CHAPTER 9

Up and Running with TensorFlow

TensorFlow is a powerful open source software library for numerical computation, particularly well suited and fine-tuned for large-scale Machine Learning. Its basic principle is simple: you first define in Python a graph of computations to perform (for example, the one in Figure 9-1), and then TensorFlow takes that graph and runs it efficiently using optimized C++ code.

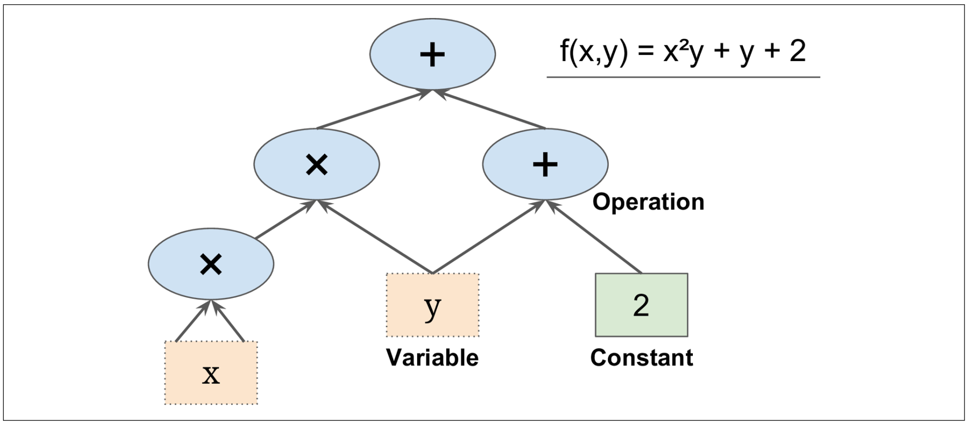


Figure 9-1. A simple computation graph

Most importantly, it is possible to break up the graph into several chunks and run them in parallel across multiple CPUs or GPUs (as shown in Figure 9-2). TensorFlow also supports distributed computing, so you can train colossal neural networks on humongous training sets in a reasonable amount of time by splitting the computations across hundreds of servers (see Chapter 12). TensorFlow can train a network with millions of parameters on a training set composed of billions of instances with millions of features each. This should come as no surprise, since TensorFlow was developed by the Google Brain team and it powers many of Google's large-scale services, such as Google Cloud Speech, Google Photos, and Google Search.

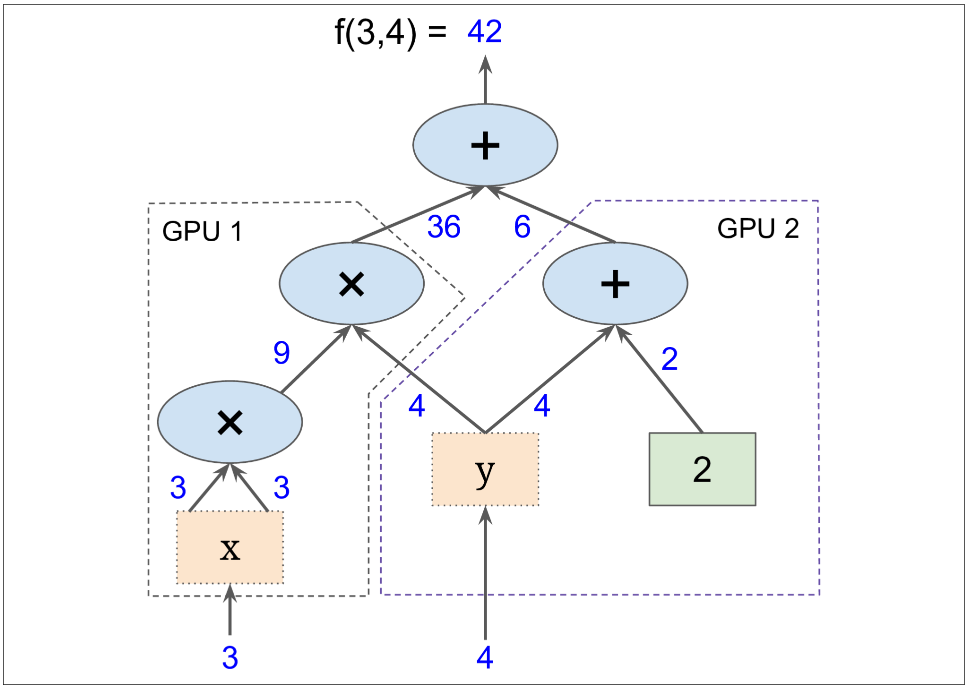


Figure 9-2. Parallel computation on multiple CPUs/GPUs/servers

When TensorFlow was open-sourced in November 2015, there were already many popular open source libraries for Deep Learning (Table 9-1 lists a few), and to be fair most of TensorFlow's features already existed in one library or another. Nevertheless, TensorFlow's clean design, scalability, flexibility,[1] and great documentation (not to mention Google's name) quickly boosted it to the top of the list. In short, TensorFlow was designed to be flexible, scalable, and production-ready, and existing frameworks arguably hit only two out of the three of these. Here are some of TensorFlow's highlights:

- It runs not only on Windows, Linux, and macOS, but also on mobile devices, including both iOS and Android.

1 TensorFlow is not limited to neural networks or even Machine Learning; you could run quantum physics simulations if you wanted.

- It provides a very simple Python API called *TF.Learn*[2] (`tensorflow.contrib.learn`), compatible with Scikit-Learn. As you will see, you can use it to train various types of neural networks in just a few lines of code. It was previously an independent project called *Scikit Flow* (or *skflow*).
- It also provides another simple API called *TF-slim* (`tensorflow.contrib.slim`) to simplify building, training, and evaluating neural networks.
- Several other high-level APIs have been built independently on top of TensorFlow, such as Keras (now available in `tensorflow.contrib.keras`) or Pretty Tensor.
- Its main Python API offers much more flexibility (at the cost of higher complexity) to create all sorts of computations, including any neural network architecture you can think of.
- It includes highly efficient C++ implementations of many ML operations, particularly those needed to build neural networks. There is also a C++ API to define your own high-performance operations.
- It provides several advanced optimization nodes to search for the parameters that minimize a cost function. These are very easy to use since TensorFlow automatically takes care of computing the gradients of the functions you define. This is called *automatic differentiating* (or *autodiff*).
- It also comes with a great visualization tool called *TensorBoard* that allows you to browse through the computation graph, view learning curves, and more.
- Google also launched a cloud service to run TensorFlow graphs.
- Last but not least, it has a dedicated team of passionate and helpful developers, and a growing community contributing to improving it. It is one of the most popular open source projects on GitHub, and more and more great projects are being built on top of it (for examples, check out the resources page on *https://www.tensorflow.org/*, or *https://github.com/jtoy/awesome-tensorflow*). To ask technical questions, you should use *http://stackoverflow.com/* and tag your question with `"tensorflow"`. You can file bugs and feature requests through GitHub. For general discussions, join the Google group.

In this chapter, we will go through the basics of TensorFlow, from installation to creating, running, saving, and visualizing simple computational graphs. Mastering these basics is important before you build your first neural network (which we will do in the next chapter).

2 Not to be confused with the TFLearn library, which is an independent project.

Table 9-1. Open source Deep Learning libraries (not an exhaustive list)

Library	API	Platforms	Started by	Year
Caffe	Python, C++, Matlab	Linux, macOS, Windows	Y. Jia, UC Berkeley (BVLC)	2013
Deeplearning4j	Java, Scala, Clojure	Linux, macOS, Windows, Android	A. Gibson, J.Patterson	2014
H2O	Python, R	Linux, macOS, Windows	H2O.ai	2014
MXNet	Python, C++, others	Linux, macOS, Windows, iOS, Android	DMLC	2015
TensorFlow	Python, C++	Linux, macOS, Windows, iOS, Android	Google	2015
Theano	Python	Linux, macOS, iOS	University of Montreal	2010
Torch	C++, Lua	Linux, macOS, iOS, Android	R. Collobert, K. Kavukcuoglu, C. Farabet	2002

Installation

Let's get started! Assuming you installed Jupyter and Scikit-Learn by following the installation instructions in Chapter 2, you can simply use pip to install TensorFlow. If you created an isolated environment using virtualenv, you first need to activate it:

```
$ cd $ML_PATH               # Your ML working directory (e.g., $HOME/ml)
$ source env/bin/activate
```

Next, install TensorFlow (if you are not using a virtualenv, you will need administrator rights, or to add the `--user` option):

```
$ pip3 install --upgrade tensorflow
```

For GPU support, you need to install `tensorflow-gpu` instead of `tensorflow`. See Chapter 12 for more details.

To test your installation, type the following command. It should output the version of TensorFlow you installed.

```
$ python3 -c 'import tensorflow; print(tensorflow.__version__)'
1.3.0
```

Creating Your First Graph and Running It in a Session

The following code creates the graph represented in Figure 9-1:

```
import tensorflow as tf

x = tf.Variable(3, name="x")
y = tf.Variable(4, name="y")
f = x*x*y + y + 2
```

That's all there is to it! The most important thing to understand is that this code does not actually perform any computation, even though it looks like it does (especially the last line). It just creates a computation graph. In fact, even the variables are not initialized yet. To evaluate this graph, you need to open a TensorFlow *session* and use it to initialize the variables and evaluate `f`. A TensorFlow session takes care of placing the operations onto *devices* such as CPUs and GPUs and running them, and it holds all the variable values.[3] The following code creates a session, initializes the variables, and evaluates, and `f` then closes the session (which frees up resources):

```
>>> sess = tf.Session()
>>> sess.run(x.initializer)
>>> sess.run(y.initializer)
>>> result = sess.run(f)
>>> print(result)
42
>>> sess.close()
```

Having to repeat `sess.run()` all the time is a bit cumbersome, but fortunately there is a better way:

```
with tf.Session() as sess:
    x.initializer.run()
    y.initializer.run()
    result = f.eval()
```

Inside the `with` block, the session is set as the default session. Calling `x.initializer.run()` is equivalent to calling `tf.get_default_session().run(x.initializer)`, and similarly `f.eval()` is equivalent to calling `tf.get_default_session().run(f)`. This makes the code easier to read. Moreover, the session is automatically closed at the end of the block.

Instead of manually running the initializer for every single variable, you can use the `global_variables_initializer()` function. Note that it does not actually perform the initialization immediately, but rather creates a node in the graph that will initialize all variables when it is run:

```
init = tf.global_variables_initializer()  # prepare an init node

with tf.Session() as sess:
    init.run()  # actually initialize all the variables
    result = f.eval()
```

Inside Jupyter or within a Python shell you may prefer to create an `InteractiveSession`. The only difference from a regular `Session` is that when an `InteractiveSession` is created it automatically sets itself as the default session, so you don't need a

3 In distributed TensorFlow, variable values are stored on the servers instead of the session, as we will see in Chapter 12.

`with` block (but you do need to close the session manually when you are done with it):

```
>>> sess = tf.InteractiveSession()
>>> init.run()
>>> result = f.eval()
>>> print(result)
42
>>> sess.close()
```

A TensorFlow program is typically split into two parts: the first part builds a computation graph (this is called the *construction phase*), and the second part runs it (this is the *execution phase*). The construction phase typically builds a computation graph representing the ML model and the computations required to train it. The execution phase generally runs a loop that evaluates a training step repeatedly (for example, one step per mini-batch), gradually improving the model parameters. We will go through an example shortly.

Managing Graphs

Any node you create is automatically added to the default graph:

```
>>> x1 = tf.Variable(1)
>>> x1.graph is tf.get_default_graph()
True
```

In most cases this is fine, but sometimes you may want to manage multiple independent graphs. You can do this by creating a new `Graph` and temporarily making it the default graph inside a `with` block, like so:

```
>>> graph = tf.Graph()
>>> with graph.as_default():
...     x2 = tf.Variable(2)
...
>>> x2.graph is graph
True
>>> x2.graph is tf.get_default_graph()
False
```

In Jupyter (or in a Python shell), it is common to run the same commands more than once while you are experimenting. As a result, you may end up with a default graph containing many duplicate nodes. One solution is to restart the Jupyter kernel (or the Python shell), but a more convenient solution is to just reset the default graph by running `tf.reset_default_graph()`.

Lifecycle of a Node Value

When you evaluate a node, TensorFlow automatically determines the set of nodes that it depends on and it evaluates these nodes first. For example, consider the following code:

```
w = tf.constant(3)
x = w + 2
y = x + 5
z = x * 3

with tf.Session() as sess:
    print(y.eval())  # 10
    print(z.eval())  # 15
```

First, this code defines a very simple graph. Then it starts a session and runs the graph to evaluate y: TensorFlow automatically detects that y depends on x, which depends on w, so it first evaluates w, then x, then y, and returns the value of y. Finally, the code runs the graph to evaluate z. Once again, TensorFlow detects that it must first evaluate w and x. It is important to note that it will *not* reuse the result of the previous evaluation of w and x. In short, the preceding code evaluates w and x twice.

All node values are dropped between graph runs, except variable values, which are maintained by the session across graph runs (queues and readers also maintain some state, as we will see in Chapter 12). A variable starts its life when its initializer is run, and it ends when the session is closed.

If you want to evaluate y and z efficiently, without evaluating w and x twice as in the previous code, you must ask TensorFlow to evaluate both y and z in just one graph run, as shown in the following code:

```
with tf.Session() as sess:
    y_val, z_val = sess.run([y, z])
    print(y_val)  # 10
    print(z_val)  # 15
```

In single-process TensorFlow, multiple sessions do not share any state, even if they reuse the same graph (each session would have its own copy of every variable). In distributed TensorFlow (see Chapter 12), variable state is stored on the servers, not in the sessions, so multiple sessions can share the same variables.

Linear Regression with TensorFlow

TensorFlow operations (also called *ops* for short) can take any number of inputs and produce any number of outputs. For example, the addition and multiplication ops each take two inputs and produce one output. Constants and variables take no input (they are called *source ops*). The inputs and outputs are multidimensional arrays, called *tensors* (hence the name "tensor flow"). Just like NumPy arrays, tensors have a type and a shape. In fact, in the Python API tensors are simply represented by NumPy ndarrays. They typically contain floats, but you can also use them to carry strings (arbitrary byte arrays).

In the examples so far, the tensors just contained a single scalar value, but you can of course perform computations on arrays of any shape. For example, the following code manipulates 2D arrays to perform Linear Regression on the California housing dataset (introduced in Chapter 2). It starts by fetching the dataset; then it adds an extra bias input feature ($x_0 = 1$) to all training instances (it does so using NumPy so it runs immediately); then it creates two TensorFlow constant nodes, `X` and `y`, to hold this data and the targets,[4] and it uses some of the matrix operations provided by TensorFlow to define `theta`. These matrix functions—`transpose()`, `matmul()`, and `matrix_inverse()`—are self-explanatory, but as usual they do not perform any computations immediately; instead, they create nodes in the graph that will perform them when the graph is run. You may recognize that the definition of `theta` corresponds to the Normal Equation ($\hat{\theta} = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$; see Chapter 4). Finally, the code creates a session and uses it to evaluate `theta`.

```
import numpy as np
from sklearn.datasets import fetch_california_housing

housing = fetch_california_housing()
m, n = housing.data.shape
housing_data_plus_bias = np.c_[np.ones((m, 1)), housing.data]

X = tf.constant(housing_data_plus_bias, dtype=tf.float32, name="X")
y = tf.constant(housing.target.reshape(-1, 1), dtype=tf.float32, name="y")
XT = tf.transpose(X)
theta = tf.matmul(tf.matmul(tf.matrix_inverse(tf.matmul(XT, X)), XT), y)

with tf.Session() as sess:
    theta_value = theta.eval()
```

The main benefit of this code versus computing the Normal Equation directly using NumPy is that TensorFlow will automatically run this on your GPU card if you have one (provided you installed TensorFlow with GPU support, of course; see Chapter 12 for more details).

4 Note that `housing.target` is a 1D array, but we need to reshape it to a column vector to compute `theta`. Recall that NumPy's `reshape()` function accepts –1 (meaning "unspecified") for one of the dimensions: that dimension will be computed based on the array's length and the remaining dimensions.

Implementing Gradient Descent

Let's try using Batch Gradient Descent (introduced in Chapter 4) instead of the Normal Equation. First we will do this by manually computing the gradients, then we will use TensorFlow's autodiff feature to let TensorFlow compute the gradients automatically, and finally we will use a couple of TensorFlow's out-of-the-box optimizers.

When using Gradient Descent, remember that it is important to first normalize the input feature vectors, or else training may be much slower. You can do this using TensorFlow, NumPy, Scikit-Learn's `StandardScaler`, or any other solution you prefer. The following code assumes that this normalization has already been done.

Manually Computing the Gradients

The following code should be fairly self-explanatory, except for a few new elements:

- The `random_uniform()` function creates a node in the graph that will generate a tensor containing random values, given its shape and value range, much like NumPy's `rand()` function.
- The `assign()` function creates a node that will assign a new value to a variable. In this case, it implements the Batch Gradient Descent step $\theta^{(\text{next step})} = \theta - \eta \nabla_{\theta}\text{MSE}(\theta)$.
- The main loop executes the training step over and over again (`n_epochs` times), and every 100 iterations it prints out the current Mean Squared Error (`mse`). You should see the MSE go down at every iteration.

```
n_epochs = 1000
learning_rate = 0.01

X = tf.constant(scaled_housing_data_plus_bias, dtype=tf.float32, name="X")
y = tf.constant(housing.target.reshape(-1, 1), dtype=tf.float32, name="y")
theta = tf.Variable(tf.random_uniform([n + 1, 1], -1.0, 1.0), name="theta")
y_pred = tf.matmul(X, theta, name="predictions")
error = y_pred - y
mse = tf.reduce_mean(tf.square(error), name="mse")
gradients = 2/m * tf.matmul(tf.transpose(X), error)
training_op = tf.assign(theta, theta - learning_rate * gradients)

init = tf.global_variables_initializer()

with tf.Session() as sess:
    sess.run(init)

    for epoch in range(n_epochs):
        if epoch % 100 == 0:
            print("Epoch", epoch, "MSE =", mse.eval())
        sess.run(training_op)

    best_theta = theta.eval()
```

Using autodiff

The preceding code works fine, but it requires mathematically deriving the gradients from the cost function (MSE). In the case of Linear Regression, it is reasonably easy, but if you had to do this with deep neural networks you would get quite a headache: it would be tedious and error-prone. You could use *symbolic differentiation* to automatically find the equations for the partial derivatives for you, but the resulting code would not necessarily be very efficient.

To understand why, consider the function $f(x)= \exp(\exp(\exp(x)))$. If you know calculus, you can figure out its derivative $f'(x) = \exp(x) \times \exp(\exp(x)) \times \exp(\exp(\exp(x)))$. If you code $f(x)$ and $f'(x)$ separately and exactly as they appear, your code will not be as efficient as it could be. A more efficient solution would be to write a function that first computes $\exp(x)$, then $\exp(\exp(x))$, then $\exp(\exp(\exp(x)))$, and returns all three. This gives you $f(x)$ directly (the third term), and if you need the derivative you can just multiply all three terms and you are done. With the naïve approach you would have had to call the `exp` function nine times to compute both $f(x)$ and $f'(x)$. With this approach you just need to call it three times.

It gets worse when your function is defined by some arbitrary code. Can you find the equation (or the code) to compute the partial derivatives of the following function? Hint: don't even try.

```
def my_func(a, b):
    z = 0
    for i in range(100):
        z = a * np.cos(z + i) + z * np.sin(b - i)
    return z
```

Fortunately, TensorFlow's autodiff feature comes to the rescue: it can automatically and efficiently compute the gradients for you. Simply replace the `gradients = ...` line in the Gradient Descent code in the previous section with the following line, and the code will continue to work just fine:

```
gradients = tf.gradients(mse, [theta])[0]
```

The `gradients()` function takes an op (in this case `mse`) and a list of variables (in this case just `theta`), and it creates a list of ops (one per variable) to compute the gradients of the op with regards to each variable. So the `gradients` node will compute the gradient vector of the MSE with regards to `theta`.

There are four main approaches to computing gradients automatically. They are summarized in Table 9-2. TensorFlow uses *reverse-mode autodiff*, which is perfect (efficient and accurate) when there are many inputs and few outputs, as is often the case in neural networks. It computes all the partial derivatives of the outputs with regards to all the inputs in just $n_{\text{outputs}} + 1$ graph traversals.

Table 9-2. Main solutions to compute gradients automatically

Technique	Nb of graph traversals to compute all gradients	Accuracy	Supports arbitrary code	Comment
Numerical differentiation	$n_{\text{inputs}} + 1$	Low	Yes	Trivial to implement
Symbolic differentiation	N/A	High	No	Builds a very different graph
Forward-mode autodiff	n_{inputs}	High	Yes	Uses *dual numbers*
Reverse-mode autodiff	$n_{\text{outputs}} + 1$	High	Yes	Implemented by TensorFlow

If you are interested in how this magic works, check out Appendix D.

Using an Optimizer

So TensorFlow computes the gradients for you. But it gets even easier: it also provides a number of optimizers out of the box, including a Gradient Descent optimizer. You can simply replace the preceding `gradients = ...` and `training_op = ...` lines with the following code, and once again everything will just work fine:

```
optimizer = tf.train.GradientDescentOptimizer(learning_rate=learning_rate)
training_op = optimizer.minimize(mse)
```

If you want to use a different type of optimizer, you just need to change one line. For example, you can use a momentum optimizer (which often converges much faster than Gradient Descent; see Chapter 11) by defining the optimizer like this:

```
optimizer = tf.train.MomentumOptimizer(learning_rate=learning_rate,
                                       momentum=0.9)
```

Feeding Data to the Training Algorithm

Let's try to modify the previous code to implement Mini-batch Gradient Descent. For this, we need a way to replace `X` and `y` at every iteration with the next mini-batch. The simplest way to do this is to use placeholder nodes. These nodes are special because they don't actually perform any computation, they just output the data you tell them to output at runtime. They are typically used to pass the training data to TensorFlow during training. If you don't specify a value at runtime for a placeholder, you get an exception.

To create a placeholder node, you must call the `placeholder()` function and specify the output tensor's data type. Optionally, you can also specify its shape, if you want to enforce it. If you specify `None` for a dimension, it means "any size." For example, the following code creates a placeholder node `A`, and also a node `B = A + 5`. When we evaluate `B`, we pass a `feed_dict` to the `eval()` method that specifies the value of `A`. Note that `A` must have rank 2 (i.e., it must be two-dimensional) and there must be three columns (or else an exception is raised), but it can have any number of rows.

```
>>> A = tf.placeholder(tf.float32, shape=(None, 3))
>>> B = A + 5
>>> with tf.Session() as sess:
...     B_val_1 = B.eval(feed_dict={A: [[1, 2, 3]]})
...     B_val_2 = B.eval(feed_dict={A: [[4, 5, 6], [7, 8, 9]]})
...
>>> print(B_val_1)
[[ 6.  7.  8.]]
>>> print(B_val_2)
[[  9.  10.  11.]
 [ 12.  13.  14.]]
```

You can actually feed the output of *any* operations, not just placeholders. In this case TensorFlow does not try to evaluate these operations; it uses the values you feed it.

To implement Mini-batch Gradient Descent, we only need to tweak the existing code slightly. First change the definition of `X` and `y` in the construction phase to make them placeholder nodes:

```
X = tf.placeholder(tf.float32, shape=(None, n + 1), name="X")
y = tf.placeholder(tf.float32, shape=(None, 1), name="y")
```

Then define the batch size and compute the total number of batches:

```
batch_size = 100
n_batches = int(np.ceil(m / batch_size))
```

Finally, in the execution phase, fetch the mini-batches one by one, then provide the value of `X` and `y` via the `feed_dict` parameter when evaluating a node that depends on either of them.

```
def fetch_batch(epoch, batch_index, batch_size):
    [...] # load the data from disk
    return X_batch, y_batch

with tf.Session() as sess:
    sess.run(init)

    for epoch in range(n_epochs):
        for batch_index in range(n_batches):
            X_batch, y_batch = fetch_batch(epoch, batch_index, batch_size)
            sess.run(training_op, feed_dict={X: X_batch, y: y_batch})
        best_theta = theta.eval()
```

We don't need to pass the value of X and y when evaluating theta since it does not depend on either of them.

Saving and Restoring Models

Once you have trained your model, you should save its parameters to disk so you can come back to it whenever you want, use it in another program, compare it to other models, and so on. Moreover, you probably want to save checkpoints at regular intervals during training so that if your computer crashes during training you can continue from the last checkpoint rather than start over from scratch.

TensorFlow makes saving and restoring a model very easy. Just create a Saver node at the end of the construction phase (after all variable nodes are created); then, in the execution phase, just call its save() method whenever you want to save the model, passing it the session and path of the checkpoint file:

```
[...]
theta = tf.Variable(tf.random_uniform([n + 1, 1], -1.0, 1.0), name="theta")
[...]
init = tf.global_variables_initializer()
saver = tf.train.Saver()

with tf.Session() as sess:
    sess.run(init)

    for epoch in range(n_epochs):
        if epoch % 100 == 0:  # checkpoint every 100 epochs
            save_path = saver.save(sess, "/tmp/my_model.ckpt")

        sess.run(training_op)

    best_theta = theta.eval()
    save_path = saver.save(sess, "/tmp/my_model_final.ckpt")
```

Restoring a model is just as easy: you create a Saver at the end of the construction phase just like before, but then at the beginning of the execution phase, instead of initializing the variables using the init node, you call the restore() method of the Saver object:

```
with tf.Session() as sess:
    saver.restore(sess, "/tmp/my_model_final.ckpt")
    [...]
```

By default a `Saver` saves and restores all variables under their own name, but if you need more control, you can specify which variables to save or restore, and what names to use. For example, the following `Saver` will save or restore only the `theta` variable under the name `weights`:

```
saver = tf.train.Saver({"weights": theta})
```

By default, the `save()` method also saves the structure of the graph in a second file with the same name plus a `.meta` extension. You can load this graph structure using `tf.train.import_meta_graph()`. This adds the graph to the default graph, and returns a `Saver` instance that you can then use to restore the graph's state (i.e., the variable values):

```
saver = tf.train.import_meta_graph("/tmp/my_model_final.ckpt.meta")

with tf.Session() as sess:
    saver.restore(sess, "/tmp/my_model_final.ckpt")
    [...]
```

This allows you to fully restore a saved model, including both the graph structure and the variable values, without having to search for the code that built it.

Visualizing the Graph and Training Curves Using TensorBoard

So now we have a computation graph that trains a Linear Regression model using Mini-batch Gradient Descent, and we are saving checkpoints at regular intervals. Sounds sophisticated, doesn't it? However, we are still relying on the `print()` function to visualize progress during training. There is a better way: enter TensorBoard. If you feed it some training stats, it will display nice interactive visualizations of these stats in your web browser (e.g., learning curves). You can also provide it the graph's definition and it will give you a great interface to browse through it. This is very useful to identify errors in the graph, to find bottlenecks, and so on.

The first step is to tweak your program a bit so it writes the graph definition and some training stats—for example, the training error (MSE)—to a log directory that TensorBoard will read from. You need to use a different log directory every time you run your program, or else TensorBoard will merge stats from different runs, which will mess up the visualizations. The simplest solution for this is to include a timestamp in the log directory name. Add the following code at the beginning of the program:

```
from datetime import datetime

now = datetime.utcnow().strftime("%Y%m%d%H%M%S")
root_logdir = "tf_logs"
logdir = "{}/run-{}/".format(root_logdir, now)
```

Next, add the following code at the very end of the construction phase:

```
mse_summary = tf.summary.scalar('MSE', mse)
file_writer = tf.summary.FileWriter(logdir, tf.get_default_graph())
```

The first line creates a node in the graph that will evaluate the MSE value and write it to a TensorBoard-compatible binary log string called a *summary*. The second line creates a `FileWriter` that you will use to write summaries to logfiles in the log directory. The first parameter indicates the path of the log directory (in this case something like *tf_logs/run-20160906091959/*, relative to the current directory). The second (optional) parameter is the graph you want to visualize. Upon creation, the `FileWriter` creates the log directory if it does not already exist (and its parent directories if needed), and writes the graph definition in a binary logfile called an *events file*.

Next you need to update the execution phase to evaluate the `mse_summary` node regularly during training (e.g., every 10 mini-batches). This will output a summary that you can then write to the events file using the `file_writer`. Here is the updated code:

```
    [...]
    for batch_index in range(n_batches):
        X_batch, y_batch = fetch_batch(epoch, batch_index, batch_size)
        if batch_index % 10 == 0:
            summary_str = mse_summary.eval(feed_dict={X: X_batch, y: y_batch})
            step = epoch * n_batches + batch_index
            file_writer.add_summary(summary_str, step)
        sess.run(training_op, feed_dict={X: X_batch, y: y_batch})
    [...]
```

Avoid logging training stats at every single training step, as this would significantly slow down training.

Finally, you want to close the `FileWriter` at the end of the program:

```
file_writer.close()
```

Now run this program: it will create the log directory and write an events file in this directory, containing both the graph definition and the MSE values. Open up a shell and go to your working directory, then type **`ls -l tf_logs/run*`** to list the contents of the log directory:

```
$ cd $ML_PATH               # Your ML working directory (e.g., $HOME/ml)
$ ls -l tf_logs/run*
total 40
-rw-r--r-- 1 ageron staff 18620 Sep 6 11:10 events.out.tfevents.1472553182.mymac
```

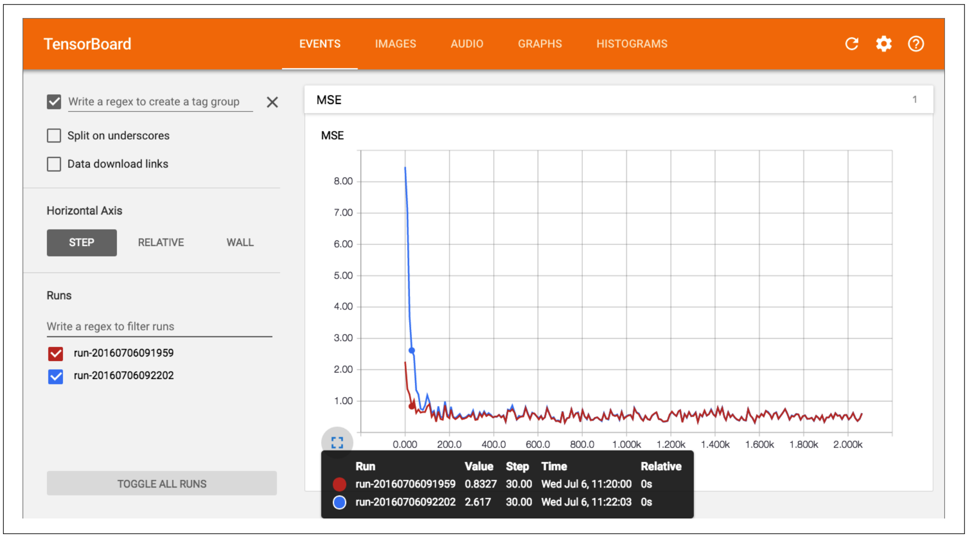
If you run the program a second time, you should see a second directory in the *tf_logs/* directory:

```
$ ls -l tf_logs/
total 0
drwxr-xr-x  3 ageron  staff  102 Sep  6 10:07 run-20160906091959
drwxr-xr-x  3 ageron  staff  102 Sep  6 10:22 run-20160906092202
```

Great! Now it's time to fire up the TensorBoard server. You need to activate your virtualenv environment if you created one, then start the server by running the `tensorboard` command, pointing it to the root log directory. This starts the TensorBoard web server, listening on port 6006 (which is "goog" written upside down):

```
$ source env/bin/activate
$ tensorboard --logdir tf_logs/
Starting TensorBoard  on port 6006
(You can navigate to http://0.0.0.0:6006)
```

Next open a browser and go to *http://0.0.0.0:6006/* (or *http://localhost:6006/*). Welcome to TensorBoard! In the Events tab you should see MSE on the right. If you click on it, you will see a plot of the MSE during training, for both runs (Figure 9-3). You can check or uncheck the runs you want to see, zoom in or out, hover over the curve to get details, and so on.



	Run	Value	Step	Time	Relative
●	run-20160706091959	0.8327	30.00	Wed Jul 6, 11:20:00	0s
●	run-20160706092202	2.617	30.00	Wed Jul 6, 11:22:03	0s

Figure 9-3. Visualizing training stats using TensorBoard

Now click on the Graphs tab. You should see the graph shown in Figure 9-4.

To reduce clutter, the nodes that have many *edges* (i.e., connections to other nodes) are separated out to an auxiliary area on the right (you can move a node back and forth between the main graph and the auxiliary area by right-clicking on it). Some parts of the graph are also collapsed by default. For example, try hovering over the `gradients` node, then click on the ⊕ icon to expand this subgraph. Next, in this subgraph, try expanding the `mse_grad` subgraph.

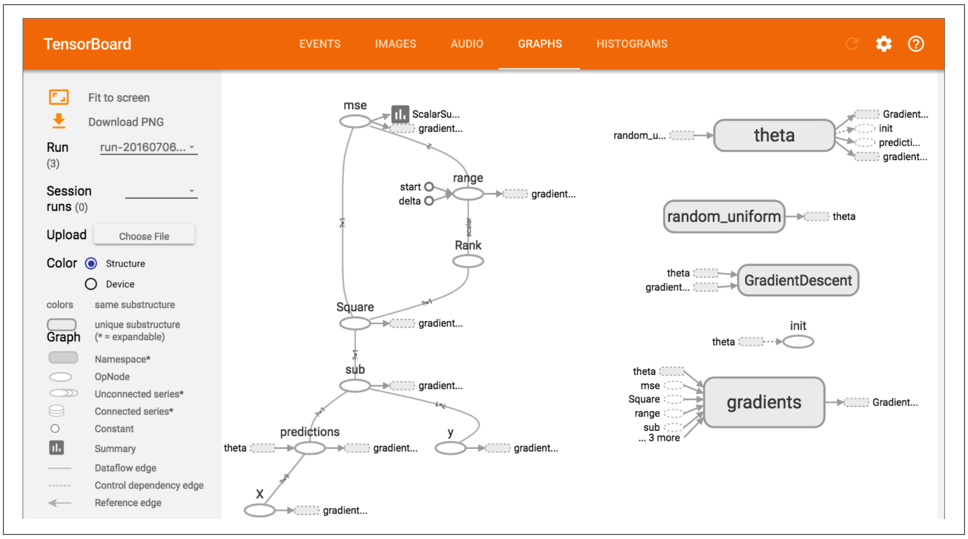


Figure 9-4. *Visualizing the graph using TensorBoard*

If you want to take a peek at the graph directly within Jupyter, you can use the `show_graph()` function available in the notebook for this chapter. It was originally written by A. Mordvintsev in his great deepdream tutorial notebook. Another option is to install E. Jang's TensorFlow debugger tool which includes a Jupyter extension for graph visualization (and more).

Name Scopes

When dealing with more complex models such as neural networks, the graph can easily become cluttered with thousands of nodes. To avoid this, you can create *name scopes* to group related nodes. For example, let's modify the previous code to define the `error` and `mse` ops within a name scope called `"loss"`:

```
with tf.name_scope("loss") as scope:
    error = y_pred - y
    mse = tf.reduce_mean(tf.square(error), name="mse")
```

The name of each op defined within the scope is now prefixed with `"loss/"`:

```
>>> print(error.op.name)
loss/sub
>>> print(mse.op.name)
loss/mse
```

In TensorBoard, the `mse` and `error` nodes now appear inside the `loss` namescope, which appears collapsed by default (Figure 9-5).

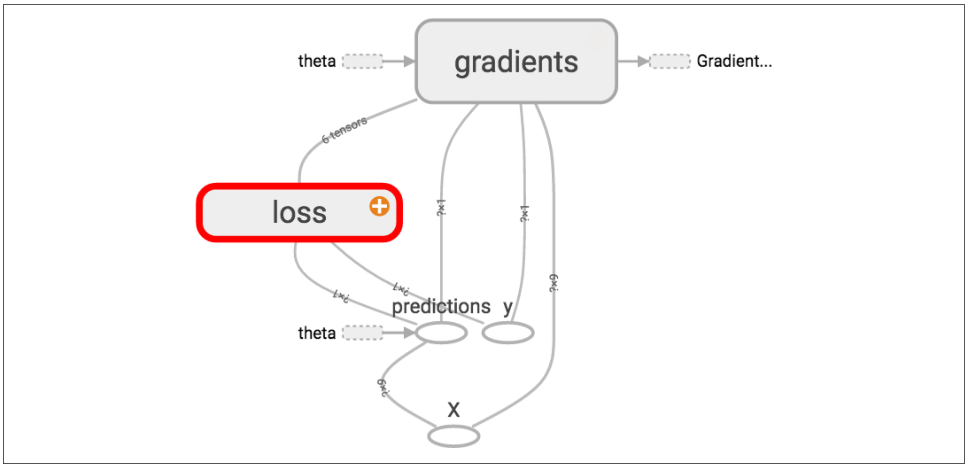


Figure 9-5. A collapsed namescope in TensorBoard

Modularity

Suppose you want to create a graph that adds the output of two *rectified linear units* (ReLU). A ReLU computes a linear function of the inputs, and outputs the result if it is positive, and 0 otherwise, as shown in Equation 9-1.

Equation 9-1. Rectified linear unit

$$h_{\mathbf{w}, b}(\mathbf{X}) = \max(\mathbf{X} \cdot \mathbf{w} + b, 0)$$

The following code does the job, but it's quite repetitive:

```
n_features = 3
X = tf.placeholder(tf.float32, shape=(None, n_features), name="X")

w1 = tf.Variable(tf.random_normal((n_features, 1)), name="weights1")
w2 = tf.Variable(tf.random_normal((n_features, 1)), name="weights2")
b1 = tf.Variable(0.0, name="bias1")
b2 = tf.Variable(0.0, name="bias2")

z1 = tf.add(tf.matmul(X, w1), b1, name="z1")
z2 = tf.add(tf.matmul(X, w2), b2, name="z2")

relu1 = tf.maximum(z1, 0., name="relu1")
relu2 = tf.maximum(z1, 0., name="relu2")

output = tf.add(relu1, relu2, name="output")
```

Such repetitive code is hard to maintain and error-prone (in fact, this code contains a cut-and-paste error; did you spot it?). It would become even worse if you wanted to add a few more ReLUs. Fortunately, TensorFlow lets you stay DRY (Don't Repeat Yourself): simply create a function to build a ReLU. The following code creates five ReLUs and outputs their sum (note that `add_n()` creates an operation that will compute the sum of a list of tensors):

```
def relu(X):
    w_shape = (int(X.get_shape()[1]), 1)
    w = tf.Variable(tf.random_normal(w_shape), name="weights")
    b = tf.Variable(0.0, name="bias")
    z = tf.add(tf.matmul(X, w), b, name="z")
    return tf.maximum(z, 0., name="relu")

n_features = 3
X = tf.placeholder(tf.float32, shape=(None, n_features), name="X")
relus = [relu(X) for i in range(5)]
output = tf.add_n(relus, name="output")
```

Note that when you create a node, TensorFlow checks whether its name already exists, and if it does it appends an underscore followed by an index to make the name unique. So the first ReLU contains nodes named `"weights"`, `"bias"`, `"z"`, and `"relu"` (plus many more nodes with their default name, such as `"MatMul"`); the second ReLU contains nodes named `"weights_1"`, `"bias_1"`, and so on; the third ReLU contains nodes named `"weights_2"`, `"bias_2"`, and so on. TensorBoard identifies such series and collapses them together to reduce clutter (as you can see in Figure 9-6).

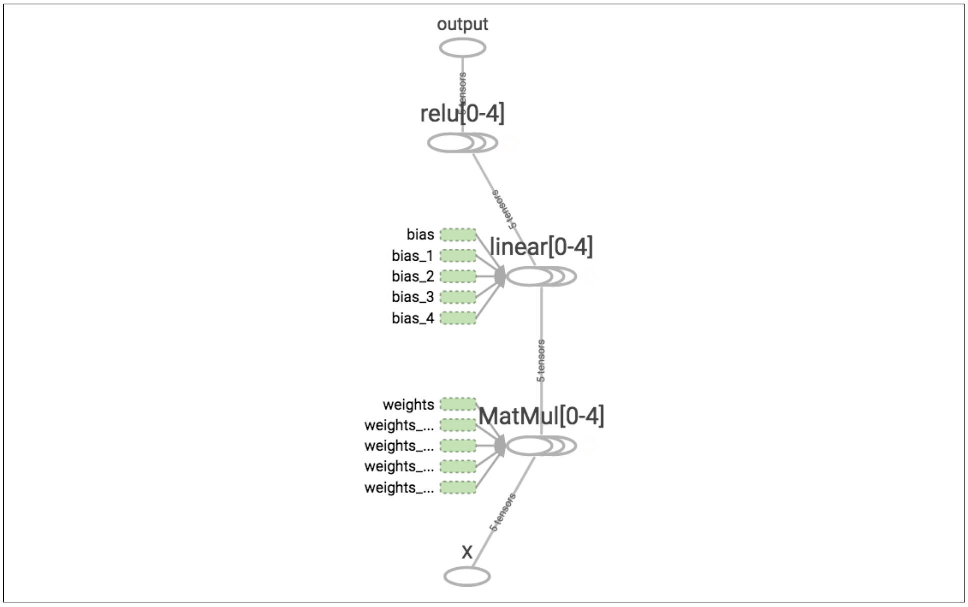


Figure 9-6. Collapsed node series

Using name scopes, you can make the graph much clearer. Simply move all the content of the `relu()` function inside a name scope. Figure 9-7 shows the resulting graph. Notice that TensorFlow also gives the name scopes unique names by appending `_1`, `_2`, and so on.

```
def relu(X):
    with tf.name_scope("relu"):
        [...]
```

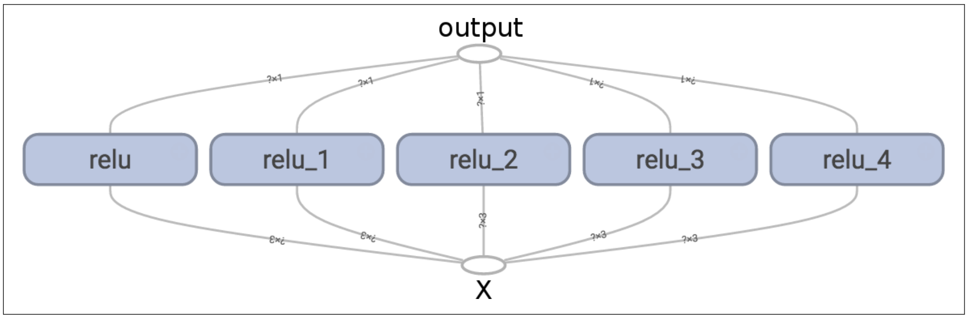


Figure 9-7. A clearer graph using name-scoped units

Sharing Variables

If you want to share a variable between various components of your graph, one simple option is to create it first, then pass it as a parameter to the functions that need it. For example, suppose you want to control the ReLU threshold (currently hardcoded to 0) using a shared `threshold` variable for all ReLUs. You could just create that variable first, and then pass it to the `relu()` function:

```
def relu(X, threshold):
    with tf.name_scope("relu"):
        [...]
        return tf.maximum(z, threshold, name="max")

threshold = tf.Variable(0.0, name="threshold")
X = tf.placeholder(tf.float32, shape=(None, n_features), name="X")
relus = [relu(X, threshold) for i in range(5)]
output = tf.add_n(relus, name="output")
```

This works fine: now you can control the threshold for all ReLUs using the `threshold` variable. However, if there are many shared parameters such as this one, it will be painful to have to pass them around as parameters all the time. Many people create a Python dictionary containing all the variables in their model, and pass it around to every function. Others create a class for each module (e.g., a `ReLU` class using class variables to handle the shared parameter). Yet another option is to set the shared variable as an attribute of the `relu()` function upon the first call, like so:

```
def relu(X):
    with tf.name_scope("relu"):
        if not hasattr(relu, "threshold"):
            relu.threshold = tf.Variable(0.0, name="threshold")
        [...]
        return tf.maximum(z, relu.threshold, name="max")
```

TensorFlow offers another option, which may lead to slightly cleaner and more modular code than the previous solutions.[5] This solution is a bit tricky to understand at first, but since it is used a lot in TensorFlow it is worth going into a bit of detail. The idea is to use the `get_variable()` function to create the shared variable if it does not exist yet, or reuse it if it already exists. The desired behavior (creating or reusing) is controlled by an attribute of the current `variable_scope()`. For example, the following code will create a variable named `"relu/threshold"` (as a scalar, since `shape=()`, and using `0.0` as the initial value):

```
with tf.variable_scope("relu"):
    threshold = tf.get_variable("threshold", shape=(),
                                initializer=tf.constant_initializer(0.0))
```

Note that if the variable has already been created by an earlier call to `get_variable()`, this code will raise an exception. This behavior prevents reusing variables by mistake. If you want to reuse a variable, you need to explicitly say so by setting the variable scope's `reuse` attribute to `True` (in which case you don't have to specify the shape or the initializer):

```
with tf.variable_scope("relu", reuse=True):
    threshold = tf.get_variable("threshold")
```

This code will fetch the existing `"relu/threshold"` variable, or raise an exception if it does not exist or if it was not created using `get_variable()`. Alternatively, you can set the `reuse` attribute to `True` inside the block by calling the scope's `reuse_variables()` method:

```
with tf.variable_scope("relu") as scope:
    scope.reuse_variables()
    threshold = tf.get_variable("threshold")
```

Once `reuse` is set to `True`, it cannot be set back to `False` within the block. Moreover, if you define other variable scopes inside this one, they will automatically inherit `reuse=True`. Lastly, only variables created by `get_variable()` can be reused this way.

5 Creating a `ReLU` class is arguably the cleanest option, but it is rather heavyweight.

Now you have all the pieces you need to make the `relu()` function access the `threshold` variable without having to pass it as a parameter:

```
def relu(X):
    with tf.variable_scope("relu", reuse=True):
        threshold = tf.get_variable("threshold")  # reuse existing variable
        [...]
        return tf.maximum(z, threshold, name="max")

X = tf.placeholder(tf.float32, shape=(None, n_features), name="X")
with tf.variable_scope("relu"):  # create the variable
    threshold = tf.get_variable("threshold", shape=(),
                                initializer=tf.constant_initializer(0.0))
relus = [relu(X) for relu_index in range(5)]
output = tf.add_n(relus, name="output")
```

This code first defines the `relu()` function, then creates the `relu/threshold` variable (as a scalar that will later be initialized to `0.0`) and builds five ReLUs by calling the `relu()` function. The `relu()` function reuses the `relu/threshold` variable, and creates the other ReLU nodes.

Variables created using `get_variable()` are always named using the name of their `variable_scope` as a prefix (e.g., `"relu/threshold"`), but for all other nodes (including variables created with `tf.Variable()`) the variable scope acts like a new name scope. In particular, if a name scope with an identical name was already created, then a suffix is added to make the name unique. For example, all nodes created in the preceding code (except the `threshold` variable) have a name prefixed with `"relu_1/"` to `"relu_5/"`, as shown in Figure 9-8.

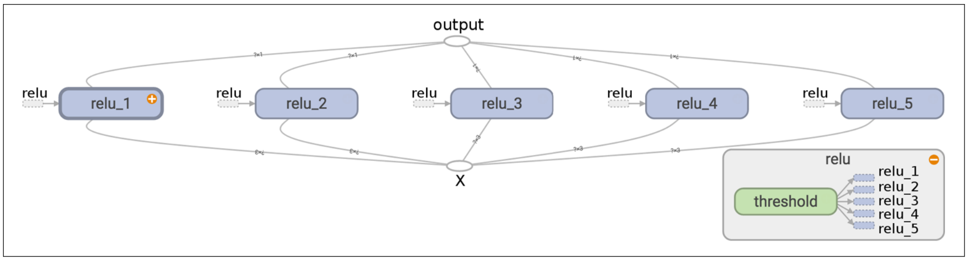


Figure 9-8. Five ReLUs sharing the threshold variable

It is somewhat unfortunate that the `threshold` variable must be defined outside the `relu()` function, where all the rest of the ReLU code resides. To fix this, the following code creates the `threshold` variable within the `relu()` function upon the first call, then reuses it in subsequent calls. Now the `relu()` function does not have to worry about name scopes or variable sharing: it just calls `get_variable()`, which will create or reuse the threshold variable (it does not need to know which is the case). The rest of the code calls relu() five times, making sure to set reuse=False on the first call, and reuse=True for the other calls.

```
def relu(X):
    threshold = tf.get_variable("threshold", shape=(),
                                initializer=tf.constant_initializer(0.0))
    [...]
    return tf.maximum(z, threshold, name="max")

X = tf.placeholder(tf.float32, shape=(None, n_features), name="X")
relus = []
for relu_index in range(5):
    with tf.variable_scope("relu", reuse=(relu_index >= 1)) as scope:
        relus.append(relu(X))
output = tf.add_n(relus, name="output")
```

The resulting graph is slightly different than before, since the shared variable lives within the first ReLU (see Figure 9-9).

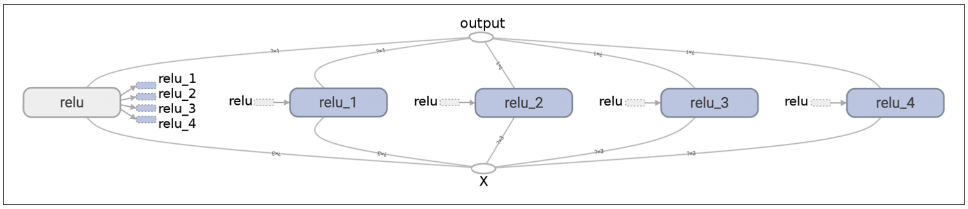


Figure 9-9. Five ReLUs sharing the threshold variable

This concludes this introduction to TensorFlow. We will discuss more advanced topics as we go through the following chapters, in particular many operations related to deep neural networks, convolutional neural networks, and recurrent neural networks as well as how to scale up with TensorFlow using multithreading, queues, multiple GPUs, and multiple servers.

Exercises

1. What are the main benefits of creating a computation graph rather than directly executing the computations? What are the main drawbacks?
2. Is the statement `a_val = a.eval(session=sess)` equivalent to `a_val = sess.run(a)`?
3. Is the statement `a_val, b_val = a.eval(session=sess), b.eval(session=sess)` equivalent to `a_val, b_val = sess.run([a, b])`?
4. Can you run two graphs in the same session?

5. If you create a graph `g` containing a variable `w`, then start two threads and open a session in each thread, both using the same graph `g`, will each session have its own copy of the variable `w` or will it be shared?
6. When is a variable initialized? When is it destroyed?
7. What is the difference between a placeholder and a variable?
8. What happens when you run the graph to evaluate an operation that depends on a placeholder but you don't feed its value? What happens if the operation does not depend on the placeholder?
9. When you run a graph, can you feed the output value of any operation, or just the value of placeholders?
10. How can you set a variable to any value you want (during the execution phase)?
11. How many times does reverse-mode autodiff need to traverse the graph in order to compute the gradients of the cost function with regards to 10 variables? What about forward-mode autodiff? And symbolic differentiation?
12. Implement Logistic Regression with Mini-batch Gradient Descent using TensorFlow. Train it and evaluate it on the moons dataset (introduced in Chapter 5). Try adding all the bells and whistles:

    - Define the graph within a `logistic_regression()` function that can be reused easily.
    - Save checkpoints using a `Saver` at regular intervals during training, and save the final model at the end of training.
    - Restore the last checkpoint upon startup if training was interrupted.
    - Define the graph using name scopes so the graph looks good in TensorBoard.
    - Add summaries to visualize the learning curves in TensorBoard.
    - Try tweaking some hyperparameters such as the learning rate or the mini-batch size and look at the shape of the learning curve.

Solutions to these exercises are available in Appendix A.

CHAPTER 10

Introduction to Artificial Neural Networks

Birds inspired us to fly, burdock plants inspired velcro, and nature has inspired many other inventions. It seems only logical, then, to look at the brain's architecture for inspiration on how to build an intelligent machine. This is the key idea that inspired *artificial neural networks* (ANNs). However, although planes were inspired by birds, they don't have to flap their wings. Similarly, ANNs have gradually become quite different from their biological cousins. Some researchers even argue that we should drop the biological analogy altogether (e.g., by saying "units" rather than "neurons"), lest we restrict our creativity to biologically plausible systems.[1]

ANNs are at the very core of Deep Learning. They are versatile, powerful, and scalable, making them ideal to tackle large and highly complex Machine Learning tasks, such as classifying billions of images (e.g., Google Images), powering speech recognition services (e.g., Apple's Siri), recommending the best videos to watch to hundreds of millions of users every day (e.g., YouTube), or learning to beat the world champion at the game of *Go* by examining millions of past games and then playing against itself (DeepMind's AlphaGo).

In this chapter, we will introduce artificial neural networks, starting with a quick tour of the very first ANN architectures. Then we will present *Multi-Layer Perceptrons* (MLPs) and implement one using TensorFlow to tackle the MNIST digit classification problem (introduced in Chapter 3).

1 You can get the best of both worlds by being open to biological inspirations without being afraid to create biologically unrealistic models, as long as they work well.

From Biological to Artificial Neurons

Surprisingly, ANNs have been around for quite a while: they were first introduced back in 1943 by the neurophysiologist Warren McCulloch and the mathematician Walter Pitts. In their landmark paper,[2] "A Logical Calculus of Ideas Immanent in Nervous Activity," McCulloch and Pitts presented a simplified computational model of how biological neurons might work together in animal brains to perform complex computations using *propositional logic*. This was the first artificial neural network architecture. Since then many other architectures have been invented, as we will see.

The early successes of ANNs until the 1960s led to the widespread belief that we would soon be conversing with truly intelligent machines. When it became clear that this promise would go unfulfilled (at least for quite a while), funding flew elsewhere and ANNs entered a long dark era. In the early 1980s there was a revival of interest in ANNs as new network architectures were invented and better training techniques were developed. But by the 1990s, powerful alternative Machine Learning techniques such as Support Vector Machines (see Chapter 5) were favored by most researchers, as they seemed to offer better results and stronger theoretical foundations. Finally, we are now witnessing yet another wave of interest in ANNs. Will this wave die out like the previous ones did? There are a few good reasons to believe that this one is different and will have a much more profound impact on our lives:

- There is now a huge quantity of data available to train neural networks, and ANNs frequently outperform other ML techniques on very large and complex problems.
- The tremendous increase in computing power since the 1990s now makes it possible to train large neural networks in a reasonable amount of time. This is in part due to Moore's Law, but also thanks to the gaming industry, which has produced powerful GPU cards by the millions.
- The training algorithms have been improved. To be fair they are only slightly different from the ones used in the 1990s, but these relatively small tweaks have a huge positive impact.
- Some theoretical limitations of ANNs have turned out to be benign in practice. For example, many people thought that ANN training algorithms were doomed because they were likely to get stuck in local optima, but it turns out that this is rather rare in practice (or when it is the case, they are usually fairly close to the global optimum).
- ANNs seem to have entered a virtuous circle of funding and progress. Amazing products based on ANNs regularly make the headline news, which pulls more

2 "A Logical Calculus of Ideas Immanent in Nervous Activity," W. McCulloch and W. Pitts (1943).

and more attention and funding toward them, resulting in more and more progress, and even more amazing products.

Biological Neurons

Before we discuss artificial neurons, let's take a quick look at a biological neuron (represented in Figure 10-1). It is an unusual-looking cell mostly found in animal cerebral cortexes (e.g., your brain), composed of a *cell body* containing the nucleus and most of the cell's complex components, and many branching extensions called *dendrites*, plus one very long extension called the *axon*. The axon's length may be just a few times longer than the cell body, or up to tens of thousands of times longer. Near its extremity the axon splits off into many branches called *telodendria*, and at the tip of these branches are minuscule structures called *synaptic terminals* (or simply *synapses*), which are connected to the dendrites (or directly to the cell body) of other neurons. Biological neurons receive short electrical impulses called *signals* from other neurons via these synapses. When a neuron receives a sufficient number of signals from other neurons within a few milliseconds, it fires its own signals.

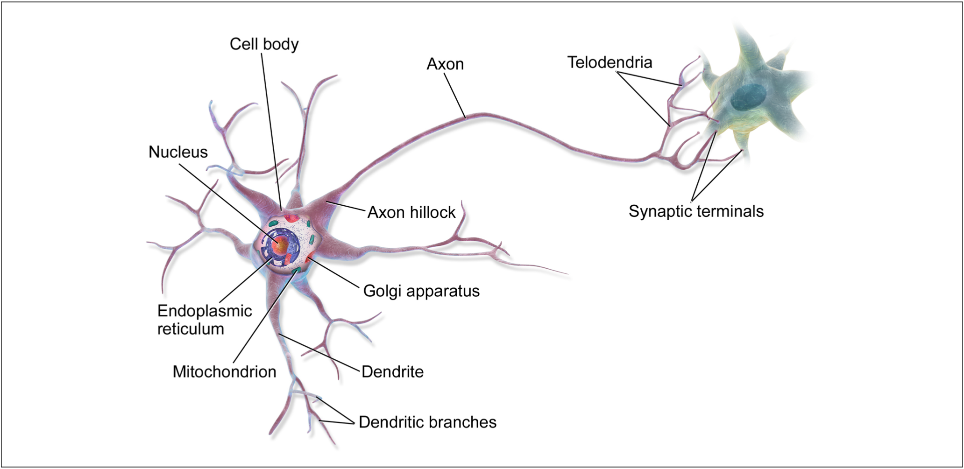


Figure 10-1. Biological neuron[3]

Thus, individual biological neurons seem to behave in a rather simple way, but they are organized in a vast network of billions of neurons, each neuron typically connected to thousands of other neurons. Highly complex computations can be performed by a vast network of fairly simple neurons, much like a complex anthill can emerge from the combined efforts of simple ants. The architecture of biological neural net-

3 Image by Bruce Blaus (Creative Commons 3.0). Reproduced from *https://en.wikipedia.org/wiki/Neuron*.

works (BNN)[4] is still the subject of active research, but some parts of the brain have been mapped, and it seems that neurons are often organized in consecutive layers, as shown in Figure 10-2.

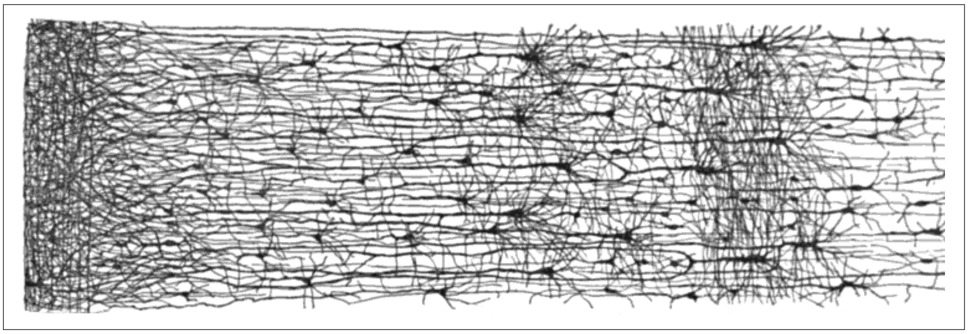


Figure 10-2. Multiple layers in a biological neural network (human cortex)[5]

Logical Computations with Neurons

Warren McCulloch and Walter Pitts proposed a very simple model of the biological neuron, which later became known as an *artificial neuron*: it has one or more binary (on/off) inputs and one binary output. The artificial neuron simply activates its output when more than a certain number of its inputs are active. McCulloch and Pitts showed that even with such a simplified model it is possible to build a network of artificial neurons that computes any logical proposition you want. For example, let's build a few ANNs that perform various logical computations (see Figure 10-3), assuming that a neuron is activated when at least two of its inputs are active.

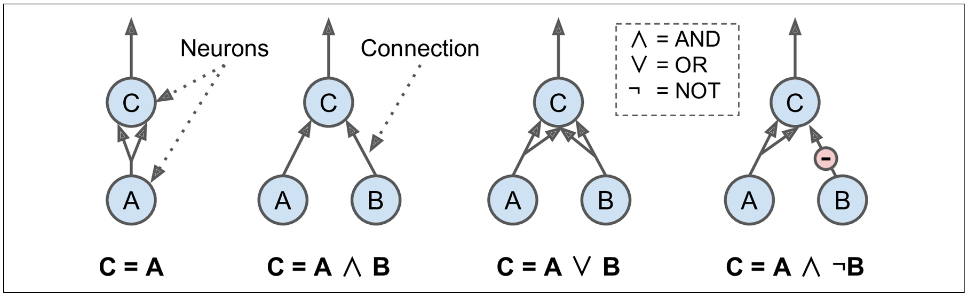


Figure 10-3. ANNs performing simple logical computations

4 In the context of Machine Learning, the phrase "neural networks" generally refers to ANNs, not BNNs.

5 Drawing of a cortical lamination by S. Ramon y Cajal (public domain). Reproduced from *https://en.wikipedia.org/wiki/Cerebral_cortex*.

- The first network on the left is simply the identity function: if neuron A is activated, then neuron C gets activated as well (since it receives two input signals from neuron A), but if neuron A is off, then neuron C is off as well.
- The second network performs a logical AND: neuron C is activated only when both neurons A and B are activated (a single input signal is not enough to activate neuron C).
- The third network performs a logical OR: neuron C gets activated if either neuron A or neuron B is activated (or both).
- Finally, if we suppose that an input connection can inhibit the neuron's activity (which is the case with biological neurons), then the fourth network computes a slightly more complex logical proposition: neuron C is activated only if neuron A is active and if neuron B is off. If neuron A is active all the time, then you get a logical NOT: neuron C is active when neuron B is off, and vice versa.

You can easily imagine how these networks can be combined to compute complex logical expressions (see the exercises at the end of the chapter).

The Perceptron

The *Perceptron* is one of the simplest ANN architectures, invented in 1957 by Frank Rosenblatt. It is based on a slightly different artificial neuron (see Figure 10-4) called a *linear threshold unit* (LTU): the inputs and output are now numbers (instead of binary on/off values) and each input connection is associated with a weight. The LTU computes a weighted sum of its inputs ($z = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n = \mathbf{w}^T \cdot \mathbf{x}$), then applies a *step function* to that sum and outputs the result: $h_\mathbf{w}(\mathbf{x}) = \text{step}(z) = \text{step}(\mathbf{w}^T \cdot \mathbf{x})$.

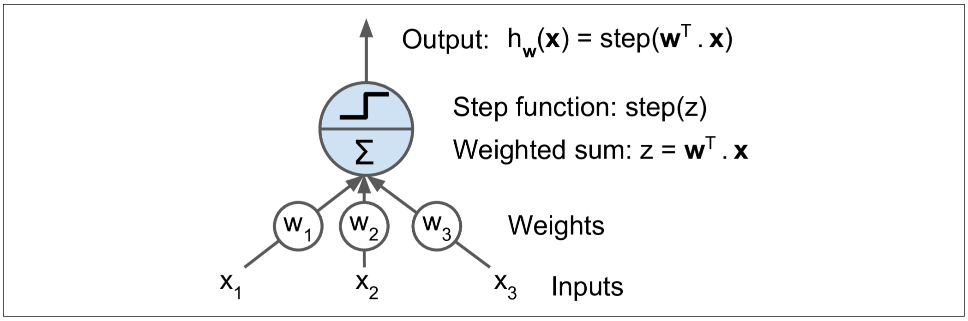

Output: $h_\mathbf{w}(\mathbf{x}) = \text{step}(\mathbf{w}^T . \mathbf{x})$
Step function: step(z)
Weighted sum: $z = \mathbf{w}^T . \mathbf{x}$
Σ
w_1
w_2
w_3
Weights
x_1
x_2
x_3
Inputs

Figure 10-4. Linear threshold unit

The most common step function used in Perceptrons is the *Heaviside step function* (see Equation 10-1). Sometimes the sign function is used instead.

Equation 10-1. Common step functions used in Perceptrons

$$\text{heaviside}\,(z) = \begin{cases} 0 & \text{if } z < 0 \\ 1 & \text{if } z \ge 0 \end{cases} \qquad \text{sgn}\,(z) = \begin{cases} -1 & \text{if } z < 0 \\ 0 & \text{if } z = 0 \\ +1 & \text{if } z > 0 \end{cases}$$

A single LTU can be used for simple linear binary classification. It computes a linear combination of the inputs and if the result exceeds a threshold, it outputs the positive class or else outputs the negative class (just like a Logistic Regression classifier or a linear SVM). For example, you could use a single LTU to classify iris flowers based on the petal length and width (also adding an extra bias feature $x_0 = 1$, just like we did in previous chapters). Training an LTU means finding the right values for w_0, w_1, and w_2 (the training algorithm is discussed shortly).

A Perceptron is simply composed of a single layer of LTUs,[6] with each neuron connected to all the inputs. These connections are often represented using special passthrough neurons called *input neurons*: they just output whatever input they are fed. Moreover, an extra bias feature is generally added ($x_0 = 1$). This bias feature is typically represented using a special type of neuron called a *bias neuron*, which just outputs 1 all the time.

A Perceptron with two inputs and three outputs is represented in Figure 10-5. This Perceptron can classify instances simultaneously into three different binary classes, which makes it a multioutput classifier.

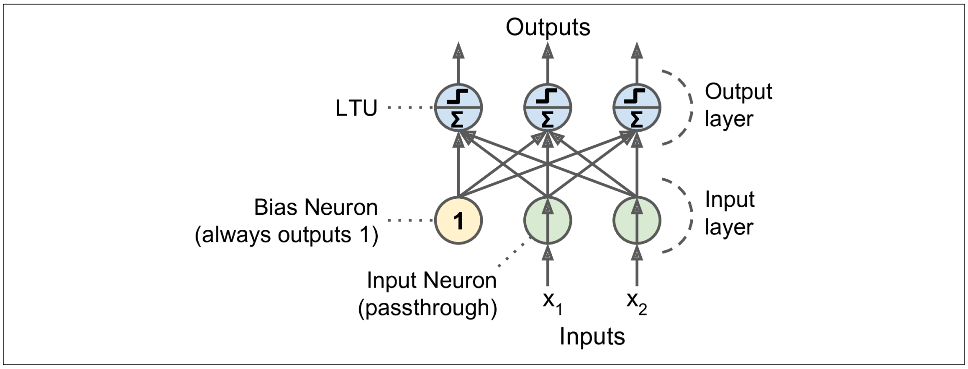


Figure 10-5. Perceptron diagram

So how is a Perceptron trained? The Perceptron training algorithm proposed by Frank Rosenblatt was largely inspired by *Hebb's rule*. In his book *The Organization of Behavior*, published in 1949, Donald Hebb suggested that when a biological neuron

6 The name *Perceptron* is sometimes used to mean a tiny network with a single LTU.

often triggers another neuron, the connection between these two neurons grows stronger. This idea was later summarized by Siegrid Löwel in this catchy phrase: "Cells that fire together, wire together." This rule later became known as Hebb's rule (or *Hebbian learning*); that is, the connection weight between two neurons is increased whenever they have the same output. Perceptrons are trained using a variant of this rule that takes into account the error made by the network; it does not reinforce connections that lead to the wrong output. More specifically, the Perceptron is fed one training instance at a time, and for each instance it makes its predictions. For every output neuron that produced a wrong prediction, it reinforces the connection weights from the inputs that would have contributed to the correct prediction. The rule is shown in Equation 10-2.

Equation 10-2. Perceptron learning rule (weight update)

$$w_{i,j}^{(\text{next step})} = w_{i,j} + \eta\left(y_j - \hat{y}_j\right)x_i$$

- $w_{i,j}$ is the connection weight between the ith input neuron and the jth output neuron.
- x_i is the ith input value of the current training instance.
- $\hat{y}_j$ is the output of the jth output neuron for the current training instance.
- y_j is the target output of the jth output neuron for the current training instance.
- η is the learning rate.

The decision boundary of each output neuron is linear, so Perceptrons are incapable of learning complex patterns (just like Logistic Regression classifiers). However, if the training instances are linearly separable, Rosenblatt demonstrated that this algorithm would converge to a solution.[7] This is called the *Perceptron convergence theorem*.

Scikit-Learn provides a `Perceptron` class that implements a single LTU network. It can be used pretty much as you would expect—for example, on the iris dataset (introduced in Chapter 4):

```python
import numpy as np
from sklearn.datasets import load_iris
from sklearn.linear_model import Perceptron

iris = load_iris()
X = iris.data[:, (2, 3)]  # petal length, petal width
y = (iris.target == 0).astype(np.int)  # Iris Setosa?
```

7 Note that this solution is generally not unique: in general when the data are linearly separable, there is an infinity of hyperplanes that can separate them.

```
per_clf = Perceptron(random_state=42)
per_clf.fit(X, y)

y_pred = per_clf.predict([[2, 0.5]])
```

You may have recognized that the Perceptron learning algorithm strongly resembles Stochastic Gradient Descent. In fact, Scikit-Learn's `Perceptron` class is equivalent to using an `SGDClassifier` with the following hyperparameters: `loss="perceptron"`, `learning_rate="constant"`, `eta0=1` (the learning rate), and `penalty=None` (no regularization).

Note that contrary to Logistic Regression classifiers, Perceptrons do not output a class probability; rather, they just make predictions based on a hard threshold. This is one of the good reasons to prefer Logistic Regression over Perceptrons.

In their 1969 monograph titled *Perceptrons*, Marvin Minsky and Seymour Papert highlighted a number of serious weaknesses of Perceptrons, in particular the fact that they are incapable of solving some trivial problems (e.g., the *Exclusive OR* (XOR) classification problem; see the left side of Figure 10-6). Of course this is true of any other linear classification model as well (such as Logistic Regression classifiers), but researchers had expected much more from Perceptrons, and their disappointment was great: as a result, many researchers dropped *connectionism* altogether (i.e., the study of neural networks) in favor of higher-level problems such as logic, problem solving, and search.

However, it turns out that some of the limitations of Perceptrons can be eliminated by stacking multiple Perceptrons. The resulting ANN is called a *Multi-Layer Perceptron* (MLP). In particular, an MLP can solve the XOR problem, as you can verify by computing the output of the MLP represented on the right of Figure 10-6, for each combination of inputs: with inputs (0, 0) or (1, 1) the network outputs 0, and with inputs (0, 1) or (1, 0) it outputs 1.

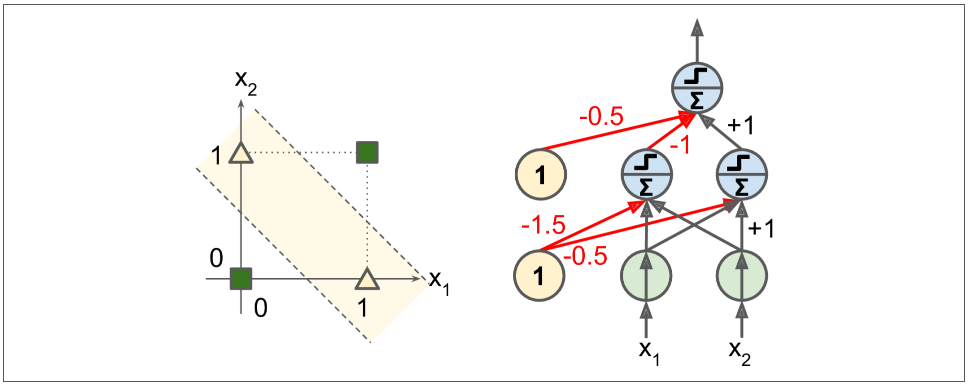


Figure 10-6. XOR classification problem and an MLP that solves it

Multi-Layer Perceptron and Backpropagation

An MLP is composed of one (passthrough) input layer, one or more layers of LTUs, called *hidden layers*, and one final layer of LTUs called the *output layer* (see Figure 10-7). Every layer except the output layer includes a bias neuron and is fully connected to the next layer. When an ANN has two or more hidden layers, it is called a *deep neural network* (DNN).

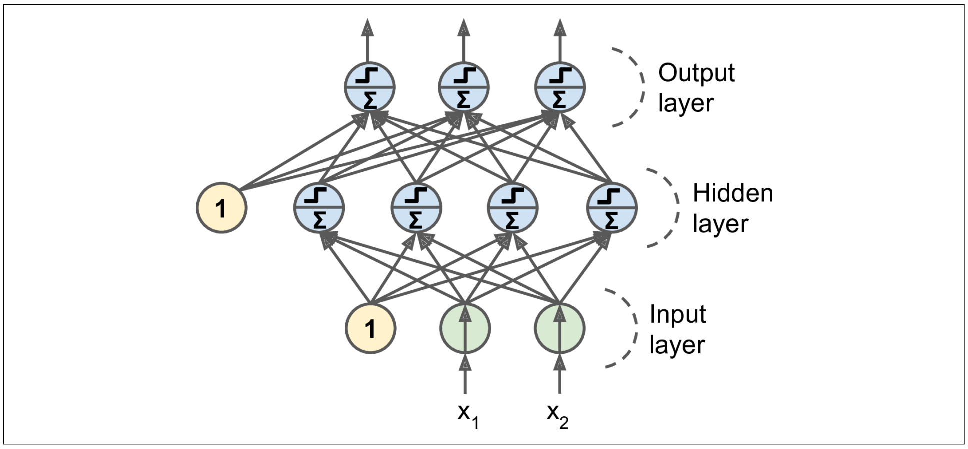


Figure 10-7. Multi-Layer Perceptron

For many years researchers struggled to find a way to train MLPs, without success. But in 1986, D. E. Rumelhart et al. published a groundbreaking article[8] introducing the *backpropagation* training algorithm.[9] Today we would describe it as Gradient Descent using reverse-mode autodiff (Gradient Descent was introduced in Chapter 4, and autodiff was discussed in Chapter 9).

For each training instance, the algorithm feeds it to the network and computes the output of every neuron in each consecutive layer (this is the forward pass, just like when making predictions). Then it measures the network's output error (i.e., the difference between the desired output and the actual output of the network), and it computes how much each neuron in the last hidden layer contributed to each output neuron's error. It then proceeds to measure how much of these error contributions came from each neuron in the previous hidden layer—and so on until the algorithm reaches the input layer. This reverse pass efficiently measures the error gradient across all the connection weights in the network by propagating the error gradient backward in the network (hence the name of the algorithm). If you check out the

8 "Learning Internal Representations by Error Propagation," D. Rumelhart, G. Hinton, R. Williams (1986).

9 This algorithm was actually invented several times by various researchers in different fields, starting with P. Werbos in 1974.

reverse-mode autodiff algorithm in Appendix D, you will find that the forward and reverse passes of backpropagation simply perform reverse-mode autodiff. The last step of the backpropagation algorithm is a Gradient Descent step on all the connection weights in the network, using the error gradients measured earlier.

Let's make this even shorter: for each training instance the backpropagation algorithm first makes a prediction (forward pass), measures the error, then goes through each layer in reverse to measure the error contribution from each connection (reverse pass), and finally slightly tweaks the connection weights to reduce the error (Gradient Descent step).

In order for this algorithm to work properly, the authors made a key change to the MLP's architecture: they replaced the step function with the logistic function, $\sigma(z) = 1 / (1 + \exp(-z))$. This was essential because the step function contains only flat segments, so there is no gradient to work with (Gradient Descent cannot move on a flat surface), while the logistic function has a well-defined nonzero derivative everywhere, allowing Gradient Descent to make some progress at every step. The backpropagation algorithm may be used with other *activation functions*, instead of the logistic function. Two other popular activation functions are:

The hyperbolic tangent function $\tanh(z) = 2\sigma(2z) - 1$
: Just like the logistic function it is S-shaped, continuous, and differentiable, but its output value ranges from –1 to 1 (instead of 0 to 1 in the case of the logistic function), which tends to make each layer's output more or less normalized (i.e., centered around 0) at the beginning of training. This often helps speed up convergence.

The ReLU function (introduced in Chapter 9)
: $\text{ReLU}(z) = \max(0, z)$. It is continuous but unfortunately not differentiable at $z = 0$ (the slope changes abruptly, which can make Gradient Descent bounce around). However, in practice it works very well and has the advantage of being fast to compute. Most importantly, the fact that it does not have a maximum output value also helps reduce some issues during Gradient Descent (we will come back to this in Chapter 11).

These popular activation functions and their derivatives are represented in Figure 10-8.

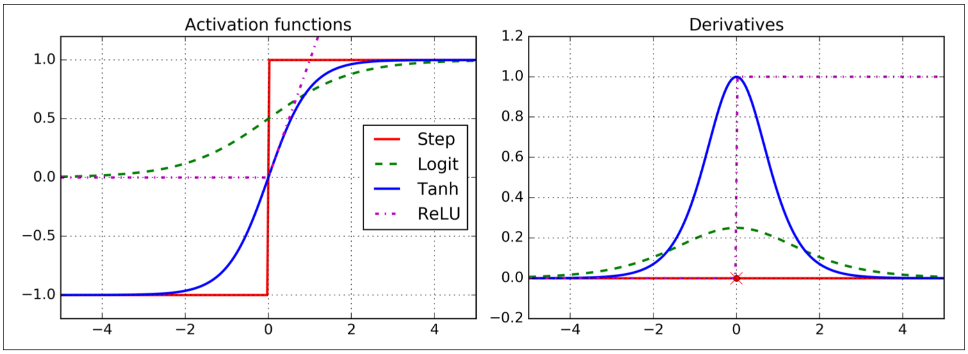


Figure 10-8. Activation functions and their derivatives

An MLP is often used for classification, with each output corresponding to a different binary class (e.g., spam/ham, urgent/not-urgent, and so on). When the classes are exclusive (e.g., classes 0 through 9 for digit image classification), the output layer is typically modified by replacing the individual activation functions by a shared *softmax* function (see Figure 10-9). The softmax function was introduced in Chapter 4. The output of each neuron corresponds to the estimated probability of the corresponding class. Note that the signal flows only in one direction (from the inputs to the outputs), so this architecture is an example of a *feedforward neural network* (FNN).

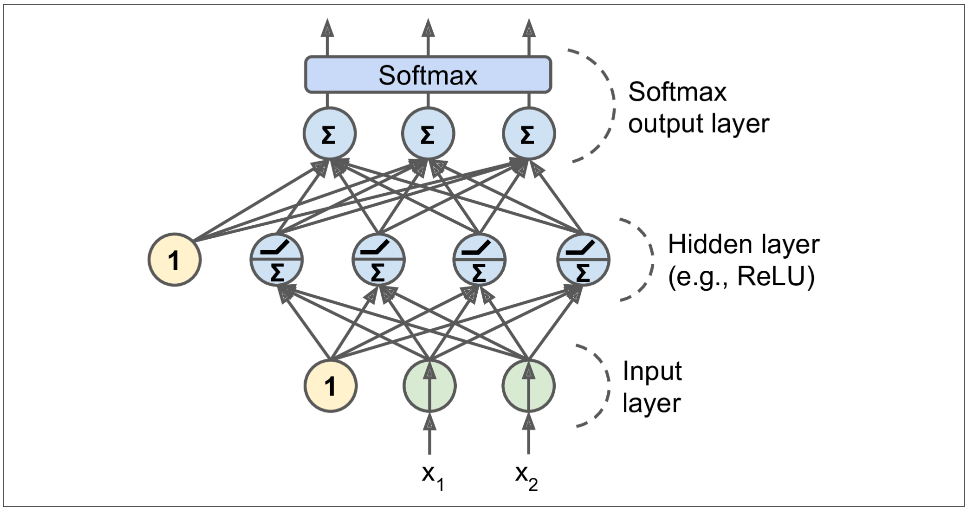


Figure 10-9. A modern MLP (including ReLU and softmax) for classification

Biological neurons seem to implement a roughly sigmoid (S-shaped) activation function, so researchers stuck to sigmoid functions for a very long time. But it turns out that the ReLU activation function generally works better in ANNs. This is one of the cases where the biological analogy was misleading.

Training an MLP with TensorFlow's High-Level API

The simplest way to train an MLP with TensorFlow is to use the high-level API TF.Learn, which offers a Scikit-Learn–compatible API. The `DNNClassifier` class makes it fairly easy to train a deep neural network with any number of hidden layers, and a softmax output layer to output estimated class probabilities. For example, the following code trains a DNN for classification with two hidden layers (one with 300 neurons, and the other with 100 neurons) and a softmax output layer with 10 neurons:

```
import tensorflow as tf

feature_cols = tf.contrib.learn.infer_real_valued_columns_from_input(X_train)
dnn_clf = tf.contrib.learn.DNNClassifier(hidden_units=[300,100], n_classes=10,
                                         feature_columns=feature_cols)
dnn_clf = tf.contrib.learn.SKCompat(dnn_clf)  # if TensorFlow >= 1.1
dnn_clf.fit(X_train, y_train, batch_size=50, steps=40000)
```

The code first creates a set of real valued columns from the training set (other types of columns, such as categorical columns, are available). Then we create the `DNNClassifier`, and we wrap it in a Scikit-Learn compatibility helper. Finally, we run 40,000 training iterations using batches of 50 instances.

If you run this code on the MNIST dataset (after scaling it, e.g., by using Scikit-Learn's `StandardScaler`), you will actually get a model that achieves around 98.2% accuracy on the test set! That's better than the best model we trained in Chapter 3:

```
>>> from sklearn.metrics import accuracy_score
>>> y_pred = dnn_clf.predict(X_test)
>>> accuracy_score(y_test, y_pred['classes'])
0.98250000000000004
```

The `tensorflow.contrib` package contains many useful functions, but it is a place for experimental code that has not yet graduated to be part of the core TensorFlow API. So the `DNNClassifier` class (and any other `contrib` code) may change without notice in the future.

Under the hood, the `DNNClassifier` class creates all the neuron layers, based on the ReLU activation function (we can change this by setting the `activation_fn` hyperparameter). The output layer relies on the softmax function, and the cost function is cross entropy (introduced in Chapter 4).

Training a DNN Using Plain TensorFlow

If you want more control over the architecture of the network, you may prefer to use TensorFlow's lower-level Python API (introduced in Chapter 9). In this section we will build the same model as before using this API, and we will implement Mini-batch Gradient Descent to train it on the MNIST dataset. The first step is the construction phase, building the TensorFlow graph. The second step is the execution phase, where you actually run the graph to train the model.

Construction Phase

Let's start. First we need to import the `tensorflow` library. Then we must specify the number of inputs and outputs, and set the number of hidden neurons in each layer:

```
import tensorflow as tf

n_inputs = 28*28  # MNIST
n_hidden1 = 300
n_hidden2 = 100
n_outputs = 10
```

Next, just like you did in Chapter 9, you can use placeholder nodes to represent the training data and targets. The shape of `X` is only partially defined. We know that it will be a 2D tensor (i.e., a matrix), with instances along the first dimension and features along the second dimension, and we know that the number of features is going to be 28 x 28 (one feature per pixel), but we don't know yet how many instances each training batch will contain. So the shape of `X` is `(None, n_inputs)`. Similarly, we know that `y` will be a 1D tensor with one entry per instance, but again we don't know the size of the training batch at this point, so the shape is `(None)`.

```
X = tf.placeholder(tf.float32, shape=(None, n_inputs), name="X")
y = tf.placeholder(tf.int64, shape=(None), name="y")
```

Now let's create the actual neural network. The placeholder `X` will act as the input layer; during the execution phase, it will be replaced with one training batch at a time (note that all the instances in a training batch will be processed simultaneously by the neural network). Now you need to create the two hidden layers and the output layer. The two hidden layers are almost identical: they differ only by the inputs they are connected to and by the number of neurons they contain. The output layer is also very similar, but it uses a softmax activation function instead of a ReLU activation function. So let's create a `neuron_layer()` function that we will use to create one layer at a time. It will need parameters to specify the inputs, the number of neurons, the activation function, and the name of the layer:

```python
def neuron_layer(X, n_neurons, name, activation=None):
    with tf.name_scope(name):
        n_inputs = int(X.get_shape()[1])
        stddev = 2 / np.sqrt(n_inputs + n_neurons)
        init = tf.truncated_normal((n_inputs, n_neurons), stddev=stddev)
        W = tf.Variable(init, name="kernel")
        b = tf.Variable(tf.zeros([n_neurons]), name="bias")
        Z = tf.matmul(X, W) + b
        if activation is not None:
            return activation(Z)
        else:
            return Z
```

Let's go through this code line by line:

1. First we create a name scope using the name of the layer: it will contain all the computation nodes for this neuron layer. This is optional, but the graph will look much nicer in TensorBoard if its nodes are well organized.
2. Next, we get the number of inputs by looking up the input matrix's shape and getting the size of the second dimension (the first dimension is for instances).
3. The next three lines create a `W` variable that will hold the weights matrix (often called the layer's *kernel*). It will be a 2D tensor containing all the connection weights between each input and each neuron; hence, its shape will be `(n_inputs, n_neurons)`. It will be initialized randomly, using a truncated[10] normal (Gaussian) distribution with a standard deviation of $2/\sqrt{\mathrm{n}_{\text{inputs}} + \mathrm{n}_{\text{neurons}}}$. Using this specific standard deviation helps the algorithm converge much faster (we will discuss this further in Chapter 11; it is one of those small tweaks to neural networks that have had a tremendous impact on their efficiency). It is important to initialize connection weights randomly for all hidden layers to avoid any symmetries that the Gradient Descent algorithm would be unable to break.[11]
4. The next line creates a `b` variable for biases, initialized to 0 (no symmetry issue in this case), with one bias parameter per neuron.
5. Then we create a subgraph to compute $\mathbf{Z} = \mathbf{X} \cdot \mathbf{W} + \mathbf{b}$. This vectorized implementation will efficiently compute the weighted sums of the inputs plus the bias term for each and every neuron in the layer, for all the instances in the batch in just one shot. Note that adding a 1D array ($\mathbf{b}$) to a 2D matrix with the same number

10 Using a truncated normal distribution rather than a regular normal distribution ensures that there won't be any large weights, which could slow down training.

11 For example, if you set all the weights to 0, then all neurons will output 0, and the error gradient will be the same for all neurons in a given hidden layer. The Gradient Descent step will then update all the weights in exactly the same way in each layer, so they will all remain equal. In other words, despite having hundreds of neurons per layer, your model will act as if there were only one neuron per layer. It is not going to fly.

of columns (**X** . **W**) results in adding the 1D array to every row in the matrix: this is called *broadcasting*.

6. Finally, if an `activation` parameter is provided, such as `tf.nn.relu` (i.e., max (0, **Z**)), then the code returns `activation(Z)`, or else it just returns `Z`.

Okay, so now you have a nice function to create a neuron layer. Let's use it to create the deep neural network! The first hidden layer takes `X` as its input. The second takes the output of the first hidden layer as its input. And finally, the output layer takes the output of the second hidden layer as its input.

```
with tf.name_scope("dnn"):
    hidden1 = neuron_layer(X, n_hidden1, name="hidden1",
                           activation=tf.nn.relu)
    hidden2 = neuron_layer(hidden1, n_hidden2, name="hidden2",
                           activation=tf.nn.relu)
    logits = neuron_layer(hidden2, n_outputs, name="outputs")
```

Notice that once again we used a name scope for clarity. Also note that `logits` is the output of the neural network *before* going through the softmax activation function: for optimization reasons, we will handle the softmax computation later.

As you might expect, TensorFlow comes with many handy functions to create standard neural network layers, so there's often no need to define your own `neuron_layer()` function like we just did. For example, TensorFlow's `tf.layers.dense()` function (previously called `tf.contrib.layers.fully_connected()`) creates a fully connected layer, where all the inputs are connected to all the neurons in the layer. It takes care of creating the weights and biases variables, named `kernel` and `bias` respectively, using the appropriate initialization strategy, and you can set the activation function using the `activation` argument. As we will see in Chapter 11, it also supports regularization parameters. Let's tweak the preceding code to use the `dense()` function instead of our `neuron_layer()` function. Simply replace the `dnn` construction section with the following code:

```
with tf.name_scope("dnn"):
    hidden1 = tf.layers.dense(X, n_hidden1, name="hidden1",
                              activation=tf.nn.relu)
    hidden2 = tf.layers.dense(hidden1, n_hidden2, name="hidden2",
                              activation=tf.nn.relu)
    logits = tf.layers.dense(hidden2, n_outputs, name="outputs")
```

Now that we have the neural network model ready to go, we need to define the cost function that we will use to train it. Just as we did for Softmax Regression in Chapter 4, we will use cross entropy. As we discussed earlier, cross entropy will penalize models that estimate a low probability for the target class. TensorFlow provides several functions to compute cross entropy. We will use `sparse_softmax_cross_entropy_with_logits()`: it computes the cross entropy based on the "logits" (i.e., the output of the network *before* going through the softmax activation function), and it expects labels in the form of integers ranging from 0 to the number of classes minus 1 (in our case, from 0 to 9). This will give us a 1D tensor containing the cross entropy for each instance. We can then use TensorFlow's `reduce_mean()` function to compute the mean cross entropy over all instances.

```
with tf.name_scope("loss"):
    xentropy = tf.nn.sparse_softmax_cross_entropy_with_logits(labels=y,
                                                              logits=logits)
    loss = tf.reduce_mean(xentropy, name="loss")
```

The `sparse_softmax_cross_entropy_with_logits()` function is equivalent to applying the softmax activation function and then computing the cross entropy, but it is more efficient, and it properly takes care of corner cases: when logits are large, floating-point rounding errors may cause the softmax output to be exactly equal to 0 or 1, and in this case the cross entropy equation would contain a log(0) term, equal to negative infinity. The `sparse_softmax_cross_entropy_with_logits()` function solves this problem by computing log(ε) instead, where ε is a tiny positive number. This is why we did not apply the softmax activation function earlier. There is also another function called `softmax_cross_entropy_with_logits()`, which takes labels in the form of one-hot vectors (instead of ints from 0 to the number of classes minus 1).

We have the neural network model, we have the cost function, and now we need to define a `GradientDescentOptimizer` that will tweak the model parameters to minimize the cost function. Nothing new; it's just like we did in Chapter 9:

```
learning_rate = 0.01

with tf.name_scope("train"):
    optimizer = tf.train.GradientDescentOptimizer(learning_rate)
    training_op = optimizer.minimize(loss)
```

The last important step in the construction phase is to specify how to evaluate the model. We will simply use accuracy as our performance measure. First, for each instance, determine if the neural network's prediction is correct by checking whether or not the highest logit corresponds to the target class. For this you can use the `in_top_k()` function. This returns a 1D tensor full of boolean values, so we need to cast these booleans to floats and then compute the average. This will give us the network's overall accuracy.

```
with tf.name_scope("eval"):
    correct = tf.nn.in_top_k(logits, y, 1)
    accuracy = tf.reduce_mean(tf.cast(correct, tf.float32))
```

And, as usual, we need to create a node to initialize all variables, and we will also create a `Saver` to save our trained model parameters to disk:

```
init = tf.global_variables_initializer()
saver = tf.train.Saver()
```

Phew! This concludes the construction phase. This was fewer than 40 lines of code, but it was pretty intense: we created placeholders for the inputs and the targets, we created a function to build a neuron layer, we used it to create the DNN, we defined the cost function, we created an optimizer, and finally we defined the performance measure. Now on to the execution phase.

Execution Phase

This part is much shorter and simpler. First, let's load MNIST. We could use Scikit-Learn for that as we did in previous chapters, but TensorFlow offers its own helper that fetches the data, scales it (between 0 and 1), shuffles it, and provides a simple function to load one mini-batch a time. Moreover, the data is already split into a training set (55,000 instances), a validation set (5,000 instances), and a test set (10,000 instances). So let's use this helper:

```
from tensorflow.examples.tutorials.mnist import input_data
mnist = input_data.read_data_sets("/tmp/data/")
```

Now we define the number of epochs that we want to run, as well as the size of the mini-batches:

```
n_epochs = 40
batch_size = 50
```

And now we can train the model:

```
with tf.Session() as sess:
    init.run()
    for epoch in range(n_epochs):
        for iteration in range(mnist.train.num_examples // batch_size):
            X_batch, y_batch = mnist.train.next_batch(batch_size)
            sess.run(training_op, feed_dict={X: X_batch, y: y_batch})
        acc_train = accuracy.eval(feed_dict={X: X_batch, y: y_batch})
        acc_val = accuracy.eval(feed_dict={X: mnist.validation.images,
                                            y: mnist.validation.labels})
        print(epoch, "Train accuracy:", acc_train, "Val accuracy:", acc_val)

    save_path = saver.save(sess, "./my_model_final.ckpt")
```

This code opens a TensorFlow session, and it runs the `init` node that initializes all the variables. Then it runs the main training loop: at each epoch, the code iterates through a number of mini-batches that corresponds to the training set size. Each mini-batch is fetched via the `next_batch()` method, and then the code simply runs the training operation, feeding it the current mini-batch input data and targets. Next, at the end of each epoch, the code evaluates the model on the last mini-batch and on the full validation set, and it prints out the result. Finally, the model parameters are saved to disk.

Using the Neural Network

Now that the neural network is trained, you can use it to make predictions. To do that, you can reuse the same construction phase, but change the execution phase like this:

```
with tf.Session() as sess:
    saver.restore(sess, "./my_model_final.ckpt")
    X_new_scaled = [...]  # some new images (scaled from 0 to 1)
    Z = logits.eval(feed_dict={X: X_new_scaled})
    y_pred = np.argmax(Z, axis=1)
```

First the code loads the model parameters from disk. Then it loads some new images that you want to classify. Remember to apply the same feature scaling as for the training data (in this case, scale it from 0 to 1). Then the code evaluates the `logits` node. If you wanted to know all the estimated class probabilities, you would need to apply the `softmax()` function to the logits, but if you just want to predict a class, you can simply pick the class that has the highest logit value (using the `argmax()` function does the trick).

Fine-Tuning Neural Network Hyperparameters

The flexibility of neural networks is also one of their main drawbacks: there are many hyperparameters to tweak. Not only can you use any imaginable *network topology* (how neurons are interconnected), but even in a simple MLP you can change the number of layers, the number of neurons per layer, the type of activation function to use in each layer, the weight initialization logic, and much more. How do you know what combination of hyperparameters is the best for your task?

Of course, you can use grid search with cross-validation to find the right hyperparameters, like you did in previous chapters, but since there are many hyperparameters to tune, and since training a neural network on a large dataset takes a lot of time, you will only be able to explore a tiny part of the hyperparameter space in a reasonable amount of time. It is much better to use randomized search, as we discussed in Chapter 2. Another option is to use a tool such as Oscar, which implements more complex algorithms to help you find a good set of hyperparameters quickly.

It helps to have an idea of what values are reasonable for each hyperparameter, so you can restrict the search space. Let's start with the number of hidden layers.

Number of Hidden Layers

For many problems, you can just begin with a single hidden layer and you will get reasonable results. It has actually been shown that an MLP with just one hidden layer can model even the most complex functions provided it has enough neurons. For a long time, these facts convinced researchers that there was no need to investigate any deeper neural networks. But they overlooked the fact that deep networks have a much higher *parameter efficiency* than shallow ones: they can model complex functions using exponentially fewer neurons than shallow nets, making them much faster to train.

To understand why, suppose you are asked to draw a forest using some drawing software, but you are forbidden to use copy/paste. You would have to draw each tree individually, branch per branch, leaf per leaf. If you could instead draw one leaf, copy/paste it to draw a branch, then copy/paste that branch to create a tree, and finally copy/paste this tree to make a forest, you would be finished in no time. Real-world data is often structured in such a hierarchical way and DNNs automatically take advantage of this fact: lower hidden layers model low-level structures (e.g., line segments of various shapes and orientations), intermediate hidden layers combine these low-level structures to model intermediate-level structures (e.g., squares, circles), and the highest hidden layers and the output layer combine these intermediate structures to model high-level structures (e.g., faces).

Not only does this hierarchical architecture help DNNs converge faster to a good solution, it also improves their ability to generalize to new datasets. For example, if you have already trained a model to recognize faces in pictures, and you now want to train a new neural network to recognize hairstyles, then you can kickstart training by reusing the lower layers of the first network. Instead of randomly initializing the weights and biases of the first few layers of the new neural network, you can initialize them to the value of the weights and biases of the lower layers of the first network. This way the network will not have to learn from scratch all the low-level structures that occur in most pictures; it will only have to learn the higher-level structures (e.g., hairstyles).

In summary, for many problems you can start with just one or two hidden layers and it will work just fine (e.g., you can easily reach above 97% accuracy on the MNIST dataset using just one hidden layer with a few hundred neurons, and above 98% accuracy using two hidden layers with the same total amount of neurons, in roughly the same amount of training time). For more complex problems, you can gradually ramp up the number of hidden layers, until you start overfitting the training set. Very complex tasks, such as large image classification or speech recognition, typically require networks with dozens of layers (or even hundreds, but not fully connected ones, as we will see in Chapter 13), and they need a huge amount of training data. However, you will rarely have to train such networks from scratch: it is much more common to reuse parts of a pretrained state-of-the-art network that performs a similar task. Training will be a lot faster and require much less data (we will discuss this in Chapter 11).

Number of Neurons per Hidden Layer

Obviously the number of neurons in the input and output layers is determined by the type of input and output your task requires. For example, the MNIST task requires 28 x 28 = 784 input neurons and 10 output neurons. As for the hidden layers, a common practice is to size them to form a funnel, with fewer and fewer neurons at each layer—the rationale being that many low-level features can coalesce into far fewer high-level features. For example, a typical neural network for MNIST may have two hidden layers, the first with 300 neurons and the second with 100. However, this practice is not as common now, and you may simply use the same size for all hidden layers—for example, all hidden layers with 150 neurons: that's just one hyperparameter to tune instead of one per layer. Just like for the number of layers, you can try increasing the number of neurons gradually until the network starts overfitting. In general you will get more bang for the buck by increasing the number of layers than the number of neurons per layer. Unfortunately, as you can see, finding the perfect amount of neurons is still somewhat of a black art.

A simpler approach is to pick a model with more layers and neurons than you actually need, then use early stopping to prevent it from overfitting (and other regularization techniques, especially *dropout*, as we will see in Chapter 11). This has been dubbed the "stretch pants" approach:[12] instead of wasting time looking for pants that perfectly match your size, just use large stretch pants that will shrink down to the right size.

Activation Functions

In most cases you can use the ReLU activation function in the hidden layers (or one of its variants, as we will see in Chapter 11). It is a bit faster to compute than other activation functions, and Gradient Descent does not get stuck as much on plateaus, thanks to the fact that it does not saturate for large input values (as opposed to the logistic function or the hyperbolic tangent function, which saturate at 1).

For the output layer, the softmax activation function is generally a good choice for classification tasks when the classes are mutually exclusive. When they are not mutually exclusive (or when there are just two classes), you generally want to use the logistic function. For regression tasks, you can simply use no activation function at all for the output layer.

12 By Vincent Vanhoucke in his Deep Learning class on Udacity.com.

This concludes this introduction to artificial neural networks. In the following chapters, we will discuss techniques to train very deep nets, and distribute training across multiple servers and GPUs. Then we will explore a few other popular neural network architectures: convolutional neural networks, recurrent neural networks, and autoencoders.[13]

Exercises

1. Draw an ANN using the original artificial neurons (like the ones in Figure 10-3) that computes $A \oplus B$ (where $\oplus$ represents the XOR operation). Hint: $A \oplus B = (A \wedge \neg B) \vee (\neg A \wedge B)$.
2. Why is it generally preferable to use a Logistic Regression classifier rather than a classical Perceptron (i.e., a single layer of linear threshold units trained using the Perceptron training algorithm)? How can you tweak a Perceptron to make it equivalent to a Logistic Regression classifier?
3. Why was the logistic activation function a key ingredient in training the first MLPs?
4. Name three popular activation functions. Can you draw them?
5. Suppose you have an MLP composed of one input layer with 10 passthrough neurons, followed by one hidden layer with 50 artificial neurons, and finally one output layer with 3 artificial neurons. All artificial neurons use the ReLU activation function.
   - What is the shape of the input matrix $\mathbf{X}$?
   - What about the shape of the hidden layer's weight vector $\mathbf{W}_h$, and the shape of its bias vector $\mathbf{b}_h$?
   - What is the shape of the output layer's weight vector $\mathbf{W}_o$, and its bias vector $\mathbf{b}_o$?
   - What is the shape of the network's output matrix $\mathbf{Y}$?
   - Write the equation that computes the network's output matrix $\mathbf{Y}$ as a function of $\mathbf{X}$, $\mathbf{W}_h$, $\mathbf{b}_h$, $\mathbf{W}_o$ and $\mathbf{b}_o$.
6. How many neurons do you need in the output layer if you want to classify email into spam or ham? What activation function should you use in the output layer? If instead you want to tackle MNIST, how many neurons do you need in the output layer, using what activation function? Answer the same questions for getting your network to predict housing prices as in Chapter 2.

13 A few extra ANN architectures are presented in Appendix E.

7. What is backpropagation and how does it work? What is the difference between backpropagation and reverse-mode autodiff?
8. Can you list all the hyperparameters you can tweak in an MLP? If the MLP overfits the training data, how could you tweak these hyperparameters to try to solve the problem?
9. Train a deep MLP on the MNIST dataset and see if you can get over 98% precision. Just like in the last exercise of Chapter 9, try adding all the bells and whistles (i.e., save checkpoints, restore the last checkpoint in case of an interruption, add summaries, plot learning curves using TensorBoard, and so on).

Solutions to these exercises are available in Appendix A.