Deep Learning / Neural Nets

Without question the biggest thing in ML and computer science right now. Is the hype real? Can you learn anything meaningful in an afternoon? How did we get to this point?

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

• Widespread parallel computing (GPUs)
• Big data training sets
Two Perspectives

There are really two common ways to view the foundations 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

Courtesy: Chris Olah
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.
Basic NN Architecture

Input Layer → Hidden Layer → Output Layer

Neuron

Synapse
Activation Function

Neurons apply activation functions at these summed inputs. Activation functions are typically non-linear.

- 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, addition and multiplication.
  - There are **Leaky** and **Noisy** variants.
Inference
The "forward" or thinking step

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)
Inference

H1 = \text{Sigmoid}(0.5 \times 1.0 + 0.9 \times -2.0 + -0.3 \times 2.0) = \text{Sigmoid}(-1.9) = .13
H2 = \text{Sigmoid}(0.5 \times 2.0 + 0.9 \times 1.0 + -0.3 \times -4.0) = \text{Sigmoid}(3.1) = .96
H3 = \text{Sigmoid}(0.5 \times 1.0 + 0.9 \times -1.0 + -0.3 \times 0.0) = \text{Sigmoid}(-0.4) = .40

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)
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Inference

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
O1 = 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 $b=0.1$:
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 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
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

It takes at least 3 units wide to pull this off, regardless of depth.

Greater depth allows us to stack these operations, and can be very effective. The gains from depth are harder to characterize.
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: \( E(w_1, w_2, w_3, \ldots, i_1, \ldots, t_1, \ldots) \). So to figure out which way, and how much, to push any particular weight, say \( w_3 \), we want to calculate \( \frac{\partial E}{\partial w_3} \).

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.

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

If we use the chain rule repeatedly across layers we can work our way backwards from the output error through the weights, adjusting them as we go. Note that this is where the requirement that activation functions must have nicely behaved derivatives comes from.

This technique makes the weight inter-dependencies much more tractable. 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.

You don't need to know the details, and this is all we have time to say, but you certainly can understand this fully if your freshman calculus isn't too rusty and you have some spare time.
Solvers

However, even this efficient process leaves us with potentially many millions of simultaneous equations to solve (real nets have a lot of weights). They are non-linear to boot. 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. Methods, often similar, 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 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.
We now know enough to attempt a problem. Only because the TensorFlow framework 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 implement a quite sophisticated and accurate convolutional neural network for this same problem.
MNIST Data

Specifically we will have a file with 55,000 of these numbers.

```
6 = [0,0,0,0,0,1,0,0,0]
```

The labels will be “one-hot vectors”, which means a 1 in the numbered slot:

```
6 = [0,0,0,0,0,1,0,0,0]
```
Make sure you are on a GPU node:

```
login006% interact -gpu
```

gpu42%

These examples assume you have the MNIST data sitting around in your current directory:

```
gpu42% ls
-rw-r--r-- 1 urbanic pscstaff 1648877 May 4 02:13 t10k-images-idx3-ubyte.gz
-rw-r--r-- 1 urbanic pscstaff  4542 May 4 02:13 t10k-labels-idx1-ubyte.gz
-rw-r--r-- 1 urbanic pscstaff  991242 May 4 02:13 train-images-idx3-ubyte.gz
-rw-r--r-- 1 urbanic pscstaff  28881 May 4 02:13 train-labels-idx1-ubyte.gz
```

To start TensorFlow:

```
gpu42% module load tensorflow/1.5_gpu
gpu42% python
```
Only “mystery” code in whole workshop!

Just reads in files as we just discussed, in batches. Easy to do but a slight digression.

```
$ python
Python 3.6.1 |Continuum Analytics, Inc.| (default, Mar 22 2017, 19:54:23)
[GCC 4.4.7 20120313 (Red Hat 4.4.7-1)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf
>>> mnist = input_data.read_data_sets(".", one_hot=True)
...  You may get some congratulatory noise here...
..........Pay it no heed.............

```

```
>>> x, y = mnist.train.next_batch(2)
>>> y[0]
array([ 0.,  0.,  0.,  0.,  1.,  0.,  0.,  0.,  0.,  0.])
>>> x[0]
array([[ 0.        ,  0.        ,  0.        ,  0.        ,  0.        ,
        0.        ,  0.        ,  0.        ,  0.        ,  0.        ,
        0.        ,  0.        ,  0.        ,  0.        ,  0.        ,
        0.        ,  0.        ,  0.        ,  0.        ,  0.        ,
        0.        ,  0.        ,  0.        ,  0.        ,  0.02352941,
        0.76470596,  0.99607849,  1.        ,  0.93725497,  0.1137255 ,
        0.        ,  0.        ,  0.        ,  0.        ,  0.        ,
        ...]))
```
The API is well documented. That is terribly unusual.
Regression MNIST

```python
$ python
Python 3.6.1 |Continuum Analytics, Inc.| (default, Mar 22 2017, 19:54:23)
[GCC 4.4.7 20120313 (Red Hat 4.4.7-1)] on linux
Type "help", "copyright", "credits" or "license" for more information.

>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf

>>> mnist = input_data.read_data_sets(".", one_hot=True)

>>> x = tf.placeholder(tf.float32, [None, 784])
>>> W = tf.Variable(tf.zeros([784, 10]))
>>> b = tf.Variable(tf.zeros([10]))
>>> y = tf.matmul(x, W) + b

>>> y_ = tf.placeholder(tf.float32, [None, 10])
```

**Placeholder**
We will use TF placeholders for inputs and outputs. We will use TF Variables for persistent data that we can calculate. NONE means this dimension can be any length.

**Image is 784 vector**
We have flattened our 28x28 image to a 1-D 784 vector. You will encounter this simplification frequently.

**b (Bias)**
A bias is often added across all inputs to eliminate some independent "background".

---

```
from tensorflow.examples.tutorials.mnist import input_data
import tensorflow as tf

mnist = input_data.read_data_sets(".", one_hot=True)

x = tf.placeholder(tf.float32, [None, 784])
W = tf.Variable(tf.zeros([784, 10]))
b = tf.Variable(tf.zeros([10]))
y = tf.matmul(x, W) + b

y_ = tf.placeholder(tf.float32, [None, 10])

cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits_v2(labels=y_, logits=y))
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)

sess = tf.InteractiveSession()
tf.global_variables_initializer().run()

for _ in range(1000):
batch_xs, batch_ys = mnist.train.next_batch(100)
sess.run(train_step, feed_dict={x: batch_xs, y_: batch_ys})

correct_prediction = tf.equal(tf.argmax(y, 1), tf.argmax(y_, 1))
accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))
print(sess.run(accuracy, feed_dict={x: mnist.test.images, y_: mnist.test.labels}))

<table>
<thead>
<tr>
<th>Digit</th>
<th>Output</th>
<th>Exponential</th>
<th>Normalized</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4.8</td>
<td>121</td>
<td>.87</td>
</tr>
<tr>
<td>1</td>
<td>-2.6</td>
<td>0.07</td>
<td>.00</td>
</tr>
<tr>
<td>2</td>
<td>2.9</td>
<td>18</td>
<td>.13</td>
</tr>
</tbody>
</table>

Given the sensible way we have constructed these outputs, the Cross Entropy Loss function is a very good way to define the error across all possibilities. Better than squared error, which we have been using until now.

Softmax Regression MNIST

GD Solver
Here we define the solver and details like step size to minimize our error.
Training Regression MNIST

```python
>> from tensorflow.examples.tutorials.mnist import input_data
>> import tensorflow as tf
>> mnist = input_data.read_data_sets(".", one_hot=True)
>>
>> x = tf.placeholder(tf.float32, [None, 784])
>> W = tf.Variable(tf.zeros([784, 10]))
>> b = tf.Variable(tf.zeros([10]))
>> y = tf.matmul(x, W) + b
>>
>> y_ = tf.placeholder(tf.float32, [None, 10])
>>
>> cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits_v2(labels=y_, logits=y))
>> train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)
>>
>> sess = tf.InteractiveSession()
>> tf.global_variables_initializer().run()
>>
>> for _ in range(1000):
>>   batch_xs, batch_ys = mnist.train.next_batch(100)
>>   sess.run(train_step, feed_dict={x: batch_xs, y_: batch_ys})
>>
>> correct_prediction = tf.equal(tf.argmax(y, 1), tf.argmax(y_, 1))
>> accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))
>> print(sess.run(accuracy, feed_dict={x: mnist.test.images, y_: mnist.test.labels}))
```

Launch
Launch the model and initialize the variables.

Train
Do 1000 iterations with batches of 100 images, labels instead of whole dataset. This is stochastic.
Testing Regression MNIST

• Argmax selects index of highest value. We end up with a list of booleans showing matches.
• Reduce that list of 0s,1s and take the mean.
• Run the graph on the test dataset to determine accuracy. No solving involved.

Result is 92%.
You may be impressed. *This is a linear matrix that knows how to read numbers by multiplying an image vector!* Or not. Consider this the most basic walkthrough of constructing a graph with TensorFlow.

We can do much better using a real NN. We will even jump quite close to the state-of-the-art and use a Convolutional Neural Net.

This will have a multi-layer structure like the deep networks we considered earlier.

It will also take advantage of the actual 2D structure of the image that we ditched so cavalierly earlier.

It will include dropout! A surprising optimization to many.
Convolutional Net

- Input Image: 1x500x500
- Normalized Image: 1x500x500
- Local Divisive Normalization
- Convolutions w/ filter bank: 20x7x7 kernels
- Pooling: 20x4x4 kernels
- Convs: 100x7x7 kernels
- Pooling: 20x4x4 kernels
- Convs: 800x7x7 kernels
- Linear Classifier
- Object Categories / Positions
- F6: Nx23x23
- at (x,y)
- at (x,y)
- at (x,y)
- C5: 200x23x23
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

\[ \begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix} \]

Edges Detector
Simplest Convolution Net

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

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 \( W_O \times H_O \times D_O \)
\[
W_O = \frac{(W_I - N + 2P)}{S+1}
\]
\[
H_O = \frac{(H_I - F + 2P)}{S+1}
\]
\[
D_O = K
\]

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.
A Sophisticated Example

These are the 96 first layer 11x11 (x3, RGB, stacked here) filters from Krizhevsky et al. (2012), a landmark advance in ImageNet classification called 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.
from tensorflow.examples.tutorials.mnist import input_data
import tensorflow as tf

mnist = input_data.read_data_sets(".", one_hot=True)
x = tf.placeholder(tf.float32, [None, 784])
y_ = tf.placeholder(tf.float32, [None, 10])
x_image = tf.reshape(x, [-1,28,28,1])

W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
b_conv1 = tf.Variable(tf.constant(0.1, shape=[32]))
h_conv1 = tf.nn.relu(tf.nn.conv2d(x_image, W_conv1, strides=[1, 1, 1, 1], padding='SAME') + b_conv1)

h_pool1 = tf.nn.max_pool(h_conv1, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')

W_conv2 = tf.Variable(tf.truncated_normal([5, 5, 32, 64], stddev=0.1))
b_conv2 = tf.Variable(tf.constant(0.1, shape=[64]))
h_conv2 = tf.nn.relu(tf.nn.conv2d(h_pool1, W_conv2, strides=[1, 1, 1, 1], padding='SAME') + b_conv2)

h_pool2 = tf.nn.max_pool(h_conv2, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')

W_fc1 = tf.Variable(tf.truncated_normal([7 * 7 * 64, 1024], stddev=0.1))
b_fc1 = tf.Variable(tf.constant(0.1, shape=[1024]))
h_pool2_flat = tf.reshape(h_pool2, [-1, 7*7*64])
h_fc1 = tf.nn.relu(tf.matmul(h_pool2_flat, W_fc1) + b_fc1)

W_fc2 = tf.Variable(tf.truncated_normal([1024, 10], stddev=0.1))
b_fc2 = tf.Variable(tf.constant(0.1, shape=[10]))
keep_prob = tf.placeholder(tf.float32)

h_fc1_drop = tf.nn.dropout(h_fc1, keep_prob)
y_conv = tf.matmul(h_fc1_drop, W_fc2) + b_fc2

cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits_v2(labels=y_, logits=y_conv))
train_step = tf.train.AdamOptimizer(1e-4).minimize(cross_entropy)
correct_prediction = tf.equal(tf.argmax(y_conv,1), tf.argmax(y_,1))
accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))

sess = tf.InteractiveSession()
sess.run(tf.global_variables_initializer())

for i in range(20000):
  batch = mnist.train.next_batch(50)
  if i%100 == 0:
    train_accuracy = accuracy.eval(feed_dict={x:batch[0], y_: batch[1], keep_prob: 1.0})
    print('step %d, training accuracy %g' % (i, train_accuracy))
  train_step.run(feed_dict={x: batch[0], y_: batch[1], keep_prob: 0.5})

test_accuracy = accuracy.eval(feed_dict={ x: mnist.test.images, y_: mnist.test.labels, keep_prob: 1.0}))
>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf

>>> mnist = input_data.read_data_sets(".", one_hot=True)

>>> x = tf.placeholder(tf.float32, [None, 784])
>>> y_ = tf.placeholder(tf.float32, [None, 10])

>>> x_image = tf.reshape(x, [-1,28,28,1])

[batch, height, width, channels]
-1 is TF for "unknown"
>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf

>>> mnist = input_data.read_data_sets(".", one_hot=True)

>>> x = tf.placeholder(tf.float32, [None, 784])
>>> y_ = tf.placeholder(tf.float32, [None, 10])

>>> x_image = tf.reshape(x, [-1, 28, 28, 1])

>>> W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
>>> b_conv1 = tf.Variable(tf.constant(0.1, shape=[32]))

>>> h_conv1 = tf.nn.relu(tf.nn.conv2d(x_image, W_conv1, strides=[1, 1, 1, 1], padding='SAME') + b_conv1)

>>> h_pool1 = tf.nn.max_pool(h_conv1, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')

---

Convolutional MNIST

The First Layer
>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf
>>>
>>> mnist = input_data.read_data_sets(".", one_hot=True)
>>> x = tf.placeholder(tf.float32, [None, 784])
>>> y_ = tf.placeholder(tf.float32, [None, 10])
>>> x_image = tf.reshape(x, [-1,28,28,1])
>>> W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
>>> b_conv1 = tf.Variable(tf.constant(0.1,shape=[32]))

We will have 32 5x5 filters in this layer
What values to initialize?
   Small random positive for weights
   Small constant for bias
>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf

>>> mnist = input_data.read_data_sets(".", one_hot=True)

>>> x = tf.placeholder(tf.float32, [None, 784])
>>> y_ = tf.placeholder(tf.float32, [None, 10])

>>> x_image = tf.reshape(x, [-1,28,28,1])

>>> W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
>>> b_conv1 = tf.Variable(tf.constant(0.1, shape=[32]))

>>> h_conv1 = tf.nn.relu(tf.nn.conv2d(x_image, W_conv1, strides=[1, 1, 1, 1], padding='SAME') + b_conv1)

Convolutional MNIST
The First Layer

TF will handle padding
More explicit in cuDNN and Caffe
Stride of 1x1
Must be same dims as X (just set depth,batch=1)
Add bias and apply our ReLU

Widely adopted around 2010!
Convolutional MNIST

The First Layer

[batch, height, width, channels]
For window size and stride.

The image we will pass to the next layer is now 14x14.

>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf

>>> mnist = input_data.read_data_sets(".", one_hot=True)

>>> x = tf.placeholder(tf.float32, [None, 784])
>>> y_ = tf.placeholder(tf.float32, [None, 10])

>>> x_image = tf.reshape(x, [-1,28,28,1])

>>> W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
>>> b_conv1 = tf.Variable(tf.constant(0.1, shape=[32]))

>>> h_conv1 = tf.nn.relu(tf.nn.conv2d(x_image, W_conv1, strides=[1, 1, 1, 1], padding='SAME') + b_conv1)

>>> h_pool1 = tf.nn.max_pool(h_conv1, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')
Convolutional MNIST

The First Layer

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>>> x_image = tf.reshape(x, [-1,28,28,1])

>>> W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
>>> b_conv1 = tf.Variable(tf.constant(0.1, shape=[32]))
>>> h_conv1 = tf.nn.relu(tf.nn.conv2d(x_image, W_conv1, strides=[1, 1, 1, 1], padding='SAME') + b_conv1)
>>> h_pool1 = tf.nn.max_pool(h_conv1, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')
Now we have 32 features coming in, and we will use 64 on this layer.

The next layer will be getting a 7x7 image.
Convolutional MNIST

Fully Connected Layer

Now we can just flatten our 64 7x7 images into one big vector for the FC layer to analyze.

We will choose 1024 neurons for this layer.
We will have a final FC layer that gets us from 1024 neurons down to our 10 possible outputs.
>>> from tensorflow.examples.tutorials.mnist import input_data
>>> import tensorflow as tf
>>> mnist = input_data.read_data_sets(".", one_hot=True)
>>> x = tf.placeholder(tf.float32, [None, 784])
>>> y_ = tf.placeholder(tf.float32, [None, 10])

>>> x_image = tf.reshape(x, [-1, 28, 28, 1])

>>> W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
>>> b_conv1 = tf.Variable(tf.constant(0.1, shape=[32]))
>>> h_conv1 = tf.nn.relu(tf.nn.conv2d(x_image, W_conv1, strides=[1, 1, 1, 1], padding='SAME') + b_conv1)
>>> h_pool1 = tf.nn.max_pool(h_conv1, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')

>>> W_conv2 = tf.Variable(tf.truncated_normal([5, 5, 32, 64], stddev=0.1))
>>> b_conv2 = tf.Variable(tf.constant(0.1, shape=[64]))
>>> h_conv2 = tf.nn.relu(tf.nn.conv2d(h_pool1, W_conv2, strides=[1, 1, 1, 1], padding='SAME') + b_conv2)
>>> h_pool2 = tf.nn.max_pool(h_conv2, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')

>>> W_fc1 = tf.Variable(tf.truncated_normal([7 * 7 * 64, 1024], stddev=0.1))
>>> b_fc1 = tf.Variable(tf.constant(0.1, shape=[1024]))
>>> h_pool2_flat = tf.reshape(h_pool2, [-1, 7*7*64])
>>> h_fc1 = tf.nn.relu(tf.matmul(h_pool2_flat, W_fc1) + b_fc1)

>>> W_fc2 = tf.Variable(tf.truncated_normal([1024, 10], stddev=0.1))
>>> b_fc2 = tf.Variable(tf.constant(0.1, shape=[10]))

>>> keep_prob = tf.placeholder(tf.float32)
>>> h_fc1_drop = tf.nn.dropout(h_fc1, keep_prob)
>>> y_conv = tf.matmul(h_fc1_drop, W_fc2) + b_fc2

>>> cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits_v2(labels=y_, logits=y_conv))
>>> train_step = tf.train.AdamOptimizer(1e-4).minimize(cross_entropy)
>>> correct_prediction = tf.equal(tf.argmax(y_conv, 1), tf.argmax(y_, 1))
>>> accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))

Convolutional MNIST
Last Steps Before Training

Just like the regression model, we will define error as cross entropy and count our correct predictions.

However this time we will use a sophisticated newer (2015) optimizer called ADAM. It is as simple as dropping it in.
Convolutional MNIST

Training

Train away for 20,000 steps in batches of 50. Notice how we turn the dropout off when we periodically check our accuracy.
>>> from tensorflow.examples.tutorials.mnist import input_data

>>> import tensorflow as tf

>>> mnist = input_data.read_data_sets(".", one_hot=True)

>>> x = tf.placeholder(tf.float32, [None, 784])
>>> y_ = tf.placeholder(tf.float32, [None, 10])

>>> x_image = tf.reshape(x, [-1,28,28,1])

>>> W_conv1 = tf.Variable(tf.truncated_normal([5, 5, 1, 32], stddev=0.1))
>>> b_conv1 = tf.Variable(tf.constant(0.1, shape=[32]))

>>> h_conv1 = tf.nn.relu(tf.nn.conv2d(x_image, W_conv1, strides=[1, 1, 1, 1], padding='SAME') + b_conv1)

>>> h_pool1 = tf.nn.max_pool(h_conv1, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')

>>> W_conv2 = tf.Variable(tf.truncated_normal([5, 5, 32, 64], stddev=0.1))
>>> b_conv2 = tf.Variable(tf.constant(0.1, shape=[64]))

>>> h_conv2 = tf.nn.relu(tf.nn.conv2d(h_pool1, W_conv2, strides=[1, 1, 1, 1], padding='SAME') + b_conv2)

>>> h_pool2 = tf.nn.max_pool(h_conv2, ksize=[1, 2, 2, 1], strides=[1, 2, 2, 1], padding='SAME')

>>> W_fc1 = tf.Variable(tf.truncated_normal([7 * 7 * 64, 1024], stddev=0.1))
>>> b_fc1 = tf.Variable(tf.constant(0.1, shape=[1024]))

>>> h_pool2_flat = tf.reshape(h_pool2, [-1, 7*7*64])

>>> h_fc1 = tf.nn.relu(tf.matmul(h_pool2_flat, W_fc1) + b_fc1)

>>> W_fc2 = tf.Variable(tf.truncated_normal([1024, 10], stddev=0.1))
>>> b_fc2 = tf.Variable(tf.constant(0.1, shape=[10]))

>>> keep_prob = tf.placeholder(tf.float32)

>>> h_fc1_drop = tf.nn.dropout(h_fc1, keep_prob)

>>> y_conv = tf.matmul(h_fc1_drop, W_fc2) + b_fc2

>>> cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits_v2(labels=y_, logits=y_conv))

>>> train_step = tf.train.AdamOptimizer(1e-4).minimize(cross_entropy)

>>> correct_prediction = tf.equal(tf.argmax(y_conv, 1), tf.argmax(y_, 1))

>>> accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))

>>> sess = tf.InteractiveSession()

>>> sess.run(tf.global_variables_initializer())

>>> for i in range(20000):
>>>  batch = mnist.train.next_batch(50)
>>>  if i%100 == 0:
>>>    train_accuracy = accuracy.eval(feed_dict={x:batch[0], y_: batch[1], keep_prob: 1.0})
>>>    print("step %d, training accuracy %g"%(i, train_accuracy))
>>>  train_step.run(feed_dict={x: batch[0], y_: batch[1], keep_prob: 0.5})

>>> test_accuracy 0.9915

We finally test against a whole difference set of test data (that is what mnist.test returns) and find that we are: 99.15% Accurate!
This *amazing, stunning, beautiful* demo from Adam Harley (now just across campus) is very similar to what we just did, but different enough to be interesting.

http://scs.ryerson.ca/~aharley/vis/conv/flat.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.
Style vs. Content

Deep Dream Generator

https://deepdreamgenerator.com/feed
There is a tool that allows us visualize our graph, data and performance more easily. It does require some instrumentation, but you may find it worthwhile.

Our CNN graph.

The time-varying behavior of our first convolutional filter.
Alternative Tools

There are a number of other tools to help you get a handle on your network performance. Perhaps the lightest weight method is to enable graph tracing.

```python
from tensorflow.python.client import timeline

options = tf.RunOptions(trace_level=tf.RunOptions.FULL_TRACE)
run_metadata = tf.RunMetadata()
sess.run(res, options=options, run_metadata=run_metadata)

fetched_timeline = timeline.Timeline(run_metadata.step_stats)
chrome_trace = fetched_timeline.generate_chrome_trace_format()
with open('timeline_01.json', 'w') as tracefile:
    tracefile.write(chrome_trace)
```

In a Chrome browser, go to chrome://tracing. In the upper left corner, you will find Load button. Press it and load your JSON file.

A lightweight debugger is tfdbg. To add support in our example, we simply wrap the Session object with a debugger wrapper. You can activate the tfdbg CLI with the --debug flag at the command line.

```python
from tensorflow.python import debug as tf_debug

sess = tf_debug.LocalCLIDebugWrapperSession(sess)
```
Optimization

The tools may give you some idea of where opportunities for improvement lie. There are many ways to speed up training, and the list of techniques and APIs is constantly growing. Here are a few commonly applicable techniques.

Input

The feed_dicts that we use are slow - they are actual Python. We should instead use the TensorFlow Dataset API (tf.data). This allows pipelining, aggregating from multiple files, and pre-processing. It will also offload much of this work to the CPU. Note that older versions of code may use the deprecated Queue API.

Training

There are many training optimization methods, and most of them are somewhat architecture or dataset dependent. There are some that have fairly general applicability, and which have become widely adopted. One is batch normalization.

I mentioned that normalizing an input dataset (say color balance on images) can make life easier on the network. If you think about how this helps the input layer, you might ask why we don't apply this to deeper layers. Indeed we can. The general idea is to prevent any activation from going very high or low, and the general technique is to track and apply a mean and standard deviation adjustment at each layer (keep the mean activation close to 0 and the activation standard deviation close to 1). It can be as simple as applying `tf.layers.batch_normalization()` to each layer's output (before the activation).
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.

Of course there are capabilities built into TensorFlow (and other frameworks) to enable this. For TensorFlow there is a build in Distributed TensorFlow API. It can be a little tricky, and currently has bottlenecks at very large scale.

An alternative that is both lighter-weight (in terms of code modifications) and has demonstrated very good performance on tens of thousands of GPUs is Horovod.

```
# Pin GPU to be used to process local rank (one GPU per process)
config = tf.ConfigProto()
config.gpu_options.visible_device_list = str(hvd.local_rank())

# Build model...
loss = ...
opt = tf.train.AdagradOptimizer(0.01)

# Add Horovod Distributed Optimizer
opt = hvd.DistributedOptimizer(opt)

# Add hook to broadcast variables from rank 0 to all other processes during initialization.
hooks = [hvd.BroadcastGlobalVariablesHook(0)]

# Make training operation
train_op = opt.minimize(loss)

# The MonitoredTrainingSession takes care of session initialization, restoring, etc. with
# tf.train.MonitoredTrainingSession(checkpoint_dir="/tmp/train_logs", config=config,
# hooks=hooks) as mon_sess:
while not mon_sess.should_stop():
    # Perform synchronous training.
    mon_sess.run(train_op)
```

Horovod: fast and easy distributed deep learning in TensorFlow
Alexander Sergeev, Mike Del Balso
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**
So far we have focused on images, and their classification. You know that deep learning has had success across a wide, and rapidly expanding, number of domains. Even our digit recognition task could be more sophisticated:

- **Classification** (What we did)
- **Localization** (Where is the digit?)
- **Detection** (Are there digits? How many?)
- **Segmentation** (Which pixels are the digits?)

These tasks would call for different network designs. This is where our Day 3 would begin.

Alas, we don't have a Day 3, but we can introduce you to the building blocks that enable these networks as well as those used for so many other applications.
So far, we have used Fully Connected and Convolutional layers. These are ubiquitous, but there are many others:

- Fully Connected (FC)
- Convolutional (CNN)
- Residual (ResNet) [Feed forward]
- Recurrent (RNN), [Feedback, but has vanishing gradients so...]
- Long Short Term Memory (LSTM)
- Bidirectional RNN
- Restricted Boltzmann Machine

Two of these are particularly common...
Very Effective Layers

Residual Neural Net (ResNet)
- Helps preserve reasonable gradients for very deep networks
- Very effective at imagery
- Used by AlphaGo Zero (40 residual CNN layers) in place of previous complex dual network
- 100s of layers common, Pushing 1000

Recurrent Neural Net
Wouldn't feedback help us with problems with context?

But the gradients get very small for longer memory.

Long Short Term Memory (LSTM)
- Has an actual memory cell
- And a "forget" input
- Many variants*
- *LSTM: A Search Space Odyssey (Greff, et. al.)
- Winning all the competitions.
Architectures

With these layers, we can build countless different networks (and use TensorFlow to define them). Again, this is "3rd day" material, but we present them here and you should feel competent to research them yourself.
Learning Approaches

**Supervised Learning**
- How you learned colors.
- What we have been doing just now.
- Used for: image recognition, tumor identification, segmentation.
- Requires labeled data.
- Lots of it. Augmenting helps.

**Reinforcement Learning**
- How you learned to walk.
- Requires goals (maybe long term, i.e. arbitrary delays between action and reward).
- Used for: Go (AlphaGo Zero), robot motion, video games.

**Unsupervised Learning**
- (Maybe) how you learned to see.
- What we did earlier with clustering and our recommender.
- Find patterns in data, compress data into model, find reducible representation of data.
- Used for: Learning from unlabeled data.

All of these have been done with and without deep learning. DL has moved to the forefront of all of these.
“Theoretician’s Nightmare”

That is paraphrasing Yann LeCun, the godfather of Deep Learning.

If it feels like this is an oddly empirical branch of computer science, you are spot on.

Many of these techniques were developed through experimentation, and many of them are not amenable to classical analysis. A theoretician would suggest that non-convex loss functions are at the heart of the matter, and that situation isn’t getting better as many of the latest techniques have made this much worse.

You may also have noticed that many of the techniques we have used today have very recent provenance. This is true throughout the field. Rarely is the undergraduate researcher so reliant upon results groundbreaking papers of a few years ago.

My own humble observation: Deep Learning looks a lot like late 19th century chemistry. There is a weak theoretical basis, but significant experimental breakthroughs of great utility. The lesson from that era was "expect a lot more perspiration than inspiration."
You now have a Toolbox

The reason that we have attempted this ridiculously ambitious workshop is that the field has reached a level of maturity where the tools can encapsulate much of the complexity in black boxes.

One should not be ashamed to use a well-designed black box. Indeed it would be foolish for you to write your own FFT or eigensolver math routines. Besides wasting time, you won’t reach the efficiency of a professionally tuned tool.

On the other hand, most programmers using those tools have been exposed to the basics of the theory, and could dig out their old textbook explanation of how to cook up an FFT. This provides some baseline level of judgement in using tools provided by others.

You are treading on newer ground. However this means there are still major discoveries to be made using these tools in fresh applications.

Any one particularly exciting dimension to this whole situation is that exploring hyperparameters has been very fruitful. The toolbox allows you to do just that.
Other Toolboxes
You have a plethora of alternatives available as well. You are now in a position to appreciate some comparisons.

<table>
<thead>
<tr>
<th>Package</th>
<th>Applications</th>
<th>Language</th>
<th>Strengths</th>
</tr>
</thead>
<tbody>
<tr>
<td>TensorFlow</td>
<td>Neural Nets</td>
<td>Python, C++</td>
<td>Very popular.</td>
</tr>
<tr>
<td>Caffe</td>
<td>Neural Nets</td>
<td>Python, C++</td>
<td>Many research projects and publications. 2.0 more TF-like.</td>
</tr>
<tr>
<td>Spark MLLIB</td>
<td>Classification, Regression, Clustering, etc.</td>
<td>Python, Scala, Java, R</td>
<td>Very scalable. Widely used in serious applications. Lots of plugins to DL frameworks: TensorFrames, TF on Spark, CaffeOnSpark, Keras Elephas.</td>
</tr>
<tr>
<td>Scikit-Learn</td>
<td>Classification, Regression, Clustering</td>
<td>Python</td>
<td></td>
</tr>
<tr>
<td>cuDNN</td>
<td>Neural Nets</td>
<td>C++, GPU-based</td>
<td>Used in many other frameworks: TF, Caffe, etc.</td>
</tr>
<tr>
<td>Theano</td>
<td>Neural Nets</td>
<td>Python</td>
<td>Lower level numerical routines. NumPy-esque.</td>
</tr>
<tr>
<td>Torch / PyTorch</td>
<td>Neural Nets</td>
<td>Lua (PyTorch=Python)</td>
<td>Was dynamic graphs (now in TF), but big things coming in 1.0, like Caffe 2 merge.</td>
</tr>
<tr>
<td>Keras</td>
<td>Neural Nets</td>
<td>Python (on top of TF, Theano)</td>
<td>Higher level approach.</td>
</tr>
<tr>
<td>Digits</td>
<td>Neural Nets</td>
<td>“Caffe”, GPU-based</td>
<td>Used with other frameworks (only Caffe at moment).</td>
</tr>
</tbody>
</table>
from __future__ import print_function
import keras
from keras.datasets import mnist
from keras.models import Sequential
from keras.layers import Dense, Dropout, Flatten, Conv2D, MaxPooling2D
from keras import backend as K

batch_size = 128
num_classes = 10
epochs = 12

# input image dimensions
img_rows, img_cols = 28, 28

# the data, split between train and test sets
(x_train, y_train), (x_test, y_test) = mnist.load_data()

if K.image_data_format() == 'channels_first':
    x_train = x_train.reshape(x_train.shape[0], 1, img_rows, img_cols)
    x_test = x_test.reshape(x_test.shape[0], 1, img_rows, img_cols)
    input_shape = (1, img_rows, img_cols)
else:
    x_train = x_train.reshape(x_train.shape[0], img_rows, img_cols, 1)
    x_test = x_test.reshape(x_test.shape[0], img_rows, img_cols, 1)
    input_shape = (img_rows, img_cols, 1)

x_train = x_train.astype('float32')
x_test = x_test.astype('float32')
x_train /= 255
x_test /= 255

# convert class vectors to binary class matrices
y_train = keras.utils.to_categorical(y_train, num_classes)
y_test = keras.utils.to_categorical(y_test, num_classes)

model = Sequential()
model.add(Conv2D(32, kernel_size=(3, 3), activation='relu', input_shape=input_shape))
model.add(Conv2D(64, (3, 3), activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Dropout(0.25))
model.add(Flatten())
model.add(Dense(128, activation='relu'))
model.add(Dense(num_classes, activation='softmax'))
model.compile(loss=keras.losses.categorical_crossentropy, optimizer=keras.optimizers.Adadelta(), metrics=['accuracy'])

model.fit(x_train, y_train, batch_size=batch_size, epochs=epochs, verbose=1, validation_data=(x_test, y_test))
score = model.evaluate(x_test, y_test, verbose=0)
print('Test loss:', score[0])
print('Test accuracy:', score[1])

Slightly smaller than our network, but same idea.
From https://github.com/keras-team/keras/blob/master/examples/mnist_cnn.py
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.

CIFAR
The CIFAR-10 dataset consists of 60,000 32x32 color images in 10 classes (airplane, auto, bird, cat, dog, ship, etc.) with 6,000 images per class. There are 50,000 training images and 10,000 test images.

ImageNet
150,000 photographs, collected from flickr and other search engines, hand labeled with the presence or absence of 1000 object categories. Competition: http://image-net.org/challenges/LSVRC/2017/

Kaggle Challenge
Many datasets of great diversity (crime, plants, sports, stocks, etc). https://www.kaggle.com/datasets
There are always multiple currently running competitions you can enter. Competitions: https://www.kaggle.com/competitions

Officially ended in 2017
Because of victory!
Demos

Ray-traced videogames soon? Recurrent CNN.

Demos

Style vs. Content: A little more subtle

Grab it at https://github.com/NVIDIA/FastPhotoStyle
Model-Free Prediction of Large Spatiotemporally Chaotic Systems from Data: A Reservoir Computing Approach

Jaideep Pathak, Brian Hunt, Michelle Girvan, Zhixin Lu, and Edward Ott

Phys. Rev. Lett. 120, 024102 – Published 12 January 2018
This talk has benefited from the generous use of materials from NVIDIA and Christopher Olah in particular.

The NVIDIA materials were drawn from their excellent Deep Learning Institute

https://developer.nvidia.com/teaching-kits

Christopher Olah’s blog is insightful and not to be missed if you are interested in this field.

http://colah.github.io/

Juergen Schmidhuber, one of the giants in the field, has written the definitive summary (up through 2014) of the deep learning history and landscape:

Deep Learning in Neural Networks: An Overview

Other materials used as credited.
Any code examples used were substantially modified from the original.
Anything not otherwise mentioned follows Apache License 2.0.