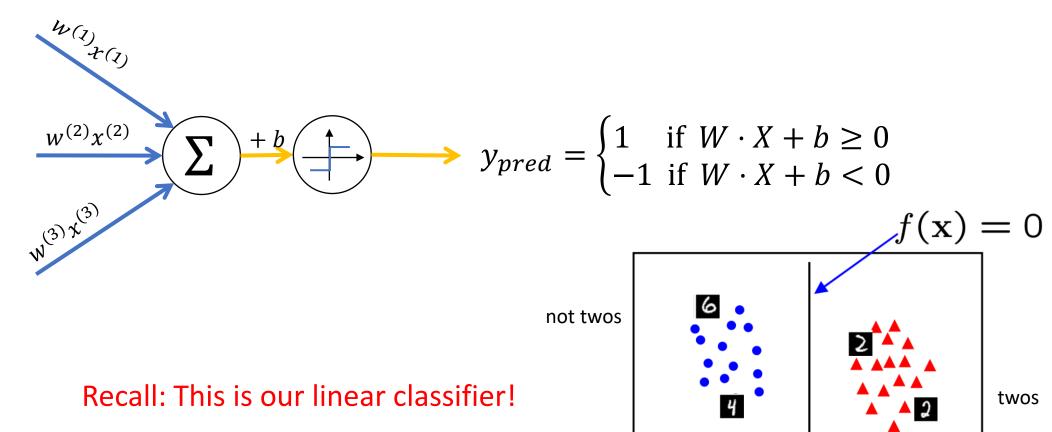
The perceptron

A perceptron is an algorithm for binary (linear!) classification.



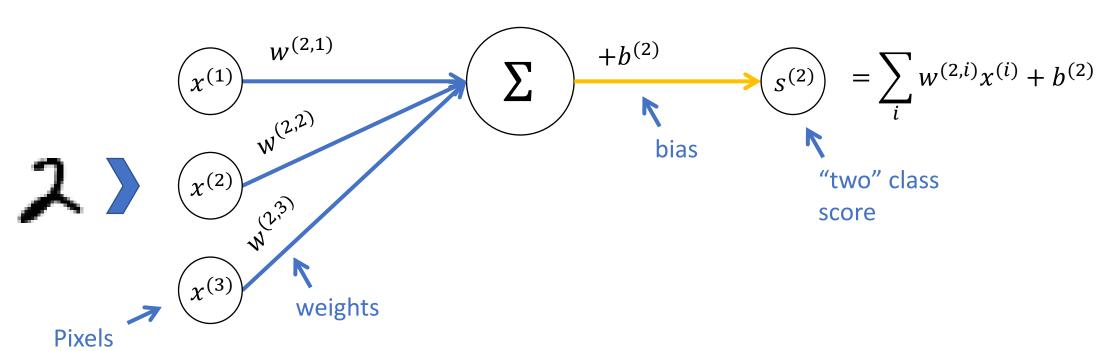
The perceptron

A perceptron is an algorithm for binary (linear!) classification.

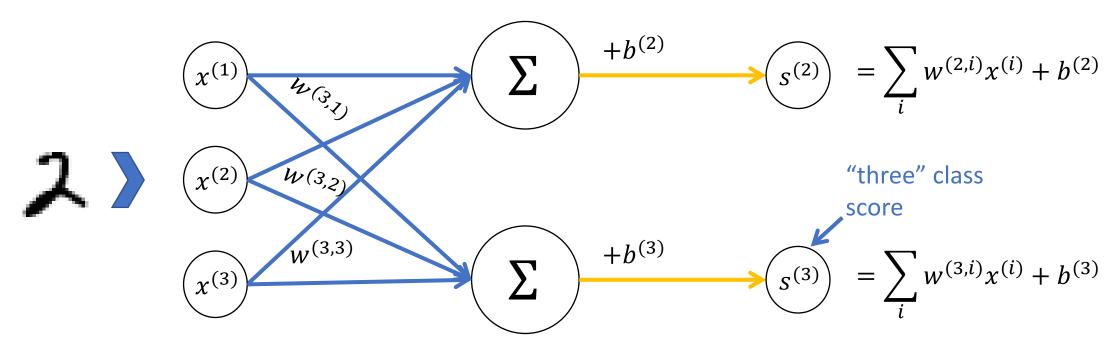


13

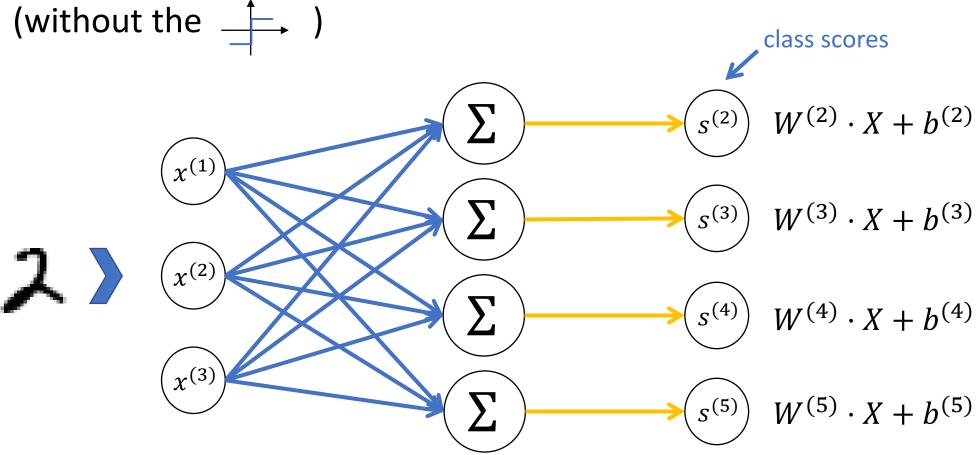
We can build a multi-class linear classifier as multiple perceptrons (without the \rightarrow)



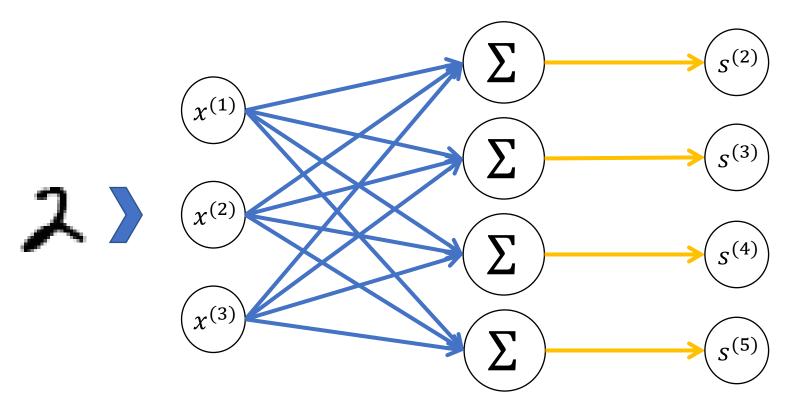
We can build a multi-class linear classifier as multiple perceptrons (without the \rightarrow)



We can build a multi-class linear classifier as multiple perceptrons



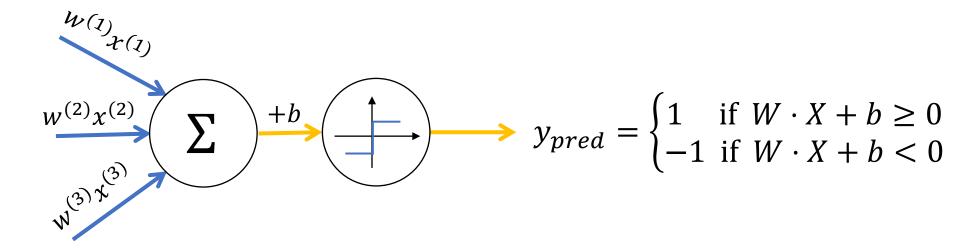
We can build a multi-class linear classifier as multiple perceptrons (without the \rightarrow)



Last time, we saw we can get all the class scores with a matrix multiplication

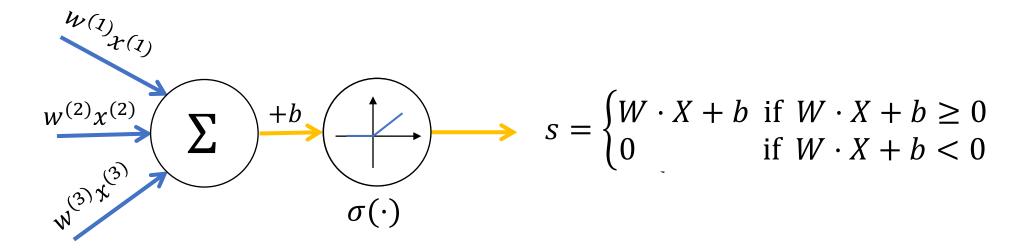
$$S = W \times X + b$$

Our perceptron can only represent linearly separable data. But, a network of perceptrons can represent more complex functions.



One more problem: This function is not differentiable!

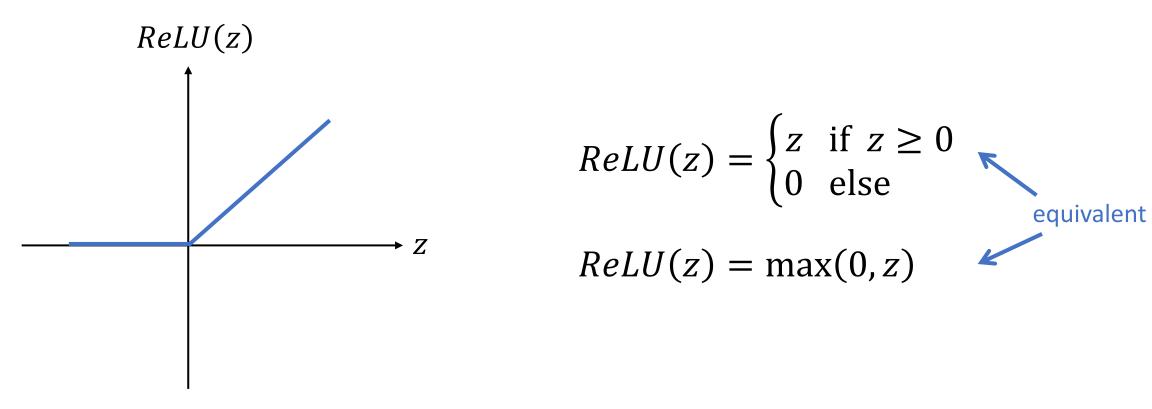
We'll replace with a continuous function, which will allow us to take the derivative of our loss function and apply Gradient Descent.



Our new function $\sigma(\cdot)$ is called the activation function.

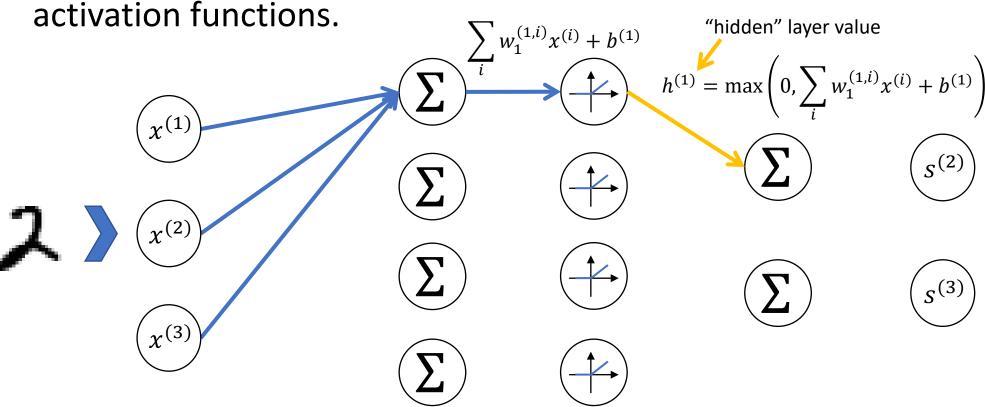
Activation functions

We will be using the **ReLU activation function** (Rectified Linear Unit). This is one of the most common choices in modern neural networks.

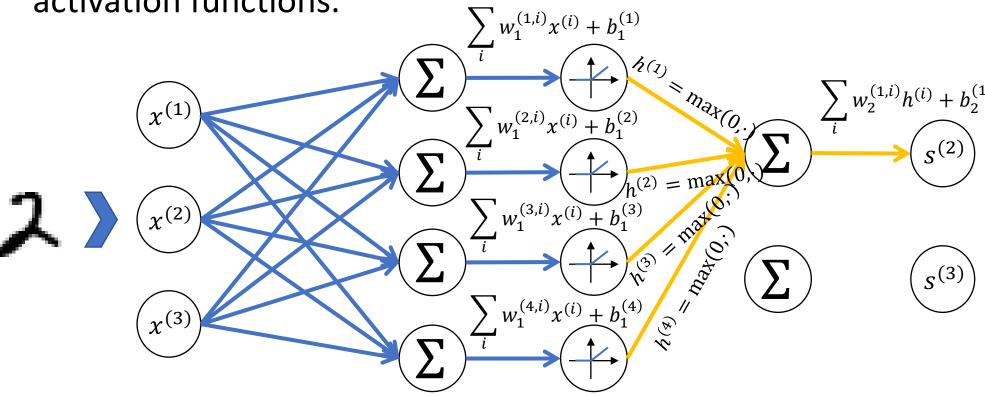


We can stack up multiple "neurons" made up of linear functions and activation functions.

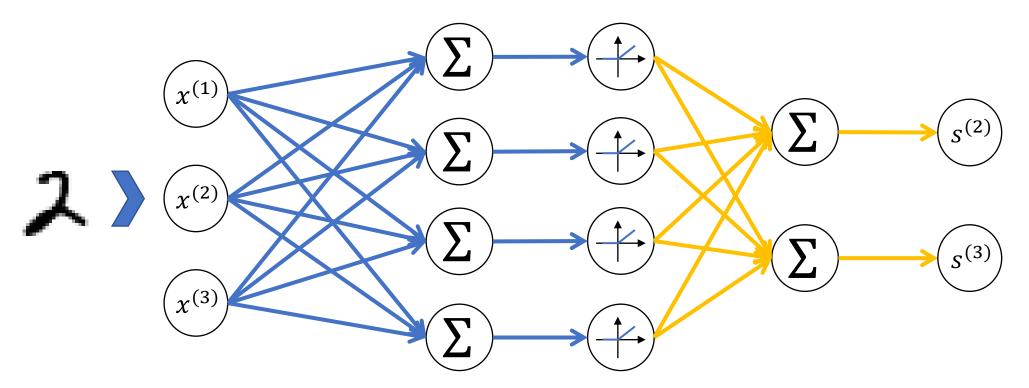
"bidden" layer value



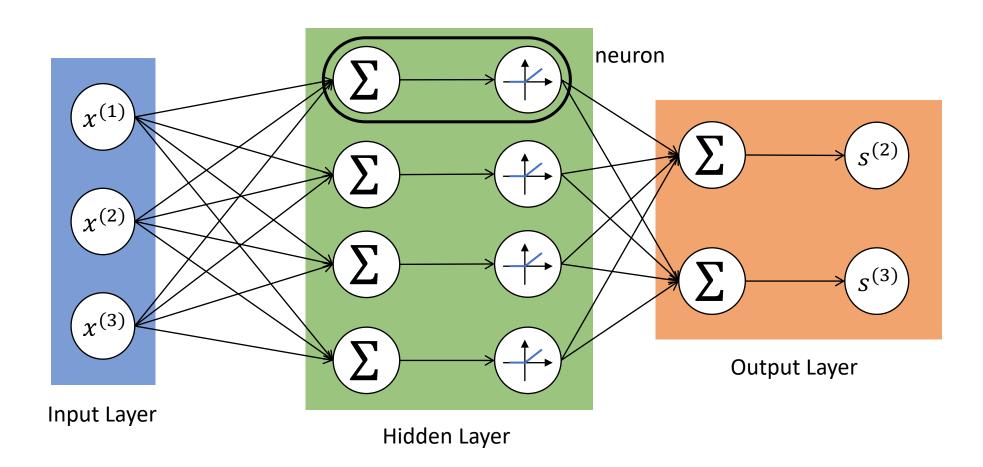
We can stack up multiple "neurons" made up of linear functions and activation functions.



We can stack up multiple "neurons" made up of linear functions and activation functions.



Our final two-layer neural network looks like this:



Fully Connected Neural Network

We call this a "fully connected" network because each node is connected to all nodes in the previous layer.

$$W_1 \times X + b_1$$

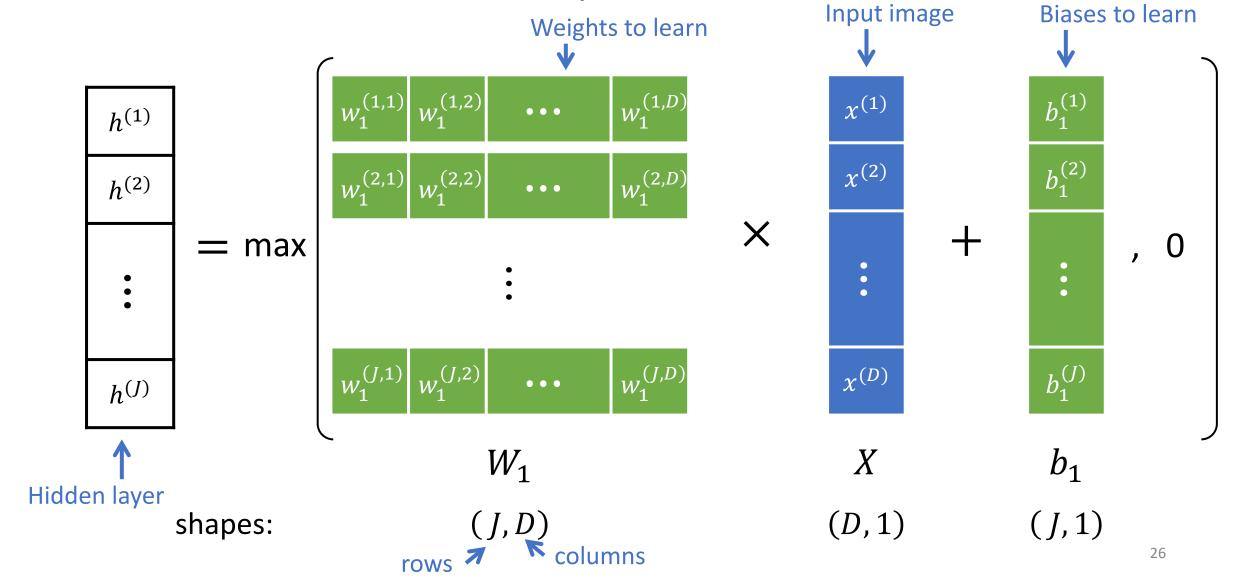
$$W_2 \times H + b_2$$

$$X^{(1)}$$

$$X^{(2)}$$

$$X^{(3)}$$

$$X^$$



Recall: Matrix Multiplication in Julia

```
julia> A = [1 2 3; 4 5 6; 7 8 9; 10 11 12]
4×3 Matrix{Int64}:
          6
          9
 10 11 12
julia> size(A)
(4, 3)
julia> B = [3 3; 2 2; 1 1]
3×2 Matrix{Int64}:
julia> size(B)
(3, 2)
iulia>
```

```
julia> A * B
4×2 Matrix{Int64}:
  10  10
  28  28
  46  46
  64  64

julia> size(A * B)
(4, 2)

julia>
```

Legal!

The inner dimensions match:

$$(4, 3) \times (3, 2) \rightarrow (4, 2)$$

Recall: Matrix Multiplication in Julia

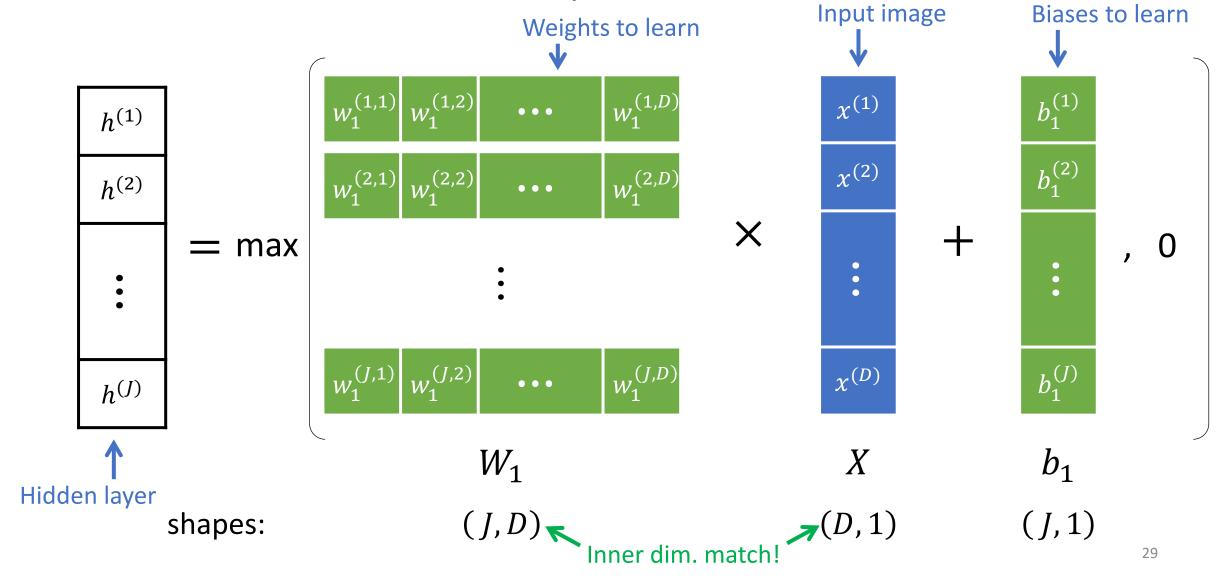
```
julia> A = [1 2 3; 4 5 6; 7 8 9; 10 11 12]
4×3 Matrix{Int64}:
 10 11 12
julia> size(A)
(4, 3)
julia> C = [1 1 1; 2 2 2]
2×3 Matrix{Int64}:
1 1 1
2 2 2
julia> size(C)
(2, 3)
```

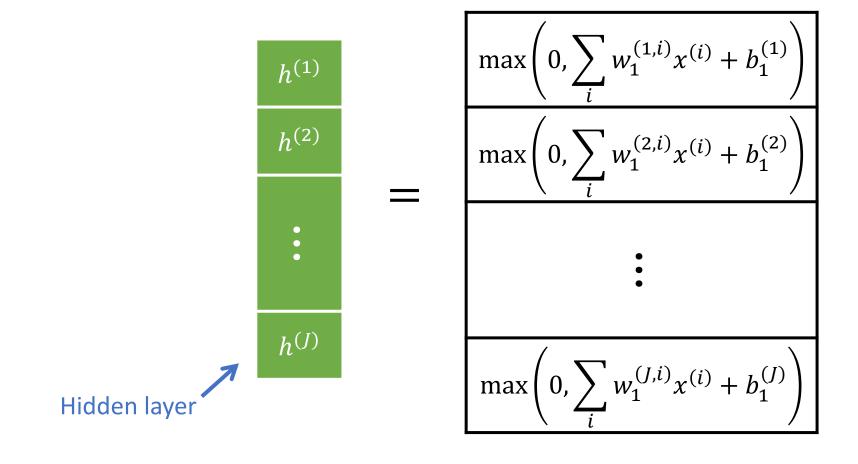
```
julia> A * C
ERROR: DimensionMismatch("matrix A has dimension
s (4,3), matrix B has dimensions (2,3)")
Stacktrace:
[1] _generic_matmatmul!(C::Matrix{Int64}, tA::C
har, tB::Char, A::Matrix{Int64}, B::Matrix{Int64}
}, _add::LinearAlgebra.MulAddMul{true, true, Boo
l, Bool})
@ LinearAlgebra C:\buildbot\worker\package_wi
n64\build\usr\share\julia\stdlib\v1.6\LinearAlge
bra\src\matmul.jl:814
```

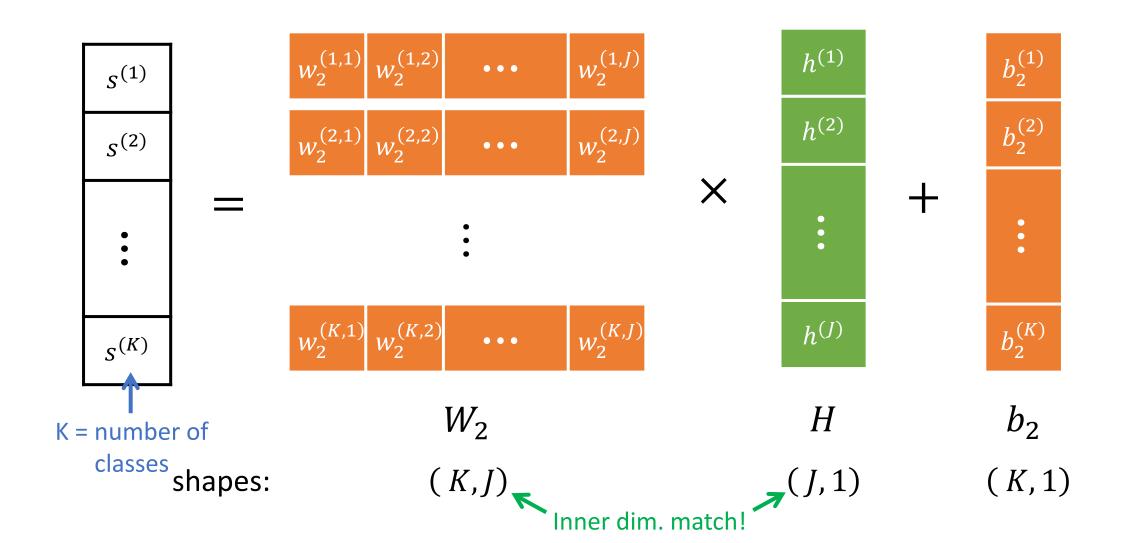
Illegal ⊗

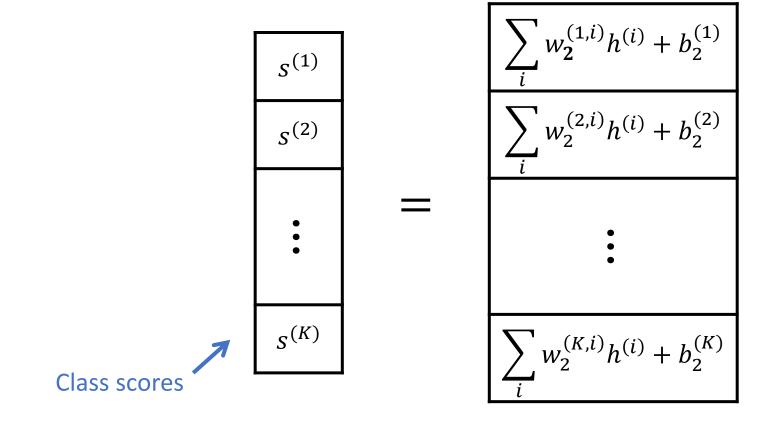
The inner dimensions don't match:

 $(4, 3) \times (2, 3) \rightarrow Fails!$









We can write a two-layer neural network as one big matrix multiplication:

scores =
$$W_2 \times \max(0, W_1 \times X + b_1) + b_2$$

First linear layer

Why do we need an activation function?

Let's look at our neural network equation:

$$scores = W_2 \times max(0, W_1 \times X + b_1) + b_2$$

What if we removed the activation function?

$$scores = W_2 \times (W_1 \times X + b_1) + b_2$$

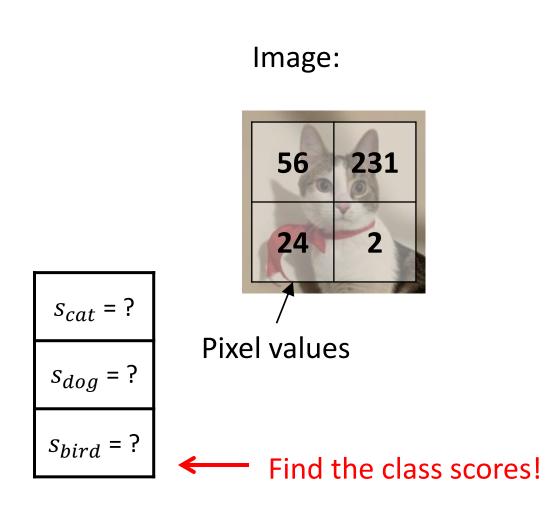
$$= (W_2 \times W_1) \times X + (W_2 \times b_1 + b_2)$$
This is still just a linear classifier!

Exercise:

Parameters:

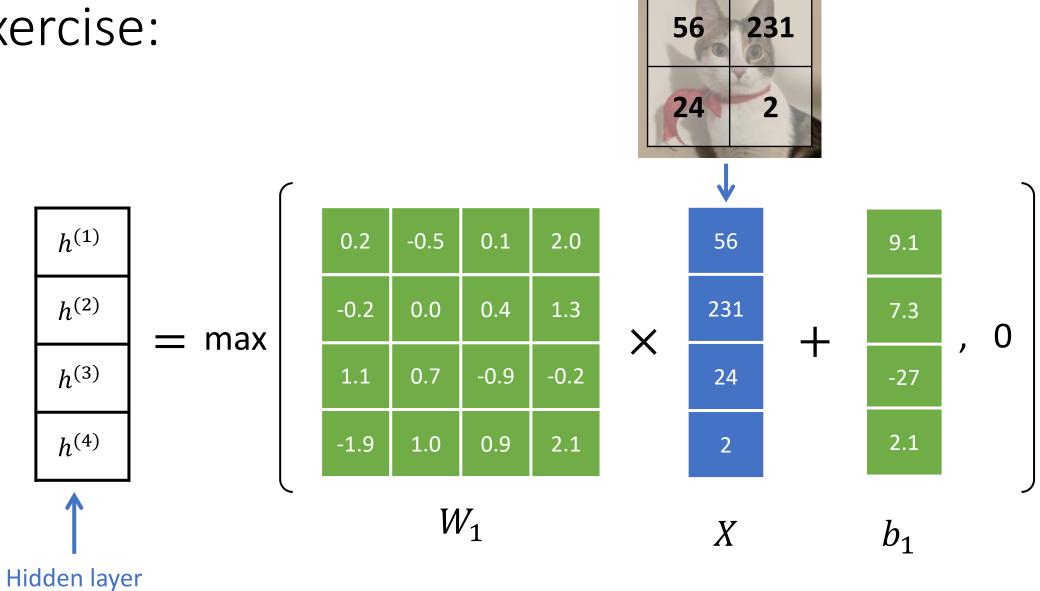
 W_1

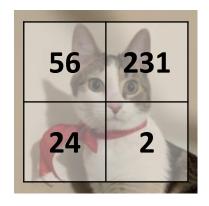
 W_2



0.2	-0.5	0.1	2.0	b_1	9.1
-0.2	0.0	0.4	1.3		7.3
1.1	0.7	-0.9	-0.2		-27
-1.9	1.0	0.9	2.1		2.1
0.8	0.9	0.0	1.4	b_2	-32
0.3	-0.3	2.2	-1.2		14
0.6	0.7	-0.1	-0.6		19

Exercise:





```
h^{(1)}
```

 $h^{(2)}$

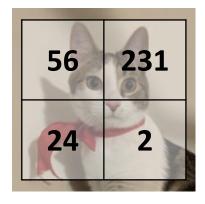
 $h^{(3)}$

 $h^{(4)}$

```
julia> X = [56; 231; 24; 2]
4-element Vector{Int64}:
 56
 231
 24
  2
julia> W1 = [0.2 -0.5 0.1 2.0; -0.2 0.0 0.4 1.3; 1.1 0.7 -0.9 -0.2; -1.9 1.0 0.9 2.1]
4×4 Matrix{Float64}:
 0.2 -0.5 0.1 2.0
           0.4 1.3
 -0.2 0.0
 1.1
      0.7 -0.9 -0.2
 -1.9
      1.0
           0.9 2.1
julia> b1 = [9.1; 7.3; -27; 2.1]
4-element Vector{Float64}:
  9.1
  7.3
 -27.0
  2.1
iulia>
```

```
julia> W1 * X + b1
```

$$H = \max(0, W_1 \times X + b_1)$$



$$h^{(1)} = 0$$

$$h^{(2)} = 8.3$$

$$h^{(3)} = 174.3$$

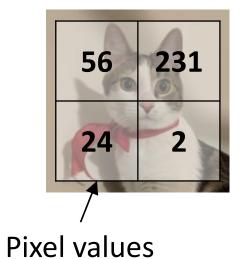
$$h^{(4)} = 152.5$$

```
julia> X = [56; 231; 24; 2]
4-element Vector{Int64}:
 56
 231
 24
  2
julia> W1 = [0.2 -0.5 0.1 2.0; -0.2 0.0 0.4 1.3; 1.1 0.7 -0.9 -0.2; -1.9 1.0 0.9 2.1]
4×4 Matrix{Float64}:
 0.2 -0.5 0.1 2.0
 -0.2 0.0 0.4 1.3
 1.1 0.7 -0.9 -0.2
 -1.9 1.0 0.9 2.1
julia> b1 = [9.1; 7.3; -27; 2.1]
4-element Vector{Float64}:
  9.1
  7.3
 -27.0
  2.1
iulia>
```

```
julia> W1 * X + b1
4-element Vector{Float64}:
   -88.8
    8.29999999999999
174.2999999999998
152.5
```

```
julia> H = max.(0, W1 * X + b1)
4-element Vector{Float64}:
    0.0
    8.2999999999999
174.299999999998
152.5
julia>
```

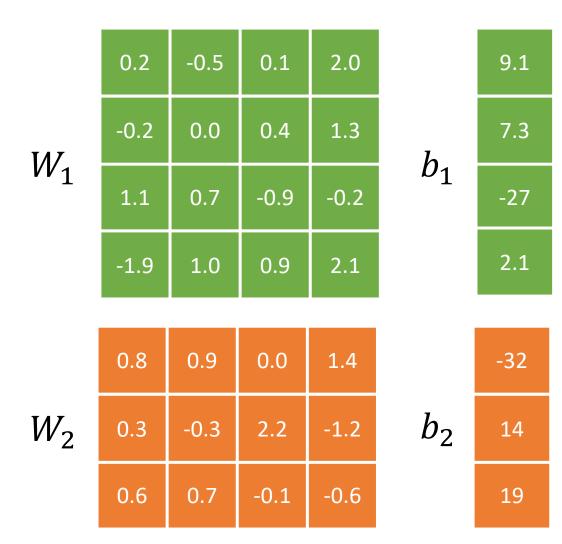
Image:

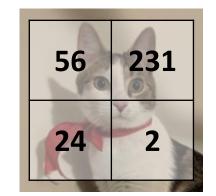


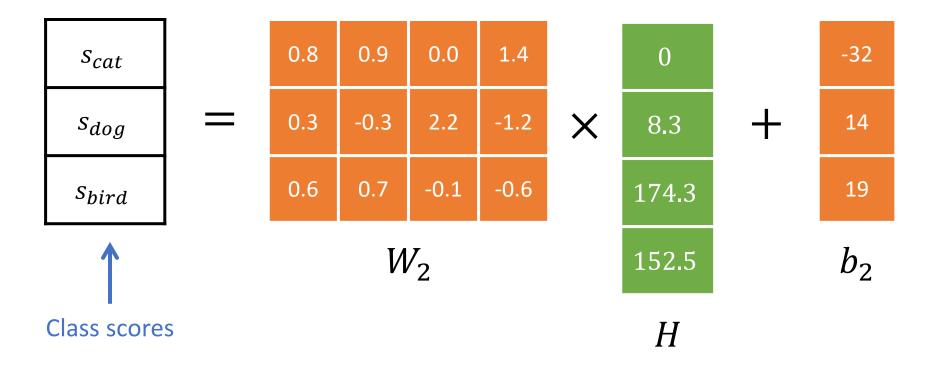
$s_{cat} = ?$	
$s_{dog} = ?$	

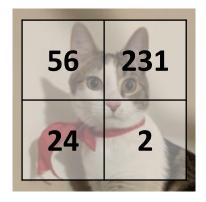
$$s_{bird} = ?$$

Parameters:









 s_{cat}

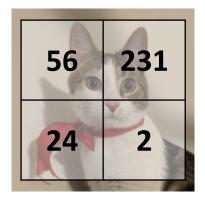
 S_{dog}

 S_{bird}

```
julia> W2 = [0.8 0.9 0.0 1.4; 0.3 -0.3 2.2 -1.2; 0.6 0.7 -0.1 -0.6]
3×4 Matrix{Float64}:
    0.8     0.9     0.0     1.4
    0.3     -0.3     2.2     -1.2
    0.6     0.7     -0.1     -0.6

julia> b2 = [-32; 14; 19]
3-element Vector{Int64}:
    -32
    14
    19
```

$$W_2 \times H + b_2$$



$$s_{cat} = 188.97$$



$$s_{dog} = 211.97$$

$$s_{bird} = -84.12$$

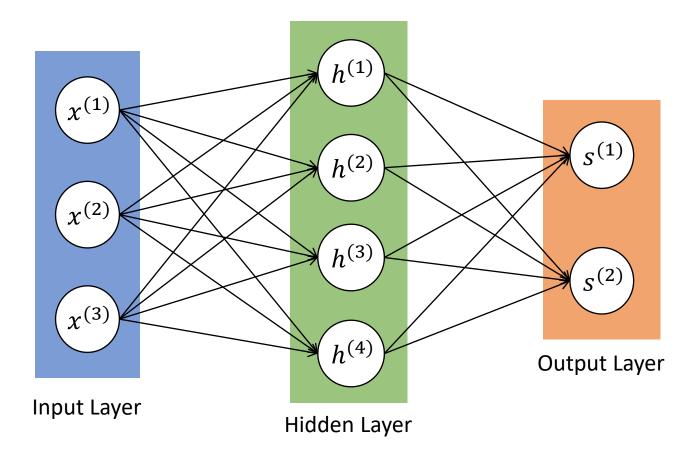
```
julia> W2 = [0.8 0.9 0.0 1.4; 0.3 -0.3 2.2 -1.2; 0.6 0.7 -0.1 -0.6]
3×4 Matrix{Float64}:
    0.8     0.9     0.0     1.4
    0.3     -0.3     2.2     -1.2
    0.6     0.7     -0.1     -0.6

julia> b2 = [-32; 14; 19]
3-element Vector{Int64}:
    -32
    14
    19
```

```
julia> argmax(scores)
2
julia>
```

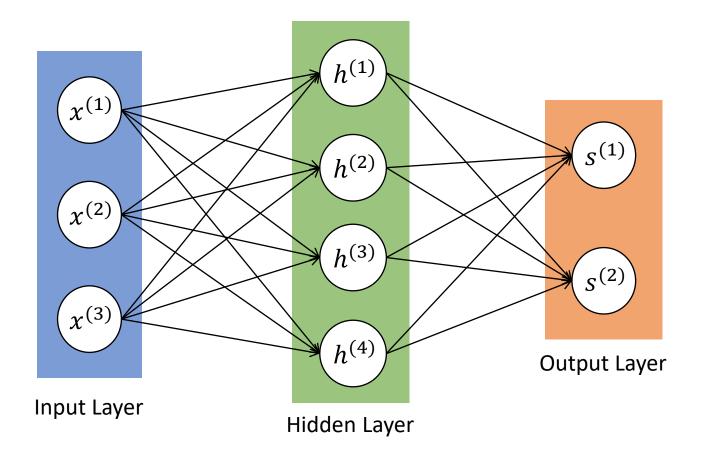
Predicted class: 2 = dog

This is a two-layer neural network (the input layer isn't counted).

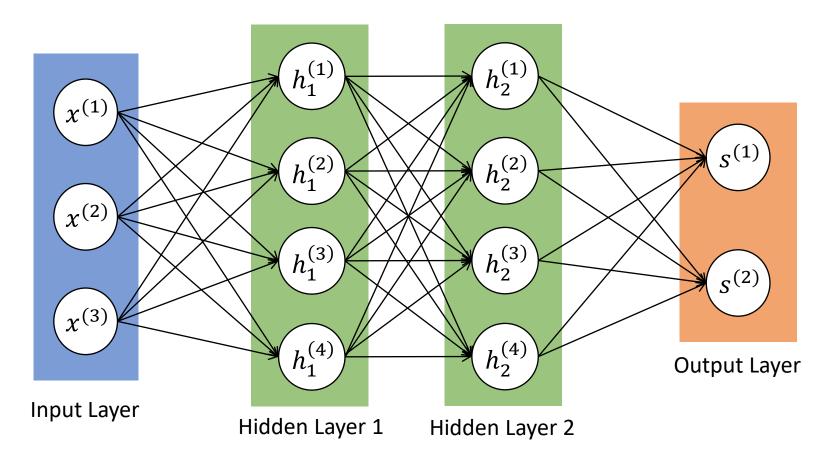


Parameters to learn: W_1, W_2, b_1, b_2

$$scores = W_2 \times max(0, W_1 \times X + b_1) + b_2$$

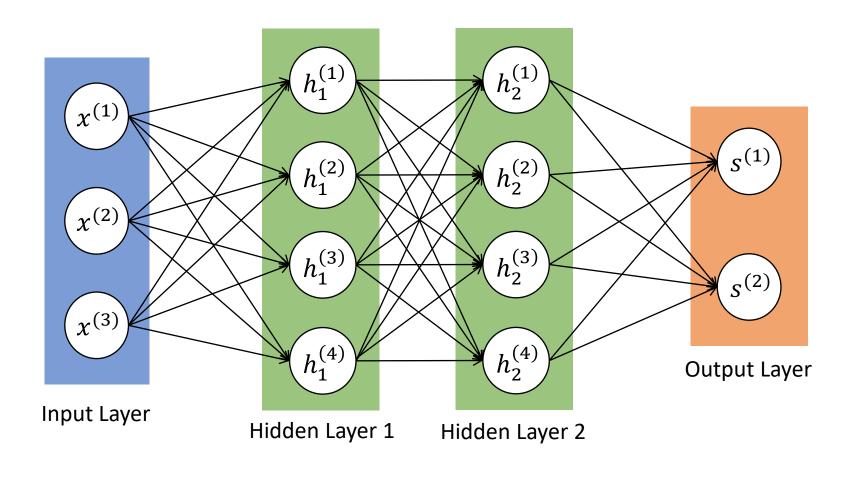


A three-layer neural network looks like this:



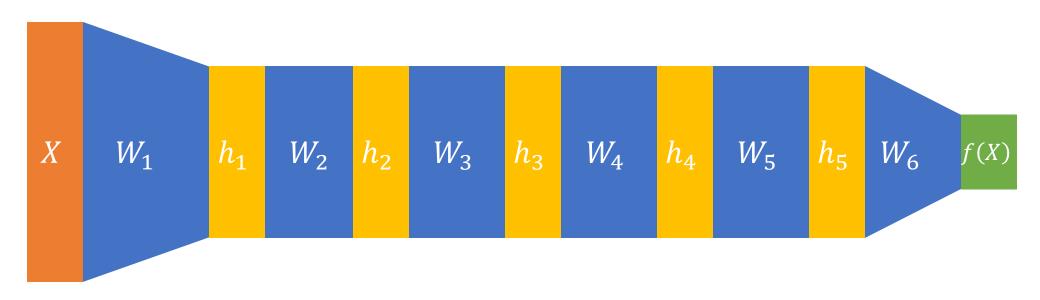
Parameters to learn: $W_1, W_2, W_3, b_1, b_2, b_3$

scores = $W_3 \times \max(0, W_2 \times \max(0, W_1 \times X + b_1) + b_2) + b_3$



Deep Neural Networks

The number of hidden layers and the size of each hidden layer are hyperparameters we need to pick.



Back to Project 4...

P4.3: Forward Pass

We call the computation of the scores the **forward pass** because we are moving *forward* through the graph.

Loss Function

We already have a function to tell us how good we are doing at classifying our images: the SVM loss!

Incorrect class score
$$L = \sum_{\forall i \setminus y} \begin{cases} f_i(X) + \Delta - f_y(X) & \text{if } f_y(X) < f_i(X) + \Delta \\ 0 & \text{otherwise} \end{cases}$$

In English: For each incorrect class, add its loss to the total, if it wasn't less than the correct class by the margin.

We will reuse the same loss function as for the linear classifier!

Regularization

We will apply regularization to the weight matrix just like in the linear classifier.

But this time, we have two weight matrices!

$$L_{reg}(W_1,W_2) = \alpha \left(\sum_{i=1}^{D\times J} \left(w_1^{(i)}\right)^2 + \sum_{i=1}^{J\times K} \left(w_2^{(i)}\right)^2\right)$$
Regularization coefficient Sum of all the squared weights in the weight matrices

P4.3: Loss & Regularization

This will look very similar to the loss function in the linear classifier!

```
function nn_svm_loss(params, X, y, reg=0)
   W1, b1 = params["W1"], params["b1"]
   W2, b2 = params["W2"], params["b2"]
   N, D = size(X)

    Replace with your computed value.

   scores, hidden = nothing, nothing
   # TODO: Use the nn forward() function to perform the forward pass, then
   # calculate the svm loss. Remember the regularization term on both
   # weight matrices.
                                                                     Your turn!
   # Get the gradients.
   grads = nn svm grad(params, X, y, scores, hidden, reg)
                                                                     Calculate the loss here.
   return loss, grads
end
                                       Provided gradient computation
```

Updating the Weights

We know that our fully connected neural network is differentiable, so we can analytically calculate the gradients for each parameter.

Gradients are provided for you in P4.3.

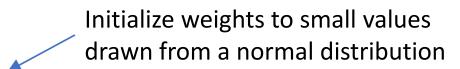
Updating the Weights

We know that our fully connected neural network is differentiable, so we can analytically calculate the gradients for each parameter.

Gradients are provided for you in P4.3.

We can use Gradient Descent to update W_1 , b_1 , W_2 and b_2 just like we did in P4.2 (no bias trick this time!)

Training algorithm:



```
W1, W2 ← randn(J, D)*eps, randn(K, J)*eps
b1, b2 ← zeros(J), zeros(K) ← Initialize biases to zero
for iteration in 1:N do:
   loss = SVM_loss(W1, W2, b1, b2, X, y)
   dW1,dW2,db1,db2 = nn_grads(W1,W2,b1,b2,X,y)
   W1 = W1 - step_size * dW1
   b1 = b1 - step_size * db1
   W2 = W2 - step_size * dW2
   b2 = b2 - step_size * db2
```

Training algorithm:

Initialize weights to small values drawn from a normal distribution

```
W1, W2 \leftarrow randn(J, D)*eps, randn(K, J)*eps
b1, b2 \leftarrow zeros(J), zeros(K) Initialize biases to zero
for iteration in 1:N do:
loss = SVM_loss(W1, W2, b1, b2, X, y)
dW1,dW2,db1,db2 = nn_grads(W1,W2,b1,b2,X,y)
W1 = W1 - step_size * dW1
b1 = b1 - step_size * dW1
W2 = W2 - step_size * dW2
b2 = b2 - step_size * db2
```

Training algorithm:

Initialize weights to small values drawn from a normal distribution

```
W1, W2 \leftarrow randn(J, D) *eps, randn(K, J) *eps
         b1, b2 \leftarrow zeros(J), zeros(K) \leftarrow Initialize biases to zero
                                                                    Sample a
         for iteration in 1:N do:
                                                                     batch!
               loss = SVM loss (W1, W2, b1, b2, X, y) \leftarrow Calculate the loss.
For a fixed number
               dW1, dW2, db1, db2 = nn grads(W1, W2, b1, b2, X, y)
of iterations...
               W1 = W1 - step size * dW1
               b1 = b1 - step size * db1
               W2 = W2 - step size * dW2
               b2 = b2 - step size * db2
```

Training algorithm:

Initialize weights to small values drawn from a normal distribution

b2 = b2 - step size * db2

Training algorithm:

Initialize weights to small values drawn from a normal distribution

b2 = b2 - step_size * db2 Update the parameters with gradient descent

```
function train nn(params, X, y, num classes, lr=0.01, reg=1e-3, batch=20, num iters=100, print freq=100)
   N, D = size(X)
   losses = zeros(num iters)
   for it in 1:num iters
       # TODO: Sample a random batch, calculate the loss and gradients, and update
       # all the weights in params. Place the loss for this iteration at
       # losses[it].
                                                                                        Your turn!
       if it % print freq == 0
                                                                                        Write the training loop
           println("Iteration ", it, ": average loss = ", sum(losses) / it)
       end
                                                                                        here.
   end
   return losses, params
end
```

Tuning hyperparameters

The regularization coefficient and learning rate need to be tuned, like in P4.2.

The number of nodes (or neurons) in the hidden layer can also be tuned.

See last lecture (Lecture 12 on Optimization) for how to tune parameters.

```
# Define constants.
hidden dims = 36
num iters = 1500
                    hyperparameters
batch = 20
reg = 1e-5
lr = 1e-1
# Initialize weights.
W1 = 1e-4 * randn(DIM, hidden dims)
b1 = zeros(1, hidden dims)
W2 = 1e-4 * randn(hidden dims, num classes)
b2 = zeros(1, num_classes)
params = Dict([("W1", W1), ("b1", b1), ("W2", W2), ("b2", b2)])
# Train the network.
losses, params = train nn(params, x train, y train, num classes, lr, reg, batch, num iters)
# Plot the losses.
plot(1:num_iters, losses)
                              This line calls your training function.
```

params contains the optimized

weights when it's finished.

Backpropagation is an algorithm to compute gradients of arbitrarily large networks.

It uses the **chain rule** (from calculus).

Backpropagation is an algorithm to compute gradients of arbitrarily large networks.

Step 1: Express a function as a graph.

$$f(x,y,z) = (x + y) \cdot z$$

$$y$$

$$+ q = x + y$$

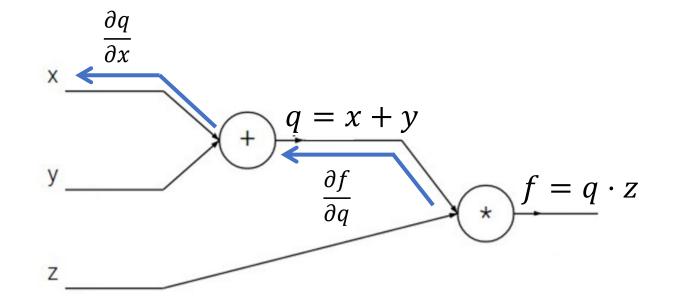
$$* f = q$$

Backpropagation is an algorithm to compute gradients of arbitrarily large networks.

Step 2: Compute gradients.

$$f(x, y, z) = (x + y) \cdot z$$

$$\frac{\partial f}{\partial x} = \frac{\partial q}{\partial x} \frac{\partial f}{\partial q} = 1 \cdot z$$
The chain rule!

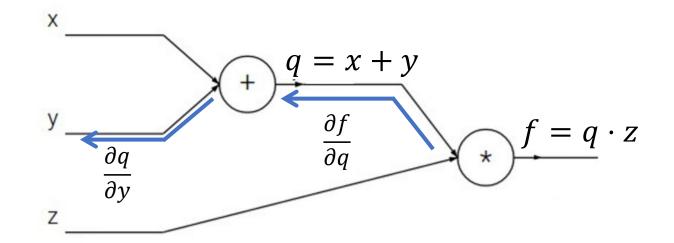


Backpropagation is an algorithm to compute gradients of arbitrarily large networks.

Step 2: Compute gradients.

$$f(x,y,z) = (x+y) \cdot z$$

$$\frac{\partial f}{\partial y} = \frac{\partial q}{\partial y} \frac{\partial f}{\partial q} = 1 \cdot z$$

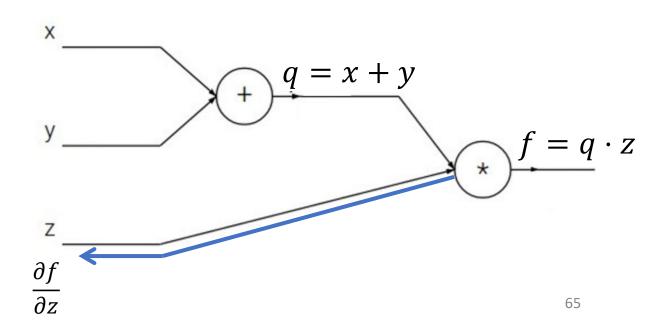


Backpropagation is an algorithm to compute gradients of arbitrarily large networks.

Step 2: Compute gradients.

$$f(x, y, z) = (x + y) \cdot z$$

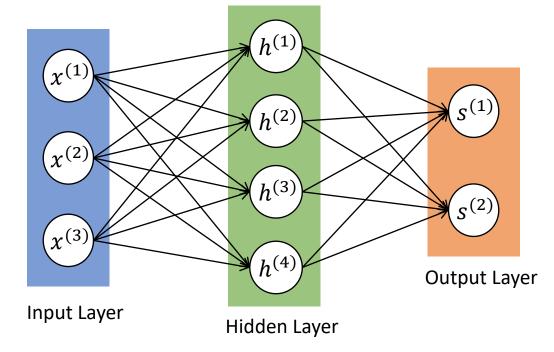
$$\frac{\partial f}{\partial z} = q$$



Backpropagation is an algorithm to compute gradients of arbitrarily large networks.

Instead of computing the derivative of the loss for a huge network, compute the gradient of each layer with respect to the input.

Then we can *propagate* the gradients backwards through the graph.

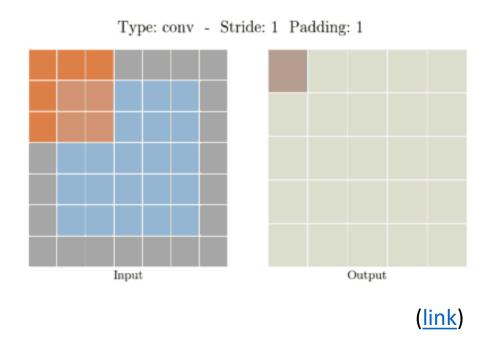


Where to go from here: Convolutional Neural Networks

Many modern deep learning methods for computer vision use Convolutional Neural Networks (CNNs).

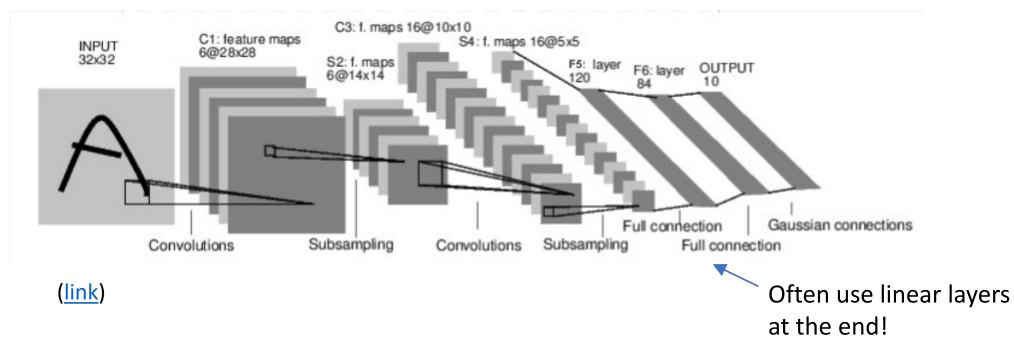
Instead of flattening the image into a vector and having a giant weight matrix, we slide a *kernel* across the image. This is a **convolution**.

This model assumes that parts of the image close to each other likely have similar features.



Where to go from here: Convolutional Neural Networks

Many modern deep learning methods for computer vision use Convolutional Neural Networks (CNNs).



Further Reading:

- CS231n on Neural Networks
 - https://cs231n.github.io/neural-networks-1/
- Prof. Patrick Winston explains Neural Nets (<u>YouTube</u>)
- <u>PyTorch</u> is a great library (in Python) for implementing neural networks