Deep Learning

In An Afternoon

John Urbanic

Parallel Computing Scientist
Pittsburgh Supercomputing Center

Unprecedented Disruption

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

10 years ago

"Neural nets will enable real time ray tracing."

"Neural nets will do protein folding."

Science Fiction. Word salad.

5 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.



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



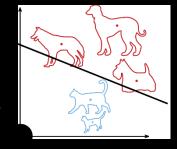
Two Perspectives

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

• Inspired by biological models.



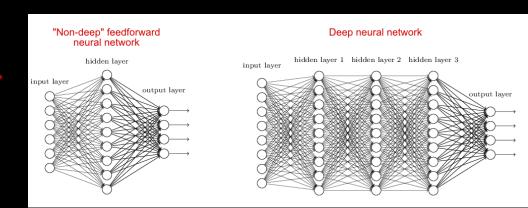
• An evolution of classic ML techniques (the perceptron).



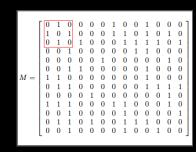
They are both fair and useful. We'll give each a thin slice of our attention before we move on to the actual implementation. You can decide which perspective works for you.



Modeled After The Brain

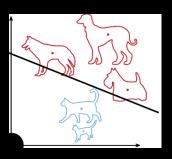






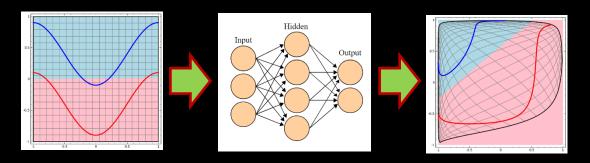
As a Highly Dimensional Non-linear Classifier

Perceptron



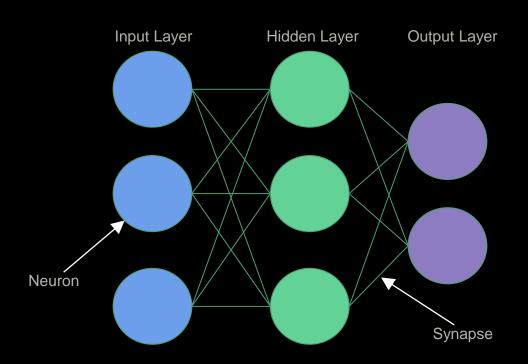
No Hidden Layer Linear

Network



Hidden Layers Nonlinear

Basic NN Architecture

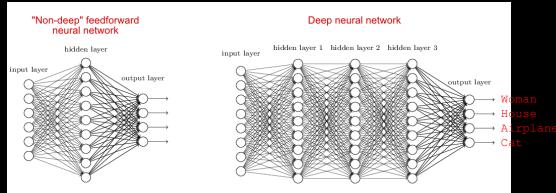


In Practice

How many inputs?



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



How deep?

100+ layers have become common.

How many outputs?



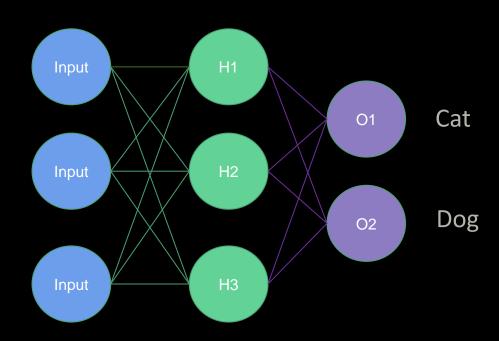
Might be an entire image.

Or could be discreet set of classification possibilities.

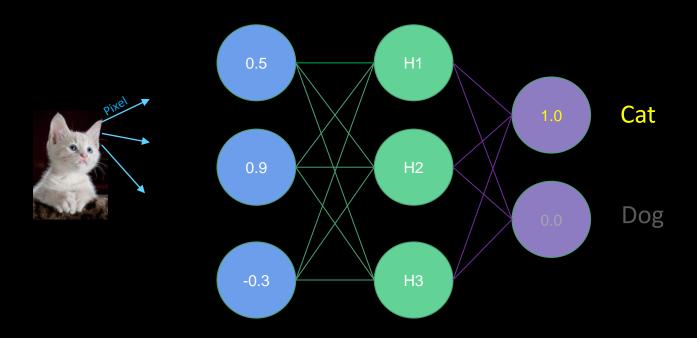
<u>Inference</u>

The "forward" or thinking step



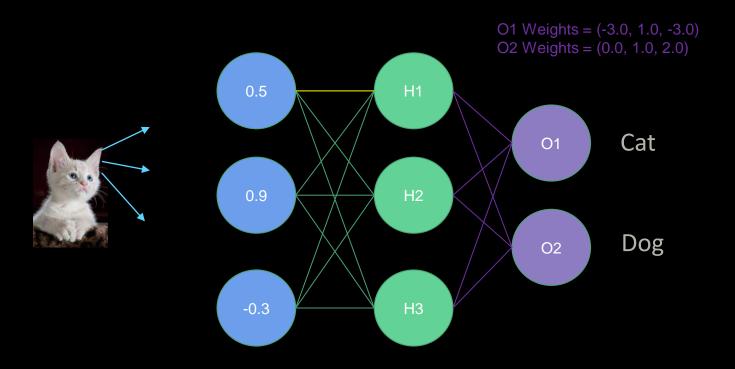


Inference Input and Output Layers



Inference

Weights or Parameters



H1 Weights = (1.0, -2.0, 2.0)

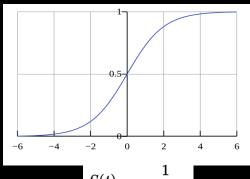
H2 Weights = (2.0, 1.0, -4.0)

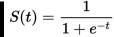
H3 Weights = (1.0, -1.0, 0.0)

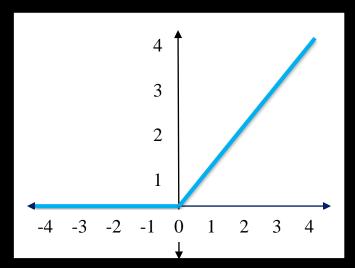
Activation Function

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.
- 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.

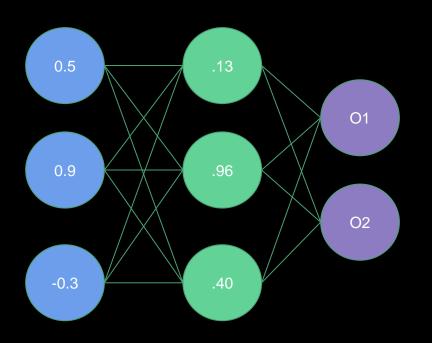






Inference

Multiply, Add, do something non-linear.



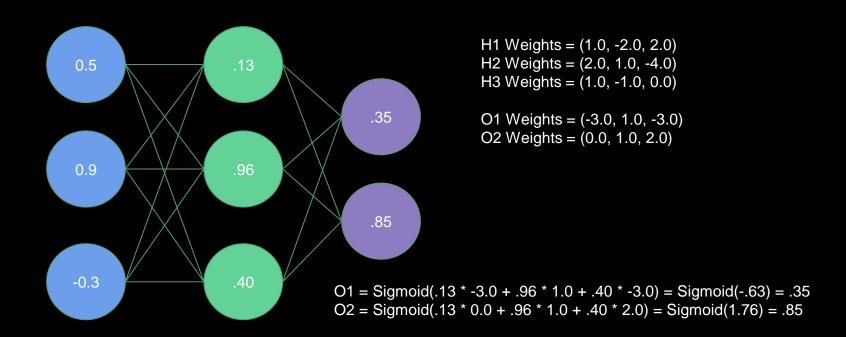
H1 Weights = (1.0, -2.0, 2.0) H2 Weights = (2.0, 1.0, -4.0) H3 Weights = (1.0, -1.0, 0.0)

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(0.5 * 1.0 + 0.9 * -1.0 + -0.3 * 0.0) = Sigmoid(0.5 * 1.0 + 0.9 * -1.0 + -0.3 * 0.0) = Sigmoid(0.5 * 1.0 + 0.9 * -1.0 + -0.3 * 0.0) = Sigmoid(0.5 * 1.0 + 0.9 * -1.0 + -0.3 * 0.0) = Sigmoid(0.5 * 1.0 + 0.9 * -1.0 + -0.3 * 0.0)

Inference

Then do it again.

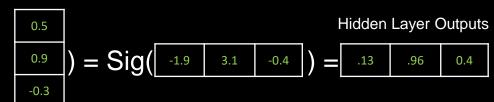


As A Matrix Operation

Hidden Layer Weights

Sig(2.0 1.0 -2.0 2.0 1.0 -4.0 1.0 -1.0 0.0

Inputs



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:



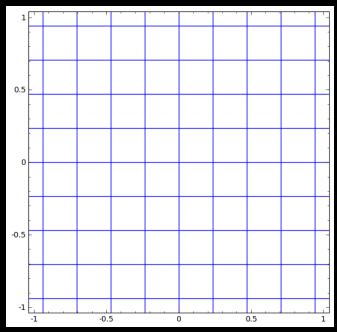
Linear + Nonlinear

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*.

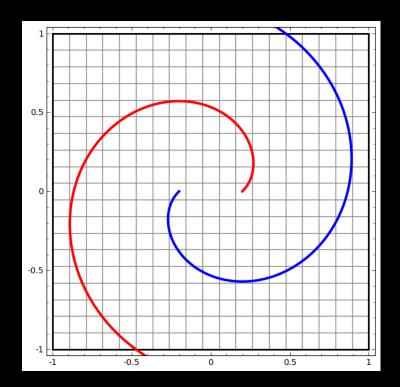
The bias provides the *translation*.

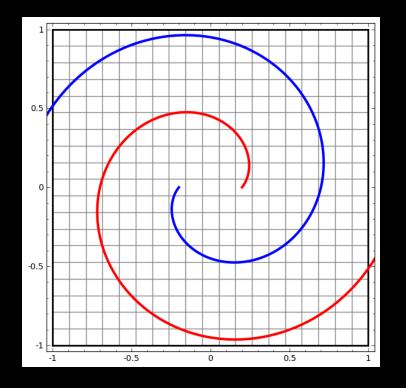
The activation function provides the warp.



Linear + Nonlinear

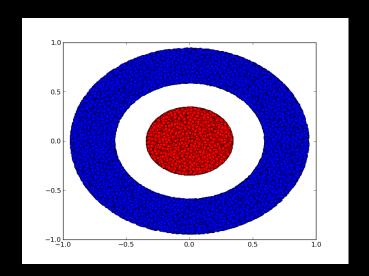
These are two very simple networks untangling spirals. Note that the second does not succeed. With more substantial networks these would both be trivial.





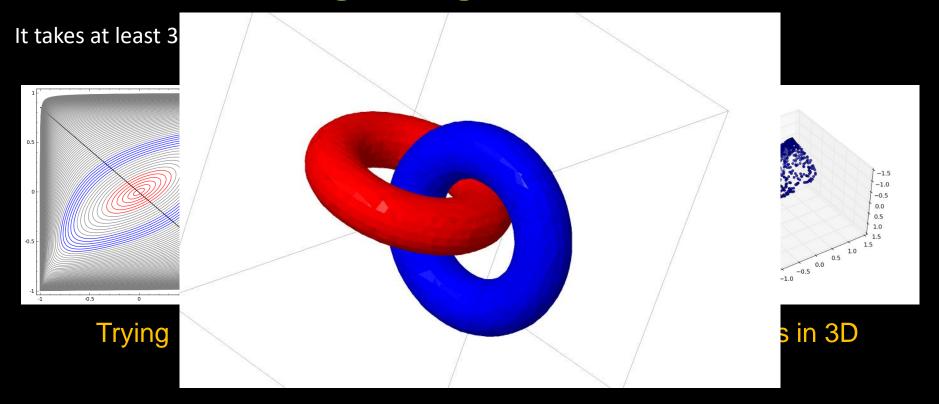
Width of Network

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?

Working In Higher Dimensions



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

Theoretically

Universal Approximation Theorem: A 1-hidden-layer feedforward network of this type can approximate any function¹, given enough width².

Not really that useful as:

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

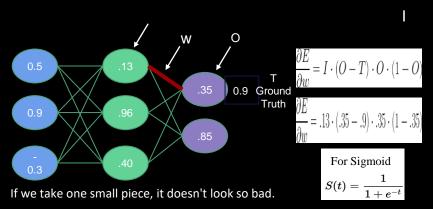
¹⁾ Borel measurable. Basically, mostly continuous and bounded.

²⁾ Could be exponential number of hidden units, with one unit required for each distinguishable input configuration.

Training Neural Networks

So how do we find these magic weights? We want to minimize the error on our training data. Given labeled inputs, select weights that generate the smallest average error on the outputs.

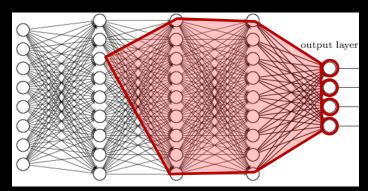
We know that the output is a function of the weights: $E(w_1, w_2, w_3, ... i_1, ... t_1, ...)$. So to figure out which way, and how much, to push any particular weight, say w_3 , we want to calculate $\frac{\partial E}{\partial w_3}$



Note that the role of the gradient, $\frac{\partial B}{\partial w_3}$, here means that it becomes a problem if it vanishes. This is an issue for very deep networks.

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.

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

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

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.

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.

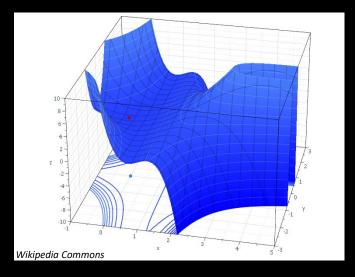
Solvers

However, even this efficient technique leaves us with potentially many millions of simultaneous equations to solve (real nets have a lot of weights). And the solution space is non-convex. Fortunately, this isn't a new problem created by deep learning, so we have options from the world of numerical methods.

The standard has been *gradient descent*. Variations of this 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.

Nevertheless, we don't expect to ever find the actual global minimum.



We could/should find the 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*.

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...
>>>
```

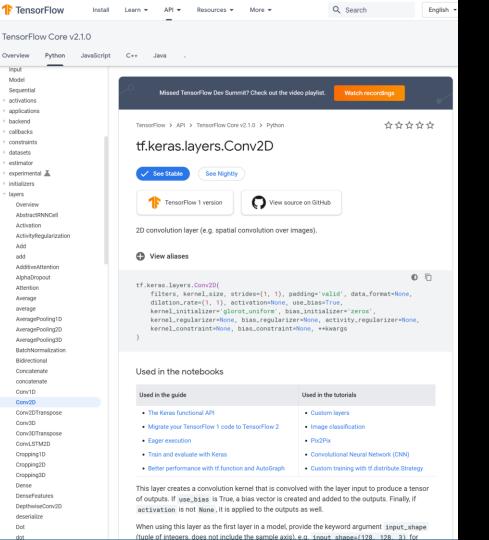
Two Other Ways To Play Along

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())
```



Input Model Sequential

activations

backend

callbacks constraints

datasets estimator

initializers layers

add

Average

average

Conv1D

Conv2D

Conv3D

Dense

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

import mages
```

```
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]))
                               Digit: 4
```

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.astvpe('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,	======================================	========

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))
```

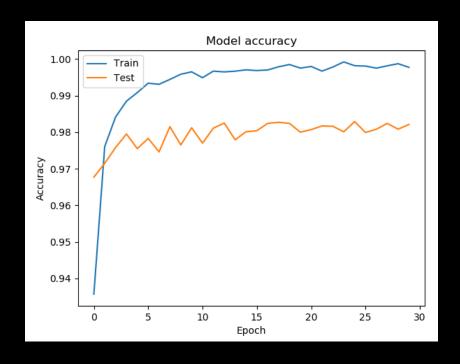


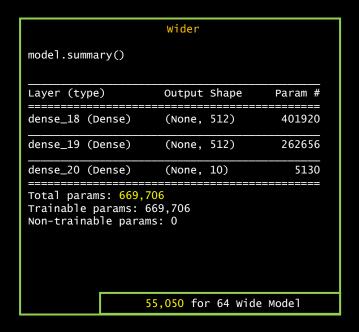
Let's Go Wider

```
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
```





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



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

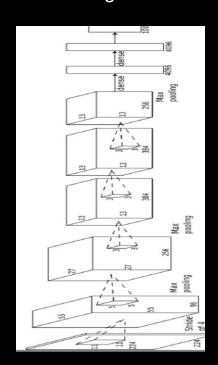
- Overfitting
- Vanishing gradients

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.

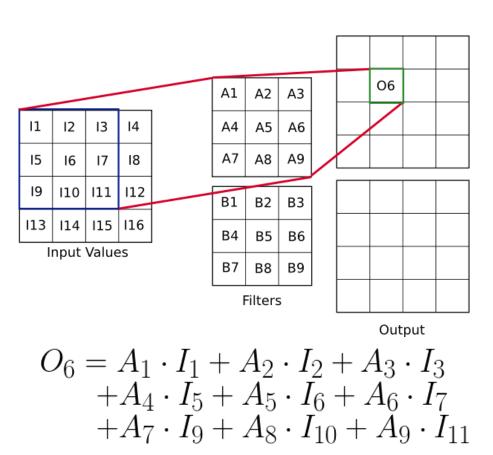
Image Recognition Done Right: CNNs

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



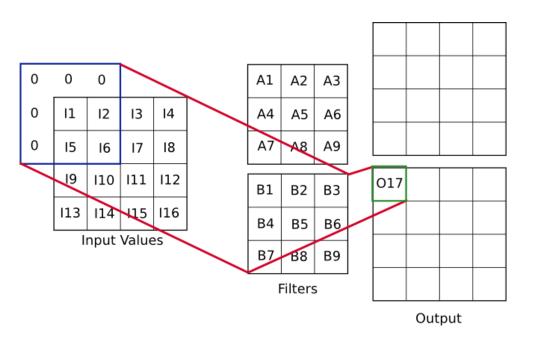


Convolution



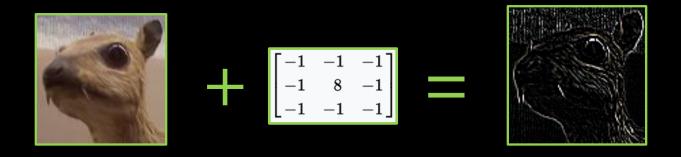
Convolution

Boundary and Index Accounting



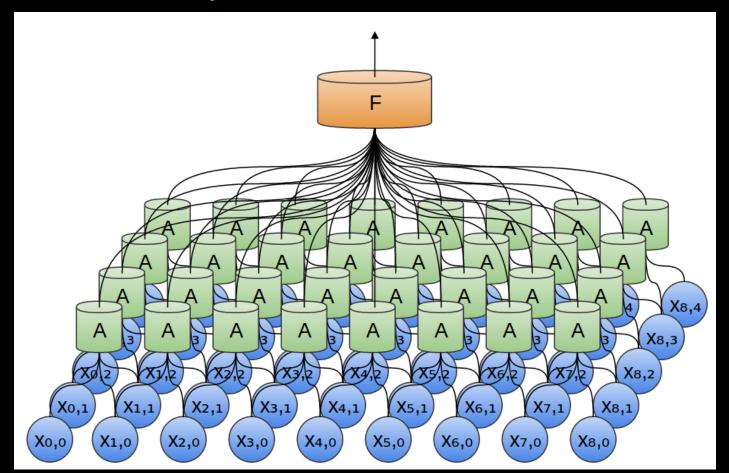
$$O_{17} = B_5 \cdot I_1 + B_6 \cdot I_2 + B_8 \cdot I_5 + B_9 \cdot I_6$$

Straight Convolution

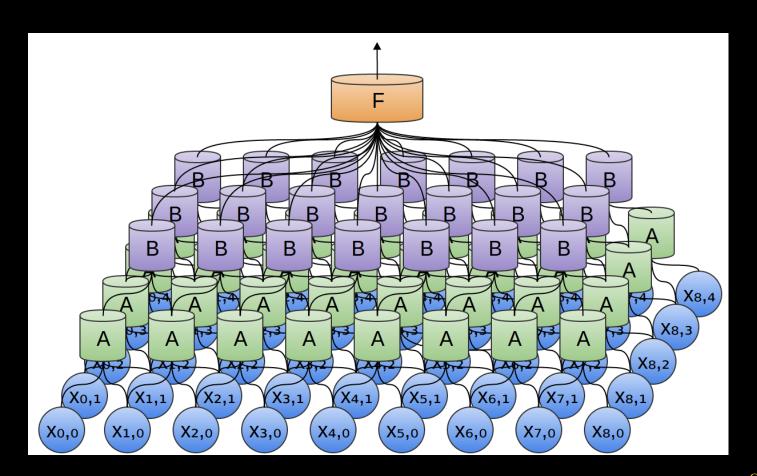


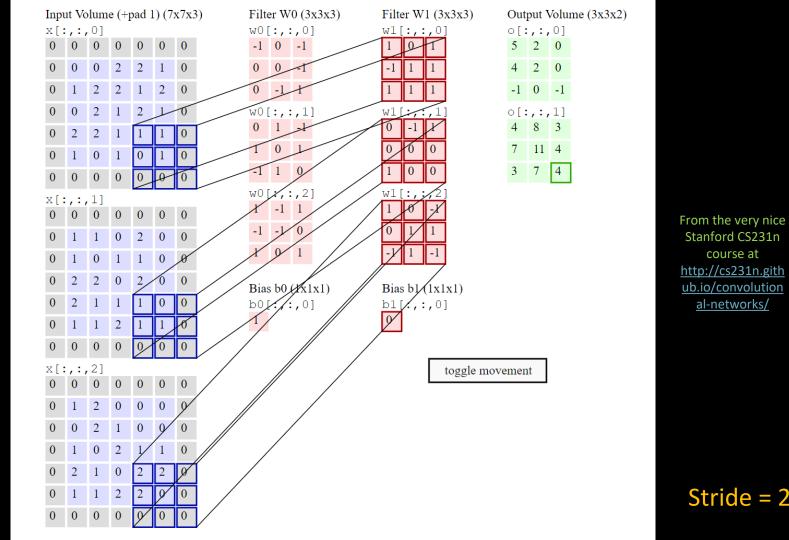
Edge Detector

Simplest Convolution Net



Stacking Convolutions





Stanford CS231n

course at

al-networks/

Stride = 2

n

n

Convolution Math

Each Convolutional Layer:

Inputs a volume of size $W_1 \times H_1 \times D_1$ (D is depth)

Requires four hyperparameters:

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

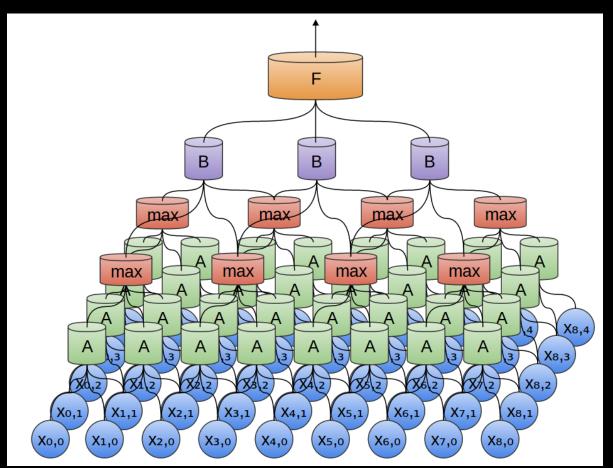
Produces a volume of size
$$W_O \times H_O \times D_O$$

 $W_O = (W_I - N + 2P) / S + 1$
 $H_O = (H_I - F + 2P) / S + 1$
 $D_O = K$

This requires N·N·D_I weights per filter, for a total of N·N·D_I·K weights and K biases

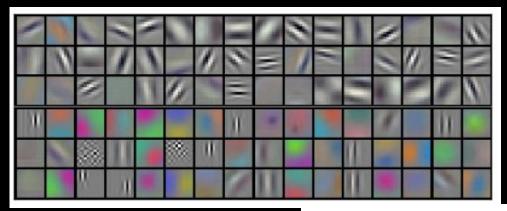
In the output volume, the d-th depth slice (of size $W_O \times H_O$) is the result of performing a convolution of the d-th filter over the input volume with a stride of S, and then offset by d-th bias.

Pooling

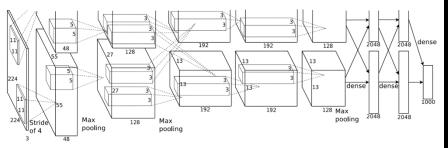


A Groundbreaking Example

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

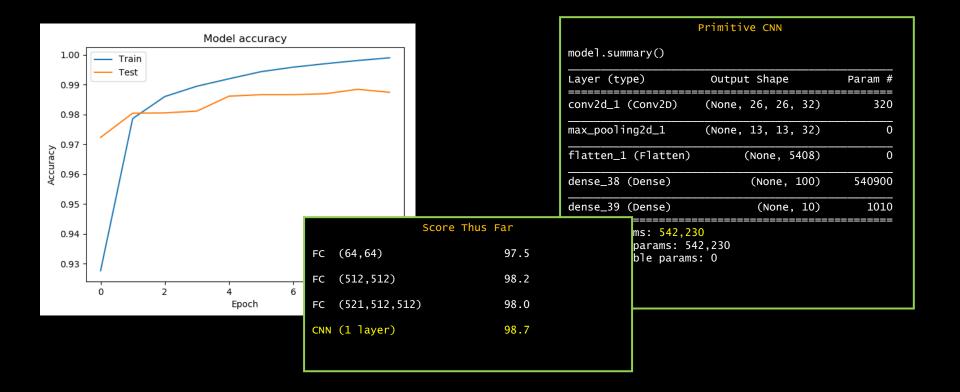
model = tf.keras.Sequential([
    tf.keras.layers.Conv2D(32, (3,3), activation='relu', input_shape=(28,28,1)),
    tf.keras.layers.MaxPooling2D(2,2),
    tf.keras.layers.Platten(),
    tf.keras.layers.Platten(),
    tf.keras.layers.Dense(100, activation='relu'),
    tf.keras.layers.Dense(100, activation='relu'),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

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

```
. . . .
```

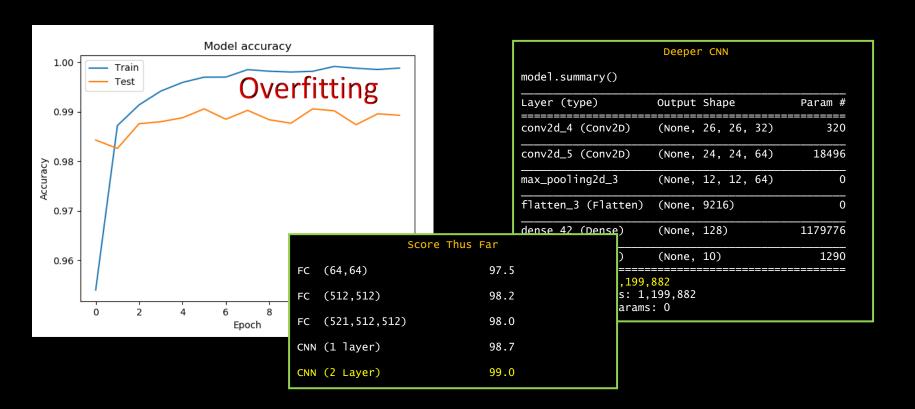


Scaling Up The CNN

```
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

```
....
```



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.



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.

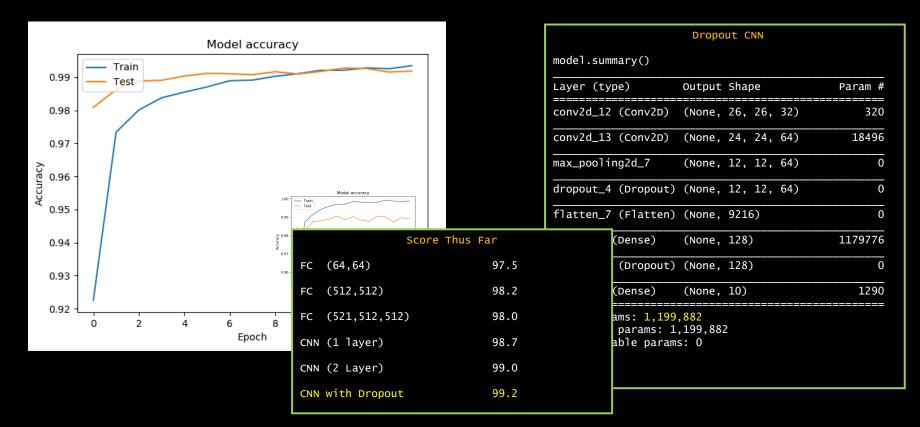
CNN With Dropout

```
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),
                                                                                                          Parameter is fraction to drop.
    tf.keras.layers.Flatten(),
    tf.keras.layers.Dense(128, activation='relu'),
    tf.keras.layers.Dropout(0.5),
    tf.keras.layers.Dense(10, activation='softmax')
1))
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))
```

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

Help From Dropout

```
....
```



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 micromanage 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

```
. . . .
```



Real Time 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

2



Downsampled drawing: 2

First guess:

Second guess: (

Layer visibility

put layer SI

Convolution layer 1 SI

Convolution layer 2 St

Downsampling layer 2 Sh

Fully-connected layer 1 Shi

ully-connected layer 2

utput laver

0123456789







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.

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:

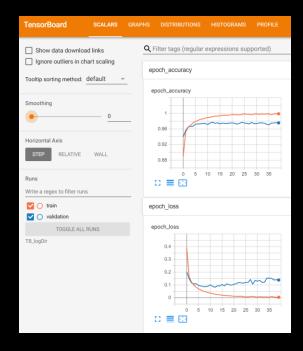
ssh -2 -Nf -L 6006:127.0.0.1:6006 br014.bridges2.psc.edu

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

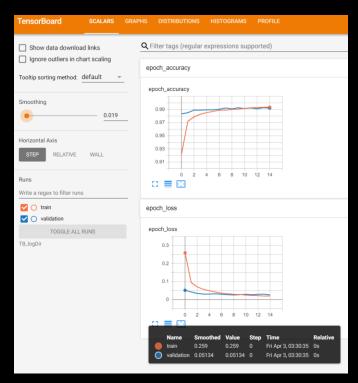
ssh -2 -Nf -L 6006:r001.ib.bridges2.psc.edu:6006 br014.bridges2.psc.edu

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 <u>real-time</u> as the model runs. This can be very useful for you to monitor overfitting.



Our First Model 64 Wide FC



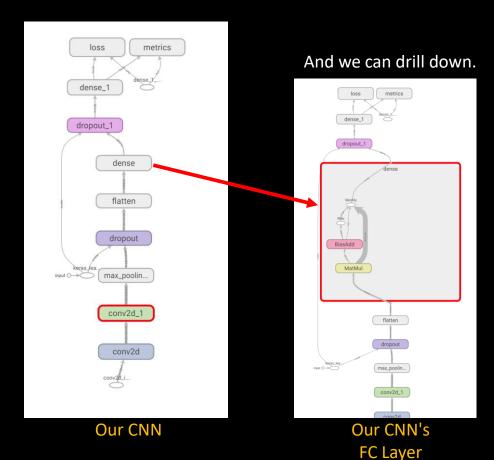
Our CNN

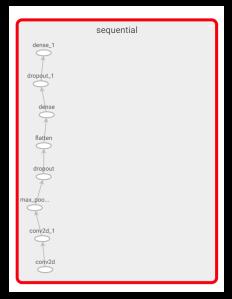
TensorBoard Graph Views

We can explore the architecture of the deep learning graphs we have constructed.



Our First Model 64 Wide FC



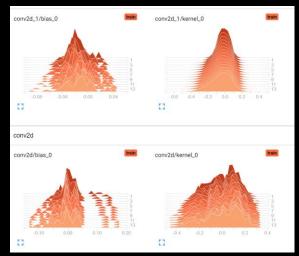


Keras
"Conceptual
Model"
View
of CNN

TensorBoard Parameter Visualization

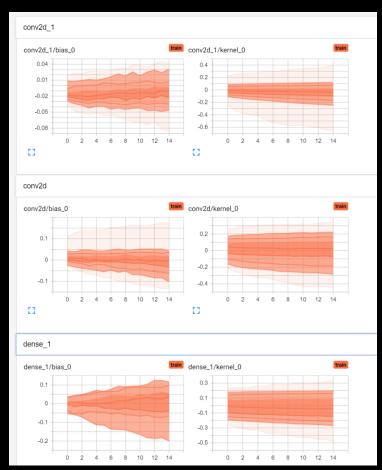
And we can observe the time evolution of our weights and biases, or at least their distributions.

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



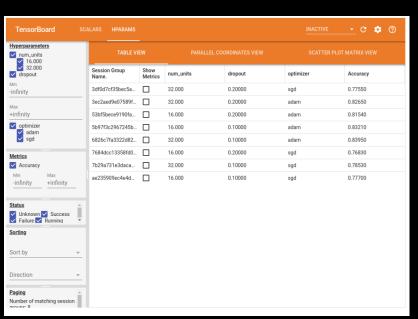
Histogram View

Distribution View



TensorBoard Add Ons

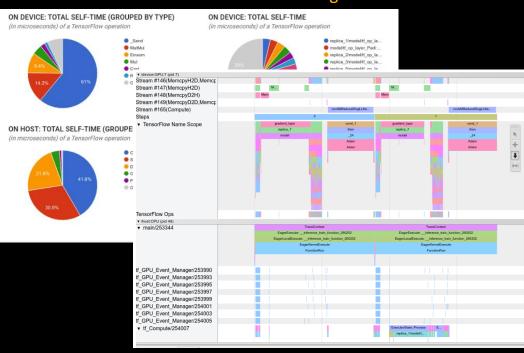
TensorBoard has lots of extended capabilities. Two particularly useful and powerful ones are Hyperparameter Search and Performance Profiling.



Hyperparameter Search

Requires some scripting on your part. Look at https://www.tensorflow.org/tensorboard/hyperparameter_t uning_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.

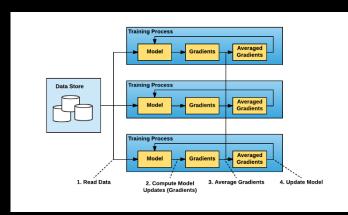
Scaling Up

You may have the idea that deep learning has a voracious appetite for GPU cycles. That is absolutely the case, and the leading edge of research is currently limited by available resources. Researchers routinely use many GPUs to train a model. Conversely, the largest resources demand that you use them in a parallel fashion. There are capabilities built into TensorFlow, the MirroredStrategy.

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

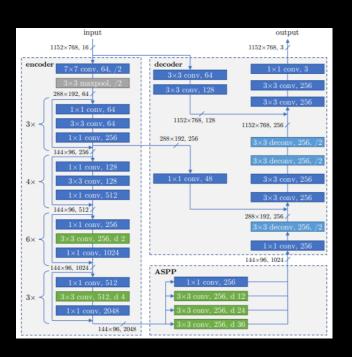


Horovod: fast and easy distributed deep learning in TensorFlow Alexander Sergeev, Mike Del Balso

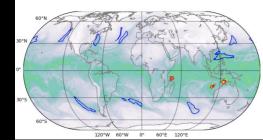
You can find a full example of using Horovod with a Keras MNIST code at: https://horovod.readthedocs.io/en/latest/keras.html

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



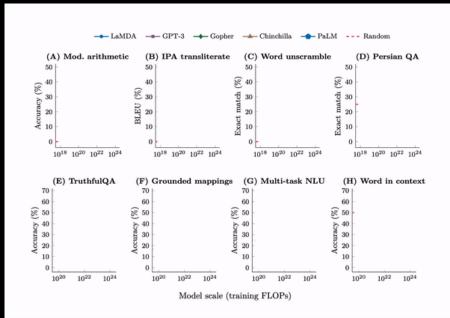
Emergent Capability

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.

However, 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.

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 How many samples do we need? Our MNIST network has learned to recognize ve This is another hyperparameter (yes), where we can only offer a vague rule of thumb. And that suggestion is What if we wanted to teach it: about 5000 per category for competence, 10 million for a real task with human performance. FREE? **Rotation Invariance** Noise Tolerance Translation Invariance Scale 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



Idiots Guide to Winning the US Open

One-Shot Learning

On the other hand, maybe I could teach adult you what a platypus is with one example. And, if you want to spot a particular mad bomber with your airport facial recognition system, you may only have one photo.

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.

```
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()))
```

from __future__ import print_function

import argparse

import torch.nn as nn

import torch

```
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)
```

'.format(

oose([

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

```
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

Boston Housing

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

CIFAR10

32x32 color images in 10 classes.



lawn_mower

CRIM per capita crime rate by town ΖN 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 ur DIS weighted distances to five Bost RAD index of accessibility to radia TAX full-value property-tax rate pe pupil-teacher ratio by town 1000(Bk - 0.63)^2 where Bk is LSTAT % lower status of the population MEDV Median value of owner-occupied

CIFAR100

1 sentence positive or negative reviews.

Like CIFAR10 but with 100 non-overlapping classes.

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

IMDB

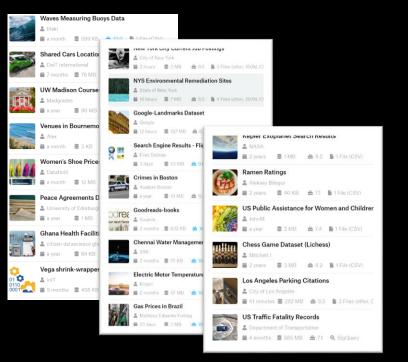
46 topics in newswire form.

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 20,000 datasets:



and competitions:

