Deep Learning In An Afternoon

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Unprecedented Disruption

In the history of science, I defy you to find a similarly quick paradigm shift.

12 years ago

"Neural nets will enable real time ray tracing." Science Fiction.

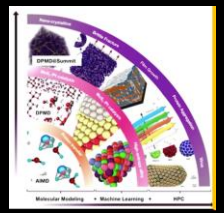
"Neural nets will do protein folding." Word salad.

8 years ago

"Neural nets will do CFD." Well, maybe someday, but not soon.

Today

Neural net enabled algorithms are the best way to do protein folding.



2024 Nobel in Chemistry

2024 Nobel in Physics was AI too!

Tomorrow

Skynet will kill us all. Or at least steal our jobs.

Why Now?

The ideas have been around for decades. Two components came together in the past 15 years to enable astounding progress:

Widespread parallel computing (GPUs)

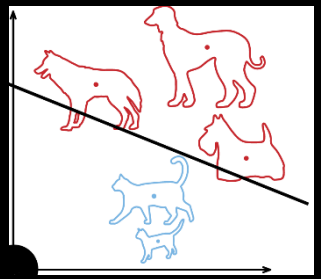
Big data training sets

Two Perspectives

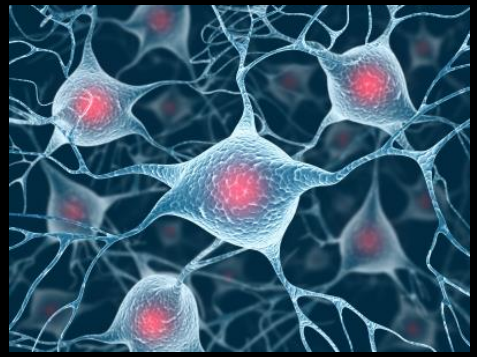
There are really two common ways to view the fundaments of deep learning.

- Inspired by biological models.

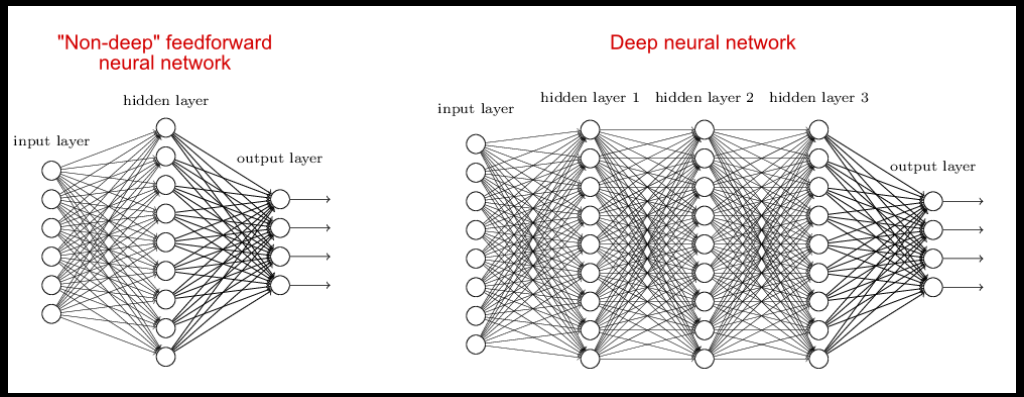
- An evolution of classic ML techniques (the perceptron).



They are both fair and useful. We'll give each a thin slice of our attention before we move on to the actual implementation. You can decide which perspective works for you.



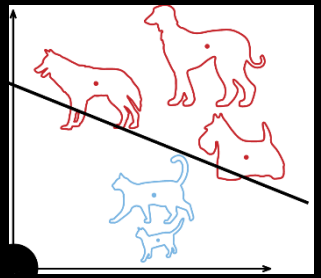
Modeled After The Brain



$$M = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

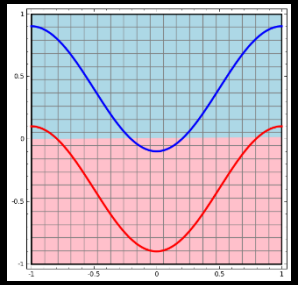
As a Highly Dimensional Non-linear Classifier

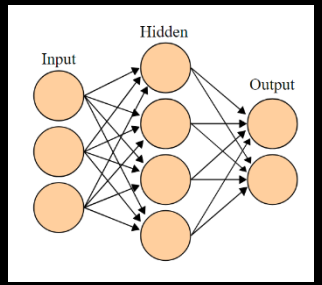
Perceptron

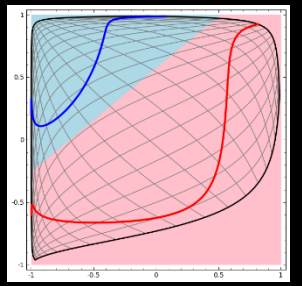


No Hidden Layer
Linear

Network



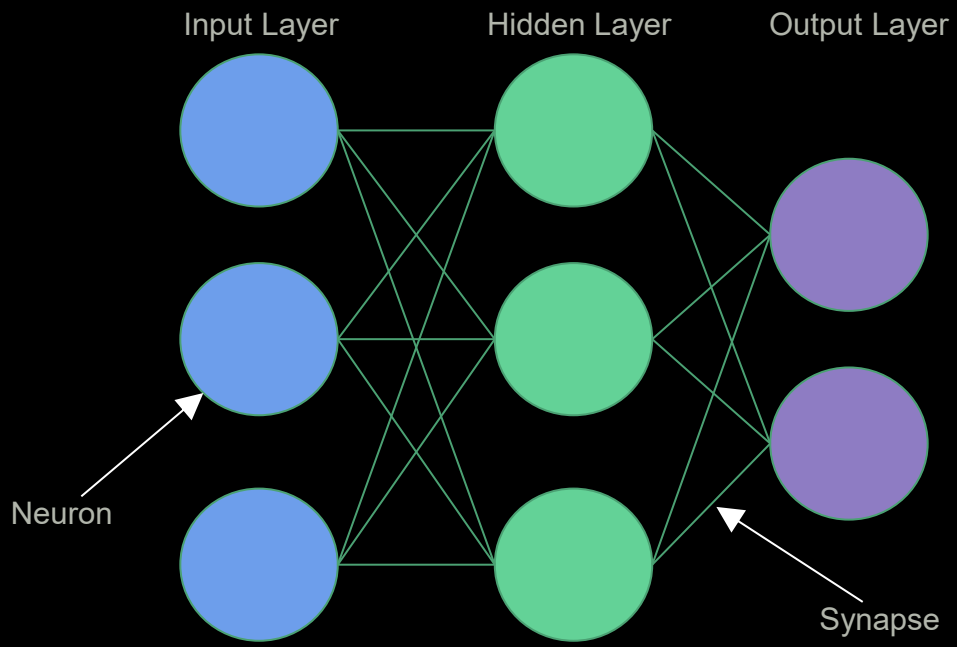




Hidden Layers
Nonlinear

Courtesy: Chris Olah

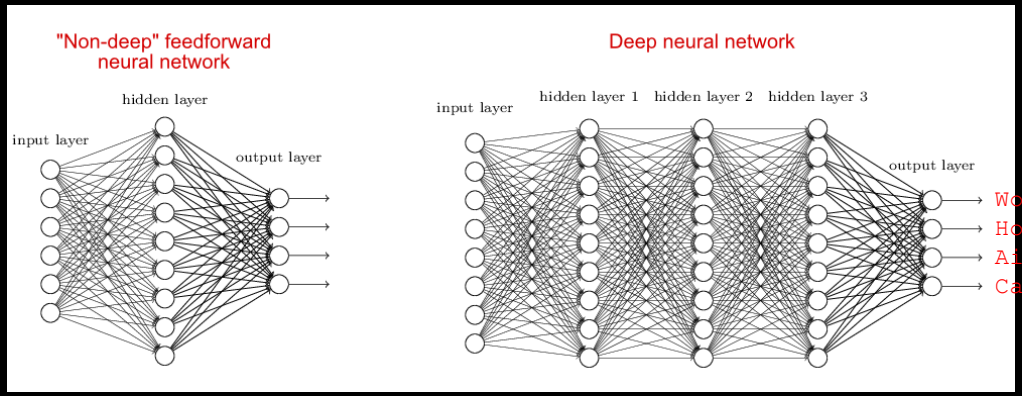
Basic NN Architecture



In Practice

How many inputs?

For an image it could be one (or 3) per pixel.



How deep?

100+ layers have become common.

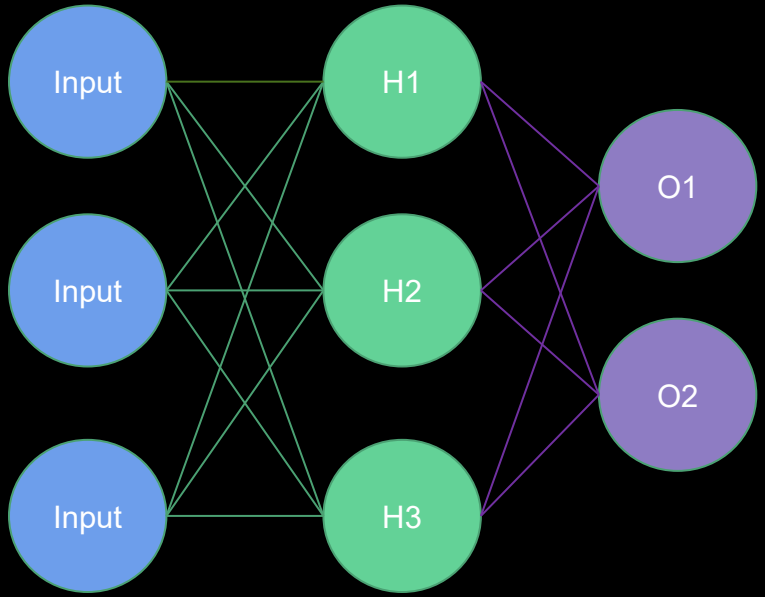
How many outputs?

Might be an entire image.

Or could be discreet set of classification possibilities.

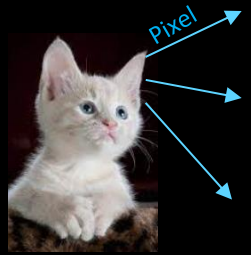
Inference

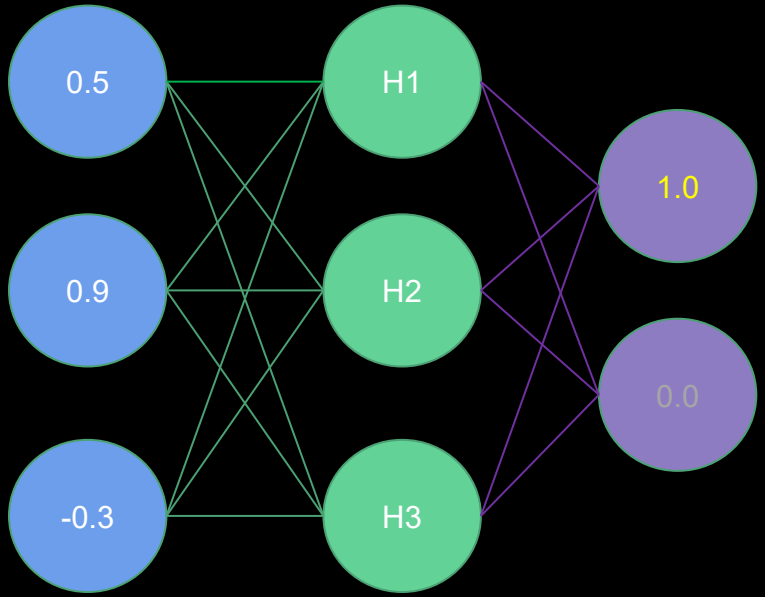
The "forward" or thinking step



Inference

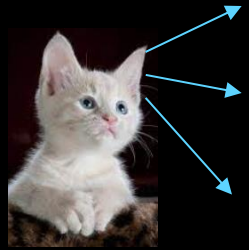
Input and Output Layers

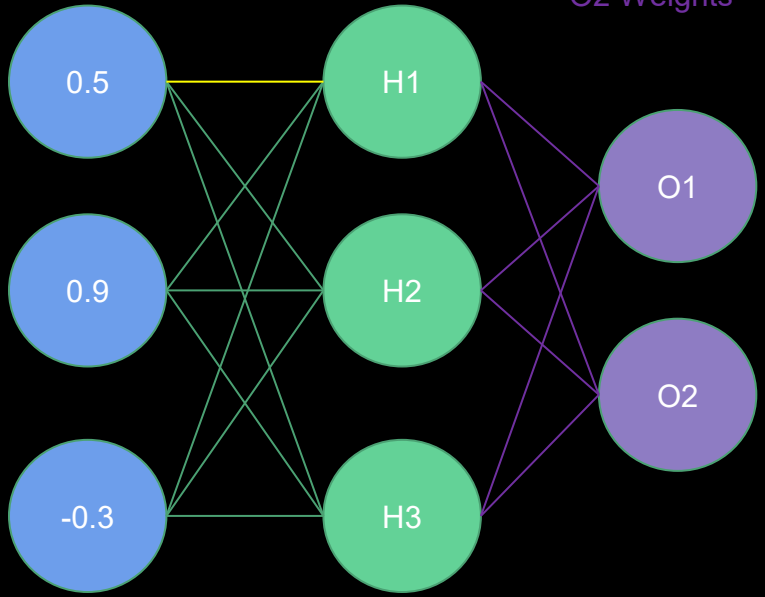




Inference

Weights or Parameters





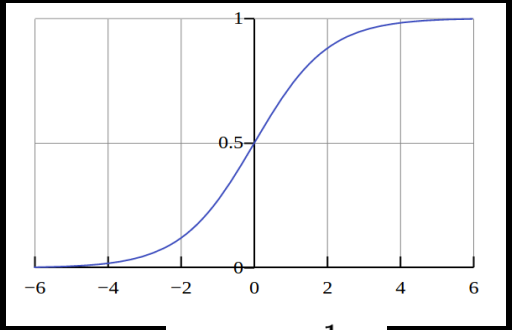
O1 Weights = (-3.0, 1.0, -3.0)
O2 Weights = (0.0, 1.0, 2.0)

H1 Weights = (1.0, -2.0, 2.0)
H2 Weights = (2.0, 1.0, -4.0)
H3 Weights = (1.0, -1.0, 0.0)

Activation Function

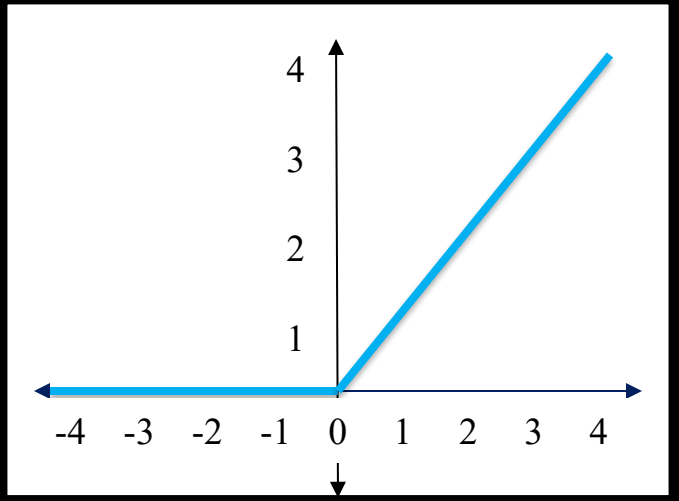
Neurons apply activation functions at these summed inputs. Activation functions are typically non-linear. There are countless possibilities. In reality, there are really only a few popular families:

- The Sigmoid function produces a value between 0 and 1, so it is intuitive when a probability is desired, and was almost standard for many years.



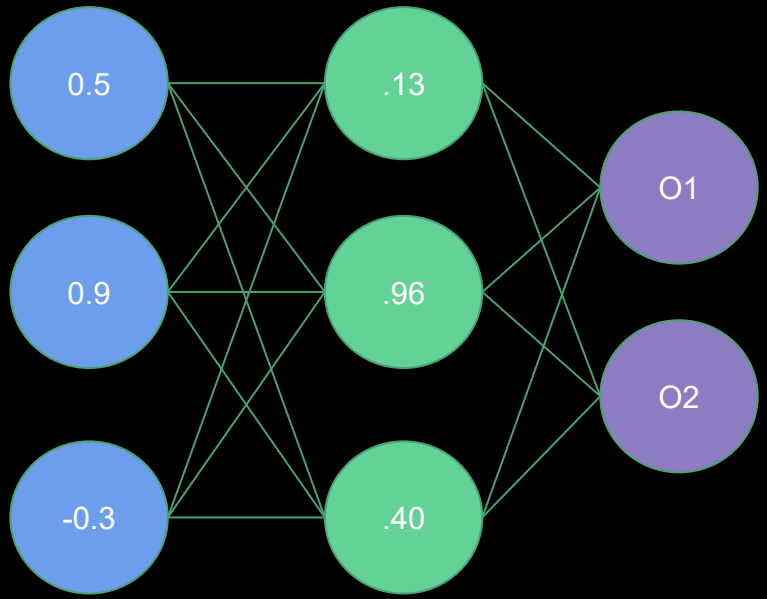
$$S(t) = \frac{1}{1 + e^{-t}}$$

- The Rectified Linear activation function is zero when the input is negative and is equal to the input when the input is positive. Rectified Linear activation functions are currently the most popular activation function as they are more efficient than the sigmoid or hyperbolic tangent.
    - Sparse activation: In a randomly initialized network, only 50% of hidden units are active.
    - Better gradient propagation: Fewer vanishing gradient problems compared to sigmoidal activation functions that saturate in both directions.
    - Efficient computation: Only comparison, maybe addition and multiplication for variants.
    - There are Leaky and Noisy variants.



Inference

Multiply, Add, do something non-linear.



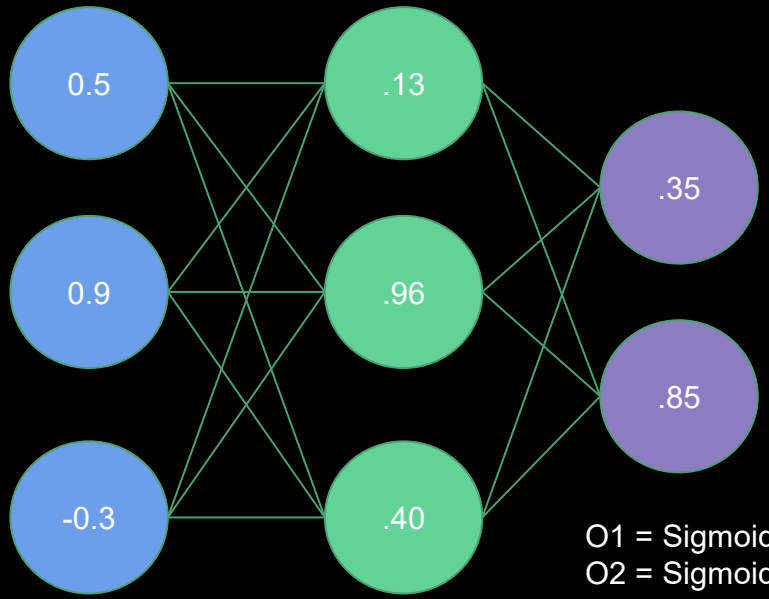
H1 Weights = (1.0, -2.0, 2.0)
H2 Weights = (2.0, 1.0, -4.0)
H3 Weights = (1.0, -1.0, 0.0)

O1 Weights = (-3.0, 1.0, -3.0)
O2 Weights = (0.0, 1.0, 2.0)

H1 = Sigmoid(0.5 * 1.0 + 0.9 * -2.0 + -0.3 * 2.0) = Sigmoid(-1.9) = .13
H2 = Sigmoid(0.5 * 2.0 + 0.9 * 1.0 + -0.3 * -4.0) = Sigmoid(3.1) = .96
H3 = Sigmoid(0.5 * 1.0 + 0.9 * -1.0 + -0.3 * 0.0) = Sigmoid(-0.4) = .40

Inference

Then do it again.



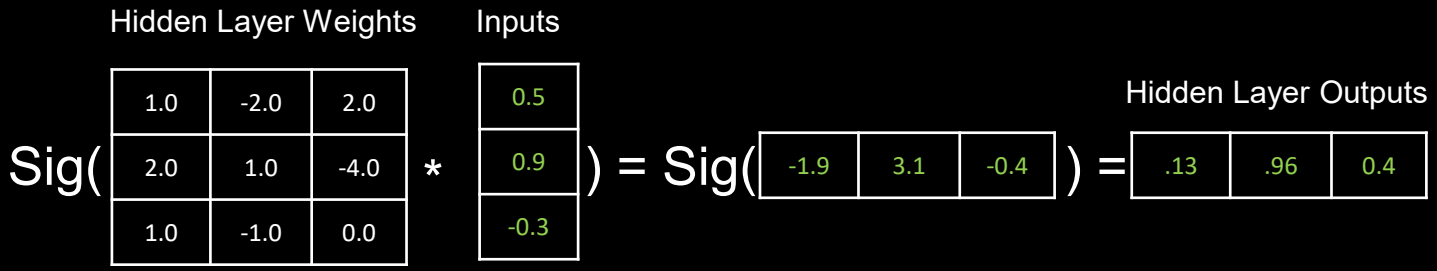
H1 Weights = (1.0, -2.0, 2.0)
H2 Weights = (2.0, 1.0, -4.0)
H3 Weights = (1.0, -1.0, 0.0)

O1 Weights = (-3.0, 1.0, -3.0)
O2 Weights = (0.0, 1.0, 2.0)

O1 = Sigmoid(.13 * -3.0 + .96 * 1.0 + .40 * -3.0) = Sigmoid(-.63) = .35
O2 = Sigmoid(.13 * 0.0 + .96 * 1.0 + .40 * 2.0) = Sigmoid(1.76) = .85

As A Matrix Operation

H1 Weights = (1.0, -2.0, 2.0)
H2 Weights = (2.0, 1.0, -4.0)
H3 Weights = (1.0, -1.0, 0.0)

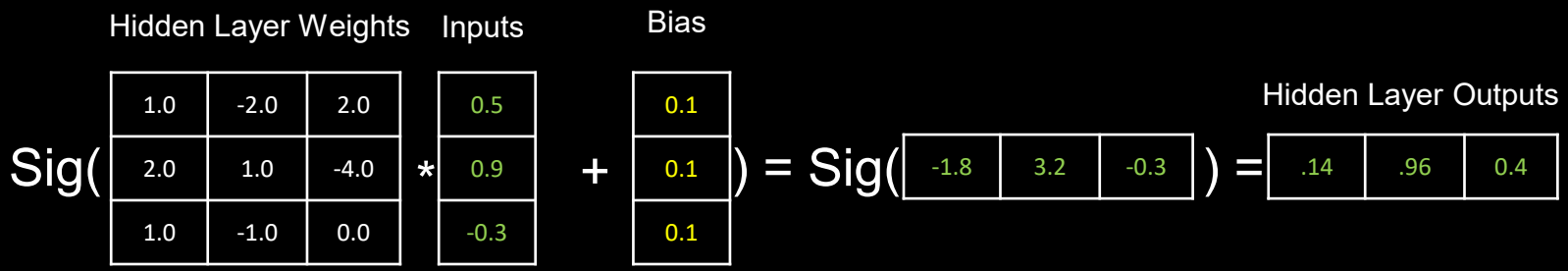


Now this looks like something that we can pump through a GPU.

Biases

It is also very useful to be able to offset our inputs by some constant. You can think of this as centering the activation function, or translating the solution (next slide). We will call this constant the *bias*, and it there will often be one value per layer.

Our math for the previously calculated layer now looks like this with bias=0.1:



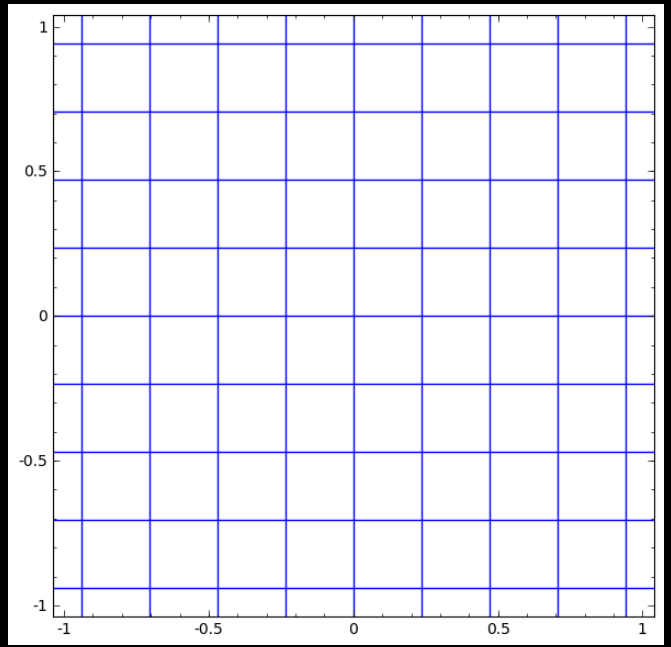
Linear + Nonlinear

The magic formula for a neural net is that, at each layer, we apply linear operations (which look naturally like linear algebra matrix operations) and then pipe the final result through some kind of final nonlinear activation function. The combination of the two allows us to do very general transforms.

The matrix multiply provides the *skew, rotation* and *scale*.

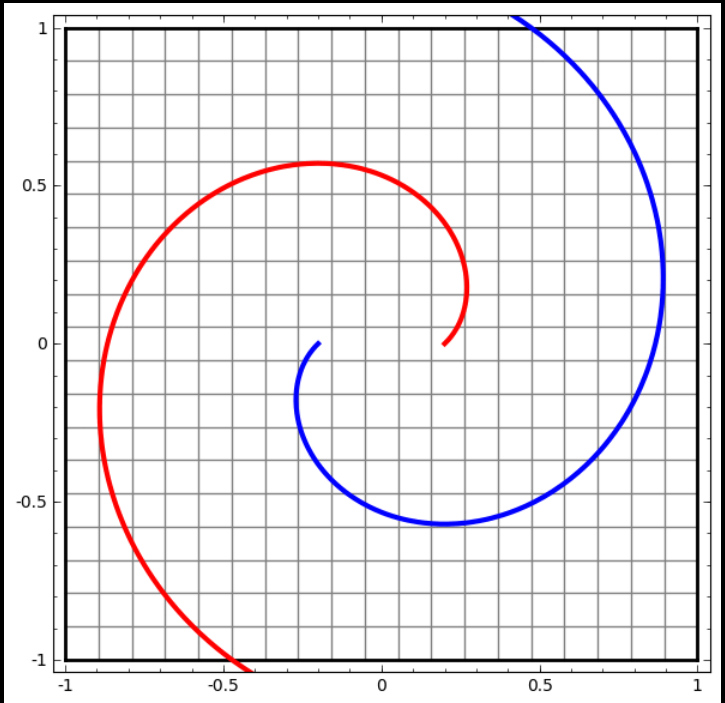
The bias provides the *translation*.

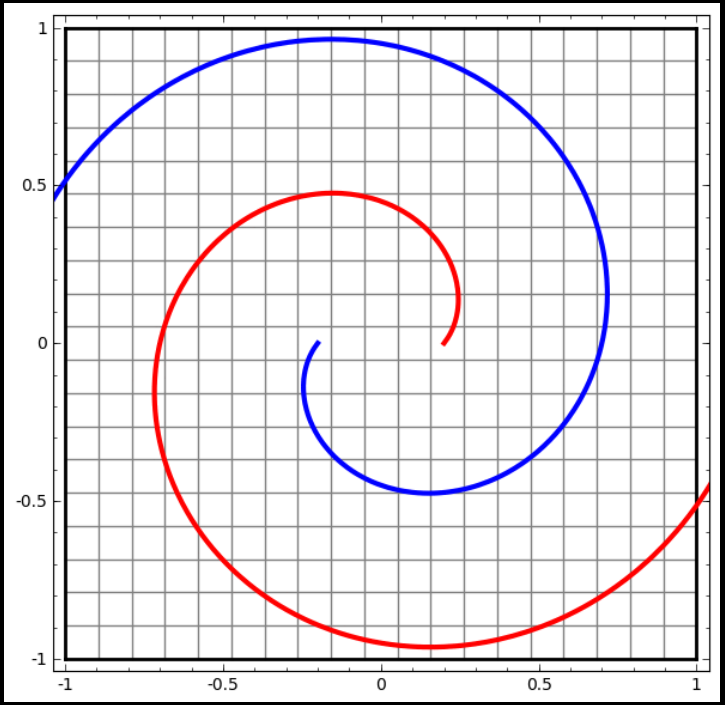
The activation function provides the *warp*.



Linear + Nonlinear

These are two very simple networks untangling spirals. Note that the second does not succeed. With more substantial networks these would both be trivial.

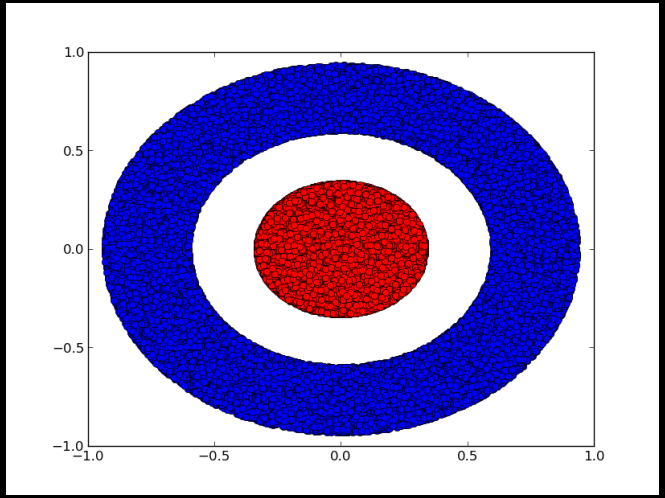




Courtesy: Chris Olah

Width of Network

A very underappreciated fact about networks is that the width of any layer determines how many dimensions it can work in. This is valuable even for lower dimension problems. How about trying to classify (separate) this dataset:

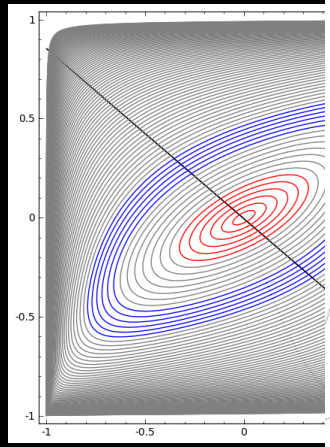


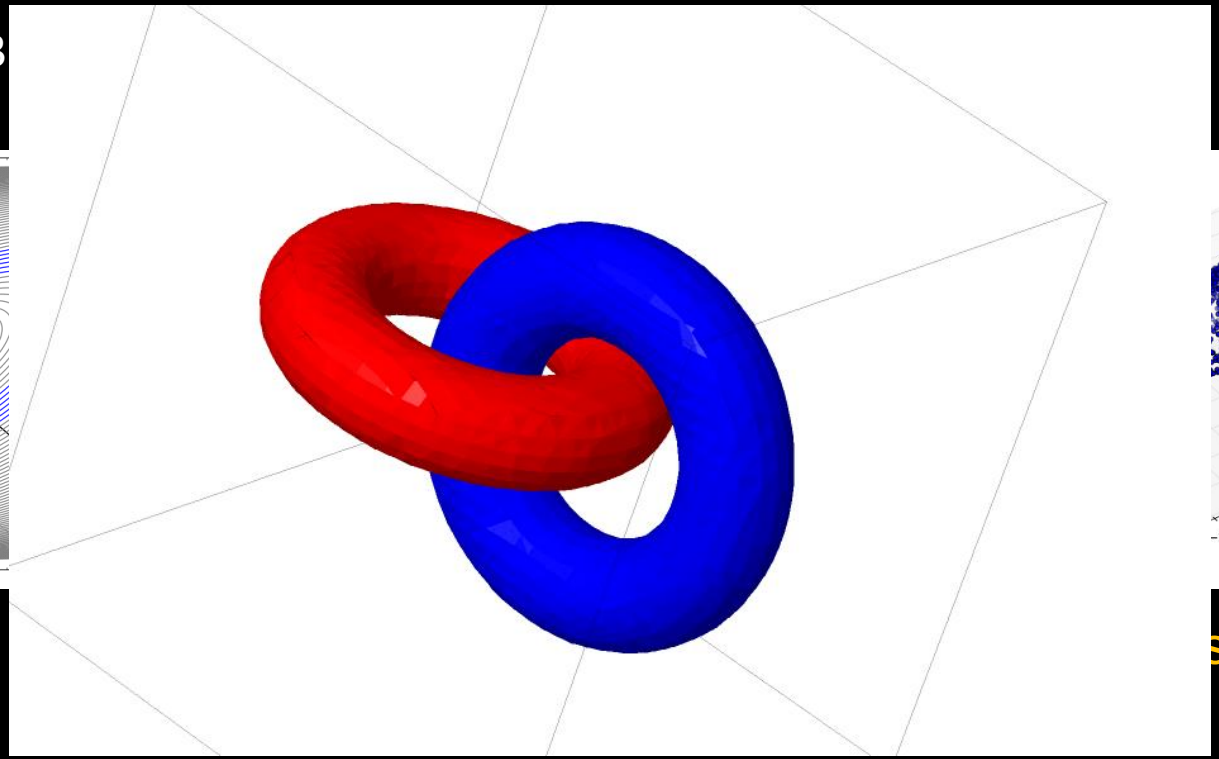
Can a neural net do this with twisting and deforming? What good does it do to have more than two dimensions with a 2D dataset?

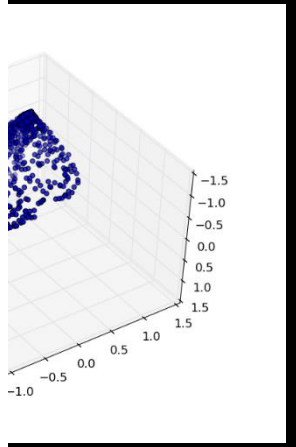
Courtesy: Chris Olah

Working In Higher Dimensions

It takes at least 3







Trying

s in 3D

Greater depth allows us to stack these operations, and can be very effective. The gains from depth are harder to characterize.

Courtesy: Chris Olah

Theoretically

Universal Approximation Theorem: A 1-hidden-layer feedforward network of this type can approximate any function[1], given enough width[2].

Not really that useful as:

- Width could be enormous.
- Doesn't tell us how to find the correct weights.

1) Borel measurable. Basically, mostly continuous and bounded.
2) Could be exponential number of hidden units, with one unit required for each distinguishable input configuration.

How Do We Find These Magic Weights? Training!

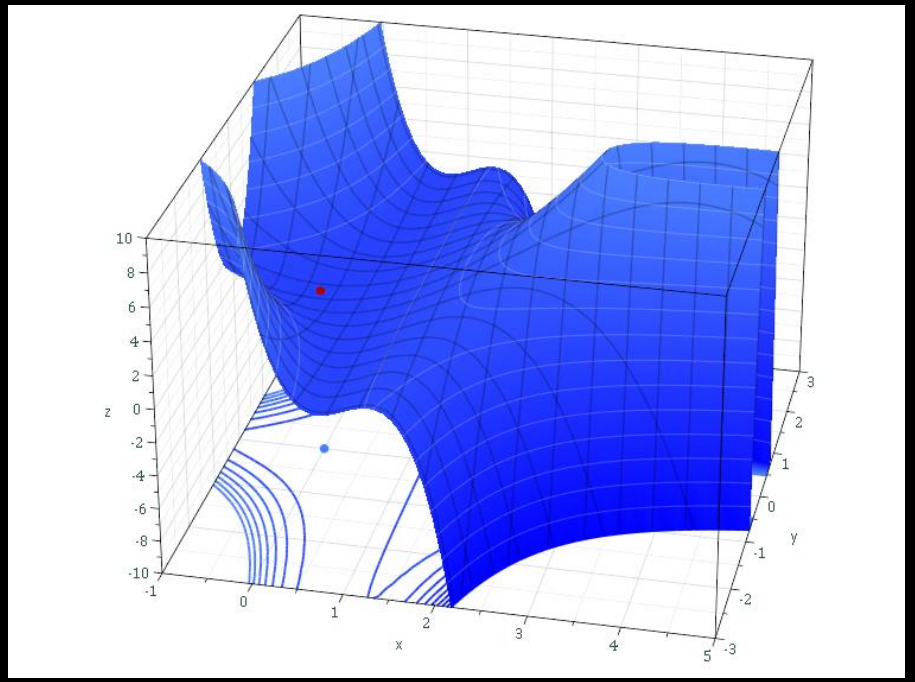
Our objective, mathematically, is really quite simple to state. *Given the loss as a function of weights, find the weight values that minimize the loss.*

If we had only two weights in our whole network, the picture would look like this.

We want to find the lowest point in our landscape.

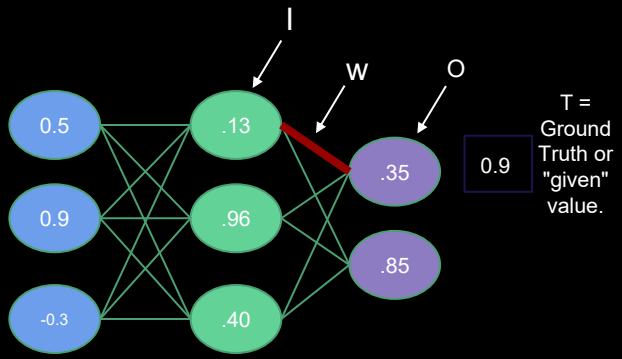
One obvious first step would be to descend the gradient from our current values. This should at least lead us to a better loss.

To do this gradient descent, we need some method of finding the gradients, $\frac{\partial E}{\partial w}$



Finding the gradients

For a tiny network, we could just write out the equations and use a little calculus. From our previous example we have all the math we need to find $\frac{\partial E}{\partial w}$ for one of the final weights.



$$\frac{\partial E}{\partial w} = I \cdot (O - T) \cdot O \cdot (1 - O)$$

$$\frac{\partial E}{\partial w} = .13 \cdot (.35 - .9) \cdot .35 \cdot (1 - .35)$$

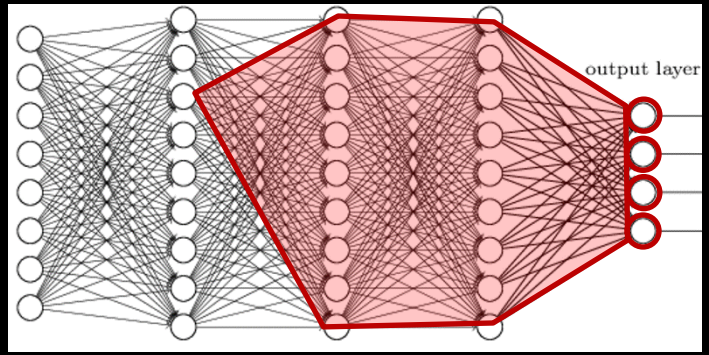
Using our Sigmoid activation function

$$S(t) = \frac{1}{1 + e^{-t}}$$

With just this information, we have some idea of which way to adjust W. But, when we get deeper into a more realistic network, the expressions get more complex...

Back-Propagation

In a useful network, the chain rule results in a lot of factors for any given weight adjustment.



There are a lot of dependencies going on here. It isn't obvious that there is a viable way to do this in very large networks.

From the fantastic *Deep Learning*, Goodfellow, Bengio and Courville.

$$\frac{\partial u^{(n)}}{\partial u^{(j)}} = \sum_{\substack{\text{path } (u^{(\pi_1)}, u^{(\pi_2)}, \ldots, u^{(\pi_t)}), \\ \text{from } \pi_1 = j \text{ to } \pi_t = n}} \prod_{k=2}^{t} \frac{\partial u^{(\pi_k)}}{\partial u^{(\pi_{k-1})}}.$$

Not as scary as it looks. There are really just two pieces. The sum represents all the possible paths, and the product operator is because each of the pieces along any path multiply each other.

Since the number of paths from one node to a distant node can grow exponentially in the length of these paths, the number of terms in the above sum, which is the number of such paths, can grow exponentially with depth. A large cost would be incurred because the same computation for the subfactors would be redone many times. To avoid such recomputation, back-propagation works as a table-filling algorithm that stores intermediate results and avoids repeating many common subexpressions. This is a version of *dynamic programing*, which you may have heard of.

Back-propagation Full Story

If you have 30 minutes, and remember freshman calculus, you can understand the complete details of the algorithm. I heartily recommend one of these.

An elegant perspective on this can be found from Chris Olah at
http://colah.github.io/posts/2015-08-Backprop .

With basic calculus you can readily work through the details. You can find an excellent explanation from the renowned *3Blue1Brown* at
https://www.youtube.com/watch?v=Ilg3gGewQ5U .

To be honest, many people are happy to leave the details to TensorFlow, or whatever package they are using. Just don't think it is beyond your understanding.

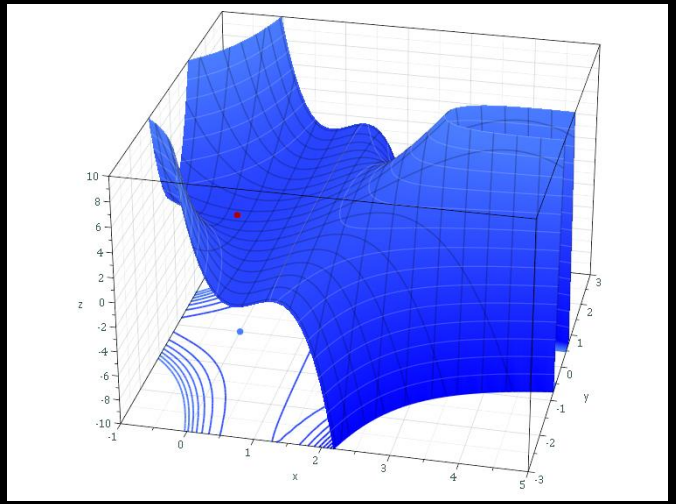
Gradient Descent

We now have gradients to push us in the right direction, and we can use the well-known numerical technique of *gradient descent*.

This is still a challenging situation, as our landscape has many local minimums that we could get trapped in on our way to finding a better one. We don't even hope to find the ideal global minimum.

Many variations have arisen that perform better for deep learning applications. TensorFlow will allow us to use these interchangeably; and we will.

Most interesting recent methods incorporate *momentum* to help get over a local minimum. Momentum and *step size (or learning rate)* are the two *hyperparameters* we will encounter later.



Again, just two weights.

We could/should find the current error for all the training data before updating the weights (an *epoch*). However it is usually much more efficient to use a *stochastic* approach, sampling a random subset of the data, updating the weights, and then repeating with another *mini-batch*. This is called *Stochastic Gradient Descent*.

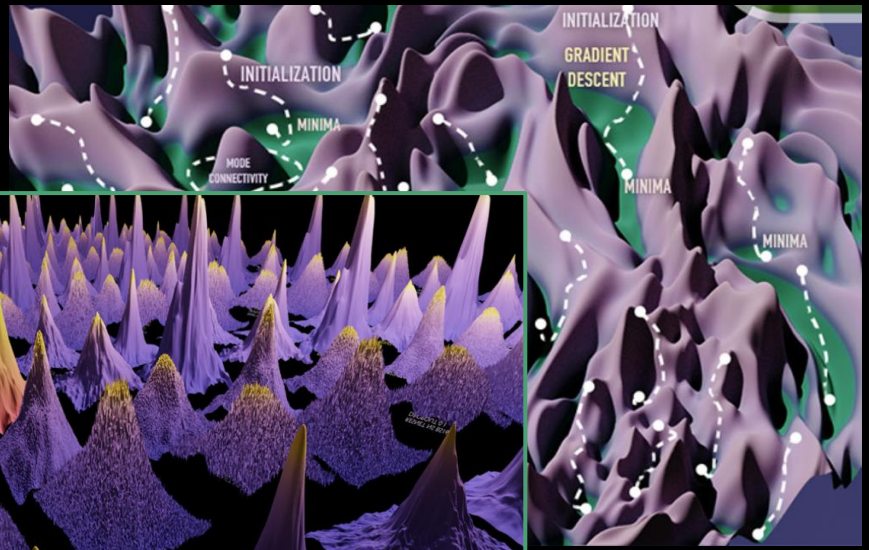
Problem Solved?

You should expect to struggle with these hyperparameters to get good performance. Why? Because these landscapes have many local minimums. For a long time this was considered an unsolvable obstacle.

For once, adding in more (many more!) helps us. There become many more "es given valley.

For the topologically inclined, we have points than pits because we only need hessian to be negative, instead of all po

Mini-batches also have an impact, as ea along a different landscape, shaking thi



Visuals by Javier Ideami @ losslandscape.com
Go there!

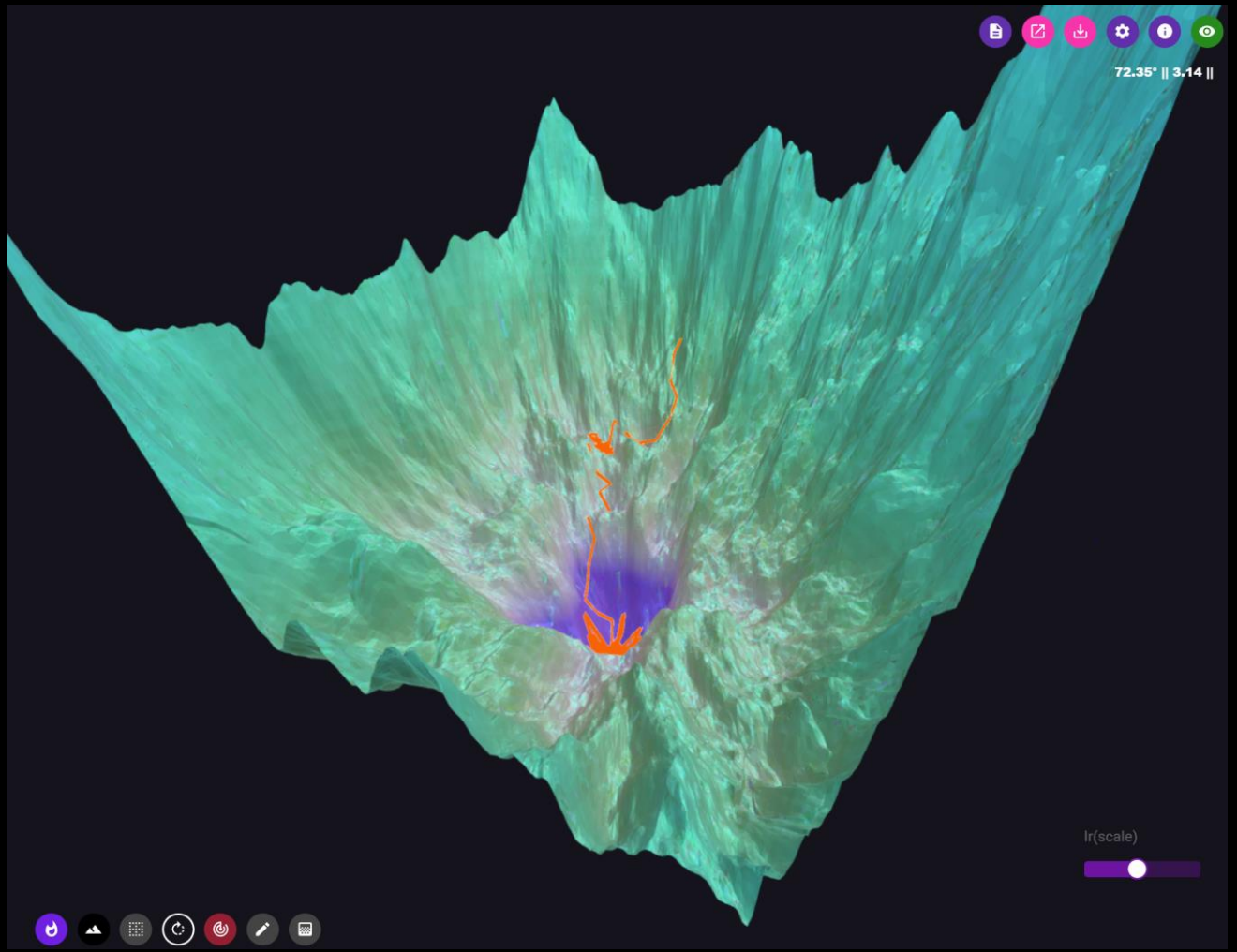
* This is not a rigorous assertion. A counterexample is protein folding. We know a very good approximate energy function, and it has many degrees of freedom, but you simply cannot obtain the folded structure by doing gradient descent.

Incredible Demo

We're going to try a live demo here, but you should visit this site and play around with it yourself. There is a lot of insight to be had.

https://losslandscape.com/explorer

Again, from the awesome Javier Ideami @ losslandscape.com



Going To Play Along?

Make sure you are on a GPU node:

```
bridges2-login014% interact -gpu
v001%
```

Load the TensorFlow 2 Container:

```
v001% singularity shell --nv  /ocean/containers/ngc/tensorflow/tensorflow_23.04-tf2-py3.sif
```

And start TensorFlow:

```
Singularity> python
Python 3.8.10 (default, Mar 13 2023, 10:26:41)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license"
>>> import tensorflow
>>> ...some congratulatory noise...
>>>
```

Two Other Ways To Play Along

From inside the container, and in the right example directory,run the python programs from the command line:

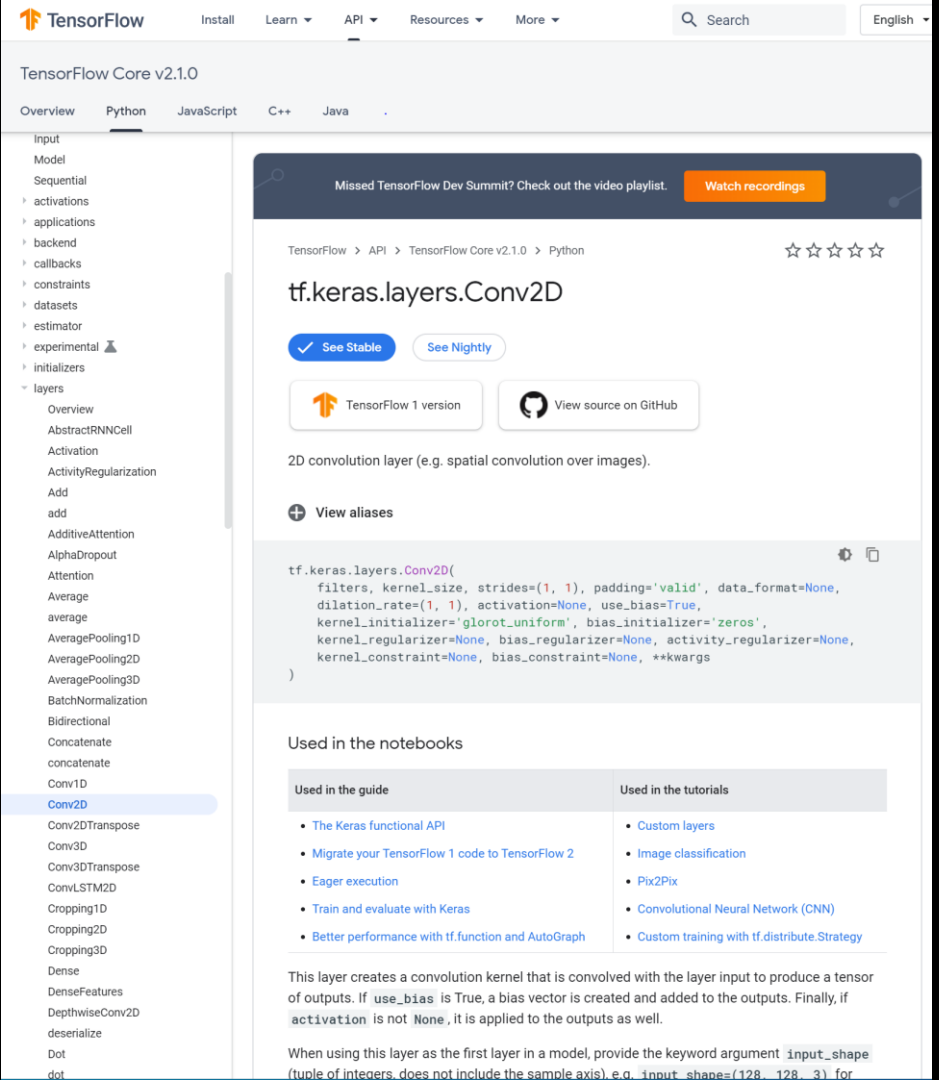
```
Singularity> python CNN_Dropout.py
```

or invoke them from within the python shell:

```
>>> exec(open("./CNN_Dropout.py").read())
```

TensorFlow or PyTorch or...?

Documentation



The API is well documented.

That is terribly unusual.

Take advantage and keep a browser open as you develop.

MNIST

We now know enough to attempt a problem. Only because the TensorFlow framework, and the Keras API, fills in a lot of the details that we have glossed over. That is one of its functions.

Our problem will be character recognition. We will learn to read handwritten digits by training on a large set of 28x28 greyscale samples.

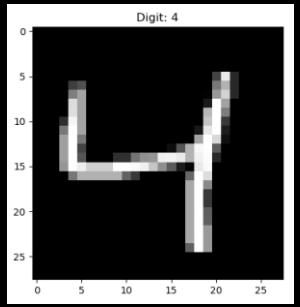
First we'll do this with the simplest possible model just to show how the TensorFlow framework functions. Then we will gradually implement our way to a quite sophisticated and accurate convolutional neural network for this same problem.

Getting Into MNIST

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()


train_images = train_images.reshape(60000, 784)
test_images  = test_images.reshape(10000, 784)

test_images  = test_images.astype('float32')
train_images = train_images.astype('float32')

test_images  /= 255
train_images /= 255
```

matplotlib bonus insight

```
import matplotlib.pyplot as plt

plt.imshow(train_images[2], cmap=plt.get_cmap('gray'),
interpolation='none')
plt.title("Digit: {}".format(train_labels[2]))
```



Defining Our Network

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()


train_images = train_images.reshape(60000, 784)
test_images  = test_images.reshape(10000, 784)

test_images  = test_images.astype('float32')
train_images = train_images.astype('float32')

test_images  /= 255
train_images /= 255


model = tf.keras.Sequential([
  tf.keras.layers.Dense(64, activation='relu', input_shape=(784,)),
  tf.keras.layers.Dense(64, activation='relu'),
  tf.keras.layers.Dense(10, activation='softmax'),
])
```

Starting from zero?

In general, initialization values are hard to pin down analytically. Values might help optimization but hurt generalization, or vice versa.

The only certainty is you need to have different values to break the symmetry, or else units in the same layer, with the same inputs, would track each other.

Practically, we just pick some "reasonable" values.

```
model.summary()
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_6 (Dense)              (None, 64)                50240
_________________________________________________________________
dense_7 (Dense)              (None, 64)                4160
_________________________________________________________________
dense_8 (Dense)              (None, 10)                650
=================================================================
Total params: 55,050
Trainable params: 55,050
Non-trainable params: 0
```

Softmax

Why Softmax?

The values coming out of our matrix operations can have large, and negative values. We would like our solution vector to be conventional probabilities that sum to 1.0. An effective way to normalize our outputs is to use the popular *Softmax* function. Let's look at an example with just three possible digits:

Digit	Output	Exponential	Normalized
0	4.8	121	.87
1	-2.6	0.07	.00
2	2.9	18	.13

Solving For Weights

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()


train_images = train_images.reshape(60000, 784)
test_images  = test_images.reshape(10000, 784)

test_images  = test_images.astype('float32')
train_images = train_images.astype('float32')

test_images  /= 255
train_images /= 255


model = tf.keras.Sequential([
  tf.keras.layers.Dense(64, activation='relu', input_shape=(784,)),
  tf.keras.layers.Dense(64, activation='relu'),
  tf.keras.layers.Dense(10, activation='softmax'),
])


model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])
```

Cross Entropy

Given the sensible way we have constructed these outputs, the Cross Entropy Loss function is a good way to define the error across all possibilities. Better than squared error, which we have been using until now. It is defined as $-\Sigma\ y\_\ \log\ y$, or if this really is a "0", $y\_=(1,0,0)$, and

$$-1\log(0.87) - 0\log(0.0001) - 0\log(0.13) = -\log(0.87) = -0.13$$

It somewhat penalizes a slightly wrong guess, or an "unconfident" right guess, and greatly penalizes a very wrong guess.

You can also think that it "undoes" the Softmax, if you want.

Training

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()


train_images = train_images.reshape(60000, 784)
test_images  = test_images.reshape(10000, 784)

test_images  = test_images.astype('float32')
train_images = train_images.astype('float32')

test_images  /= 255
train_images /= 255



model = tf.keras.Sequential([
  tf.keras.layers.Dense(64, activation='relu', input_shape=(784,)),
  tf.keras.layers.Dense(64, activation='relu'),
  tf.keras.layers.Dense(10, activation='softmax'),
])


model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])



history = model.fit(train_images, train_labels, batch_size=128, epochs=40, verbose=1, validation_data=(test_images, test_labels))
```

Results

matplotlib bonus insight

```
history = model.fit(train_images, ..., ...)

plt.plot(history.history['accuracy'])
plt.plot(history.history['val_accuracy'])
plt.title('Model accuracy')
plt.ylabel('Accuracy')
plt.xlabel('Epoch')
plt.legend(['Train', 'Test'], loc='upper

plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.title('Model loss')
plt.ylabel('Loss')
plt.xlabel('Epoch')
plt.legend(['Train', 'Test'], loc='upper
plt.show()
```

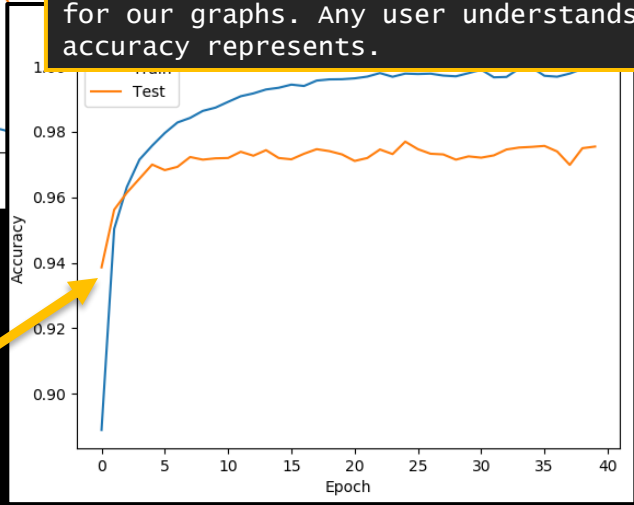
```
/sample - loss: 0.3971 - accuracy:

/sample - loss: 0.1696 - accuracy:
```

Accuracy or Loss?

Loss is the "mathematical" value we have specified in our model to use for parameter fitting.

Accuracy is simply how many we get right when we test our model as an application. It might not apply to a non-classification problem (think *Stable Diffusion*) and it doesn't capture how much right or wrong we are (we could be very confident that a dog is a cat).

The two are normally closely related and track each other. We will choose Accuracy for our graphs. Any user understands what accuracy represents.



0.9755

Why would the test accuracy *ever* be better than the training (as momentarily happens here)?

The training value is the average over each batch, and the test value is only at the end of the epoch, when the model tends to be at least slightly better.

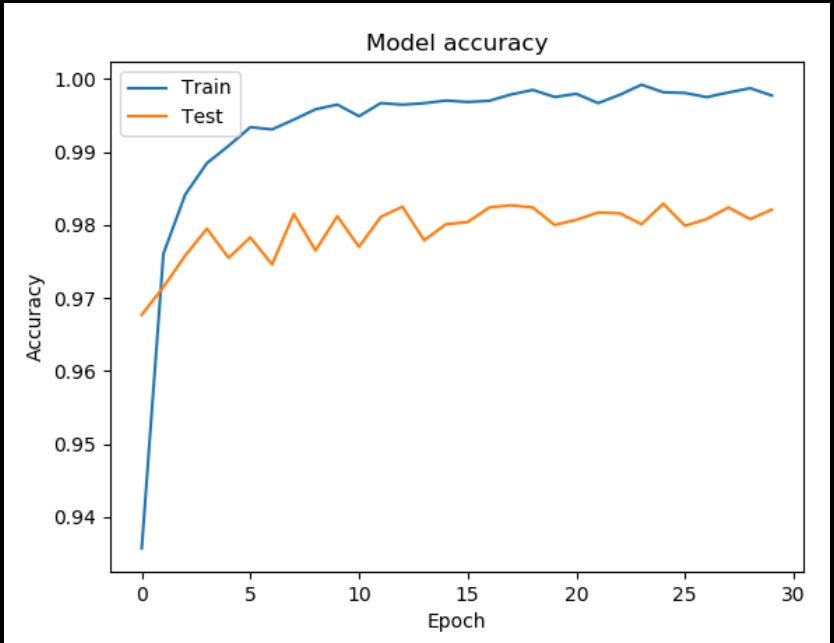
Latter on we will see that regularization techniques (which are only turned on for training) also add to this effect.

Let's Go Wider

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()

train_images = train_images.reshape(60000, 784)
test_images  = test_images.reshape(10000, 784)

test_images  = test_images.astype('float32')
train_images = train_images.astype('float32')

test_images  /= 255
train_images /= 255

model = tf.keras.Sequential([
  tf.keras.layers.Dense(512, activation='relu', input_shape=(784,)),
  tf.keras.layers.Dense(512, activation='relu'),
  tf.keras.layers.Dense(10, activation='softmax'),
])


model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])


model.fit(train_images, train_labels, batch_size=128, epochs=30, verbose=1, validation_data=(test_images, test_labels))
```

Wider Results

```
....
....
Epoch 30/30
60000/60000 [==============================] - 2s 32us/sample - loss: 0.0083 - accuracy: 0.9977 - val_loss: 0.1027 - val_accuracy: 0.9821
```



Wider

```
model.summary()

_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_18 (Dense)             (None, 512)               401920
_________________________________________________________________
dense_19 (Dense)             (None, 512)               262656
_________________________________________________________________
dense_20 (Dense)             (None, 10)                5130
=================================================================
Total params: 669,706
Trainable params: 669,706
Non-trainable params: 0
```

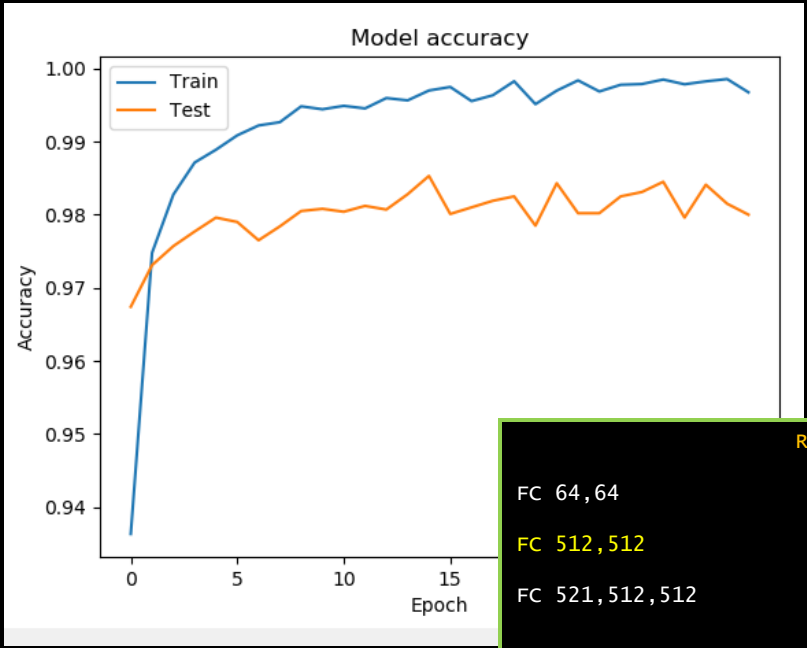
55,050 for 64 Wide Model

Maybe Deeper?

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()

train_images = train_images.reshape(60000, 784)
test_images  = test_images.reshape(10000, 784)

test_images  = test_images.astype('float32')
train_images = train_images.astype('float32')

test_images  /= 255
train_images /= 255

model = tf.keras.Sequential([
  tf.keras.layers.Dense(512, activation='relu', input_shape=(784,)),
  tf.keras.layers.Dense(512, activation='relu'),
  tf.keras.layers.Dense(512, activation='relu'),
  tf.keras.layers.Dense(10, activation='softmax'),
])


model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])


model.fit(train_images, train_labels, batch_size=128, epochs=30, verbose=1, validation_data=(test_images, test_labels))
```

Wide And Deep Results

```
....
....
60000/60000 [==============================] - 3s 45us/sample - loss: 0.0119 - accuracy: 0.9967 - val_loss: 0.1183 - val_accuracy: 0.9800
```



Deep and Wide

```
model.summary()
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_24 (Dense)             (None, 512)               401920
_________________________________________________________________
dense_25 (Dense)             (None, 512)               262656
_________________________________________________________________
dense_26 (Dense)             (None, 512)               262656
_________________________________________________________________
dense_27 (Dense)             (None, 10)                5130
=================================================================
Total params: 932,362
s: 932,362
arams: 0
```

Recap

FC 64,64	97.5
FC 512,512	98.2
FC 521,512,512	98.0

Brute Force Does Not Work

You usually can't just brute force your way into success. Beyond the obvious time and memory costs, you are opening yourself up to

- Overfitting
- Vanishing gradients

We will have to be smarter than "bigger is better" about choosing our hyperparameters. One very smart thing to do is to choose a more appropriate architecture.

Image Recognition Done Right: CNNs

AlexNet won the 2012 ImageNet LSVRC and changed the DL world.

4M	FULL CONNECT
16M	FULL 4096/ReLU
37M	FULL 4096/ReLU
	MAX POOLING
442K	CONV 3x3/ReLU
1.3M	CONV 3x3ReLU
884K	CONV 3x3/ReLU
	MAX POOLING 2x2sub
	LOCAL CONTRAST NORM
307K	CONV 11x11/ReLU
	MAX POOL 2x2sub
	LOCAL CONTRAST NORM
35K	CONV 11x11/ReLU

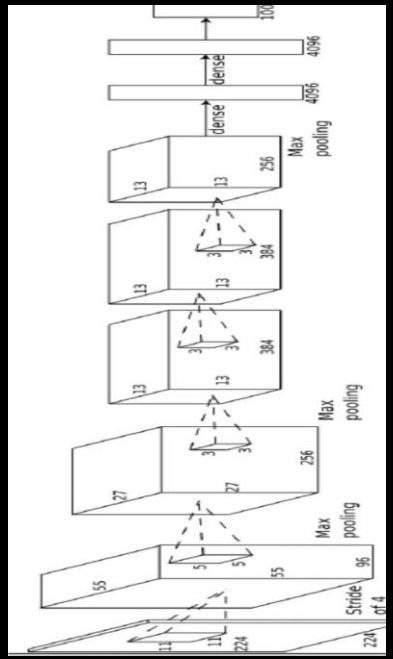
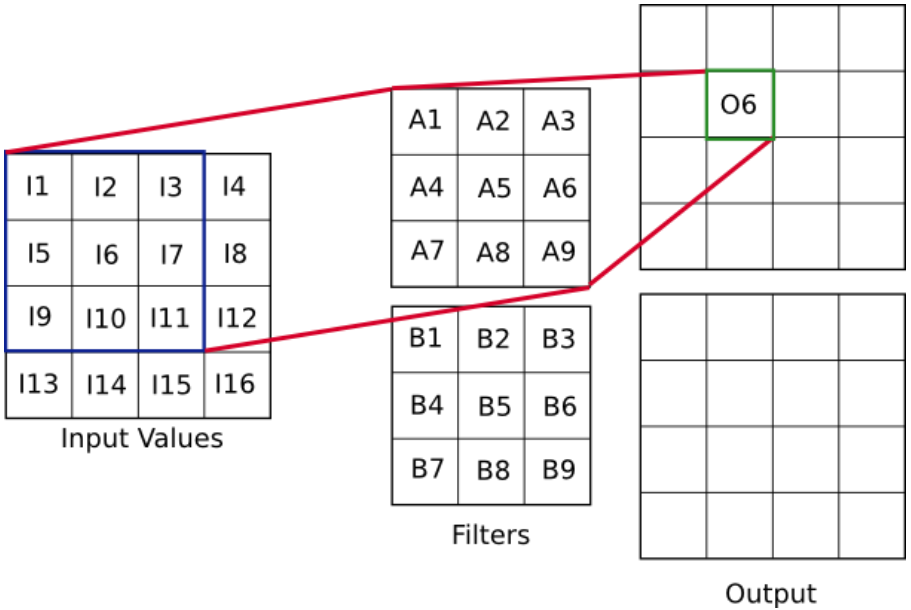


Image Object Recognition [Krizhevsky, Sutskever, Hinton 2012]

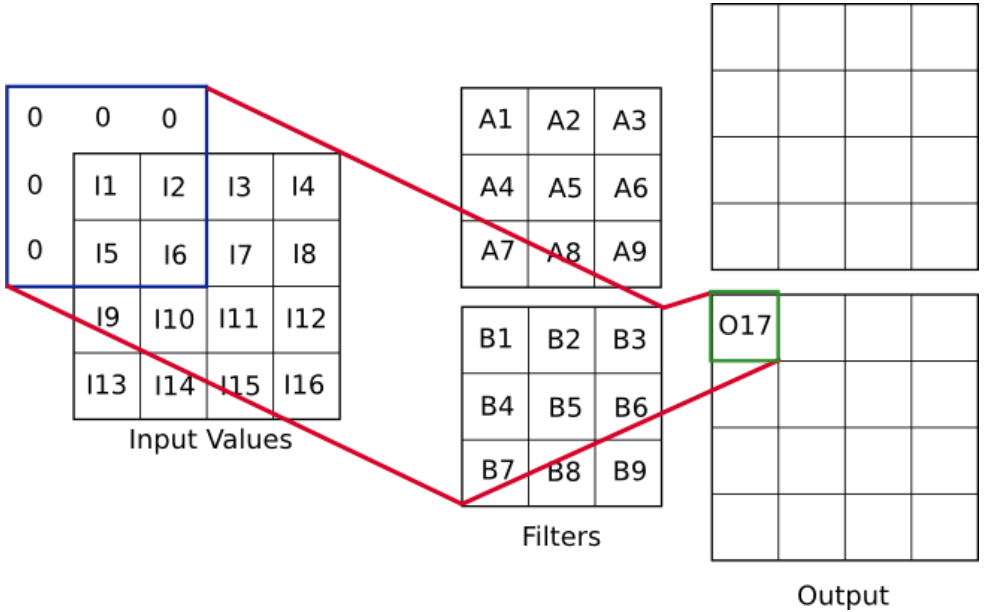
Convolution



$$O_6 = A_1 \cdot I_1 + A_2 \cdot I_2 + A_3 \cdot I_3 + A_4 \cdot I_5 + A_5 \cdot I_6 + A_6 \cdot I_7 + A_7 \cdot I_9 + A_8 \cdot I_{10} + A_9 \cdot I_{11}$$

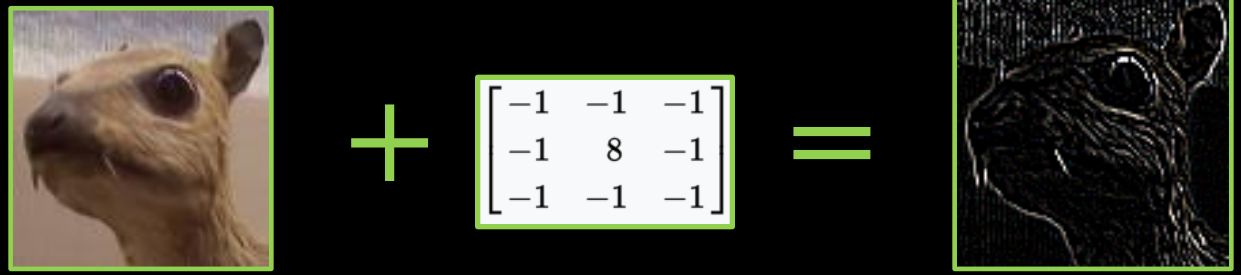
Convolution

Boundary and Index Accounting



$$O_{17} = B_5 \cdot I_1 + B_6 \cdot I_2 + B_8 \cdot I_5 + B_9 \cdot I_6$$

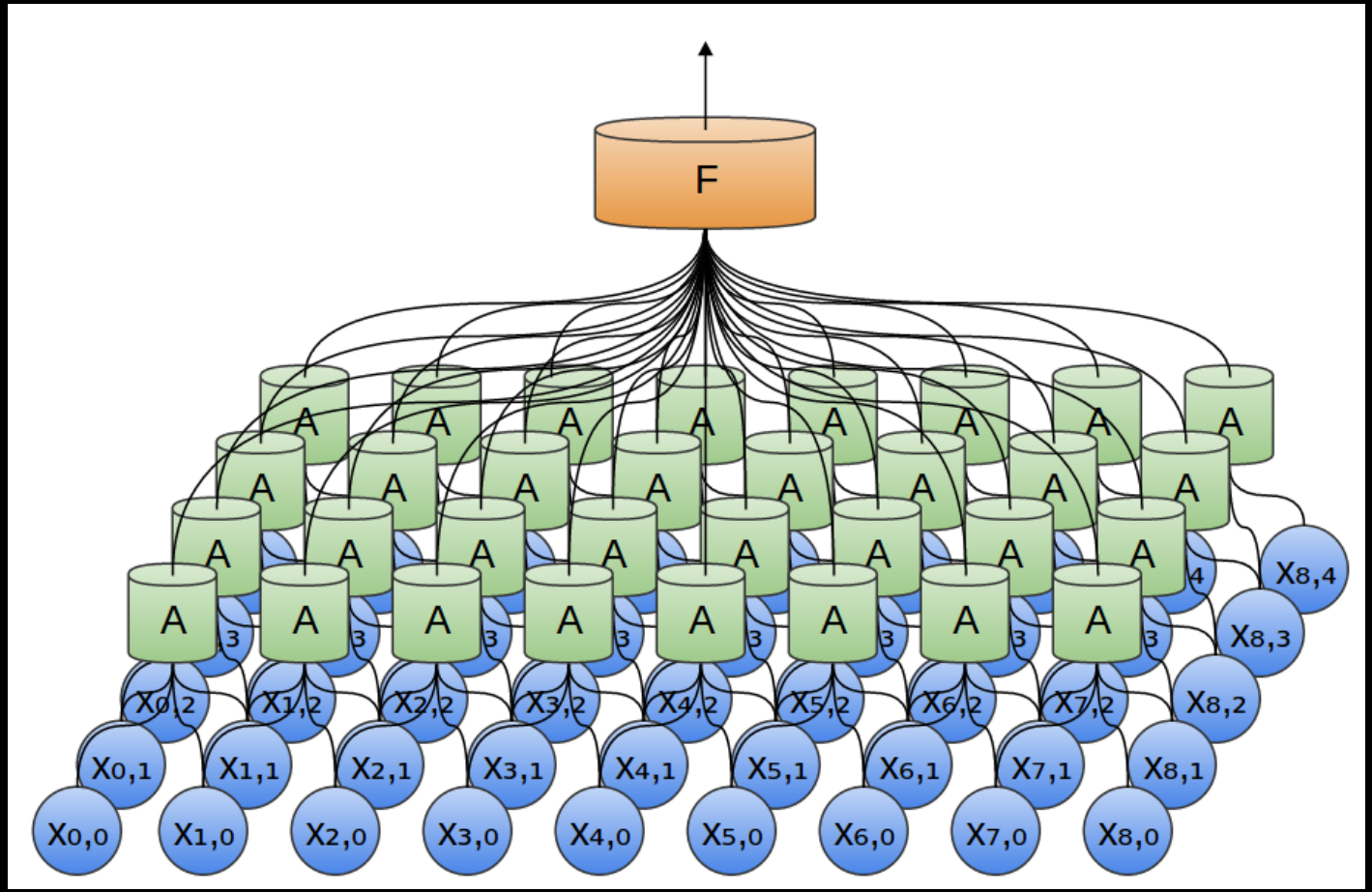
Straight Convolution



Edge Detector

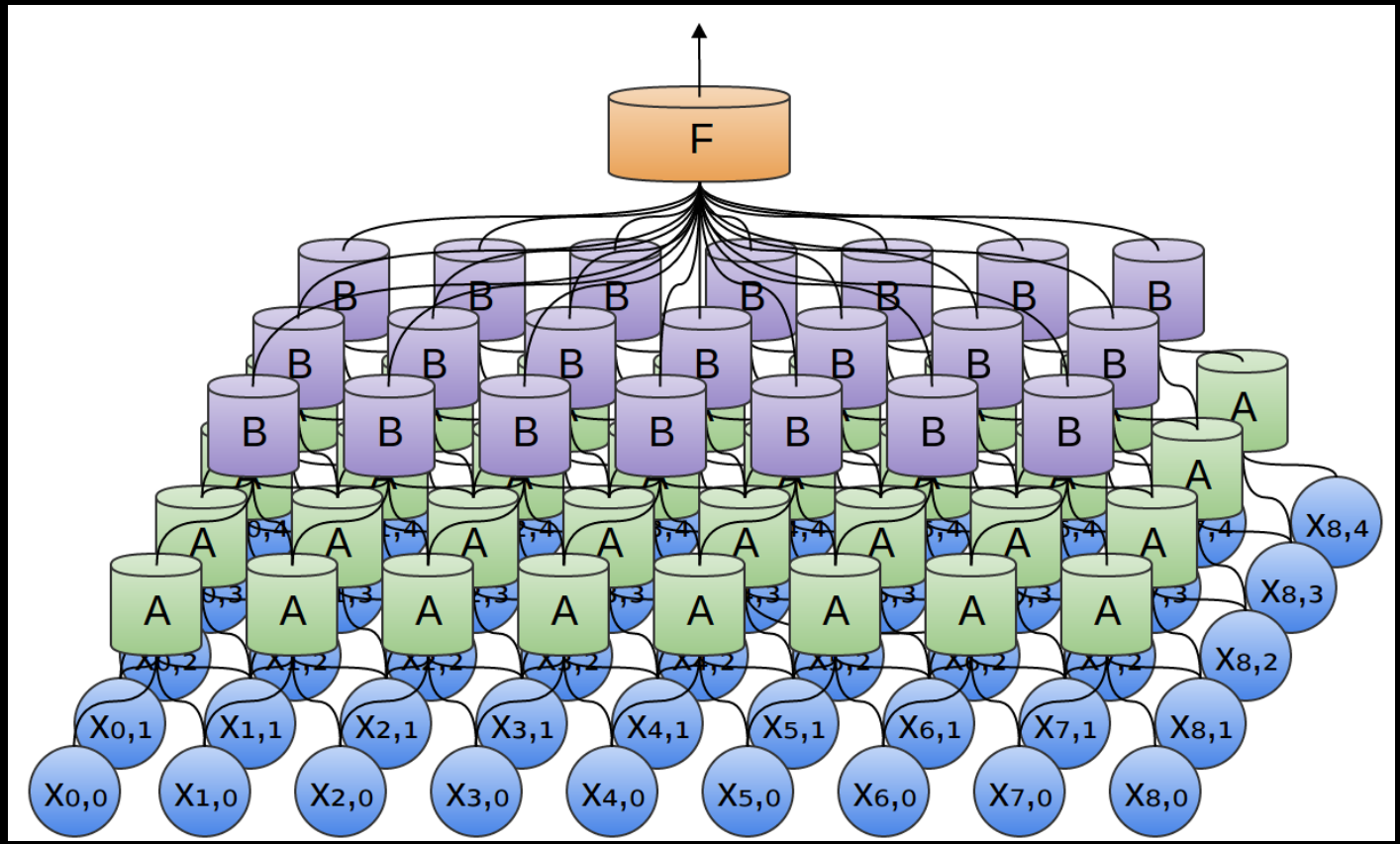
Images: Wikipedia

Simplest Convolution Net



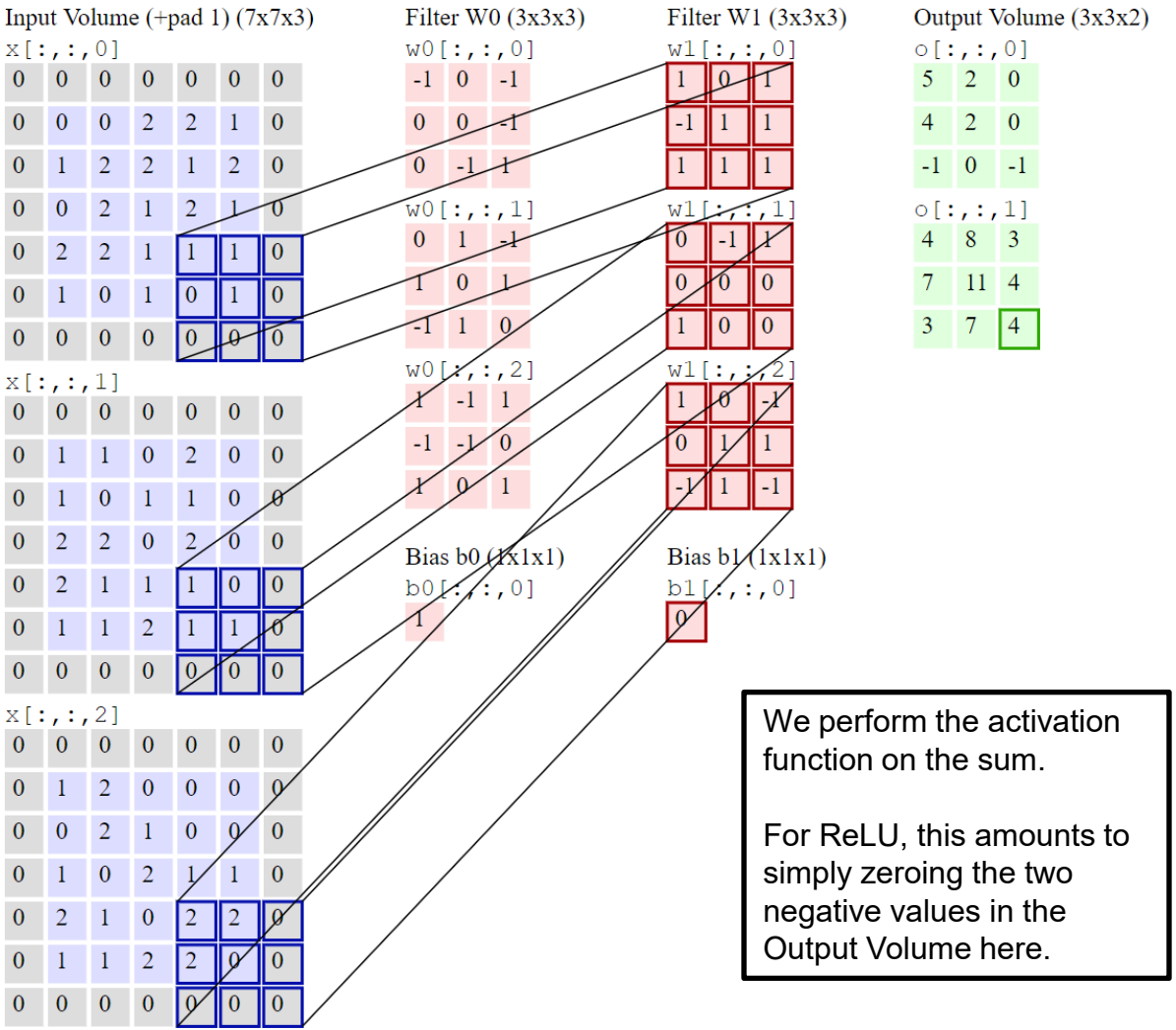
Courtesy: Chris Olah

Stacking Convolutions



Courtesy: Chris Olah

Convolution



From the very nice Stanford CS231n course at http://cs231n.github.io/convolutional-networks/

We perform the activation function on the sum.

For ReLU, this amounts to simply zeroing the two negative values in the Output Volume here.

Stride = 2

Convolution Math

Each Convolutional Layer:

Inputs a volume of size $W_I \times H_I \times D_I$ (D is depth)

Requires four hyperparameters:

- Number of filters K
- their spatial extent N
- the stride S
- the amount of padding P

Produces a volume of size $W_O \times H_O \times D_O$

$W_O = (W_I - N + 2P) / S+1$

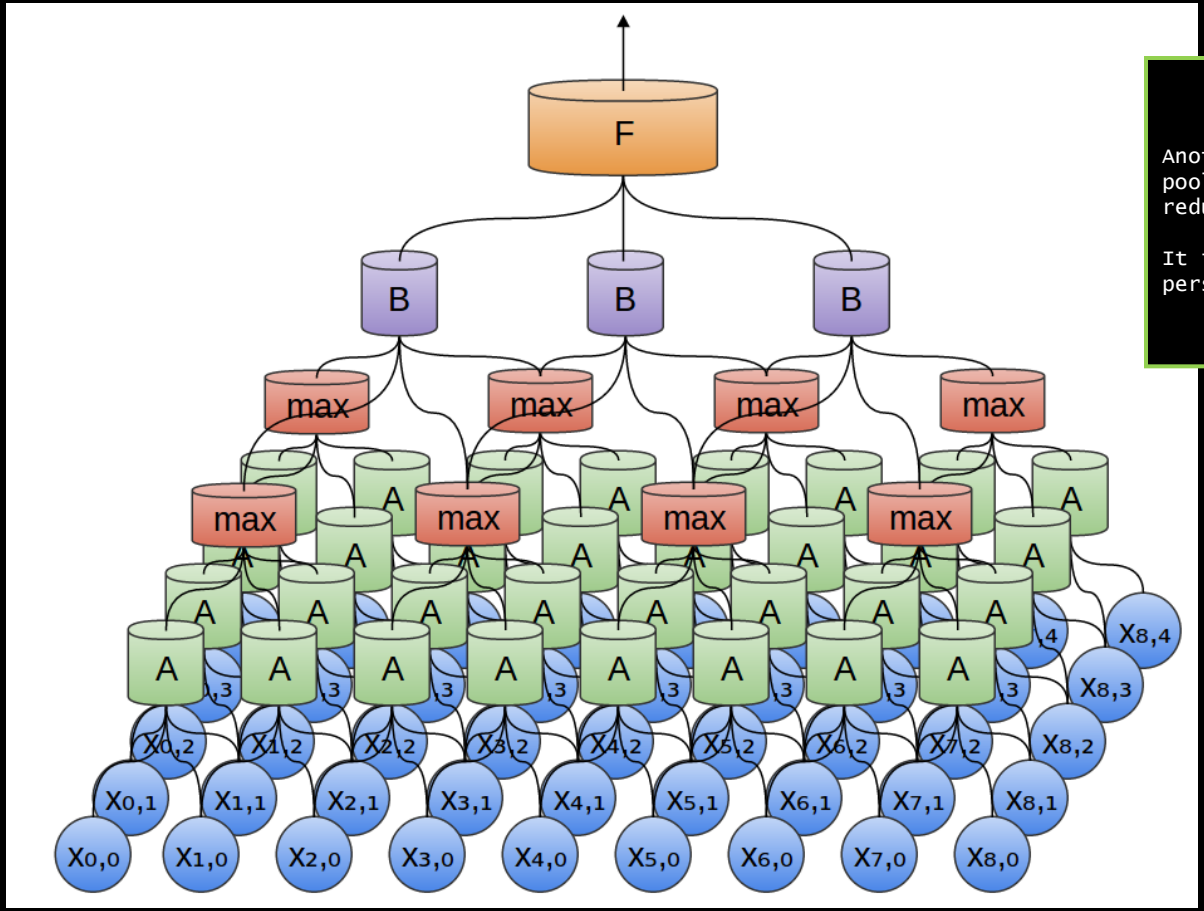
$H_O = (H_I - F + 2P) / S+1$

$D_O = K$

This requires $N \cdot N \cdot D_I$ weights per filter, for a total of $N \cdot N \cdot D_I \cdot K$ weights and K biases

In the output volume, the d-th depth slice (of size $W_O \times H_O$) is the result of performing a convolution of the d-th filter over the input volume with a stride of S, and then offset by d-th bias.

Pooling



Another Dimensionality Reduction!

Another very valid perspective is that pooling is a simple dimensionality reduction.

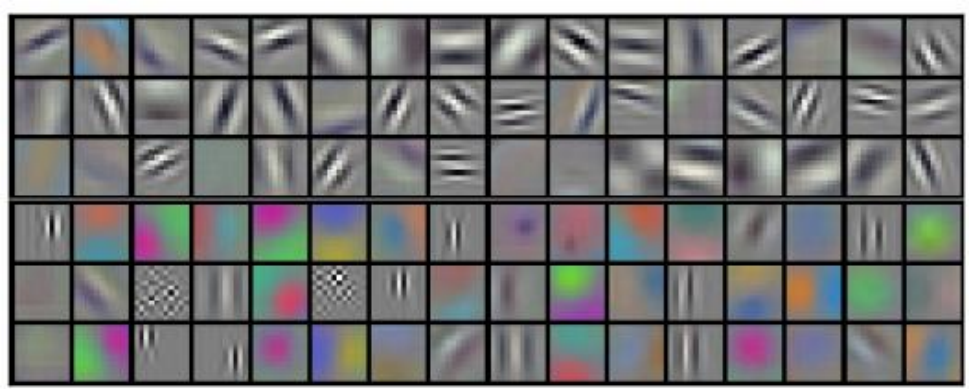
It is very helpful to posses these different perspectives.

We don't use an activation function when pooling.

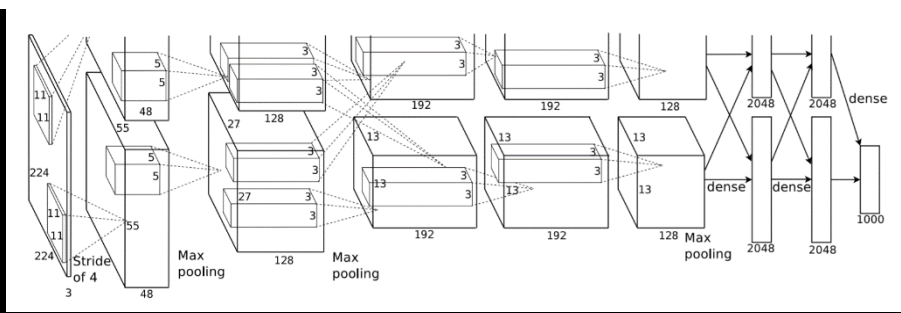
Courtesy: Chris Olah

A Groundbreaking Example

These are the 96 first layer 11x11 (x3, RGB, stacked here) filters from AlexNet.



Among the several novel techniques combined in this work (such as aggressive use of ReLU), they used dual GPUs, with different flows for each, communicating only at certain layers. A result is that the bottom GPU consistently specialized on color information, and the top did not.



This is your brain on CNNs.

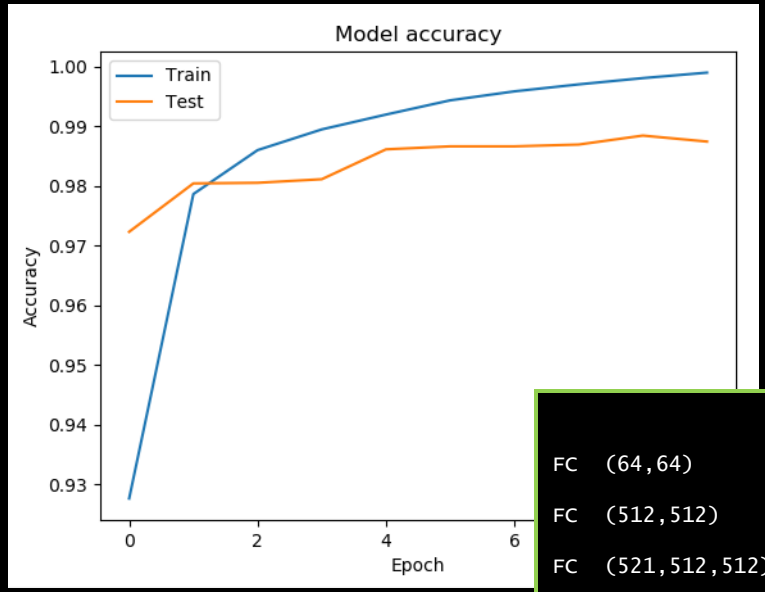
One of countless "illusions" I could provoke your own CNNs with.

Let's Start Small

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()

train_images = train_images.reshape(60000, 28, 28, 1)
test_images = test_images.reshape(10000, 28, 28, 1)
train_images, test_images = train_images/255, test_images/255

model = tf.keras.Sequential([
    tf.keras.layers.Conv2D(32, (3,3), activation='relu', input_shape=(28,28,1)),
    tf.keras.layers.MaxPooling2D(2,2),
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(100, activation='relu'),
    tf.keras.layers.Dense(10, activation='softmax')
])

model.compile(optimizer=tf.keras.optimizers.SGD(lr=0.01, momentum=0.9), loss='sparse_categorical_crossentropy', metrics=['accuracy'])


model.fit(train_images, train_labels, batch_size=32, epochs=10, verbose=1, validation_data=(test_images, test_labels))
```

Early CNN Results

```
....
....
Epoch 10/10
60000/60000 [==============================] - 12s 198us/sample - loss: 0.0051 - accuracy: 0.9989 - val_loss: 0.0424 - val_accuracy: 0.9874
```



Primitive CNN

```
model.summary()
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d_1 (Conv2D)            (None, 26, 26, 32)        320
_________________________________________________________________
max_pooling2d_1              (None, 13, 13, 32)        0
_________________________________________________________________
flatten_1 (Flatten)          (None, 5408)              0
_________________________________________________________________
dense_38 (Dense)             (None, 100)               540900
_________________________________________________________________
dense_39 (Dense)             (None, 10)                1010
=================================================================
ms: 542,230
params: 542,230
ble params: 0
```

Score Thus Far

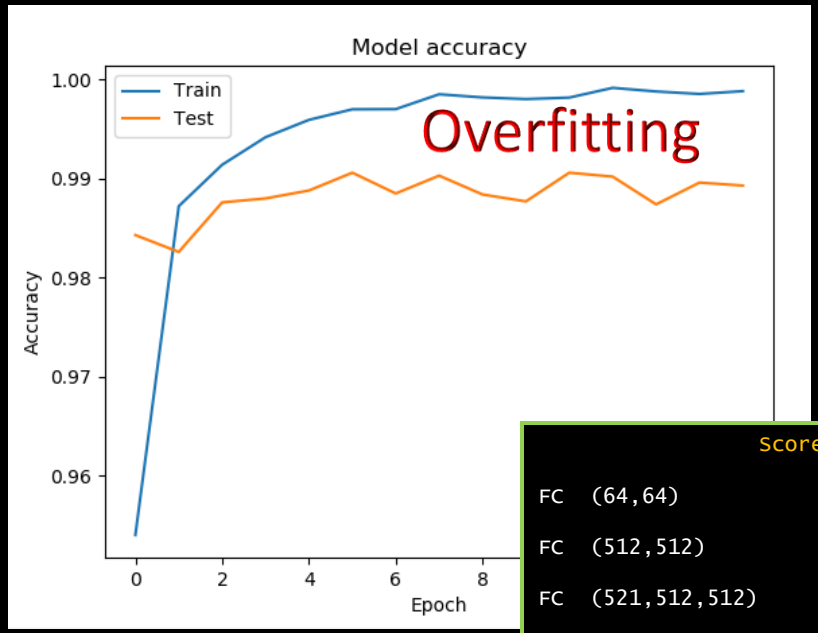
FC	(64,64)	97.5
FC	(512,512)	98.2
FC	(521,512,512)	98.0
CNN	(1 layer)	98.7

Scaling Up The CNN

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()

train_images = train_images.reshape(60000, 28, 28, 1)
test_images = test_images.reshape(10000, 28, 28, 1)
train_images, test_images = train_images/255, test_images/255

model = tf.keras.Sequential([
    tf.keras.layers.Conv2D(32, (3,3), activation='relu', input_shape=(28,28,1)),
    tf.keras.layers.Conv2D(64, (3,3), activation='relu'),
    tf.keras.layers.MaxPooling2D(2,2),
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(128, activation='relu'),
    tf.keras.layers.Dense(10, activation='softmax')
])

model.compile(optimizer=tf.keras.optimizers.SGD(lr=0.01, momentum=0.9), loss='sparse_categorical_crossentropy', metrics=['accuracy'])


model.fit(train_images, train_labels, batch_size=32, epochs=10, verbose=1, validation_data=(test_images, test_labels))
```

Deeper CNN Results

```
....
....
Epoch 15/15
60000/60000 [==============================] - 34s 566us/sample - loss: 0.0052 - accuracy: 0.9985 - val_loss: 0.0342 - val_accuracy: 0.9903
```



Deeper CNN

```
model.summary()
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d_4 (Conv2D)            (None, 26, 26, 32)        320
_________________________________________________________________
conv2d_5 (Conv2D)            (None, 24, 24, 64)        18496
_________________________________________________________________
max_pooling2d_3              (None, 12, 12, 64)        0
_________________________________________________________________
flatten_3 (Flatten)          (None, 9216)              0
_________________________________________________________________
dense_42 (Dense)             (None, 128)               1179776
_________________________________________________________________
                             (None, 10)                1290
=================================================================
,199,882
s: 1,199,882
arams: 0
```

Score Thus Far

FC	(64,64)	97.5
FC	(512,512)	98.2
FC	(521,512,512)	98.0
CNN	(1 layer)	98.7
CNN	(2 Layer)	99.0

Overfitting = Memorization

We now have enough parameters that the network is prone to memorizing instead of learning. This will only get worse as our larger and smarter networks grow into billions of parameters.

Cat

Dog

Dog

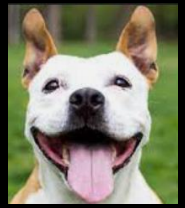
Cat

Cat

Dog

Dog

Dog



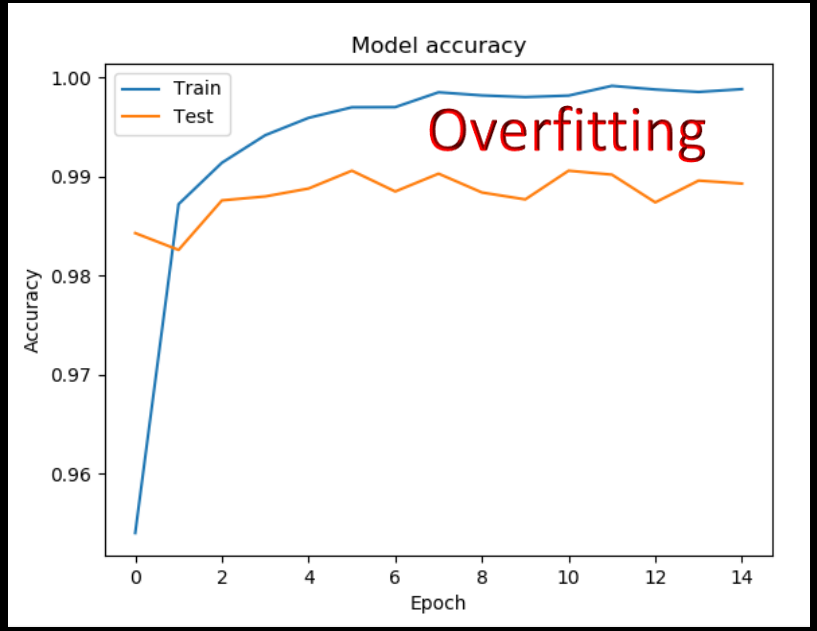
Dog

Dog

Cat

Cat

Dropout



As we know by now, we need some form of regularization to help with the overfitting. One seemingly crazy way to do this is the relatively new technique (introduced by the venerable Geoffrey Hinton in 2012) of Dropout.

Some view it as an ensemble method that trains multiple data models simultaneously. One neat perspective of this analysis-defying technique comes from Jürgen Schmidhuber, another innovator in the field; under certain circumstances, it could also be viewed as a form of training set augmentation: effectively, more and more informative complex features are removed from the training data.

CNN With Dropout

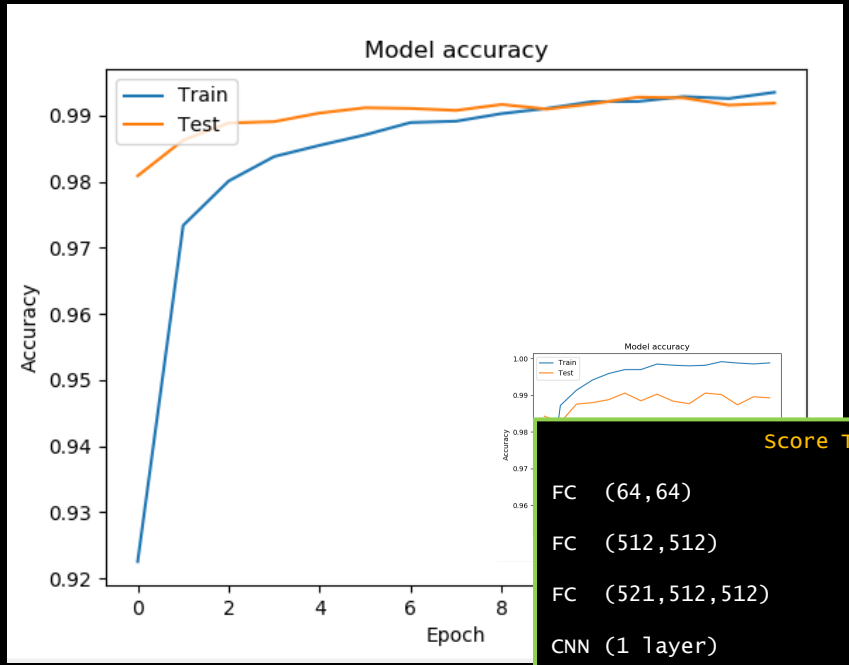
```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()

train_images = train_images.reshape(60000, 28, 28, 1)
test_images = test_images.reshape(10000, 28, 28, 1)
train_images, test_images = train_images/255, test_images/255

model = tf.keras.Sequential([
    tf.keras.layers.Conv2D(32, (3,3), activation='relu', input_shape=(28,28,1)),
    tf.keras.layers.Conv2D(64, (3,3), activation='relu'),
    tf.keras.layers.MaxPooling2D(2,2),
    tf.keras.layers.Dropout(0.25),
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(128, activation='relu'),
    tf.keras.layers.Dropout(0.5),
    tf.keras.layers.Dense(10, activation='softmax')
])

model.compile(optimizer=tf.keras.optimizers.SGD(lr=0.01, momentum=0.9), loss='sparse_categorical_crossentropy', metrics=['accuracy'])


model.fit(train_images, train_labels, batch_size=32, epochs=10, verbose=1, validation_data=(test_images, test_labels))
```

Parameter is fraction to *drop*.

Drop out is not used in the final, trained, network. Similarly, it is automatically disabled here during testing.

Help From Dropout

```
....
....
Epoch 15/15
60000/60000 [==============================] - 40s 667us/sample - loss: 0.0187 - accuracy: 0.9935 - val_loss: 0.0301 - val_accuracy: 0.9919
```



Dropout CNN

```
model.summary()
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d_12 (Conv2D)           (None, 26, 26, 32)        320
_________________________________________________________________
conv2d_13 (Conv2D)           (None, 24, 24, 64)        18496
_________________________________________________________________
max_pooling2d_7              (None, 12, 12, 64)        0
_________________________________________________________________
dropout_4 (Dropout)          (None, 12, 12, 64)        0
_________________________________________________________________
flatten_7 (Flatten)          (None, 9216)              0
_________________________________________________________________
(Dense)                      (None, 128)               1179776
_________________________________________________________________
(Dropout)                    (None, 128)               0
_________________________________________________________________
(Dense)                      (None, 10)                1290
=================================================================
ams: 1,199,882
 params: 1,199,882
able params: 0
```

Score Thus Far

FC	(64,64)	97.5
FC	(512,512)	98.2
FC	(521,512,512)	98.0
CNN	(1 layer)	98.7
CNN	(2 Layer)	99.0
CNN with Dropout		99.2

Batch Normalization

Another "between layers" layer that is quite popular is Batch Normalization. This technique really helps with vanishing or exploding gradients. So it is better with deeper networks.

- Maybe not so compatible with Dropout, but the subject of research (and debate).
- Maybe Apply Dropout after all BN layers: https://arxiv.org/pdf/1801.05134.pdf
- Before or after non-linear activation function? Oddly, also open to debate. But, it may be more appropriate after the activation function if for s-shaped functions like the hyperbolic tangent and logistic function, and before the activation function for activations that result in non-Gaussian distributions like ReLU.

How could we apply it before of after our activation function if we wanted to? We haven't been peeling our layers apart, but we can micro-manage more if we want to:

```
model.add(tf.keras.layers.Conv2D(64, (3, 3), use_bias=False))
model.add(tf.keras.layers.BatchNormalization())
model.add(tf.keras.layers.Activation("relu"))

model.add(tf.keras.layers.Conv2D(64, kernel_size=3, strides=2, padding="same"))
model.add(tf.keras.layers.LeakyReLU(alpha=0.2))
model.add(tf.keras.layers.BatchNormalization(momentum=0.8))
```

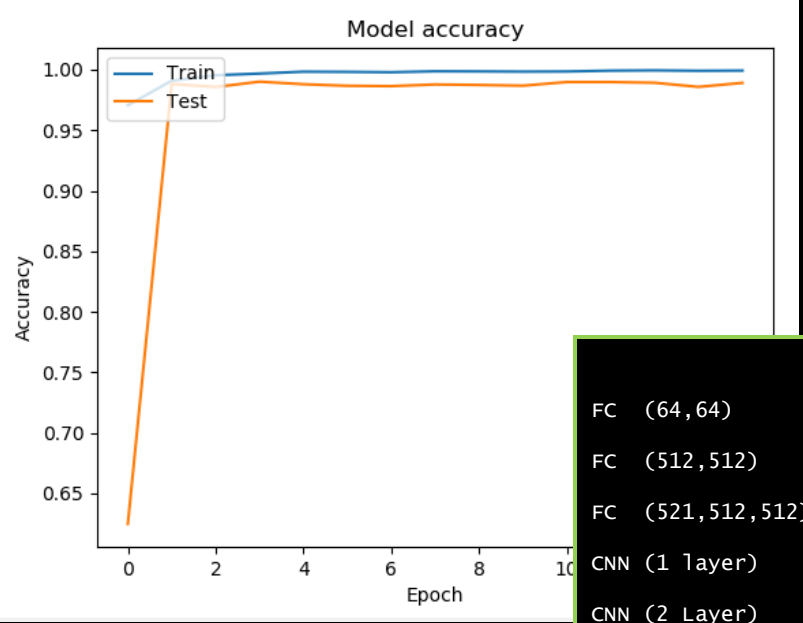
There are also normalizations that work on single samples instead of batches, so better for recurrent networks. In TensorFlow we have Group Normalization, Instance Normalization and Layer Normalization.

Trying Batch Normalization

```
import tensorflow as tf

mnist = tf.keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()

train_images = train_images.reshape(60000, 28, 28, 1)
test_images = test_images.reshape(10000, 28, 28, 1)
train_images, test_images = train_images/255, test_images/255

model = tf.keras.Sequential([
    tf.keras.layers.Conv2D(32, (3,3), activation='relu', input_shape=(28,28,1)),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Conv2D(64, (3,3), activation='relu'),
    tf.keras.layers.MaxPooling2D(2,2),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(128, activation='relu'),
    tf.keras.layers.BatchNormalization(),
    tf.keras.layers.Dense(10, activation='softmax')
])

model.compile(optimizer=tf.keras.optimizers.SGD(lr=0.01, momentum=0.9), loss='sparse_categorical_crossentropy', metrics=['accuracy'])


model.fit(train_images, train_labels, batch_size=32, epochs=10, verbose=1, validation_data=(test_images, test_labels))
```

Not So Helpful

```
....
....
Epoch 15/15
60000/60000 [==============================] - 50s 834us/sample - loss: 0.0027 - accuracy: 0.9993 - val_loss: 0.0385 - val_accuracy: 0.9891
```



Score Thus Far

FC (64,64)	97.5
FC (512,512)	98.2
FC (521,512,512)	98.0
CNN (1 layer)	98.7
CNN (2 Layer)	99.0
CNN with Dropout	99.2
Batch Normalization	98.9

Batch Normalization CNN

```
model.summary()
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d_2 (Conv2D)            (None, 26, 26, 32)        320
_________________________________________________________________
batch_normalization          (None, 26, 26, 32)        128
_________________________________________________________________
conv2d_3 (Conv2D)            (None, 24, 24, 64)        18496
_________________________________________________________________
max_pooling2d_1              (None, 12, 12, 64)        0
_________________________________________________________________
tation_1                     (None, 12, 12, 64)        256
_________________________________________________________________
tten)                        (None, 9216)              0
_________________________________________________________________
)                            (None, 128)               1179776
_________________________________________________________________
tation_2                     (Batch (None, 128)        512
_________________________________________________________________
)                            (None, 10)                1290
=================================================================
1,200,778
ms: 1,200,330
params: 448
```

Another Fantastic Demo

This *amazing, stunning, beautiful* demo from Adam Harley is very similar to what we just did, but different enough to be interesting.

https://aharley.github.io/nn_vis/cnn/2d.html

It is worth experiment with. Note that this is an excellent demonstration of how efficient the forward network is. You are getting very real-time analysis from a lightweight web program. Training it took some time.

Draw your number here

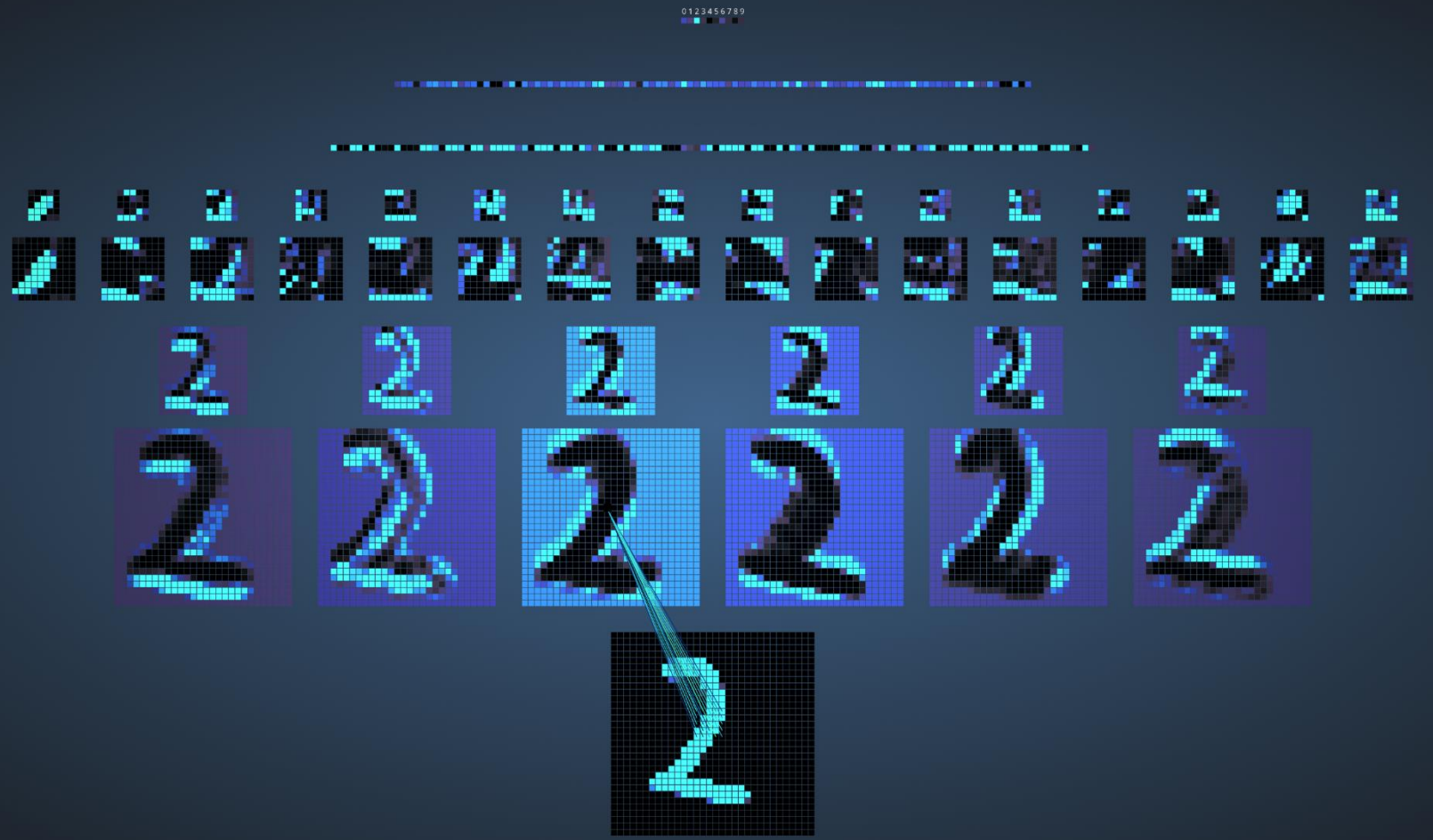
Downsampled drawing: 2

First guess: 2

Second guess: 0

Layer visibility

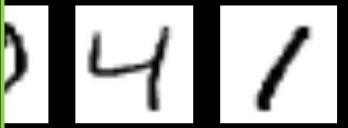
Input layer	Show
Convolution layer 1	Show
Downsampling layer 1	Show
Convolution layer 2	Show
Downsampling layer 2	Show
Fully-connected layer 1	Show
Fully-connected layer 2	Show
Output layer	Show



Data Augmentation

As I've mentioned, labeled data is valuable. This type of *supervised learning* often requires human-labeled data. Getting more out of our expensive data is very desirable. More datapoints generally equals better accuracy. The process of generating more training data from our existing pool is called *Data Augmentation*, and is an extremally common technique, especially for classification

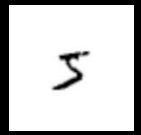
Our MNIST network has learned to recognize ve



What if we wanted to teach it:

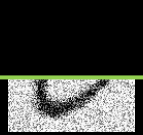
How many samples do we need?

This is another hyperparameter (yes), where we can only offer a vague rule of thumb. And that suggestion is about 5000 per category for competence, 10 million for a real task with human performance.



Scale Invariance

Rotation Invariance



Noise Tolerance

Translation Invariance

You can see how straightforward and mechanical this is. And yet very effective. You will often see detailed explanations of the data augmentation techniques employed in any given project.

Note that tf.image makes many of these processes very convenient.

Stupid Neural Nets

Why can't they learn like we do? Can't I just tell you a fact, or an algorithm, and you can just "get it" it without countless iteration?

English for Infants

On the other hand, maybe I could teach adu
particular mad bomber with your airport fac

How did you learn the English "rules"?

He wrote a fantastic follow-up, with some other surprisingly complex rules that we all somehow "know", but were never taught.

https://www.bbc.com/culture/article/20160908-the-language-rules-we-know-but-dont-know-we-know

There is such a thing as "one-shot" (or N-shot) learning. But it is harder, requires more specialized techniques, and is straying into the area of unsupervised learning. We will come back to this, but it is no magic bullet for sparse data.

Adding TensorBoard To Your Code

TensorBoard is a very versatile tool that allows us multiple types of insight into our TensorFlow codes. We need only add a callback into the model to activate the necessary logging.

```
...
...

model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])

tensorboard_callback = tf.keras.callbacks.TensorBoard(log_dir='TB_logDir', histogram_freq=1)

history = model.fit(train_images, train_labels, batch_size=128, epochs=15, verbose=1,
        validation_data=(test_images, test_labels), callbacks=[tensorboard_callback])
...
...
```

TensorBoard runs as a server, because it has useful run-time capabilities, and requires you to start it separately, and to access it via a browser.

Somewhere else:

```
tensorboard --logdir=TB_logD
```

Somewhere else:

```
Start your Browser and point it at port 6006: http://localhost:6006/
```

If you are running on Bridges login nodes, from your computer something like:

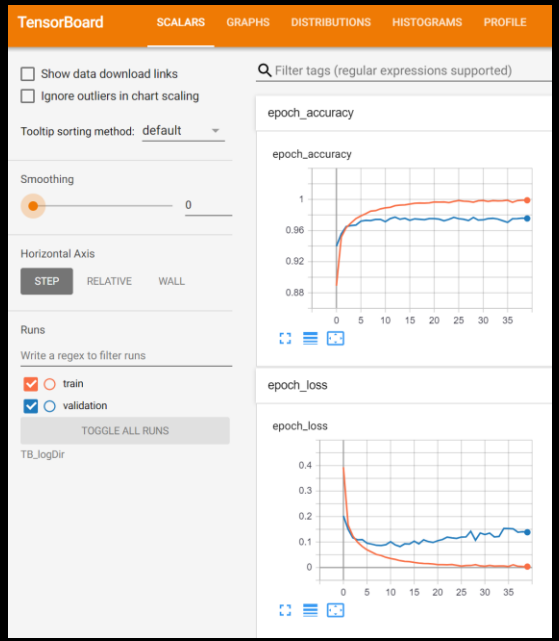
ssh -2 -Nf -L 6006:127.0.0.1:6006 br014.bridges2.psc.edu

If you are running on a Bridges compute nodes, you need to use the compute's IB address/hostname, for example:

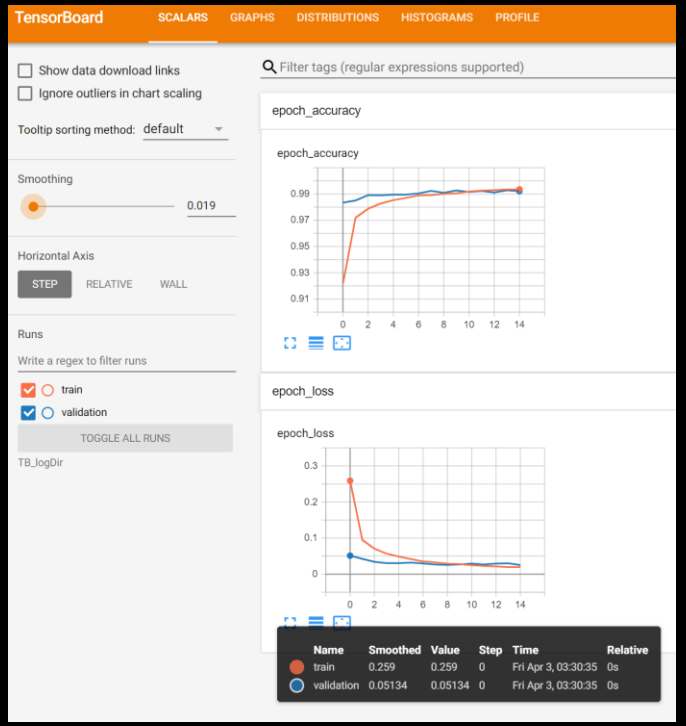
ssh -2 -Nf -L 6006:r001.ib.bridges2.psc.edu:6006 br014.bridges2.psc.edu

TensorBoard Analysis

The most obvious thing we can do is to look at our training loss. Note that TB is happy to do this in *real-time* as the model runs. This can be very useful for you to monitor overfitting.



Our First Model
64 Wide FC



Our CNN

Early Stopping

Of course, manual monitoring is not he only way to prevent needless training after the loss has plateaued. There are numerous ways in any framework to enable early stopping.

The most common is to add the *EarlyStopping* callback to your training loop.

```
tf.keras.callbacks.EarlyStopping(
    monitor='val_loss',
    min_delta=0,
    patience=0,
    verbose=0,
    mode='auto',
    baseline=None,
    restore_best_weights=False,
    start_from_epoch=0
)
```

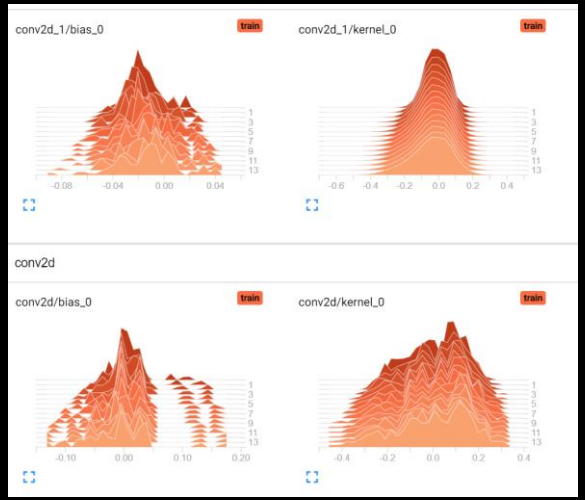
`monitor`	Quantity to be monitored. Defaults to `"val_loss"`.
`min_delta`	Minimum change in the monitored quantity to qualify as an improvement, i.e. an absolute change of less than min_delta, will count as no improvement. Defaults to `0`.
`patience`	Number of epochs with no improvement after which training will be stopped. Defaults to `0`.
`verbose`	Verbosity mode, 0 or 1. Mode 0 is silent, and mode 1 displays messages when the callback takes an action. Defaults to `0`.
`mode`	One of `{"auto", "min", "max"}`. In `min` mode, training will stop when the quantity monitored has stopped decreasing; in `"max"` mode it will stop when the quantity monitored has stopped increasing; in `"auto"` mode, the direction is automatically inferred from the name of the monitored quantity. Defaults to `"auto"`.
`baseline`	Baseline value for the monitored quantity. If not `None`, training will stop if the model doesn't show improvement over the baseline. Defaults to `None`.
`restore_best_weights`	Whether to restore model w… . If `False`, the model weights o… ed regardless of the performan… training will run for `patien`… aults to `False`.
`start_from_epoch`	Number of epochs to wait before starting to monitor improvement. This allows for a warm-up period in which no improvement is expected and thus training will not be stopped. Defaults to `0`.

Note that early stopping can also be considered a form of regularization. We are preventing overfitting by stopping the training before it descends into pure memorization.

TensorBoard Parameter Visualization

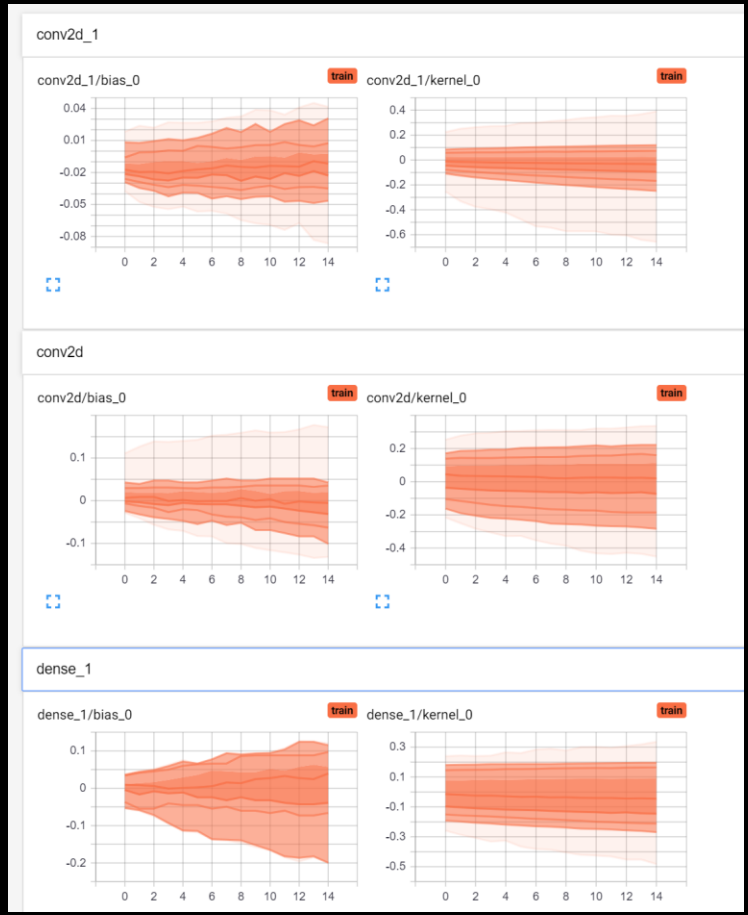
And we can observe the time evolution of our weights and biases, or at least their distributions.

This can be very telling, but requires some deeper application and architecture dependent understanding.



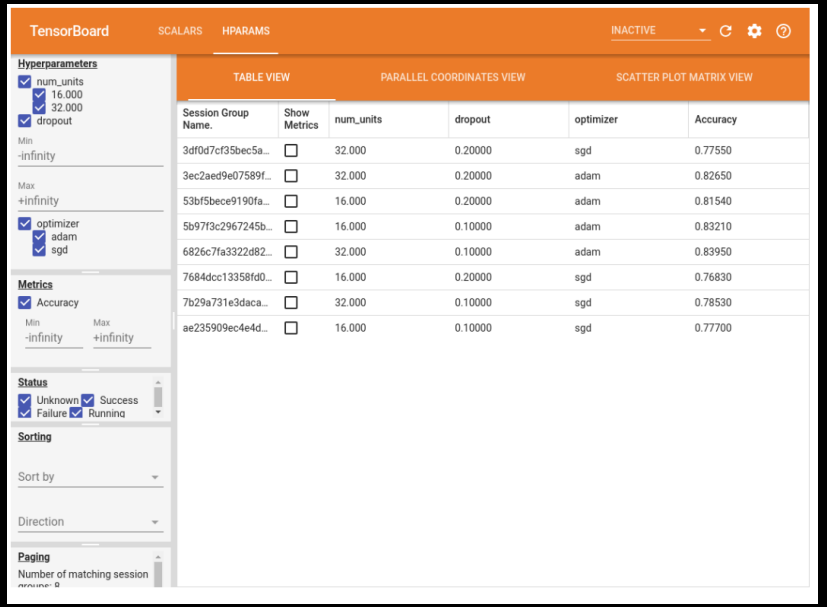
Histogram View

Distribution View



TensorBoard Add Ons

TensorBoard has lots of extended capabilities. Two particularly useful and powerful ones are Hyperparameter Search and Performance Profiling.



Hyperparameter Search

Requires some scripting on your part. Look at https://www.tensorflow.org/tensorboard/hyperparameter_tuning_with_hparams for a good introduction.

Performance Profiling

Going beyond basics, like IO time, requires integration of hardware specific tools. This is well covered if you are using NVIDIA, otherwise you may have a little experimentation to do. The end result is a user friendly interface and valuable guidance.

Scaling

If one GPU is good, more must be better! This is largely true, and you will notice our GPU nodes are stuffed full with 4 or more GPUs each.

You might also notice that most of the machines in the "Top 10" have a lot of GPUs in them. They deliver most of the FLOPS for scientific codes, but are also an enviable Deep Learning resource.

You might have noticed that most of the interesting leading-edge research seems to involve a lot of GPUs these days.

And the very public battles in the Large Language Model space seem to be about who can get their hands on the largest GPU clusters.

How might you reach these levels of capability?

And what about those scaling limitations I mentioned earlier?

Actually a Crypto miner. We hate these guys for hoarding our GPUs!!!

Data Parallelism

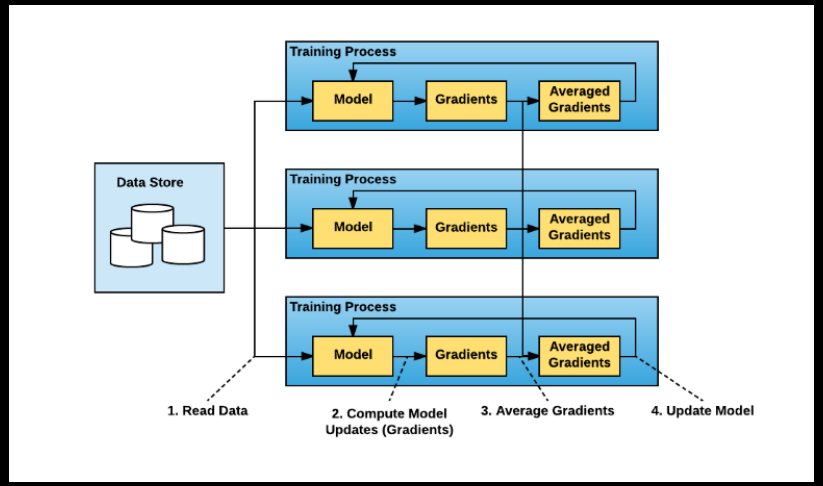
One early technique to utilize multiple GPUs was to independently train an *ensemble* of GPUs on the same task, and then have them vote on the answer. This method does work, but then the end user needs to have an ensemble of their own GPUs. This is not ideal for an application that you wish to run on your phone, or in a self-driving car.

It would be better if we could use a lot of GPUs for the training step, but end up with one great set of parameters that will fit on a single GPU when we are done. Then our users don't need to own supercomputers.

One technique to achieve this is to use *Data Parallelism* so that each GPU trains on a separate batch of data, and at the end of that batch we average the collective wisdom of all of these GPUs to arrive at our new and improved parameters.

Now when we finish we have one super set of parameters that fits on a single GPU.

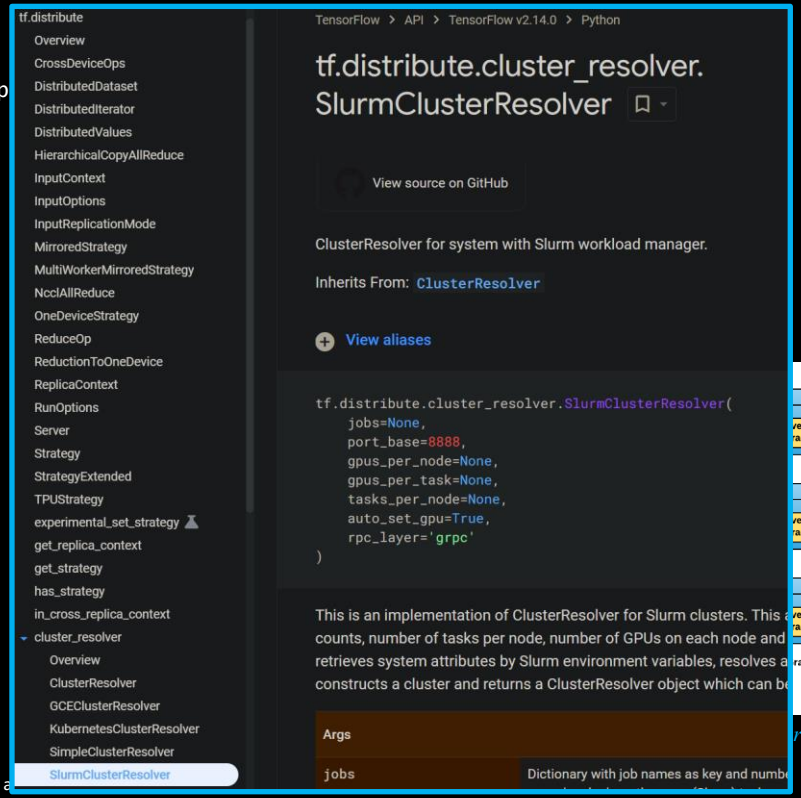
This gradient averaging requires an *all-reduce*, which can be quite expensive given the number of weights involved.



TensorFlow Scalability

This is very straightforward to implement in TensorFlow using the MirroredStrategy on a single node with multiple GPUs, or MultiWorkerMirroredStrategy across multiple nodes.

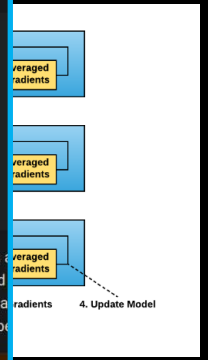
```
strategy = tf.distribute.MirroredStrategy()
with strategy.scope():
    model = tf.keras.Sequential([
        tf.keras.layers.Dropout(rate=0.2, input_shape=X.shap
        tf.keras.layers.Dense(units=64, activation='relu'),
        ...
    ])
    model.compile(...)
model.fit(...)
```



An alternative that has proven itself at extreme scale is *Horovod*.

MNIST with Horovod!

```
# Horovod: initialize Horovod.
hvd.init()

# Horovod: pin GPU to be used to process local rank (one GPU per process)
config = tf.ConfigProto()
config.gpu_options.allow_growth = True
config.gpu_options.visible_device_list = str(hvd.local_rank())
K.set_session(tf.Session(config=config))
...
# Horovod: adjust number of epochs based on number of GPUs.
epochs = int(math.ceil(12.0 / hvd.size()))
...
# Horovod: adjust learning rate based on number of GPUs.
opt = keras.optimizers.Adadelta(1.0 * hvd.size())
...
# Horovod: add Horovod Distributed Optimizer.
opt = hvd.DistributedOptimizer(opt)
...
model.compile(loss=keras.losses.categorical_crossentropy,optimizer=opt,metrics=['a

callbacks = [hvd.callbacks.BroadcastGlobalVariablesCallback(0),]
if hvd.rank() == 0: callbacks.append(keras.callbacks.ModelCheckpoint('./checkpoint-
{epoch}.h5'))
```

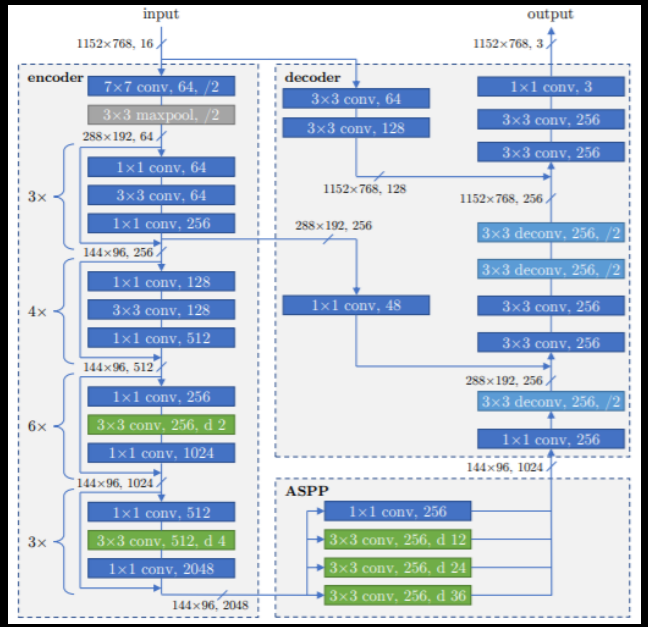


rning in TensorFlow

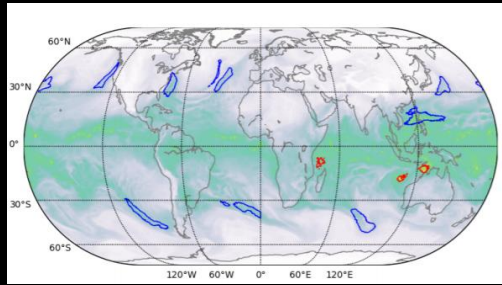
You can find a full example of using Horovod with a Keras MNIST code at:
https://horovod.readthedocs.io/en/latest/keras.html

Scaling Up Massively

Horovod demonstrates its excellent scalability with a Climate Analytics code that won the Gordon Bell prize in 2018. It predicts Tropical Cyclones and Atmospheric River events based upon climate models. It shows not only the reach of deep learning in the sciences, but the scale at which networks can be trained.



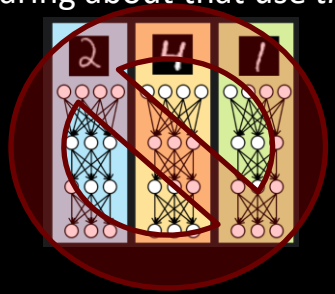
- *1.13 ExaFlops (mixed precision) peak training performance*
- *On 4560 6 GPU nodes (27,360 GPUs total)*
- *High-accuracy (harder when predicting "no hurricane today" is 98% accurate), solved with weighted loss function.*
- *Layers each have different learning rate*



Exascale Deep Learning for Climate Analytics
Kurth, et. al.

Model Parallelism

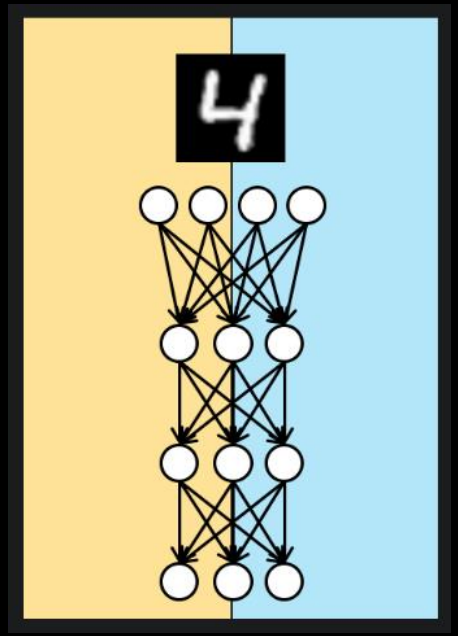
What about all these LLMs you have been hearing about that use *trillions* of parameters? Now, we don't have enough memory to fit the whole model on one GPU.



Instead we spread the parts of the model around (mostly their parameters, but could also be different sections of a more complex model) by using *Model Parallelism.*

The most popular way to do this in TensorFlow is via the *Mesh TensorFlow* API.

And, we can mix the way we distribute these parameters, layers, pipelines and model branches in various hybrid methods as well.



From the Chainer *docs on their parallelism API. Yet another DL framework.*

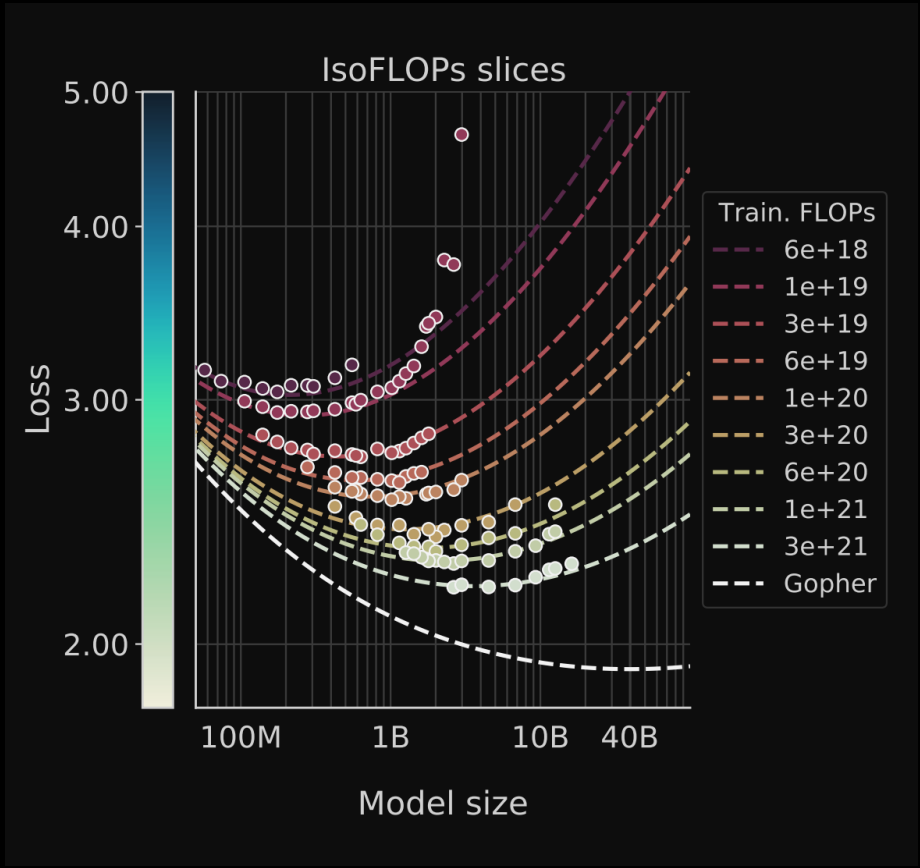
Scaling of LLMs

For LLMs that have been designed to scale well (avoiding overfitting and vanishing gradients, for example), we find that performance is a predictable function of:

- The dataset size
- The number of parameters

And these curves show no signs of ending yet.

So, in these applications we do expect better performance through brute force scaling.



Training Compute-Optimal Large Language Models
Hoffmann et. al.

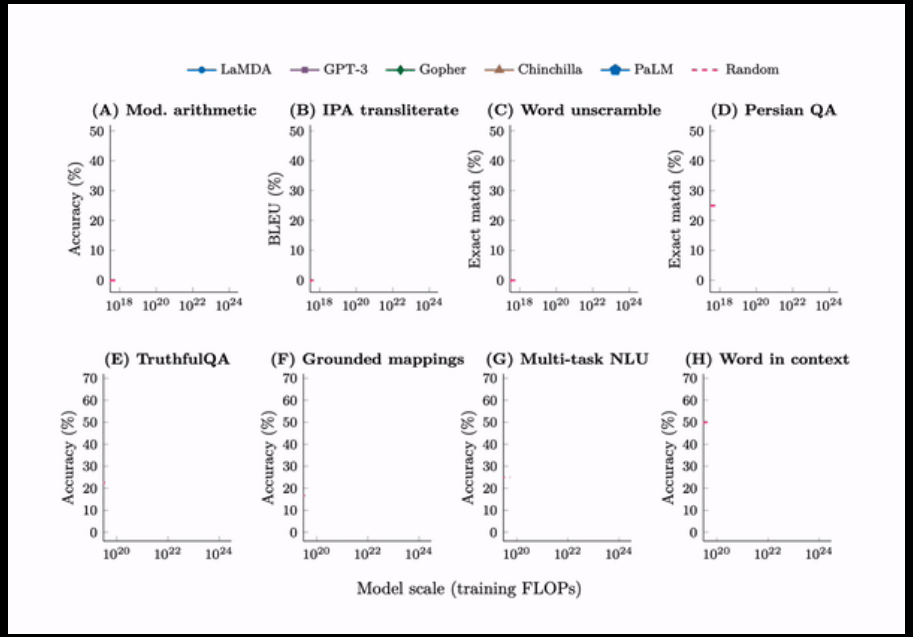
Emergent Capability

An emergent ability as an ability that is not present in small models but develops as the model is scaled. These might be unanticipated.

Some areas of science are familiar with this idea (physics and biology, for sure). In computer science this concept has largely been a novelty (Conway's Game of Life is a notable example). In Deep Learning, it has become a very significant phenomena.

Once again, bear in mind that many of the principles we have mentioned (overfitting, vanishing gradients, etc.) mean that brute force scaling is not going to be a default route to better performance.

Instead, understanding of those principles will allow you the option to scale.



https://www.jasonwei.net/blog/emergence
Also a good associated paper.

PyTorch?

```
import os
os.environ["KERAS_BACKEND"] = "torch"

import keras

mnist = keras.datasets.mnist
(train_images, train_labels), (test_images, test_labels) = mnist.load_data()

train_images = train_images.reshape(60000, 28, 28, 1)
test_images = test_images.reshape(10000, 28, 28, 1)
train_images, test_images = train_images/255, test_images/255

model = keras.Sequential([
    keras.layers.Conv2D(32, (3,3), activation='relu', input_shape=(28,28,1)),
    keras.layers.Conv2D(64, (3,3), activation='relu'),
    keras.layers.MaxPooling2D(2,2),
    keras.layers.Dropout(0.25),
    keras.layers.Flatten(),
    keras.layers.Dense(128, activation='relu'),
    keras.layers.Dropout(0.5),
    keras.layers.Dense(10, activation='softmax')
])

model.compile(optimizer='adam', loss='sparse_categorical_crossentropy', metrics=['accuracy'])

model.fit(train_images, train_labels, batch_size=128, epochs=15, verbose=1, validation_data=(test_images, test_labels))
```

This could be done in the shell.

Use the Latest Environment

```
interact -p GPU-shared --gres=gpu:h100-80:1

singularity shell --nv /ocean/containers/ngc/pytorch/pytorch_latest.sif
```

```python
from __future__ import print_function
import argparse
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim
from torchvision import datasets, transforms
from torch.optim.lr_scheduler import StepLR


class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 32, 3, 1)
        self.conv2 = nn.Conv2d(32, 64, 3, 1)
        self.dropout1 = nn.Dropout2d(0.25)
        self.dropout2 = nn.Dropout2d(0.5)
        self.fc1 = nn.Linear(9216, 128)
        self.fc2 = nn.Linear(128, 10)

    def forward(self, x):
        x = self.conv1(x)
        x = F.relu(x)
        x = self.conv2(x)
        x = F.relu(x)
        x = F.max_pool2d(x, 2)
        x = self.dropout1(x)
        x = torch.flatten(x, 1)
        x = self.fc1(x)
        x = F.relu(x)
        x = self.dropout2(x)
        x = self.fc2(x)
        output = F.log_softmax(x, dim=1)
        return output


def train(args, model, device, train_loader, optimizer, epoch):
    model.train()
    for batch_idx, (data, target) in enumerate(train_loader):
        data, target = data.to(device), target.to(device)
        optimizer.zero_grad()
        output = model(data)
        loss = F.nll_loss(output, target)
        loss.backward()
        optimizer.step()
        if batch_idx % args.log_interval == 0:
            print('Train Epoch: {} [{}/{} ({:.0f}%)]\tLoss: {:.6f}'.format(
                epoch, batch_idx * len(data), len(train_loader.dataset),
                100. * batch_idx / len(train_loader), loss.item()))
```

```python
def test(args, model, device, test_loader):
    model.eval()
    test_loss = 0
    correct = 0
    with torch.no_grad():
        for data, target in test_loader:
            data, target = data.to(device), target.to(device)
            output = model(data)
            test_loss += F.nll_loss(output, target, reduction='sum').item()  # sum up batch loss
            pred = output.argmax(dim=1, keepdim=True)  # get the index of the max log-probability
            correct += pred.eq(target.view_as(pred)).sum().item()

    test_loss /= len(test_loader.dataset)
```

```
n'.format(
```

```
pose([
```

Old School PyTorch CNN MNIST

Not a fair comparison of terseness as this version has a lot of extra flexibility.

From:
https://github.com/pytorch/examples/blob/master/mnist/main.py

```python
    model = Net().to(device)
    optimizer = optim.Adadelta(model.parameters(), lr=args.lr)

    scheduler = StepLR(optimizer, step_size=1, gamma=args.gamma)
    for epoch in range(1, args.epochs + 1):
        train(args, model, device, train_loader, optimizer, epoch)
        test(args, model, device, test_loader)
        scheduler.step()

    if args.save_model:
        torch.save(model.state_dict(), "mnist_cnn.pt")


if __name__ == '__main__':
    main()
```

Exercises

We are going to leave you with a few substantial problems that you are now equipped to tackle. Feel free to use your extended workshop access to work on these, and remember that additional time is an easy Startup Allocation away. Of course everything we have done is standard and you can work on these problems in any reasonable environment.

You may have wondered what else was to be found at tf.keras.datasets. The answer is many interesting problems. The obvious follow-on is:

Fashion MNIST

These are 60,000 training images, and 10,000 test images of 10 types of clothing, in 28x28 greyscale. Sound familiar? A more challenging drop-in for MNIST.

More tf.keras.datasets Fun

CRIM	per capita crime rate by town
ZN	proportion of residential land
INDUS	proportion of non-retail busine
CHAS	Charles River dummy variable (=
NOX	nitric oxides concentration (pa
RM	average number of rooms per dwe
AGE	proportion of owner-occupied un
DIS	weighted distances to five Bost
RAD	index of accessibility to radia
TAX	full-value property-tax rate pe
PTRATIO	pupil-teacher ratio by town
B	1000(Bk - 0.63)^2 where Bk is t
LSTAT	% lower status of the populatio
MEDV	Median value of owner-occupied

Boston Housing Predict housing prices base upon crime, zoning, pollution, etc.

CIFAR10 32x32 color images in 10 classes.

CIFAR100 Like CIFAR10 but with 100 non-overlapping classes.

IMDB 1 sentence positive or negative reviews.

I have been known to fall asleep during films, but this...
Mann photographs the Alberta Rocky Mountains in a superb fashion...
This is the kind of film for a snowy Sunday afternoon...

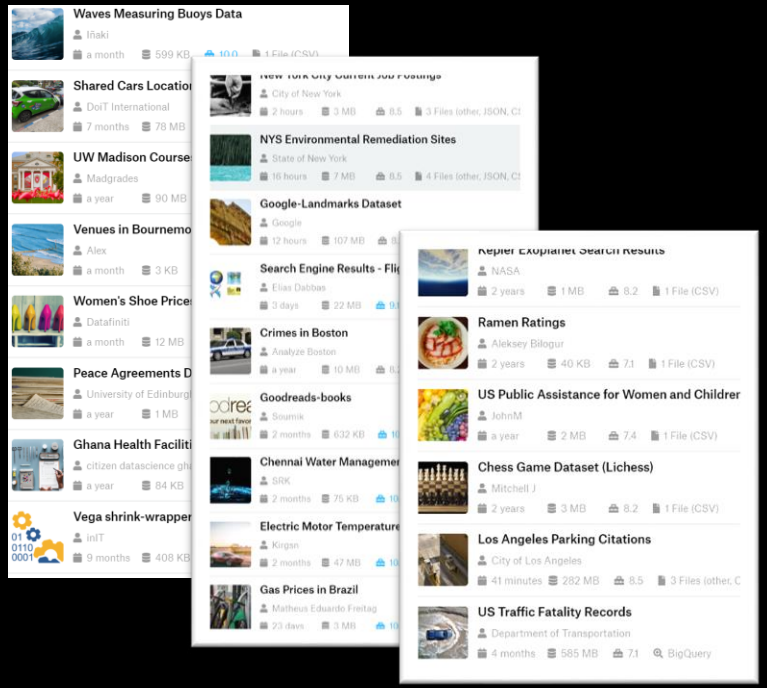
Reuters 46 topics in newswire form.

Its december acquisition of space co it expects earnings per share in 1987 of 1 15 to 1 30 dlrs per share up from 70 cts in 1986 the company said pretax net should rise to nine to 10 mln dlrs from six mln dlrs in 1986 and rental operation revenues to 19 to 22 mln dlrs from 12 5 mln dlrs it said cash flow per share this year should be 2 50 to three dlrs reuters...

Endless Exercises

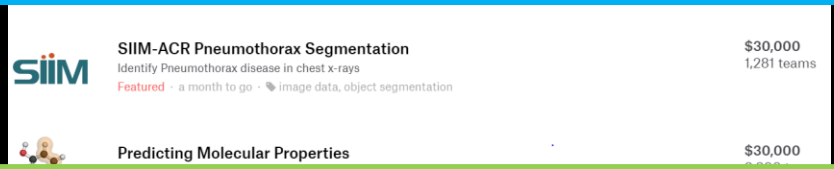
Kaggle Challenge

The benchmark driven nature of deep learning research, and its competitive consequences, have found a nexus at Kaggle.com. There you can find over 500,000 datasets:



Hugging Face

- Also a lot of datasets (450,000)
- and models (1,900,000)
- No competitions
- A little more profit driven
- and a lot more advanced/confusing.



Including this one: