STAT679
Computing for Data Science and Statistics

Lecture 19: TensorFlow, continued

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

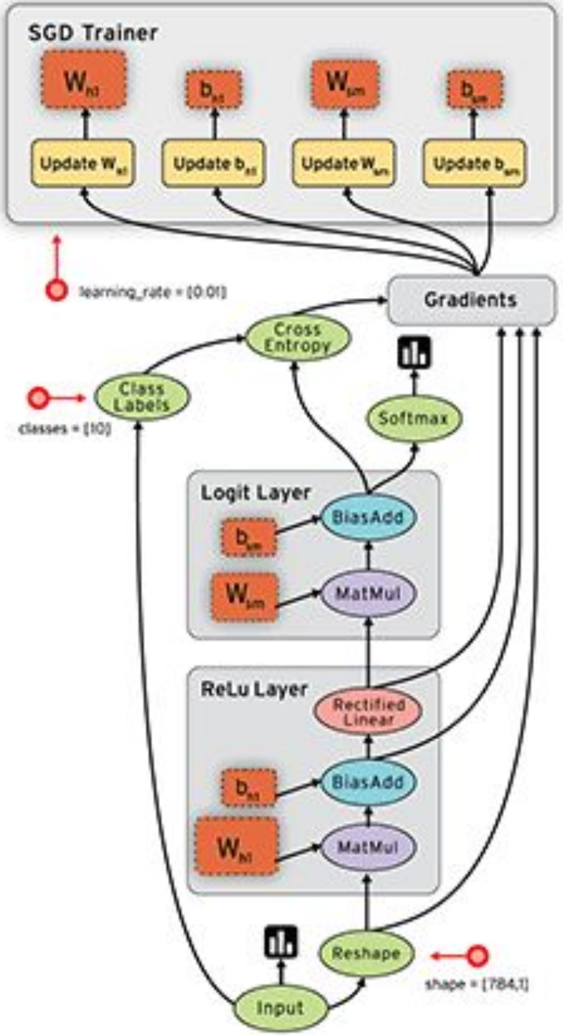
In previous lecture:

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)

As of TF version 2, working with `tf.Graph` directly is deprecated

Instead we use `tf.function` objects

But there is still a `tf.Graph` object lurking behind the scenes!

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

https://www.tensorflow.org/api_docs/python/tf/function

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

Encoded as 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:

Math operations (trigonometric functions, special functions, logicals)

Matrix operations (matrix-vector multiplication, decompositions)

Reduce operations (e.g., summing or taking the mean along an axis)

Tensor operations: +,-,*,/

```python
import tensorflow as tf

a = tf.constant(5, dtype=tf.float32)
b = tf.constant(3.1415, dtype=tf.float32)
c = tf.constant(2, dtype=tf.float32)

def silly_pyfunction(x,y,z):
    return x/a + b*y - c*z
silly = tf.function(silly_pyfunction)

print(silly([4,3,2,1], [2,3,4,5], [1,1,2,2]))
```

```
tf.Tensor([ 5.083   8.0245  8.966  11.9075], shape=(4,), dtype=float32)
```

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

```python
x = tf.constant(1, dtype=tf.float32)
y = tf.constant(0, dtype=tf.float32)
x/y
```

```
<tf.Tensor: shape=(), dtype=float32, numpy=inf>
```

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

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

```
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)
print( c.numpy() )
```

```
[[ 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)
```

```
---------------------------------------------------------------------------
InvalidArgumentError                      Traceback (most recent call last)
<ipython-input-9-715b0435c363> in <module>
      1 M1 = tf.constant([[1,0,1],[0,1,1]], dtype=tf.float32)
      2 M2 = tf.constant([[1,0,1,1],[0,0,1,1]], dtype=tf.float32)
----> 3 R = tf.matmul(M1,M2)
        ...

~/.local/lib/python3.8/site-packages/six.py in raise_from(value, from_value)

InvalidArgumentError: Matrix size-incompatible: In[0]: [2,3], In[1]: [2,4] [Op:MatMul]
```

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

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```

```
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      ...

~/.local/lib/python3.8/site-pac

InvalidArgumentError: Matrix size-incompatible: In[0]: [2,3], In[1]: [2,4] [Op:MatMul]
```

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/api_docs/python/tf/linalg/matmul

More matrix operations in TF: `tf.linalg`

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

`tf.linalg.det`: computes determinant of a matrix

`tf.linalg.inv`: computes inverse of a matrix

`tf.linalg.solve`: solves Ax = b

`tf.linalg.matrix_transpose`: transposes a matrix

`tf.linalg.cholesky(...)`: computes Cholesky decomposition
https://en.wikipedia.org/wiki/Cholesky_decomposition

Element-wise operations in TF

TF element-wise operations are just like Numpy universal functions

Examples:

`tf.math.abs()`: computes absolute value

`tf.math.acos()`: computes arccosine

`tf.math.cos()`: computes cosine

`tf.math.exp()`: computes exponential

`tf.math.log()`: computes logarithm

`tf.math.sigmoid()`: computes sigmoid function

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

```python
r = tf.constant(-5, dtype=tf.float32)
c = tf.constant(1+1j, dtype=tf.complex64)

print( tf.math.abs(r) )
print( tf.math.abs(c) )
```

```
tf.Tensor(5.0, shape=(), dtype=float32)
tf.Tensor(1.4142135, shape=(), dtype=float32)
```

Element-wise comparisons in TF

TF supports element-wise comparisons of tensors

`tf.math.less()`, `tf.math.less_equal()`,
`tf.math.greater()`, `tf.math.greater_equal()`
`tf.math.equal()`, `tf.math.not_equal()`

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

`tf.math.logical_and()`
`tf.math.logical_or()`
`tf.math.logical_xor()`
Also supported: `tf.math.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 convolutional NN on the same data
   Using the `tf.keras` API, which hides much of the low-level operations

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…)

Pared-down demo code:

http://pages.stat.wisc.edu/~kdlevin/teaching/Spring2021/STAT679/democode/softmax_mnist_demo.ipynb

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

Recognizing MNIST Digits

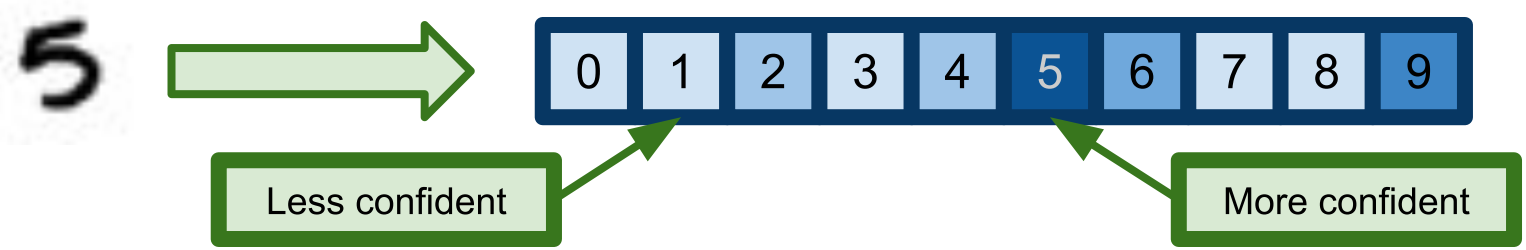
Goal: given an image, classify what digit it represents.

= 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: $\sigma_j(z) = \dfrac{e^{z_j}}{\sum_i e^{z_i}}$

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...

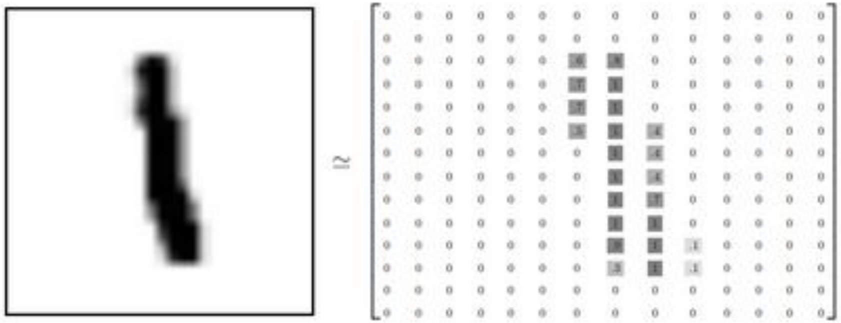


Image credit: TensorFlow tutorial

...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

```
class SoftmaxModel(tf.Module):
    def __init__(self, d_data, d_class):
        super().__init__()
        self.W = tf.Variable(tf.random.normal(shape=[d_class,d_data]), dtype=tf.float32)
        self.b = tf.Variable(tf.random.normal(shape=[d_class]), dtype=tf.float32)
    def __call__(self, x):
        z = tf.linalg.matvec( self.W, x) + self.b
        return tf.nn.softmax( z )

classifier = SoftmaxModel( 784, 10 )
```

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

Image credit: TensorFlow v1 tutorial

Building the model

Our model outputs a 10-dimensional probability. So `W` should map a vector to a 10-vector.

```python
class SoftmaxModel(tf.Module):
    def __init__(self, d_data, d_class):
        super().__init__()
        self.W = tf.Variable(tf.random.normal(shape=[d_class,d_data]), dtype=tf.float32)
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    def __call__(self, x):
        z = tf.linalg.matvec( self.W, x) + self.b
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classifier = SoftmaxModel( 784, 10 )
```

Bias term is same dimension as `Wx`.

Each row of `x` is going to be a single observation, a 784-dimensional vector (28-by-28 image has 784 pixels).

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

Image credit: TensorFlow v1 tutorial

Training the model: choosing a loss function

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

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Sum over digits 0 to 9

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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: building more of the graph

We'll read the truth into `ytrue`, while `y_pred` will be our model's predicted labels.

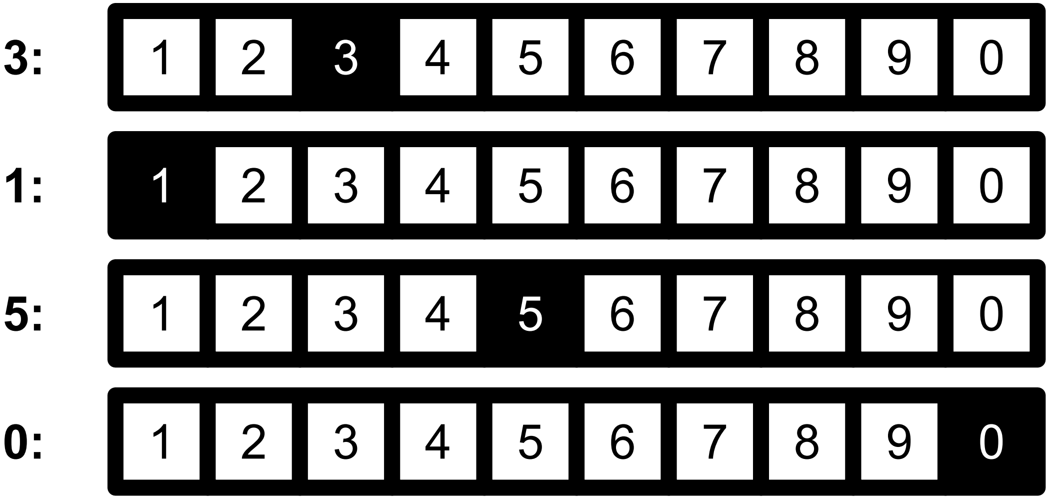
```
def crossent_loss(y_true, y_pred):
    crossents = tf.keras.losses.categorical_crossentropy(y_true, y_pred)
    return tf.reduce_mean( crossents )
```

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



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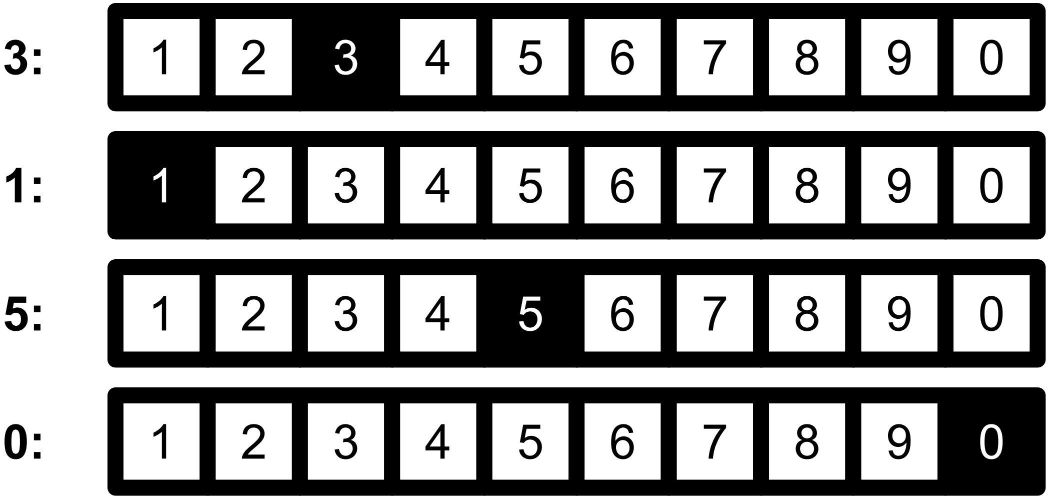

Note: this is a case where it's good to use the `tf.SparseTensor` object. If K is really big, it's expensive to store all those 0s! In our application, K=10, so it's no big deal, but in, for example, NLP, K=1e6 is not uncommon.

Training the model

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

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

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    return tf.reduce_mean( crossents )
```

Training the model

Take the gradient of the loss with respect to the model parameters, update accordingly. This pattern should look familiar from the previous lecture.

```
def train(model, images, labels, learning_rate):

    with tf.GradientTape() as t:
        current_loss = crossent_loss(labels, model(images))

    dW, db = t.gradient(current_loss, [model.W, model.b])

    model.W.assign_sub(learning_rate * dW)
    model.b.assign_sub(learning_rate * db)
```

```
def training_loop(model, x, y, epochs=1):
    for e in range(epochs):
        ds = tf.data.Dataset.from_tensor_slices( (x, y) )
        ds = ds.shuffle( x.shape[0] ).batch(100)
        for (xbatch,ybatch) in ds:
            train(model, xbatch, ybatch, learning_rate=0.5)
    predicted = model(x)
    train_loss = crossent_loss(y, predicted)
    train_acc = accuracy( y, predicted )
    print("Final state: train_loss=%2.5f, train_acc=%2.5f" %
                  (train_loss, train_acc) )
```

Training the model

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    print("Final state: train_loss=%2.5f, train_acc=%2.5f" %
                (train_loss, train_acc) )
```

The `tf.data.Dataset` object provides tools for working with data, including shuffling and batching.

Instead of evaluating the loss on all 60K training elements for every gradient step, we are using a small subset of the data (called a **batch**).

More information: https://www.tensorflow.org/api_docs/python/tf/data/Dataset

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    dW, db = t.gradient(current_loss, [model.W, model.b])

    model.W.assign_sub(learning_rate * dW)
    model.b.assign_sub(learning_rate * db)
```

Iterate over all of the batches. Each is a set of 100 (image,label) pairs.

```python
def training_loop(model, x, y, epochs=1):
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            train(model, xbatch, ybatch, learning_rate=0.5)
    predicted = model(x)
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    train_acc = accuracy( y, predicted )
    print("Final state: train_loss=%2.5f, train_acc=%2.5f" %
                (train_loss, train_acc) )
```

Each “epoch”, we will go through the dataset once.

Instead of evaluating the loss on all 60K training elements for every gradient step, we are using a small subset of the data (called a **batch**).

More information: https://www.tensorflow.org/api_docs/python/tf/data/Dataset

Training the model

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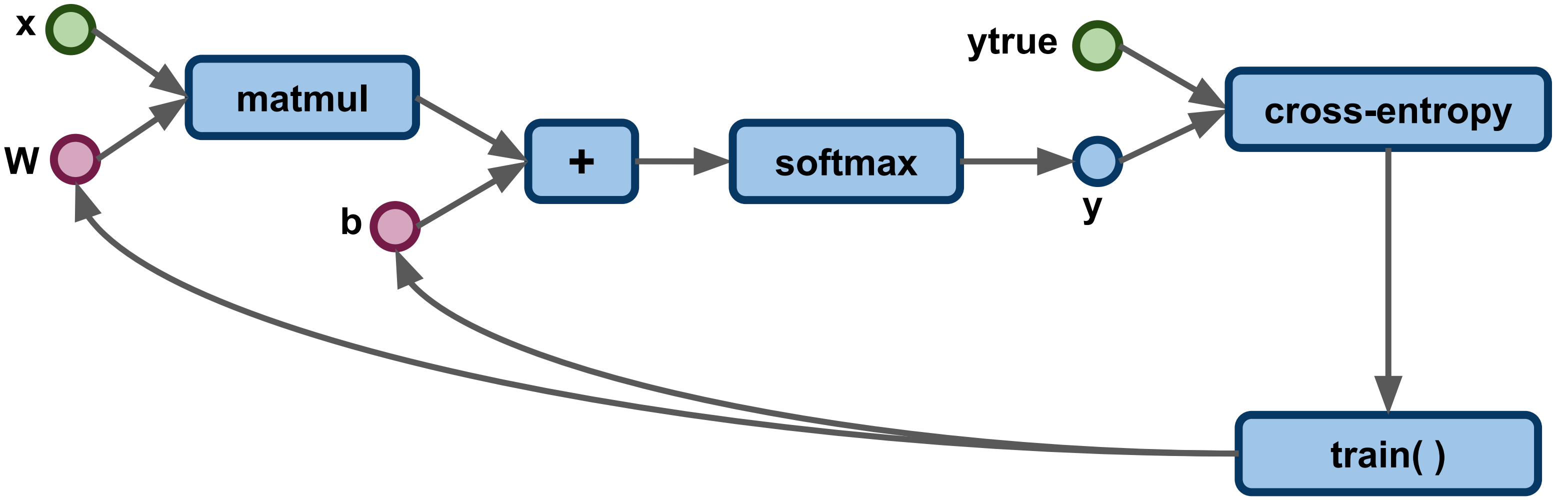
    predicted = model(x)
    train_loss = crossent_loss(y, predicted)
    train_acc = accuracy( y, predicted )
    print("Final state: train_loss=%2.5f, train_acc=%2.5f" %
                  (train_loss, train_acc) )
```

Print out the model accuracy and the loss, evaluated on the input data.

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://www.tensorflow.org/tensorboard/graphs

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)

What fraction of the labels did we get right?

```
def accuracy( y_true, y_pred ):
    hits = tf.math.equal( tf.math.argmax(y_true,1), tf.math.argmax(y_pred,1) )
    hits = tf.cast( hits, dtype=tf.float32 )
    return tf.reduce_mean( hits )
```

To "undo" the one-hot encoding, we take the argmax.

Putting it all together

TF includes the MNIST data. We just need to load it, rescale it and flatten the images using `tf.reshape`

```
mnist = tf.keras.datasets.mnist

(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0
```

TF MNIST pixels are integers 0 to 255. Rescale to be in [0,1]

```
train_shape = x_train.shape
x_train = tf.reshape( x_train, [train_shape[0], 28*28] )
test_shape = x_test.shape
x_test = tf.reshape( x_test, [test_shape[0], 28*28] )
```

Reshape the data so that each 28-by-28 image is now a 784-dimensional vector.

```
classifier =  SoftmaxModel( 784, 10 )
training_loop( classifier, x_train, y_train, 20 )
```

```
Final state: train_loss=0.29206, train_acc=0.92160
```

```
accuracy( y_test, classifier(x_test))
```

```
<tf.Tensor: shape=(), dtype=float32, numpy=0.913>
```

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(x_train, y_train), (x_test, y_test) = mnist.load_data()
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```
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test_shape = x_test.shape
x_test = tf.reshape( x_test, [test_shape[0], 28*28] )
```

```
classifier =  SoftmaxModel( 784, 10 )
training_loop( classifier, x_train, y_train, 20 )
```

```
Final state: train_loss=0.29206, train_acc=0.92160
```

```
accuracy( y_test, classifier(x_test))
```

```
<tf.Tensor: shape=(), dtype=float32, numpy=0.913>
```

Initialize the softmax classifier and fit it to the training data.

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

Putting it all together

```
mnist = tf.keras.datasets.mnist

(x_train, y_train), (x_test, y_test) = mnist.load_data()
x_train, x_test = x_train / 255.0, x_test / 255.0
```

```
train_shape = x_train.shape
x_train = tf.reshape( x_train, [train_shape[0], 28*28] )
test_shape = x_test.shape
x_test = tf.reshape( x_test, [test_shape[0], 28*28] )
```

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```

```
accuracy( y_test, classifier(x_test))
```

```
<tf.Tensor: shape=(), dtype=float32, numpy=0.913>
```

Accuracy on test data is a bit worse than train. This is normal. We fit the model to the train data. On the other hand, the model has never seen the test data before.

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

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**

Output of unit

Activation function

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

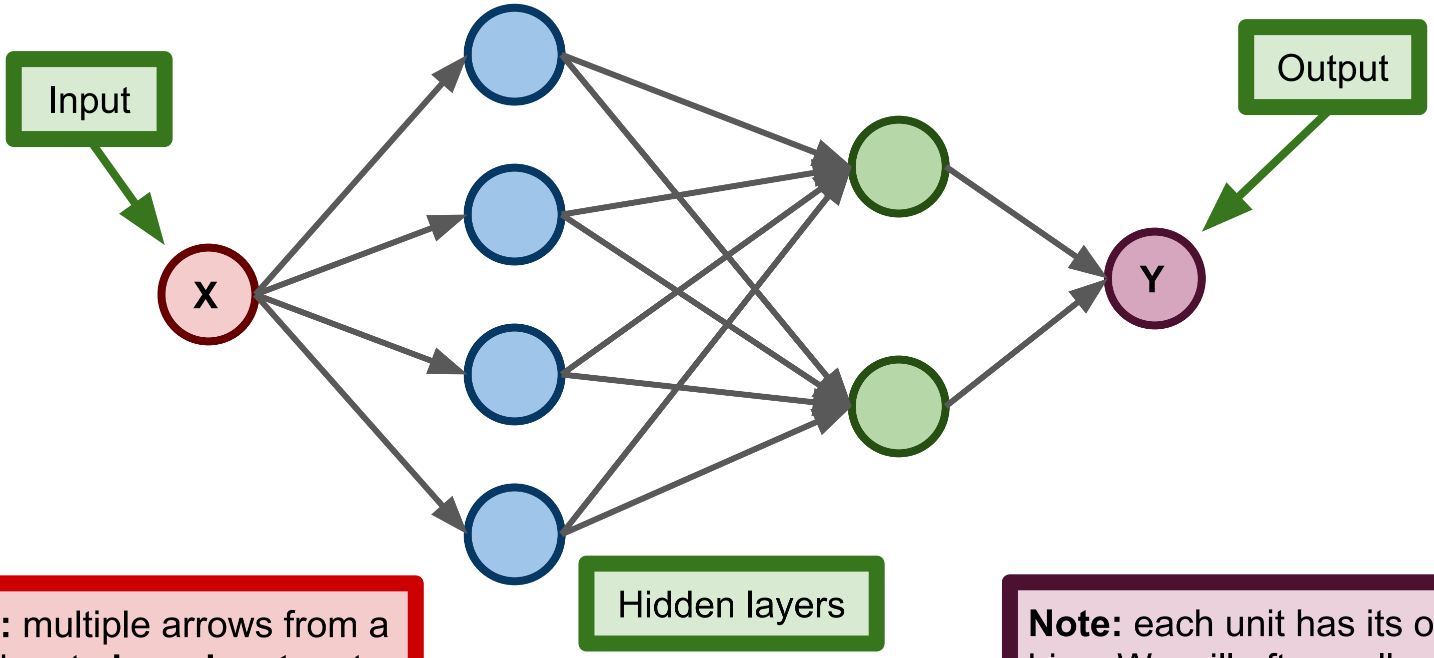
Weights

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)

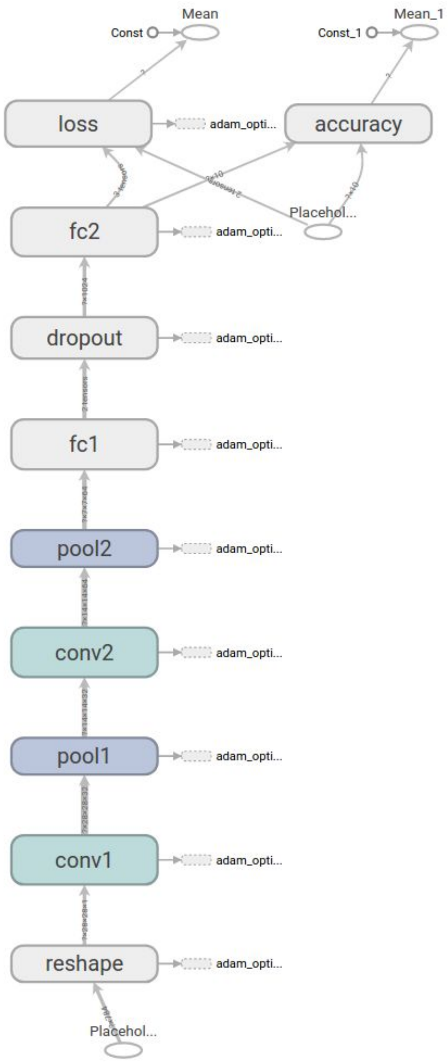
Deep (many layers)

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

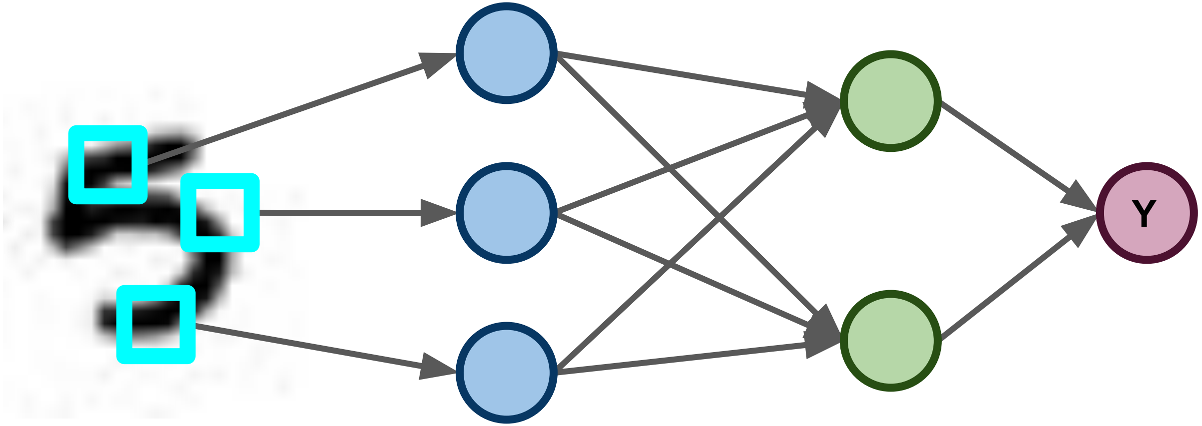
Still a linear operation

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

Convolution: receptive fields



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:

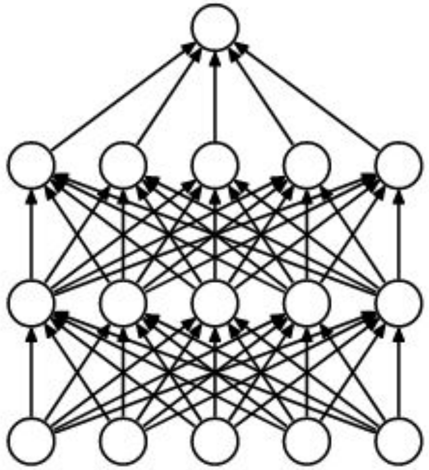
- Max pooling: report maximum value over the outputs
- (weighted) average: take weighted average over the outputs
  - Weighted according to, e.g., distance from center of receptive field

Dropout

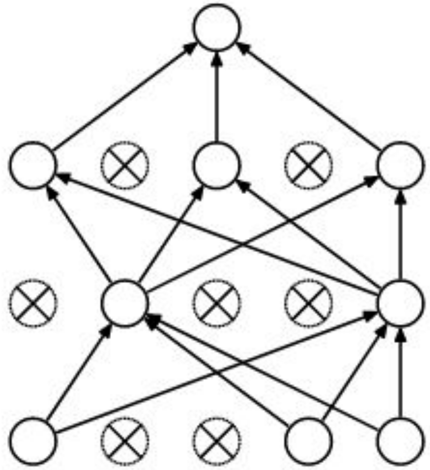
Common technique for regularization (avoiding overfitting)

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

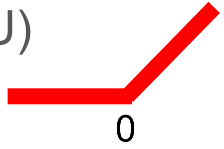
Building the Neural Net

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://pages.stat.wisc.edu/~kdlevin/teaching/Spring2021/STAT679/democode/cnn_mnist_demo.ipynb