Using the Prediction Service

Under the hood, AI Platform just runs TF Serving, so in principle you could use the same code as earlier, if you knew which URL to query. There's just one problem: GCP also takes care of encryption and authentication. Encryption is based on SSL/TLS, and authentication is token-based: a secret authentication token must be sent to the server in every request. So before your code can use the prediction service (or any other GCP service), it must obtain a token. We will see how to do this shortly, but first you need to configure authentication and give your application the appropriate access rights on GCP. You have two options for authentication:

- Your application (i.e., the client code that will query the prediction service) could authenticate using user credentials with your own Google login and password. Using user credentials would give your application the exact same rights as on GCP, which is certainly way more than it needs. Moreover, you would have to deploy your credentials in your application, so anyone with access could steal your credentials and fully access your GCP account. In short, do not choose this option; it is only needed in very rare cases (e.g., when your application needs to access its user's GCP account).
- The client code can authenticate with a *service account*. This is an account that represents an application, not a user. It is generally given very restricted access rights: strictly what it needs, and no more. This is the recommended option.

So, let's create a service account for your application: in the navigation menu, go to IAM & admin → Service accounts, then click Create Service Account, fill in the form (service account name, ID, description), and click Create (see Figure 19-7). Next, you must give this account some access rights. Select the ML Engine Developer role: this will allow the service account to make predictions, and not much more. Optionally, you can grant some users access to the service account (this is useful when your GCP user account is part of an organization, and you wish to authorize other users in the organization to deploy applications that will be based on this service account or to manage the service account itself). Next, click Create Key to export the service account's private key, choose JSON, and click Create. This will download the private key in the form of a JSON file. Make sure to keep it private!

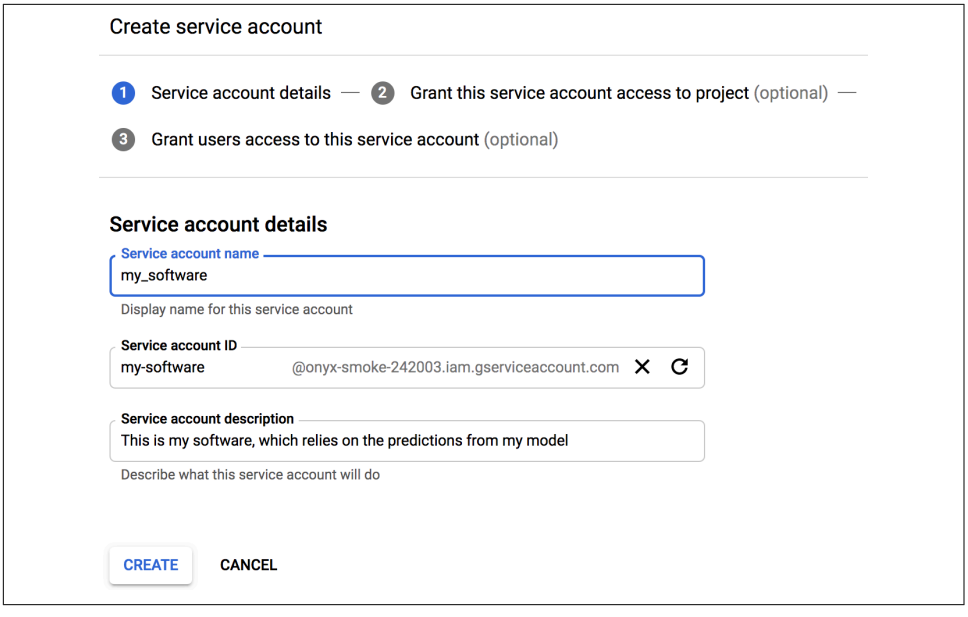


Figure 19-7. Creating a new service account in Google IAM

Great! Now let's write a small script that will query the prediction service. Google provides several libraries to simplify access to its services:

Google API Client Library
: This is a fairly thin layer on top of *OAuth 2.0* (for the authentication) and REST. You can use it with all GCP services, including AI Platform. You can install it using pip: the library is called `google-api-python-client`.

Google Cloud Client Libraries
: These are a bit more high-level: each one is dedicated to a particular service, such as GCS, Google BigQuery, Google Cloud Natural Language, and Google Cloud Vision. All these libraries can be installed using pip (e.g., the GCS Client Library is called `google-cloud-storage`). When a client library is available for a given service, it is recommended to use it rather than the Google API Client Library, as it implements all the best practices and will often use gRPC rather than REST, for better performance.

At the time of this writing there is no client library for AI Platform, so we will use the Google API Client Library. It will need to use the service account's private key; you can tell it where it is by setting the `GOOGLE_APPLICATION_CREDENTIALS` environment variable, either before starting the script or within the script like this:

```
import os

os.environ["GOOGLE_APPLICATION_CREDENTIALS"] = "my_service_account_key.json"
```

If you deploy your application to a virtual machine on Google Cloud Engine (GCE), or within a container using Google Cloud Kubernetes Engine, or as a web application on Google Cloud App Engine, or as a microservice on Google Cloud Functions, and if the `GOOGLE_APPLICATION_CREDENTIALS` environment variable is not set, then the library will use the default service account for the host service (e.g., the default GCE service account, if your application runs on GCE).

Next, you must create a resource object that wraps access to the prediction service:[7]

```
import googleapiclient.discovery

project_id = "onyx-smoke-242003" # change this to your project ID
model_id = "my_mnist_model"
model_path = "projects/{}/models/{}".format(project_id, model_id)
ml_resource = googleapiclient.discovery.build("ml", "v1").projects()
```

Note that you can append `/versions/0001` (or any other version number) to the `model_path` to specify the version you want to query: this can be useful for A/B testing or for testing a new version on a small group of users before releasing it widely (this is called a *canary*). Next, let's write a small function that will use the resource object to call the prediction service and get the predictions back:

```
def predict(X):
    input_data_json = {"signature_name": "serving_default",
                       "instances": X.tolist()}
    request = ml_resource.predict(name=model_path, body=input_data_json)
    response = request.execute()
    if "error" in response:
        raise RuntimeError(response["error"])
    return np.array([pred[output_name] for pred in response["predictions"]])
```

The function takes a NumPy array containing the input images and prepares a dictionary that the client library will convert to the JSON format (as we did earlier). Then it prepares a prediction request, and executes it; it raises an exception if the response contains an error, or else it extracts the predictions for each instance and bundles them in a NumPy array. Let's see if it works:

```
>>> Y_probas = predict(X_new)
>>> np.round(Y_probas, 2)
array([[0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 1.  , 0.  , 0.  ],
       [0.  , 0.  , 0.99, 0.01, 0.  , 0.  , 0.  , 0.  , 0.  , 0.  ],
       [0.  , 0.96, 0.01, 0.  , 0.  , 0.  , 0.  , 0.01, 0.01, 0.  ]])
```

7 If you get an error saying that module `google.appengine` was not found, set `cache_discovery=False` in the call to the `build()` method; see *https://stackoverflow.com/q/55561354*.

Yes! You now have a nice prediction service running on the cloud that can automatically scale up to any number of QPS, plus you can query it from anywhere securely. Moreover, it costs you close to nothing when you don't use it: you'll pay just a few cents per month per gigabyte used on GCS. And you can also get detailed logs and metrics using Google Stackdriver.

But what if you want to deploy your model to a mobile app? Or to an embedded device?

Deploying a Model to a Mobile or Embedded Device

If you need to deploy your model to a mobile or embedded device, a large model may simply take too long to download and use too much RAM and CPU, all of which will make your app unresponsive, heat the device, and drain its battery. To avoid this, you need to make a mobile-friendly, lightweight, and efficient model, without sacrificing too much of its accuracy. The TFLite library provides several tools[8] to help you deploy your models to mobile and embedded devices, with three main objectives:

- Reduce the model size, to shorten download time and reduce RAM usage.
- Reduce the amount of computations needed for each prediction, to reduce latency, battery usage, and heating.
- Adapt the model to device-specific constraints.

To reduce the model size, TFLite's model converter can take a SavedModel and compress it to a much lighter format based on FlatBuffers. This is an efficient cross-platform serialization library (a bit like protocol buffers) initially created by Google for gaming. It is designed so you can load FlatBuffers straight to RAM without any preprocessing: this reduces the loading time and memory footprint. Once the model is loaded into a mobile or embedded device, the TFLite interpreter will execute it to make predictions. Here is how you can convert a SavedModel to a FlatBuffer and save it to a *.tflite* file:

```
converter = tf.lite.TFLiteConverter.from_saved_model(saved_model_path)
tflite_model = converter.convert()
with open("converted_model.tflite", "wb") as f:
    f.write(tflite_model)
```

You can also save a tf.keras model directly to a FlatBuffer using `from_keras_model()`.

8 Also check out TensorFlow's Graph Transform Tools for modifying and optimizing computational graphs.

The converter also optimizes the model, both to shrink it and to reduce its latency. It prunes all the operations that are not needed to make predictions (such as training operations), and it optimizes computations whenever possible; for example, $3 \times a + 4 \times a + 5 \times a$ will be converted to $(3 + 4 + 5) \times a$. It also tries to fuse operations whenever possible. For example, Batch Normalization layers end up folded into the previous layer's addition and multiplication operations, whenever possible. To get a good idea of how much TFLite can optimize a model, download one of the pretrained TFLite models, unzip the archive, then open the excellent Netron graph visualization tool and upload the *.pb* file to view the original model. It's a big, complex graph, right? Next, open the optimized *.tflite* model and marvel at its beauty!

Another way you can reduce the model size (other than simply using smaller neural network architectures) is by using smaller bit-widths: for example, if you use half-floats (16 bits) rather than regular floats (32 bits), the model size will shrink by a factor of 2, at the cost of a (generally small) accuracy drop. Moreover, training will be faster, and you will use roughly half the amount of GPU RAM.

TFLite's converter can go further than that, by quantizing the model weights down to fixed-point, 8-bit integers! This leads to a fourfold size reduction compared to using 32-bit floats. The simplest approach is called *post-training quantization*: it just quantizes the weights after training, using a fairly basic but efficient symmetrical quantization technique. It finds the maximum absolute weight value, m, then it maps the floating-point range $-m$ to $+m$ to the fixed-point (integer) range –127 to +127. For example (see Figure 19-8), if the weights range from –1.5 to +0.8, then the bytes –127, 0, and +127 will correspond to the floats –1.5, 0.0, and +1.5, respectively. Note that 0.0 always maps to 0 when using symmetrical quantization (also note that the byte values +68 to +127 will not be used, since they map to floats greater than +0.8).

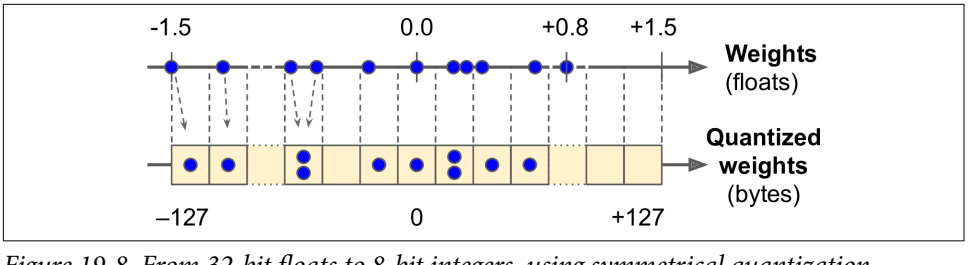


Figure 19-8. From 32-bit floats to 8-bit integers, using symmetrical quantization

To perform this post-training quantization, simply add `OPTIMIZE_FOR_SIZE` to the list of converter optimizations before calling the `convert()` method:

```
converter.optimizations = [tf.lite.Optimize.OPTIMIZE_FOR_SIZE]
```

This technique dramatically reduces the model's size, so it's much faster to download and store. However, at runtime the quantized weights get converted back to floats before they are used (these recovered floats are not perfectly identical to the original

floats, but not too far off, so the accuracy loss is usually acceptable). To avoid recomputing them all the time, the recovered floats are cached, so there is no reduction of RAM usage. And there is no reduction either in compute speed.

The most effective way to reduce latency and power consumption is to also quantize the activations so that the computations can be done entirely with integers, without the need for any floating-point operations. Even when using the same bit-width (e.g., 32-bit integers instead of 32-bit floats), integer computations use less CPU cycles, consume less energy, and produce less heat. And if you also reduce the bit-width (e.g., down to 8-bit integers), you can get huge speedups. Moreover, some neural network accelerator devices (such as the Edge TPU) can only process integers, so full quantization of both weights and activations is compulsory. This can be done post-training; it requires a calibration step to find the maximum absolute value of the activations, so you need to provide a representative sample of training data to TFLite (it does not need to be huge), and it will process the data through the model and measure the activation statistics required for quantization (this step is typically fast).

The main problem with quantization is that it loses a bit of accuracy: it is equivalent to adding noise to the weights and activations. If the accuracy drop is too severe, then you may need to use *quantization-aware training*. This means adding fake quantization operations to the model so it can learn to ignore the quantization noise during training; the final weights will then be more robust to quantization. Moreover, the calibration step can be taken care of automatically during training, which simplifies the whole process.

I have explained the core concepts of TFLite, but going all the way to coding a mobile app or an embedded program would require a whole other book. Fortunately, one exists: if you want to learn more about building TensorFlow applications for mobile and embedded devices, check out the O'Reilly book *TinyML: Machine Learning with TensorFlow on Arduino and Ultra-Low Power Micro-Controllers*, by Pete Warden (who leads the TFLite team) and Daniel Situnayake.

TensorFlow in the Browser

What if you want to use your model in a website, running directly in the user's browser? This can be useful in many scenarios, such as:

- When your web application is often used in situations where the user's connectivity is intermittent or slow (e.g., a website for hikers), so running the model directly on the client side is the only way to make your website reliable.
- When you need the model's responses to be as fast as possible (e.g., for an online game). Removing the need to query the server to make predictions will definitely reduce the latency and make the website much more responsive.
- When your web service makes predictions based on some private user data, and you want to protect the user's privacy by making the predictions on the client side so that the private data never has to leave the user's machine.[9]

For all these scenarios, you can export your model to a special format that can be loaded by the TensorFlow.js JavaScript library. This library can then use your model to make predictions directly in the user's browser. The TensorFlow.js project includes a `tensorflowjs_converter` tool that can convert a TensorFlow SavedModel or a Keras model file to the *TensorFlow.js Layers* format: this is a directory containing a set of sharded weight files in binary format and a *model.json* file that describes the model's architecture and links to the weight files. This format is optimized to be downloaded efficiently on the web. Users can then download the model and run predictions in the browser using the TensorFlow.js library. Here is a code snippet to give you an idea of what the JavaScript API looks like:

```
import * as tf from '@tensorflow/tfjs';
const model = await tf.loadLayersModel('https://example.com/tfjs/model.json');
const image = tf.fromPixels(webcamElement);
const prediction = model.predict(image);
```

Once again, doing justice to this topic would require a whole book. If you want to learn more about TensorFlow.js, check out the O'Reilly book *Practical Deep Learning for Cloud, Mobile, and Edge*, by Anirudh Koul, Siddha Ganju, and Meher Kasam.

Next, we will see how to use GPUs to speed up computations!

9 If you're interested in this topic, check out *federated learning*.

Using GPUs to Speed Up Computations

In Chapter 11 we discussed several techniques that can considerably speed up training: better weight initialization, Batch Normalization, sophisticated optimizers, and so on. But even with all of these techniques, training a large neural network on a single machine with a single CPU can take days or even weeks.

In this section we will look at how to speed up your models by using GPUs. We will also see how to split the computations across multiple devices, including the CPU and multiple GPU devices (see Figure 19-9). For now we will run everything on a single machine, but later in this chapter we will discuss how to distribute computations across multiple servers.

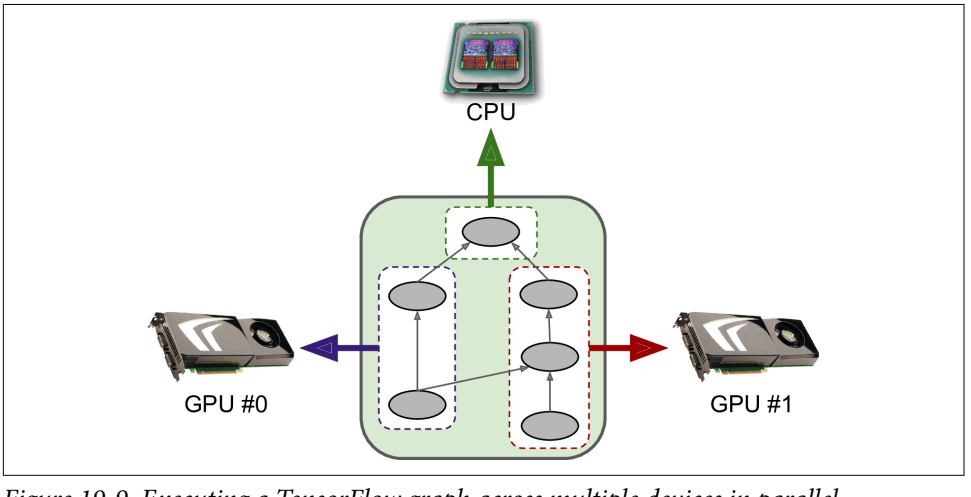


Figure 19-9. Executing a TensorFlow graph across multiple devices in parallel

Thanks to GPUs, instead of waiting for days or weeks for a training algorithm to complete, you may end up waiting for just a few minutes or hours. Not only does this save an enormous amount of time, but it also means that you can experiment with various models much more easily and frequently retrain your models on fresh data.

You can often get a major performance boost simply by adding GPU cards to a single machine. In fact, in many cases this will suffice; you won't need to use multiple machines at all. For example, you can typically train a neural network just as fast using four GPUs on a single machine rather than eight GPUs across multiple machines, due to the extra delay imposed by network communications in a distributed setup. Similarly, using a single powerful GPU is often preferable to using multiple slower GPUs.

The first step is to get your hands on a GPU. There are two options for this: you can either purchase your own GPU(s), or you can use GPU-equipped virtual machines on the cloud. Let's start with the first option.

Getting Your Own GPU

If you choose to purchase a GPU card, then take some time to make the right choice. Tim Dettmers wrote an excellent blog post to help you choose, and he updates it regularly: I encourage you to read it carefully. At the time of this writing, TensorFlow only supports Nvidia cards with CUDA Compute Capability 3.5+ (as well as Google's TPUs, of course), but it may extend its support to other manufacturers. Moreover, although TPUs are currently only available on GCP, it is highly likely that TPU-like cards will be available for sale in the near future, and TensorFlow may support them. In short, make sure to check TensorFlow's documentation to see what devices are supported at this point.

If you go for an Nvidia GPU card, you will need to install the appropriate Nvidia drivers and several Nvidia libraries.[10] These include the *Compute Unified Device Architecture* library (CUDA), which allows developers to use CUDA-enabled GPUs for all sorts of computations (not just graphics acceleration), and the *CUDA Deep Neural Network* library (cuDNN), a GPU-accelerated library of primitives for DNNs. cuDNN provides optimized implementations of common DNN computations such as activation layers, normalization, forward and backward convolutions, and pooling (see Chapter 14). It is part of Nvidia's Deep Learning SDK (note that you'll need to create an Nvidia developer account in order to download it). TensorFlow uses CUDA and cuDNN to control the GPU cards and accelerate computations (see Figure 19-10).

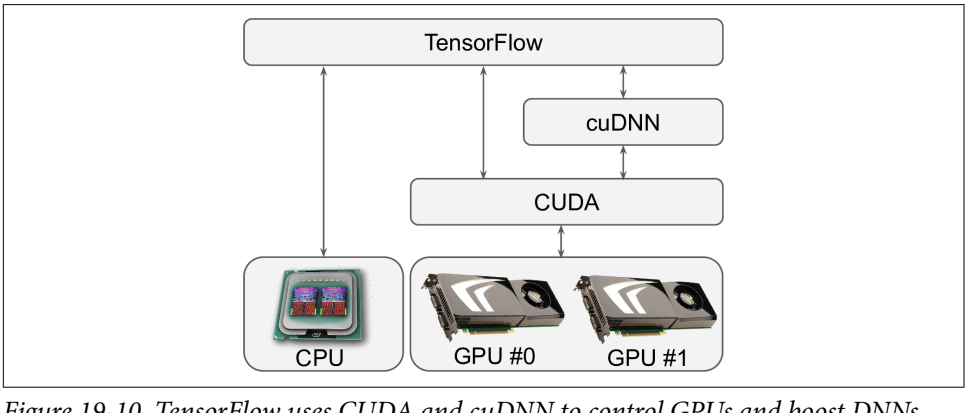


Figure 19-10. TensorFlow uses CUDA and cuDNN to control GPUs and boost DNNs

10 Please check the docs for detailed and up-to-date installation instructions, as they change quite often.

Once you have installed the GPU card(s) and all the required drivers and libraries, you can use the `nvidia-smi` command to check that CUDA is properly installed. It lists the available GPU cards, as well as processes running on each card:

```
$ nvidia-smi
Sun Jun  2 10:05:22 2019
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 418.67       Driver Version: 410.79       CUDA Version: 10.0     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Tesla T4            Off  | 00000000:00:04.0 Off |                    0 |
| N/A   61C    P8    17W /  70W |      0MiB / 15079MiB |      0%      Default |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
```

At the time of this writing, you'll also need to install the GPU version of TensorFlow (i.e., the `tensorflow-gpu` library); however, there is ongoing work to have a unified installation procedure for both CPU-only and GPU machines, so please check the installation documentation to see which library you should install. In any case, since installing every required library correctly is a bit long and tricky (and all hell breaks loose if you do not install the correct library versions), TensorFlow provides a Docker image with everything you need inside. However, in order for the Docker container to have access to the GPU, you will still need to install the Nvidia drivers on the host machine.

To check that TensorFlow actually sees the GPUs, run the following tests:

```
>>> import tensorflow as tf
>>> tf.test.is_gpu_available()
True
>>> tf.test.gpu_device_name()
'/device:GPU:0'
>>> tf.config.experimental.list_physical_devices(device_type='GPU')
[PhysicalDevice(name='/physical_device:GPU:0', device_type='GPU')]
```

The `is_gpu_available()` function checks whether at least one GPU is available. The `gpu_device_name()` function gives the first GPU's name: by default, operations will

run on this GPU. The `list_physical_devices()` function returns the list of all available GPU devices (just one in this example).[11]

Now, what if you don't want to invest time and money in getting your own GPU card? Just use a GPU VM on the cloud!

Using a GPU-Equipped Virtual Machine

All major cloud platforms now offer GPU VMs, some preconfigured with all the drivers and libraries you need (including TensorFlow). Google Cloud Platform enforces various GPU quotas, both worldwide and per region: you cannot just create thousands of GPU VMs without prior authorization from Google.[12] By default, the worldwide GPU quota is zero, so you cannot use any GPU VMs. Therefore, the very first thing you need to do is to request a higher worldwide quota. In the GCP console, open the navigation menu and go to IAM & admin → Quotas. Click Metric, click None to uncheck all locations, then search for "GPU" and select "GPUs (all regions)" to see the corresponding quota. If this quota's value is zero (or just insufficient for your needs), then check the box next to it (it should be the only selected one) and click "Edit quotas." Fill in the requested information, then click "Submit request." It may take a few hours (or up to a few days) for your quota request to be processed and (generally) accepted. By default, there is also a quota of one GPU per region and per GPU type. You can request to increase these quotas too: click Metric, select None to uncheck all metrics, search for "GPU," and select the type of GPU you want (e.g., NVIDIA P4 GPUs). Then click the Location drop-down menu, click None to uncheck all metrics, and click the location you want; check the boxes next to the quota(s) you want to change, and click "Edit quotas" to file a request.

Once your GPU quota requests are approved, you can in no time create a VM equipped with one or more GPUs by using Google Cloud AI Platform's *Deep Learning VM Images*: go to *https://homl.info/dlvm*, click View Console, then click "Launch on Compute Engine" and fill in the VM configuration form. Note that some locations do not have all types of GPUs, and some have no GPUs at all (change the location to see the types of GPUs available, if any). Make sure to select TensorFlow 2.0 as the framework, and check "Install NVIDIA GPU driver automatically on first startup." It is also a good idea to check "Enable access to JupyterLab via URL instead of SSH": this will make it very easy to start a Jupyter notebook running on this GPU VM, powered by

11 Many code examples in this chapter use experimental APIs. They are very likely to be moved to the core API in future versions. So if an experimental function fails, try simply removing the word `experimental`, and hopefully it will work. If not, then perhaps the API has changed a bit; please check the Jupyter notebook, as I will ensure it contains the correct code.

12 Presumably, these quotas are meant to stop bad guys who might be tempted to use GCP with stolen credit cards to mine cryptocurrencies.

JupyterLab (this is an alternative web interface to run Jupyter notebooks). Once the VM is created, scroll down the navigation menu to the Artificial Intelligence section, then click AI Platform → Notebooks. Once the Notebook instance appears in the list (this may take a few minutes, so click Refresh once in a while until it appears), click its Open JupyterLab link. This will run JupyterLab on the VM and connect your browser to it. You can create notebooks and run any code you want on this VM, and benefit from its GPUs!

But if you just want to run some quick tests or easily share notebooks with your colleagues, then you should try Colaboratory.

Colaboratory

The simplest and cheapest way to access a GPU VM is to use *Colaboratory* (or *Colab*, for short). It's free! Just go to *https://colab.research.google.com/* and create a new Python 3 notebook: this will create a Jupyter notebook, stored on your Google Drive (alternatively, you can open any notebook on GitHub, or on Google Drive, or you can even upload your own notebooks). Colab's user interface is similar to Jupyter's, except you can share and use the notebooks like regular Google Docs, and there are a few other minor differences (e.g., you can create handy widgets using special comments in your code).

When you open a Colab notebook, it runs on a free Google VM dedicated to that notebook, called a *Colab Runtime* (see Figure 19-11). By default the Runtime is CPU-only, but you can change this by going to Runtime → "Change runtime type," selecting GPU in the "Hardware accelerator" drop-down menu, then clicking Save. In fact, you could even select TPU! (Yes, you can actually use a TPU for free; we will talk about TPUs later in this chapter, though, so for now just select GPU.)

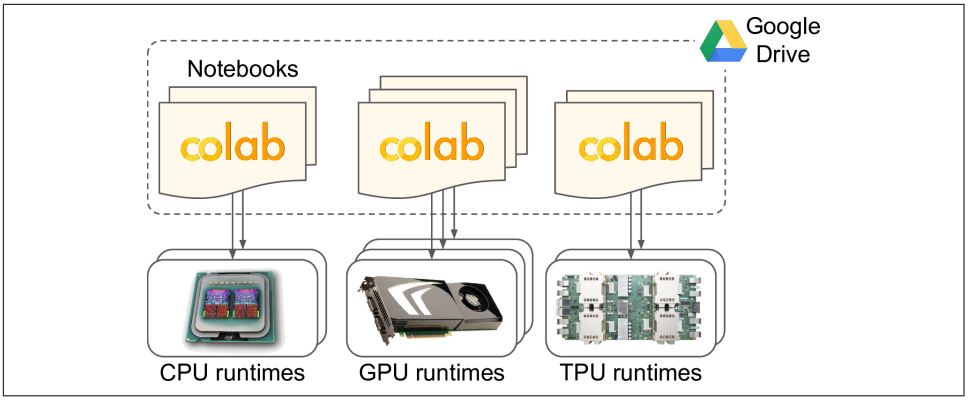


Figure 19-11. Colab Runtimes and notebooks

Colab does have some restrictions: first, there is a limit to the number of Colab notebooks you can run simultaneously (currently 5 per Runtime type). Moreover, as the FAQ states, "Colaboratory is intended for interactive use. Long-running background computations, particularly on GPUs, may be stopped. Please do not use Colaboratory for cryptocurrency mining." Also, the web interface will automatically disconnect from the Colab Runtime if you leave it unattended for a while (~30 minutes). When you reconnect to the Colab Runtime, it may have been reset, so make sure you always export any data you care about (e.g., download it or save it to Google Drive). Even if you never disconnect, the Colab Runtime will automatically shut down after 12 hours, as it is not meant for long-running computations. Despite these limitations, it's a fantastic tool to run tests easily, get quick results, and collaborate with your colleagues.

Managing the GPU RAM

By default TensorFlow automatically grabs all the RAM in all available GPUs the first time you run a computation. It does this to limit GPU RAM fragmentation. This means that if you try to start a second TensorFlow program (or any program that requires the GPU), it will quickly run out of RAM. This does not happen as often as you might think, as you will most often have a single TensorFlow program running on a machine: usually a training script, a TF Serving node, or a Jupyter notebook. If you need to run multiple programs for some reason (e.g., to train two different models in parallel on the same machine), then you will need to split the GPU RAM between these processes more evenly.

If you have multiple GPU cards on your machine, a simple solution is to assign each of them to a single process. To do this, you can set the `CUDA_VISIBLE_DEVICES` environment variable so that each process only sees the appropriate GPU card(s). Also set the `CUDA_DEVICE_ORDER` environment variable to `PCI_BUS_ID` to ensure that

each ID always refers to the same GPU card. For example, if you have four GPU cards, you could start two programs, assigning two GPUs to each of them, by executing commands like the following in two separate terminal windows:

```
$ CUDA_DEVICE_ORDER=PCI_BUS_ID CUDA_VISIBLE_DEVICES=0,1 python3 program_1.py
# and in another terminal:
$ CUDA_DEVICE_ORDER=PCI_BUS_ID CUDA_VISIBLE_DEVICES=3,2 python3 program_2.py
```

Program 1 will then only see GPU cards 0 and 1, named `/gpu:0` and `/gpu:1` respectively, and program 2 will only see GPU cards 2 and 3, named `/gpu:1` and `/gpu:0` respectively (note the order). Everything will work fine (see Figure 19-12). Of course, you can also define these environment variables in Python by setting `os.environ["CUDA_DEVICE_ORDER"]` and `os.environ["CUDA_VISIBLE_DEVICES"]`, as long as you do so before using TensorFlow.

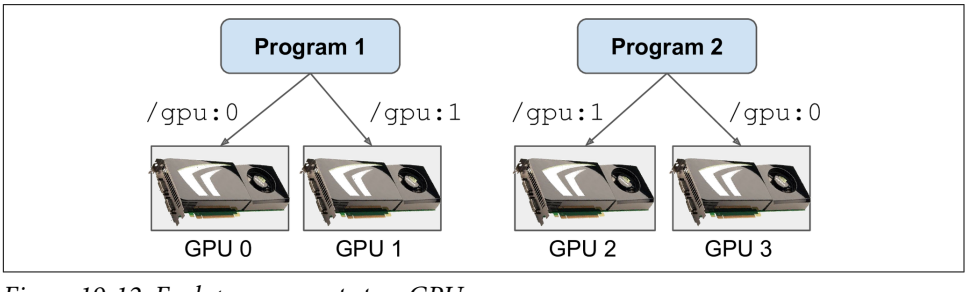


Figure 19-12. Each program gets two GPUs

Another option is to tell TensorFlow to grab only a specific amount of GPU RAM. This must be done immediately after importing TensorFlow. For example, to make TensorFlow grab only 2 GiB of RAM on each GPU, you must create a *virtual GPU device* (also called a *logical GPU device*) for each physical GPU device and set its memory limit to 2 GiB (i.e., 2,048 MiB):

```
for gpu in tf.config.experimental.list_physical_devices("GPU"):
    tf.config.experimental.set_virtual_device_configuration(
        gpu,
        [tf.config.experimental.VirtualDeviceConfiguration(memory_limit=2048)])
```

Now (supposing you have four GPUs, each with at least 4 GiB of RAM) two programs like this one can run in parallel, each using all four GPU cards (see Figure 19-13).

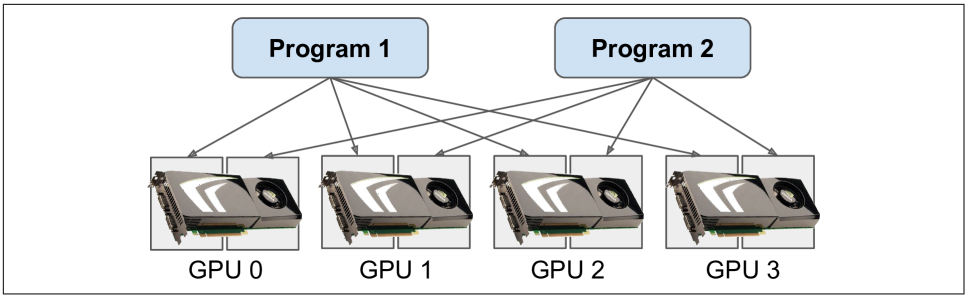


Figure 19-13. Each program gets all four GPUs, but with only 2 GiB of RAM on each GPU

If you run the `nvidia-smi` command while both programs are running, you should see that each process holds 2 GiB of RAM on each card:

```
$ nvidia-smi
[...]
+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Type   Process name                             Usage      |
|=============================================================================|
|    0      2373      C   /usr/bin/python3                          2241MiB |
|    0      2533      C   /usr/bin/python3                          2241MiB |
|    1      2373      C   /usr/bin/python3                          2241MiB |
|    1      2533      C   /usr/bin/python3                          2241MiB |
[...]
```

Yet another option is to tell TensorFlow to grab memory only when it needs it (this also must be done immediately after importing TensorFlow):

```
for gpu in tf.config.experimental.list_physical_devices("GPU"):
    tf.config.experimental.set_memory_growth(gpu, True)
```

Another way to do this is to set the `TF_FORCE_GPU_ALLOW_GROWTH` environment variable to `true`. With this option, TensorFlow will never release memory once it has grabbed it (again, to avoid memory fragmentation), except of course when the program ends. It can be harder to guarantee deterministic behavior using this option (e.g., one program may crash because another program's memory usage went through the roof), so in production you'll probably want to stick with one of the previous options. However, there are some cases where it is very useful: for example, when you use a machine to run multiple Jupyter notebooks, several of which use TensorFlow. This is why the `TF_FORCE_GPU_ALLOW_GROWTH` environment variable is set to `true` in Colab Runtimes.

Lastly, in some cases you may want to split a GPU into two or more *virtual GPUs*—for example, if you want to test a distribution algorithm (this is a handy way to try out the code examples in the rest of this chapter even if you have a single GPU, such

as in a Colab Runtime). The following code splits the first GPU into two virtual devices, with 2 GiB of RAM each (again, this must be done immediately after importing TensorFlow):

```
physical_gpus = tf.config.experimental.list_physical_devices("GPU")
tf.config.experimental.set_virtual_device_configuration(
    physical_gpus[0],
    [tf.config.experimental.VirtualDeviceConfiguration(memory_limit=2048),
     tf.config.experimental.VirtualDeviceConfiguration(memory_limit=2048)])
```

These two virtual devices will then be called `/gpu:0` and `/gpu:1`, and you can place operations and variables on each of them as if they were really two independent GPUs. Now let's see how TensorFlow decides which devices it should place variables and execute operations on.

Placing Operations and Variables on Devices

The TensorFlow whitepaper[13] presents a friendly *dynamic placer* algorithm that automagically distributes operations across all available devices, taking into account things like the measured computation time in previous runs of the graph, estimations of the size of the input and output tensors for each operation, the amount of RAM available in each device, communication delay when transferring data into and out of devices, and hints and constraints from the user. In practice this algorithm turned out to be less efficient than a small set of placement rules specified by the user, so the TensorFlow team ended up dropping the dynamic placer.

That said, tf.keras and tf.data generally do a good job of placing operations and variables where they belong (e.g., heavy computations on the GPU, and data preprocessing on the CPU). But you can also place operations and variables manually on each device, if you want more control:

- As just mentioned, you generally want to place the data preprocessing operations on the CPU, and place the neural network operations on the GPUs.
- GPUs usually have a fairly limited communication bandwidth, so it is important to avoid unnecessary data transfers in and out of the GPUs.
- Adding more CPU RAM to a machine is simple and fairly cheap, so there's usually plenty of it, whereas the GPU RAM is baked into the GPU: it is an expensive and thus limited resource, so if a variable is not needed in the next few training steps, it should probably be placed on the CPU (e.g., datasets generally belong on the CPU).

13 Martín Abadi et al., "TensorFlow: Large-Scale Machine Learning on Heterogeneous Distributed Systems" Google Research whitepaper (2015).

By default, all variables and all operations will be placed on the first GPU (named `/gpu:0`), except for variables and operations that don't have a GPU kernel:[14] these are placed on the CPU (named `/cpu:0`). A tensor or variable's `device` attribute tells you which device it was placed on:[15]

```
>>> a = tf.Variable(42.0)
>>> a.device
'/job:localhost/replica:0/task:0/device:GPU:0'
>>> b = tf.Variable(42)
>>> b.device
'/job:localhost/replica:0/task:0/device:CPU:0'
```

You can safely ignore the prefix `/job:localhost/replica:0/task:0` for now (it allows you to place operations on other machines when using a TensorFlow cluster; we will talk about jobs, replicas, and tasks later in this chapter). As you can see, the first variable was placed on GPU 0, which is the default device. However, the second variable was placed on the CPU: this is because there are no GPU kernels for integer variables (or for operations involving integer tensors), so TensorFlow fell back to the CPU.

If you want to place an operation on a different device than the default one, use a `tf.device()` context:

```
>>> with tf.device("/cpu:0"):
...     c = tf.Variable(42.0)
...
>>> c.device
'/job:localhost/replica:0/task:0/device:CPU:0'
```

The CPU is always treated as a single device (`/cpu:0`), even if your machine has multiple CPU cores. Any operation placed on the CPU may run in parallel across multiple cores if it has a multi-threaded kernel.

If you explicitly try to place an operation or variable on a device that does not exist or for which there is no kernel, then you will get an exception. However, in some cases you may prefer to fall back to the CPU; for example, if your program may run both on CPU-only machines and on GPU machines, you may want TensorFlow to ignore your `tf.device("/gpu:*")` on CPU-only machines. To do this, you can call `tf.config.set_soft_device_placement(True)` just after importing TensorFlow: when a

14 As we saw in Chapter 12, a kernel is a variable or operation's implementation for a specific data type and device type. For example, there is a GPU kernel for the `float32` `tf.matmul()` operation, but there is no GPU kernel for `int32` `tf.matmul()` (only a CPU kernel).

15 You can also use `tf.debugging.set_log_device_placement(True)` to log all device placements.

placement request fails, TensorFlow will fall back to its default placement rules (i.e., GPU 0 by default if it exists and there is a GPU kernel, and CPU 0 otherwise).

Now how exactly will TensorFlow execute all these operations across multiple devices?

Parallel Execution Across Multiple Devices

As we saw in Chapter 12, one of the benefits of using TF Functions is parallelism. Let's look at this a bit more closely. When TensorFlow runs a TF Function, it starts by analyzing its graph to find the list of operations that need to be evaluated, and it counts how many dependencies each of them has. TensorFlow then adds each operation with zero dependencies (i.e., each source operation) to the evaluation queue of this operation's device (see Figure 19-14). Once an operation has been evaluated, the dependency counter of each operation that depends on it is decremented. Once an operation's dependency counter reaches zero, it is pushed to the evaluation queue of its device. And once all the nodes that TensorFlow needs have been evaluated, it returns their outputs.

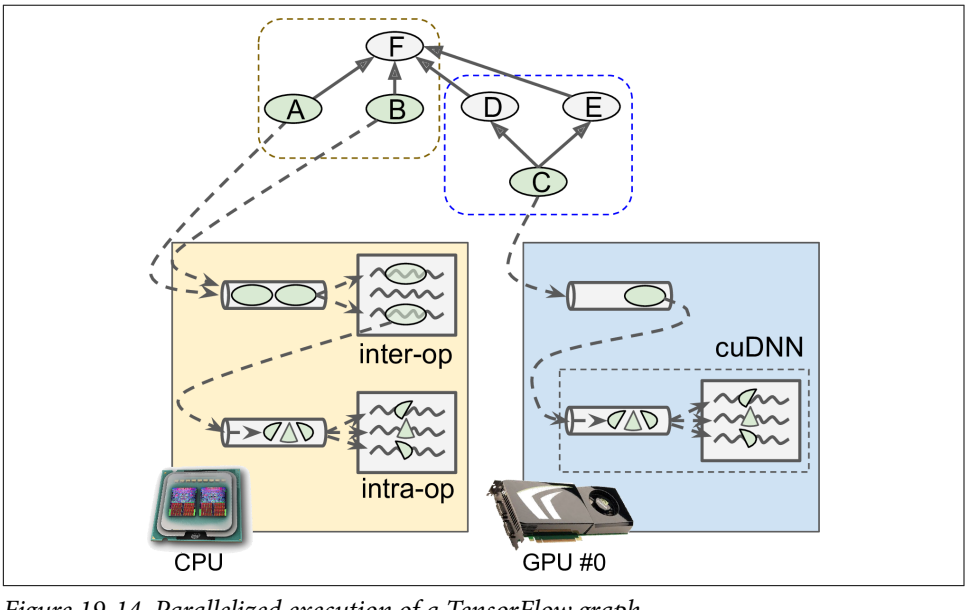


Figure 19-14. Parallelized execution of a TensorFlow graph

Operations in the CPU's evaluation queue are dispatched to a thread pool called the *inter-op thread pool*. If the CPU has multiple cores, then these operations will effectively be evaluated in parallel. Some operations have multithreaded CPU kernels: these kernels split their tasks into multiple suboperations, which are placed in another evaluation queue and dispatched to a second thread pool called the *intra-op*

thread pool (shared by all multithreaded CPU kernels). In short, multiple operations and suboperations may be evaluated in parallel on different CPU cores.

For the GPU, things are a bit simpler. Operations in a GPU's evaluation queue are evaluated sequentially. However, most operations have multithreaded GPU kernels, typically implemented by libraries that TensorFlow depends on, such as CUDA and cuDNN. These implementations have their own thread pools, and they typically exploit as many GPU threads as they can (which is the reason why there is no need for an inter-op thread pool in GPUs: each operation already floods most GPU threads).

For example, in Figure 19-14, operations A, B, and C are source ops, so they can immediately be evaluated. Operations A and B are placed on the CPU, so they are sent to the CPU's evaluation queue, then they are dispatched to the inter-op thread pool and immediately evaluated in parallel. Operation A happens to have a multithreaded kernel; its computations are split into three parts, which are executed in parallel by the intra-op thread pool. Operation C goes to GPU 0's evaluation queue, and in this example its GPU kernel happens to use cuDNN, which manages its own intra-op thread pool and runs the operation across many GPU threads in parallel. Suppose C finishes first. The dependency counters of D and E are decremented and they reach zero, so both operations are pushed to GPU 0's evaluation queue, and they are executed sequentially. Note that C only gets evaluated once, even though both D and E depend on it. Suppose B finishes next. Then F's dependency counter is decremented from 4 to 3, and since that's not 0, it does not run yet. Once A, D, and E are finished, then F's dependency counter reaches 0, and it is pushed to the CPU's evaluation queue and evaluated. Finally, TensorFlow returns the requested outputs.

An extra bit of magic that TensorFlow performs is when the TF Function modifies a stateful resource, such as a variable: it ensures that the order of execution matches the order in the code, even if there is no explicit dependency between the statements. For example, if your TF Function contains `v.assign_add(1)` followed by `v.assign(v * 2)`, TensorFlow will ensure that these operations are executed in that order.

You can control the number of threads in the inter-op thread pool by calling `tf.config.threading.set_inter_op_parallelism_threads()`. To set the number of intra-op threads, use `tf.config.threading.set_intra_op_parallelism_threads()`. This is useful if you want do not want TensorFlow to use all the CPU cores or if you want it to be single-threaded.[16]

16 This can be useful if you want to guarantee perfect reproducibility, as I explain in this video, based on TF 1.

With that, you have all you need to run any operation on any device, and exploit the power of your GPUs! Here are some of the things you could do:

- You could train several models in parallel, each on its own GPU: just write a training script for each model and run them in parallel, setting `CUDA_DEVICE_ORDER` and `CUDA_VISIBLE_DEVICES` so that each script only sees a single GPU device. This is great for hyperparameter tuning, as you can train in parallel multiple models with different hyperparameters. If you have a single machine with two GPUs, and it takes one hour to train one model on one GPU, then training two models in parallel, each on its own dedicated GPU, will take just one hour. Simple!
- You could train a model on a single GPU and perform all the preprocessing in parallel on the CPU, using the dataset's `prefetch()` method[17] to prepare the next few batches in advance so that they are ready when the GPU needs them (see Chapter 13).
- If your model takes two images as input and processes them using two CNNs before joining their outputs, then it will probably run much faster if you place each CNN on a different GPU.
- You can create an efficient ensemble: just place a different trained model on each GPU so that you can get all the predictions much faster to produce the ensemble's final prediction.

But what if you want to *train* a single model across multiple GPUs?

Training Models Across Multiple Devices

There are two main approaches to training a single model across multiple devices: *model parallelism*, where the model is split across the devices, and *data parallelism*, where the model is replicated across every device, and each replica is trained on a subset of the data. Let's look at these two options closely before we train a model on multiple GPUs.

Model Parallelism

So far we have trained each neural network on a single device. What if we want to train a single neural network across multiple devices? This requires chopping the model into separate chunks and running each chunk on a different device.

17 At the time of this writing it only prefetches the data to the CPU RAM, but you can use `tf.data.experimental.prefetch_to_device()` to make it prefetch the data and push it to the device of your choice so that the GPU does not waste time waiting for the data to be transferred.

Unfortunately, such model parallelism turns out to be pretty tricky, and it really depends on the architecture of your neural network. For fully connected networks, there is generally not much to be gained from this approach (see Figure 19-15). Intuitively, it may seem that an easy way to split the model is to place each layer on a different device, but this does not work because each layer needs to wait for the output of the previous layer before it can do anything. So perhaps you can slice it vertically—for example, with the left half of each layer on one device, and the right part on another device? This is slightly better, since both halves of each layer can indeed work in parallel, but the problem is that each half of the next layer requires the output of both halves, so there will be a lot of cross-device communication (represented by the dashed arrows). This is likely to completely cancel out the benefit of the parallel computation, since cross-device communication is slow (especially when the devices are located on different machines).

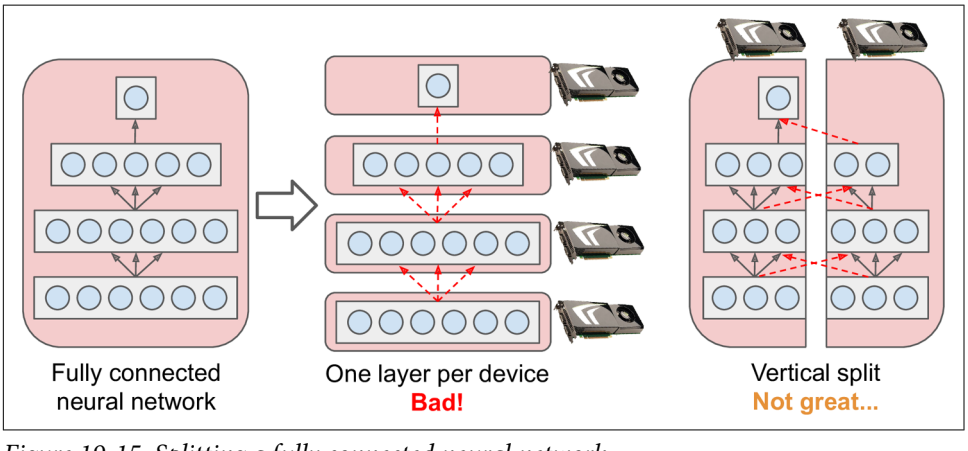


Figure 19-15. Splitting a fully connected neural network

Some neural network architectures, such as convolutional neural networks (see Chapter 14), contain layers that are only partially connected to the lower layers, so it is much easier to distribute chunks across devices in an efficient way (Figure 19-16).

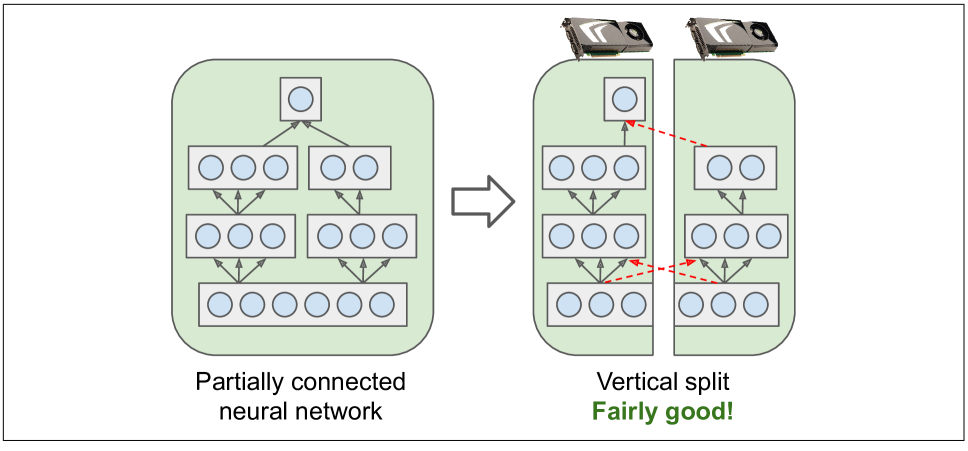


Figure 19-16. Splitting a partially connected neural network

Deep recurrent neural networks (see Chapter 15) can be split a bit more efficiently across multiple GPUs. If you split the network horizontally by placing each layer on a different device, and you feed the network with an input sequence to process, then at the first time step only one device will be active (working on the sequence's first value), at the second step two will be active (the second layer will be handling the output of the first layer for the first value, while the first layer will be handling the second value), and by the time the signal propagates to the output layer, all devices will be active simultaneously (Figure 19-17). There is still a lot of cross-device communication going on, but since each cell may be fairly complex, the benefit of running multiple cells in parallel may (in theory) outweigh the communication penalty. However, in practice a regular stack of `LSTM` layers running on a single GPU actually runs much faster.

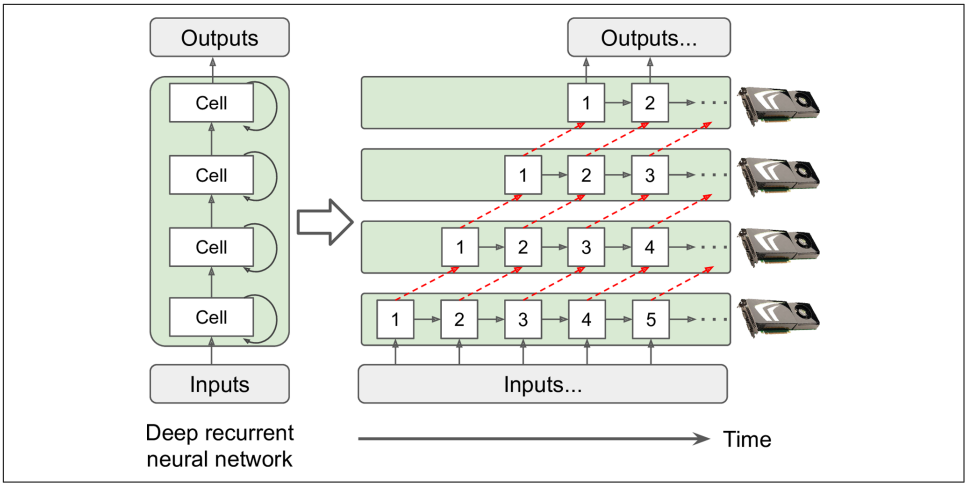


Figure 19-17. Splitting a deep recurrent neural network

In short, model parallelism may speed up running or training some types of neural networks, but not all, and it requires special care and tuning, such as making sure that devices that need to communicate the most run on the same machine.[18] Let's look at a much simpler and generally more efficient option: data parallelism.

Data Parallelism

Another way to parallelize the training of a neural network is to replicate it on every device and run each training step simultaneously on all replicas, using a different mini-batch for each. The gradients computed by each replica are then averaged, and the result is used to update the model parameters. This is called *data parallelism*. There are many variants of this idea, so let's look at the most important ones.

Data parallelism using the mirrored strategy

Arguably the simplest approach is to completely mirror all the model parameters across all the GPUs and always apply the exact same parameter updates on every GPU. This way, all replicas always remain perfectly identical. This is called the *mirrored strategy*, and it turns out to be quite efficient, especially when using a single machine (see Figure 19-18).

18 If you are interested in going further with model parallelism, check out Mesh TensorFlow.

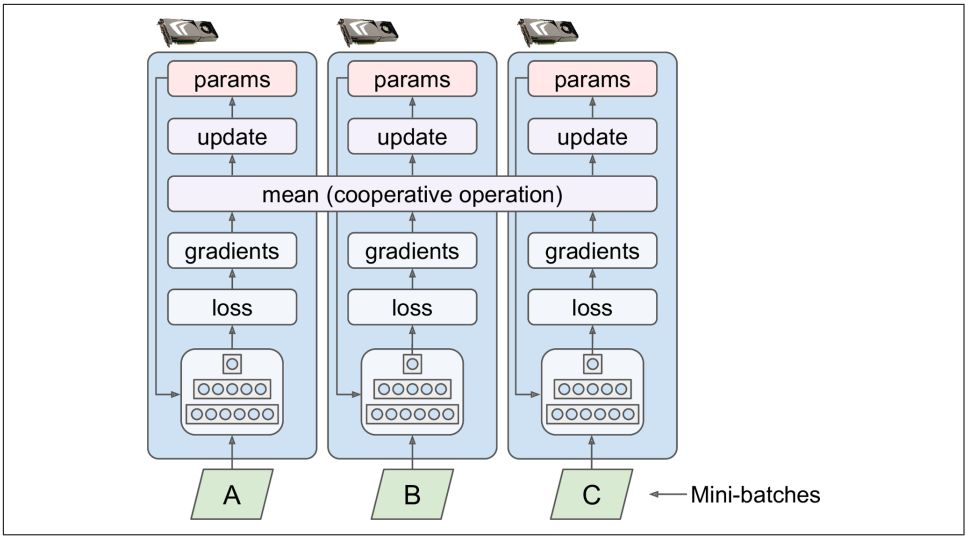


Figure 19-18. Data parallelism using the mirrored strategy

The tricky part when using this approach is to efficiently compute the mean of all the gradients from all the GPUs and distribute the result across all the GPUs. This can be done using an *AllReduce* algorithm, a class of algorithms where multiple nodes collaborate to efficiently perform a reduce operation (such as computing the mean, sum, and max), while ensuring that all nodes obtain the same final result. Fortunately, there are off-the-shelf implementations of such algorithms, as we will see.

Data parallelism with centralized parameters

Another approach is to store the model parameters outside of the GPU devices performing the computations (called *workers*), for example on the CPU (see Figure 19-19). In a distributed setup, you may place all the parameters on one or more CPU-only servers called *parameter servers*, whose only role is to host and update the parameters.

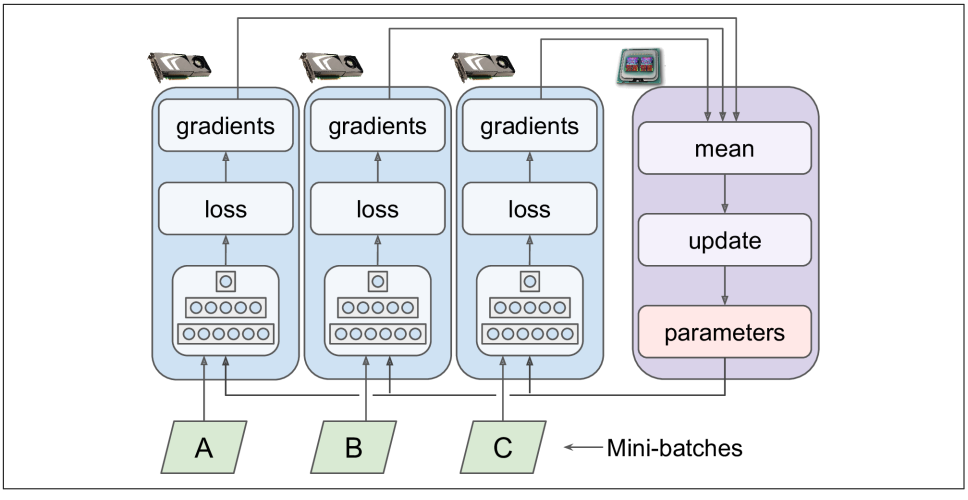


Figure 19-19. Data parallelism with centralized parameters

Whereas the mirrored strategy imposes synchronous weight updates across all GPUs, this centralized approach allows either synchronous or asynchronous updates. Let's see the pros and cons of both options.

Synchronous updates. With *synchronous updates*, the aggregator waits until all gradients are available before it computes the average gradients and passes them to the optimizer, which will update the model parameters. Once a replica has finished computing its gradients, it must wait for the parameters to be updated before it can proceed to the next mini-batch. The downside is that some devices may be slower than others, so all other devices will have to wait for them at every step. Moreover, the parameters will be copied to every device almost at the same time (immediately after the gradients are applied), which may saturate the parameter servers' bandwidth.

To reduce the waiting time at each step, you could ignore the gradients from the slowest few replicas (typically ~10%). For example, you could run 20 replicas, but only aggregate the gradients from the fastest 18 replicas at each step, and just ignore the gradients from the last 2. As soon as the parameters are updated, the first 18 replicas can start working again immediately, without having to wait for the 2 slowest replicas. This setup is generally described as having 18 replicas plus 2 *spare replicas*.[19]

19 This name is slightly confusing because it sounds like some replicas are special, doing nothing. In reality, all replicas are equivalent: they all work hard to be among the fastest at each training step, and the losers vary at every step (unless some devices are really slower than others). However, it does mean that if a server crashes, training will continue just fine.

Asynchronous updates. With asynchronous updates, whenever a replica has finished computing the gradients, it immediately uses them to update the model parameters. There is no aggregation (it removes the "mean" step in Figure 19-19) and no synchronization. Replicas work independently of the other replicas. Since there is no waiting for the other replicas, this approach runs more training steps per minute. Moreover, although the parameters still need to be copied to every device at every step, this happens at different times for each replica, so the risk of bandwidth saturation is reduced.

Data parallelism with asynchronous updates is an attractive choice because of its simplicity, the absence of synchronization delay, and a better use of the bandwidth. However, although it works reasonably well in practice, it is almost surprising that it works at all! Indeed, by the time a replica has finished computing the gradients based on some parameter values, these parameters will have been updated several times by other replicas (on average $N - 1$ times, if there are N replicas), and there is no guarantee that the computed gradients will still be pointing in the right direction (see Figure 19-20). When gradients are severely out-of-date, they are called *stale gradients*: they can slow down convergence, introducing noise and wobble effects (the learning curve may contain temporary oscillations), or they can even make the training algorithm diverge.

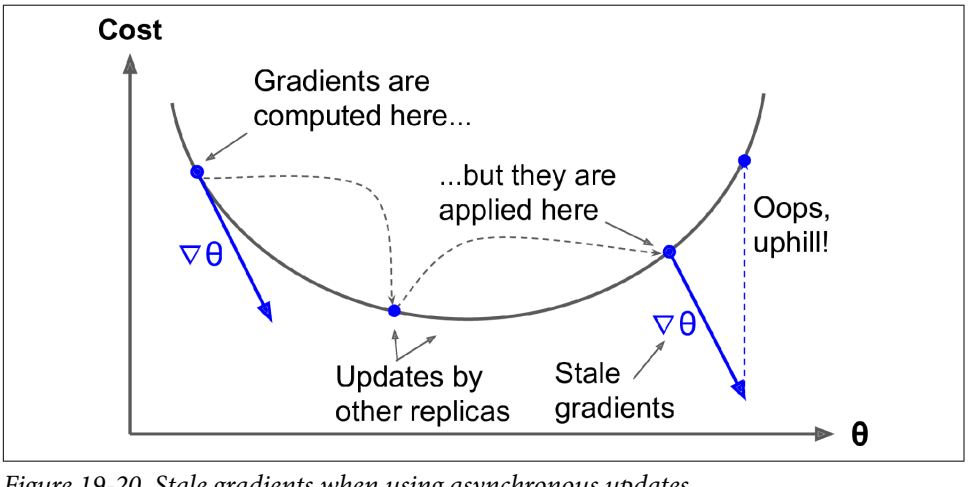


Figure 19-20. Stale gradients when using asynchronous updates

There are a few ways you can reduce the effect of stale gradients:

- Reduce the learning rate.
- Drop stale gradients or scale them down.
- Adjust the mini-batch size.

- Start the first few epochs using just one replica (this is called the *warmup phase*). Stale gradients tend to be more damaging at the beginning of training, when gradients are typically large and the parameters have not settled into a valley of the cost function yet, so different replicas may push the parameters in quite different directions.

A paper published by the Google Brain team in 2016[20] benchmarked various approaches and found that using synchronous updates with a few spare replicas was more efficient than using asynchronous updates, not only converging faster but also producing a better model. However, this is still an active area of research, so you should not rule out asynchronous updates just yet.

Bandwidth saturation

Whether you use synchronous or asynchronous updates, data parallelism with centralized parameters still requires communicating the model parameters from the parameter servers to every replica at the beginning of each training step, and the gradients in the other direction at the end of each training step. Similarly, when using the mirrored strategy, the gradients produced by each GPU will need to be shared with every other GPU. Unfortunately, there always comes a point where adding an extra GPU will not improve performance at all because the time spent moving the data into and out of GPU RAM (and across the network in a distributed setup) will outweigh the speedup obtained by splitting the computation load. At that point, adding more GPUs will just worsen the bandwidth saturation and actually slow down training.

For some models, typically relatively small and trained on a very large training set, you are often better off training the model on a single machine with a single powerful GPU with a large memory bandwidth.

Saturation is more severe for large dense models, since they have a lot of parameters and gradients to transfer. It is less severe for small models (but the parallelization gain is limited) and for large sparse models, where the gradients are typically mostly zeros and so can be communicated efficiently. Jeff Dean, initiator and lead of the Google Brain project, reported typical speedups of 25–40× when distributing computations across 50 GPUs for dense models, and a 300× speedup for sparser models trained across 500 GPUs. As you can see, sparse models really do scale better. Here are a few concrete examples:

20 Jianmin Chen et al., "Revisiting Distributed Synchronous SGD," arXiv preprint arXiv:1604.00981 (2016).

- Neural machine translation: 6× speedup on 8 GPUs
- Inception/ImageNet: 32× speedup on 50 GPUs
- RankBrain: 300× speedup on 500 GPUs

Beyond a few dozen GPUs for a dense model or few hundred GPUs for a sparse model, saturation kicks in and performance degrades. There is plenty of research going on to solve this problem (exploring peer-to-peer architectures rather than centralized parameter servers, using lossy model compression, optimizing when and what the replicas need to communicate, and so on), so there will likely be a lot of progress in parallelizing neural networks in the next few years.

In the meantime, to reduce the saturation problem, you probably want to use a few powerful GPUs rather than plenty of weak GPUs, and you should also group your GPUs on few and very well interconnected servers. You can also try dropping the float precision from 32 bits (`tf.float32`) to 16 bits (`tf.bfloat16`). This will cut in half the amount of data to transfer, often without much impact on the convergence rate or the model's performance. Lastly, if you are using centralized parameters, you can shard (split) the parameters across multiple parameter servers: adding more parameter servers will reduce the network load on each server and limit the risk of bandwidth saturation.

OK, now let's train a model across multiple GPUs!

Training at Scale Using the Distribution Strategies API

Many models can be trained quite well on a single GPU, or even on a CPU. But if training is too slow, you can try distributing it across multiple GPUs on the same machine. If that's still too slow, try using more powerful GPUs, or add more GPUs to the machine. If your model performs heavy computations (such as large matrix multiplications), then it will run much faster on powerful GPUs, and you could even try to use TPUs on Google Cloud AI Platform, which will usually run even faster for such models. But if you can't fit any more GPUs on the same machine, and if TPUs aren't for you (e.g., perhaps your model doesn't benefit much from TPUs, or perhaps you want to use your own hardware infrastructure), then you can try training it across several servers, each with multiple GPUs (if this is still not enough, as a last resort you can try adding some model parallelism, but this requires a lot more effort). In this section we will see how to train models at scale, starting with multiple GPUs on the same machine (or TPUs) and then moving on to multiple GPUs across multiple machines.

Luckily, TensorFlow comes with a very simple API that takes care of all the complexity for you: the *Distribution Strategies API*. To train a Keras model across all available GPUs (on a single machine, for now) using data parallelism with the mirrored

strategy, create a `MirroredStrategy` object, call its `scope()` method to get a distribution context, and wrap the creation and compilation of your model inside that context. Then call the model's `fit()` method normally:

```
distribution = tf.distribute.MirroredStrategy()

with distribution.scope():
    mirrored_model = keras.models.Sequential([...])
    mirrored_model.compile([...])

batch_size = 100 # must be divisible by the number of replicas
history = mirrored_model.fit(X_train, y_train, epochs=10)
```

Under the hood, tf.keras is distribution-aware, so in this `MirroredStrategy` context it knows that it must replicate all variables and operations across all available GPU devices. Note that the `fit()` method will automatically split each training batch across all the replicas, so it's important that the batch size be divisible by the number of replicas. And that's all! Training will generally be significantly faster than using a single device, and the code change was really minimal.

Once you have finished training your model, you can use it to make predictions efficiently: call the `predict()` method, and it will automatically split the batch across all replicas, making predictions in parallel (again, the batch size must be divisible by the number of replicas). If you call the model's `save()` method, it will be saved as a regular model, *not* as a mirrored model with multiple replicas. So when you load it, it will run like a regular model, on a single device (by default GPU 0, or the CPU if there are no GPUs). If you want to load a model and run it on all available devices, you must call `keras.models.load_model()` within a distribution context:

```
with distribution.scope():
    mirrored_model = keras.models.load_model("my_mnist_model.h5")
```

If you only want to use a subset of all the available GPU devices, you can pass the list to the `MirroredStrategy`'s constructor:

```
distribution = tf.distribute.MirroredStrategy(["/gpu:0", "/gpu:1"])
```

By default, the `MirroredStrategy` class uses the *NVIDIA Collective Communications Library* (NCCL) for the AllReduce mean operation, but you can change it by setting the `cross_device_ops` argument to an instance of the `tf.distribute.HierarchicalCopyAllReduce` class, or an instance of the `tf.distribute.ReductionToOneDevice` class. The default NCCL option is based on the `tf.distribute.NcclAllReduce` class, which is usually faster, but this depends on the number and types of GPUs, so you may want to give the alternatives a try.[21]

21 For more details on AllReduce algorithms, read this great post by Yuichiro Ueno, and this page on scaling with NCCL.

If you want to try using data parallelism with centralized parameters, replace the `MirroredStrategy` with the `CentralStorageStrategy`:

```
distribution = tf.distribute.experimental.CentralStorageStrategy()
```

You can optionally set the `compute_devices` argument to specify the list of devices you want to use as workers (by default it will use all available GPUs), and you can optionally set the `parameter_device` argument to specify the device you want to store the parameters on (by default it will use the CPU, or the GPU if there is just one).

Now let's see how to train a model across a cluster of TensorFlow servers!

Training a Model on a TensorFlow Cluster

A *TensorFlow cluster* is a group of TensorFlow processes running in parallel, usually on different machines, and talking to each other to complete some work—for example, training or executing a neural network. Each TF process in the cluster is called a *task*, or a *TF server*. It has an IP address, a port, and a type (also called its *role* or its *job*). The type can be either `"worker"`, `"chief"`, `"ps"` (parameter server), or `"evaluator"`:

- Each *worker* performs computations, usually on a machine with one or more GPUs.
- The *chief* performs computations as well (it is a worker), but it also handles extra work such as writing TensorBoard logs or saving checkpoints. There is a single chief in a cluster. If no chief is specified, then the first worker is the chief.
- A *parameter server* only keeps track of variable values, and it is usually on a CPU-only machine. This type of task is only used with the `ParameterServerStrategy`.
- An *evaluator* obviously takes care of evaluation.

To start a TensorFlow cluster, you must first specify it. This means defining each task's IP address, TCP port, and type. For example, the following *cluster specification* defines a cluster with three tasks (two workers and one parameter server; see Figure 19-21). The cluster spec is a dictionary with one key per job, and the values are lists of task addresses (*IP:port*):

```
cluster_spec = {
    "worker": [
        "machine-a.example.com:2222",  # /job:worker/task:0
        "machine-b.example.com:2222"   # /job:worker/task:1
    ],
    "ps": ["machine-a.example.com:2221"] # /job:ps/task:0
}
```

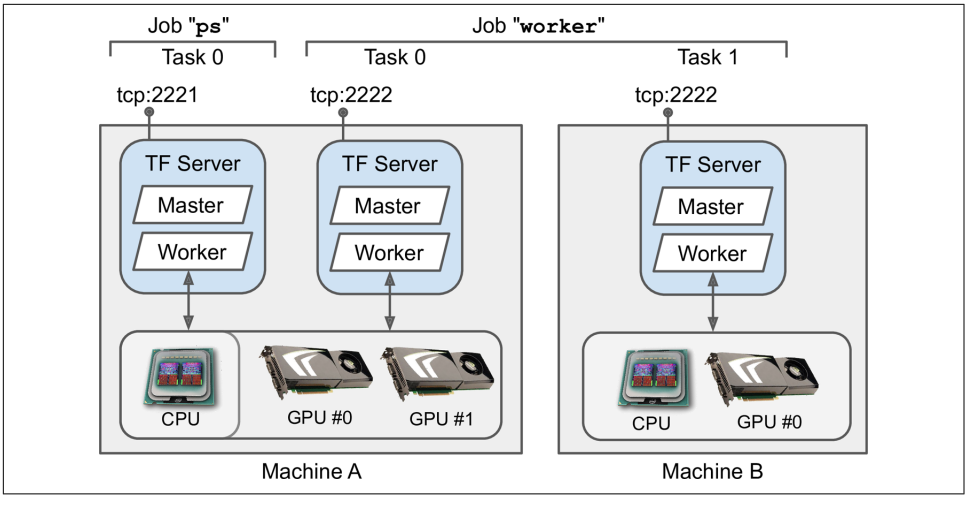


Figure 19-21. TensorFlow cluster

In general there will be a single task per machine, but as this example shows, you can configure multiple tasks on the same machine if you want (if they share the same GPUs, make sure the RAM is split appropriately, as discussed earlier).

By default, every task in the cluster may communicate with every other task, so make sure to configure your firewall to authorize all communications between these machines on these ports (it's usually simpler if you use the same port on every machine).

When you start a task, you must give it the cluster spec, and you must also tell it what its type and index are (e.g., worker 0). The simplest way to specify everything at once (both the cluster spec and the current task's type and index) is to set the `TF_CONFIG` environment variable before starting TensorFlow. It must be a JSON-encoded dictionary containing a cluster specification (under the `"cluster"` key) and the type and index of the current task (under the `"task"` key). For example, the following `TF_CONFIG` environment variable uses the cluster we just defined and specifies that the task to start is the first worker:

```
import os
import json

os.environ["TF_CONFIG"] = json.dumps({
    "cluster": cluster_spec,
    "task": {"type": "worker", "index": 0}
})
```

In general you want to define the `TF_CONFIG` environment variable outside of Python, so the code does not need to include the current task's type and index (this makes it possible to use the same code across all workers).

Now let's train a model on a cluster! We will start with the mirrored strategy—it's surprisingly simple! First, you need to set the `TF_CONFIG` environment variable appropriately for each task. There should be no parameter server (remove the "ps" key in the cluster spec), and in general you will want a single worker per machine. Make extra sure you set a different task index for each task. Finally, run the following training code on every worker:

```
distribution = tf.distribute.experimental.MultiWorkerMirroredStrategy()

with distribution.scope():
    mirrored_model = keras.models.Sequential([...])
    mirrored_model.compile([...])

batch_size = 100 # must be divisible by the number of replicas
history = mirrored_model.fit(X_train, y_train, epochs=10)
```

Yes, that's exactly the same code we used earlier, except this time we are using the `MultiWorkerMirroredStrategy` (in future versions, the `MirroredStrategy` will probably handle both the single machine and multimachine cases). When you start this script on the first workers, they will remain blocked at the AllReduce step, but as soon as the last worker starts up training will begin, and you will see them all advancing at exactly the same rate (since they synchronize at each step).

You can choose from two AllReduce implementations for this distribution strategy: a ring AllReduce algorithm based on gRPC for the network communications, and NCCL's implementation. The best algorithm to use depends on the number of workers, the number and types of GPUs, and the network. By default, TensorFlow will apply some heuristics to select the right algorithm for you, but if you want to force one algorithm, pass `CollectiveCommunication.RING` or `CollectiveCommunication.NCCL` (from `tf.distribute.experimental`) to the strategy's constructor.

If you prefer to implement asynchronous data parallelism with parameter servers, change the strategy to `ParameterServerStrategy`, add one or more parameter servers, and configure `TF_CONFIG` appropriately for each task. Note that although the workers will work asynchronously, the replicas on each worker will work synchronously.

Lastly, if you have access to TPUs on Google Cloud, you can create a `TPUStrategy` like this (then use it like the other strategies):

```
resolver = tf.distribute.cluster_resolver.TPUClusterResolver()
tf.tpu.experimental.initialize_tpu_system(resolver)
tpu_strategy = tf.distribute.experimental.TPUStrategy(resolver)
```

If you are a researcher, you may be eligible to use TPUs for free; see *https://tensorflow.org/tfrc* for more details.

You can now train models across multiple GPUs and multiple servers: give yourself a pat on the back! If you want to train a large model, you will need many GPUs, across many servers, which will require either buying a lot of hardware or managing a lot of cloud VMs. In many cases, it's going to be less hassle and less expensive to use a cloud service that takes care of provisioning and managing all this infrastructure for you, just when you need it. Let's see how to do that on GCP.

Running Large Training Jobs on Google Cloud AI Platform

If you decide to use Google AI Platform, you can deploy a training job with the same training code as you would run on your own TF cluster, and the platform will take care of provisioning and configuring as many GPU VMs as you desire (within your quotas).

To start the job, you will need the `gcloud` command-line tool, which is part of the Google Cloud SDK. You can either install the SDK on your own machine, or just use the Google Cloud Shell on GCP. This is a terminal you can use directly in your web browser; it runs on a free Linux VM (Debian), with the SDK already installed and preconfigured for you. The Cloud Shell is available anywhere in GCP: just click the Activate Cloud Shell icon at the top right of the page (see Figure 19-22).

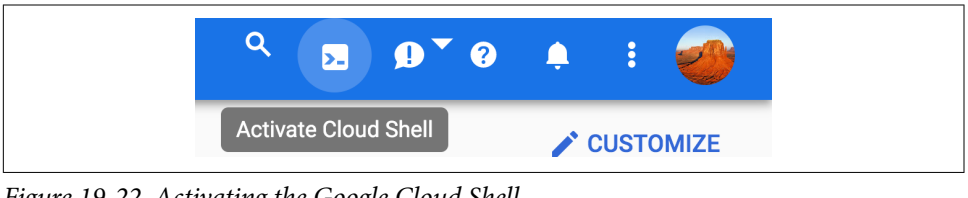


Figure 19-22. Activating the Google Cloud Shell

If you prefer to install the SDK on your machine, once you have installed it, you need to initialize it by running `gcloud init`: you will need to log in to GCP and grant access to your GCP resources, then select the GCP project you want to use (if you have more than one), as well as the region where you want the job to run. The `gcloud` command gives you access to every GCP feature, including the ones we used earlier. You don't have to go through the web interface every time; you can write scripts that start or stop VMs for you, deploy models, or perform any other GCP action.

Before you can run the training job, you need to write the training code, exactly like you did earlier for a distributed setup (e.g., using the `ParameterServerStrategy`). AI Platform will take care of setting `TF_CONFIG` for you on each VM. Once that's done, you can deploy it and run it on a TF cluster with a command line like this:

```
$ gcloud ai-platform jobs submit training my_job_20190531_164700 \
    --region asia-southeast1 \
    --scale-tier PREMIUM_1 \
    --runtime-version 2.0 \
    --python-version 3.5 \
    --package-path /my_project/src/trainer \
    --module-name trainer.task \
    --staging-bucket gs://my-staging-bucket \
    --job-dir gs://my-mnist-model-bucket/trained_model \
    --
    --my-extra-argument1 foo --my-extra-argument2 bar
```

Let's go through these options. The command will start a training job named `my_job_20190531_164700`, in the `asia-southeast1` region, using a `PREMIUM_1` *scale tier*: this corresponds to 20 workers (including a chief) and 11 parameter servers (check out the other available scale tiers). All these VMs will be based on AI Platform's 2.0 runtime (a VM configuration that includes TensorFlow 2.0 and many other packages)[22] and Python 3.5. The training code is located in the */my_project/src/trainer* directory, and the `gcloud` command will automatically bundle it into a pip package and upload it to GCS at *gs://my-staging-bucket*. Next, AI Platform will start several VMs, deploy the package to them, and run the `trainer.task` module. Lastly, the `--job-dir` argument and the extra arguments (i.e., all the arguments located after the `--` separator) will be passed to the training program: the chief task will usually use the `--job-dir` argument to find out where to save the final model on GCS, in this case at *gs://my-mnist-model-bucket/trained_model*. And that's it! In the GCP console, you can then open the navigation menu, scroll down to the Artificial Intelligence section, and open AI Platform → Jobs. You should see your job running, and if you click it you will see graphs showing the CPU, GPU, and RAM utilization for every task. You can click View Logs to access the detailed logs using Stackdriver.

If you place the training data on GCS, you can create a `tf.data.TextLineDataset` or `tf.data.TFRecordDataset` to access it: just use the GCS paths as the filenames (e.g., *gs://my-data-bucket/my_data_001.csv*). These datasets rely on the `tf.io.gfile` package to access files: it supports both local files and GCS files (but make sure the service account you use has access to GCS).

22 At the time of this writing, the 2.0 runtime is not yet available, but it should be ready by the time you read this. Check out the list of available runtimes.

If you want to explore a few hyperparameter values, you can simply run multiple jobs and specify the hyperparameter values using the extra arguments for your tasks. However, if you want to explore many hyperparameters efficiently, it's a good idea to use AI Platform's hyperparameter tuning service instead.

Black Box Hyperparameter Tuning on AI Platform

AI Platform provides a powerful Bayesian optimization hyperparameter tuning service called Google Vizier.[23] To use it, you need to pass a YAML configuration file when creating the job (`--config tuning.yaml`). For example, it may look like this:

```
trainingInput:
  hyperparameters:
    goal: MAXIMIZE
    hyperparameterMetricTag: accuracy
    maxTrials: 10
    maxParallelTrials: 2
    params:
      - parameterName: n_layers
        type: INTEGER
        minValue: 10
        maxValue: 100
        scaleType: UNIT_LINEAR_SCALE
      - parameterName: momentum
        type: DOUBLE
        minValue: 0.1
        maxValue: 1.0
        scaleType: UNIT_LOG_SCALE
```

This tells AI Platform that we want to maximize the metric named `"accuracy"`, the job will run a maximum of 10 trials (each trial will run our training code to train the model from scratch), and it will run a maximum of 2 trials in parallel. We want it to tune two hyperparameters: the `n_layers` hyperparameter (an integer between 10 and 100) and the `momentum` hyperparameter (a float between 0.1 and 1.0). The `scaleType` argument specifies the prior for the hyperparameter value: `UNIT_LINEAR_SCALE` means a flat prior (i.e., no a priori preference), while `UNIT_LOG_SCALE` says we have a prior belief that the optimal value lies closer to the max value (the other possible prior is `UNIT_REVERSE_LOG_SCALE`, when we believe the optimal value to be close to the min value).

The `n_layers` and `momentum` arguments will be passed as command-line arguments to the training code, and of course it is expected to use them. The question is, how will the training code communicate the metric back to the AI Platform so that it can

23 Daniel Golovin et al., "Google Vizier: A Service for Black-Box Optimization," *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining* (2017): 1487–1495.

decide which hyperparameter values to use during the next trial? Well, AI Platform just monitors the output directory (specified via `--job-dir`) for any event file (introduced in Chapter 10) containing summaries for a metric named `"accuracy"` (or whatever metric name is specified as the `hyperparameterMetricTag`), and it reads those values. So your training code simply has to use the `TensorBoard()` callback (which you will want to do anyway for monitoring), and you're good to go!

Once the job is finished, all the hyperparameter values used in each trial and the resulting accuracy will be available in the job's output (available via the AI Platform → Jobs page).

AI Platform jobs can also be used to efficiently execute your model on large amounts of data: each worker can read part of the data from GCS, make predictions, and save them to GCS.

Now you have all the tools and knowledge you need to create state-of-the-art neural net architectures and train them at scale using various distribution strategies, on your own infrastructure or on the cloud—and you can even perform powerful Bayesian optimization to fine-tune the hyperparameters!

Exercises

1. What does a SavedModel contain? How do you inspect its content?
2. When should you use TF Serving? What are its main features? What are some tools you can use to deploy it?
3. How do you deploy a model across multiple TF Serving instances?
4. When should you use the gRPC API rather than the REST API to query a model served by TF Serving?
5. What are the different ways TFLite reduces a model's size to make it run on a mobile or embedded device?
6. What is quantization-aware training, and why would you need it?
7. What are model parallelism and data parallelism? Why is the latter generally recommended?
8. When training a model across multiple servers, what distribution strategies can you use? How do you choose which one to use?
9. Train a model (any model you like) and deploy it to TF Serving or Google Cloud AI Platform. Write the client code to query it using the REST API or the gRPC

API. Update the model and deploy the new version. Your client code will now query the new version. Roll back to the first version.

10. Train any model across multiple GPUs on the same machine using the `MirroredStrategy` (if you do not have access to GPUs, you can use Colaboratory with a GPU Runtime and create two virtual GPUs). Train the model again using the `CentralStorageStrategy` and compare the training time.
11. Train a small model on Google Cloud AI Platform, using black box hyperparameter tuning.

Thank You!

Before we close the last chapter of this book, I would like to thank you for reading it up to the last paragraph. I truly hope that you had as much pleasure reading this book as I had writing it, and that it will be useful for your projects, big or small.

If you find errors, please send feedback. More generally, I would love to know what you think, so please don't hesitate to contact me via O'Reilly, through the *ageron/handson-ml2* GitHub project, or on Twitter at @aureliengeron.

Going forward, my best advice to you is to practice and practice: try going through all the exercises (if you have not done so already), play with the Jupyter notebooks, join Kaggle.com or some other ML community, watch ML courses, read papers, attend conferences, and meet experts. It also helps tremendously to have a concrete project to work on, whether it is for work or for fun (ideally for both), so if there's anything you have always dreamt of building, give it a shot! Work incrementally; don't shoot for the moon right away, but stay focused on your project and build it piece by piece. It will require patience and perseverance, but when you have a walking robot, or a working chatbot, or whatever else you fancy to build, it will be immensely rewarding.

My greatest hope is that this book will inspire you to build a wonderful ML application that will benefit all of us! What will it be?

—Aurélien Géron, June 17, 2019

APPENDIX A

Exercise Solutions

Solutions to the coding exercises are available in the online Jupyter notebooks at *https://github.com/ageron/handson-ml2*.

Chapter 1: The Machine Learning Landscape

1. Machine Learning is about building systems that can learn from data. Learning means getting better at some task, given some performance measure.
2. Machine Learning is great for complex problems for which we have no algorithmic solution, to replace long lists of hand-tuned rules, to build systems that adapt to fluctuating environments, and finally to help humans learn (e.g., data mining).
3. A labeled training set is a training set that contains the desired solution (a.k.a. a label) for each instance.
4. The two most common supervised tasks are regression and classification.
5. Common unsupervised tasks include clustering, visualization, dimensionality reduction, and association rule learning.
6. Reinforcement Learning is likely to perform best if we want a robot to learn to walk in various unknown terrains, since this is typically the type of problem that Reinforcement Learning tackles. It might be possible to express the problem as a supervised or semisupervised learning problem, but it would be less natural.
7. If you don't know how to define the groups, then you can use a clustering algorithm (unsupervised learning) to segment your customers into clusters of similar customers. However, if you know what groups you would like to have, then you

can feed many examples of each group to a classification algorithm (supervised learning), and it will classify all your customers into these groups.

8. Spam detection is a typical supervised learning problem: the algorithm is fed many emails along with their labels (spam or not spam).
9. An online learning system can learn incrementally, as opposed to a batch learning system. This makes it capable of adapting rapidly to both changing data and autonomous systems, and of training on very large quantities of data.
10. Out-of-core algorithms can handle vast quantities of data that cannot fit in a computer's main memory. An out-of-core learning algorithm chops the data into mini-batches and uses online learning techniques to learn from these mini-batches.
11. An instance-based learning system learns the training data by heart; then, when given a new instance, it uses a similarity measure to find the most similar learned instances and uses them to make predictions.
12. A model has one or more model parameters that determine what it will predict given a new instance (e.g., the slope of a linear model). A learning algorithm tries to find optimal values for these parameters such that the model generalizes well to new instances. A hyperparameter is a parameter of the learning algorithm itself, not of the model (e.g., the amount of regularization to apply).
13. Model-based learning algorithms search for an optimal value for the model parameters such that the model will generalize well to new instances. We usually train such systems by minimizing a cost function that measures how bad the system is at making predictions on the training data, plus a penalty for model complexity if the model is regularized. To make predictions, we feed the new instance's features into the model's prediction function, using the parameter values found by the learning algorithm.
14. Some of the main challenges in Machine Learning are the lack of data, poor data quality, nonrepresentative data, uninformative features, excessively simple models that underfit the training data, and excessively complex models that overfit the data.
15. If a model performs great on the training data but generalizes poorly to new instances, the model is likely overfitting the training data (or we got extremely lucky on the training data). Possible solutions to overfitting are getting more data, simplifying the model (selecting a simpler algorithm, reducing the number of parameters or features used, or regularizing the model), or reducing the noise in the training data.
16. A test set is used to estimate the generalization error that a model will make on new instances, before the model is launched in production.

17. A validation set is used to compare models. It makes it possible to select the best model and tune the hyperparameters.
18. The train-dev set is used when there is a risk of mismatch between the training data and the data used in the validation and test datasets (which should always be as close as possible to the data used once the model is in production). The train-dev set is a part of the training set that's held out (the model is not trained on it). The model is trained on the rest of the training set, and evaluated on both the train-dev set and the validation set. If the model performs well on the training set but not on the train-dev set, then the model is likely overfitting the training set. If it performs well on both the training set and the train-dev set, but not on the validation set, then there is probably a significant data mismatch between the training data and the validation + test data, and you should try to improve the training data to make it look more like the validation + test data.
19. If you tune hyperparameters using the test set, you risk overfitting the test set, and the generalization error you measure will be optimistic (you may launch a model that performs worse than you expect).

Chapter 2: End-to-End Machine Learning Project

See the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

Chapter 3: Classification

See the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

Chapter 4: Training Models

1. If you have a training set with millions of features you can use Stochastic Gradient Descent or Mini-batch Gradient Descent, and perhaps Batch Gradient Descent if the training set fits in memory. But you cannot use the Normal Equation or the SVD approach because the computational complexity grows quickly (more than quadratically) with the number of features.
2. If the features in your training set have very different scales, the cost function will have the shape of an elongated bowl, so the Gradient Descent algorithms will take a long time to converge. To solve this you should scale the data before training the model. Note that the Normal Equation or SVD approach will work just fine without scaling. Moreover, regularized models may converge to a suboptimal solution if the features are not scaled: since regularization penalizes large weights, features with smaller values will tend to be ignored compared to features with larger values.

3. Gradient Descent cannot get stuck in a local minimum when training a Logistic Regression model because the cost function is convex.[1]
4. If the optimization problem is convex (such as Linear Regression or Logistic Regression), and assuming the learning rate is not too high, then all Gradient Descent algorithms will approach the global optimum and end up producing fairly similar models. However, unless you gradually reduce the learning rate, Stochastic GD and Mini-batch GD will never truly converge; instead, they will keep jumping back and forth around the global optimum. This means that even if you let them run for a very long time, these Gradient Descent algorithms will produce slightly different models.
5. If the validation error consistently goes up after every epoch, then one possibility is that the learning rate is too high and the algorithm is diverging. If the training error also goes up, then this is clearly the problem and you should reduce the learning rate. However, if the training error is not going up, then your model is overfitting the training set and you should stop training.
6. Due to their random nature, neither Stochastic Gradient Descent nor Mini-batch Gradient Descent is guaranteed to make progress at every single training iteration. So if you immediately stop training when the validation error goes up, you may stop much too early, before the optimum is reached. A better option is to save the model at regular intervals; then, when it has not improved for a long time (meaning it will probably never beat the record), you can revert to the best saved model.
7. Stochastic Gradient Descent has the fastest training iteration since it considers only one training instance at a time, so it is generally the first to reach the vicinity of the global optimum (or Mini-batch GD with a very small mini-batch size). However, only Batch Gradient Descent will actually converge, given enough training time. As mentioned, Stochastic GD and Mini-batch GD will bounce around the optimum, unless you gradually reduce the learning rate.
8. If the validation error is much higher than the training error, this is likely because your model is overfitting the training set. One way to try to fix this is to reduce the polynomial degree: a model with fewer degrees of freedom is less likely to overfit. Another thing you can try is to regularize the model—for example, by adding an ℓ_2 penalty (Ridge) or an ℓ_1 penalty (Lasso) to the cost function. This will also reduce the degrees of freedom of the model. Lastly, you can try to increase the size of the training set.

1 If you draw a straight line between any two points on the curve, the line never crosses the curve.

9. If both the training error and the validation error are almost equal and fairly high, the model is likely underfitting the training set, which means it has a high bias. You should try reducing the regularization hyperparameter α.
10. Let's see:
    - A model with some regularization typically performs better than a model without any regularization, so you should generally prefer Ridge Regression over plain Linear Regression.
    - Lasso Regression uses an ℓ_1 penalty, which tends to push the weights down to exactly zero. This leads to sparse models, where all weights are zero except for the most important weights. This is a way to perform feature selection automatically, which is good if you suspect that only a few features actually matter. When you are not sure, you should prefer Ridge Regression.
    - Elastic Net is generally preferred over Lasso since Lasso may behave erratically in some cases (when several features are strongly correlated or when there are more features than training instances). However, it does add an extra hyperparameter to tune. If you want Lasso without the erratic behavior, you can just use Elastic Net with an `l1_ratio` close to 1.
11. If you want to classify pictures as outdoor/indoor and daytime/nighttime, since these are not exclusive classes (i.e., all four combinations are possible) you should train two Logistic Regression classifiers.
12. See the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

Chapter 5: Support Vector Machines

1. The fundamental idea behind Support Vector Machines is to fit the widest possible "street" between the classes. In other words, the goal is to have the largest possible margin between the decision boundary that separates the two classes and the training instances. When performing soft margin classification, the SVM searches for a compromise between perfectly separating the two classes and having the widest possible street (i.e., a few instances may end up on the street). Another key idea is to use kernels when training on nonlinear datasets.
2. After training an SVM, a *support vector* is any instance located on the "street" (see the previous answer), including its border. The decision boundary is entirely determined by the support vectors. Any instance that is *not* a support vector (i.e., is off the street) has no influence whatsoever; you could remove them, add more instances, or move them around, and as long as they stay off the street they won't affect the decision boundary. Computing the predictions only involves the support vectors, not the whole training set.

3. SVMs try to fit the largest possible "street" between the classes (see the first answer), so if the training set is not scaled, the SVM will tend to neglect small features (see Figure 5-2).
4. An SVM classifier can output the distance between the test instance and the decision boundary, and you can use this as a confidence score. However, this score cannot be directly converted into an estimation of the class probability. If you set `probability=True` when creating an SVM in Scikit-Learn, then after training it will calibrate the probabilities using Logistic Regression on the SVM's scores (trained by an additional five-fold cross-validation on the training data). This will add the `predict_proba()` and `predict_log_proba()` methods to the SVM.
5. This question applies only to linear SVMs since kernelized SVMs can only use the dual form. The computational complexity of the primal form of the SVM problem is proportional to the number of training instances m, while the computational complexity of the dual form is proportional to a number between m^2 and m^3. So if there are millions of instances, you should definitely use the primal form, because the dual form will be much too slow.
6. If an SVM classifier trained with an RBF kernel underfits the training set, there might be too much regularization. To decrease it, you need to increase `gamma` or `C` (or both).
7. Let's call the QP parameters for the hard margin problem $\mathbf{H}'$, $\mathbf{f}'$, $\mathbf{A}'$, and $\mathbf{b}'$ (see "Quadratic Programming" on page 167). The QP parameters for the soft margin problem have m additional parameters ($n_p = n + 1 + m$) and m additional constraints ($n_c = 2m$). They can be defined like so:
   - $\mathbf{H}$ is equal to $\mathbf{H}'$, plus m columns of 0s on the right and m rows of 0s at the bottom: $\mathbf{H} = \begin{pmatrix} \mathbf{H}' & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{pmatrix}$
   - $\mathbf{f}$ is equal to $\mathbf{f}'$ with m additional elements, all equal to the value of the hyperparameter C.
   - $\mathbf{b}$ is equal to $\mathbf{b}'$ with m additional elements, all equal to 0.
   - $\mathbf{A}$ is equal to $\mathbf{A}'$, with an extra $m \times m$ identity matrix $\mathbf{I}_m$ appended to the right, $-*\mathrm{I}*_m$ just below it, and the rest filled with 0s: $\mathbf{A} = \begin{pmatrix} \mathbf{A}' & \mathbf{I}_m \\ \mathbf{0} & -\mathbf{I}_m \end{pmatrix}$

For the solutions to exercises 8, 9, and 10, please see the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

Chapter 6: Decision Trees

1. The depth of a well-balanced binary tree containing m leaves is equal to $\log_2(m)$,[2] rounded up. A binary Decision Tree (one that makes only binary decisions, as is the case with all trees in Scikit-Learn) will end up more or less well balanced at the end of training, with one leaf per training instance if it is trained without restrictions. Thus, if the training set contains one million instances, the Decision Tree will have a depth of $\log_2(10^6) \approx 20$ (actually a bit more since the tree will generally not be perfectly well balanced).
2. A node's Gini impurity is generally lower than its parent's. This is due to the CART training algorithm's cost function, which splits each node in a way that minimizes the weighted sum of its children's Gini impurities. However, it is possible for a node to have a higher Gini impurity than its parent, as long as this increase is more than compensated for by a decrease in the other child's impurity. For example, consider a node containing four instances of class A and one of class B. Its Gini impurity is $1 - (1/5)^2 - (4/5)^2 = 0.32$. Now suppose the dataset is one-dimensional and the instances are lined up in the following order: A, B, A, A, A. You can verify that the algorithm will split this node after the second instance, producing one child node with instances A, B, and the other child node with instances A, A, A. The first child node's Gini impurity is $1 - (1/2)^2 - (1/2)^2 = 0.5$, which is higher than its parent's. This is compensated for by the fact that the other node is pure, so its overall weighted Gini impurity is $2/5 \times 0.5 + 3/5 \times 0 = 0.2$, which is lower than the parent's Gini impurity.
3. If a Decision Tree is overfitting the training set, it may be a good idea to decrease `max_depth`, since this will constrain the model, regularizing it.
4. Decision Trees don't care whether or not the training data is scaled or centered; that's one of the nice things about them. So if a Decision Tree underfits the training set, scaling the input features will just be a waste of time.
5. The computational complexity of training a Decision Tree is $O(n \times m \log(m))$. So if you multiply the training set size by 10, the training time will be multiplied by $K = (n \times 10m \times \log(10m)) / (n \times m \times \log(m)) = 10 \times \log(10m) / \log(m)$. If $m = 10^6$, then $K \approx 11.7$, so you can expect the training time to be roughly 11.7 hours.
6. Presorting the training set speeds up training only if the dataset is smaller than a few thousand instances. If it contains 100,000 instances, setting `presort=True` will considerably slow down training.

For the solutions to exercises 7 and 8, please see the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

2 $\log_2$ is the binary log; $\log_2(m) = \log(m) / \log(2)$.

Chapter 7: Ensemble Learning and Random Forests

1. If you have trained five different models and they all achieve 95% precision, you can try combining them into a voting ensemble, which will often give you even better results. It works better if the models are very different (e.g., an SVM classifier, a Decision Tree classifier, a Logistic Regression classifier, and so on). It is even better if they are trained on different training instances (that's the whole point of bagging and pasting ensembles), but if not this will still be effective as long as the models are very different.
2. A hard voting classifier just counts the votes of each classifier in the ensemble and picks the class that gets the most votes. A soft voting classifier computes the average estimated class probability for each class and picks the class with the highest probability. This gives high-confidence votes more weight and often performs better, but it works only if every classifier is able to estimate class probabilities (e.g., for the SVM classifiers in Scikit-Learn you must set `probability=True`).
3. It is quite possible to speed up training of a bagging ensemble by distributing it across multiple servers, since each predictor in the ensemble is independent of the others. The same goes for pasting ensembles and Random Forests, for the same reason. However, each predictor in a boosting ensemble is built based on the previous predictor, so training is necessarily sequential, and you will not gain anything by distributing training across multiple servers. Regarding stacking ensembles, all the predictors in a given layer are independent of each other, so they can be trained in parallel on multiple servers. However, the predictors in one layer can only be trained after the predictors in the previous layer have all been trained.
4. With out-of-bag evaluation, each predictor in a bagging ensemble is evaluated using instances that it was not trained on (they were held out). This makes it possible to have a fairly unbiased evaluation of the ensemble without the need for an additional validation set. Thus, you have more instances available for training, and your ensemble can perform slightly better.
5. When you are growing a tree in a Random Forest, only a random subset of the features is considered for splitting at each node. This is true as well for Extra-Trees, but they go one step further: rather than searching for the best possible thresholds, like regular Decision Trees do, they use random thresholds for each feature. This extra randomness acts like a form of regularization: if a Random Forest overfits the training data, Extra-Trees might perform better. Moreover, since Extra-Trees don't search for the best possible thresholds, they are much faster to train than Random Forests. However, they are neither faster nor slower than Random Forests when making predictions.

6. If your AdaBoost ensemble underfits the training data, you can try increasing the number of estimators or reducing the regularization hyperparameters of the base estimator. You may also try slightly increasing the learning rate.
7. If your Gradient Boosting ensemble overfits the training set, you should try decreasing the learning rate. You could also use early stopping to find the right number of predictors (you probably have too many).

For the solutions to exercises 8 and 9, please see the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

Chapter 8: Dimensionality Reduction

1. The main motivations for dimensionality reduction are:

   - To speed up a subsequent training algorithm (in some cases it may even remove noise and redundant features, making the training algorithm perform better)
   - To visualize the data and gain insights on the most important features
   - To save space (compression)

   The main drawbacks are:

   - Some information is lost, possibly degrading the performance of subsequent training algorithms.
   - It can be computationally intensive.
   - It adds some complexity to your Machine Learning pipelines.
   - Transformed features are often hard to interpret.

2. The curse of dimensionality refers to the fact that many problems that do not exist in low-dimensional space arise in high-dimensional space. In Machine Learning, one common manifestation is the fact that randomly sampled high-dimensional vectors are generally very sparse, increasing the risk of overfitting and making it very difficult to identify patterns in the data without having plenty of training data.
3. Once a dataset's dimensionality has been reduced using one of the algorithms we discussed, it is almost always impossible to perfectly reverse the operation, because some information gets lost during dimensionality reduction. Moreover, while some algorithms (such as PCA) have a simple reverse transformation procedure that can reconstruct a dataset relatively similar to the original, other algorithms (such as T-SNE) do not.

4. PCA can be used to significantly reduce the dimensionality of most datasets, even if they are highly nonlinear, because it can at least get rid of useless dimensions. However, if there are no useless dimensions—as in a Swiss roll dataset—then reducing dimensionality with PCA will lose too much information. You want to unroll the Swiss roll, not squash it.
5. That's a trick question: it depends on the dataset. Let's look at two extreme examples. First, suppose the dataset is composed of points that are almost perfectly aligned. In this case, PCA can reduce the dataset down to just one dimension while still preserving 95% of the variance. Now imagine that the dataset is composed of perfectly random points, scattered all around the 1,000 dimensions. In this case roughly 950 dimensions are required to preserve 95% of the variance. So the answer is, it depends on the dataset, and it could be any number between 1 and 950. Plotting the explained variance as a function of the number of dimensions is one way to get a rough idea of the dataset's intrinsic dimensionality.
6. Regular PCA is the default, but it works only if the dataset fits in memory. Incremental PCA is useful for large datasets that don't fit in memory, but it is slower than regular PCA, so if the dataset fits in memory you should prefer regular PCA. Incremental PCA is also useful for online tasks, when you need to apply PCA on the fly, every time a new instance arrives. Randomized PCA is useful when you want to considerably reduce dimensionality and the dataset fits in memory; in this case, it is much faster than regular PCA. Finally, Kernel PCA is useful for nonlinear datasets.
7. Intuitively, a dimensionality reduction algorithm performs well if it eliminates a lot of dimensions from the dataset without losing too much information. One way to measure this is to apply the reverse transformation and measure the reconstruction error. However, not all dimensionality reduction algorithms provide a reverse transformation. Alternatively, if you are using dimensionality reduction as a preprocessing step before another Machine Learning algorithm (e.g., a Random Forest classifier), then you can simply measure the performance of that second algorithm; if dimensionality reduction did not lose too much information, then the algorithm should perform just as well as when using the original dataset.
8. It can absolutely make sense to chain two different dimensionality reduction algorithms. A common example is using PCA to quickly get rid of a large number of useless dimensions, then applying another much slower dimensionality reduction algorithm, such as LLE. This two-step approach will likely yield the same performance as using LLE only, but in a fraction of the time.

For the solutions to exercises 9 and 10, please see the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

Chapter 9: Unsupervised Learning Techniques

1. In Machine Learning, clustering is the unsupervised task of grouping similar instances together. The notion of similarity depends on the task at hand: for example, in some cases two nearby instances will be considered similar, while in others similar instances may be far apart as long as they belong to the same densely packed group. Popular clustering algorithms include K-Means, DBSCAN, agglomerative clustering, BIRCH, Mean-Shift, affinity propagation, and spectral clustering.
2. The main applications of clustering algorithms include data analysis, customer segmentation, recommender systems, search engines, image segmentation, semi-supervised learning, dimensionality reduction, anomaly detection, and novelty detection.
3. The elbow rule is a simple technique to select the number of clusters when using K-Means: just plot the inertia (the mean squared distance from each instance to its nearest centroid) as a function of the number of clusters, and find the point in the curve where the inertia stops dropping fast (the "elbow"). This is generally close to the optimal number of clusters. Another approach is to plot the silhouette score as a function of the number of clusters. There will often be a peak, and the optimal number of clusters is generally nearby. The silhouette score is the mean silhouette coefficient over all instances. This coefficient varies from +1 for instances that are well inside their cluster and far from other clusters, to –1 for instances that are very close to another cluster. You may also plot the silhouette diagrams and perform a more thorough analysis.
4. Labeling a dataset is costly and time-consuming. Therefore, it is common to have plenty of unlabeled instances, but few labeled instances. Label propagation is a technique that consists in copying some (or all) of the labels from the labeled instances to similar unlabeled instances. This can greatly extend the number of labeled instances, and thereby allow a supervised algorithm to reach better performance (this is a form of semi-supervised learning). One approach is to use a clustering algorithm such as K-Means on all the instances, then for each cluster find the most common label or the label of the most representative instance (i.e., the one closest to the centroid) and propagate it to the unlabeled instances in the same cluster.
5. K-Means and BIRCH scale well to large datasets. DBSCAN and Mean-Shift look for regions of high density.
6. Active learning is useful whenever you have plenty of unlabeled instances but labeling is costly. In this case (which is very common), rather than randomly selecting instances to label, it is often preferable to perform active learning, where human experts interact with the learning algorithm, providing labels for

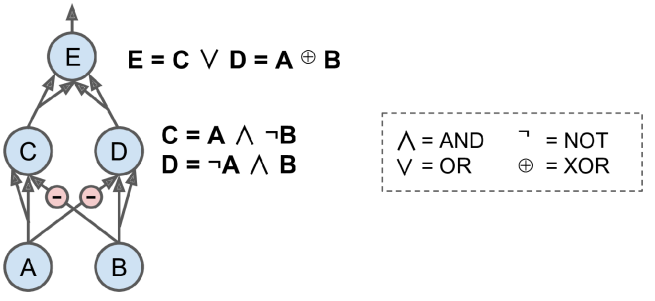
specific instances when the algorithm requests them. A common approach is uncertainty sampling (see the description in "Active Learning" on page 255).

7. Many people use the terms *anomaly detection* and *novelty detection* interchangeably, but they are not exactly the same. In anomaly detection, the algorithm is trained on a dataset that may contain outliers, and the goal is typically to identify these outliers (within the training set), as well as outliers among new instances. In novelty detection, the algorithm is trained on a dataset that is presumed to be "clean," and the objective is to detect novelties strictly among new instances. Some algorithms work best for anomaly detection (e.g., Isolation Forest), while others are better suited for novelty detection (e.g., one-class SVM).
8. A Gaussian mixture model (GMM) is a probabilistic model that assumes that the instances were generated from a mixture of several Gaussian distributions whose parameters are unknown. In other words, the assumption is that the data is grouped into a finite number of clusters, each with an ellipsoidal shape (but the clusters may have different ellipsoidal shapes, sizes, orientations, and densities), and we don't know which cluster each instance belongs to. This model is useful for density estimation, clustering, and anomaly detection.
9. One way to find the right number of clusters when using a Gaussian mixture model is to plot the Bayesian information criterion (BIC) or the Akaike information criterion (AIC) as a function of the number of clusters, then choose the number of clusters that minimizes the BIC or AIC. Another technique is to use a Bayesian Gaussian mixture model, which automatically selects the number of clusters.

For the solutions to exercises 10 to 13, please see the Jupyter notebooks available at *https://github.com/ageron/handson-ml2*.

Chapter 10: Introduction to Artificial Neural Networks with Keras

1. Visit the TensorFlow Playground and play around with it, as described in this exercise.
2. Here is a neural network based on the original artificial neurons that computes $A \oplus B$ (where $\oplus$ represents the exclusive OR), using the fact that $A \oplus B = (A \wedge \neg B) \vee (\neg A \wedge B)$. There are other solutions—for example, using the fact that $A \oplus B = (A \vee B) \wedge \neg(A \wedge B)$, or the fact that $A \oplus B = (A \vee B) \wedge (\neg A \vee \wedge B)$, and so on.



3. A classical Perceptron will converge only if the dataset is linearly separable, and it won't be able to estimate class probabilities. In contrast, a Logistic Regression classifier will converge to a good solution even if the dataset is not linearly separable, and it will output class probabilities. If you change the Perceptron's activation function to the logistic activation function (or the softmax activation function if there are multiple neurons), and if you train it using Gradient Descent (or some other optimization algorithm minimizing the cost function, typically cross entropy), then it becomes equivalent to a Logistic Regression classifier.
4. The logistic activation function was a key ingredient in training the first MLPs because its derivative is always nonzero, so Gradient Descent can always roll down the slope. When the activation function is a step function, Gradient Descent cannot move, as there is no slope at all.
5. Popular activation functions include the step function, the logistic (sigmoid) function, the hyperbolic tangent (tanh) function, and the Rectified Linear Unit (ReLU) function (see Figure 10-8). See Chapter 11 for other examples, such as ELU and variants of the ReLU function.
6. Considering the MLP described in the question, 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, where all artificial neurons use the ReLU activation function: ..The shape of the input matrix $\mathbf{X}$ is $m \times 10$, where m represents the training batch size.
   a. The shape of the hidden layer's weight vector $\mathbf{W}_h$ is 10×50, and the length of its bias vector $\mathbf{b}_h$ is 50.
   b. The shape of the output layer's weight vector $\mathbf{W}_o$ is 50×3, and the length of its bias vector $\mathbf{b}_o$ is 3.
   c. The shape of the network's output matrix $\mathbf{Y}$ is $m \times 3$.
   d. $Y^* = \text{ReLU}(\text{ReLU}(\mathbf{X}\,\mathbf{W}_h + \mathbf{b}_h)\,\mathbf{W}_o + \mathbf{b}_o)$. Recall that the ReLU function just sets every negative number in the matrix to zero. Also note that when you are adding a bias vector to a matrix, it is added to every single row in the matrix, which is called *broadcasting*.

7. To classify email into spam or ham, you just need one neuron in the output layer of a neural network—for example, indicating the probability that the email is spam. You would typically use the logistic activation function in the output layer when estimating a probability. If instead you want to tackle MNIST, you need 10 neurons in the output layer, and you must replace the logistic function with the softmax activation function, which can handle multiple classes, outputting one probability per class. If you want your neural network to predict housing prices like in Chapter 2, then you need one output neuron, using no activation function at all in the output layer.[3]
8. Backpropagation is a technique used to train artificial neural networks. It first computes the gradients of the cost function with regard to every model parameter (all the weights and biases), then it performs a Gradient Descent step using these gradients. This backpropagation step is typically performed thousands or millions of times, using many training batches, until the model parameters converge to values that (hopefully) minimize the cost function. To compute the gradients, backpropagation uses reverse-mode autodiff (although it wasn't called that when backpropagation was invented, and it has been reinvented several times). Reverse-mode autodiff performs a forward pass through a computation graph, computing every node's value for the current training batch, and then it performs a reverse pass, computing all the gradients at once (see Appendix D for more details). So what's the difference? Well, backpropagation refers to the whole process of training an artificial neural network using multiple backpropagation steps, each of which computes gradients and uses them to perform a Gradient Descent step. In contrast, reverse-mode autodiff is just a technique to compute gradients efficiently, and it happens to be used by backpropagation.
9. Here is a list of all the hyperparameters you can tweak in a basic MLP: the number of hidden layers, the number of neurons in each hidden layer, and the activation function used in each hidden layer and in the output layer.[4] In general, the ReLU activation function (or one of its variants; see Chapter 11) is a good default for the hidden layers. For the output layer, in general you will want the logistic activation function for binary classification, the softmax activation function for multiclass classification, or no activation function for regression.

3 When the values to predict can vary by many orders of magnitude, you may want to predict the logarithm of the target value rather than the target value directly. Simply computing the exponential of the neural network's output will give you the estimated value (since $\exp(\log v) = v$).

4 In Chapter 11 we discuss many techniques that introduce additional hyperparameters: type of weight initialization, activation function hyperparameters (e.g., the amount of leak in leaky ReLU), Gradient Clipping threshold, type of optimizer and its hyperparameters (e.g., the momentum hyperparameter when using a `MomentumOptimizer`), type of regularization for each layer and regularization hyperparameters (e.g., dropout rate when using dropout), and so on.