Neural network programming: NN frameworks

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You can get the code and slides for today's class at the SciNet Education web page.

`https://support.scinet.utoronto.ca/education`

Click on the link for the class, and look under "File Storage" and find the file "frameworks.pdf".

This class will cover the following topics:

- Review some of the available neural network frameworks.
- Redo the MNIST example using Keras.
- Introduce Keras' functional syntax.

We will be using Keras for the rest of the course. You will need to get it installed. If you have problems, let me know.

A review of last class

Recall what we did last class.

- We built a neural network, consisting of three layers: an input layer, a single hidden layer, and an output layer.

- We defined a cost function, which measured the inaccuracy of the neural network's predictions.

- We used backpropagation to calculate the derivatives of the cost function with respect to the weights and biases.

- Using gradient descent, we trained the network to identify images from the MNIST data set.

However, we built all the parts of the network by hand. There are better ways to do this.

Neural network frameworks

Now that we have a sense of how neural networks work, we're ready to switch gears and use a 'framework'. Why would we do that?

- Coding your own networks from scratch can be a bit of work. (Though it's easier and cleaner if you use classes.)
- Neural network (NN) frameworks have been specifically designed to solve NN problems.
- Python, of course, is not a high-performance language.
- The neural networks which are built using frameworks are compiled before being used, thus being much faster than Python.
- The NN frameworks are also designed to use GPUs, which make things significantly faster than just using CPUs.

The training of neural networks is particularly well suited to GPUs.

Theano

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Let's review several of the more-popular NN frameworks out there. First is the Theano programming package.

- Theano is not strictly a NN framework. It was designed to handle multi-dimensional array manipulation.
- Developed by the LISA/MILA lab at the Université de Montréal.
- Written in Python; uses a numpy-like syntax, but generates C code which is compiled before being used.
- Supports symbolic differentiation.
- Is the grand-daddy of NN programming approaches.
- No longer under development.

Though previously commonly used in NN programming, it's essentially no longer used since it is no longer being developed.

TensorFlow

TensorFlow is Google's NN framework.

- Released as open source in November 2015.
- The second-generation machine-learning framework developed internally at Google, successor to DistBelief.
- More flexible than some other neural network frameworks.
- Capable of running on multiple cores and GPUs.
- Provides APIs for Python, C++, Java and other languages.
- Can be a bit of challenge to learn (many ways to do the same thing).
- With Tensorflow 2.0, Keras has become the main API.

This framework is popular, though not necessarily the fastest.

Caffe was developed as part of a Ph.D. project at U.C. Berkeley.

- Stands for Convolutional Architecture for Fast Feature Embedding.

- Currently maintained by the Berkeley Vision and Learning Center.

- Written in C++, but has Python and MATLAB interfaces.

- Particularly strong in the image-recognition and analysis area.

- Weaker if you're not doing convolution networks (we'll get to this next week), meaning you're studying text, sound, or time series.

- Only a few native input formats, and only one native output format, HDF5 (though you can get around this using the Python interface).

This is a commonly-encountered framework wherever images are being used.

Another framework used for neural networks is Torch.

- First released in 2002. Quite mature at this point.
- Written in Lua. Never heard of Lua? Welcome to the club.
- Pytorch was release by Facebook in January 2018.
- Like Theano, Torch is more flexible than just NN. It is more of a generic scientific computing framework.
- Very strong on GPUs.
- Very fast. Often the fastest depending on the problem being considered.
- Limited visualization capabilities.
- Used and maintained by Facebook, Twitter and other high-profile companies.

This framework is growing in popularity, through the pytorch interface.

There are other frameworks which you may run into.

- Microsoft Cognitive Toolkit (previously CNTK).
- Apache MXNet, used by Amazon for cloud deep learning.
- Deeplearning4j, a Java-based NN framework.
- PaddlePaddle, Baidu's NN framework.

And of course, many others.

Keras

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We will use Keras on top of your favourite backend.

- Keras is a NN framework, but it's only the top-most level.

- More accurately, it's an API standard for creating neural networks.

- It runs on top of a 'back end': Theano, TensorFlow, CNTK, MXNet, TypeScript, JavaScript, PlaidML, Scala, CoreML, and others.

- Because it's a proper framework, all of the NN goodies you need are already built into it.

- Very popular; designed for fast development of networks.

- Is compatible with both Python 2 and 3.

- By default it will try to use TensorFlow on the back end; you may switch it if you wish.
  - On Macs/Linux, edit your $HOME/.keras/keras.json file.
  - On Windows, edit your %USERPROFILE%/.keras/keras.json file.
  - You can also set the KERAS_BACKEND environment variable.

- Use the usual "pip install keras" to install it from the Linux command line.

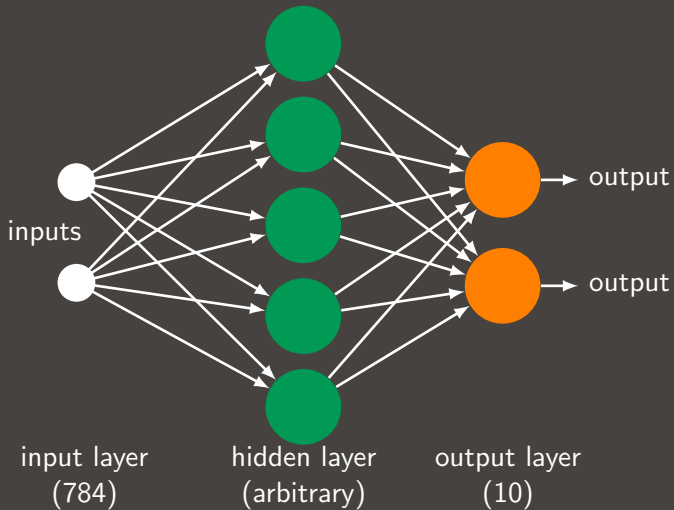Because it is so commonly used, the MNIST data set is built into most NN frameworks.

Keras is no different, so we'll just grab it from Keras directly.

```
In [1]:
In [1]: from keras.datasets import mnist
Using Theano backend.
In [2]:
In [2]: (x_train, y_train), (x_test, y_test) = \
                mnist.load_data()
In [3]:
In [3]: x_train.shape
Out[3]: (60000, 28, 28)
In [4]:
```

Prepping the data

As with last time, we need the data in a specific format:

- Instead of 28 x 28, we flatten the data into a 784-element vector.

- We only take the first 500 data points for training, to be consistent with last class.

- The labels must be changed to a categorical format (one-hot encoding).

```
In [4]:
In [4]: import keras.utils as ku
In [5]:
In [5]: x_train = x_train[0:500, :, :].reshape(500, 784)
In [6]: x_test = x_test[0:100, :, :].reshape(100, 784)
In [7]:
In [7]: y_train = ku.to_categorical(y_train[0:500], 10)
In [8]: y_test = ku.to_categorical(y_test[0:100], 10)
In [9]:
```

Our neural network

inputs

output

output

input layer
(784)

hidden layer
(arbitrary)

output layer
(10)

Our network using Keras

Let us re-implement our second network using Keras.

- A "Sequential" model means the layers are stacked on one another in a linear fashion.

- A "Dense" ("fully-connected") layer is the regular layer we've been using.

- Use "input_dim" in the first layer to indicate the shape of the incoming data.

- The "activation" is the output function of the neuron.

- The "name" of the layer is optional.

```python
# model1.py
import keras.models as km
import keras.layers as kl

def get_model(numnodes):
  model = km.Sequential()
  model.add(kl.Dense(numnodes, input_dim = 784,
    activation = 'sigmoid', name = 'hidden'))
  model.add(kl.Dense(10, name = 'output',
    activation = 'sigmoid'))
  return model
```

```
In [9]: import model1 as m1
In [10]: model = m1.get_model(30)
In [11]: model.output_shape
Out[11]: (None, 10)
In [12]:
```

```
In [12]:
In [12]: model.summary()
Layer (type)                   Output Shape              Param #
=================================================================
hidden (Dense)                 (None, 30)                23550

_____
output (Dense)                 (None, 10)                310
=================================================================
Total params:  23,860
Trainable params:  23,860
Non-trainable params:  0

_____
In [13]:
```

Plotting the model

Keras allows you the ability to plot your model. This is sometimes helpful if your model gets complicated.

Note that you will need to install the 'pydots' package for this to work.

```
In [13]:
In [13]: ku.plot_model(model, to_file = 'mymodel.pdf')
In [14]:
```

The weird number which represents the input layer is actually a bug in Keras. It only occurs when you don't specify the input layer explicitly, which you don't when you use km.Sequential().

Our network using Keras, continued more
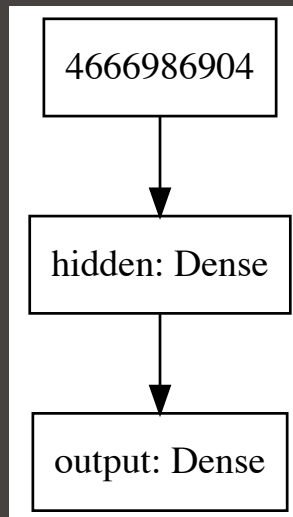
```
In [14]:
In [14]: model.compile(optimizer = 'sgd', metrics = ['accuracy'], loss = "mean_squared_error")
In [15]:
In [15]: fit = model.fit(x_train, y_train, epochs = 1000, batch_size = 5, verbose = 2)
Epoch 1/1000
0s - loss: 0.1963 - acc: 0.1170
Epoch 2/1000
0s - loss: 0.1338 - acc: 0.1720
.
.
Epoch 999/1000
0s - loss: 0.0394 - acc: 0.8440
Epoch 1000/1000
0s - loss: 0.0394 - acc: 0.8440
In [16]:
```

About that optimization flag

The optimization flag was set to "sgd".

- This stands for "Stochastic Gradient Descent".
- This is similar to regular gradient descent that we used previously.
  - Regular gradient descent is ridiculously slow on large amounts of data.
  - To speed things up, SGD uses a randomly-selected subset of the data (a "batch") to update the coefficients.
  - This is repeated many times, using different batches, until all of the data has been used. This is called an "epoch".
- In practise, regular gradient descent is never used, stochastic gradient descent is used instead, since it's so much faster.
- The only real advantage of regular gradient descent is that it's easier to code, which is why I used it in previous classes.

Our network using Keras, notes

Some notes about the compilation of the model.

- We must specify the loss (cost) function with the "loss" argument.

- We must specify the optimization algorithm, using the "optimizer" flag.

- The optimizer can be generic ('sgd'), as in this example, or you can specify parameters using the optimizers in the keras.optimizers module.

- I sometimes specify the optimizer explicitly so that I can specify the value of η (using 'lr', the 'learning rate').

- The 'metrics' argument is optional, but is needed if you want the accuracy to be printed.

Plotting the training

The fit.history dictionary contains useful information about the training. Sometimes plotting can give you some insight into the quality of the training, and whether or not it's finished.

```
In [16]:
In [16]: import matplotlib.pyplot as plt
In [17]: plt.plot(fit.history['acc'])
In [18]: plt.xlabel('Epoch')
In [19]: plt.ylabel('Accuracy')
In [20]:
```
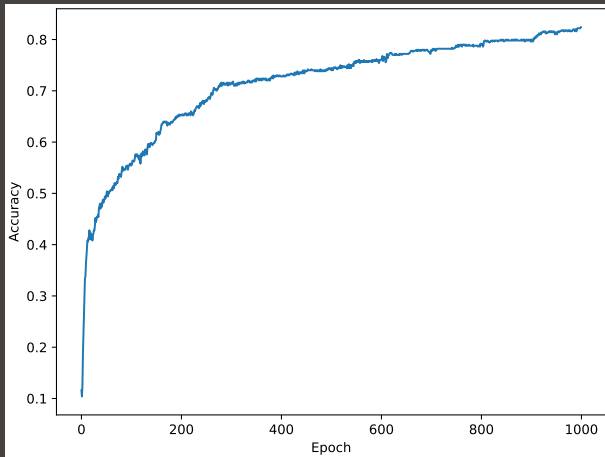
Now check against the test data.

We see the over-fitting rearing its head (84% versus 62%).

We can do better! That will be the goal of next class.

```
In [20]:
In [21]: score = model.evaluate(x_test, y_test)
In [22]:
In [22]: score
Out[22]: [0.056402873396873471, 0.62]
In [23]:
```

Our network using Keras, different syntax

```python
# model1.py
import keras.models as km
import keras.layers as kl

def get_model(numnodes):

  model = km.Sequential()

  model.add(kl.Dense(numnodes, input_dim = 784,
    activation = 'sigmoid', name = 'hidden'))

  model.add(kl.Dense(10, name = 'output',
    activation = 'sigmoid'))

  return model
```

Keras has two syntaxes available for creating networks.

```python
# model2.py
import keras.models as km, keras.layers as kl

def get_model(numnodes):

  input_image = kl.Input(shape = (784,),
    name = 'input')

  x = kl.Dense(numnodes, name = 'hidden',
    activation = 'sigmoid')(input_image)

  x = kl.Dense(10, name = 'output',
    activation = 'sigmoid')(x)

  model = km.Model(inputs = input_image,
    outputs = x)

  return model
```

Keras' functional syntax

The second syntax is known as the 'functional' syntax. Why would such a thing be available?

- The original syntax, using model = km.Sequential() works fine, assuming you have a single input, a single output, and all layers lay in a sequence.

- But what do you do if you have multiple inputs and outputs?

- In a later class, we'll do an example of a network which takes two inputs: input data, and a requested number. The sequential networks can't handle this sort of input without combining the input together at the input stage, which may not make sense.

- The functional syntax allows you to create networks which have multiple inputs and outputs.

- It also gives you the ability to combine the output of layers within the network.

- Options for combining layer outputs include concatenating, multipling/dividing, adding/subtracting, etc.

input 1

input 2

output 1

output 2

Training with multiple outputs: an aside
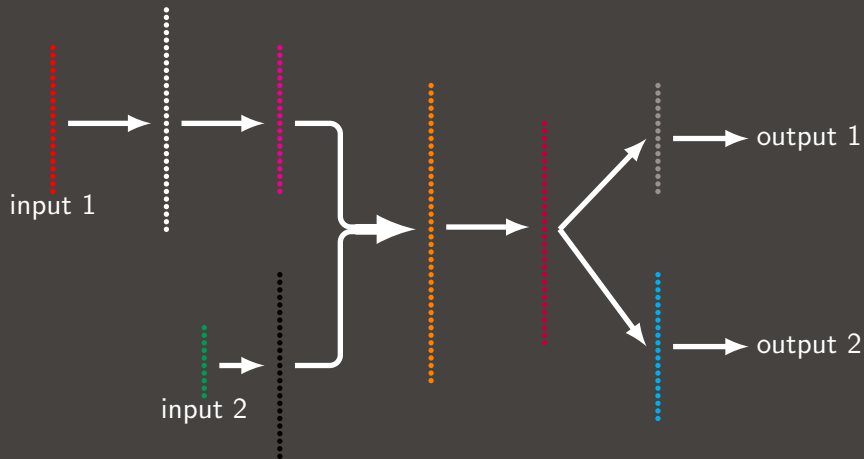
As you might imagine, if you have multiple outputs the training of your network is going to get complicated. There are several ways the training of such networks can be specified.

- The first is to specify multiple loss functions, one for each output. This is done by putting a list of loss functions into your compile command (loss = ['mean_squared_error', 'categorical_crossentropy'])

- You can also scale how much emphasis to put on one output versus another, using the 'loss_weights' argument to the compile function (loss_weights = [1.0, 0.2]).

- You can also define your own custom loss functions. These take two arguments (y_true and y_pred), and return the loss value.

There is lots of flexibility available for setting up the loss functions. We will use this functionality later in the course.

The next steps

We can do better. What's the plan? There are a few simple approaches:

- Use more data.
- Change the activation function.
- Change the cost function.
- Change the optimization algorithm.
- Change the way things are initialized.
- Add regularization, to try to deal with the over-fitting.

We'll try some of these next class, but there are also some not-so-simple approaches:

- Completely overhaul the network strategy.

We'll take a look at this next week.

The next steps, an aside

There are alot of things we can tweak to make the network do better on the testing data. How do we know what to do?

- In many ways, implementing a network is an art.

- Certain forms and functions and parameters are known to lead to certain types of behaviour, and thus are used in certain situations.

- Choosing the correct values of parameters can often seem like a matter of trial-and-error.

- And choosing the correct activation functions, number of nodes, can also seem like trial-and-error.

- But there are more-sophisticated ways of finding the optimum parameter choices. We may discuss this in a later class.

Practise is often needed to know how to approach various types of problems. Consult your colleagues, and the literature.

Linky goodness

Keras:

- `https://keras.io`

Other frameworks:

- `http://deeplearning.net/software/theano`
- `https://www.tensorflow.org`
- `http://caffe.berkeleyvision.org`
- `http://torch.ch`