# Quantessentials

## Getting started with deep learning in TensorFlow

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**Revisiting the topic of deep learning**

Following the expert call on deep learning with Prof Matthew Dixon, we come back to the topic from an implementation point of view. We provide an introduction to Google's *TensorFlow* – one of the most popular and powerful libraries for deep learning.

**Getting started with TensorFlow**

In its core, TensorFlow operates on a graph representation of a computational problem, in which the nodes correspond to mathematical operations, while the edges represent data that flows between the nodes (hence the name). We introduce the objects needed to construct a feed-forward neural network using the low-level API of the library (TensorFlow Core), show how to train such a model and display summary statistics in the visualisation tool *TensorBoard*.

**Building models quickly with higher level APIs**

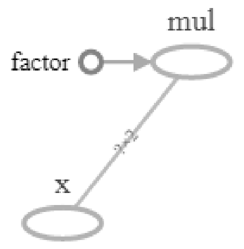
TensorFlow Core gives complete control over a model by letting the user to create the entire computational graph. However, what's needed in most cases is something "off the shelf" that allows you to build and experiment with models quickly. There are a number of high-level APIs that hide a lot of the technical detail. Here we provide an example of a network built with *Keras* running on top of TensorFlow, but also able to use Microsoft's CNTK and Theano.

# What's TensorFlow?

The expert call on Deep learning (Oct 2017) provided us with the intuition behind machine learning models and gave an introduction to some of the theory behind neural networks. The aim of this report is to revisit the topic from an implementation viewpoint and introduce the reader to Google's *TensorFlow* – arguably the most popular library for deep learning for both research and production purposes.

TensorFlow operates on a **graph** representation of an underlying computational task (and can therefore be used for other kinds of maths problems, such as general optimisation or solving PDEs). Every node in the graph represents a mathematical operation, such as addition or computing gradients, while edges represent the data that feeds into a computation (see Figure 1).

**Figure 1: Simple computation graph**




Source: UBS Quant, generated with TensorBoard. The graph represents the mathematical operation of multiplying a multidimensional array called $x$ by a constant called $factor$.

Once a dataflow graph is constructed it has to be evaluated in a TensorFlow session on a local or remote set of devices. This process is regarded as relatively **low-level** programming; however there are a number of high-level APIs that hide the details of graphs and sessions such as *Keras* or TensorFlow's *Estimator*. In this note we show examples using the low-level API in order to understand the fundamental principles of TensorFlow Core, which will give insights into how the higher level APIs work internally. We will then use Keras to implement the portfolio returns example from the expert call.

The biggest problem with deep learning is it is very data hungry. This limits its use to some extent within finance. Tick data is very amenable as an input into a deep learning network; daily data might be the limit.

In a new departure for us we have put all the code into a Jupyter Notebook which is available on UBS Neo at [LINK].

## Installing TensorFlow

TensorFlow provides APIs for multiple programming languages and there are third party packages for a few more (including R from RStudio). All of the examples in this note were written in Python (version 3.5.2) and using the CPU-only version of the library.

The easiest way we found to install and run TensorFlow under Windows was using the mechanisms provided from Anaconda. With Anaconda, getting the library *should be* as simple as running:

```
conda install tensorflow
```

in the command line. The alternative is to use native `pip`, which in theory *should also be straightforward*. For further details and installation on other operating systems we refer the reader TensorFlow's guide.

# Basic objects and operations

The central unit in TensorFlow is the **tensor**, which can be thought of as a multidimensional array containing data. Each tensor has a *shape* (dimensionality of the array and size of each dimension), which may or may not be known, and *type*, which is common to all the elements in the tensor. The main types of tensors are:

*(1) constants*, *(2) placeholders* and *(3) variables*, which we introduce with examples below.

**Constants**, as the name suggests, are things that once defined don't change in the future. These have to be initialised with a specific value (not a mathematical operation) and become part of the underlying graph. The way to define them is using the constructor `tf.constant`, demonstrated in Figure 2, where we create two constants of float type (note the decimal point).

**Figure 2: Constants**

```
import tensorflow as tf
tf.reset_default_graph()
### Constants ###
const1 = tf.constant(7., name = "const1")
const2 = tf.constant(3., name = "const2")

# What's the type of a constant?
print("Type of a constant: {}".format(type(const1)))

# What if we try to print it or add the two together?
print("const1 = {}".format(const1))
Sum = const1 + const2
print("Sum = {}".format(Sum))
Product = const1 * const2
print("Product = {}".format(Product))
```

```
Type of a constant: <class 'tensorflow.python.framework.ops.Tensor'>
const1 = Tensor("const1:0", shape=(), dtype=float32)
Sum = Tensor("add:0", shape=(), dtype=float32)
Product = Tensor("mul:0", shape=(), dtype=float32)
```

Source: UBS Quant.

If we print or try to add the two constants together, the result is not the same if these were regular Python objects, namely `const1 = 7.0` and `Sum = 10.0`. The output of these two operations only gives us information about the resulting objects (their name, shape and type)[1].

As mentioned in the introduction, to get the output from a computation it needs to be evaluated in an active TensorFlow session. The code above only defines the computation graph (displayed in Figure 3). We set up a session and evaluate the graph in Figure 4.

[1] The sum `const1 + const2` is equivalent to `tf.add(const1, const2)`. All basic maths operations implicitly call a corresponding `tf.-` method.

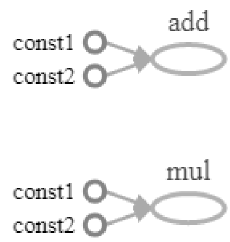
**Figure 4: Evaluating operations in a session**

```
# All operations have to be evaluated in active TF session
with tf.Session() as sess:
    # print the two constants:
    print("const1 = {}, const2 = {}".format(
            sess.run(const1), sess.run(const2)))

    # Sum of the two constants:
    print("Sum = {}".format(sess.run(Sum)))

    # Product of the two constants:
    print("Product = {}".format(sess.run(Product)))
```

```
const1 = 7.0, const2 = 3.0
Sum = 10.0
Product = 21.0
```

Source: UBS Quant.

**Figure 3: Computation graph**




Source: UBS Quant, generated with TensorBoard. The graph is set-up in Figure 2 and evaluated in Figure 4.

The second special type of tensor we look at is the **placeholder**. Placeholders are used to feed external data into a computation and therefore allow you to create a graph without the underlying data. The syntax to define a placeholder and perform operations with it is demonstrated in Figure 5. It is important to set the data type (`dtype`) and the shape argument. Typically, the size of the data (number of observations) changes, but the dimensionality (number of features) is constant. In the example below, the placeholder $x$ is a two-dimensional tensor of an arbitrary size. When evaluating an operation that depends on one or more placeholders, values for all of them need to be supplied as a dictionary via the `feed_dict` argument.

**Figure 5: Placeholders**

```
### Placeholders ###
x = tf.placeholder(dtype = tf.float32, shape = [None, 2])
output = const1 * x

x_values = [[7, 5], [3, 1]]
with tf.Session() as sess:
    print("Multiply by const1:\n {}".format(
            sess.run(output, feed_dict = {x: x_values})))
```

```
Multiply by const1:
 [[ 49.  35.]
 [ 21.   7.]]
```

Source: UBS Quant.

## Linear regression with TensorFlow

The easiest way to introduce the last type of special tensors – **variables**, is by building a model. We use a simple linear regression, $Y = \alpha + \beta X + \epsilon$, as an example to also introduce the rest of the objects we'll need for deep learning: *initialiser*, *loss* and *optimiser*. The true model is:

$$Y = 2 + 3X + N(0,1) \tag{1}$$

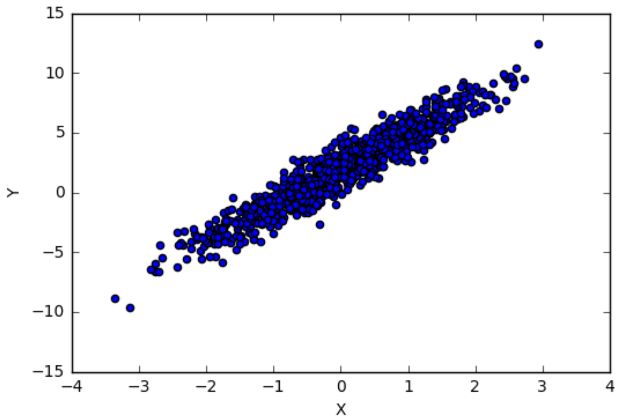
To generate random samples from this model we use the function defined in Figure 6, while Figure 7 shows realisations from it.

**Figure 6: Generating random samples**

```
import numpy as np
import scipy as sp
import matplotlib.pyplot as plt

def get_training_samples(n = 1000):
    x = sp.randn(n, 1)
    y = 2 + 3 * x + sp.randn(n, 1)
    return(x, y)

# Generate some samples and plot them:
batch_x, batch_y = get_training_samples()

plt.scatter(batch_x, batch_y)
plt.xlabel("X")
plt.ylabel("Y")
plt.show()
```

Source: UBS Quant.

**Figure 7: Sample data**




Source: UBS Quant.

In this setting, the two parameters – $\alpha$ and $\beta$, are the *variables* we wish to optimise over, given some training samples ($\boldsymbol{x}$, $\mathbf{y}_{\text{true}}$). To this end, we define two variables – $a$ and $b$ with initial values of 1. In the low-level API of TensorFlow variables must be explicitly initialised before they can be used in computations; `tf.global_variables_initializer()` initialises all variables at once. Since we will be feeding training data in the graph we also create a placeholder for the input $\boldsymbol{x}$ and finally specify the linear model as $y = a + b \cdot x$.

**Figure 8: Variables in a simple linear regression**

```
### Variables ###
a = tf.Variable(initial_value = 1, name = "alpha", dtype = tf.float32)
b = tf.Variable(initial_value = 1, name = "beta", dtype = tf.float32)
# Define a variable initialiser
init = tf.global_variables_initializer()

# Pleaceholder for x
x = tf.placeholder(dtype = tf.float32, shape = [None, 1], name = "x")

# Specify the linear model model:
y = a + b * x
```

Source: UBS Quant.

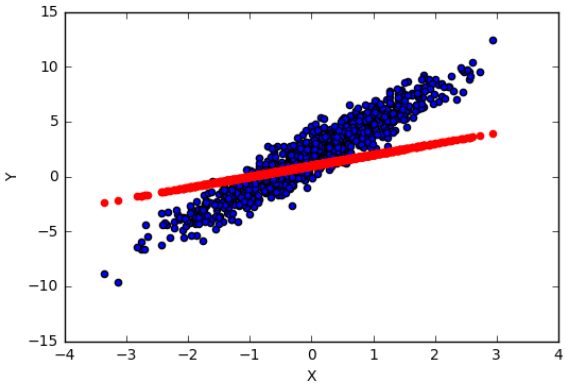
We evaluate the graph with the initial values of the two variables below. Note that the output `y` is a function of the placeholder `x`, so values for it must be fed into the graph via the `feed_dict` argument.

**Figure 9: Evaluate a model**

```
with tf.Session() as sess:
    #  initialise a and b
    init.run()

    # evaluate y
    test_y = y.eval(feed_dict = {x: batch_x})

    # Plot the data and fitted values
    plt.scatter(batch_x, batch_y)
    plt.scatter(batch_x, test_y, color = "red")
    plt.xlabel("X")
    plt.ylabel("Y")
    plt.show()
```

Source: UBS Quant.

**Figure 10: Original data and fitted values**




Source: UBS Quant.

To assess and improve the model we need to implement a *loss* function. The standard loss for regression problems is the Mean Squared Error (MSE), which is readily available in Tensorflow's losses module. Recall that MSE is a function of the true and the predicted values. So far we haven't used the true values in the graph, so the first thing to do is define another placeholder to feed $y_{tue}$. Notice that `loss`, defined in Figure 11, depends on two placeholders: `x` and `y_true`, so both have to be supplied when evaluating it.

**Figure 11: Define and evaluate loss**

```
# create a placeholder for y_true!
y_true = tf.placeholder(dtype = tf.float32, shape = [None, 1],
                        name = "y_true")
# loss: MSE between y and y_true
loss = tf.losses.mean_squared_error(y, y_true)
```

```
with tf.Session() as sess:
    init.run() # initialise variables
    batch_x, batch_y = get_training_samples()
    # calculate loss:
    print(loss.eval(feed_dict = {x: batch_x, y_true: batch_y}))
```

```
6.08897
```

Source: UBS Quant.

The final step is to minimise the loss. TensorFlow provides a number of (in our opinion, very good) optimisers in its train module. For this simple problem we use a generic gradient descent and specify the loss function to be optimised.

**Figure 12: Optimiser**

```
opti = tf.train.GradientDescentOptimizer(
    learning_rate = 0.01).minimize(loss = loss)
```

```
with tf.Session() as sess:
    init.run()
    for i in range(500):
        batch_x, batch_y = get_training_samples()
        # optimise
        opti.run(feed_dict = {x: batch_x, y_true: batch_y})
    print("Estimates: a = {} b = {}".format(a.eval(), b.eval()))
    print("Loss: {}".format(loss.eval({x: batch_x, y_true: batch_y})))
```

```
Estimates: a = 1.9995245933532715 b = 3.002850294113159
Loss: 1.041538119316101
```

Source: UBS Quant.

We can see from the output that the parameters were learnt correctly ($\alpha = 2$ and $\beta = 3$) and that the loss is as expected equal to 1 (since the error term has a variance of 1).

## Deep learning

For an overview of recap of deep learning we refer the reader to our note Introduction to Deep Learning.

We begin by developing a neural network to learn the following function:

$$Y(x) = \begin{cases} \sin(2\pi x), & 0 \leq x \leq 0.75 \\ -1, & 0.75 < x \leq 1 \end{cases}$$

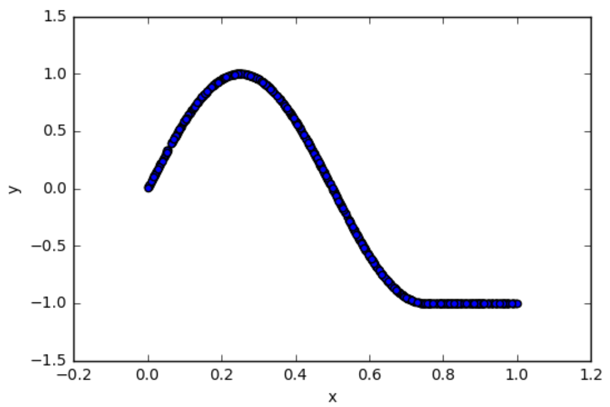
The aim of this example will be to demonstrate the low-level API syntax for constructing feed-forward neural networks, their ability to learn non-linear relationships and also introduce *TensorBoard* – a tool that makes it easier to understand and debug complex graphs.

**Figure 13: Non-linear function to learn**

```
def get_training_samples(n = 1000):
    x = sp.rand(n, 1)  #  random uniforms
    y = np.sin(x * 2 * np.pi)
    y[x > 0.75] = -1
    return(x, y)

batch_x, batch_y = get_training_samples()
plt.scatter(batch_x, batch_y)
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

Source: UBS Quant.

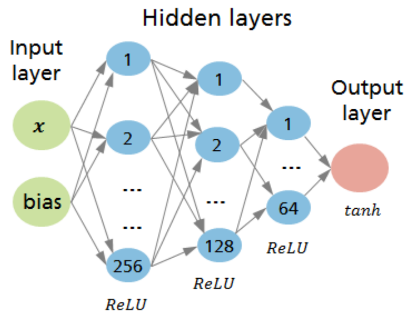
**Figure 14: Non-linear function to learn**




Source: UBS Quant.

The first step is to define the network architecture. There is only one feature in this example, namely $x$, taking values between 0 and 1. The input layer therefore consists of only two neurons – the input $x$ and a bias term. We use 3 hidden layers with decreasing number of nodes (256, 128 and 64) and a Rectified Linear Unit ($ReLU$) activation function in each of them. Since this is a regression problem, the output layer consists of a single node. We use our knowledge on the range of the function that we are trying to learn – namely $[-1, 1]$, and set the activation to be the hyperbolic tangent[2] (see Figure 15).

**Figure 15: Network architecture**




Source: UBS Quant.

The code in Figure 16 defines the network architecture described above in a very similar way to the linear regression example. In particular, we start by creating a placeholder for the input $x$, which feeds into the first hidden layer, `hl_1`; every other hidden layer and the output layer take the results from the previous one. Although a standard gradient descent optimiser will work just fine in this example, adaptive methods, such as *Adam* or *Adagrad* optimisers, achieve better results in highly non-linear problems and are thus preferable when training (deep) networks. Finally, we construct an initialiser for the variables in the model (weights and biases) which we have implicitly defined via `tf.layers.dense`.

**Figure 16: Setting up a feed-forward, fully connected neural network with 3 hidden layers**

```
# A placeholder to feed-in the inputs
x = tf.placeholder(tf.float32, shape = [None, 1], name = "x")

### Hidden layers ###
# The first layer takes x as input
hl_1 = tf.layers.dense(inputs = x, units = 256, activation = tf.nn.relu,
                       name = "layer1")
# Every other layer takes the previous one as input
hl_2 = tf.layers.dense(inputs = hl_1, units = 128, activation = tf.nn.relu,
                       name = "layer2")
hl_3 = tf.layers.dense(inputs = hl_2, units = 64, activation = tf.nn.relu,
                       name = "layer3")
# Output layer
y_pred = tf.layers.dense(inputs = hl_3, units = 1, activation = tf.nn.tanh)
# Loss, optimiser, initialiser
y_true = tf.placeholder(tf.float32, shape = [None, 1], name = "y_true")
loss = tf.losses.mean_squared_error(y_true, y_pred)
opti = tf.train.AdagradOptimizer(learning_rate = 0.01).minimize(loss)
init = tf.global_variables_initializer()
```

Source: UBS Quant.

We can export a *summary* about the model using TensorFlow's summary module. For example, if we want to plot the values of the loss function at each iteration, we can collect them by attaching `tf.summary.scalar` to `loss`. We then construct a FileWriter, specifying a log-directory as an input, which is the directory where the data will be stored. The FileWriter also accepts `Graph` as an input; if it is provided TensorBoard will also visualise the underlying computation graph. The third and final step is to write the summary data to disk at the end of each iteration of the optimization process (see Figure 17).

[2] Note on activation functions: as a rough guidance is to use ReLU or ELU activation functions in the hidden layers, as these do not suffer from the "vanishing gradient" problem; for output layer the most commonly used activation functions are the identity for regression (as the output tends to be unbounded) and softmax for classification problems.

**Figure 17: Writing summaries in TensorBoard and evaluating the graph**

```
### Adding a summary to TensorBoard ###
import time
tf.summary.scalar("loss", loss)
summ = tf.summary.merge_all()

## Run the model
with tf.Session() as sess:
    init.run()
    # Define a filewriter, specifying the directory and the graph
    fw =  tf.summary.FileWriter("C:/Users/DI/TF/neural/{}/".format(
            int(time.time())), sess.graph)

    for i in range(10000):
        batch_x, batch_y = get_training_samples(500)
        opti.run(feed_dict = {y_true: batch_y, x: batch_x})
        # Write the summary
        fw.add_summary(summ.eval({y_true: batch_y, x: batch_x}),
                       global_step = i)

    plt.scatter(batch_x, y_pred.eval({x: batch_x}))
    plt.show()
```

**Step 1: Add the loss to summary**

**Step 2: Create a FileWriter; don't forget to change the log-directory**

**Step 3: Evaluate the loss at each iteration and add to summary**

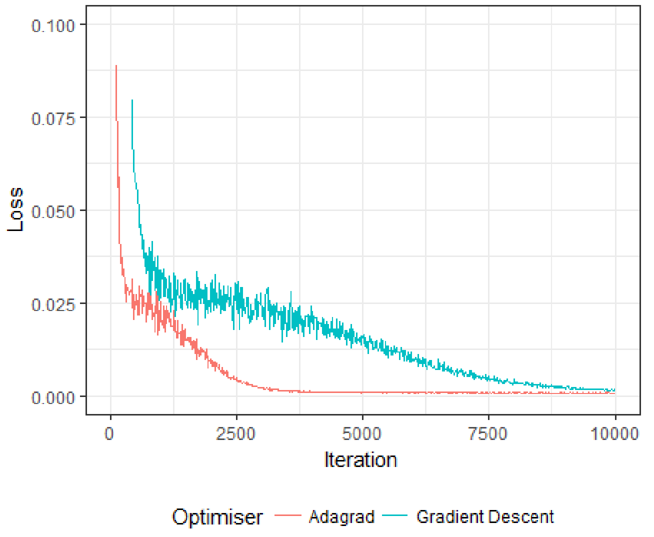
Source: UBS Quant. The lines highlighted in red are used to set-up summaries in TensorBoard.

Once the optimisation has started, we can launch TensorBoard by running the following command in the terminal/command line:

```
tensorboard  --logdir path_to_logdirectory
```

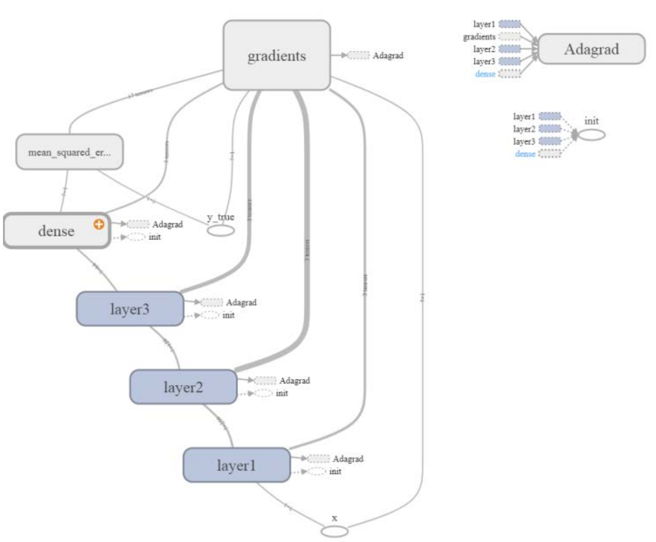
where `path_to_logdirectory` is the same as directory that was passed to the FileWriter. To view TensorBoard go to `localhost:6006` in your web-browser[3]. Under the "Scalars" tab you should be able to see a chart with the loss function (note that you can also download the data as csv or json), while the computation graph can be viewed under the "Graphs" tab.

**Figure 18: Losses**




Source: UBS Quant. To demonstrate the difference that an optimiser can make we fitted the neural network from Figure 16 using the more sophisticated Adagrad and the simpler Gradient Descent.

**Figure 19: Computation graph of the neural network**




Source: UBS Quant, generated with TensorBoard. Note that you can expand any subgraph by clicking on the orange plus sign in the top right corner.

[3] May not work in Internet Explorer.

## Portfolio returns example

In this section we reproduce the example from the expert call on deep learning. We consider $n$ stocks with returns $r_i(t)$, equally weighted in a portfolio, so that its return is:

$$r_P(t) = \sum_{i=1}^{n} w_{i,t} r_i(t), \;\; w_{i,t} = \frac{1}{n}$$

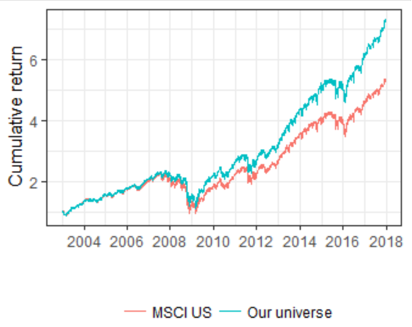
The observed data, which is also the set of features we use as inputs, consists of the daily historical returns of all the stocks. The target is a categorical variable, labelled as:

$$Y_t = \begin{cases} 1, & r_p(t+1) > \epsilon \\ 0, & |r_p(t+1)| \leq \epsilon \\ -1, & r_p(t+1) < -\epsilon \end{cases}$$

where $\epsilon$ is a threshold determined from the training data to avoid class imbalance. In other words, we would like to make a decision on whether to buy, stay out of or sell the entire portfolio, based on a prediction of the direction of the next day portfolio return.

The universe of stocks we consider consists of MSCI US, restricted to those companies which have price data throughout the period from January 2003 through November 2017 (i.e. we admit look-ahead bias, see Figure 20). We do not provide the data to run this example (for both technical and compliance issues) and therefore in order to run the examples below the reader will need to create a pandas dataframe with stocks as columns.

**Figure 20: Portfolio return**




Source: UBS Quant, MSCI.

We implement the model with the Keras, still running with TensorFlow as backend[4]. Despite being much higher level the package is very flexible, allowing the user to experiment with network architectures much quicker.

The code in Figure 21 loads the relevant libraries and data. The function `get_samples`, defined in the Jupyter notebook, performs the required transformations on the data, including subsets of it, and will also be used in a rolling forecasting experiment.

[4] Keras can also run on top of Microsoft's CNTK and Theano.

**Figure 21: Load libraries and data**

```
import numpy as np
import pandas as pd
import keras
from keras.layers import Dense
from keras.models import Sequential
from keras.utils import to_categorical

market_data = pd.read_csv("portfolio_returns\market_data_tf.csv")

(target_train, predictors_train, predictors_test,
     target_test) = get_samples(window = market_data.shape[0] - 1)

n_cols = predictors_train.shape[1]
n_labels = target_train.shape[1]
```

```
Using TensorFlow backend.
```

Source: UBS Quant.

We begin by setting up a neural network with three hidden layers and "tapered" feed-forward architecture (200, 100 and 50 neurons in each layer). The way to do that in Keras is shown in Figure 22, which compared to the low-level API of TensorFlow (Figure 16) is more straightforward and less verbose. There are two main differences:

- No need to specify placeholders for inputs that feed into the graph
- Learning process configuration (i.e. details on what loss and optimiser to use) is done via the `compile` method, instead of constructing separate loss and optimiser objects.

**Figure 22: Setting up feed-forward neural network with 3 hidden layers in Keras**

```
### Set up a sequential (feed-forward) network with 3 hidden layers ###
model = Sequential()

# Add 3 dense (fully-connected) layers and the output layer
model.add(Dense(200, activation = "relu", input_shape = (n_cols, ), name = "layer1"))
model.add(Dense(100, activation = "relu", input_shape = (n_cols, ), name = "layer2"))
model.add(Dense(50, activation = "relu", input_shape = (n_cols, ), name = "layer3"))
model.add(Dense(3, activation = "softmax", name = "output"))

# Loss, optimizer are specified when compiling the model
model.compile(optimizer="adam", loss="categorical_crossentropy", metrics=["accuracy"])
```

Source: UBS Quant. Compare to Figure 16 which uses TensorFlow's low-level API.

By default Keras prints out details about the model that is being fitted, such as training and validation loss for each epoch. We also print the accuracy by passing it to the `metrics` argument in the `compile` method.

The final step is to fit the model, which is done via the `fit` method. This is where we feed the data into the graph. There are a number of other arguments, such as how long to train the model (number of epochs) and whether or not to split the data into a test and validation sets. In the example below (Figure 23) we specify a train/test split of 80/20 and display details about model performance in the last epoch of training. We can see that the in-sample accuracy is quite impressive at

97%; however, looking at validation accuracy (34%) we can conclude that the model has overfit the data[5].

**Figure 23: Fitting a network and setting up TensorBoard in Keras**

```
### Fit the model & write to TensorBoard ###
# Create TensorBaord summaries
vis = keras.callbacks.TensorBoard("C:/Users/DI/TF/port_ret/{}/".format(int(time.time())))

# And finally run the optimisation, passing <vis> to callbacks
model.fit(predictors_train, target_train, epochs = 20, batch_size = 200,
          validation_split = 0.2, callbacks = [vis])
```

```
Epoch 20/20
3017/3017 [==============================] - 0s - loss: 0.1337 - acc: 0.9751 - val_loss: 2.21
63 - val_acc: 0.3391
```

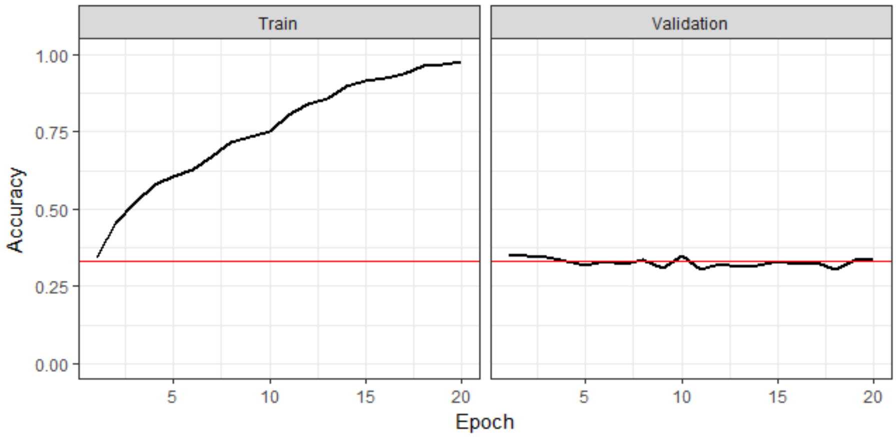
Source: UBS Quant. Compare to Figure 17 which uses TensorFlow's low-level API.

Visualising basic charts in TensorBoard with Keras is also much more straightforward. We do that by creating a `callbacks.TensorBoard` object and pass it to the `callbacks` argument when fitting the model. By default, this will plot the training and validation loss and accuracy as well as the underlying graph (these should look like the charts in Figure 24).

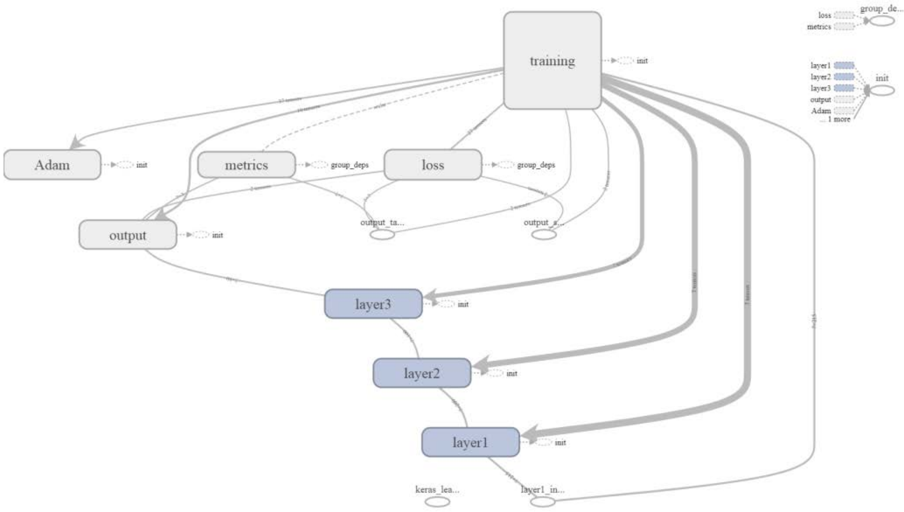
[5] Fully connected feed-forward neural networks are known for overfitting; regularisation techniques such as dropout, or more complex architectures (convolutional networks), solve this problem to a certain extent.

**Figure 24: Network summaries**

**Panel A: Training vs validation accuracy**




**Panel B: Graph**




Source: UBS Quant. Accuracy data and the graph were downloaded from TensorBoard. The red horizontal line (Panel A) is at 0.33 and indicates the expected accuracy if we were to guess any of the 3 states at random.

We can make predictions with the neural network using the `predict` method, passing an array containing values for the set of features used to build the model. In the example below we calculate the in-sample accuracy using the entire dataset.

**Figure 25: In-sample predictions**

```
preds_in = model.predict(predictors_train)
(np.argmax(preds_in, axis = 1) == np.argmax(target_train, axis = 1)).mean()
```

```
0.85312831389183452
```

Source: UBS Quant. The in-sample accuracy of the neural network is 85%.

To perform the rolling forecasting experiment, we only need to wrap the above code in a for-loop and feed the relevant data when fitting the model. The code to do this was relegated to the associated Jupyter Notebook. As one would expect, the out-of-sample predictive power of the model is very similar to the one achieved on the validation set (slightly above 33%) as the model doesn't take into account the temporal structure of the data.

We note that the results that we get are in agreement with the comments made in the expert call, namely that much more (e.g. higher-frequency than daily) is needed for deep learning to become useful.

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