STATS 507
Data Analysis in Python

Lecture 25: TensorFlow II

TensorFlow

Previous lecture: Introduction to TensorFlow

- `tf.Tensor` objects represent tensors
- Tensors are combined into a computational graph
  - Captures the computational operations to be carried out at runtime

This lecture: Advanced TF

- More detail on the computational graph and `tf.Tensor` objects
- **Lab:** recognizing MNIST handwritten digits

Recall: TensorFlow as DataFlow

Computational graph: how data “flows” through program

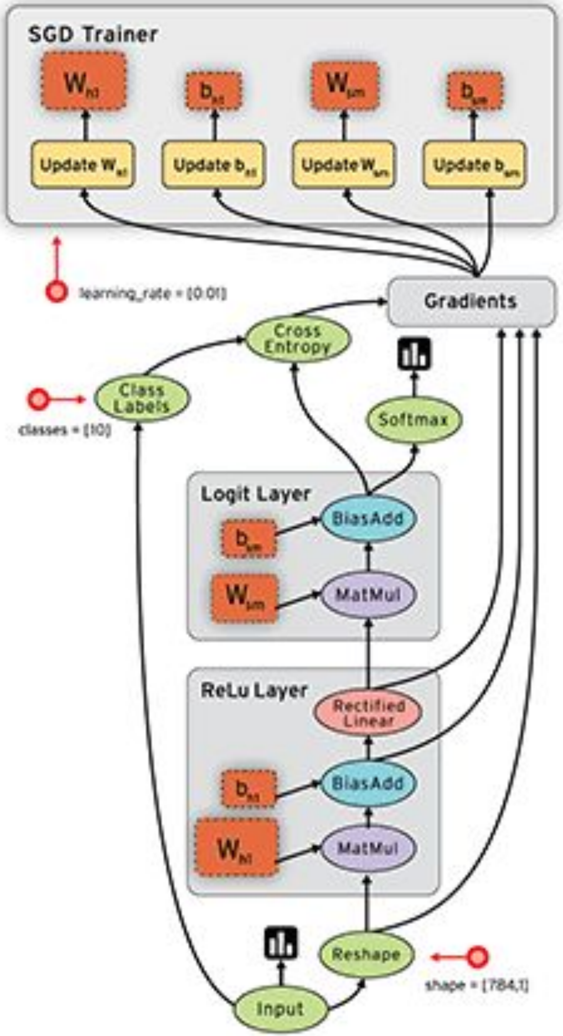
In previous lecture:

We were a bit fast and loose with nodes and edges

Strictly speaking:

Nodes are operations (`tf.Operation`)

Edges are tensors (`tf.Tensor`)



More on the Computational Graph

`tf.Graph`

Special class provided by TF to represent a computational graph

Contains `tf.Operation` objects and `tf.Tensor` objects

...and keeps track of how they interact (i.e., the graph structure itself)

When you define tensors in TF, a graph is built for you automatically

Called the **default graph**

At all times, *some* graph is the default graph

Call `tf.get_default_graph()` to access it

More: https://www.tensorflow.org/versions/r1.14/api_docs/python/tf/Graph

More on the Computational Graph

`tf.Tensor`

(Already familiar to you)

Represents a tensor, i.e., data on which to perform computations

`tf.Operation`

TF class that represents a computation performed on zero or more tensors

Also a node in a computational graph

Tensor operations

Previous lecture: we saw different ways of creating tensors…

...but not much in the way of how to do things with them.

Example functions available in TF:

`tf.abs(...)`: computes absolute value of a tensor

`tf.add_n(...)`: adds two or more tensors, element-wise

`tf.cholesky(...)`: computes Cholesky decomposition

https://en.wikipedia.org/wiki/Cholesky_decomposition

`tf.exp(...)`: computes exponential, element-wise

`tf.less(...)`: evaluates x < y, element-wise

`tf.sigmoid(...)`: computes sigmoid function element-wise

https://en.wikipedia.org/wiki/Sigmoid_function

Tensor operations: +,-,*,/

```
import tensorflow as tf
sess = tf.Session()

a = tf.constant(5, dtype=tf.float32)
b = tf.constant(3.1415, dtype=tf.float32)
c = tf.constant(2, dtype=tf.float32)
x = tf.placeholder(tf.float32)
y = tf.placeholder(tf.float32)
z = tf.placeholder(tf.float32)
ans = x/a + b*y - c*z

print(sess.run(ans, {x: [4,3,2,1], y: [2,3,4,5], z: [1,1,2,2]}))
sess.close()
```

```
[  5.08300018   8.02449989   8.9659996   11.90750027]
```

`+,-,*,/` short for `tf.add()`, `tf.subtract()`, `tf.multiply()`, `tf.divide()`, respectively.

```
sess = tf.Session()
divbyzero = x/y
print(sess.run(divbyzero, {x:1, y:0}))
```

```
inf
```

Note: Division by zero results in `inf`, rather than `nan`.

Matrix multiplication in TF: `tf.matmul()`

```
sess = tf.Session()
M = tf.constant([[1,0,1],[0,1,1],[1,1,0]], dtype=tf.float32)
oneThruNine = tf.constant([[1,2,3],[4,5,6],[7,8,9]], dtype=tf.float32)
c = tf.matmul(oneThruNine, M)
with sess.as_default():
    print(c.eval())
```

```
[[  4.   5.   3.]
 [ 10.  11.   9.]
 [ 16.  17.  15.]]
```

`tf.matmul(A,B)` multiplies tensors `A` and `B`, as matrices, provided their ranks and types agree.

```
M1 = tf.constant([[1,0,1],[0,1,1]], dtype=tf.float32)
M2 = tf.constant([[1,0,1,1],[0,0,1,1]], dtype=tf.float32)
R = tf.matmul(M1,M2)
```

```
---------------------------------------------------------------------------
ValueError                                Traceback (most recent call last)
<ipython-input-88-73edd2aef228> in <module>()
```

...

```
661     if missing_shape_fn:
```

```
ValueError: Dimensions must be equal, but are 3 and 2 for 'MatMul_13' (op: 'MatMul') with input shapes: [2,3], [2,4].
```

Matrix multiplication in TF: `tf.matmul()`

```
sess = tf.Session()
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    print(c.eval())
```

```
[[  4.   5.   3.]
 [ 10.  11.   9.]
 [ 16.  17.  15.]]
```

`tf.matmul(A,B)` multiplies tensors `A` and `B`, as matrices, provided their ranks and types agree.

```
M1 = tf.constant([[1,0,1],[0,1,1]], dtype=tf.float32)
M2 = tf.constant([[1,0,1,1],[0,0,1,1]], dtype=tf.float32)
R = tf.matmul(M1,M2)
```

```
-------------------------
ValueError
<ipython-input-88-73edd2
    ...
661    if missing_shape_fn:
```

Note: `tf.matmul()` can be used to multiply tensors of arbitrary rank. Using appropriate flags, we can transpose/adjoint the arguments as we please.
https://www.tensorflow.org/versions/r1.14/api_docs/python/tf/linalg/matmul

```
ValueError: Dimensions must be equal, but are 3 and 2 for 'MatMul_13' (op: 'MatMul') with input shapes: [2,3], [2,4].
```

More matrix operations in TF

`tf.matrix_diag`: picks out diagonal of a matrix (or other tensor)

`tf.matrix_determinant`: computes determinant of a matrix

`tf.matrix_inverse`: computes inverse of a matrix

`tf.matrix_solve`: solves Ax = b

`tf.matrix_transpose`: transposes a matrix

Element-wise operations in TF

TF element-wise operations are just like Numpy universal functions

Examples:

- `tf.abs()`: computes absolute value
- `tf.acos()`: computes arccosine
- `tf.cos()`: computes cosine
- `tf.exp()`: computes exponential
- `tf.log()`: computes logarithm
- `tf.sigmoid()`: computes sigmoid function
  https://en.wikipedia.org/wiki/Sigmoid_function

```
real = tf.constant(-5, dtype=tf.float32)
cx = tf.constant(1+1j, dtype=tf.complex64)
z = tf.abs(cx)
with sess.as_default():
    print(tf.abs(real).eval())
    print(z.eval())
```

```
5.0
1.41421
```

Element-wise comparisons in TF

TF supports element-wise comparisons of tensors

`tf.less()`, `tf.less_equal()`,

`tf.greater()`, `tf.greater_equal()`

`tf.equal()`, `tf.not_equal()`

Logical (operate on tensors with `dtype=bool`)

`tf.logical_and()`

`tf.logical_or()`

`tf.logical_xor()`

Also supported: `tf.logical_not()`, but this isn't a comparison

So, TF has a lot of stuff going on!

“low-level” TF API makes lots of powerful tools available

...almost too many!

I just wanted to train a neural net!
Why do I have to worry about all this stuff?!

Rest of Lecture: Lab

1) We'll use softmax regression to classify handwritten digits
   Using the low-level API that we discussed last lecture

2) We'll build and train a simple NN on the same data
   Also using the low-level API
   So you can see why many people just use the `tf.estimator` API!

Workshop: Recognizing MNIST Digits

MNIST is a famous computer vision data set

28-by-28 greyscale images of hand-written digits

https://en.wikipedia.org/wiki/MNIST_database

Each image is labeled according to what digit it represents

2012: 0.23 percent error rate: https://arxiv.org/abs/1202.2745

(there has probably been improvement in this number since then…)

Follow along:

https://github.com/tensorflow/docs/blob/master/site/en/r1/tutorials/estimators/cnn.ipynb

Pared-down demo code:

http://www-personal.umich.edu/~klevin/teaching/Fall2019/STATS507/tf_demo/softmax_mnist.ipynb

Image credit: Wyss, König, and Verschure (2003)

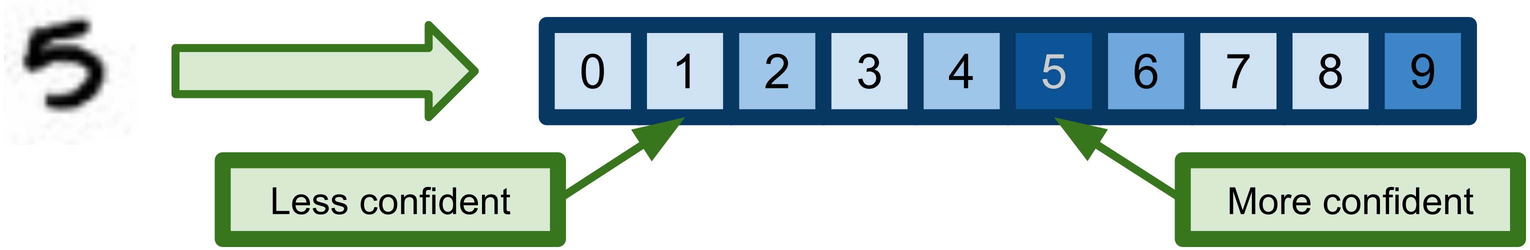
Recognizing MNIST Digits

Goal: given an image, classify what digit it represents.

= 5?
= 9?

In particular, we'll build a model that outputs a vector of probabilities

`i`-th entry of vector will be model's confidence that image is digit `i`.



Softmax Regression

Generalizes logistic regression to categorical variables with >2 values

Softmax function: $\sigma_j(z) = \frac{e^{z_j}}{\sum_i e^{z_i}}$

Probability that the observation is from category **j**

Model parameters

Our model will assign probabilities to digits as $\mathbb{P}[Y = j] = \sigma_j(WX + b)$

Observed data

More information:
https://en.wikipedia.org/wiki/Multinomial_logistic_regression
https://en.wikipedia.org/wiki/Softmax_function
C. M. Bishop (2006). *Pattern Recognition and Machine Learning*. Springer.

The Plan

Represent 28-by-28 images by flattened 784-dimensional vectors

Apply softmax regression to vectors

- Learn weights `W` and bias `b`
- Train on a training set of labeled images

Evaluate learned model on test set

Flattening the data

Images are most naturally represented as matrices...

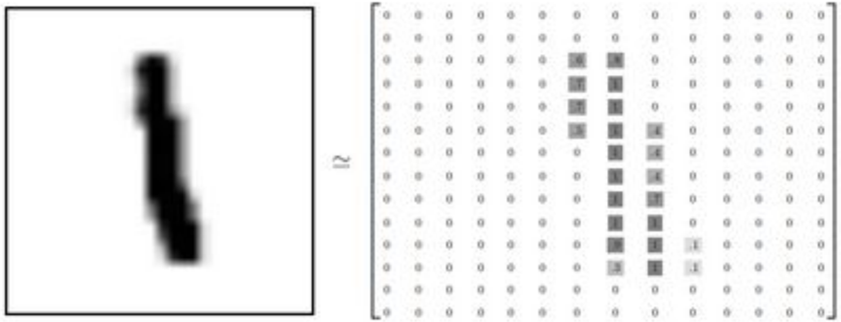


Image credit: TensorFlow tutorial

...but softmax regression requires vector inputs.

Solution: “unroll” image into a vector. It doesn’t matter how we do this, so long as we’re consistent. That is, so long as every image is flattened to a vector in the **same way**.

Building the model

```python
import tensorflow as tf
x = tf.placeholder(tf.float32, [None, 784])
W = tf.Variable(tf.zeros([784, 10]))
b = tf.Variable(tf.zeros([10]))
y = tf.nn.softmax(tf.matmul(x, W) + b)
```

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \text{softmax}\left(\begin{bmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

Image credit: TensorFlow tutorial

Building the model

```python
import tensorflow as tf
x = tf.placeholder(tf.float32, [None, 784])
W = tf.Variable(tf.zeros([784, 10]))
b = tf.Variable(tf.zeros([10]))
y = tf.nn.softmax(tf.matmul(x, W) + b)
```

Each row of `x` is going to be a single observation, each of which is 784-dimensional vector (28-by-28 image has 784 pixels), but we don't know how many rows `x` will have, yet.

`W` is a matrix of weights. We are computing `xW`, so for matrix multiplication to make sense rows of `W` must agree with columns of `x`. Our model outputs a 10-dimensional probability, so 10 columns is what we want.

Bias term is same dimension as `Wx`.

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \text{softmax}\left(\begin{bmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$

Image credit: TensorFlow tutorial

Training the model

To train our model, we need to choose a loss function

We’ll use cross-entropy: https://en.wikipedia.org/wiki/Cross_entropy

Related to the KL divergence

$$H_{y'}(y) = \sum_i y'_i \log y_i$$

Sum over digits 0 to 9

The true distribution

Our model

Training the model

To train our model, we need to choose a loss function

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Related to the KL divergence

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Sum over digits 0 to 9

The true distribution

Our model

Note: the formula above is the sum for **one** observation. Our actual loss function will be a sum of these sums: for each training example, we need to sum of over the 10 digits.

Training the model

To train our model, we need to choose a loss function

We'll use cross-entropy: https://en.wikipedia.org/wiki/Cross_entropy

Related to the KL divergence

$$H_{y'}(y) = \sum_i y'_i \log y_i$$

```
cross_entropy = tf.reduce_mean(-tf.reduce_sum(ytrue * tf.log(y), reduction_indices=[1]))
```

Training the model

To train our model, we need to choose a loss function

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"True" y

Our model

```
cross_entropy = tf.reduce_mean(-tf.reduce_sum(ytrue * tf.log(y), reduction_indices=[1]))
```

Tells TF to take the mean across the **second** axis.

Training the model

To train our model, we need to choose a loss function

We'll use cross-entropy: https://en.wikipedia.org/wiki/Cross_entropy

Related to the KL divergence

$$H_{y'}(y) = \sum_i y'_i \log y_i$$

"True" y

Our model

```
cross_entropy = tf.reduce_mean(-tf.reduce_sum(ytrue * tf.log(y), reduction_indices=[1]))
```

Note: it turns out that it's more efficient and more numerically stable to use TF built-in function for cross-entropy, but this is how we would implement it if we had to.

Tells TF to take the mean across the **second** axis.

Training the model: building more of the graph

We'll read the truth into `ytrue`. Again, we don't know how many training instances there will be.

```
ytrue = tf.placeholder(tf.float32, [None, 10])
cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits(labels=ytrue, logits=y))
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)
```

Specify the gradient descent step. This operation encodes a single gradient step in trying to minimize the cross-entropy.

Specify the **learning rate**, which controls the step size in our gradient descent algorithm.

Training the model: building more of the graph

We'll read the truth into `ytrue`. Again, we don't know how many training instances there will be.

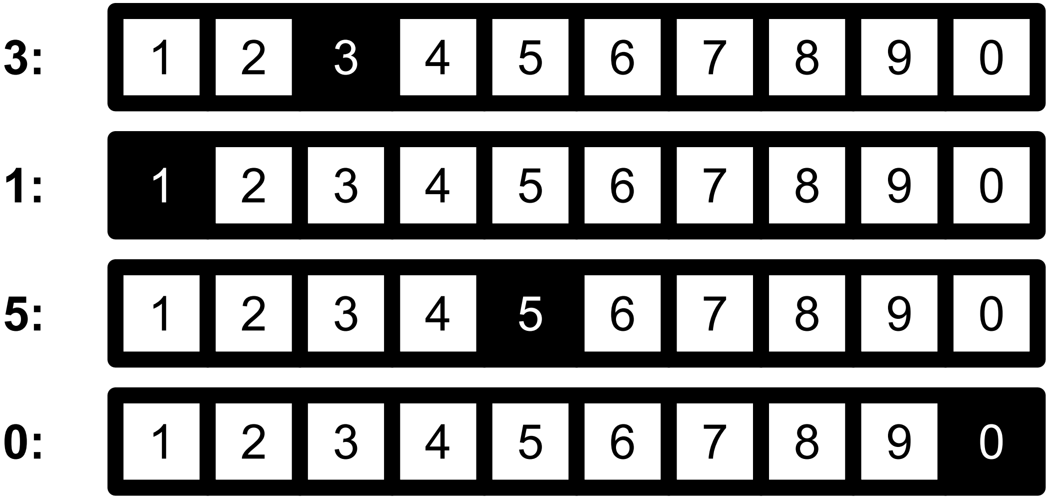
```
ytrue = tf.placeholder(tf.float32, [None, 10])
cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits(labels=ytrue, logits=y))
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)
```

Note: we are using what is called a **one-hot** encoding in the true labels `ytrue`.

Aside: one-hot encodings

In ML, it is common to represent categorical variables by vectors

- K possible values for the variable
- represent by a K-dimensional vector
- Object of k-th category represented by vector with k-th entry 1, rest 0



Aside: one-hot encodings

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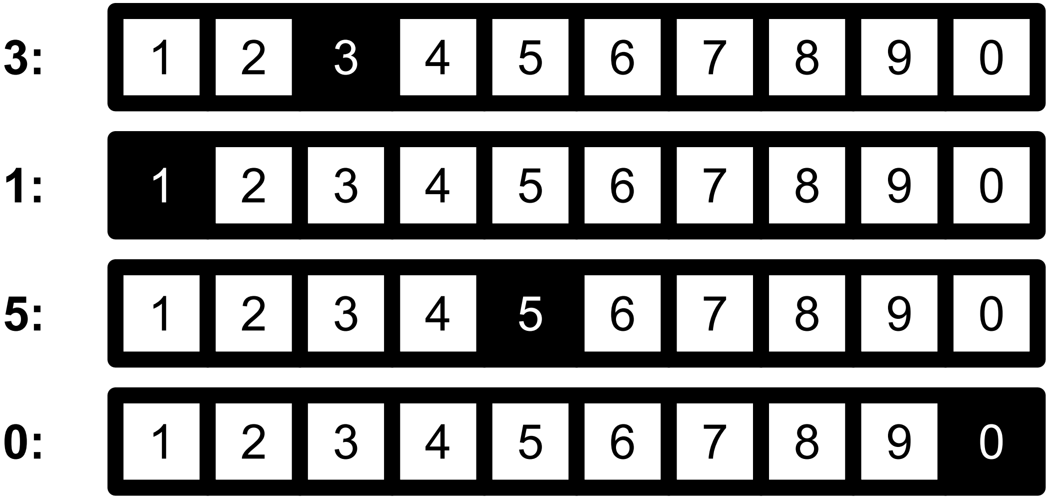


Note: this is a case where it's good to use the `tf.SparseTensor` object. If K is really big, it's expensive to store all those 0s! In our application, K=10, so it's no big deal, but in, for example, NLP, K=1e6 is not uncommon.

Training the model: building more of the graph

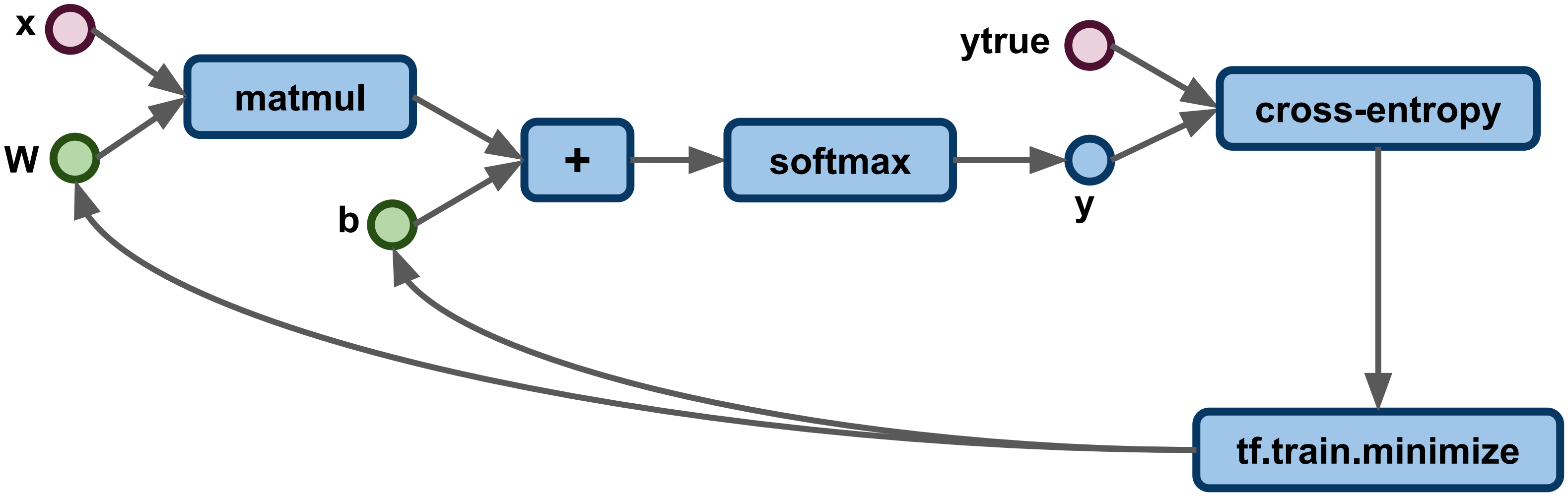
We'll read the truth into `ytrue`. Again, we don't know how many training instances there will be.

```
ytrue = tf.placeholder(tf.float32, [None, 10])
cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits(labels=ytrue, logits=y))
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)
```

Note: TensorFlow supplies a number of other optimization routines
https://www.tensorflow.org/api_guides/python/train#Optimizers

Running the Computational Graph

Here's the graph we've built, so far:



Note: this is a simplification of the graph that TF would build for you. You can view the actual graph using TensorBoard: https://github.com/tensorflow/docs/blob/master/site/en/r1/guide/graph_viz.md

Putting it all together

```
from tensorflow.examples.tutorials.mnist import input_data
data_dir = "data_dir"
mnist = input_data.read_data_sets(data_dir, one_hot=True)
```

```
Extracting data_dir/train-images-idx3-ubyte.gz
Extracting data_dir/train-labels-idx1-ubyte.gz
Extracting data_dir/t10k-images-idx3-ubyte.gz
Extracting data_dir/t10k-labels-idx1-ubyte.gz
```

```
ytrue = tf.placeholder(tf.float32, [None, 10])
cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits(labels=ytrue, logits=y))
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)
```

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

for _ in range(5000):
    batch_xs, batch_ys = mnist.train.next_batch(100)
    sess.run(train_step, feed_dict={x: batch_xs, ytrue: batch_ys})
```

Putting it all together

TF includes code for downloading MNIST data. We just need to tell it what directory to save it in.

```
from tensorflow.examples.tutorials.mnist import input_data
data_dir = "data_dir"
mnist = input_data.read_data_sets(data_dir, one_hot=True)
```

```
Extracting data_dir/train-images-idx3-ubyte.gz
Extracting data_dir/train-labels-idx1-ubyte.gz
Extracting data_dir/t10k-images-idx3-ubyte.gz
Extracting data_dir/t10k-labels-idx1-ubyte.gz
```

Build the computational graph (`x`, `y`, `W`, `b` omitted for space)

```
ytrue = tf.placeholder(tf.float32, [None, 10])
cross_entropy = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits(labels=ytrue, logits=y)
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)
```

Start session, take 5000 gradient steps. Use a **batched** approach. Each gradient step is based on a small subset of the **training data**.

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

for _ in range(5000):
    batch_xs, batch_ys = mnist.train.next_batch(100)
    sess.run(train_step, feed_dict={x: batch_xs, ytrue: batch_ys})
```

Assessing the model: test data

Once we've trained a model, how do we tell if it's good?

Use train/test split

- Data set aside ahead of time, which the model hasn't seen before
- Train on one set of data (train data), evaluate on another (test data)

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

```
0.9221
```

Now we're using the **test data** instead of the training data.

Workshop II: Better Digit Recognition with NNs

Can we do better than 92% accuracy?

One obvious flaw:

Our softmax regression doesn’t use structure of the image

How we vectorized our image didn’t matter!

Two options:

1) Write down a better model
2) Use a neural net!

Crash Course: Neural Nets

Output of unit

Activation function

Biologically-inspired computing model

Inputs processed by units ("neurons")

- Each unit outputs a function of some inputs
- Units apply linear functions to their inputs...
- ...followed by a nonlinear **activation function**

$$f(x) = K\left(\sum_i w_i g_i(x)\right)$$

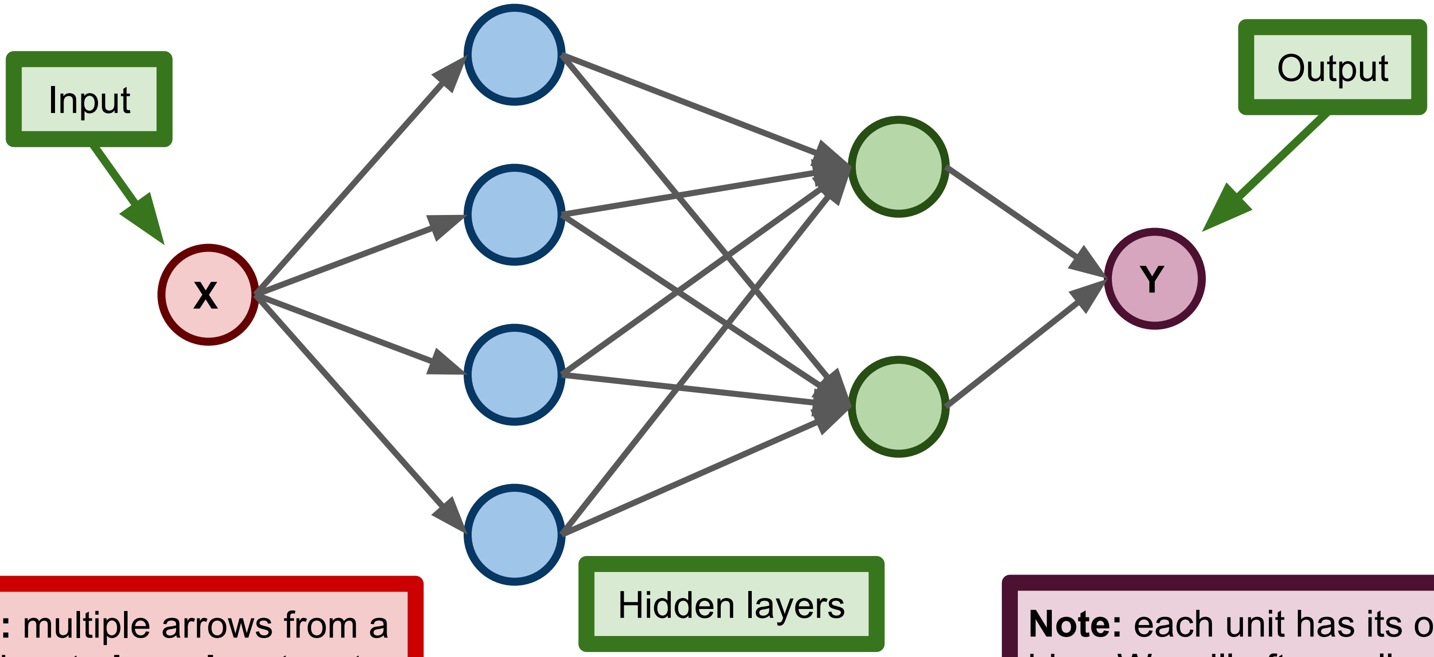
Weights

Inputs to unit

Goal: build a model that approximates some function

- **Ex:** input is an audio signal, output is a (prob. dist. over) word label
- **Ex:** input is English text, output is (prob. dist. over) French text
- **Ex:** input is an image, output is (prob. dist. over) label

Crash Course: Neural Nets



Note: multiple arrows from a unit denote **broadcast**, not different outputs.

Note: each unit has its own weight and bias. We will often collect the weights and biases from a single layer into a single tensor or pair of tensors.

Crash Course: Neural Nets

Early NNs: perceptron (Rosenblatt, 1957)

- Single-layer of computation
- Can only learn linearly separable functions
- https://en.wikipedia.org/wiki/Perceptron

$$f(x) = \begin{cases} 1 & \text{if } w \cdot x + b > 0 \\ 0 & \text{otherwise} \end{cases}$$

Multilayer perceptron (MLP)

- Multiple layers of units, can learn more complicated functions (e.g., XOR)
- https://en.wikipedia.org/wiki/Multilayer_perceptron

Feed-forward vs recurrent neural net (RNN)

- Feed-forward network is an acyclic graph
- RNN can have units whose outputs feed back to earlier units

Convolutional Neural Nets (CNNs)

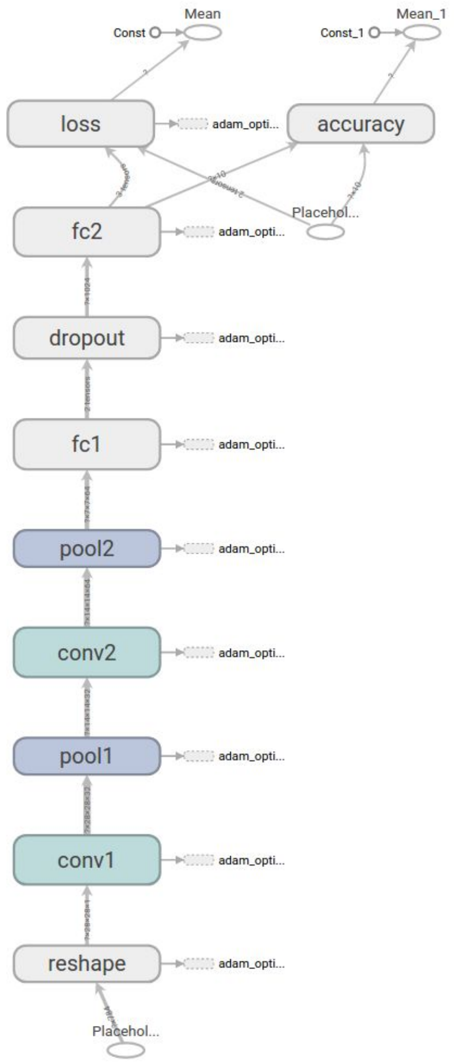
Deep (many layers)

Feed-forward (NN connections are acyclic)

Three basic types of layers:

- Convolutional
- Pooling
- Fully connected

Dropout “layer” provides regularization



Convolution

(Based on) an operation from signal processing

Roughly speaking, convolution computes response of a system to an input

https://en.wikipedia.org/wiki/Convolution

Typical NNs: units apply matrix multiplication followed by nonlinearity

CNN: units apply convolution instead of matrix multiplication

Still a linear operation

In image processing, units apply convolution to their **receptive fields**

Biologically inspired: e.g., neurons in visual cortex respond selectively

https://en.wikipedia.org/wiki/Receptive_field

Pooling

Typical setup: pass output of one unit to next layer

Pooling replaces this with a **summary statistic**

- Input to next layer is a function of several units from previous layer
- Example: pool adjacent pixels in an image

Common pooling operations:

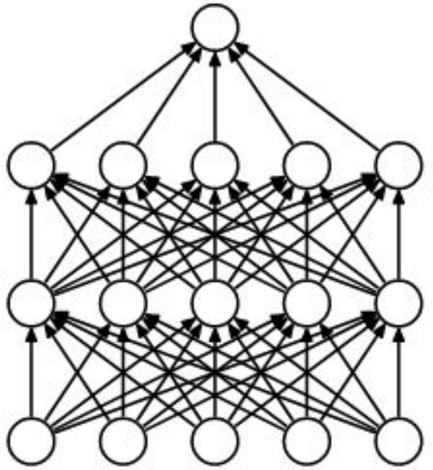
- Max pooling: report maximum value over the outputs
- (weighted) average: take weighted average over the outputs
  - Weighted according to, e.g., distance from center of receptive field

Dropout

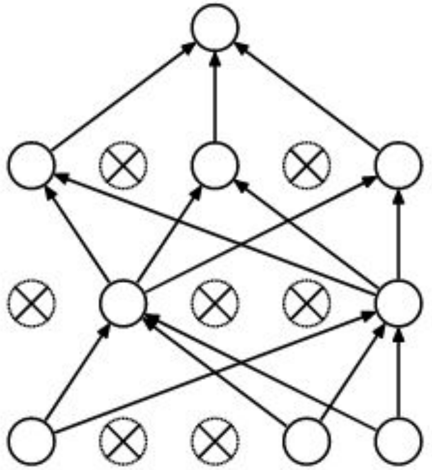
Common technique for regularization (avoiding overfitting)

At each training step, randomly choose some units to drop

- These units do not contribute to the network computation
- Forces other weights to “compensate”, introduces redundancy across units



(a) Standard Neural Net



(b) After applying dropout.

Image credit: Srivastava, et al (2014)
This is the paper in which dropout was initially suggested.
https://www.cs.toronto.edu/~hinton/absps/JMLRdropout.pdf

Building the Neural Net

Four layers
- Two convolutional layers
- Two fully-connected layers
- Dropout between FC layers

Nonlinearity: We'll use Rectified Linear Unit (RELU)
https://en.wikipedia.org/wiki/Rectifier_(neural_networks)

Pooling: max-pooling over 2-by-2 squares

Jupyter notebook:
http://www-personal.umich.edu/~klevin/teaching/Fall2019/STATS507/tf_demo/cnn_mnist.ipynb