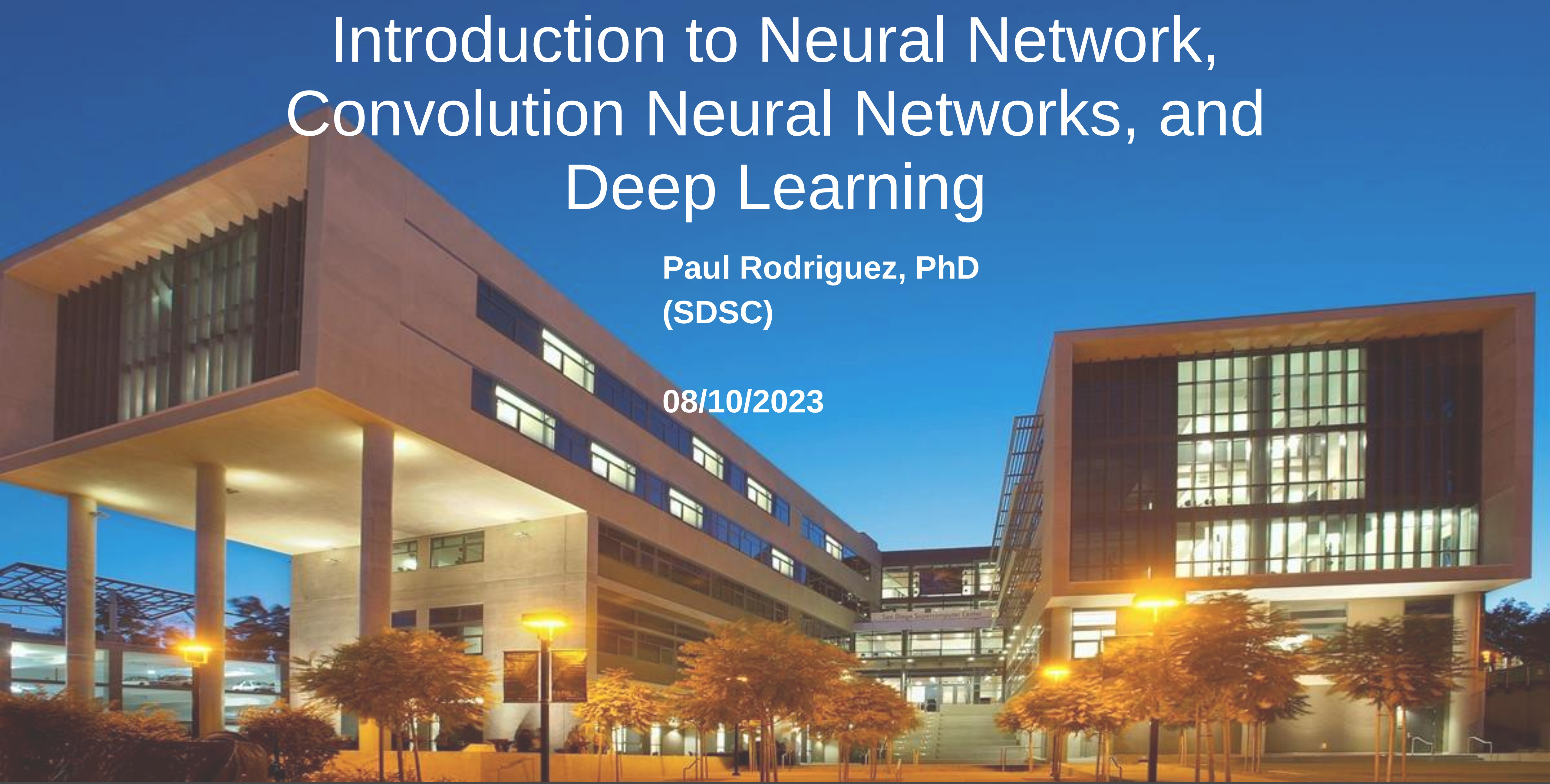
Introduction to Neural Network, Convolution Neural Networks, and Deep Learning

Paul Rodriguez, PhD
(SDSC)

08/10/2023



SDSC SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

Schedule overview

Mai Nguyen, Paul Rodriguez

- **Yesterday - Scaling**
  - R on HPC
  - Spark

- **Todoay – Deep Learning**
  - Part 1A Intro to NN/CNN/Deep Learning
  - Part 1B Practical Guidelines and Multinode execution
  - DL Layers and Models
  - DL Transfer Learning
  - DL Functional API, Special Connections, Transformers

Outline

- **Part I A**

Overview of Neural Networks (aka Multilayer Perceptron)

Convolution Neural Networks and Scaling

Exercise, MNIST classification

- **Part I B**

Practical Guidelines: Hyperparameters, Workflows, GPUs

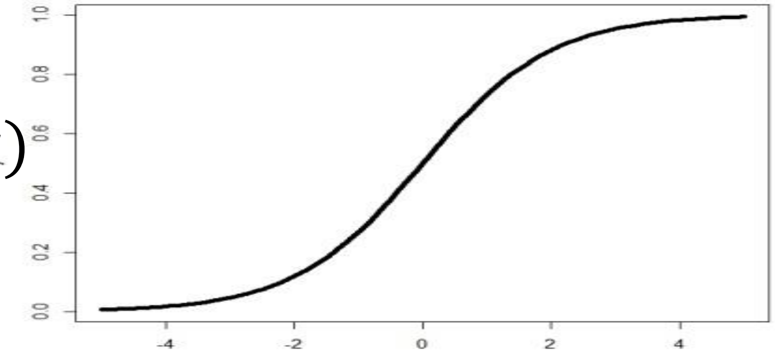
Exercise, Multinode MNIST

Logistic Regression to Neural Network

$$f(x, b, w) = \frac{\exp^{(b+w*x)}}{1+\exp^{(b+wx)}} = \frac{1}{1+exp^{(-(b+wx))}}$$

for parameters: $b = 0 \;\; , \; w_1 = 1$

$y = f(x)$



x

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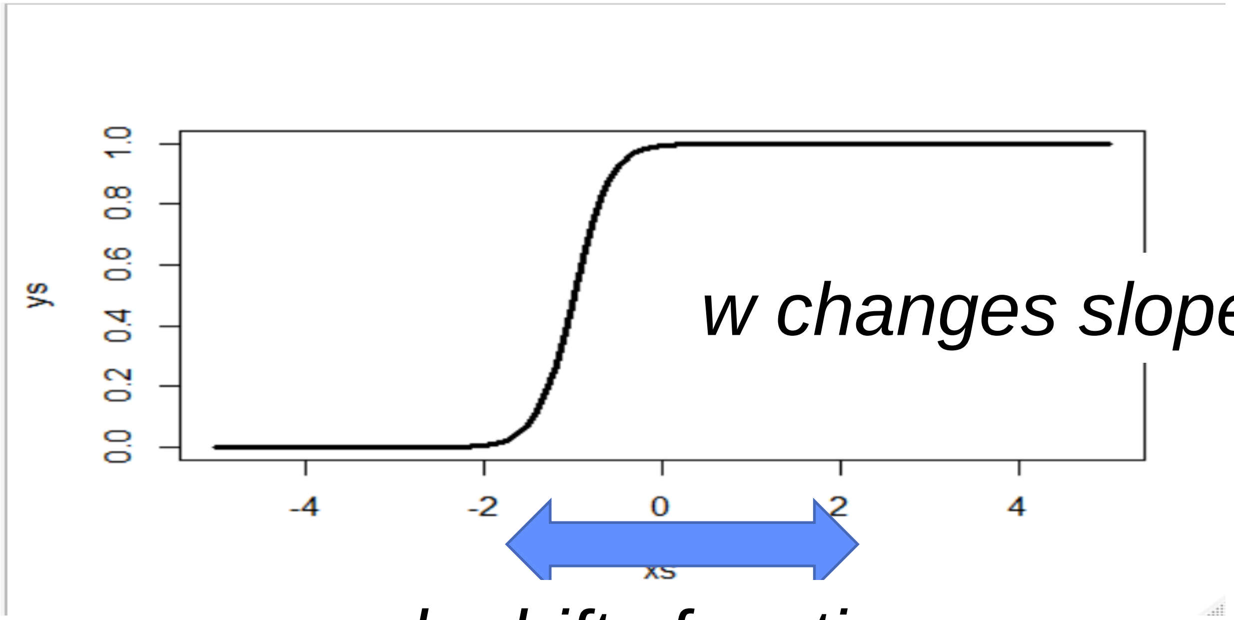
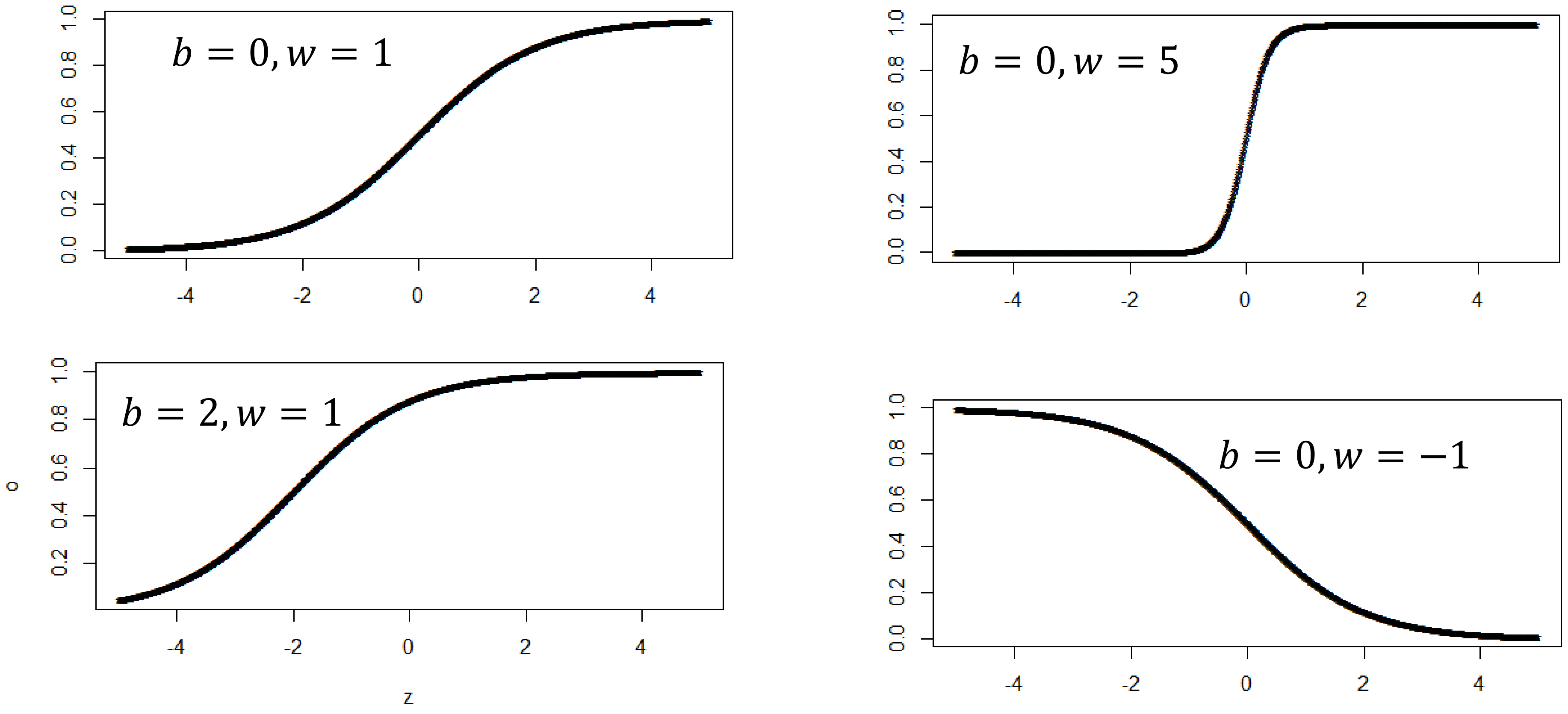


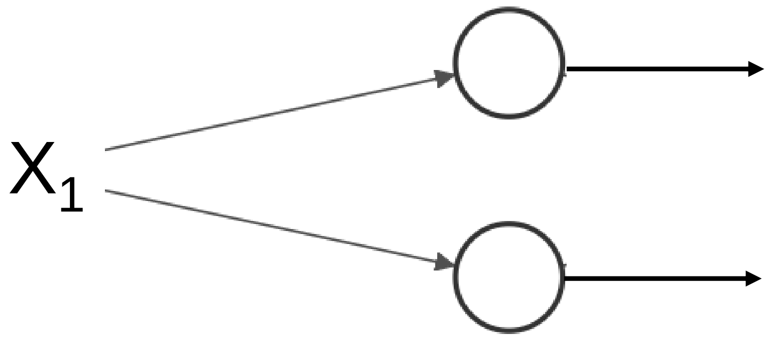
w changes slope

b shifts function

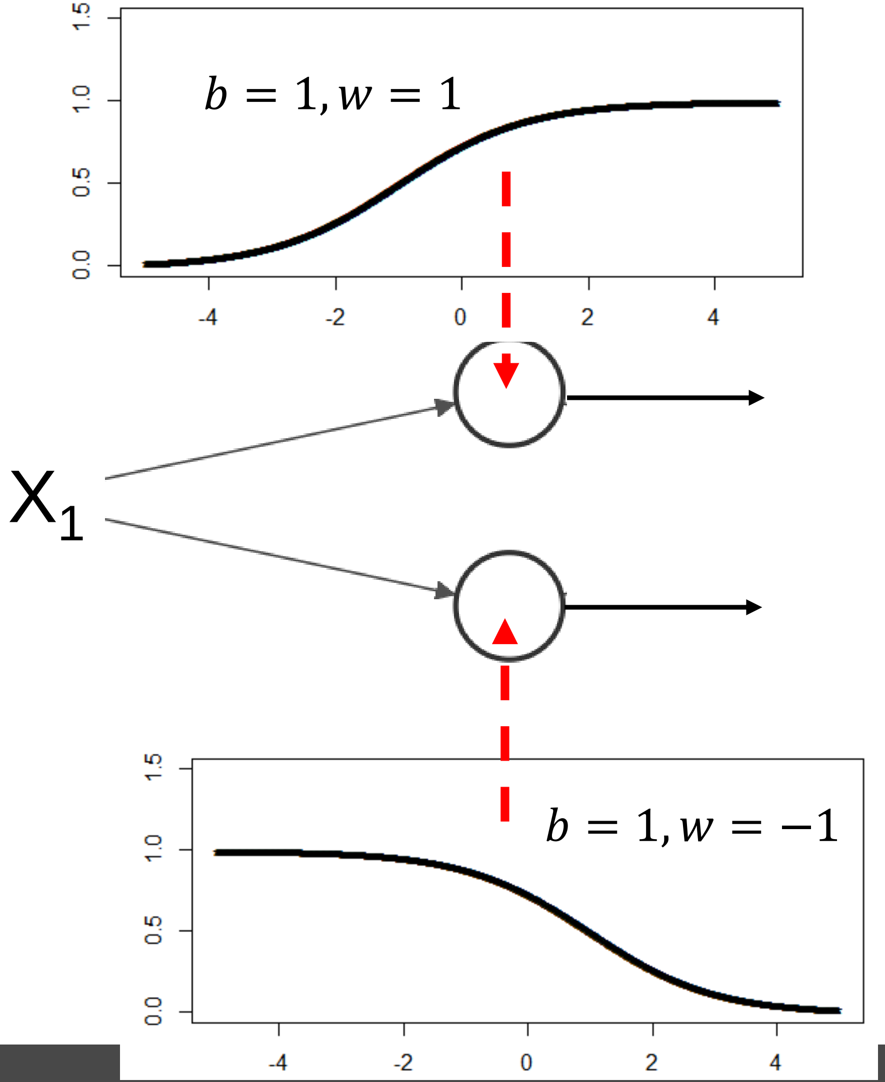
Logistic function w/various weights



Example: 1 input into 2 logistic units



Example: 1 input into 2 logistic units with these activations



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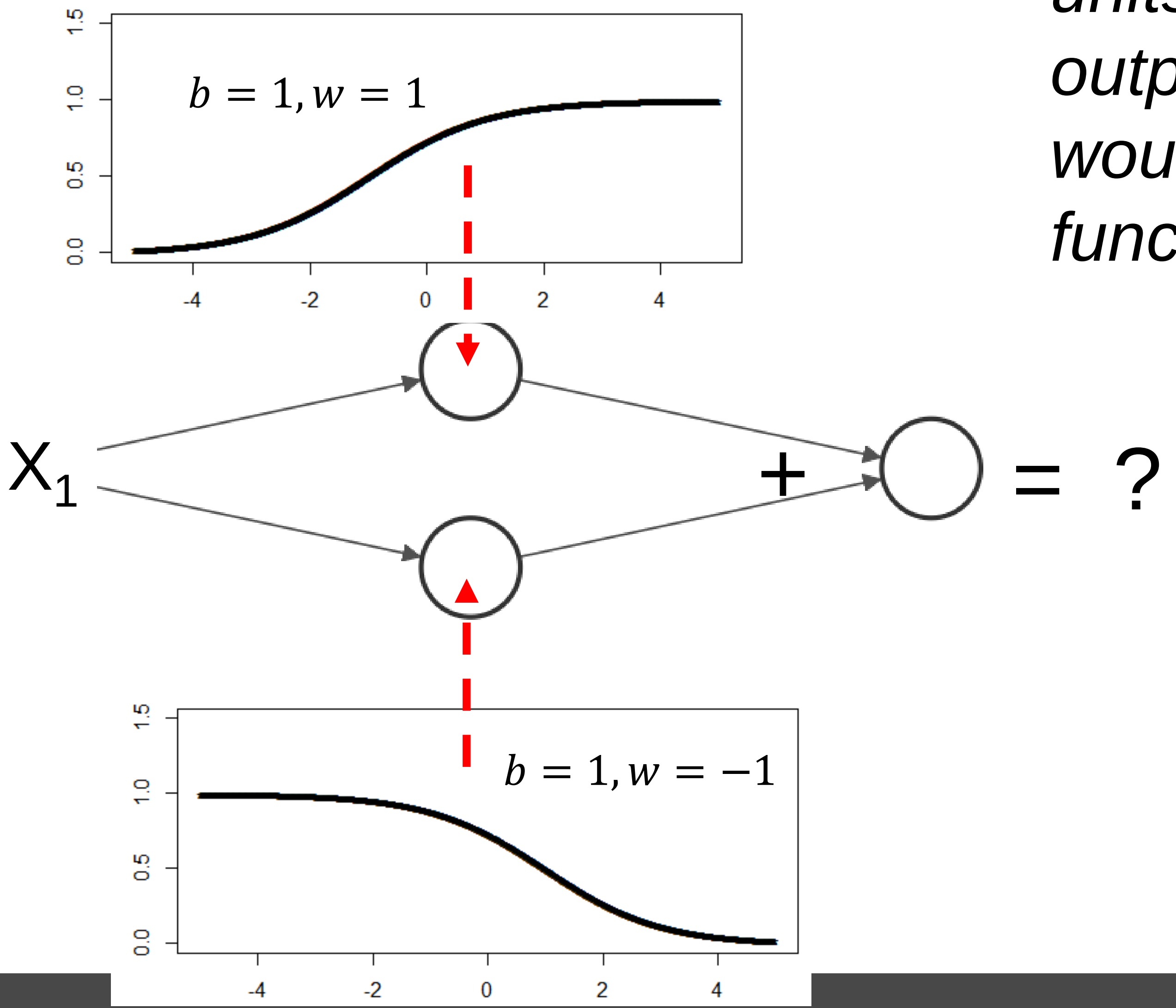
If you add these 2 units into a final output unit what would the output function look like?



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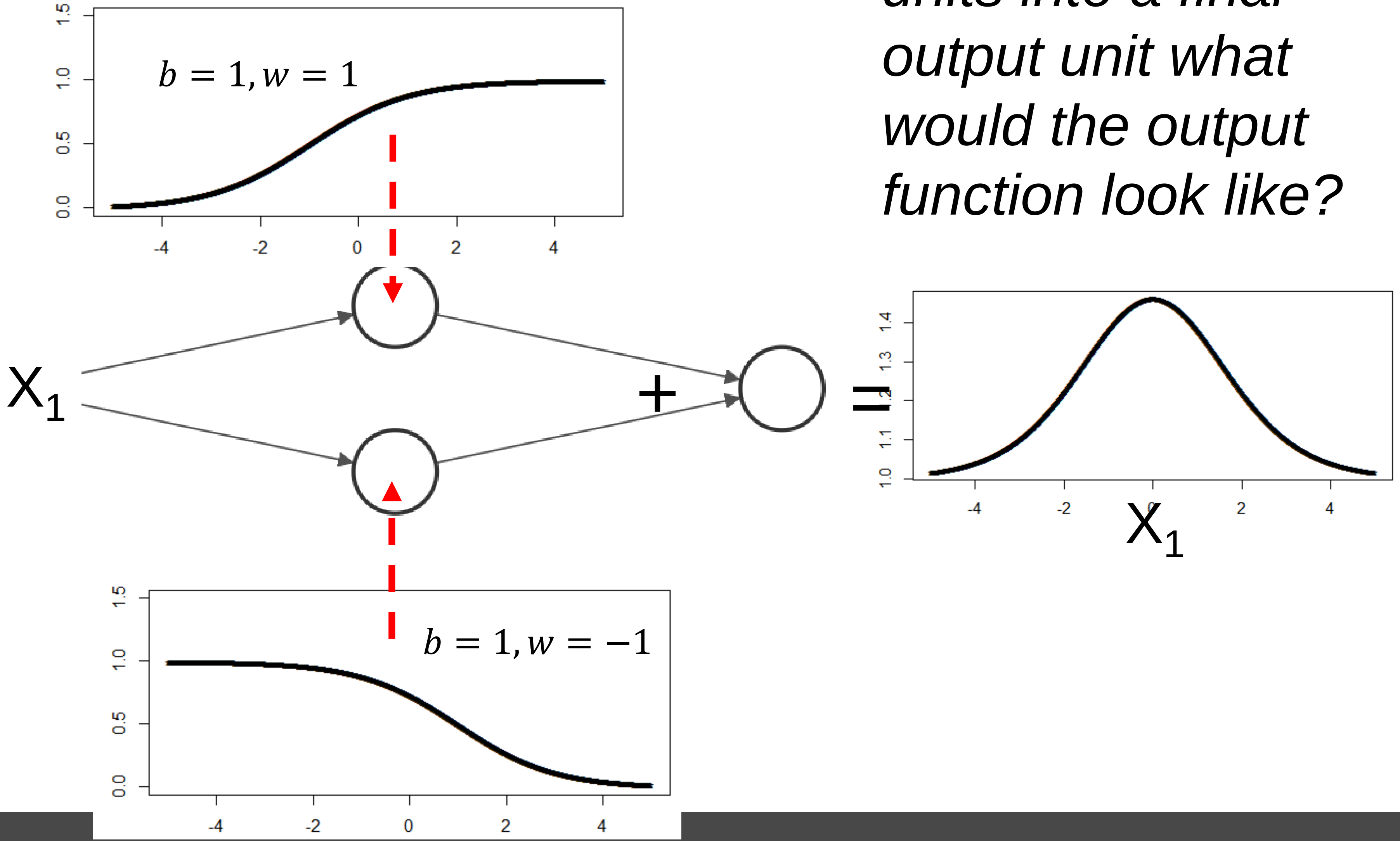
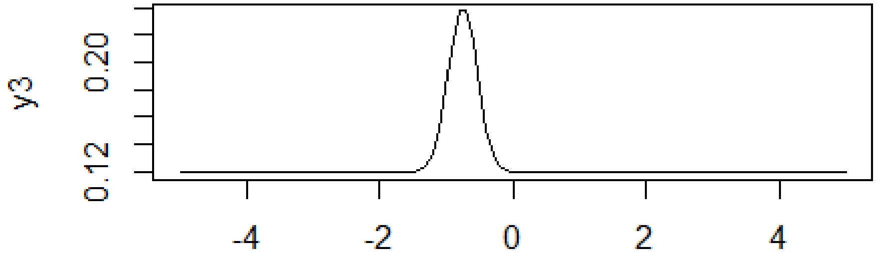
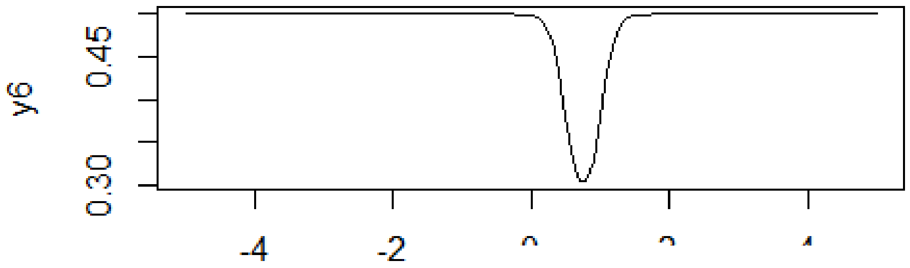


Higher level function combinations

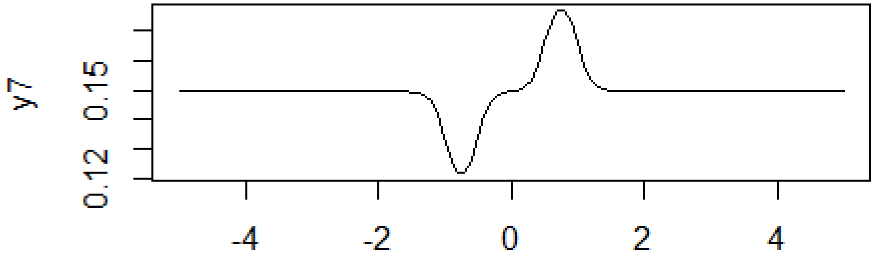
```
x=seq(-5,5,.1)
y1=1/(1+exp(10+   10*x))
y2=1/(1+exp(-5+(-10)*x))
y3=1/(1+exp(1+1*y1+1*y2))
plot(x,y3,type="l")
```




```
y4=1/(1+exp(10+ (-10)*x))
y5=1/(1+exp(-5+(10)*x))
y6=1/(1+exp(1-1*y4-1*y5))
plot(x,y6,type="l")
```




```
y7=1/(1+exp(1+2*y3+1*y6))
plot(x,y7,type="l")
```



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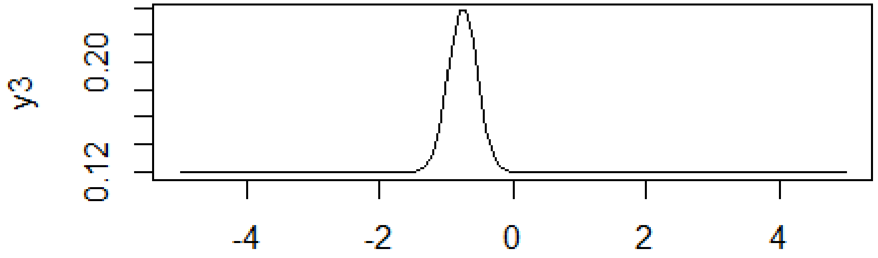

Multiple layer networks can represent any logical or real-valued functions (unbiased, but potential to overfit)

```
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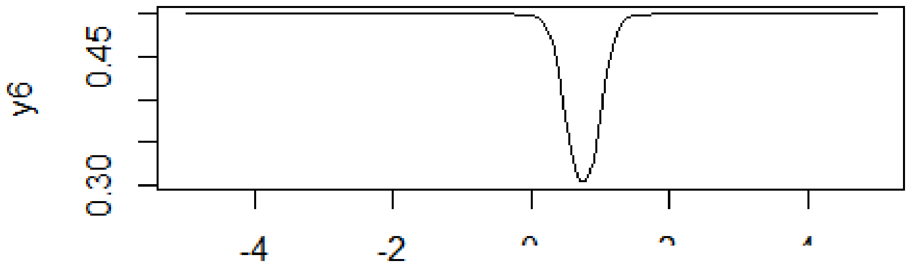


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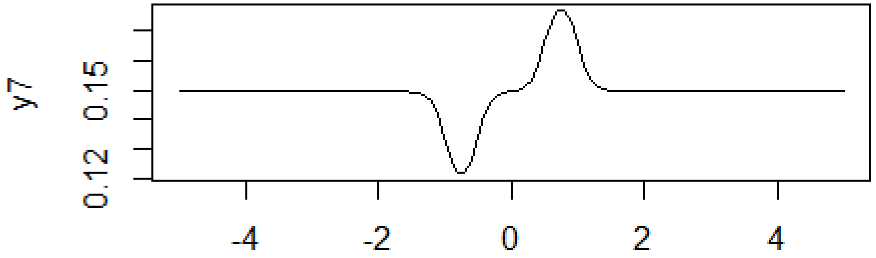

Logistic to Neural Network model

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Draw out function as a little graph, 1 input

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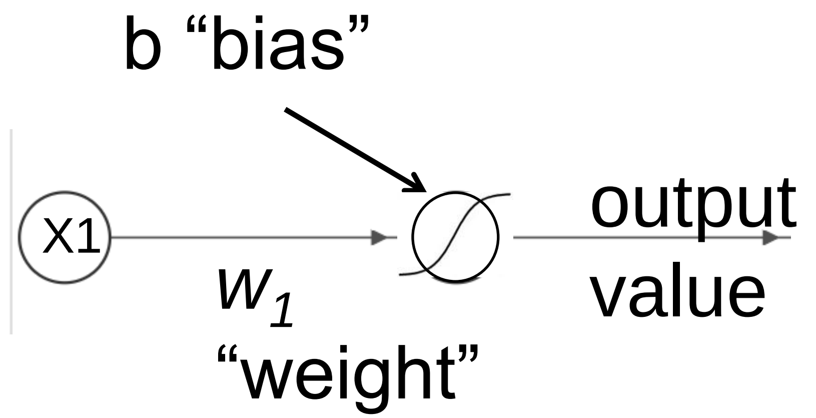

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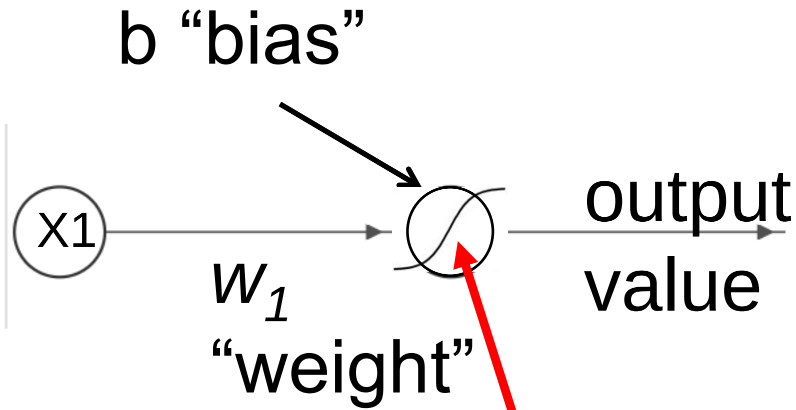
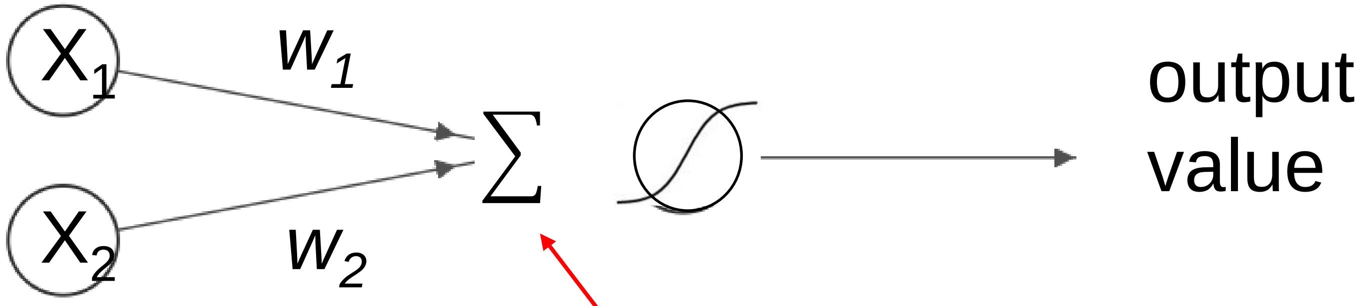


Draw out function as a little graph, 1 input

logistic function will transform input to output – call it the ‘activation’ function

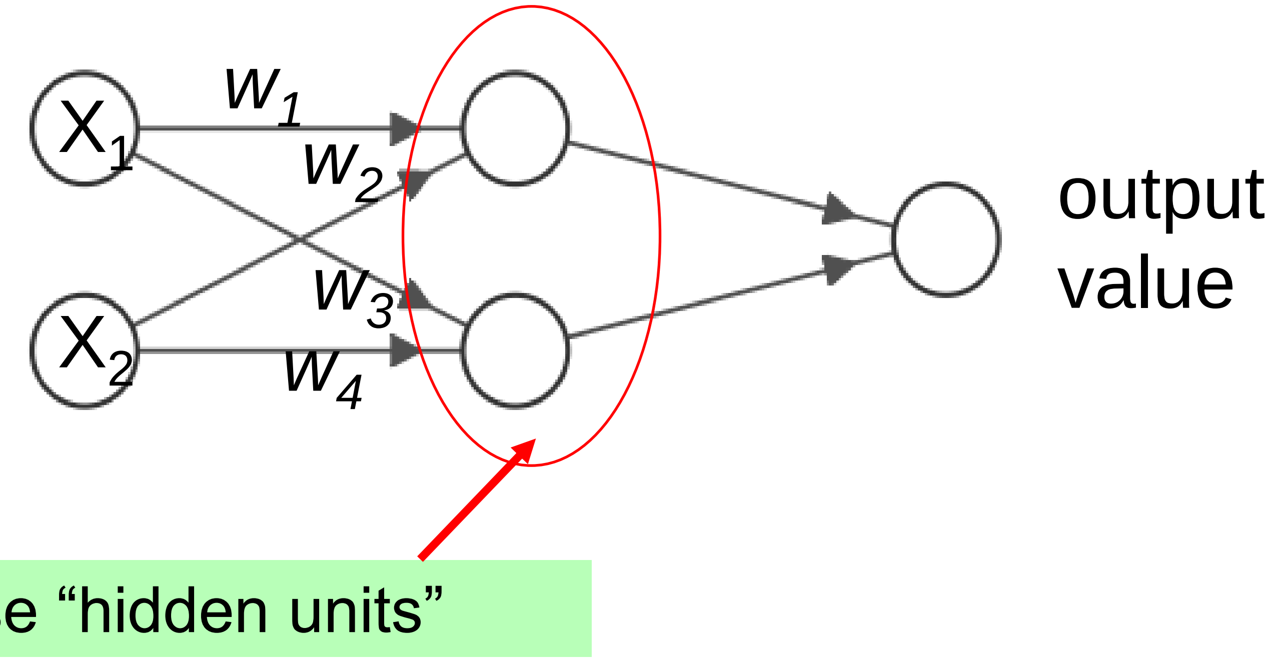
Using 2 input units, the graph model would be:



$b + w1\ x1 + w2\ x2$

We usually don't draw the bias.
We assume inputs*weights are summed (a dot product)

Using 2 input units, 2 intermediate units, and 1 output:



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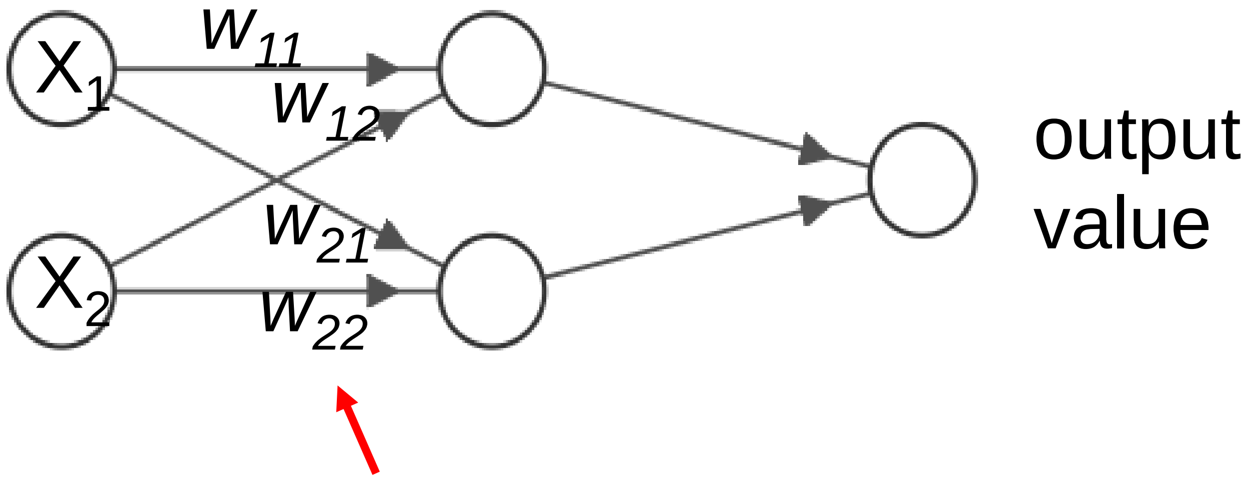
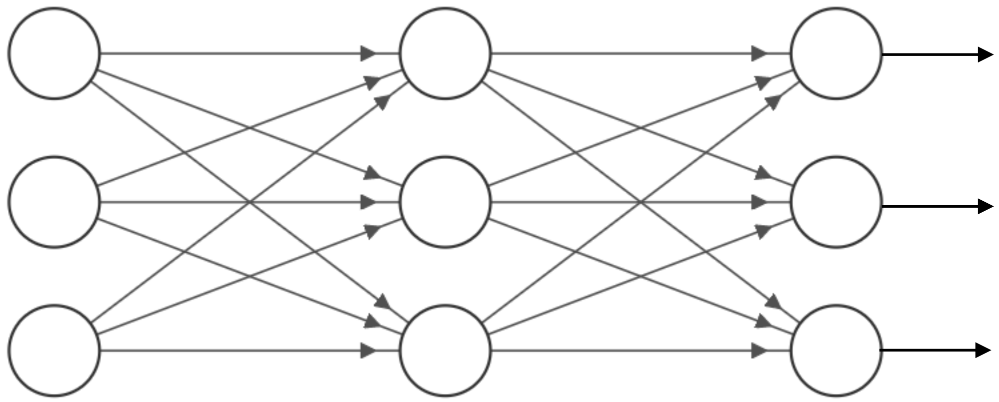


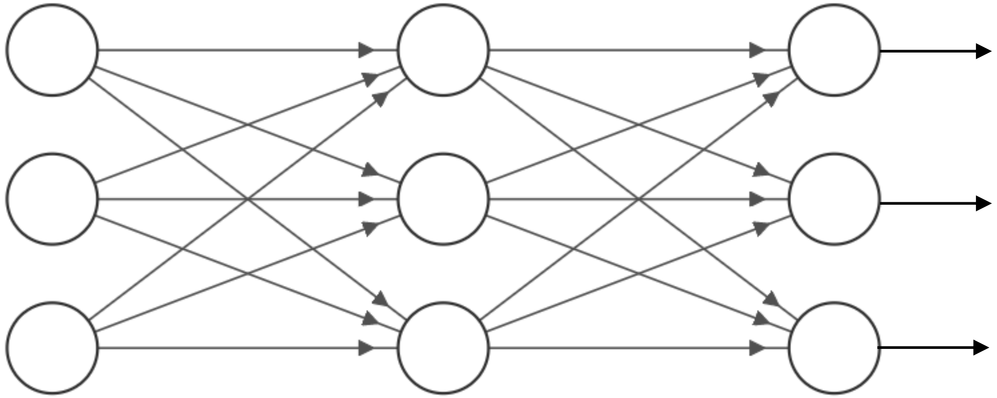
For X a Px1 vector, we can set up indices in a weight matrix so that: W*X = incoming activations from previous layer

More generally, we can add a hidden layer, and have many inputs and outputs



A “Multilayer Perceptron”

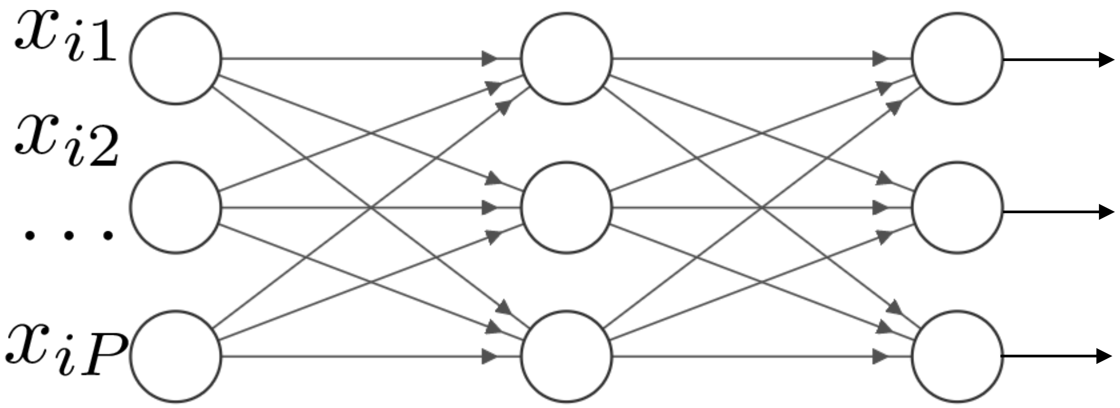
1 Input layer   1 Hidden layer   1 Output



A “Multilayer Perceptron”

1 Input layer   1 Hidden layer   1 Output

P input units for each input *i*

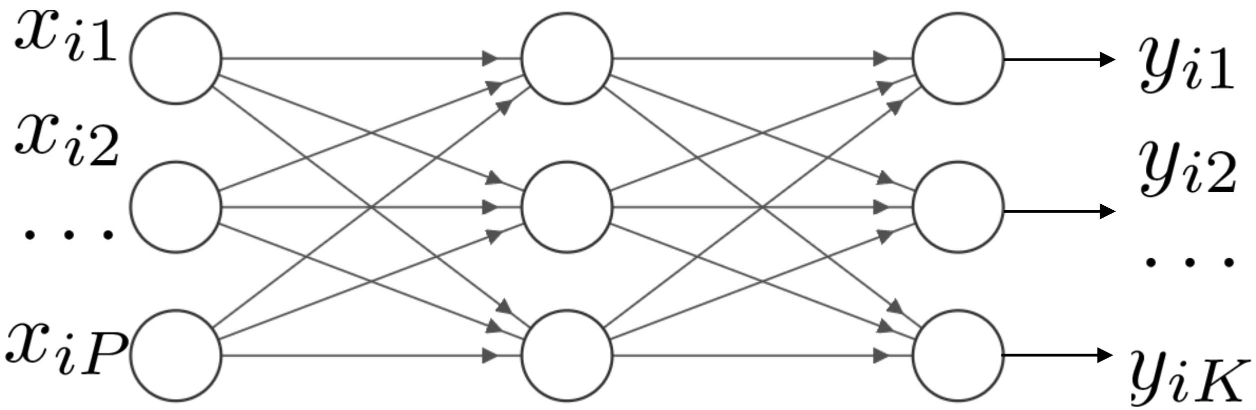


A “Multilayer Perceptron”

1 Input layer

1 Hidden layer

1 Output



P input units for each input *i*

M hidden units

K output units

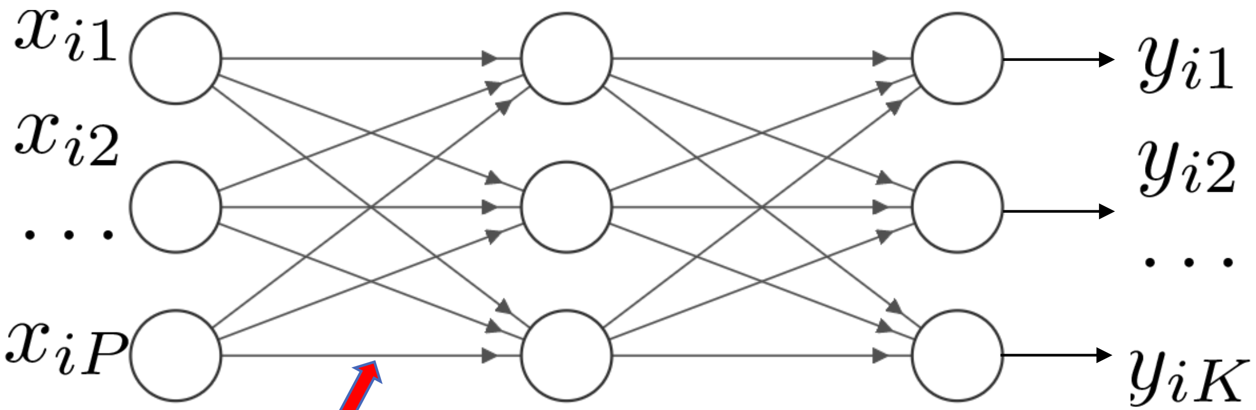
A “Multilayer Perceptron”

1 Input layer

1 Hidden layer

1 Output

P input units for each input *i*

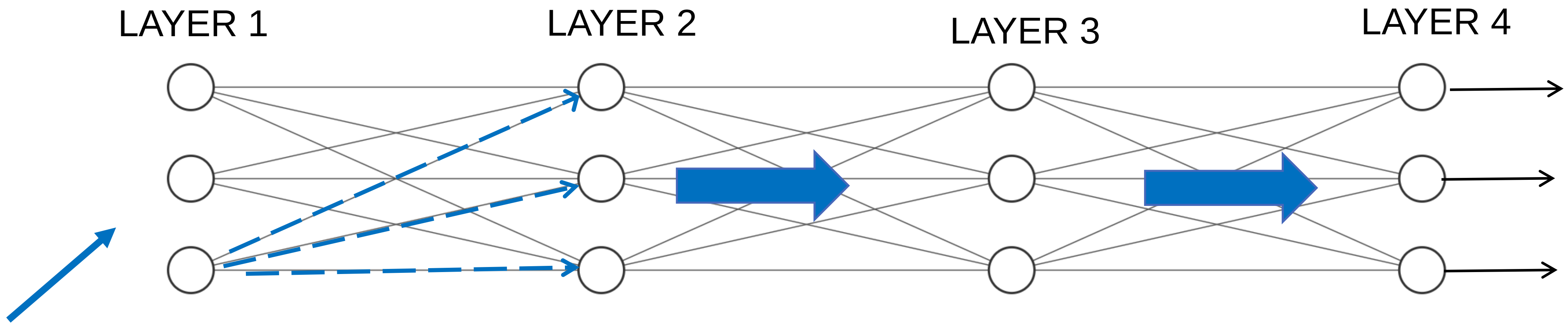


K output units

M hidden units

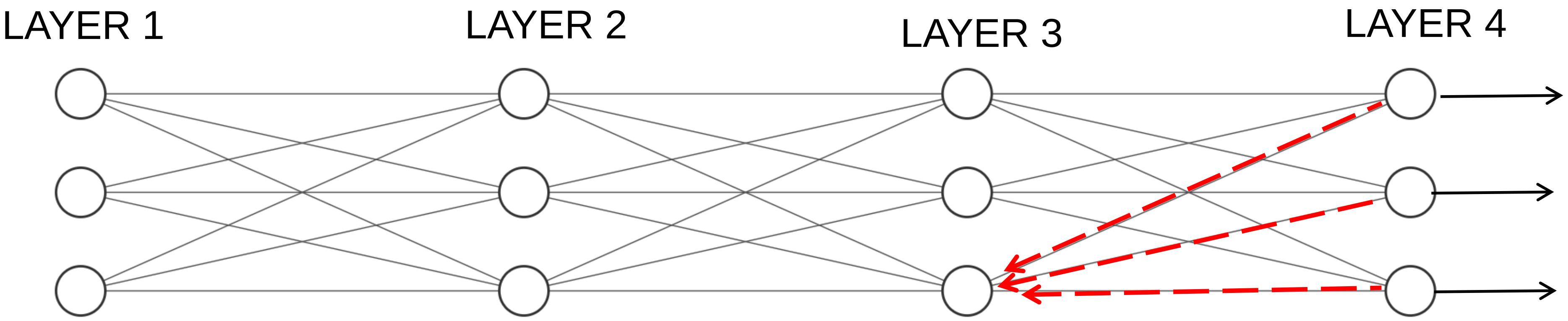
1 weight parameter for each connection

Algorithm steps



1. FORWARD PROPAGATE AN ENTIRE BATCH OF INPUTS

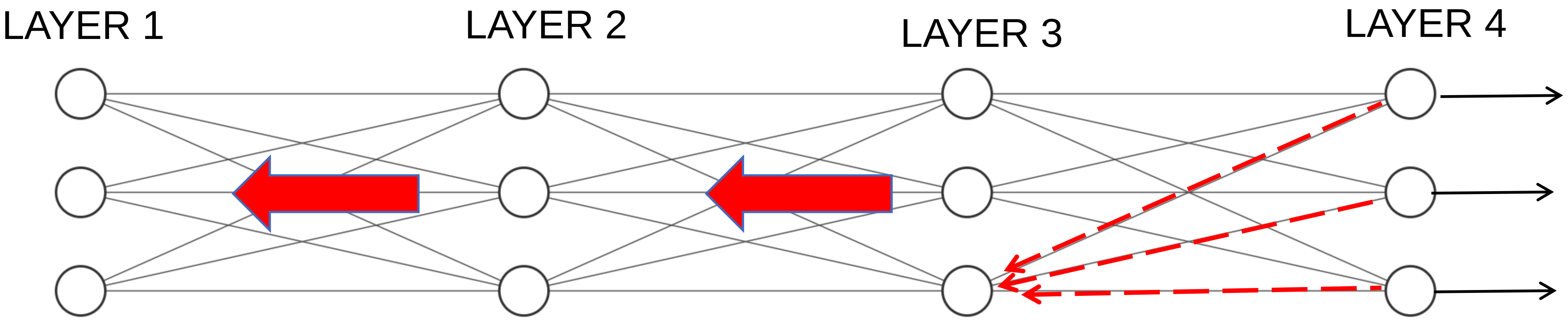
Algorithm steps



2. BACKWARD PROPAGATE ERROR FOR WHOLE BATCH USING DERIVATIVE CHAIN RULE:

$$\frac{dE}{dw_{mp}} = \sum_{k}^{K} \frac{dE_k}{d\hat{y}_k} \frac{d\hat{y}_k}{da_k} \frac{da_k}{dh_m} \frac{dh_m}{da_m} \frac{da_m}{dw_{mp}}$$

Algorithm steps and Vanishing Gradients



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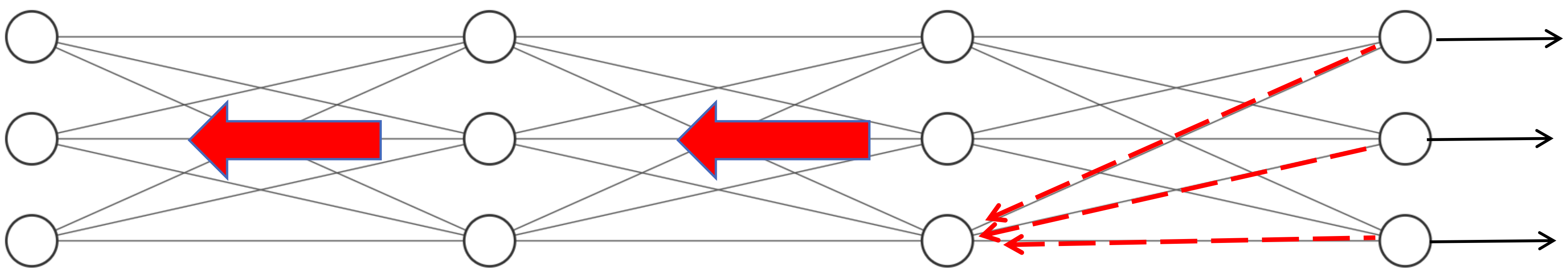
Note: As you go farther back, the error information gets diluted and the error gradient starts 'vanishing'

Algorithm steps and Vanishing Gradients



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Note: As you go farther back, the error information gets diluted and the error gradient starts 'vanishing'

A different activation function helps …

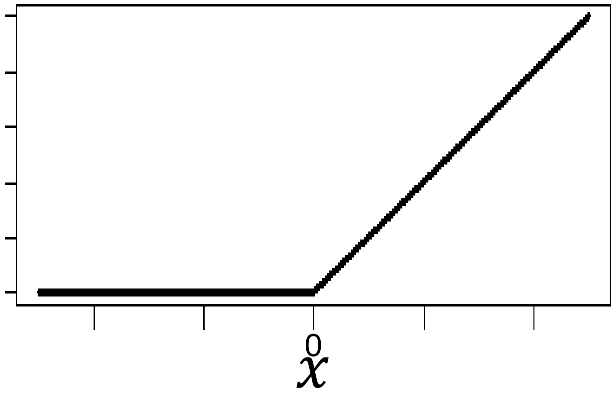
The rectified linear unit (RELU)

RELU activation function

It is unscaled (bad!)

But *df/da* is constant (good!)

RELU (rectified linear unit)



$$f(a) = \begin{cases} a & a > 0 \\ 0 & a <= 0 \end{cases}$$

where $a = XW$

Overall, RELU mitigates vanishing gradients

The Neural Network Algorithm

INITIALIZE weights to small value (for example: +/- <0.3)

LOOP until stopping criterion:

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UPDATE WEIGHTS: ***w*** **←** ***w*** – ***learning_rate*** $* \ \frac{dL}{dw}$

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STOP: when validation error reaches minimum or after a max number of epochs

The Neural Network Algorithm [and heuristics]

INITIALIZE weights to small value (for example: +/- <0.3)

LOOP until stopping criterion:

[work in batches of input]

FORWARD PROPAGATION: calculate all node activations

BACKWARD PROPAGATION: calculate all error derivatives to ***minimize Loss***

UPDATE WEIGHTS: $w \leftarrow w - \text{learning\_rate} * \frac{dL}{dw}$

[adapt learning rate, use momentum]

STOP: when validation error reaches minimum or after a max number of epochs

[several metrics of loss are possible]

Neural Network main options to choose:

- 1 Architecture: number of hidden units & layers
- 2 Optimizer and learning rate
- 3 Loss function depends on task
- Note: more hidden layers, more hidden units => more potential for overfitting

terminology and cheat sheet on output activations (for reference):

Type of Problem	Y outputs	Output Activation Function (this gives a SCORE= $\hat{Y}$)	Output PREDICTION (what you decide to predict)	Output Loss Function	Evaluative Measure
Regression: map into K real valued predictions	if $Y \in (-\infty, +\infty)^K$	$\hat{Y} = XW$	$\hat{Y}$	Sum Squared Error (SSE)	Mean Squared Error (MSE)
Multivariate output of 0's and 1's	if $Y \in [0,1]^K$	$\hat{Y} = \frac{1}{1+exp^{-(XW)}}$	1 or 0	SSE	MSE
Binary Classification	if $Y \in \{0,1\}$	$\hat{Y} = \frac{1}{1+exp^{-(XW)}}$	A probability given by $\hat{Y}$: $P(y=1\|x)$	Cross Entropy $L = -ylog(\hat{y}) - (1-y)(log(\hat{y}))$	Accuracy, ROC
Multiclassification	if $Y \in \{0,1\}^K$	$\hat{Y}_k = \frac{exp^{-(XW_k)}}{\sum_k exp^{-(XW_k)}}$	Max class	Cross Entropy $L = -\sum_k y_k log(\hat{y_k})$	Accuracy

Summary:

Pro:

- Multilayer Perceptron, and Neural Networks in general, are flexible powerful learners
- Hidden layers learn a nonlinear transformation of input

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- Multilayer Perceptron, and Neural Networks in general, are flexible powerful learners
- Hidden layers learn a nonlinear transformation of input

Con:

- Lots of parameters
- Hard to interpret
- Needs more data

A neural network can discover visual features using ‘convolutions’

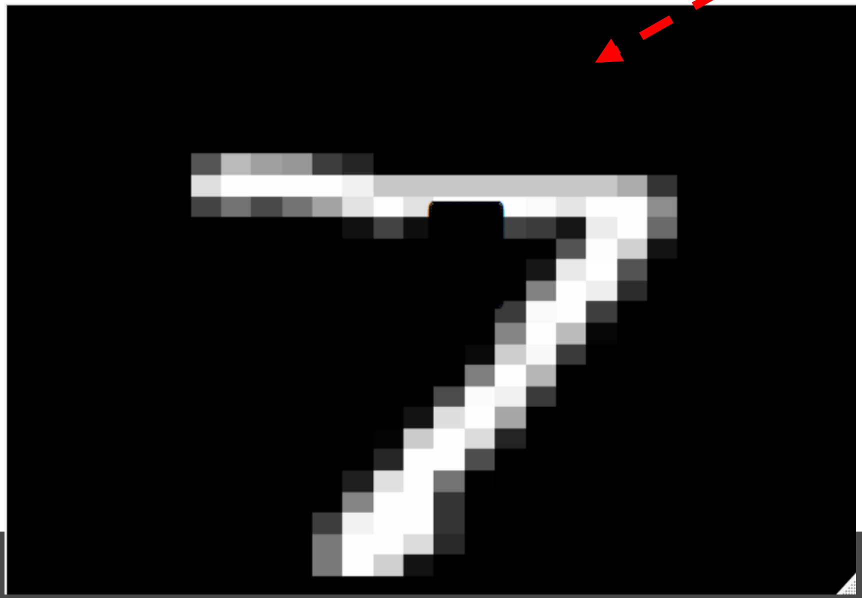
Next: Image classification of digits

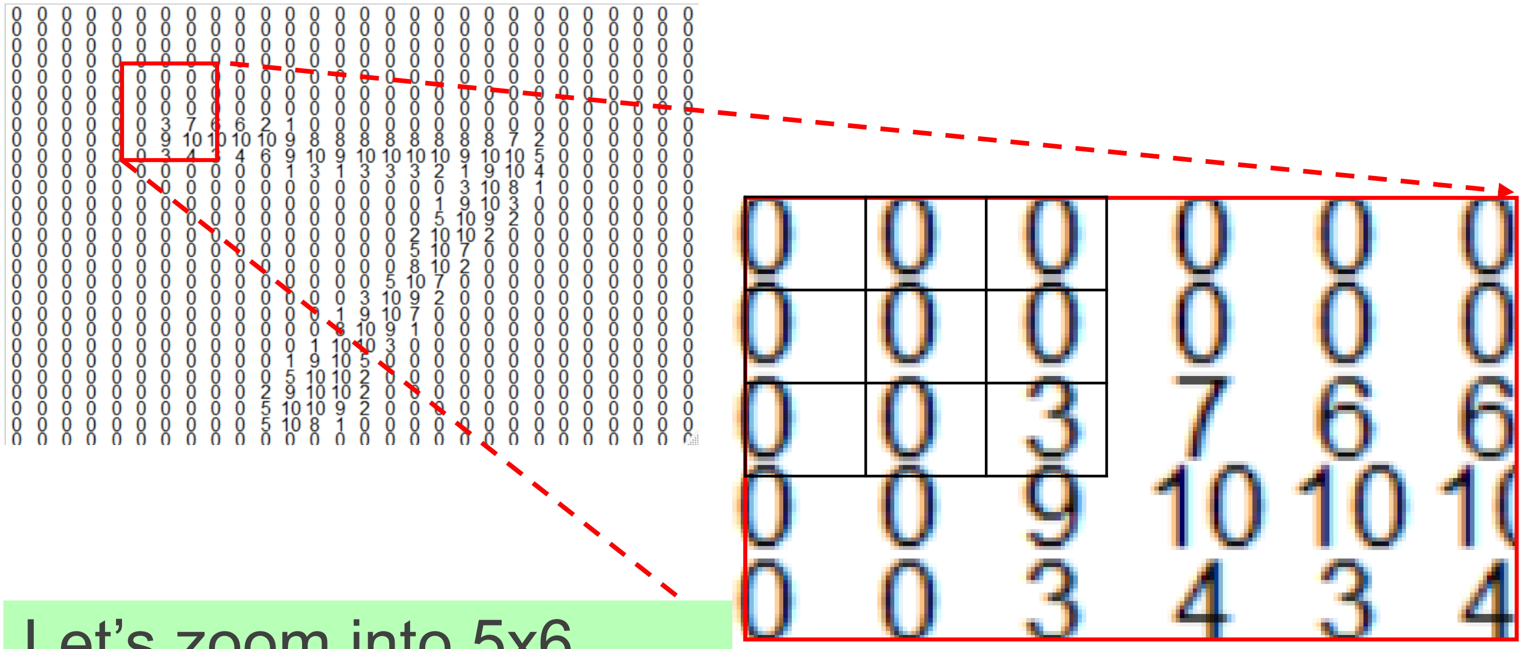
Image features

- **MNIST - A database of handwritten printed digits**

  (National Inst. of Standards and Technology)

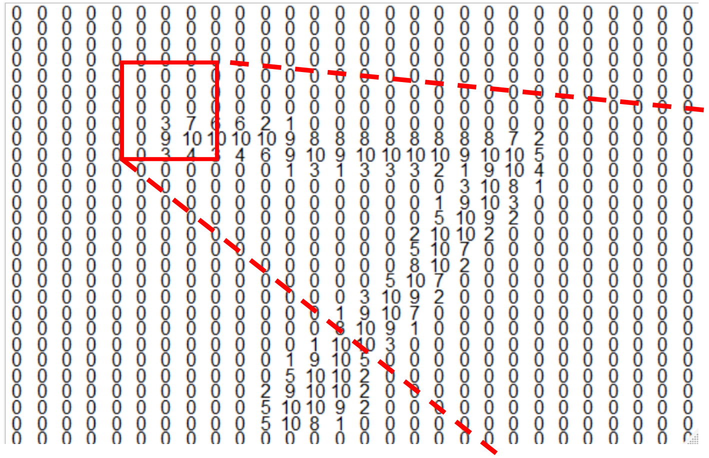
How to classify digits?





Let’s zoom into 5x6 window of pixels near the tip of ‘7’

Take a 3x3 patch of pixels and apply a ‘filter’ template – designed to find an edge



0	0	0	0	0	0
0	0	0	0	0	0
0	0	3	7	6	6
0	0	9	10	10	10
0	0	3	4	3	4

X

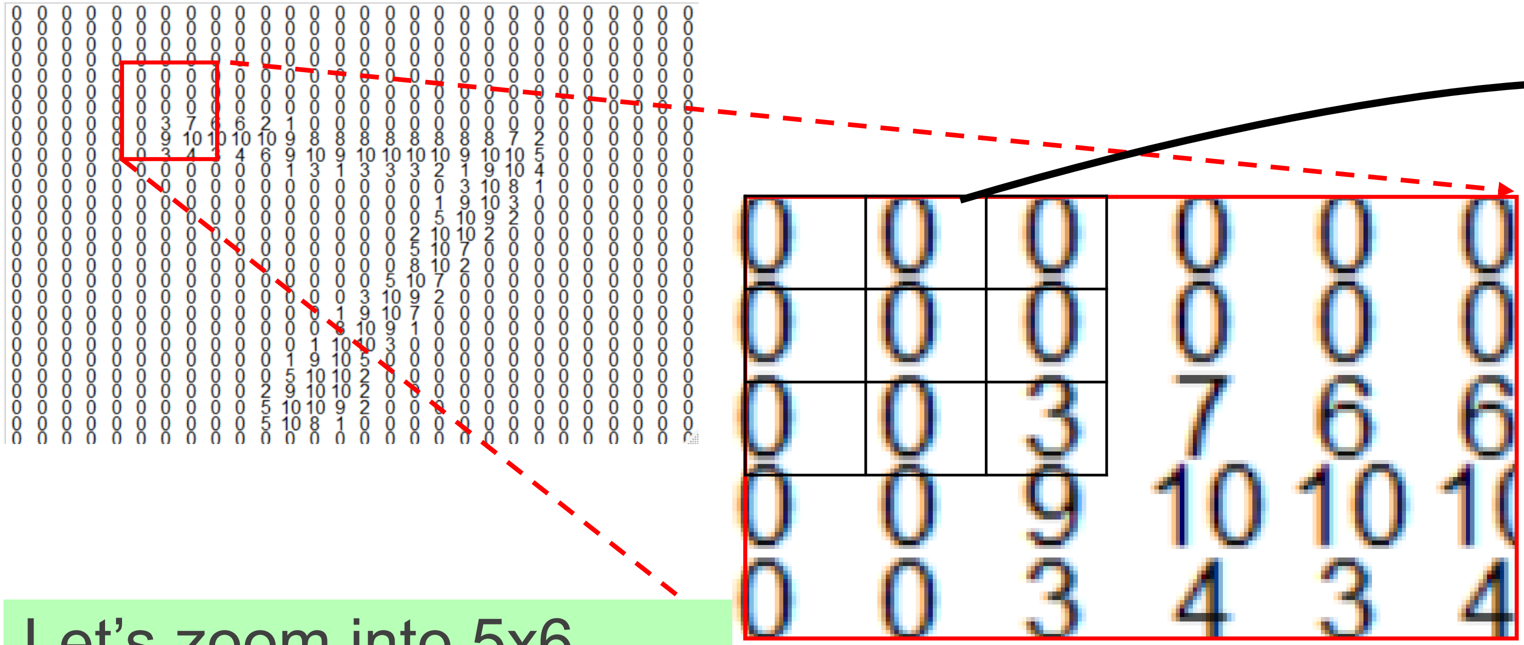
-1	0	+1
-1	0	+1
-1	0	+1

1. Multiply 3x3 patch of pixels with 3x3 filter

Let’s zoom into 5x6 window of pixels near the tip of ‘7’

Take a 3x3 patch of pixels and apply a ‘filter’ template – designed to find an edge

(our weight parameters)



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X

-1	0	+1
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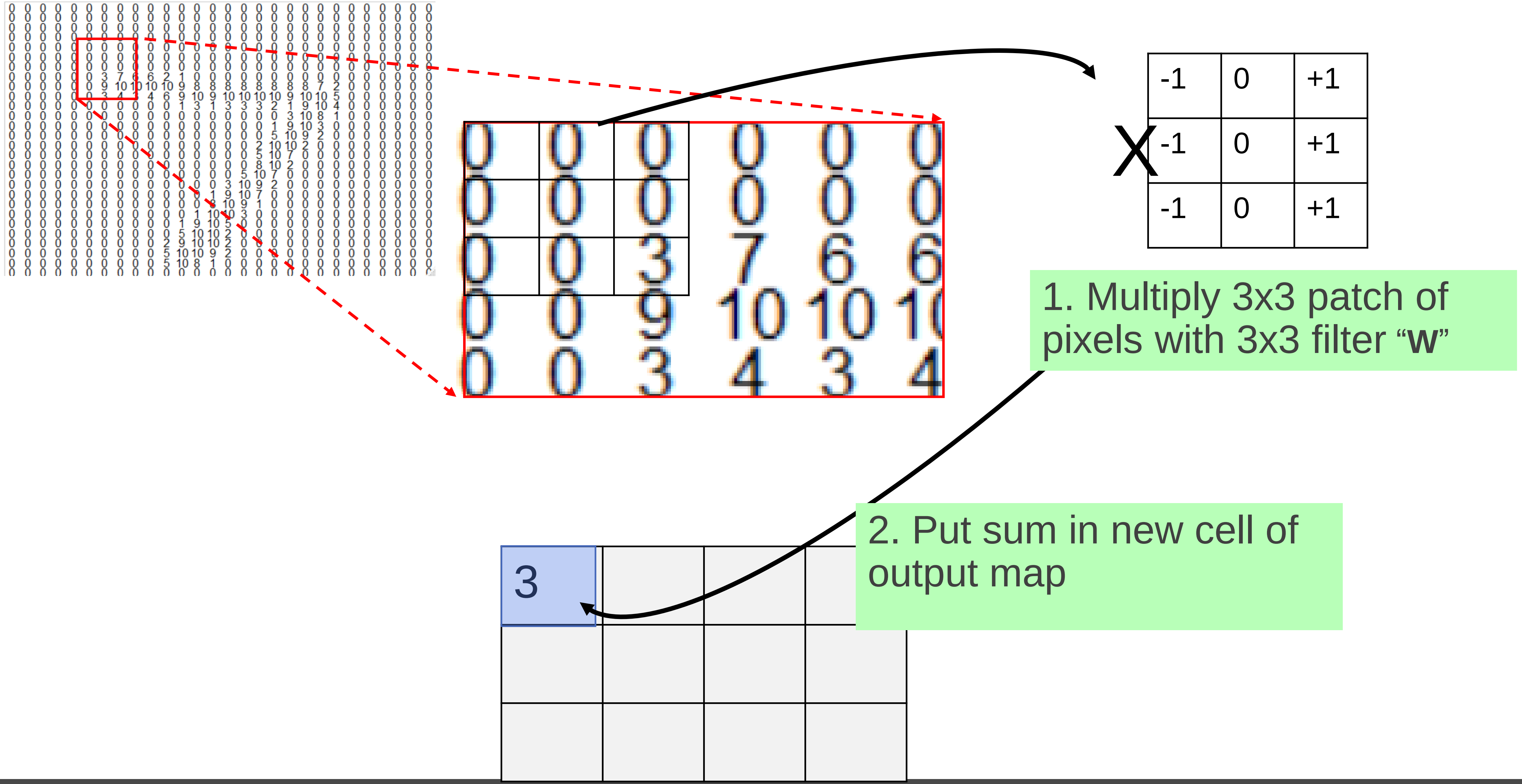
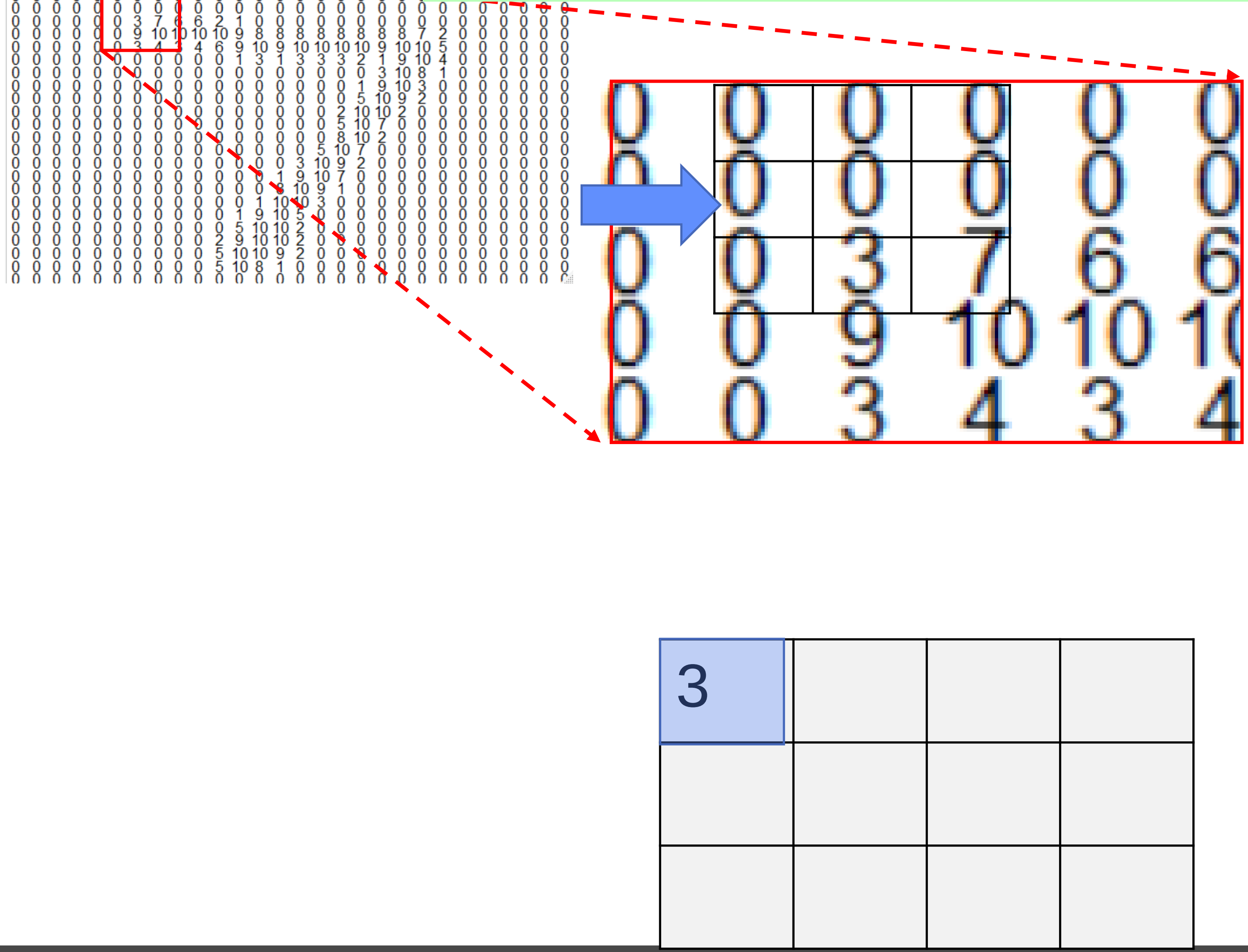
1. Multiply 3x3 patch of pixels with 3x3 filter “**W**”


0 0 0 0 0 0
0 0 0 0 0 0
0 0 3 7 6 6
0 0 9 10 10 10
0 0 3 4 3 4
X
-1 0 +1
-1 0 +1
-1 0 +1
1. Multiply 3x3 patch of pixels with 3x3 filter "**w**"
2. Put sum in new cell of output map
3

3. Slide filter horizontally to get next output value



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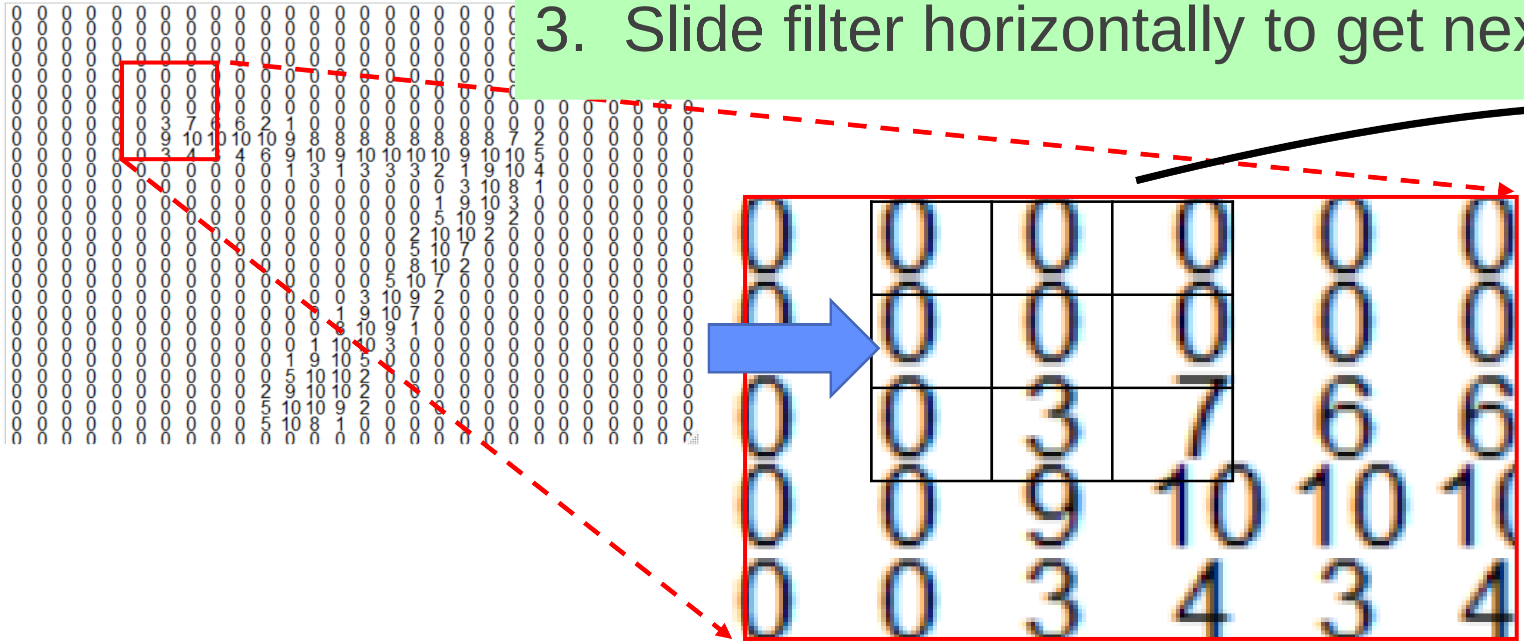

X

-1	0	+1
-1	0	+1
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3	7		

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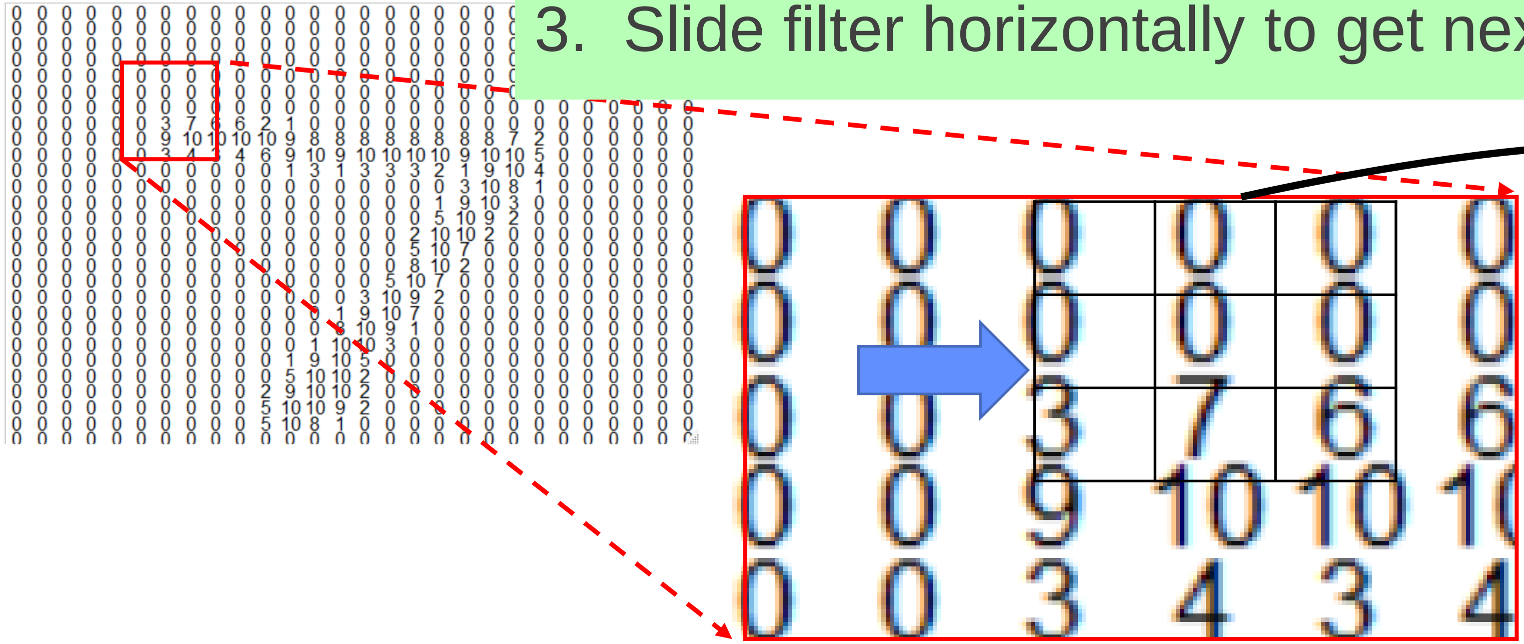

X

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-1	0	+1

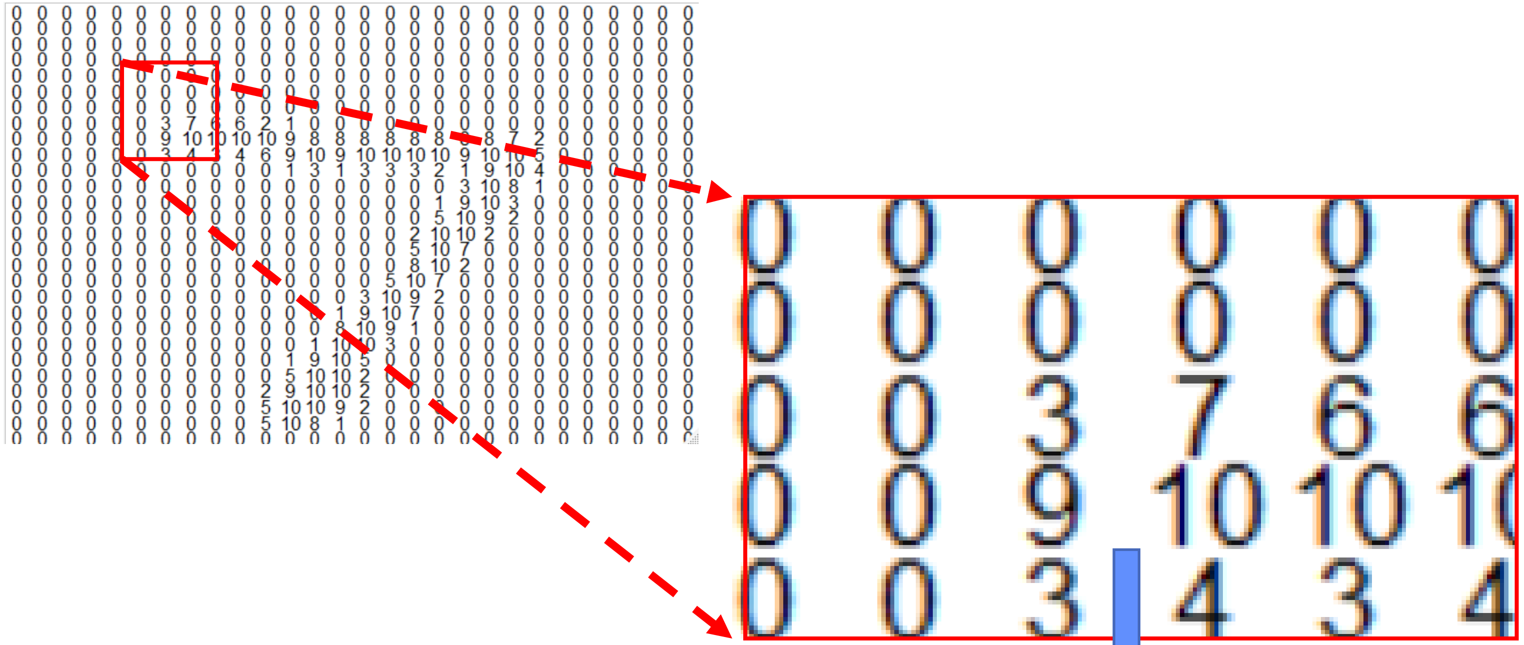
1. Multiply 3x3 patch of pixels with 3x3 filter “**W**”

2. Put sum in new cell of output map

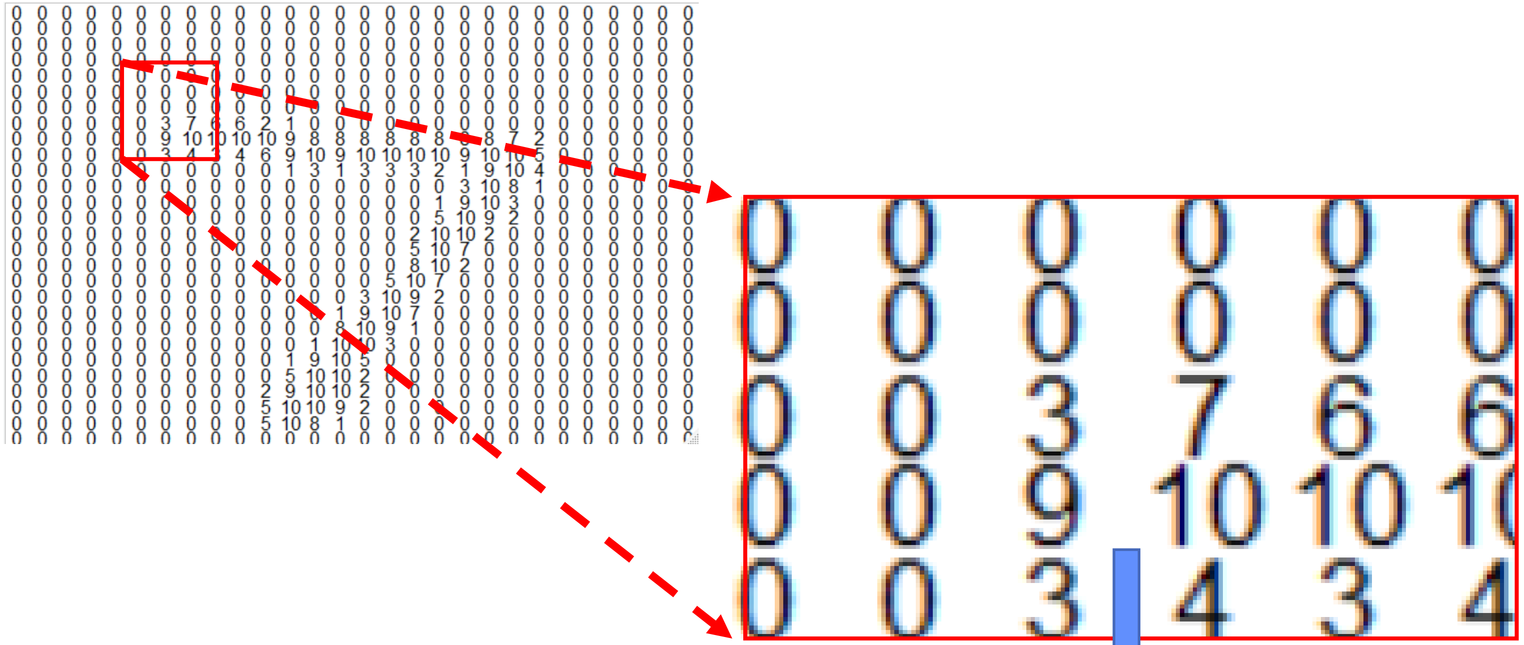
3	7	3	

NOTE: sliding a filter is known as a “convolution” operation

After vertical and horizontal sliding the 5x6 patch is now a 3x5 ***feature map.***



3	7	3	-1
12	17	4	-1
15	21	4	-1



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What do the highest values in the feature map represent?

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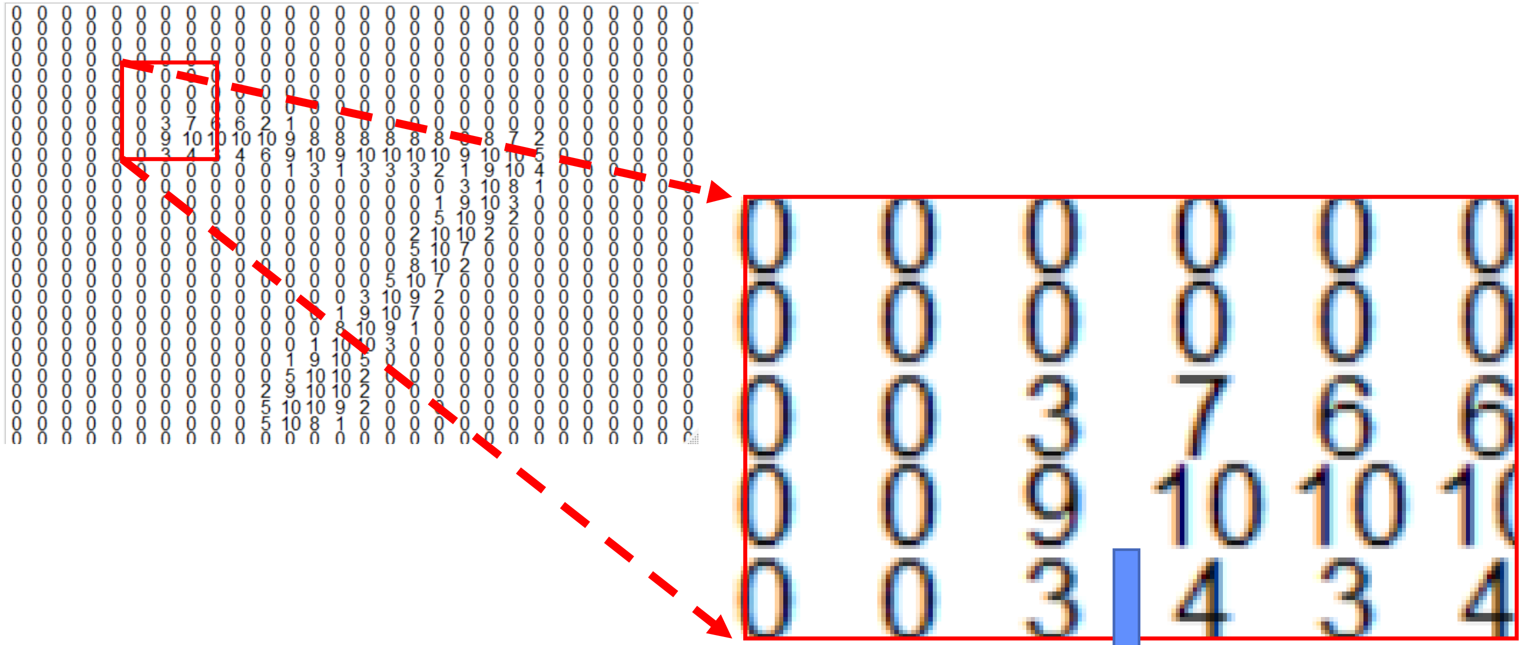
12	17	4	-1
15	21	4	-1



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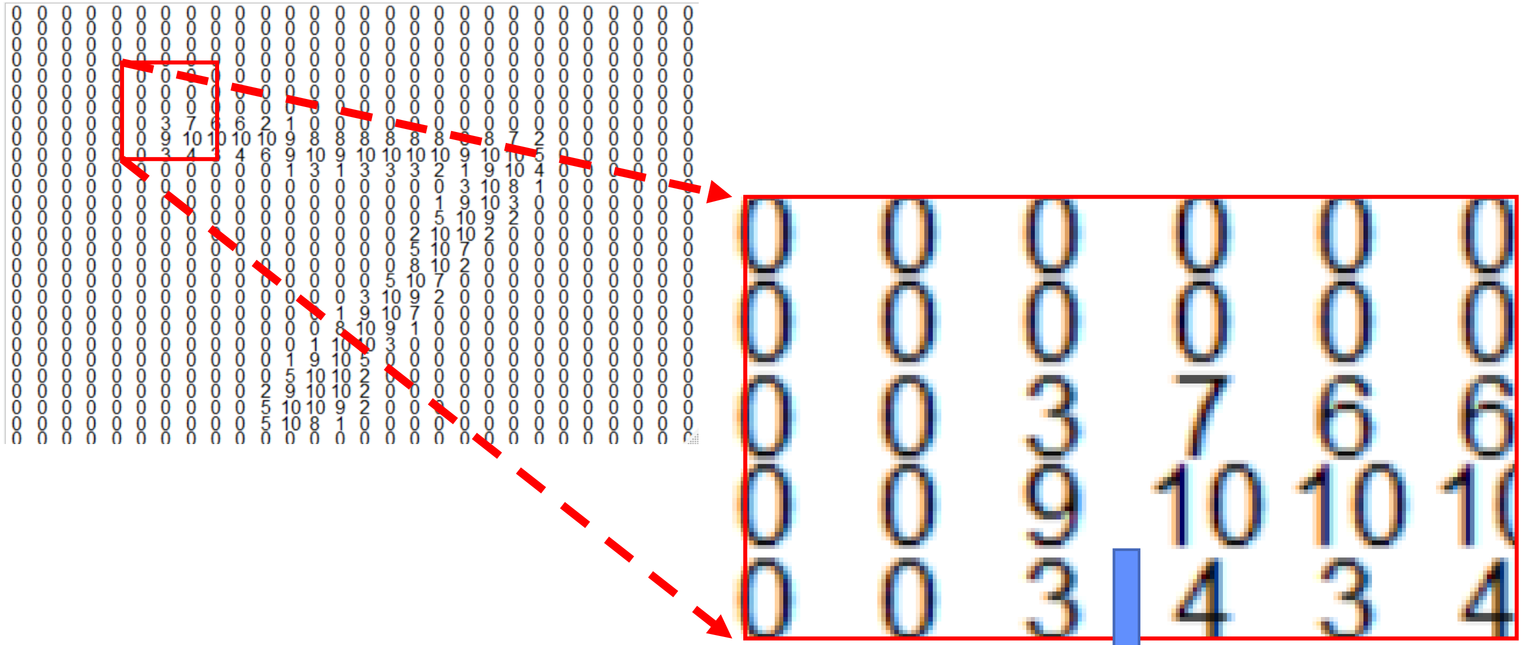
Optional next step:

Use another filter, and take maximum over elements - “max pooling”



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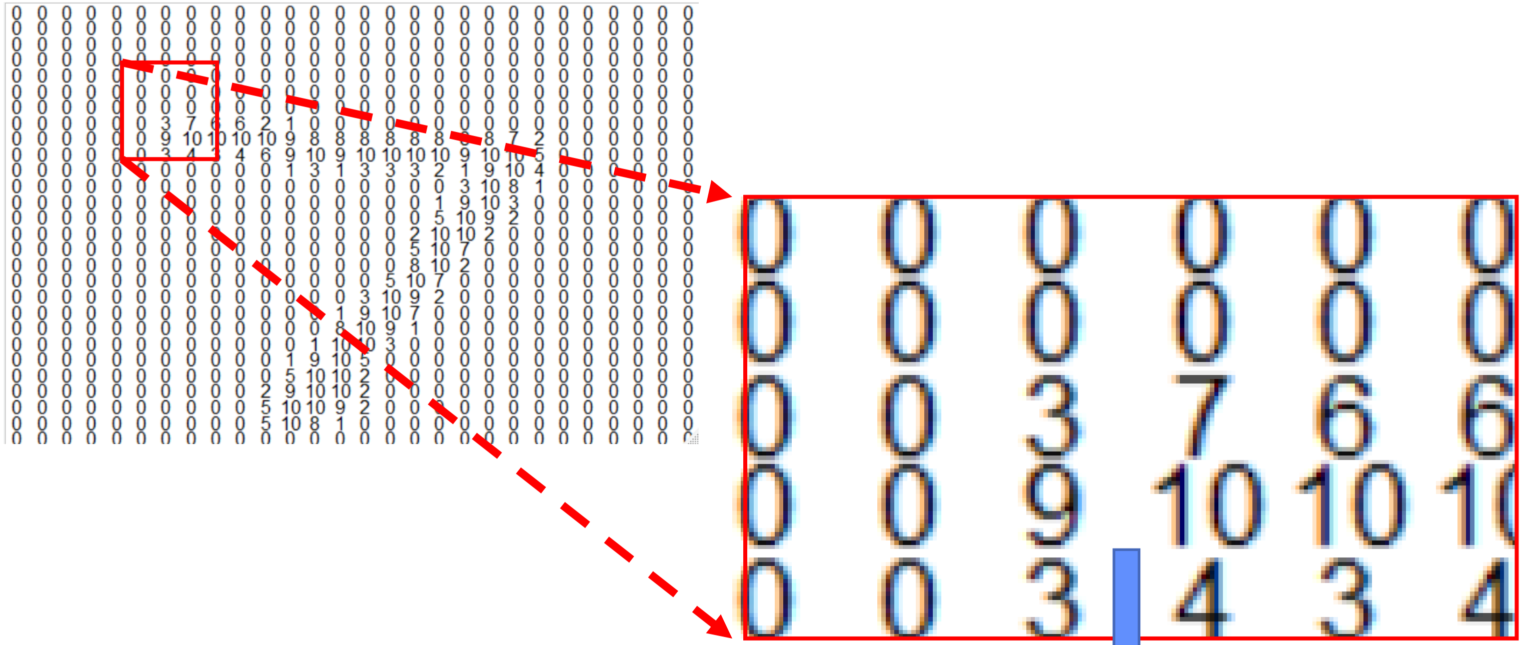
2x2 filter has max=17

17		



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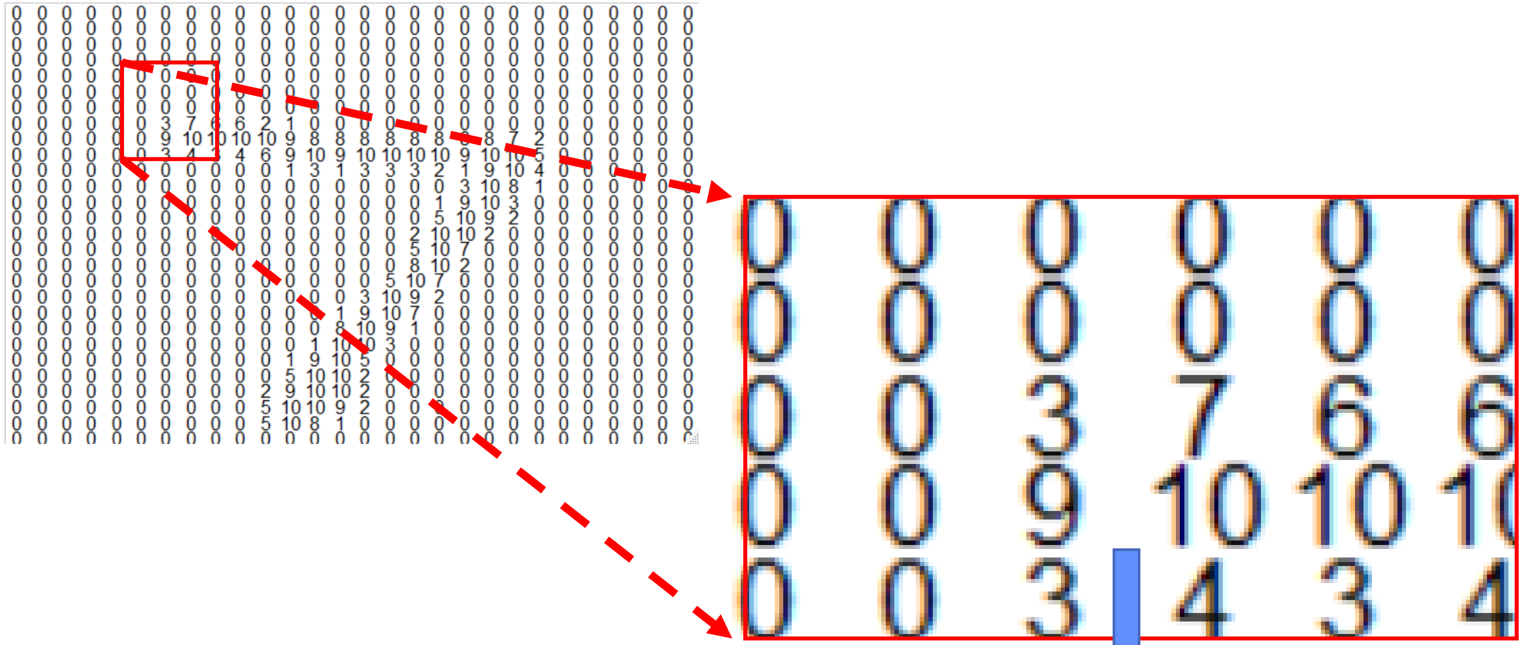
Optional next step:

Use another filter, and take maximum over elements - “max pooling”

Slide filter …

17	17	4
21	21	4

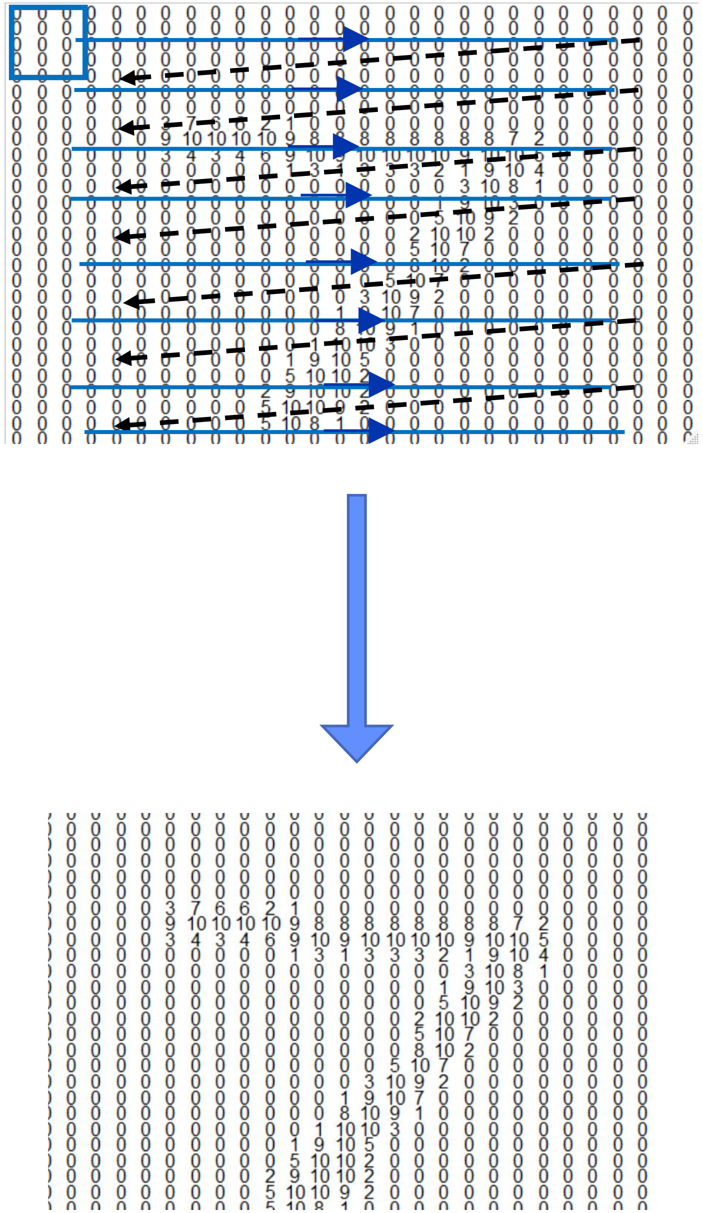


3	7	3	-1
12	17	4	-1
15	21	4	-1

Slide filter …

17	17	4
21	21	4

*After convolution and pooling,the 5x6 patch is **transformed** into a 2x3 feature map of ‘edge gradients’*



A convolution of one filter is applied to the entire image across and down.

The entire 28x28 input is ***transformed*** *into a smaller feature map of ‘edge gradients’*

Pooling is optionally applied

Convolution Neural Network (CNN)

In CNNs the filter values are weight parameters that are learned (**feature discovery**)

W_{11}	W_{12}	W_{13}
W_{21}	W_{22}	W_{23}
W_{31}	W_{32}	W_{33}

Convolution Neural Network (CNN)

In CNNs the filter values are weight parameters that are learned (**feature discovery**)

W_{11}	W_{12}	W_{13}
W_{21}	W_{22}	W_{23}
W_{31}	W_{32}	W_{33}

A convolution layer is a set of feature maps, where each map is derived from convolution of 1 filter with input

Convolution Neural Network (CNN)

More hyperparameters:

Size of filter (smaller is more general)

Convolution Neural Network (CNN)

More hyperparameters:

Size of filter (smaller, like 3x3, is more general)

Number of pixels to slide over (1 or 2 is usually fine)

Convolution Neural Network (CNN)

More hyperparameters:

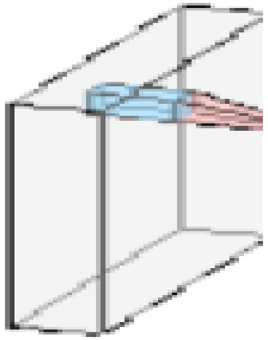
- Size of filter (smaller, like 3x3, is more general)
- Number of pixels to slide over (1 or 2 is usually fine)
- Max pooling or not (usually some pooling layers)
- Number of filters (depends on the problem!)

- **A large CNN example**

Convolution with image

- **Make 1 layer, using HxWx3 image (3 for Red,Green,Blue channels)**

Crop or resize image as needed

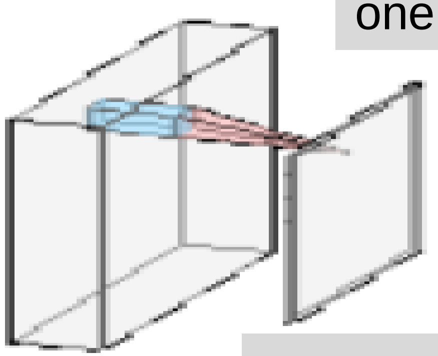


224x224x3

Convolution with image

- **Make 1 layer, using HxWx3 image (3 for RGB channels)**

Crop or
resize
image as
needed



one 3x3x3 filter

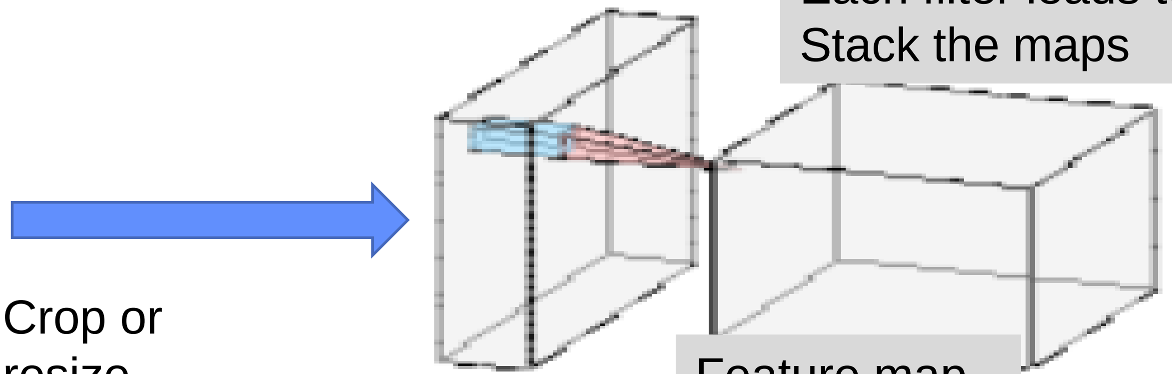
224x224x
3

Feature map
Size depends
on filter size
and slide
parameter

Convolution with image

- **Make 1 layer, using HxWx3 image (3 for RGB channels)**

Crop or resize image as needed



224x224x3

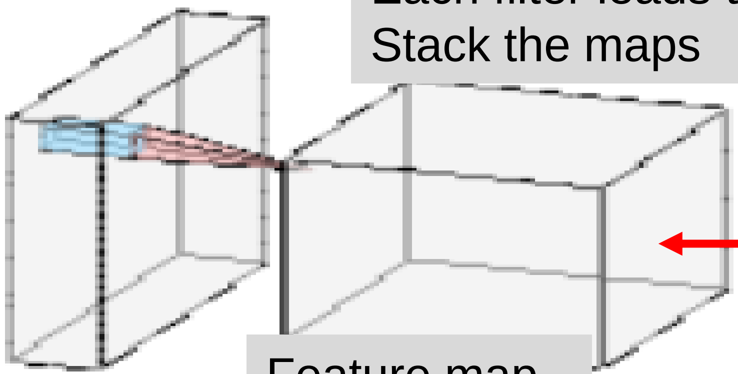
Repeat for many filters, all 3x3x3.
Each filter leads to 1 feature map
Stack the maps

Feature map
Size depends on filter size and slide parameter

Convolution with image

- **Make 1 layer, using HxWx3 image (3 for RGB channels)**

Crop or resize image as needed



224x224x3

Repeat for many filters, all 3x3x3.
Each filter leads to 1 feature map
Stack the maps

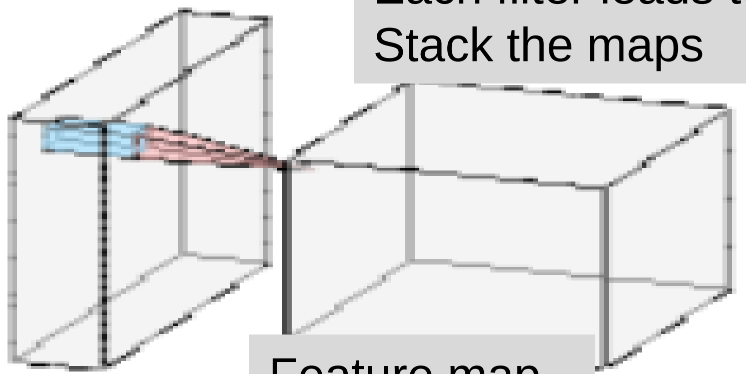
Feature map
Size depends on filter size and slide parameter

This is a "convolution layer"
The thickness is the number of different feature maps, sometimes called 'channels' or 'number of filters' or 'depth'

Convolution with image

- **Make 1 layer, using HxWx3 image (3 for RGB channels)**

Crop or
resize
image as
needed



224x224x
3

Repeat for many filters, all 3x3x3.
Each filter leads to 1 feature map
Stack the maps

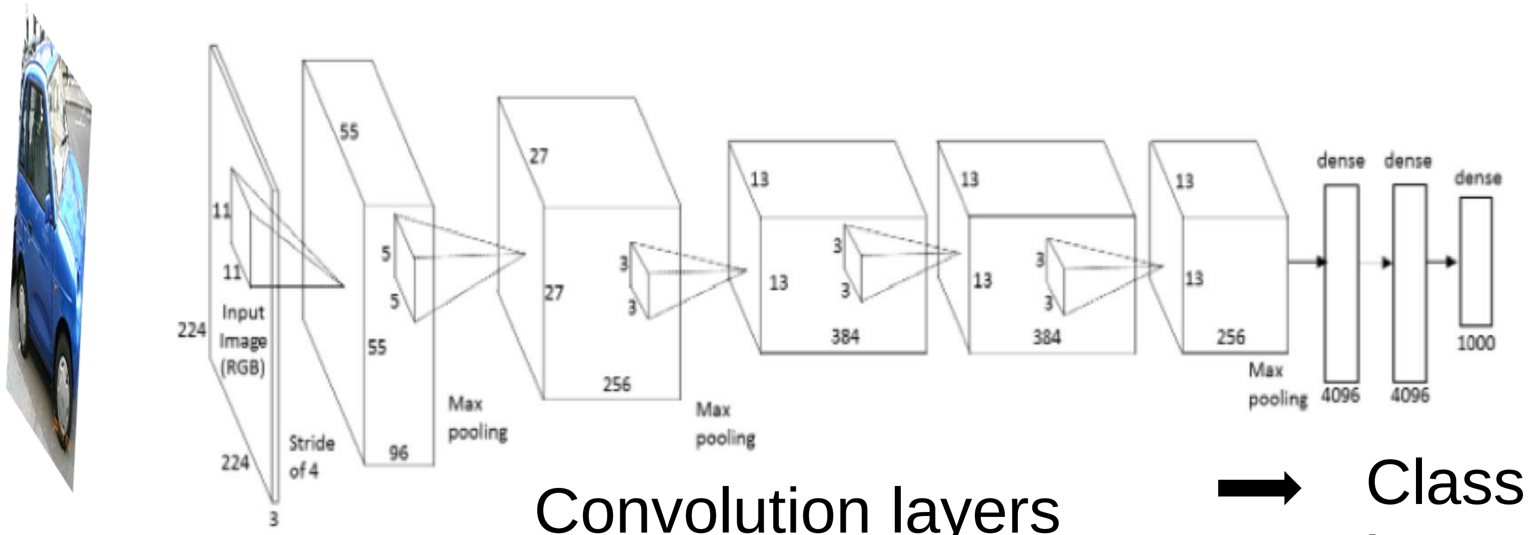
Feature map
Size depends
on filter size
and slide
parameter

Add a next convolution layer
The filter size is HxWx num-of-filters-previous-layer

Also, add a layer of max-pool to down sample a feature map

Large Scale Versions

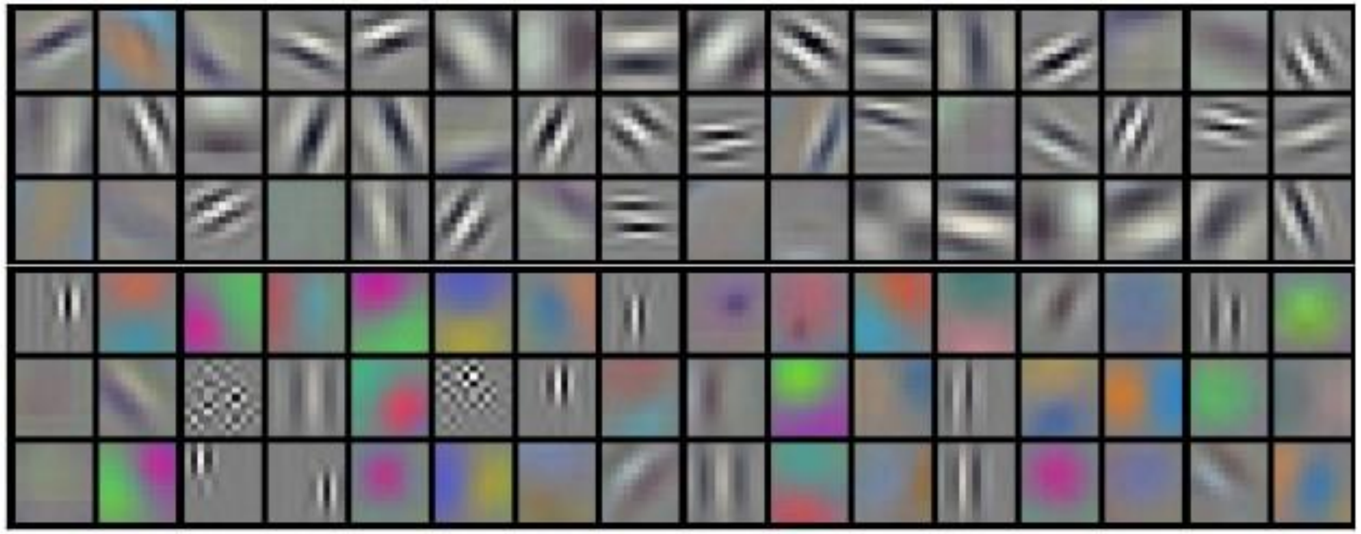
- **Large Convolution Networks – Alexnet, VGG19, ResNet, GoogLeNet, …**



Convolution layers ➡ Classification layers and output

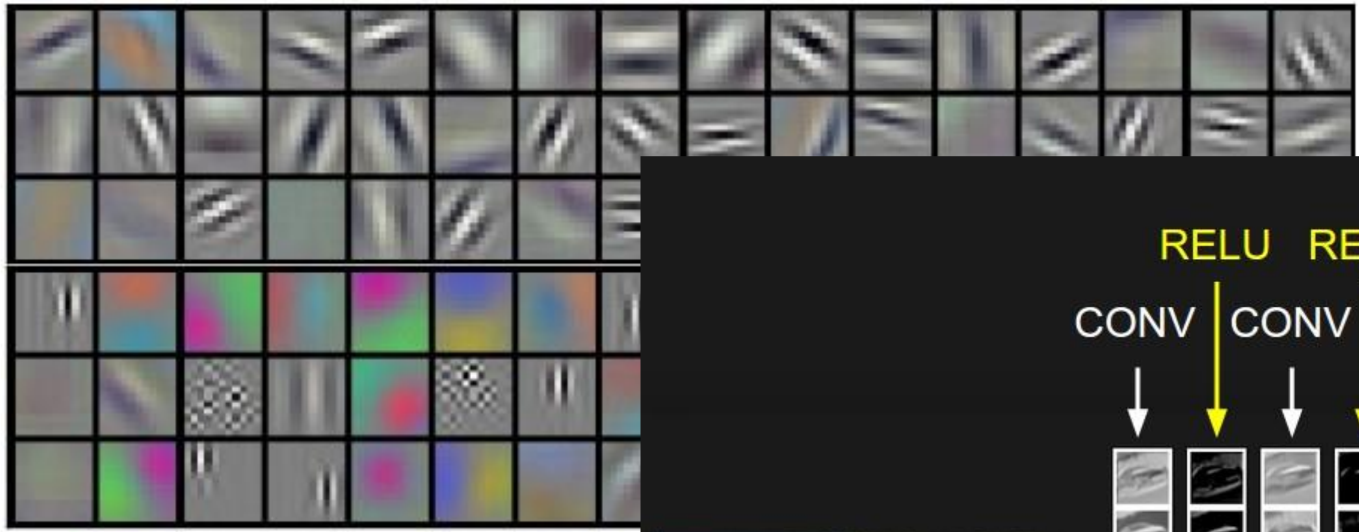
What Learned Convolutions Look Like

First convolution layer filters are simple features

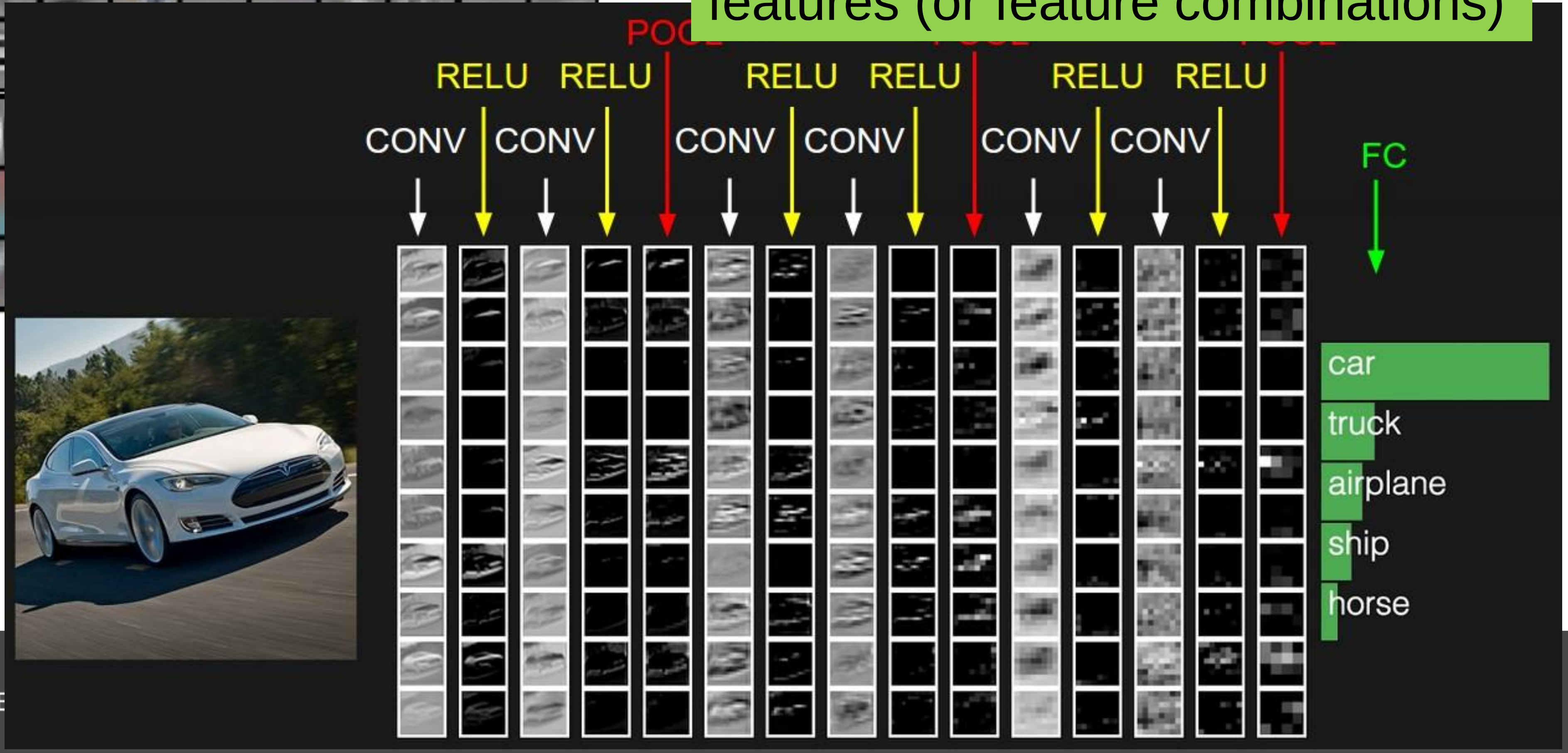


What Learned Convolutions

First convolution layer filters are simple features



Higher layers are more abstract features (or feature combinations)



Convolution Neural Network Summary

CNNs works because convolution layers have a special architecture and function – it is biased to do certain kind of transformations

Low layers have less filters that represent simple local features for all classes

Higher layers have more filters that cover large regions that represent object class features

What is deep learning?

Deep learning refers to learning complex and varied transformations of the input

Deep learning refers to **discovering** useful features of the input

Deep learning is a neural network with many layers

Where to go from here

- Find relevant examples to your domain or task
- Tensorflow has many examples with tutorials in their documentation
- Tensorflow hub and model examples have code and pretrained models

https://tfhub.dev/google/imagenet/inception_v1/classification/4

https://keras.io/examples/

- **Next, notebook exercise**

Exercise CNN for Digit Classification

- The 'hello world' of CNNs

- It uses MNIST dataset and Keras/Tensorflow

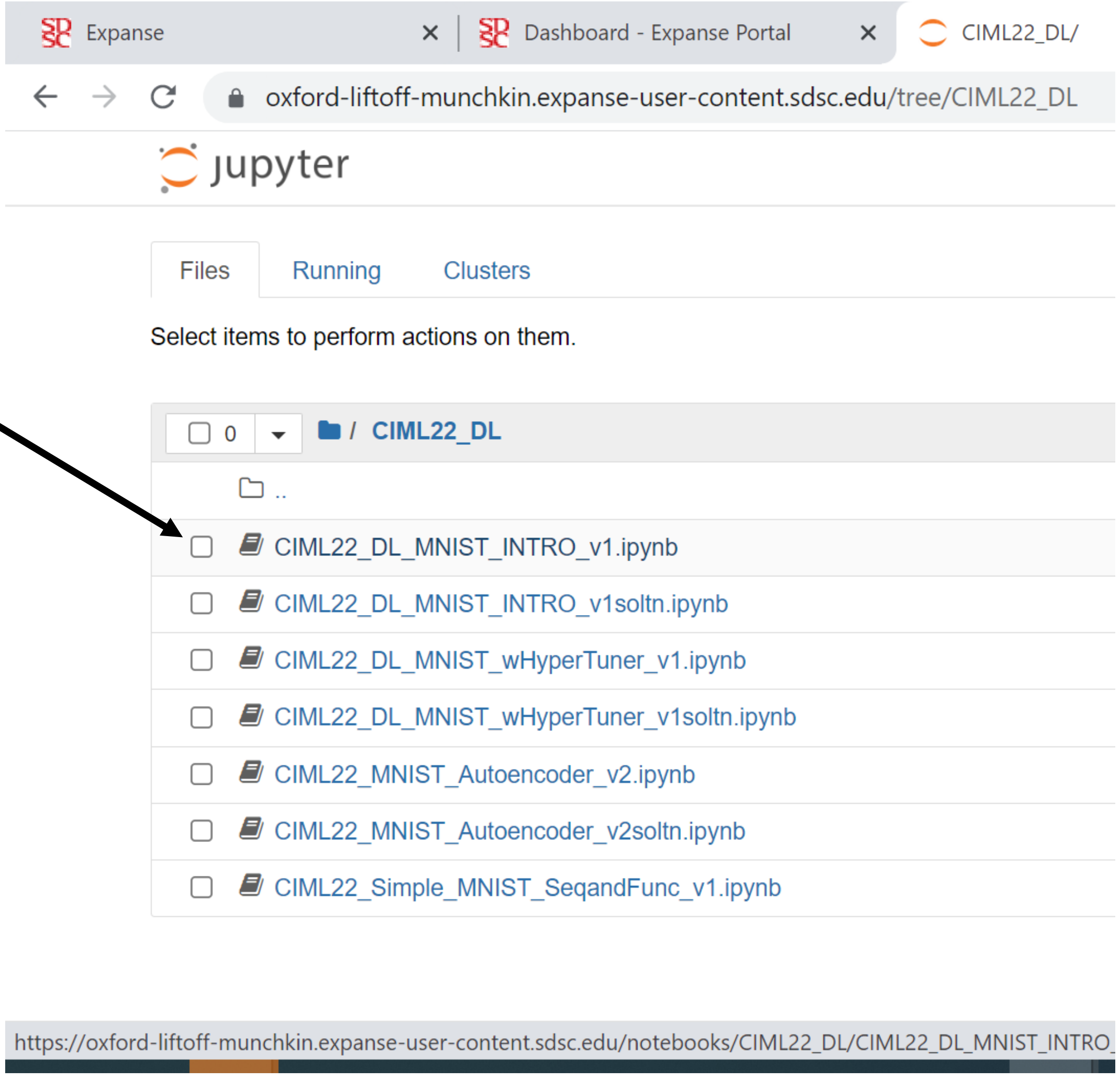
- Goal: Get familiar with Keras and CNN layers coding, and CNN solutions

- We will login and start a notebook

(see next pages for quick overview)

In jupyter notebook session open the MNIST_Intro notebook

Follow instructions in the notebook



Keras code for a convolution neural nework

```
# --------------Set up Model ---------------------
def build_model(numfilters):
    mymodel = keras.models.Sequential()
    mymodel.add(keras.layers.Convolution2D(numfilters,      #<<<< ------ 1
                                  (3, 3),
                                  strides=1,
                                  data_format="channels_last",
                                  activation='relu',
                                  input_shape=(28,28,1)))
    #add another conv layer?   mymodel.add(keras.layers.Convolution2D( ...

    mymodel.add(keras.layers.MaxPooling2D(pool_size=(2,2),strides=2,data_format="channels_la
    mymodel.add(keras.layers.Flatten())            #reorganize 2DxFilters output into 1D

    #---------------Now add final classification layers
    mymodel.add(keras.layers.Dense(32, activation='relu'))
    mymodel.add(keras.layers.Dense(10, activation='softmax'))

    # --------- Now configure model algorithm -----
    mymodel.compile(loss='categorical_crossentropy',
              optimizer=keras.optimizers.Adam(learning_rate=0.001),
```

A sequential model

Add convolution layer

Add max pooling, then flatten into a vector for classification layers

- Remember every layer has some input, ouput
- Keras figures out the shapes
- Not every layer in Keras has trainable parameters – like which ones above?

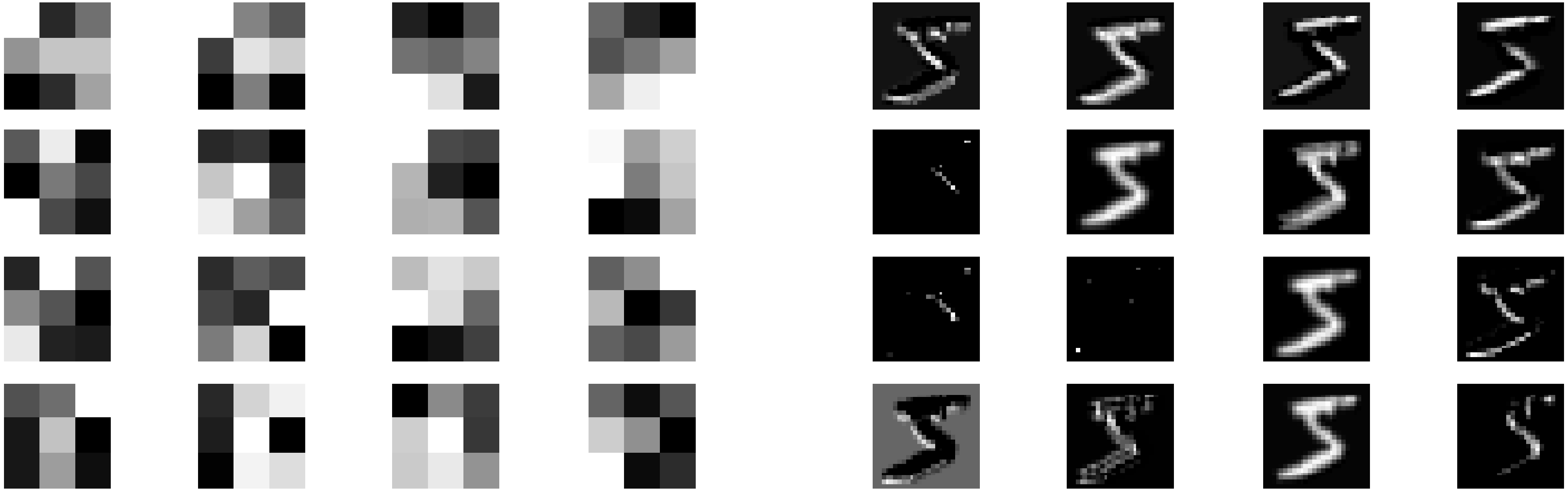
Zooming in on keras convolution layers statements

Use 16 filters, each of size 3x3

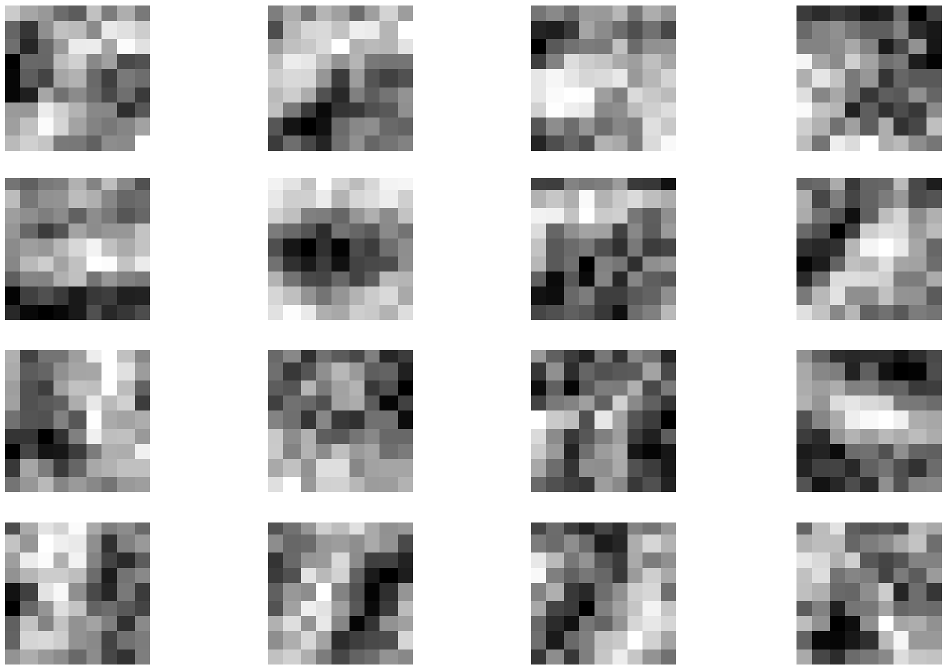
```
my_model.add(tf.keras.layers.Convolution2D(filters=16,
                                           kernel_size=(3, 3),
                                           strides=1,
                                           data_format="channels_last",
                                           activation='relu',
                                           input_shape=(28,28,1)))
```

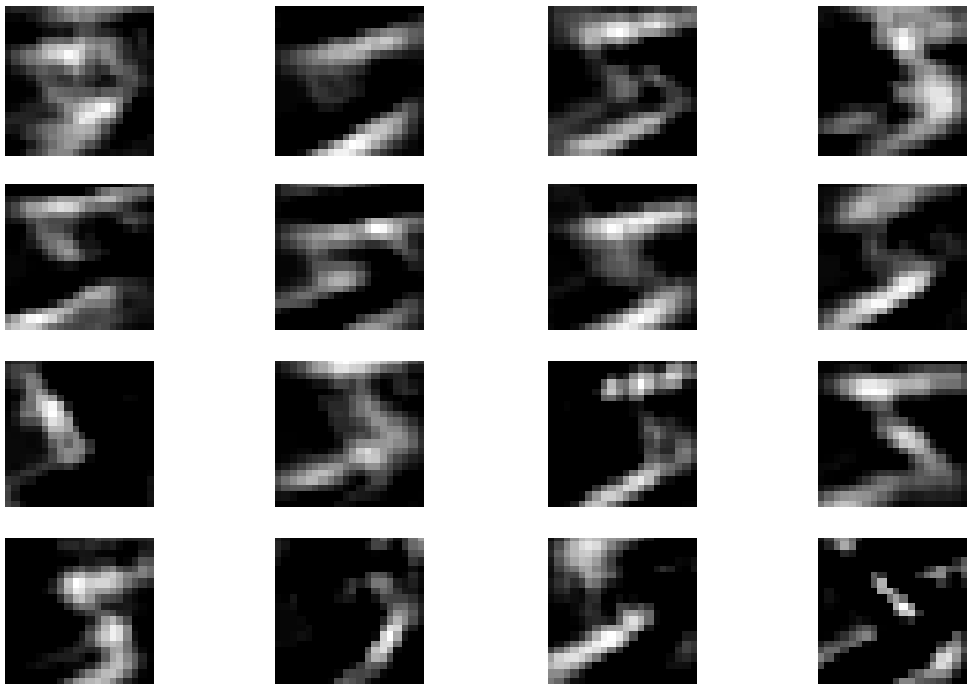
Input shape does not include number of images

Exercise notes: 3x3 first convolution layer filter and activation



9x9 first convolution layer filter and activation





End