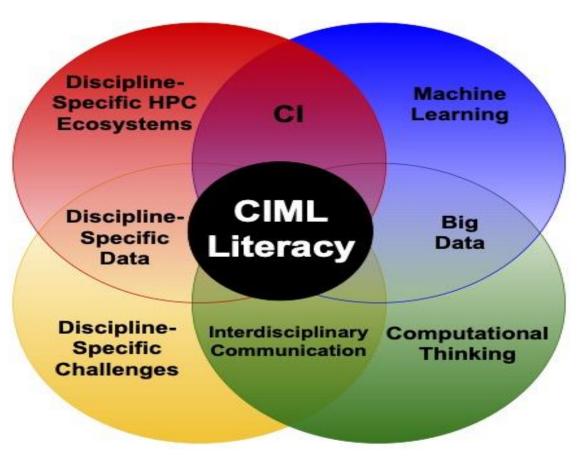
Introduction to Neural Network, Convolution Neural Networks, and Deep Learning

July, 2022

Paul Rodriguez, PhD (SDSC)



Outline

- Overview of Neural Networks (aka Multilayer Perceptron)
- Convolution Neural Networks
- Basic Keras commands for building, training CNNs - exercise
- Hyperparameters and Tuning and workflows exercise

2nd session

4.3 Deep Learning 10:05 AM – 10:50 AM

[Here, I am going to do the basic CNN tutorial, but more of an exercise than tutorial, meaning they will have to fill in code parts more on their own. I am also going to do some tutorial/demo with the hyperparameter tuner tool, so that's a new thing, but it follows the slides I did in the webinar]

Practical things to Consider, aka, new stuff for the extended tutorial,

- MNIST exercise/tutorial with Keras on Expanse
- Hyperparameter Tuning, keras tuner, tutorial
- Setting up configurations with yaml demo/tutorial
- Sample Workflow, batch job -> yaml file -> hyperparam search ->model demo



to get neural network:

Consider the Logistic Function

(aka sigmoid)

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

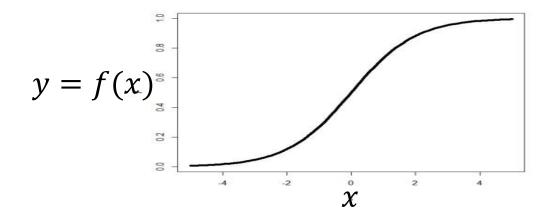
to get neural network:

Consider the Logistic Function

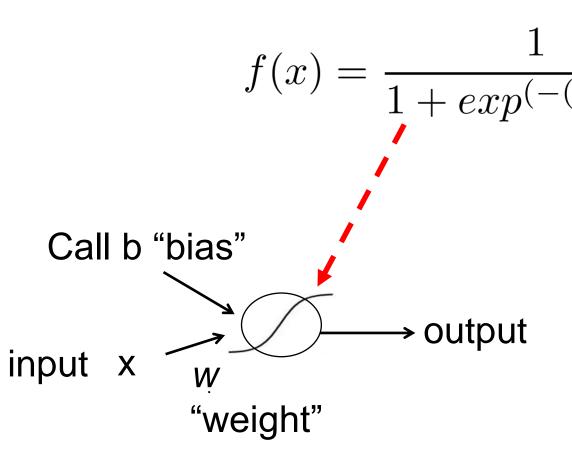
(aka sigmoid)

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

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



Make a graphical description of Logistic Function



this node (or unit) will transform input to output with logistic activation function

Make a graphical description of Logistic Function

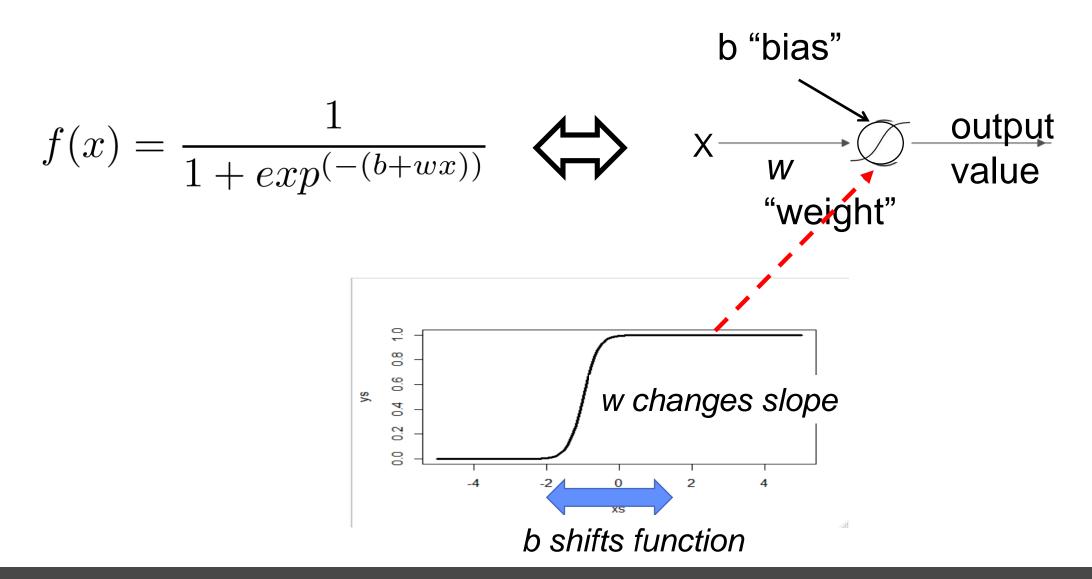
$$f(x) = \frac{1}{1 + exp^{(-)}}$$
Call b "bias"
output input x "weight"

this node (or unit) will transform input to output with logistic activation function

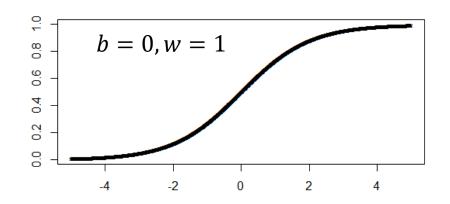
Goal: given some data X and outputs Y find *w* & *b* so that output =1 when Y=1

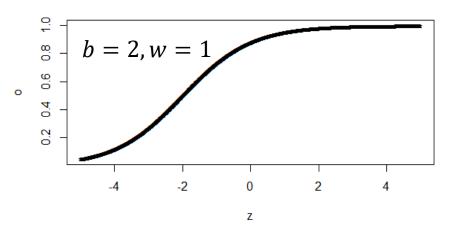
How does changing parameters affect the function?

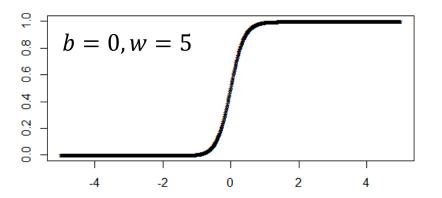
How does changing parameters affect the function?

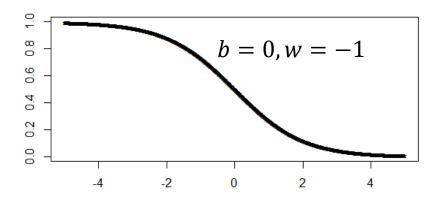


Logistic function w/various weights

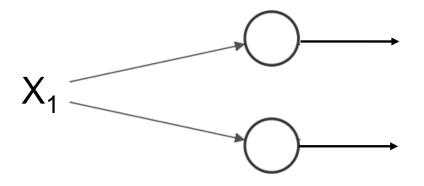




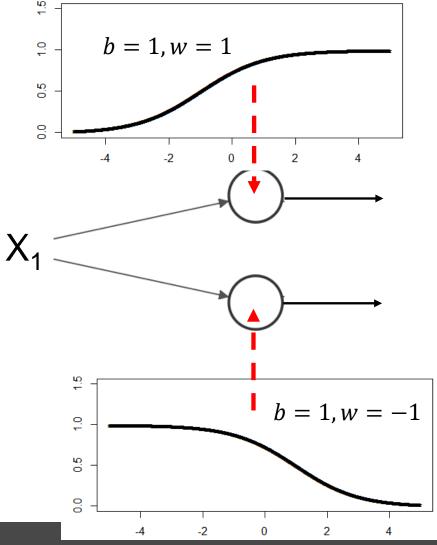




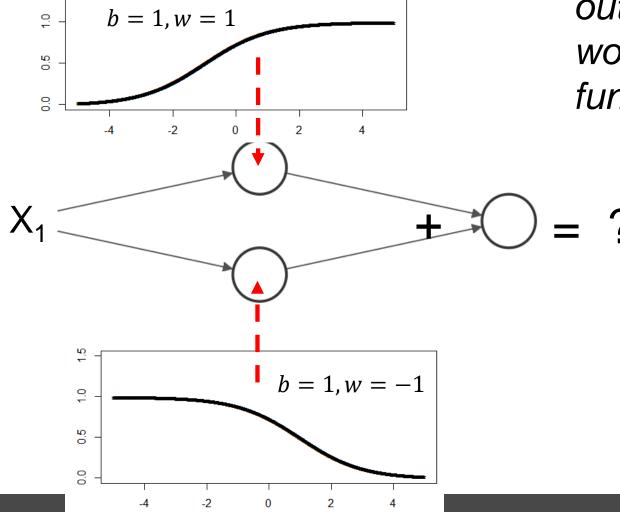
Example: 1 input into 2 logistic units



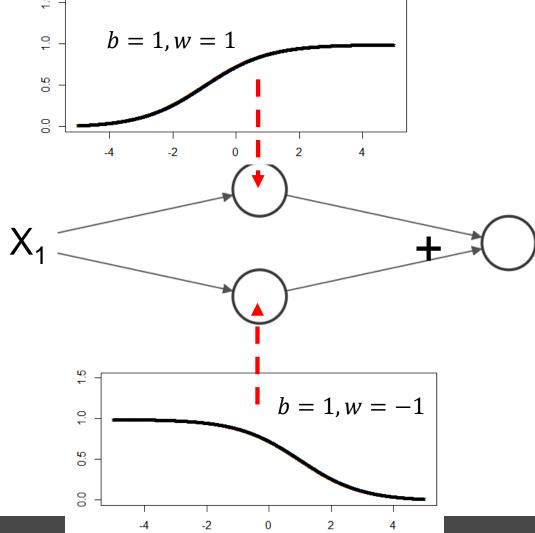
Example: 1 input into 2 logistic units with these activations



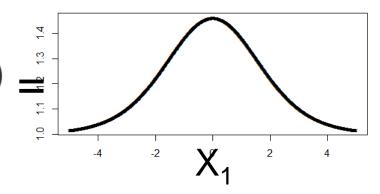
Example: 1 input into 2 logistic units with these activations



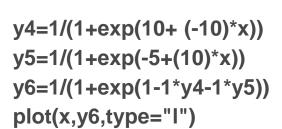
Example: 1 input into 2 logistic units with these activations

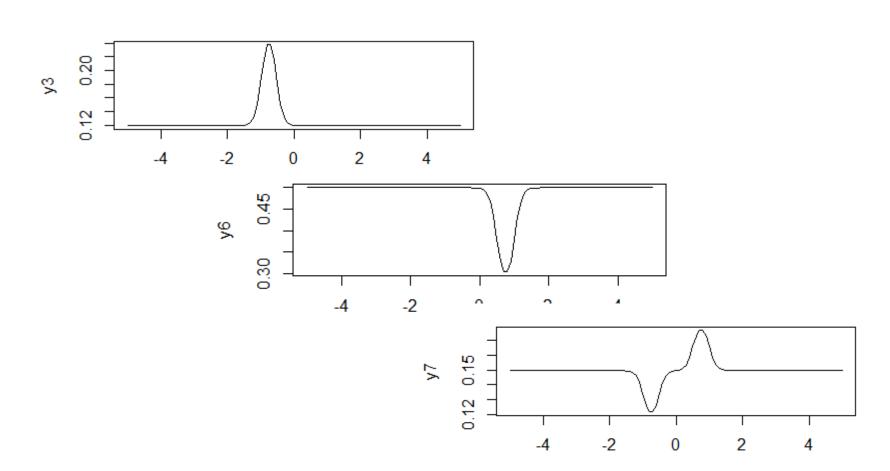


If you add these 2 units into a final output unit what would the output function look like?

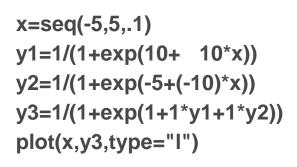


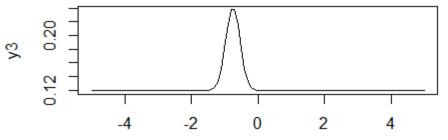
Higher level function combinations



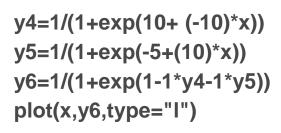


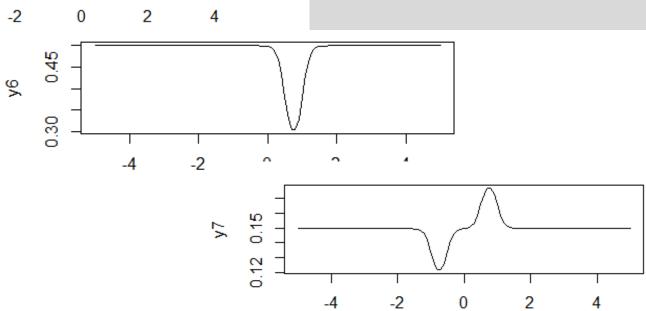
Higher level function combinations

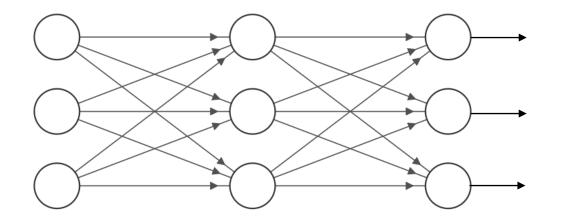




Multiple layer networks can represent any logical or realvalued functions (unbiased, but potential to overfit)

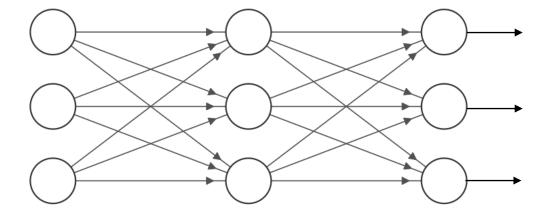




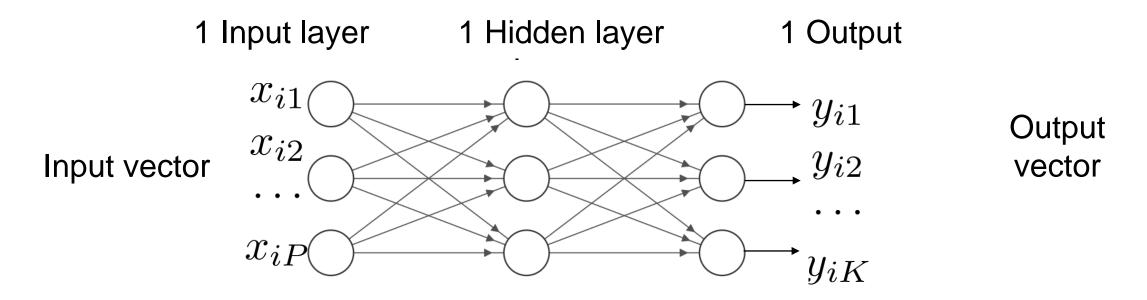


Multilayer Perceptron

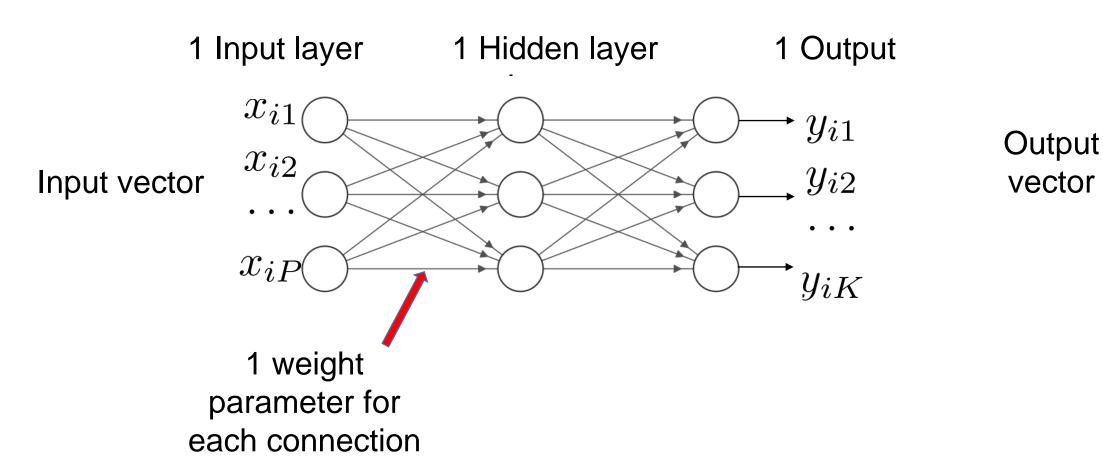
1 Input layer 1 Hidden layer 1 Output



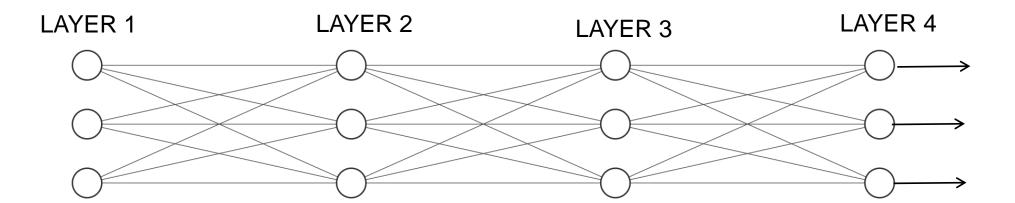
Multilayer Perceptron



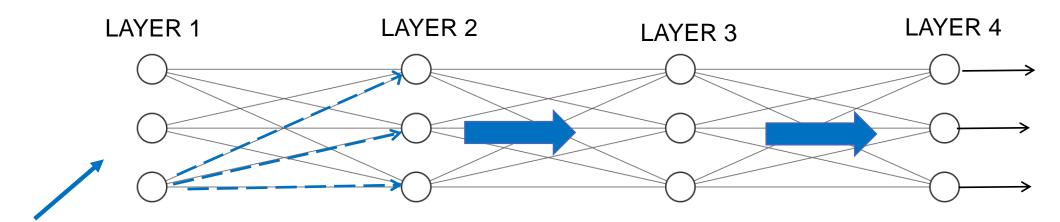
Multilayer Perceptron



First step: choose layers, connectivity, and activations



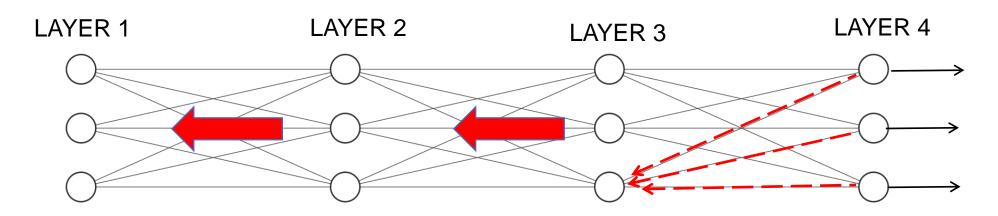
Algorithm steps:



1. FORWARD PROPAGATE ACTIVATION:

apply input data x_i, calculate all node activations

Algorithm steps:



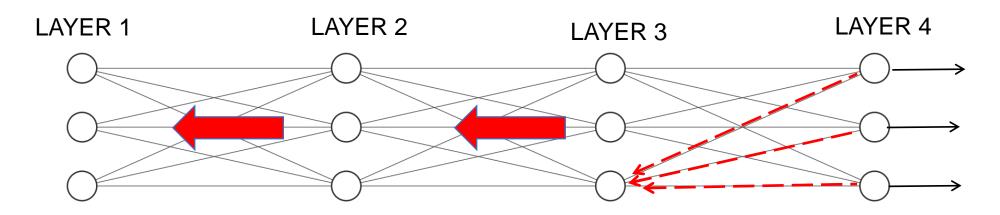
1. FORWARD PROPAGATE ACTIVATION:

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2. BACKWARD PROPAGATE ERROR:

calculate Error (or Loss) derivatives, dE/dY, pass it back to lower layer

algorithm steps:



1. FORWARD PROPAGATE ACTIVATION:

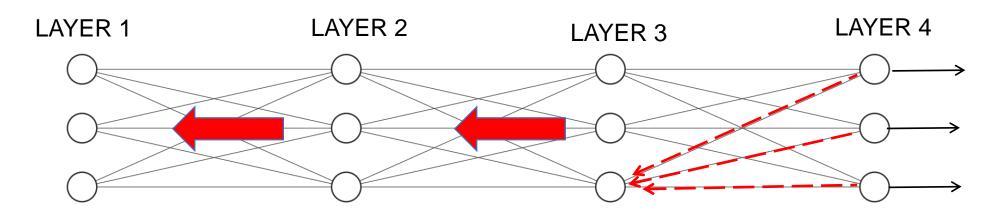
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calculate Error (or Loss) derivatives, dE/dY, pass it back to lower layer

For hidden layers use chain rule: (dE/dY dY/dH₃ dH₃/dH₂ etc...) needs a summation of previous layer

algorithm steps:



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apply input data x_i , calculate all node activations

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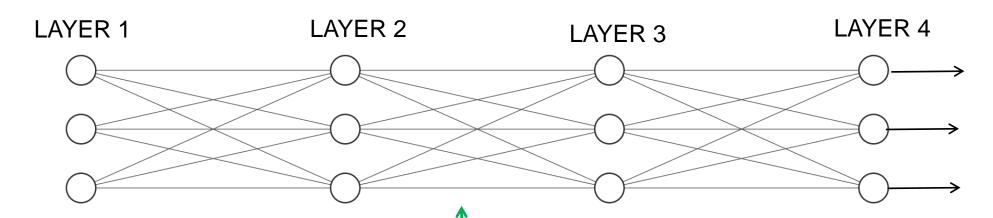
calculate Error (or Loss) derivatives, dE/dY, pass it back to lower layer

For hidden layers use chain rule: (dE/dY dY/dH₃ dH₃/dH₂ etc...) needs a summation of previous layers

Beware: error signals get diluted as you go backward - the 'vanishing gradient' problem



algorithm steps:



1. FORWARD PROPAGATE ACTIVATION:

apply input data x_i, calculate all node activations

2. BACKWARD PROPAGATE ERROR:

calculate Error (or Loss) derivatives (dE/dY) pass it back to lower layer

3. Update weights and bias terms

$$w_{ji} = w_{ji} - \eta \frac{dE}{dw_{ji}}$$

INITIALIZE WEIGHTS (small random values)

INITIALIZE WEIGHTS

LOOP until stopping criterion:

FORWARD PROPAGATION: calculate all node activations

INITIALIZE WEIGHTS

LOOP until stopping criterion:

FORWARD PROPAGATION: calculate all node activations

BACKWARD PROPAGATION: calculate all derivatives to minimize Loss (dL)

INITIALIZE WEIGHTS

LOOP until stopping criterion:

FORWARD PROPAGATION: calculate all node activations

BACKWARD PROPAGATION: calculate all derivatives to minimize Loss (dL)

UPDATE WEIGHTS: $w \leftarrow w - learning_rate * \frac{aL}{dw}$

INITIALIZE WEIGHTS

LOOP until stopping criterion:

FORWARD PROPAGATION: calculate all node activations

BACKWARD PROPAGATION: calculate all derivatives to minimize Loss (dL)

UPDATE WEIGHTS: $w \leftarrow w - learning_rate * \frac{aL}{dw}$

STOP: when validation loss reaches minimum or converges

NN Algorithm [heuristics, options to learn faster and/or better]

INITIALIZE WEIGHTS [use truncated distributions]

LOOP until stopping criterion: [work in batches of input]

FORWARD PROPAGATION: calculate all node activations

BACKWARD PROPAGATION: calculate all derivatives to minimize Loss (dL)

UPDATE WEIGHTS: $w \leftarrow w - learning_rate * \frac{aL}{dw}$

[adapt learning rate, use momentum]

STOP: when validation loss reaches minimum or converges

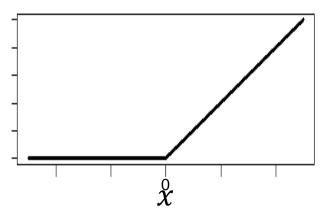
[several metrics of loss are possible]



A heuristic for deep networks

RELU (rectified linear

RELU activation function



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

where a = XW

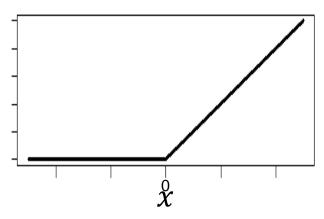
A heuristic for deep networks

RELU activation function

It is unscaled (bad!)

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

RELU (rectified linear



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

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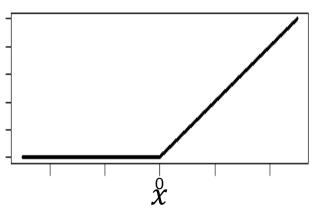
A heuristic for deep networks

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RELU activation function

It is unscaled (bad!)

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



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

where a = XW

RELU helps mitigates vanishing gradients

Summary:

Pro:

Neural Networks in general, are flexible, powerful learners Hidden layers learn a nonlinear transformation of input Many heuristics about what works

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Neural Networks in general, are flexible, powerful learners Hidden layers learn a nonlinear transformation of input Many heuristics about what works

Con:

Hard to interpret

Needs more data

Lots of parameters



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



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

Deep learning refers to discovering useful features of the input



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



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Image features

MNIST - A database of handwritten printed digits

(National Inst. of Standards and Technology)



Image features

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How to classify digits?



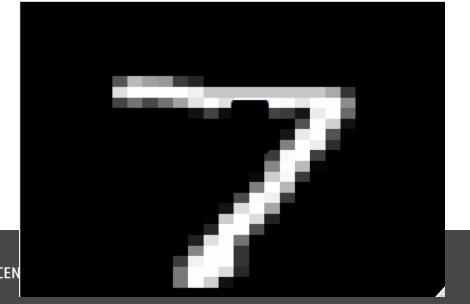
Image features

MNIST - A database of handwritten printed digits

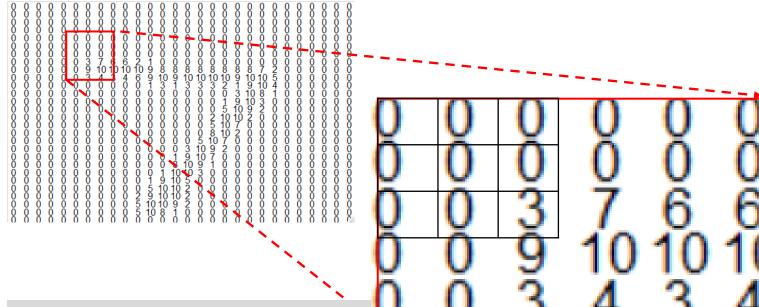
(National Inst. of Standards and Technology)

0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 7 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9

How to classify digits?

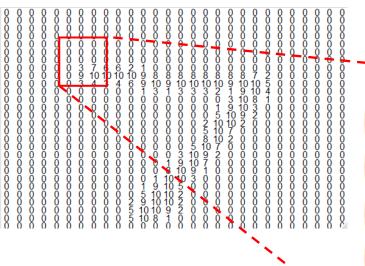


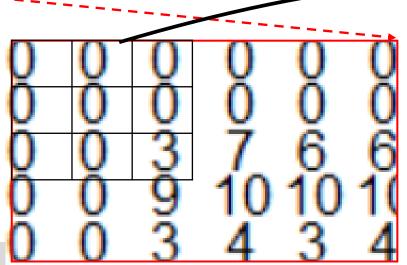




Let's zoom into 5x6 window of pixels near the tip of '7'

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



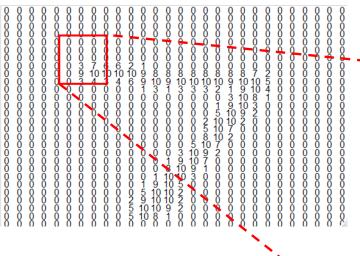


	-1	0	+1
X	-1	0	+1
	-1	0	+1

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



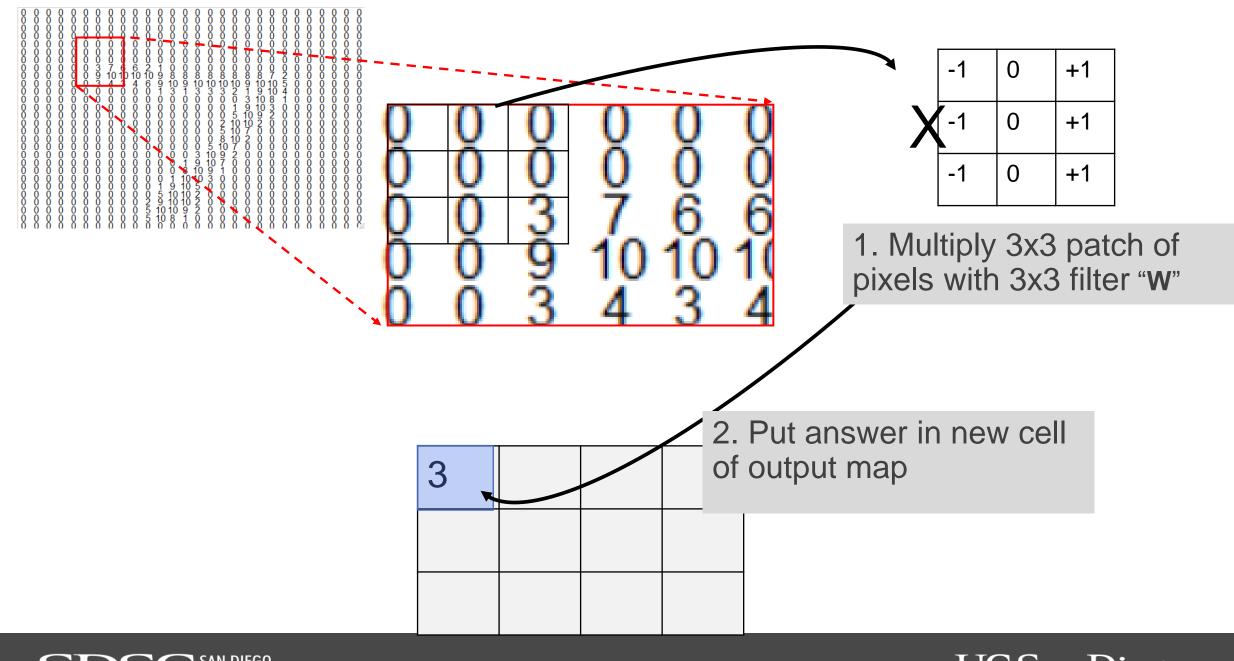
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 7 6 6 0 0 9 10 10 10 (our weight parameters)

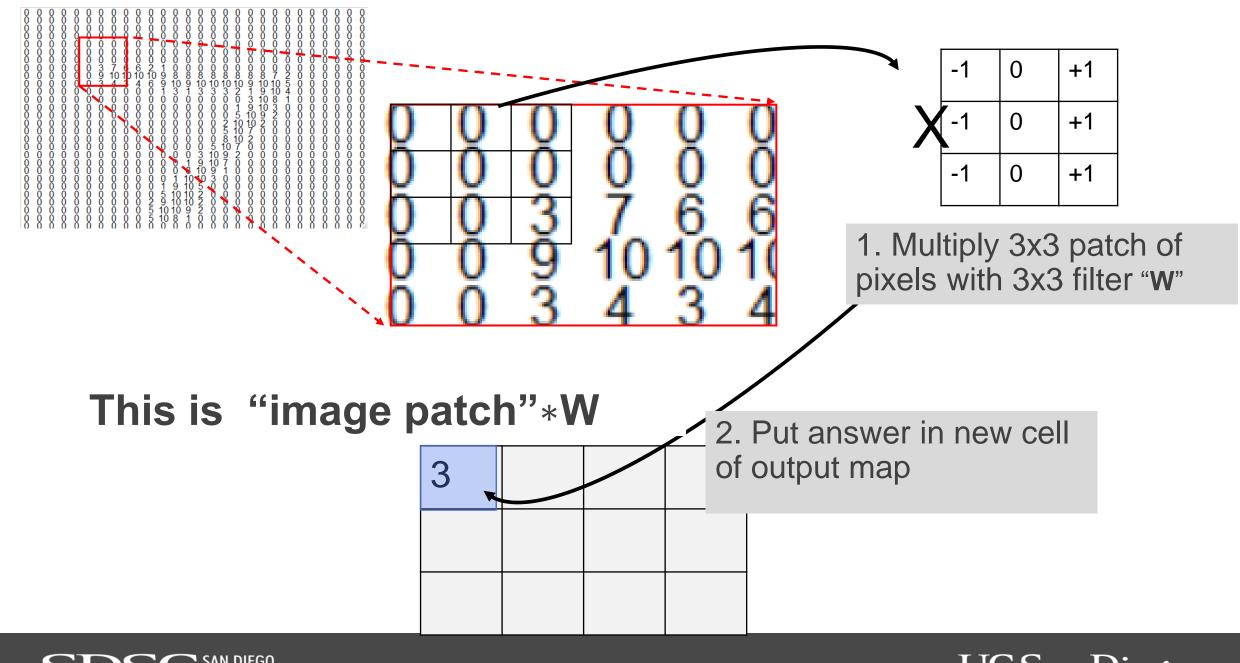
-1 0 +1 -1 0 +1 -1 0 +1

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

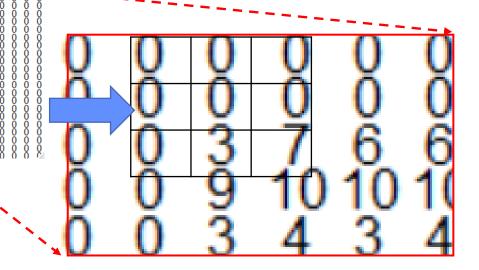
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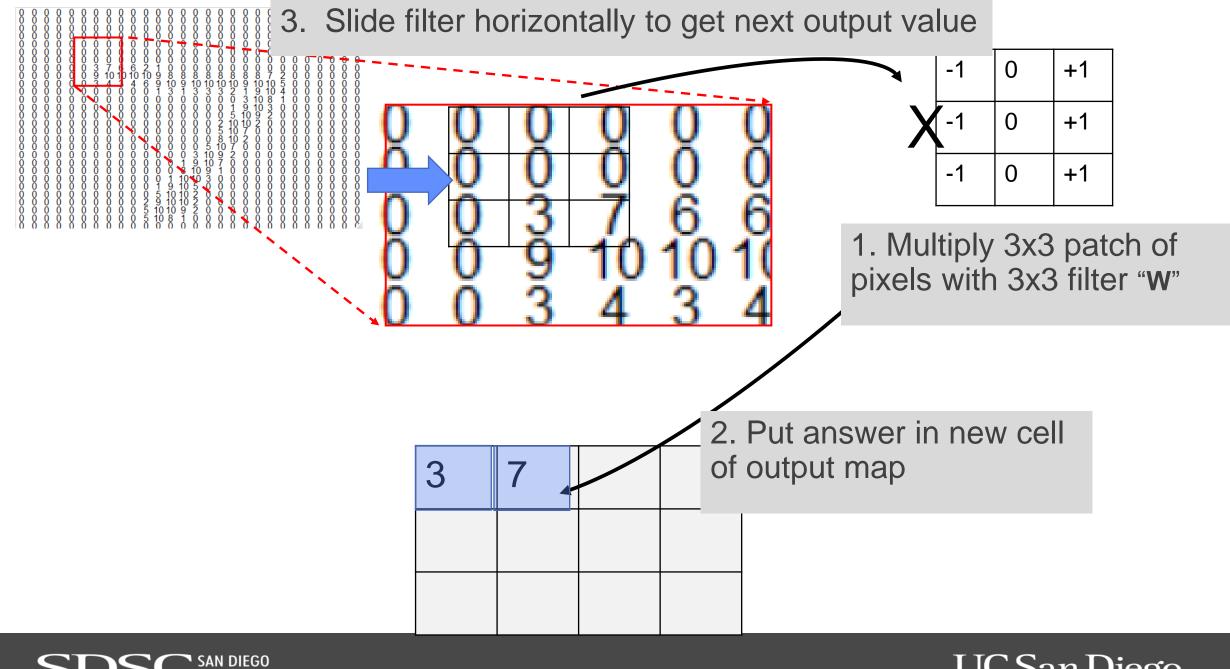


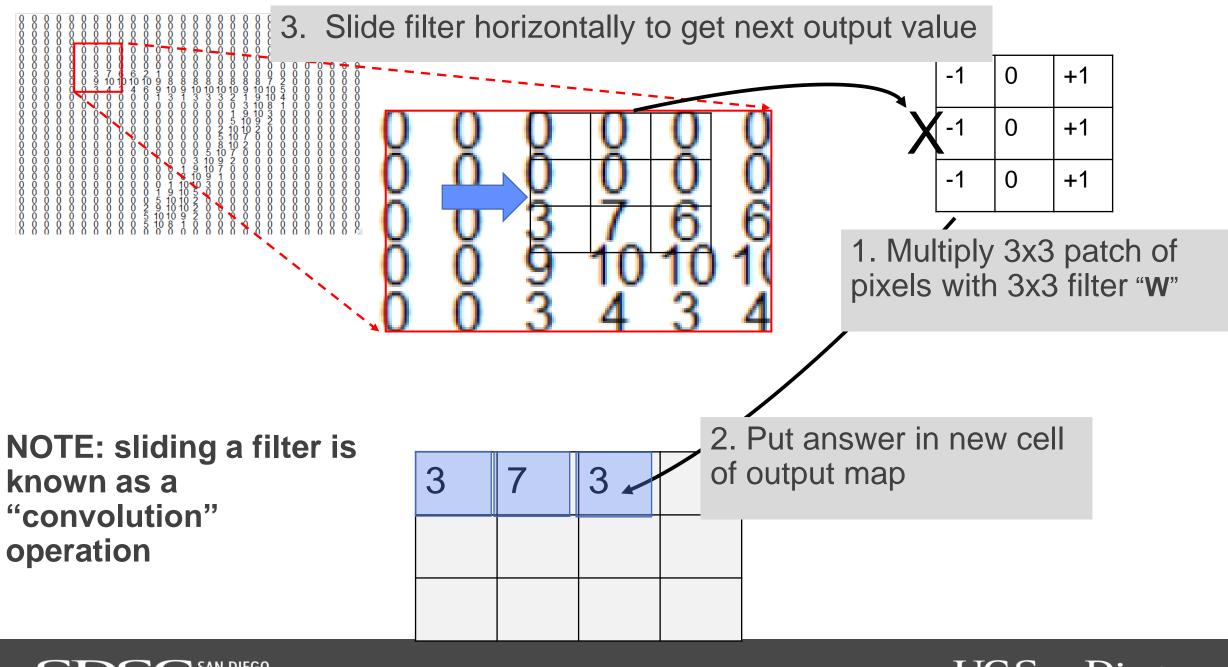


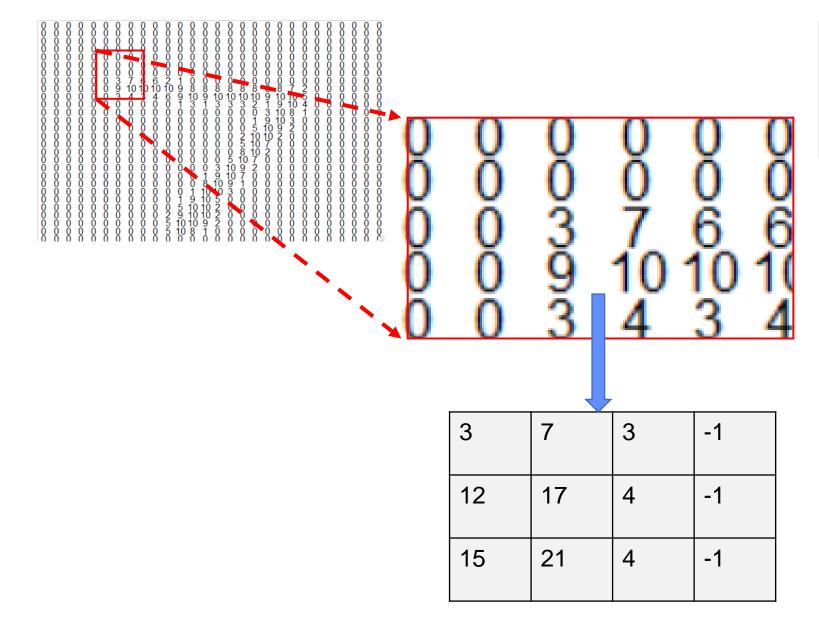
3. Slide filter horizontally to get next output value



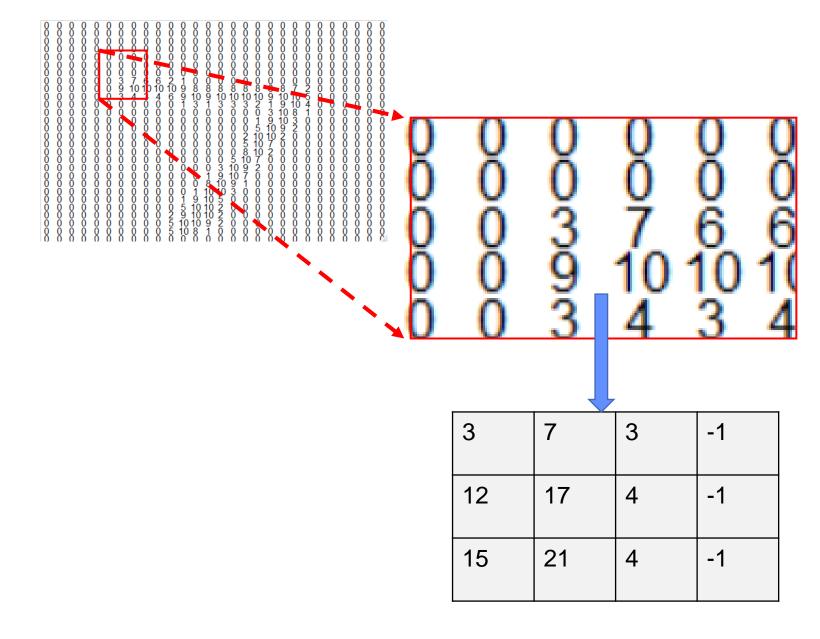
3		





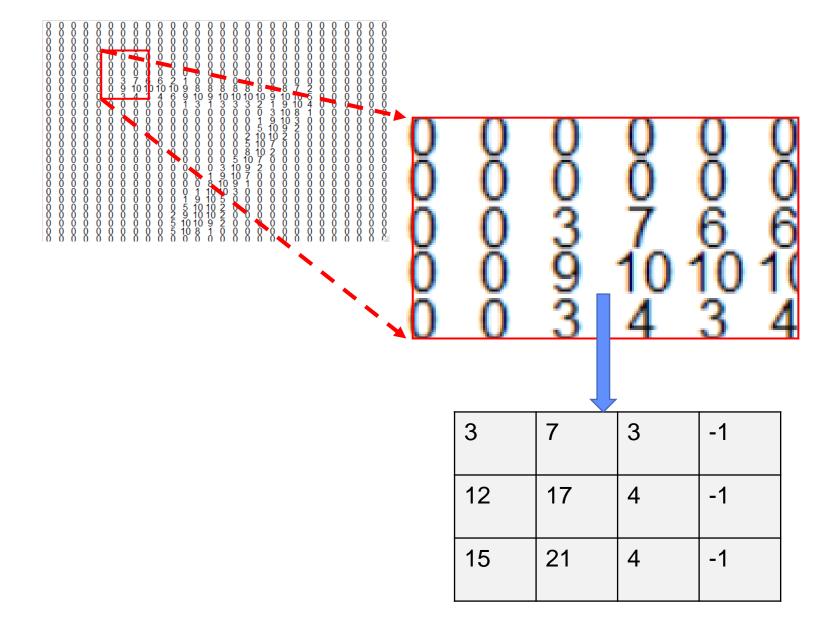


After vertical and horizontal sliding the 5x6 patch is now a 3x5 feature map.



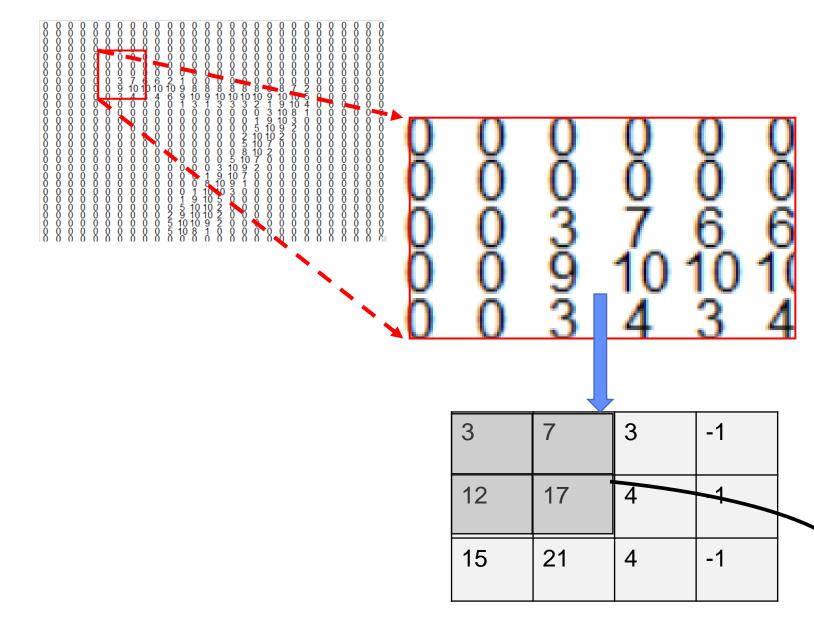
After vertical and horizontal sliding the 5x6 patch is now a 3x5 **feature map.**

What do the highest values in the feature map represent?



Optional next step:

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



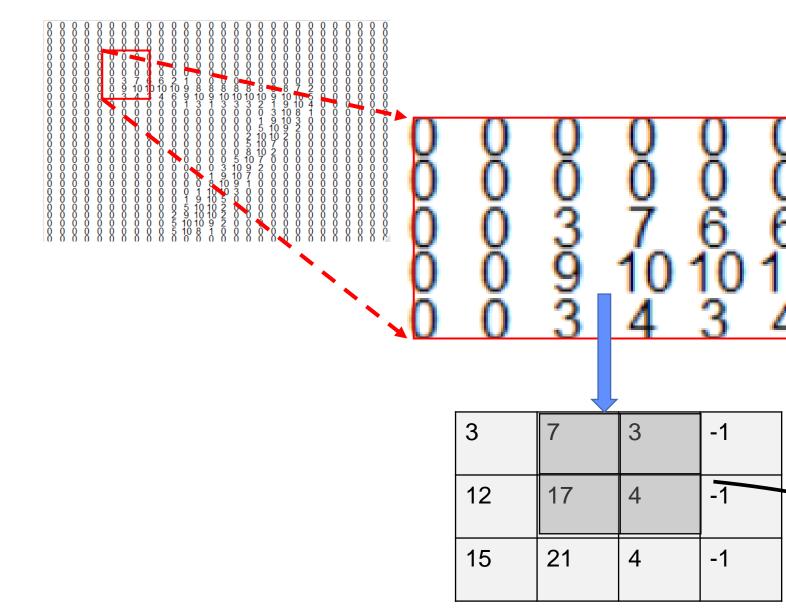
Optional next step:

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

2x2 filter has max=17

17



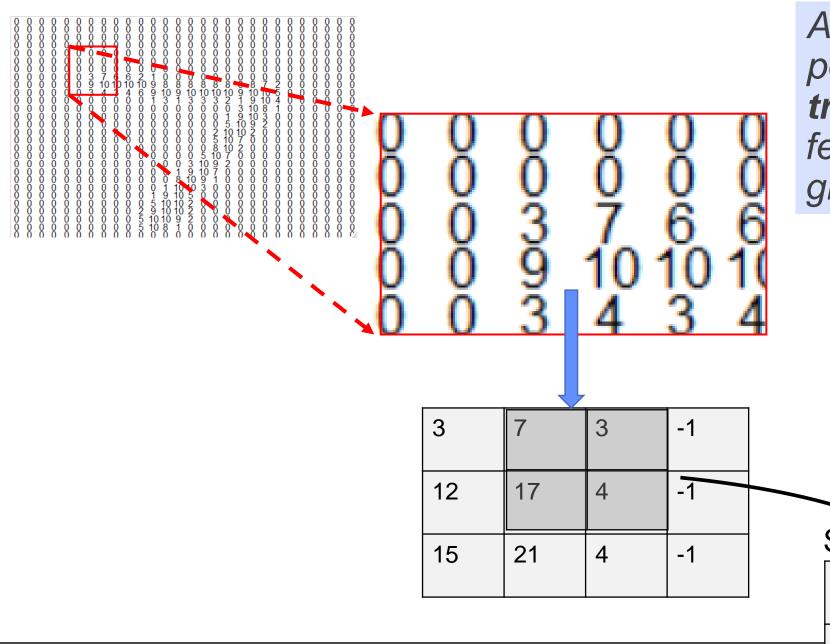


Optional next step:

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

Slide filter ...

17	17	4
21	21	4



After convolution and pooling 5x6 patch is **transformed** into a 2x3 feature map of 'edge gradients'

Slide filter ...

17	17	4
21	21	4

Feature engineering

In Computer Vision there are many kinds of edge detectors and many ways to scale them

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

But building features is hard, so if you have enough data ...

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

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

More hyperparameters:

Size of filter (smaller is more general)

More hyperparameters:

Size of filter (smaller is more general)

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

fine)



More hyperparameters:

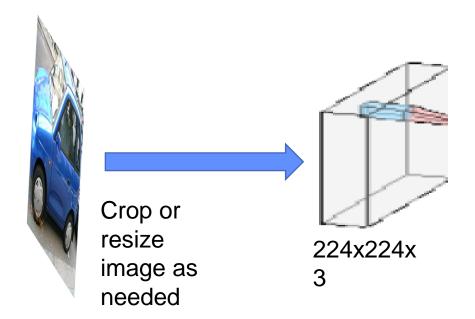
Size of filter (smaller is more general)

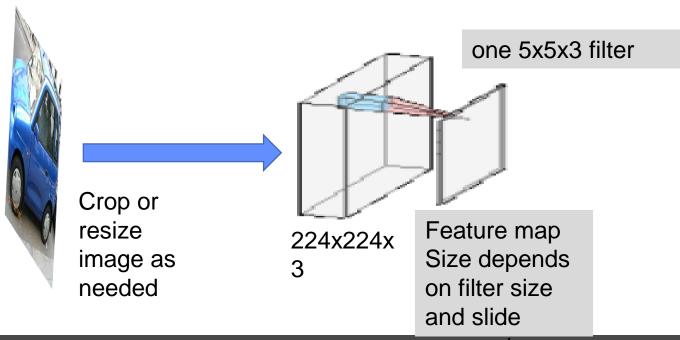
Number of pixels to slide over (1 or 2 is usually fine)

Number of filters (depends on the problem!)

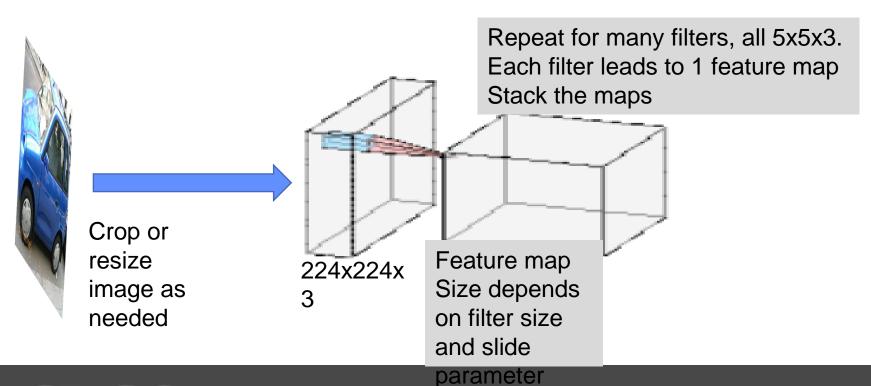
Max pooling or not (usually some pooling layers)



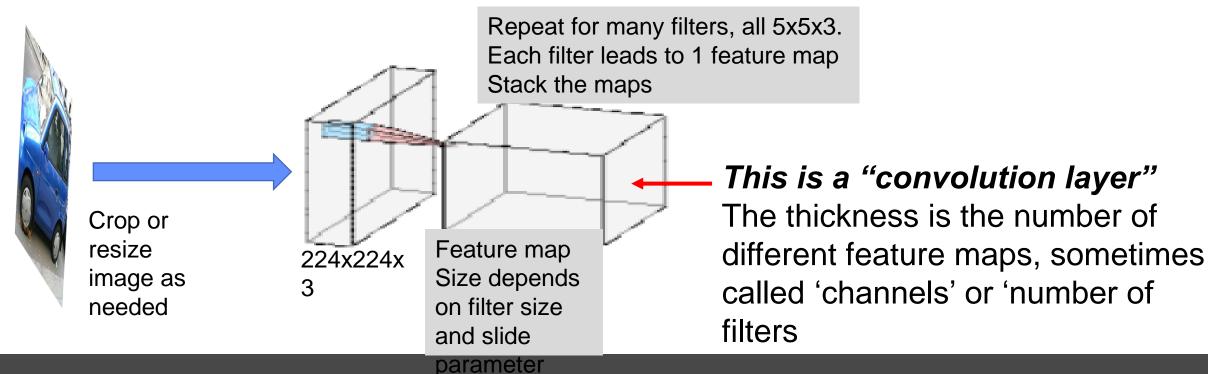




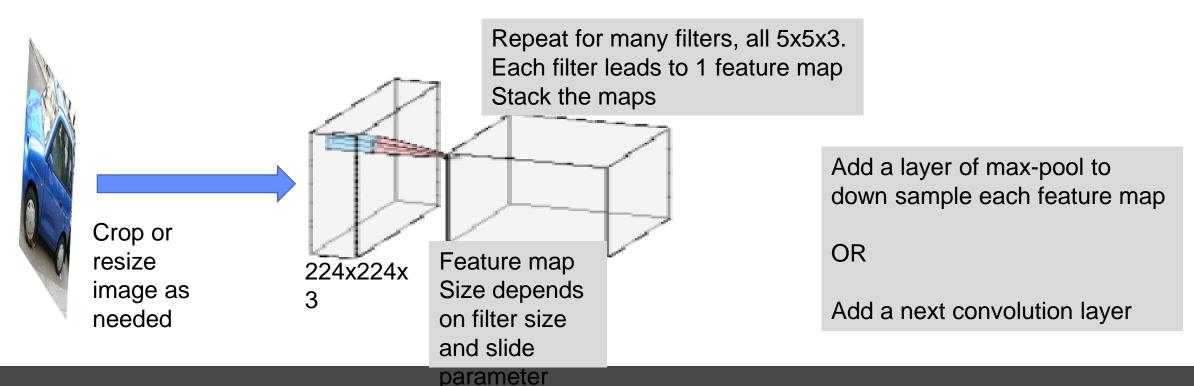












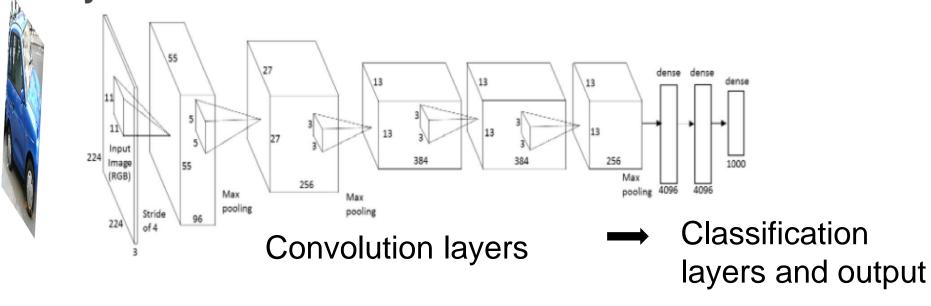


Large Scale Versions

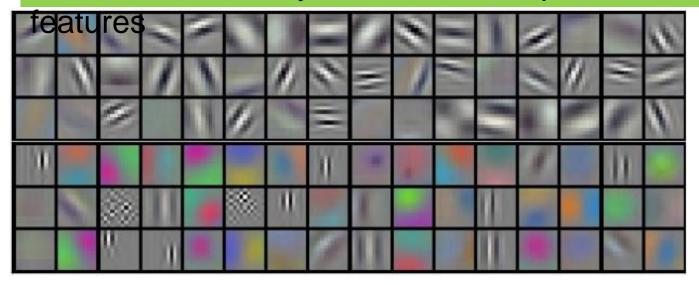
 Large (deep) Convolution Networks are turning out to be feasible with GPUs (some are 100+ layers)

Need large amounts of data and many heuristics to avoid overfitting and

increase efficiency



First convolution layer filters are simple

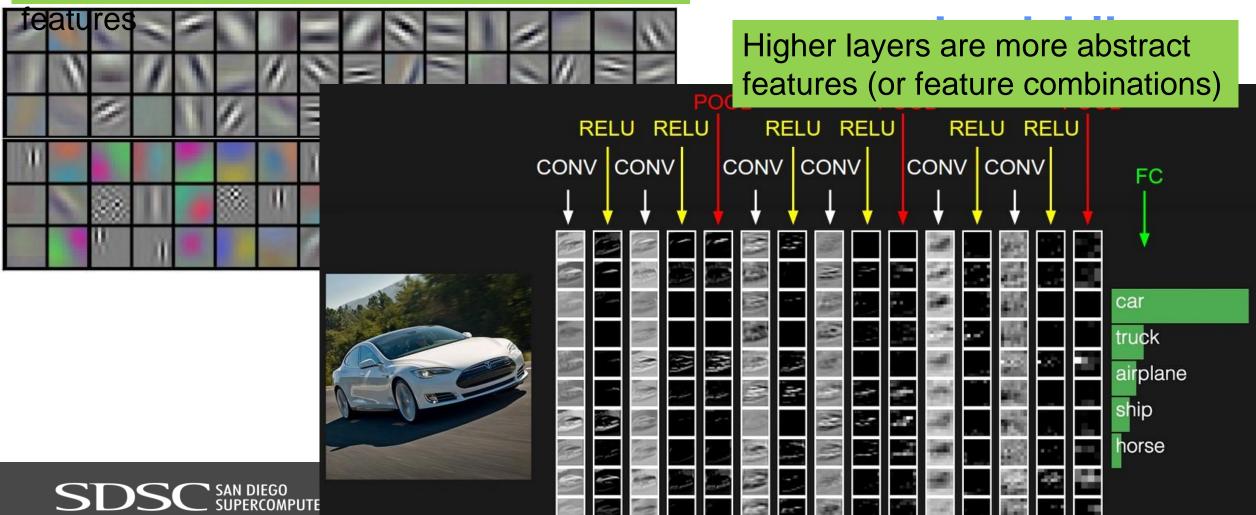


What Learned Convolutions Look Like



First convolution layer filters are simple

What Learned Convolutions



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



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Exercise CNN for Digit Classification

- The 'hello world' of CNNs
- Uses MNIST dataset and Keras



```
Widgets
View
       Insert
               Cell
                      Kernel
                                         Help
               ► Run ■ C
                                                 ::::::
 import warnings
   warnings.filterwarnings("ignore")
   import tensorflow as tf
   tf.get logger().setLevel('ERROR')
   #load and prepare data
    (x train, y train), (x test, y test) = tf.keras.datasets.mnist.load data()
                                         = x train / 255.0, x test / 255.0
   x train, x test
   #specify the neural network model and optimization
   my model = tf.keras.models.Sequential([
                          tf.keras.layers.Flatten(input shape=(28, 28)),
                           tf.keras.layers.Dense(10) ])
              = tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True)
   loss
   optimizer = tf.keras.optimizers.SGD(learning rate=0.01)
   my model.compile(optimizer=optimizer, loss=loss, metrics=['accuracy'])
   #fit the model
   fit history= my model.fit(x train, y train, epochs=5, batch size=128)
   #evaluate the fit
   my model.evaluate(x test, y test)
```

A basic model workflow in 4 steps

load/prepare data

define a model

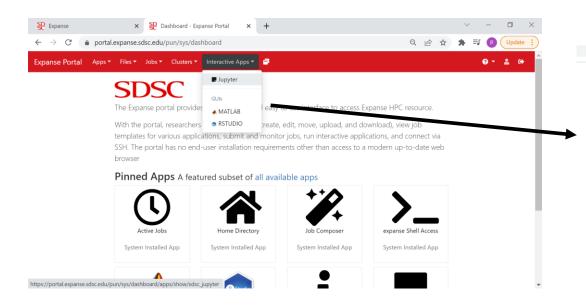
fit a model

test the model

Zooming in on keras.models statements

Zooming in on keras convolution layers statements

Use 16 filters, each of size 3x3



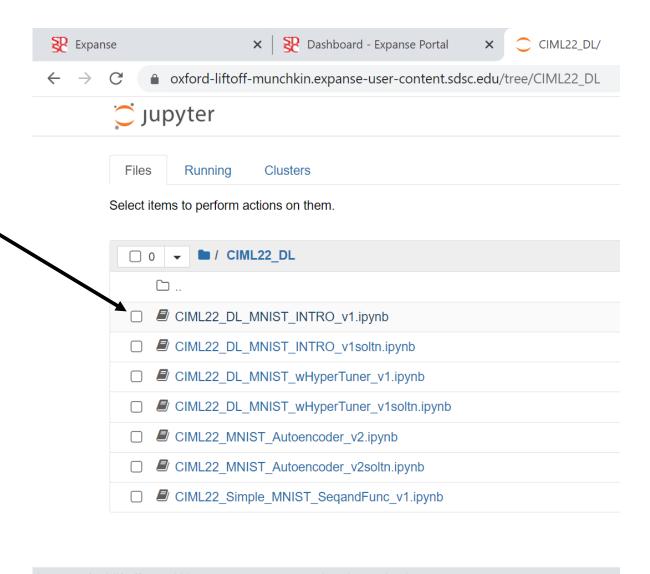
Expanse user portal: launch a jupyter notebook session (with compute or shared is OK)



	sds184		
	Partition (Please choose the gpu, gpu-shared, or gpu-preempt as the partition if using gpus):		
71 7	compute		
Account:	Time limit (min):		
	120		
Partition (Please cho			
shared	Number of cores:		
	128		
Time limit (min):	Memory required per node (GB):		
120	246		
Number of cores:			
	GPUs (optional):		
16	0		
Memory required pe	Singularity Image File Location: (Use your own or to include from existing container library at /cm/shared/apps/container e.g.,		
16	/cm/shared/apps/containers/singularity/pytorch/pytorch-latest.sif)		
	/cm/shared/apps/containers/singularity/tensorflow/tensorflow-latest.sif		
GPUs (optional):			
0	Environment modules to be loaded (E.g., to use latest version of system Anaconda3 include cpu,gcc,anaconda3):		
	singularitypro/3.9		
Singularity Image Fi /cm/shared/apps/co	Conda Environment (Enter your own conda environment if any):		
/cm/shared/apps/co			
Environment modul	Reservation:		
singularitypro/3.9	ciml-day1		
Conda Environment	Qo\$:		
Conda Environment			
Reservation:	Working directory:		
	home		
	Type:		
QoS:	Notebook		
Working directory:			
home			
Type:			
Notebook	 50		
1 1			

In jupyter notebook session open the MNIST_Intro notebook

Follow instructions in the notebook



 $https://oxford-liftoff-munchkin.expanse-user-content.sdsc.edu/notebooks/CIML22_DL/CIML22_DL_MNIST_INTRO INTRO IN$

Outline

- Overview of Neural Networks (aka Multilayer Perceptron)
- Convolution Neural Networks
- Basic Keras commands for building, training CNNs - exercise
- Hyperparameters and Tuning and workflows exercise



Things to think about for running a project

- Choosing Hyperparameters a bit of exploration and exploitation
- Need to figure out efficient Job workflow
- On HPC, CPU work fine for many cases, you will want to use GPUs for 'large' models and/or large datasets.
- Model saves and/or checkpoints are available in tensorflow; tensorboard available but needs to be secure (ask for details)

Choosing Hyperparameters

Generally:

```
architecture (layers, units, activation, filters, ...)
algorithm (learning rate, optimizer, epochs, ...)
efficient learning (batch size, normalization, initialization, ...)
```

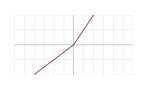
- Some options are determined by task: loss function, CNN vs MLP, ...
- Use what works, from related work or the latest recommendations,

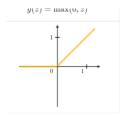
Some general recommendations (with caveats)

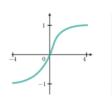
 From Hands-On Machine Learning, Keras, and TensorFlow, 2nd Ed, 2019, Géron,

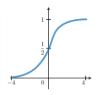
pg 338 Activations: Scaled-ELU > ELU > leaky ReLU > ReLU > tanh > logistic"











pg 359 Optimizer tradeoffs speed vs quality: * is bad *** is good

Table 11-2. Optimizer comparison

Class	Convergence speed	Convergence quality
SGD	*	***
SGD(momentum=)	**	***
SGD(momentum=, nesterov=True)	**	***
Adagrad	***	* (stops too early)
RMSprop	***	** or ***
Adam	***	** or ***
Nadam	***	** or ***
AdaMax	***	** or ***



Hyperparameters Search

- Can take a long time, hard to find global optimal
- Start with small data, short runs to get sense of range of good parameter values
- Easy but possibly time-consuming method: grid search over uniformly spaced values
- Do "exploration" then "exploitation", search wide then search deep Keras Tuner functions can help with the wide search

Hyperparameter Search Tool

Keras Hypertuner class implements several search strategies:

Hyperband is like a tournament competition of hyperparameter configurations, with incremental training, to weed out worse ones

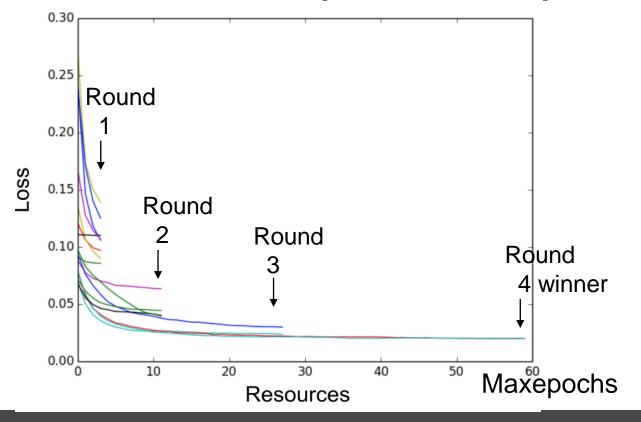
RandomSearch will search randomly through the space of configurations and try to find better regions

Bayesian optimization is like function approximation to pick out next configuration



Hyperband Bracket

Each round runs several network configurations for small number of epochs Several rounds with increasing epochs make up a bracket Several brackets are run to end up with several possible overall winners.



Note, you could run a small grid search around hyperband winners to confirm performance

Keras Tuner code snippet

Set up function to make the model

Set up hyperparameter choices

Define 'tuner' object; tuner search uses the model fit function

```
def build_model_hp(hp):
  hp_numfilters = hp.Int('hpnumfilters',min_value=8,max_value=32,step=4
  #your variable name ^^^ the parameter name in the hp object
def build model(numfilters,activation choice): #<<----add code: if yo</pre>
                                          list and change code t
    mymodel = keras.models.Sequential()
    mymodel.add(keras.layers.Convolution2D(numfilters,
                                    (3, 3),
                                    strides=1
tuner = kt.Hyperband(build_model_hp,
                     objective = 'val_accuracy',
                     max epochs = num max epochs,
                     factor
                                = 3.
                     hyperband_iterations=10,
                     directory = dirname,
                     overwrite =True, #overwrite directo
                     project_name='hyperbandtest',
                     executions per trial=5, #to try severe
                     seed
                                 =777)
```

Workflow and Organizing Jobs

Job Level: What makes sense to include in each job?

Model Level: run & test model for each parameter configuration

Data Level: loop through cross validation datasets (if applicable)

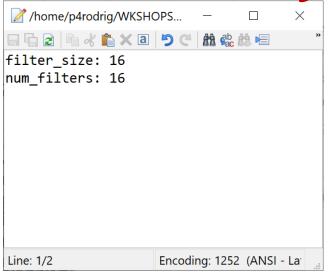
- Consider how long each a model runs for 1 configuration of hyperparameters for 1 dataset
- Organize jobs into reasonable chunks of work
- For large models consider model-checkpoints



Organizing Configurations – one way

Code snippet: using 'YAML' file to set up hyperparameter configuration

Create text file with "Parameter: Value" pairs



Read file as python dictionary

```
import yaml
with open("./modelrun_args.yaml", "r") as f:
    my_yaml=yaml.safe_load(f) #this returns a python dictionary

filter_size=my_yaml.get("filter_size")
num_filters=my_yaml.get("num_filters")
print('arguments, filter_size:',filter_size,' num_filters',num_filters)
```

Example slurm job script and execution for Expanse

You could also modify or set up parameters; and save yaml files for each run

```
#!/usr/bin/env bash
#SBATCH --job-name =mnist0522
#SBATCH --account=sds164
#SBATCH --partition=compute
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=128
#SBATCH --time=00:10:00
#SBATCH --output=myjoboutput.o%j.%N.out
module purge
module load singularitypro
module list
echo "filter_size: 3 " > modelrun_args.yaml
echo "num_filters: 16 " >> modelrun_args.yaml
singularity exec --bind /expanse,/scratch --nv \
  /cm/shared/apps/containers/singularity/tensorflow/tensorflow-latest.s
  python3 Intro mnist cnn2 forbatch.py > mymnist stdoutput.txt
```

```
02 EXP-05192022]$
02 EXP-05192022]$ sbatch run-job-tf-compute.sbatch
job 12502781
)2 EXP-05192022]$ squeue --me
BID PARTITION
                  NAME
                           USER ST
                                          TIME
                                                NODES NODELIST (REASON)
781
     compute =mnist05 p4rodrig PD
                                          0:00
                                                     1 (Priority)
     compute galyleo- p4rodrig R
                                                     1 \exp{-13-06}
                                         26:03
)2 EXP-05192022]$
```

Python Notebook vs Scripts

- On HPC you may want to run batch jobs on a script not a notebook.
- 1 Papermill is one tool (see PRose talk)
- 2 Or, you can use "jupyter nbconvert --to script your-python.ipynb" in the batch job.

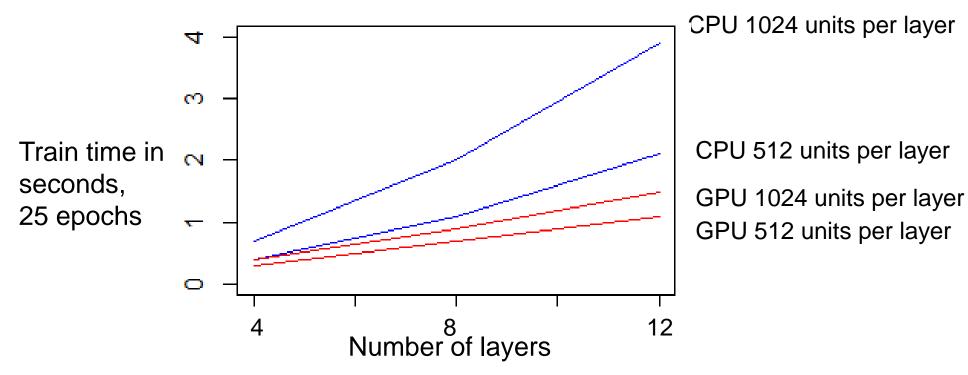
Also, turnoff plot display, save plots in files, and use a configuration file to pass in parameters

note on using GPU

- GPU node has multiple GPU devices
- By default tensforflow will run on 0th gpu device if GPU is available, otherwise it will use all CPU cores

Code snippet to check for GPU devices

GPU shared (V100) vs CPU (128 cores) For MLP with Dense Layers, 80000x200 data matrix



GPUs faster, but you might have to wait more in job queue; also some memory limits compared to CPU



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

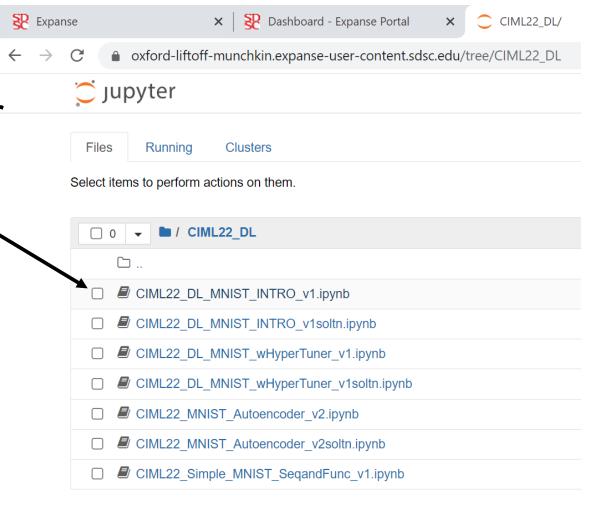
https://tfhub.dev/google/imagenet/inception_v1/classification/4

https://keras.io/examples/



In jupyter notebook session open the MNIST_wHyperTuner notebook

Follow instructions in the notebook

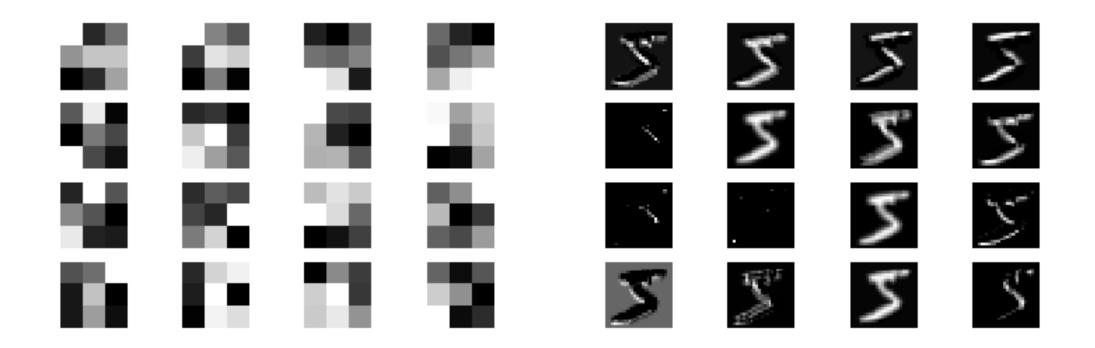


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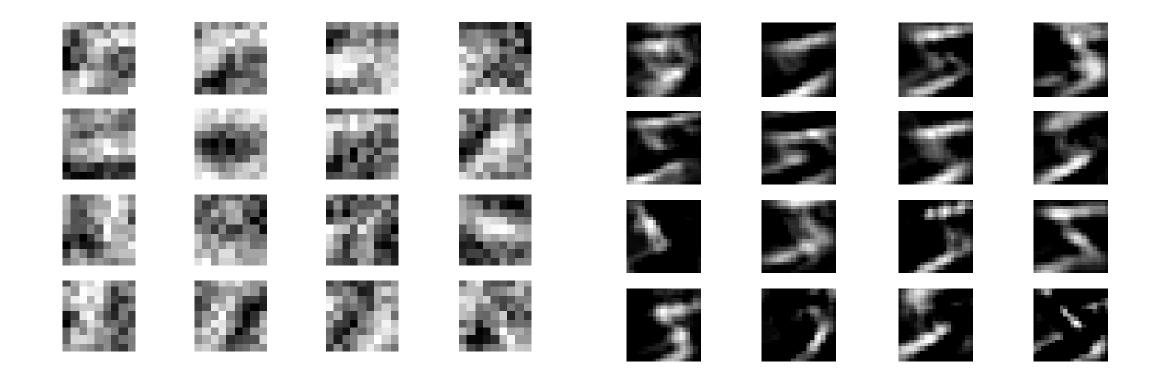
End

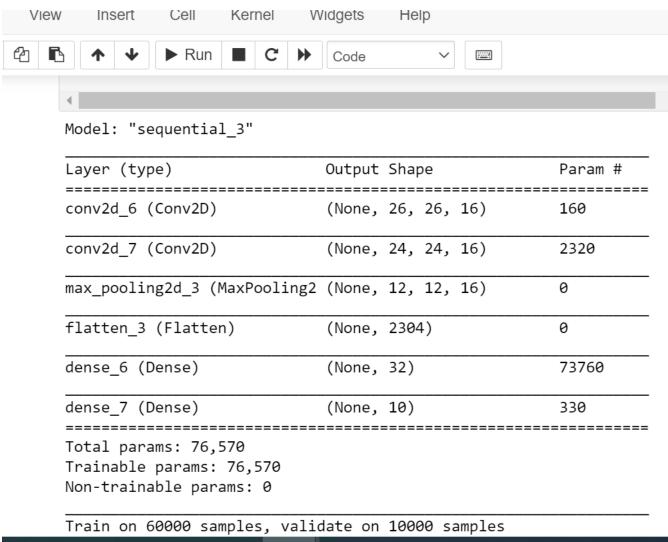


Exercise notes: 3x3 first convolution layer filter and activation



9x9 first convolution layer filter and activation





Filter_wts X num_filters + filter_bias: (3x3x1) *16 + 16*1 = 9*16+16=160