

tures can coalesce into far fewer high-level features. A typical neural network for MNIST might have 3 hidden layers, the first with 300 neurons, the second with 200, and the third with 100. However, this practice has been largely abandoned because it seems that using the same number of neurons in all hidden layers performs just as well in most cases, or even better; plus, there is only one hyperparameter to tune, instead of one per layer. That said, depending on the dataset, it can sometimes help to make the first hidden layer bigger than the others.

Just like the number of layers, you can try increasing the number of neurons gradually until the network starts overfitting. But in practice, it's often simpler and more efficient to pick a model with more layers and neurons than you actually need, then use early stopping and other regularization techniques to prevent it from overfitting. Vincent Vanhoucke, a scientist at Google, has dubbed this the “stretch pants” approach: instead of wasting time looking for pants that perfectly match your size, just use large stretch pants that will shrink down to the right size. With this approach, you avoid bottleneck layers that could ruin your model. On the flip side, if a layer has too few neurons, it will not have enough representational power to preserve all the useful information from the inputs (e.g., a layer with two neurons can only output 2D data, so if it processes 3D data, some information will be lost). No matter how big and powerful the rest of the network is, that information will never be recovered.



In general you will get more bang for your buck by increasing the number of layers instead of the number of neurons per layer.

Learning Rate, Batch Size, and Other Hyperparameters

The numbers of hidden layers and neurons are not the only hyperparameters you can tweak in an MLP. Here are some of the most important ones, as well as tips on how to set them:

Learning rate

The learning rate is arguably the most important hyperparameter. In general, the optimal learning rate is about half of the maximum learning rate (i.e., the learning rate above which the training algorithm diverges, as we saw in [Chapter 4](#)). One way to find a good learning rate is to train the model for a few hundred iterations, starting with a very low learning rate (e.g., 10^{-5}) and gradually increasing it up to a very large value (e.g., 10). This is done by multiplying the learning rate by a constant factor at each iteration (e.g., by $\exp(\log(10^6)/500)$ to go from 10^{-5} to 10 in 500 iterations). If you plot the loss as a function of the learning rate (using a log scale for the learning rate), you should see it dropping at first. But after a while, the learning rate will be too large, so the loss will shoot back up: the opti-

mal learning rate will be a bit lower than the point at which the loss starts to climb (typically about 10 times lower than the turning point). You can then reinitialize your model and train it normally using this good learning rate. We will look at more learning rate techniques in [Chapter 11](#).

Optimizer

Choosing a better optimizer than plain old Mini-batch Gradient Descent (and tuning its hyperparameters) is also quite important. We will see several advanced optimizers in [Chapter 11](#).

Batch size

The batch size can have a significant impact on your model's performance and training time. The main benefit of using large batch sizes is that hardware accelerators like GPUs can process them efficiently (see [Chapter 19](#)), so the training algorithm will see more instances per second. Therefore, many researchers and practitioners recommend using the largest batch size that can fit in GPU RAM. There's a catch, though: in practice, large batch sizes often lead to training instabilities, especially at the beginning of training, and the resulting model may not generalize as well as a model trained with a small batch size. In April 2018, Yann LeCun even tweeted "Friends don't let friends use mini-batches larger than 32," citing a [2018 paper](#)²⁴ by Dominic Masters and Carlo Luschi which concluded that using small batches (from 2 to 32) was preferable because small batches led to better models in less training time. Other papers point in the opposite direction, however; in 2017, papers by [Elad Hoffer et al.](#)²⁵ and [Priya Goyal et al.](#)²⁶ showed that it was possible to use very large batch sizes (up to 8,192) using various techniques such as warming up the learning rate (i.e., starting training with a small learning rate, then ramping it up, as we will see in [Chapter 11](#)). This led to a very short training time, without any generalization gap. So, one strategy is to try to use a large batch size, using learning rate warmup, and if training is unstable or the final performance is disappointing, then try using a small batch size instead.

Activation function

We discussed how to choose the activation function earlier in this chapter: in general, the ReLU activation function will be a good default for all hidden layers. For the output layer, it really depends on your task.

24 Dominic Masters and Carlo Luschi, "Revisiting Small Batch Training for Deep Neural Networks," arXiv preprint arXiv:1804.07612 (2018).

25 Elad Hoffer et al., "Train Longer, Generalize Better: Closing the Generalization Gap in Large Batch Training of Neural Networks," *Proceedings of the 31st International Conference on Neural Information Processing Systems* (2017): 1729–1739.

26 Priya Goyal et al., "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour," arXiv preprint arXiv:1706.02677 (2017).

Number of iterations

In most cases, the number of training iterations does not actually need to be tweaked: just use early stopping instead.



The optimal learning rate depends on the other hyperparameters—especially the batch size—so if you modify any hyperparameter, make sure to update the learning rate as well.

For more best practices regarding tuning neural network hyperparameters, check out the excellent [2018 paper](#)²⁷ by Leslie Smith.

This concludes our introduction to artificial neural networks and their implementation with Keras. In the next few chapters, we will discuss techniques to train very deep nets. We will also explore how to customize models using TensorFlow’s lower-level API and how to load and preprocess data efficiently using the Data API. And we will dive into other popular neural network architectures: convolutional neural networks for image processing, recurrent neural networks for sequential data, autoencoders for representation learning, and generative adversarial networks to model and generate data.²⁸

Exercises

1. The [TensorFlow Playground](#) is a handy neural network simulator built by the TensorFlow team. In this exercise, you will train several binary classifiers in just a few clicks, and tweak the model’s architecture and its hyperparameters to gain some intuition on how neural networks work and what their hyperparameters do. Take some time to explore the following:
 - a. The patterns learned by a neural net. Try training the default neural network by clicking the Run button (top left). Notice how it quickly finds a good solution for the classification task. The neurons in the first hidden layer have learned simple patterns, while the neurons in the second hidden layer have learned to combine the simple patterns of the first hidden layer into more complex patterns. In general, the more layers there are, the more complex the patterns can be.
 - b. Activation functions. Try replacing the tanh activation function with a ReLU activation function, and train the network again. Notice that it finds a solution

²⁷ Leslie N. Smith, “A Disciplined Approach to Neural Network Hyper-Parameters: Part 1—Learning Rate, Batch Size, Momentum, and Weight Decay,” arXiv preprint arXiv:1803.09820 (2018).

²⁸ A few extra ANN architectures are presented in [Appendix E](#).

- even faster, but this time the boundaries are linear. This is due to the shape of the ReLU function.
- c. The risk of local minima. Modify the network architecture to have just one hidden layer with three neurons. Train it multiple times (to reset the network weights, click the Reset button next to the Play button). Notice that the training time varies a lot, and sometimes it even gets stuck in a local minimum.
 - d. What happens when neural nets are too small. Remove one neuron to keep just two. Notice that the neural network is now incapable of finding a good solution, even if you try multiple times. The model has too few parameters and systematically underfits the training set.
 - e. What happens when neural nets are large enough. Set the number of neurons to eight, and train the network several times. Notice that it is now consistently fast and never gets stuck. This highlights an important finding in neural network theory: large neural networks almost never get stuck in local minima, and even when they do these local optima are almost as good as the global optimum. However, they can still get stuck on long plateaus for a long time.
 - f. The risk of vanishing gradients in deep networks. Select the spiral dataset (the bottom-right dataset under “DATA”), and change the network architecture to have four hidden layers with eight neurons each. Notice that training takes much longer and often gets stuck on plateaus for long periods of time. Also notice that the neurons in the highest layers (on the right) tend to evolve faster than the neurons in the lowest layers (on the left). This problem, called the “vanishing gradients” problem, can be alleviated with better weight initialization and other techniques, better optimizers (such as AdaGrad or Adam), or Batch Normalization (discussed in [Chapter 11](#)).
 - g. Go further. Take an hour or so to play around with other parameters and get a feel for what they do, to build an intuitive understanding about neural networks.
2. Draw an ANN using the original artificial neurons (like the ones in [Figure 10-3](#)) that computes $A \oplus B$ (where \oplus represents the XOR operation). Hint: $A \oplus B = (A \wedge \neg B \vee (\neg A \wedge B))$.
 3. Why is it generally preferable to use a Logistic Regression classifier rather than a classical Perceptron (i.e., a single layer of threshold logic units trained using the Perceptron training algorithm)? How can you tweak a Perceptron to make it equivalent to a Logistic Regression classifier?
 4. Why was the logistic activation function a key ingredient in training the first MLPs?
 5. Name three popular activation functions. Can you draw them?

6. Suppose you have an MLP composed of one input layer with 10 passthrough neurons, followed by one hidden layer with 50 artificial neurons, and finally one output layer with 3 artificial neurons. All artificial neurons use the ReLU activation function.
 - What is the shape of the input matrix \mathbf{X} ?
 - What are the shapes of the hidden layer's weight vector \mathbf{W}_h and its bias vector \mathbf{b}_h ?
 - What are the shapes of the output layer's weight vector \mathbf{W}_o and its bias vector \mathbf{b}_o ?
 - What is the shape of the network's output matrix \mathbf{Y} ?
 - Write the equation that computes the network's output matrix \mathbf{Y} as a function of \mathbf{X} , \mathbf{W}_h , \mathbf{b}_h , \mathbf{W}_o , and \mathbf{b}_o .
7. How many neurons do you need in the output layer if you want to classify email into spam or ham? What activation function should you use in the output layer? If instead you want to tackle MNIST, how many neurons do you need in the output layer, and which activation function should you use? What about for getting your network to predict housing prices, as in [Chapter 2](#)?
8. What is backpropagation and how does it work? What is the difference between backpropagation and reverse-mode autodiff?
9. Can you list all the hyperparameters you can tweak in a basic MLP? If the MLP overfits the training data, how could you tweak these hyperparameters to try to solve the problem?
10. Train a deep MLP on the MNIST dataset (you can load it using `keras.datasets.mnist.load_data()`). See if you can get over 98% precision. Try searching for the optimal learning rate by using the approach presented in this chapter (i.e., by growing the learning rate exponentially, plotting the loss, and finding the point where the loss shoots up). Try adding all the bells and whistles—save checkpoints, use early stopping, and plot learning curves using TensorBoard.

Solutions to these exercises are available in [Appendix A](#).

Training Deep Neural Networks

In [Chapter 10](#) we introduced artificial neural networks and trained our first deep neural networks. But they were shallow nets, with just a few hidden layers. What if you need to tackle a complex problem, such as detecting hundreds of types of objects in high-resolution images? You may need to train a much deeper DNN, perhaps with 10 layers or many more, each containing hundreds of neurons, linked by hundreds of thousands of connections. Training a deep DNN isn't a walk in the park. Here are some of the problems you could run into:

- You may be faced with the tricky *vanishing gradients* problem or the related *exploding gradients* problem. This is when the gradients grow smaller and smaller, or larger and larger, when flowing backward through the DNN during training. Both of these problems make lower layers very hard to train.
- You might not have enough training data for such a large network, or it might be too costly to label.
- Training may be extremely slow.
- A model with millions of parameters would severely risk overfitting the training set, especially if there are not enough training instances or if they are too noisy.

In this chapter we will go through each of these problems and present techniques to solve them. We will start by exploring the vanishing and exploding gradients problems and some of their most popular solutions. Next, we will look at transfer learning and unsupervised pretraining, which can help you tackle complex tasks even when you have little labeled data. Then we will discuss various optimizers that can speed up training large models tremendously. Finally, we will go through a few popular regularization techniques for large neural networks.

With these tools, you will be able to train very deep nets. Welcome to Deep Learning!

The Vanishing/Exploding Gradients Problems

As we discussed in [Chapter 10](#), the backpropagation algorithm works by going from the output layer to the input layer, propagating the error gradient along the way. Once the algorithm has computed the gradient of the cost function with regard to each parameter in the network, it uses these gradients to update each parameter with a Gradient Descent step.

Unfortunately, gradients often get smaller and smaller as the algorithm progresses down to the lower layers. As a result, the Gradient Descent update leaves the lower layers' connection weights virtually unchanged, and training never converges to a good solution. We call this the *vanishing gradients* problem. In some cases, the opposite can happen: the gradients can grow bigger and bigger until layers get insanely large weight updates and the algorithm diverges. This is the *exploding gradients* problem, which surfaces in recurrent neural networks (see [Chapter 15](#)). More generally, deep neural networks suffer from unstable gradients; different layers may learn at widely different speeds.

This unfortunate behavior was empirically observed long ago, and it was one of the reasons deep neural networks were mostly abandoned in the early 2000s. It wasn't clear what caused the gradients to be so unstable when training a DNN, but some light was shed in a [2010 paper](#) by Xavier Glorot and Yoshua Bengio.¹ The authors found a few suspects, including the combination of the popular logistic sigmoid activation function and the weight initialization technique that was most popular at the time (i.e., a normal distribution with a mean of 0 and a standard deviation of 1). In short, they showed that with this activation function and this initialization scheme, the variance of the outputs of each layer is much greater than the variance of its inputs. Going forward in the network, the variance keeps increasing after each layer until the activation function saturates at the top layers. This saturation is actually made worse by the fact that the logistic function has a mean of 0.5, not 0 (the hyperbolic tangent function has a mean of 0 and behaves slightly better than the logistic function in deep networks).

Looking at the logistic activation function (see [Figure 11-1](#)), you can see that when inputs become large (negative or positive), the function saturates at 0 or 1, with a derivative extremely close to 0. Thus, when backpropagation kicks in it has virtually no gradient to propagate back through the network; and what little gradient exists keeps getting diluted as backpropagation progresses down through the top layers, so there is really nothing left for the lower layers.

¹ Xavier Glorot and Yoshua Bengio, "Understanding the Difficulty of Training Deep Feedforward Neural Networks," *Proceedings of the 13th International Conference on Artificial Intelligence and Statistics* (2010): 249–256.

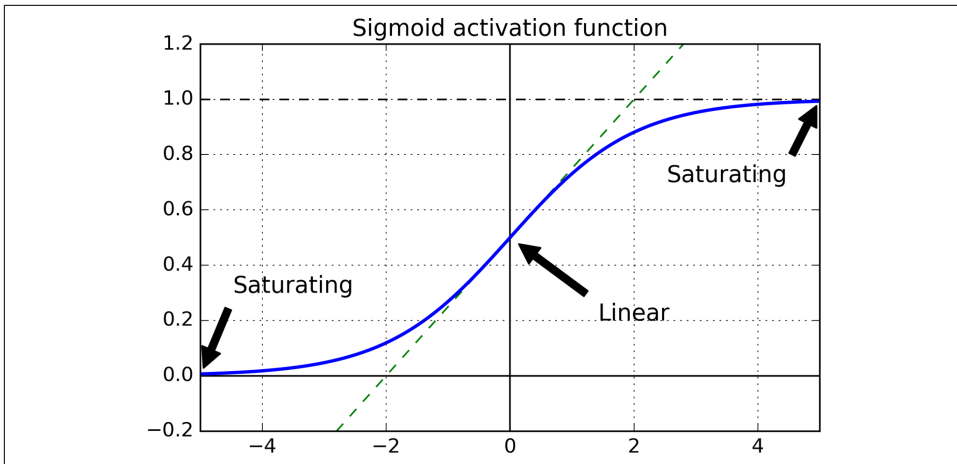


Figure 11-1. Logistic activation function saturation

Glorot and He Initialization

In their paper, Glorot and Bengio propose a way to significantly alleviate the unstable gradients problem. They point out that we need the signal to flow properly in both directions: in the forward direction when making predictions, and in the reverse direction when backpropagating gradients. We don't want the signal to die out, nor do we want it to explode and saturate. For the signal to flow properly, the authors argue that we need the variance of the outputs of each layer to be equal to the variance of its inputs,² and we need the gradients to have equal variance before and after flowing through a layer in the reverse direction (please check out the paper if you are interested in the mathematical details). It is actually not possible to guarantee both unless the layer has an equal number of inputs and neurons (these numbers are called the *fan-in* and *fan-out* of the layer), but Glorot and Bengio proposed a good compromise that has proven to work very well in practice: the connection weights of each layer must be initialized randomly as described in Equation 11-1, where $\text{fan}_{\text{avg}} = (\text{fan}_{\text{in}} + \text{fan}_{\text{out}})/2$. This initialization strategy is called *Xavier initialization* or *Glorot initialization*, after the paper's first author.

² Here's an analogy: if you set a microphone amplifier's knob too close to zero, people won't hear your voice, but if you set it too close to the max, your voice will be saturated and people won't understand what you are saying. Now imagine a chain of such amplifiers: they all need to be set properly in order for your voice to come out loud and clear at the end of the chain. Your voice has to come out of each amplifier at the same amplitude as it came in.

Equation 11-1. Glorot initialization (when using the logistic activation function)

Normal distribution with mean 0 and variance $\sigma^2 = \frac{1}{fan_{avg}}$

Or a uniform distribution between $-r$ and $+r$, with $r = \sqrt{\frac{3}{fan_{avg}}}$

If you replace fan_{avg} with fan_{in} in Equation 11-1, you get an initialization strategy that Yann LeCun proposed in the 1990s. He called it *LeCun initialization*. Genevieve Orr and Klaus-Robert Müller even recommended it in their 1998 book *Neural Networks: Tricks of the Trade* (Springer). LeCun initialization is equivalent to Glorot initialization when $fan_{in} = fan_{out}$. It took over a decade for researchers to realize how important this trick is. Using Glorot initialization can speed up training considerably, and it is one of the tricks that led to the success of Deep Learning.

Some papers³ have provided similar strategies for different activation functions. These strategies differ only by the scale of the variance and whether they use fan_{avg} or fan_{in} , as shown in Table 11-1 (for the uniform distribution, just compute $r = \sqrt{3\sigma^2}$). The initialization strategy for the ReLU activation function (and its variants, including the ELU activation described shortly) is sometimes called *He initialization*, after the paper's first author. The SELU activation function will be explained later in this chapter. It should be used with LeCun initialization (preferably with a normal distribution, as we will see).

Table 11-1. Initialization parameters for each type of activation function

Initialization	Activation functions	σ^2 (Normal)
Glorot	None, tanh, logistic, softmax	$1 / fan_{avg}$
He	ReLU and variants	$2 / fan_{in}$
LeCun	SELU	$1 / fan_{in}$

By default, Keras uses Glorot initialization with a uniform distribution. When creating a layer, you can change this to He initialization by setting `kernel_initializer="he_uniform"` or `kernel_initializer="he_normal"` like this:

```
keras.layers.Dense(10, activation="relu", kernel_initializer="he_normal")
```

If you want He initialization with a uniform distribution but based on fan_{avg} rather than fan_{in} , you can use the `VarianceScaling` initializer like this:

³ E.g., Kaiming He et al., "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification," *Proceedings of the 2015 IEEE International Conference on Computer Vision* (2015): 1026–1034.

```
he_avg_init = keras.initializers.VarianceScaling(scale=2., mode='fan_avg',
                                                  distribution='uniform')
keras.layers.Dense(10, activation="sigmoid", kernel_initializer=he_avg_init)
```

Nonsaturating Activation Functions

One of the insights in the 2010 paper by Glorot and Bengio was that the problems with unstable gradients were in part due to a poor choice of activation function. Until then most people had assumed that if Mother Nature had chosen to use roughly sigmoid activation functions in biological neurons, they must be an excellent choice. But it turns out that other activation functions behave much better in deep neural networks—in particular, the ReLU activation function, mostly because it does not saturate for positive values (and because it is fast to compute).

Unfortunately, the ReLU activation function is not perfect. It suffers from a problem known as the *dying ReLUs*: during training, some neurons effectively “die,” meaning they stop outputting anything other than 0. In some cases, you may find that half of your network’s neurons are dead, especially if you used a large learning rate. A neuron dies when its weights get tweaked in such a way that the weighted sum of its inputs are negative for all instances in the training set. When this happens, it just keeps outputting zeros, and Gradient Descent does not affect it anymore because the gradient of the ReLU function is zero when its input is negative.⁴

To solve this problem, you may want to use a variant of the ReLU function, such as the *leaky ReLU*. This function is defined as $\text{LeakyReLU}_\alpha(z) = \max(\alpha z, z)$ (see [Figure 11-2](#)). The hyperparameter α defines how much the function “leaks”: it is the slope of the function for $z < 0$ and is typically set to 0.01. This small slope ensures that leaky ReLUs never die; they can go into a long coma, but they have a chance to eventually wake up. A [2015 paper](#)⁵ compared several variants of the ReLU activation function, and one of its conclusions was that the leaky variants always outperformed the strict ReLU activation function. In fact, setting $\alpha = 0.2$ (a huge leak) seemed to result in better performance than $\alpha = 0.01$ (a small leak). The paper also evaluated the *randomized leaky ReLU* (RReLU), where α is picked randomly in a given range during training and is fixed to an average value during testing. RReLU also performed fairly well and seemed to act as a regularizer (reducing the risk of overfitting the training set). Finally, the paper evaluated the *parametric leaky ReLU* (PReLU), where α is authorized to be learned during training (instead of being a hyperparameter, it becomes a parameter that can be modified by backpropagation like any other param-

4 Unless it is part of the first hidden layer, a dead neuron may sometimes come back to life: Gradient Descent may indeed tweak neurons in the layers below in such a way that the weighted sum of the dead neuron’s inputs is positive again.

5 Bing Xu et al., “Empirical Evaluation of Rectified Activations in Convolutional Network,” arXiv preprint arXiv:1505.00853 (2015).

eter). PReLU was reported to strongly outperform ReLU on large image datasets, but on smaller datasets it runs the risk of overfitting the training set.

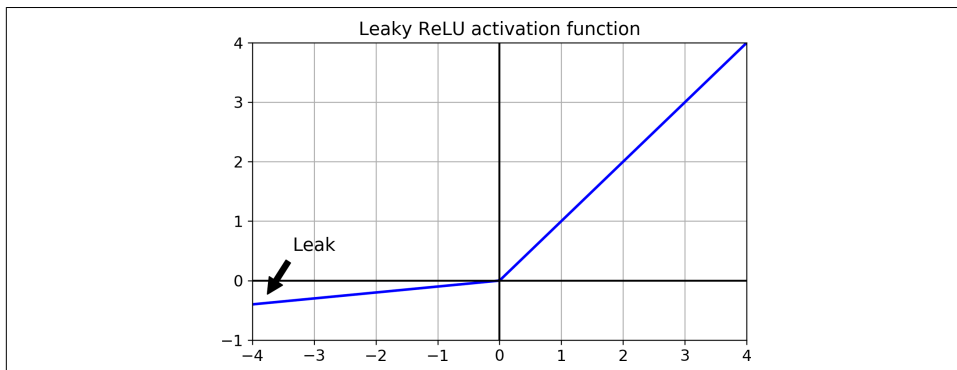


Figure 11-2. Leaky ReLU: like ReLU, but with a small slope for negative values

Last but not least, a [2015 paper](#) by Djork-Arné Clevert et al.⁶ proposed a new activation function called the *exponential linear unit* (ELU) that outperformed all the ReLU variants in the authors' experiments: training time was reduced, and the neural network performed better on the test set. [Figure 11-3](#) graphs the function, and [Equation 11-2](#) shows its definition.

Equation 11-2. ELU activation function

$$\text{ELU}_{\alpha}(z) = \begin{cases} \alpha(\exp(z) - 1) & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$

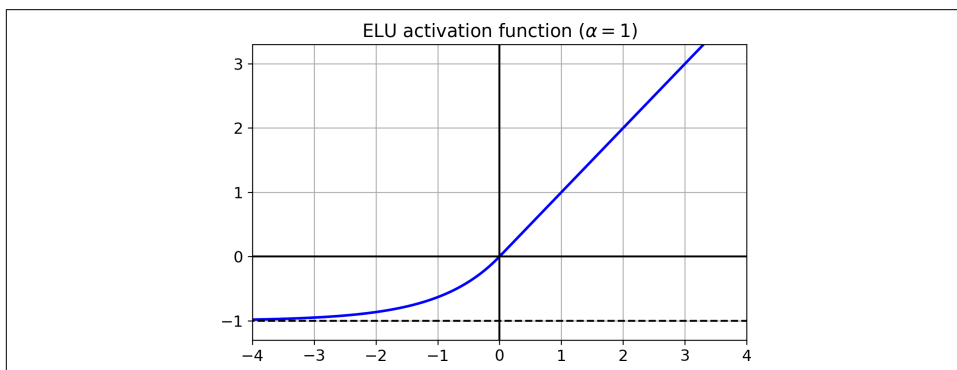


Figure 11-3. ELU activation function

⁶ Djork-Arné Clevert et al., "Fast and Accurate Deep Network Learning by Exponential Linear Units (ELUs)," *Proceedings of the International Conference on Learning Representations* (2016).

The ELU activation function looks a lot like the ReLU function, with a few major differences:

- It takes on negative values when $z < 0$, which allows the unit to have an average output closer to 0 and helps alleviate the vanishing gradients problem. The hyperparameter α defines the value that the ELU function approaches when z is a large negative number. It is usually set to 1, but you can tweak it like any other hyperparameter.
- It has a nonzero gradient for $z < 0$, which avoids the dead neurons problem.
- If α is equal to 1 then the function is smooth everywhere, including around $z = 0$, which helps speed up Gradient Descent since it does not bounce as much to the left and right of $z = 0$.

The main drawback of the ELU activation function is that it is slower to compute than the ReLU function and its variants (due to the use of the exponential function). Its faster convergence rate during training compensates for that slow computation, but still, at test time an ELU network will be slower than a ReLU network.

Then, a [2017 paper](#)⁷ by Günter Klambauer et al. introduced the Scaled ELU (SELU) activation function: as its name suggests, it is a scaled variant of the ELU activation function. The authors showed that if you build a neural network composed exclusively of a stack of dense layers, and if all hidden layers use the SELU activation function, then the network will *self-normalize*: the output of each layer will tend to preserve a mean of 0 and standard deviation of 1 during training, which solves the vanishing/exploding gradients problem. As a result, the SELU activation function often significantly outperforms other activation functions for such neural nets (especially deep ones). There are, however, a few conditions for self-normalization to happen (see the paper for the mathematical justification):

- The input features must be standardized (mean 0 and standard deviation 1).
- Every hidden layer's weights must be initialized with LeCun normal initialization. In Keras, this means setting `kernel_initializer="lecun_normal"`.
- The network's architecture must be sequential. Unfortunately, if you try to use SELU in nonsequential architectures, such as recurrent networks (see [Chapter 15](#)) or networks with *skip connections* (i.e., connections that skip layers, such as in Wide & Deep nets), self-normalization will not be guaranteed, so SELU will not necessarily outperform other activation functions.

⁷ Günter Klambauer et al., "Self-Normalizing Neural Networks," *Proceedings of the 31st International Conference on Neural Information Processing Systems* (2017): 972–981.

- The paper only guarantees self-normalization if all layers are dense, but some researchers have noted that the SELU activation function can improve performance in convolutional neural nets as well (see [Chapter 14](#)).



So, which activation function should you use for the hidden layers of your deep neural networks? Although your mileage will vary, in general $\text{SELU} > \text{ELU} > \text{leaky ReLU}$ (and its variants) $> \text{ReLU} > \tanh > \text{logistic}$. If the network's architecture prevents it from self-normalizing, then ELU may perform better than SELU (since SELU is not smooth at $z = 0$). If you care a lot about runtime latency, then you may prefer leaky ReLU. If you don't want to tweak yet another hyperparameter, you may use the default α values used by Keras (e.g., 0.3 for leaky ReLU). If you have spare time and computing power, you can use cross-validation to evaluate other activation functions, such as RReLU if your network is overfitting or PReLU if you have a huge training set. That said, because ReLU is the most used activation function (by far), many libraries and hardware accelerators provide ReLU-specific optimizations; therefore, if speed is your priority, ReLU might still be the best choice.

To use the leaky ReLU activation function, create a LeakyReLU layer and add it to your model just after the layer you want to apply it to:

```
model = keras.models.Sequential([
    ...
    keras.layers.Dense(10, kernel_initializer="he_normal"),
    keras.layers.LeakyReLU(alpha=0.2),
    ...
])
```

For PReLU, replace `LeakyRelu(alpha=0.2)` with `PReLU()`. There is currently no official implementation of RReLU in Keras, but you can fairly easily implement your own (to learn how to do that, see the exercises at the end of [Chapter 12](#)).

For SELU activation, set `activation="selu"` and `kernel_initializer="lecun_normal"` when creating a layer:

```
layer = keras.layers.Dense(10, activation="selu",
                             kernel_initializer="lecun_normal")
```

Batch Normalization

Although using He initialization along with ELU (or any variant of ReLU) can significantly reduce the danger of the vanishing/exploding gradients problems at the beginning of training, it doesn't guarantee that they won't come back during training.

In a 2015 paper,⁸ Sergey Ioffe and Christian Szegedy proposed a technique called *Batch Normalization* (BN) that addresses these problems. The technique consists of adding an operation in the model just before or after the activation function of each hidden layer. This operation simply zero-centers and normalizes each input, then scales and shifts the result using two new parameter vectors per layer: one for scaling, the other for shifting. In other words, the operation lets the model learn the optimal scale and mean of each of the layer's inputs. In many cases, if you add a BN layer as the very first layer of your neural network, you do not need to standardize your training set (e.g., using a `StandardScaler`); the BN layer will do it for you (well, approximately, since it only looks at one batch at a time, and it can also rescale and shift each input feature).

In order to zero-center and normalize the inputs, the algorithm needs to estimate each input's mean and standard deviation. It does so by evaluating the mean and standard deviation of the input over the current mini-batch (hence the name “Batch Normalization”). The whole operation is summarized step by step in Equation 11-3.

Equation 11-3. Batch Normalization algorithm

$$\begin{aligned}
 1. \quad \boldsymbol{\mu}_B &= \frac{1}{m_B} \sum_{i=1}^{m_B} \mathbf{x}^{(i)} \\
 2. \quad \boldsymbol{\sigma}_B^2 &= \frac{1}{m_B} \sum_{i=1}^{m_B} (\mathbf{x}^{(i)} - \boldsymbol{\mu}_B)^2 \\
 3. \quad \hat{\mathbf{x}}^{(i)} &= \frac{\mathbf{x}^{(i)} - \boldsymbol{\mu}_B}{\sqrt{\boldsymbol{\sigma}_B^2 + \epsilon}} \\
 4. \quad \mathbf{z}^{(i)} &= \boldsymbol{\gamma} \otimes \hat{\mathbf{x}}^{(i)} + \boldsymbol{\beta}
 \end{aligned}$$

In this algorithm:

- $\boldsymbol{\mu}_B$ is the vector of input means, evaluated over the whole mini-batch B (it contains one mean per input).
- $\boldsymbol{\sigma}_B$ is the vector of input standard deviations, also evaluated over the whole mini-batch (it contains one standard deviation per input).
- m_B is the number of instances in the mini-batch.
- $\hat{\mathbf{x}}^{(i)}$ is the vector of zero-centered and normalized inputs for instance i .

⁸ Sergey Ioffe and Christian Szegedy, “Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift,” *Proceedings of the 32nd International Conference on Machine Learning* (2015): 448–456.

- γ is the output scale parameter vector for the layer (it contains one scale parameter per input).
- \otimes represents element-wise multiplication (each input is multiplied by its corresponding output scale parameter).
- β is the output shift (offset) parameter vector for the layer (it contains one offset parameter per input). Each input is offset by its corresponding shift parameter.
- ϵ is a tiny number that avoids division by zero (typically 10^{-5}). This is called a *smoothing term*.
- $\mathbf{z}^{(i)}$ is the output of the BN operation. It is a rescaled and shifted version of the inputs.

So during training, BN standardizes its inputs, then rescales and offsets them. Good! What about at test time? Well, it's not that simple. Indeed, we may need to make predictions for individual instances rather than for batches of instances: in this case, we will have no way to compute each input's mean and standard deviation. Moreover, even if we do have a batch of instances, it may be too small, or the instances may not be independent and identically distributed, so computing statistics over the batch instances would be unreliable. One solution could be to wait until the end of training, then run the whole training set through the neural network and compute the mean and standard deviation of each input of the BN layer. These “final” input means and standard deviations could then be used instead of the batch input means and standard deviations when making predictions. However, most implementations of Batch Normalization estimate these final statistics during training by using a moving average of the layer's input means and standard deviations. This is what Keras does automatically when you use the `BatchNormalization` layer. To sum up, four parameter vectors are learned in each batch-normalized layer: γ (the output scale vector) and β (the output offset vector) are learned through regular backpropagation, and μ (the final input mean vector) and σ (the final input standard deviation vector) are estimated using an exponential moving average. Note that μ and σ are estimated during training, but they are used only after training (to replace the batch input means and standard deviations in [Equation 11-3](#)).

Ioffe and Szegedy demonstrated that Batch Normalization considerably improved all the deep neural networks they experimented with, leading to a huge improvement in the ImageNet classification task (ImageNet is a large database of images classified into many classes, commonly used to evaluate computer vision systems). The vanishing gradients problem was strongly reduced, to the point that they could use saturating activation functions such as the tanh and even the logistic activation function. The networks were also much less sensitive to the weight initialization. The authors were able to use much larger learning rates, significantly speeding up the learning process. Specifically, they note that:

Applied to a state-of-the-art image classification model, Batch Normalization achieves the same accuracy with 14 times fewer training steps, and beats the original model by a significant margin. [...] Using an ensemble of batch-normalized networks, we improve upon the best published result on ImageNet classification: reaching 4.9% top-5 validation error (and 4.8% test error), exceeding the accuracy of human raters.

Finally, like a gift that keeps on giving, Batch Normalization acts like a regularizer, reducing the need for other regularization techniques (such as dropout, described later in this chapter).

Batch Normalization does, however, add some complexity to the model (although it can remove the need for normalizing the input data, as we discussed earlier). Moreover, there is a runtime penalty: the neural network makes slower predictions due to the extra computations required at each layer. Fortunately, it's often possible to fuse the BN layer with the previous layer, after training, thereby avoiding the runtime penalty. This is done by updating the previous layer's weights and biases so that it directly produces outputs of the appropriate scale and offset. For example, if the previous layer computes $\mathbf{XW} + \mathbf{b}$, then the BN layer will compute $\gamma \otimes (\mathbf{XW} + \mathbf{b} - \mu) / \sigma + \beta$ (ignoring the smoothing term ϵ in the denominator). If we define $\mathbf{W}' = \gamma \otimes \mathbf{W} / \sigma$ and $\mathbf{b}' = \gamma \otimes (\mathbf{b} - \mu) / \sigma + \beta$, the equation simplifies to $\mathbf{XW}' + \mathbf{b}'$. So if we replace the previous layer's weights and biases (\mathbf{W} and \mathbf{b}) with the updated weights and biases (\mathbf{W}' and \mathbf{b}'), we can get rid of the BN layer (TFLite's optimizer does this automatically; see [Chapter 19](#)).



You may find that training is rather slow, because each epoch takes much more time when you use Batch Normalization. This is usually counterbalanced by the fact that convergence is much faster with BN, so it will take fewer epochs to reach the same performance. All in all, *wall time* will usually be shorter (this is the time measured by the clock on your wall).

Implementing Batch Normalization with Keras

As with most things with Keras, implementing Batch Normalization is simple and intuitive. Just add a `BatchNormalization` layer before or after each hidden layer's activation function, and optionally add a BN layer as well as the first layer in your model. For example, this model applies BN after every hidden layer and as the first layer in the model (after flattening the input images):

```

model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.BatchNormalization(),
    keras.layers.Dense(300, activation="elu", kernel_initializer="he_normal"),
    keras.layers.BatchNormalization(),
    keras.layers.Dense(100, activation="elu", kernel_initializer="he_normal"),
    keras.layers.BatchNormalization(),
    keras.layers.Dense(10, activation="softmax")
])

```

That’s all! In this tiny example with just two hidden layers, it’s unlikely that Batch Normalization will have a very positive impact; but for deeper networks it can make a tremendous difference.

Let’s display the model summary:

```

>>> model.summary()
Model: "sequential_3"

```

Layer (type)	Output Shape	Param #
=====		
flatten_3 (Flatten)	(None, 784)	0

batch_normalization_v2 (Batch Normalization)	(None, 784)	3136

dense_50 (Dense)	(None, 300)	235500

batch_normalization_v2_1 (Batch Normalization)	(None, 300)	1200

dense_51 (Dense)	(None, 100)	30100

batch_normalization_v2_2 (Batch Normalization)	(None, 100)	400

dense_52 (Dense)	(None, 10)	1010
=====		
Total params: 271,346		
Trainable params: 268,978		
Non-trainable params: 2,368		

As you can see, each BN layer adds four parameters per input: γ , β , μ , and σ (for example, the first BN layer adds 3,136 parameters, which is 4×784). The last two parameters, μ and σ , are the moving averages; they are not affected by backpropagation, so Keras calls them “non-trainable”⁹ (if you count the total number of BN parameters, $3,136 + 1,200 + 400$, and divide by 2, you get 2,368, which is the total number of non-trainable parameters in this model).

⁹ However, they are estimated during training, based on the training data, so arguably they *are* trainable. In Keras, “non-trainable” really means “untouched by backpropagation.”

Let's look at the parameters of the first BN layer. Two are trainable (by backpropagation), and two are not:

```
>>> [(var.name, var.trainable) for var in model.layers[1].variables]
[('batch_normalization_v2/gamma:0', True),
 ('batch_normalization_v2/beta:0', True),
 ('batch_normalization_v2/moving_mean:0', False),
 ('batch_normalization_v2/moving_variance:0', False)]
```

Now when you create a BN layer in Keras, it also creates two operations that will be called by Keras at each iteration during training. These operations will update the moving averages. Since we are using the TensorFlow backend, these operations are TensorFlow operations (we will discuss TF operations in [Chapter 12](#)):

```
>>> model.layers[1].updates
[<tf.Operation 'cond_2/Identity' type=Identity>,
 <tf.Operation 'cond_3/Identity' type=Identity>]
```

The authors of the BN paper argued in favor of adding the BN layers before the activation functions, rather than after (as we just did). There is some debate about this, as which is preferable seems to depend on the task—you can experiment with this too to see which option works best on your dataset. To add the BN layers before the activation functions, you must remove the activation function from the hidden layers and add them as separate layers after the BN layers. Moreover, since a Batch Normalization layer includes one offset parameter per input, you can remove the bias term from the previous layer (just pass `use_bias=False` when creating it):

```
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.BatchNormalization(),
    keras.layers.Dense(300, kernel_initializer="he_normal", use_bias=False),
    keras.layers.BatchNormalization(),
    keras.layers.Activation("elu"),
    keras.layers.Dense(100, kernel_initializer="he_normal", use_bias=False),
    keras.layers.BatchNormalization(),
    keras.layers.Activation("elu"),
    keras.layers.Dense(10, activation="softmax")
])
```

The `BatchNormalization` class has quite a few hyperparameters you can tweak. The defaults will usually be fine, but you may occasionally need to tweak the momentum. This hyperparameter is used by the `BatchNormalization` layer when it updates the exponential moving averages; given a new value \mathbf{v} (i.e., a new vector of input means or standard deviations computed over the current batch), the layer updates the running average $\hat{\mathbf{v}}$ using the following equation:

$$\hat{\mathbf{v}} \leftarrow \hat{\mathbf{v}} \times \text{momentum} + \mathbf{v} \times (1 - \text{momentum})$$

A good momentum value is typically close to 1; for example, 0.9, 0.99, or 0.999 (you want more 9s for larger datasets and smaller mini-batches).

Another important hyperparameter is `axis`: it determines which axis should be normalized. It defaults to `-1`, meaning that by default it will normalize the last axis (using the means and standard deviations computed across the *other* axes). When the input batch is 2D (i.e., the batch shape is `[batch size, features]`), this means that each input feature will be normalized based on the mean and standard deviation computed across all the instances in the batch. For example, the first BN layer in the previous code example will independently normalize (and rescale and shift) each of the 784 input features. If we move the first BN layer before the `Flatten` layer, then the input batches will be 3D, with shape `[batch size, height, width]`; therefore, the BN layer will compute 28 means and 28 standard deviations (1 per column of pixels, computed across all instances in the batch and across all rows in the column), and it will normalize all pixels in a given column using the same mean and standard deviation. There will also be just 28 scale parameters and 28 shift parameters. If instead you still want to treat each of the 784 pixels independently, then you should set `axis=[1, 2]`.

Notice that the BN layer does not perform the same computation during training and after training: it uses batch statistics during training and the “final” statistics after training (i.e., the final values of the moving averages). Let’s take a peek at the source code of this class to see how this is handled:

```
class BatchNormalization(keras.layers.Layer):
    [...]
    def call(self, inputs, training=None):
        [...]
```

The `call()` method is the one that performs the computations; as you can see, it has an extra `training` argument, which is set to `None` by default, but the `fit()` method sets it to 1 during training. If you ever need to write a custom layer, and it must behave differently during training and testing, add a `training` argument to the `call()` method and use this argument in the method to decide what to compute¹⁰ (we will discuss custom layers in [Chapter 12](#)).

`BatchNormalization` has become one of the most-used layers in deep neural networks, to the point that it is often omitted in the diagrams, as it is assumed that BN is added after every layer. But a recent [paper](#)¹¹ by Hongyi Zhang et al. may change this assumption: by using a novel *fixed-update* (fixup) weight initialization technique, the authors managed to train a very deep neural network (10,000 layers!) without BN,

10 The Keras API also specifies a `keras.backend.learning_phase()` function that should return 1 during training and 0 otherwise.

11 Hongyi Zhang et al., “Fixup Initialization: Residual Learning Without Normalization,” arXiv preprint arXiv:1901.09321 (2019).

achieving state-of-the-art performance on complex image classification tasks. As this is bleeding-edge research, however, you may want to wait for additional research to confirm this finding before you drop Batch Normalization.

Gradient Clipping

Another popular technique to mitigate the exploding gradients problem is to clip the gradients during backpropagation so that they never exceed some threshold. This is called *Gradient Clipping*.¹² This technique is most often used in recurrent neural networks, as Batch Normalization is tricky to use in RNNs, as we will see in [Chapter 15](#). For other types of networks, BN is usually sufficient.

In Keras, implementing Gradient Clipping is just a matter of setting the `clipvalue` or `clipnorm` argument when creating an optimizer, like this:

```
optimizer = keras.optimizers.SGD(clipvalue=1.0)
model.compile(loss="mse", optimizer=optimizer)
```

This optimizer will clip every component of the gradient vector to a value between -1.0 and 1.0 . This means that all the partial derivatives of the loss (with regard to each and every trainable parameter) will be clipped between -1.0 and 1.0 . The threshold is a hyperparameter you can tune. Note that it may change the orientation of the gradient vector. For instance, if the original gradient vector is $[0.9, 100.0]$, it points mostly in the direction of the second axis; but once you clip it by value, you get $[0.9, 1.0]$, which points roughly in the diagonal between the two axes. In practice, this approach works well. If you want to ensure that Gradient Clipping does not change the direction of the gradient vector, you should clip by norm by setting `clipnorm` instead of `clipvalue`. This will clip the whole gradient if its ℓ_2 norm is greater than the threshold you picked. For example, if you set `clipnorm=1.0`, then the vector $[0.9, 100.0]$ will be clipped to $[0.00899964, 0.9999595]$, preserving its orientation but almost eliminating the first component. If you observe that the gradients explode during training (you can track the size of the gradients using TensorBoard), you may want to try both clipping by value and clipping by norm, with different thresholds, and see which option performs best on the validation set.

Reusing Pretrained Layers

It is generally not a good idea to train a very large DNN from scratch: instead, you should always try to find an existing neural network that accomplishes a similar task to the one you are trying to tackle (we will discuss how to find them in [Chapter 14](#)), then reuse the lower layers of this network. This technique is called *transfer learning*.

¹² Razvan Pascanu et al., “On the Difficulty of Training Recurrent Neural Networks,” *Proceedings of the 30th International Conference on Machine Learning* (2013): 1310–1318.

It will not only speed up training considerably, but also require significantly less training data.

Suppose you have access to a DNN that was trained to classify pictures into 100 different categories, including animals, plants, vehicles, and everyday objects. You now want to train a DNN to classify specific types of vehicles. These tasks are very similar, even partly overlapping, so you should try to reuse parts of the first network (see [Figure 11-4](#)).

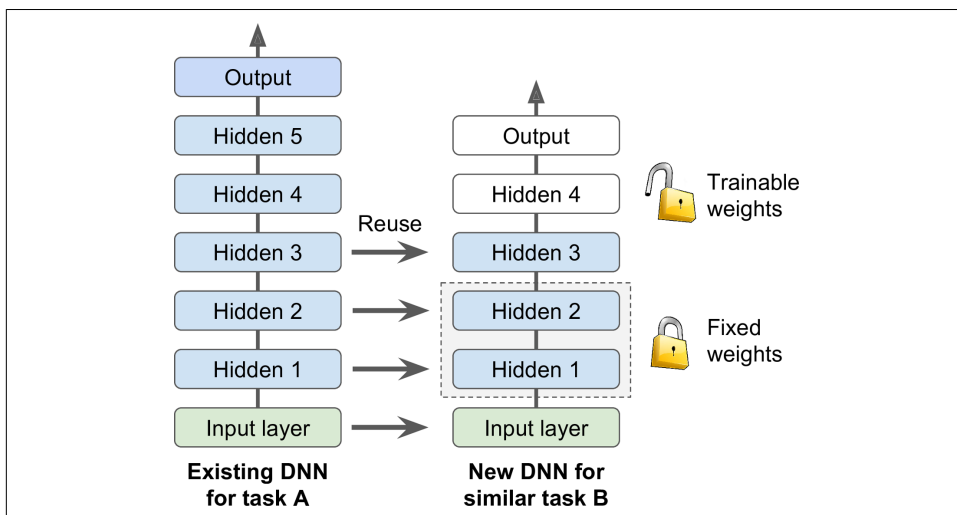


Figure 11-4. Reusing pretrained layers



If the input pictures of your new task don't have the same size as the ones used in the original task, you will usually have to add a preprocessing step to resize them to the size expected by the original model. More generally, transfer learning will work best when the inputs have similar low-level features.

The output layer of the original model should usually be replaced because it is most likely not useful at all for the new task, and it may not even have the right number of outputs for the new task.

Similarly, the upper hidden layers of the original model are less likely to be as useful as the lower layers, since the high-level features that are most useful for the new task may differ significantly from the ones that were most useful for the original task. You want to find the right number of layers to reuse.



The more similar the tasks are, the more layers you want to reuse (starting with the lower layers). For very similar tasks, try keeping all the hidden layers and just replacing the output layer.

Try freezing all the reused layers first (i.e., make their weights non-trainable so that Gradient Descent won't modify them), then train your model and see how it performs. Then try unfreezing one or two of the top hidden layers to let backpropagation tweak them and see if performance improves. The more training data you have, the more layers you can unfreeze. It is also useful to reduce the learning rate when you unfreeze reused layers: this will avoid wrecking their fine-tuned weights.

If you still cannot get good performance, and you have little training data, try dropping the top hidden layer(s) and freezing all the remaining hidden layers again. You can iterate until you find the right number of layers to reuse. If you have plenty of training data, you may try replacing the top hidden layers instead of dropping them, and even adding more hidden layers.

Transfer Learning with Keras

Let's look at an example. Suppose the Fashion MNIST dataset only contained eight classes—for example, all the classes except for sandal and shirt. Someone built and trained a Keras model on that set and got reasonably good performance (>90% accuracy). Let's call this model A. You now want to tackle a different task: you have images of sandals and shirts, and you want to train a binary classifier (positive=shirt, negative=sandal). Your dataset is quite small; you only have 200 labeled images. When you train a new model for this task (let's call it model B) with the same architecture as model A, it performs reasonably well (97.2% accuracy). But since it's a much easier task (there are just two classes), you were hoping for more. While drinking your morning coffee, you realize that your task is quite similar to task A, so perhaps transfer learning can help? Let's find out!

First, you need to load model A and create a new model based on that model's layers. Let's reuse all the layers except for the output layer:

```
model_A = keras.models.load_model("my_model_A.h5")
model_B_on_A = keras.models.Sequential(model_A.layers[:-1])
model_B_on_A.add(keras.layers.Dense(1, activation="sigmoid"))
```

Note that `model_A` and `model_B_on_A` now share some layers. When you train `model_B_on_A`, it will also affect `model_A`. If you want to avoid that, you need to *clone* `model_A` before you reuse its layers. To do this, you clone model A's architecture with `clone_model()`, then copy its weights (since `clone_model()` does not clone the weights):

```
model_A_clone = keras.models.clone_model(model_A)
model_A_clone.set_weights(model_A.get_weights())
```

Now you could train `model_B_on_A` for task B, but since the new output layer was initialized randomly it will make large errors (at least during the first few epochs), so there will be large error gradients that may wreck the reused weights. To avoid this, one approach is to freeze the reused layers during the first few epochs, giving the new layer some time to learn reasonable weights. To do this, set every layer's trainable attribute to `False` and compile the model:

```
for layer in model_B_on_A.layers[:-1]:
    layer.trainable = False

model_B_on_A.compile(loss="binary_crossentropy", optimizer="sgd",
                    metrics=["accuracy"])
```



You must always compile your model after you freeze or unfreeze layers.

Now you can train the model for a few epochs, then unfreeze the reused layers (which requires compiling the model again) and continue training to fine-tune the reused layers for task B. After unfreezing the reused layers, it is usually a good idea to reduce the learning rate, once again to avoid damaging the reused weights:

```
history = model_B_on_A.fit(X_train_B, y_train_B, epochs=4,
                          validation_data=(X_valid_B, y_valid_B))

for layer in model_B_on_A.layers[:-1]:
    layer.trainable = True

optimizer = keras.optimizers.SGD(lr=1e-4) # the default lr is 1e-2
model_B_on_A.compile(loss="binary_crossentropy", optimizer=optimizer,
                    metrics=["accuracy"])
history = model_B_on_A.fit(X_train_B, y_train_B, epochs=16,
                          validation_data=(X_valid_B, y_valid_B))
```

So, what's the final verdict? Well, this model's test accuracy is 99.25%, which means that transfer learning reduced the error rate from 2.8% down to almost 0.7%! That's a factor of four!

```
>>> model_B_on_A.evaluate(X_test_B, y_test_B)
[0.06887910133600235, 0.9925]
```

Are you convinced? You shouldn't be: I cheated! I tried many configurations until I found one that demonstrated a strong improvement. If you try to change the classes or the random seed, you will see that the improvement generally drops, or even vanishes or reverses. What I did is called "torturing the data until it confesses." When a

paper just looks too positive, you should be suspicious: perhaps the flashy new technique does not actually help much (in fact, it may even degrade performance), but the authors tried many variants and reported only the best results (which may be due to sheer luck), without mentioning how many failures they encountered on the way. Most of the time, this is not malicious at all, but it is part of the reason so many results in science can never be reproduced.

Why did I cheat? It turns out that transfer learning does not work very well with small dense networks, presumably because small networks learn few patterns, and dense networks learn very specific patterns, which are unlikely to be useful in other tasks. Transfer learning works best with deep convolutional neural networks, which tend to learn feature detectors that are much more general (especially in the lower layers). We will revisit transfer learning in [Chapter 14](#), using the techniques we just discussed (and this time there will be no cheating, I promise!).

Unsupervised Pretraining

Suppose you want to tackle a complex task for which you don't have much labeled training data, but unfortunately you cannot find a model trained on a similar task. Don't lose hope! First, you should try to gather more labeled training data, but if you can't, you may still be able to perform *unsupervised pretraining* (see [Figure 11-5](#)). Indeed, it is often cheap to gather unlabeled training examples, but expensive to label them. If you can gather plenty of unlabeled training data, you can try to use it to train an unsupervised model, such as an autoencoder or a generative adversarial network (see [Chapter 17](#)). Then you can reuse the lower layers of the autoencoder or the lower layers of the GAN's discriminator, add the output layer for your task on top, and fine-tune the final network using supervised learning (i.e., with the labeled training examples).

It is this technique that Geoffrey Hinton and his team used in 2006 and which led to the revival of neural networks and the success of Deep Learning. Until 2010, unsupervised pretraining—typically with restricted Boltzmann machines (RBMs; see [Appendix E](#))—was the norm for deep nets, and only after the vanishing gradients problem was alleviated did it become much more common to train DNNs purely using supervised learning. Unsupervised pretraining (today typically using autoencoders or GANs rather than RBMs) is still a good option when you have a complex task to solve, no similar model you can reuse, and little labeled training data but plenty of unlabeled training data.

Note that in the early days of Deep Learning it was difficult to train deep models, so people would use a technique called *greedy layer-wise pretraining* (depicted in [Figure 11-5](#)). They would first train an unsupervised model with a single layer, typically an RBM, then they would freeze that layer and add another one on top of it, then train the model again (effectively just training the new layer), then freeze the

new layer and add another layer on top of it, train the model again, and so on. Nowadays, things are much simpler: people generally train the full unsupervised model in one shot (i.e., in [Figure 11-5](#), just start directly at step three) and use autoencoders or GANs rather than RBMs.

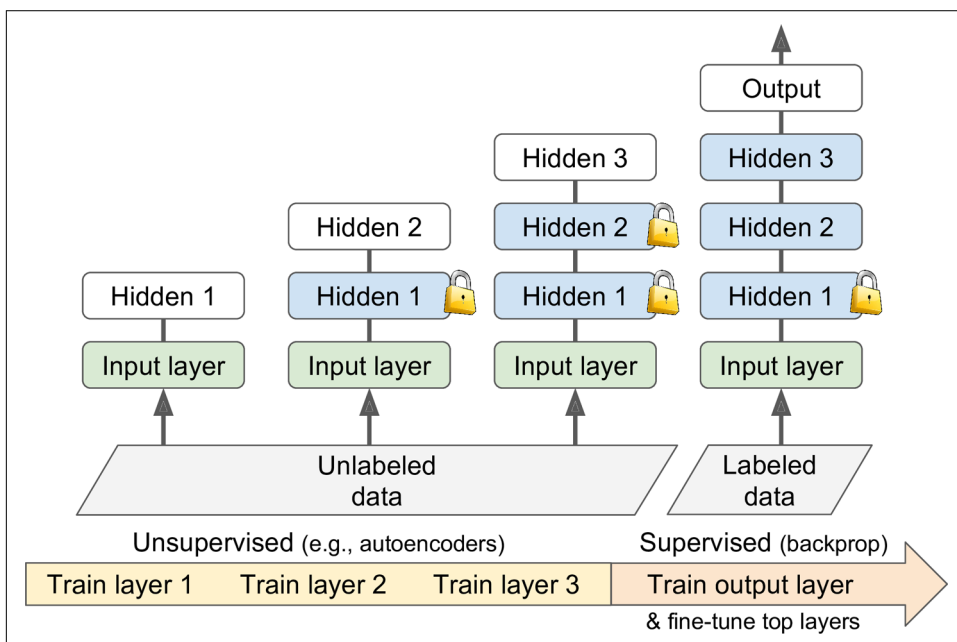


Figure 11-5. In unsupervised training, a model is trained on the unlabeled data (or on all the data) using an unsupervised learning technique, then it is fine-tuned for the final task on the labeled data using a supervised learning technique; the unsupervised part may train one layer at a time as shown here, or it may train the full model directly

Pretraining on an Auxiliary Task

If you do not have much labeled training data, one last option is to train a first neural network on an auxiliary task for which you can easily obtain or generate labeled training data, then reuse the lower layers of that network for your actual task. The first neural network's lower layers will learn feature detectors that will likely be reusable by the second neural network.

For example, if you want to build a system to recognize faces, you may only have a few pictures of each individual—clearly not enough to train a good classifier. Gathering hundreds of pictures of each person would not be practical. You could, however, gather a lot of pictures of random people on the web and train a first neural network to detect whether or not two different pictures feature the same person. Such a

network would learn good feature detectors for faces, so reusing its lower layers would allow you to train a good face classifier that uses little training data.

For *natural language processing* (NLP) applications, you can download a corpus of millions of text documents and automatically generate labeled data from it. For example, you could randomly mask out some words and train a model to predict what the missing words are (e.g., it should predict that the missing word in the sentence “What ___ you saying?” is probably “are” or “were”). If you can train a model to reach good performance on this task, then it will already know quite a lot about language, and you can certainly reuse it for your actual task and fine-tune it on your labeled data (we will discuss more pretraining tasks in [Chapter 15](#)).



Self-supervised learning is when you automatically generate the labels from the data itself, then you train a model on the resulting “labeled” dataset using supervised learning techniques. Since this approach requires no human labeling whatsoever, it is best classified as a form of unsupervised learning.

Faster Optimizers

Training a very large deep neural network can be painfully slow. So far we have seen four ways to speed up training (and reach a better solution): applying a good initialization strategy for the connection weights, using a good activation function, using Batch Normalization, and reusing parts of a pretrained network (possibly built on an auxiliary task or using unsupervised learning). Another huge speed boost comes from using a faster optimizer than the regular Gradient Descent optimizer. In this section we will present the most popular algorithms: momentum optimization, Nesterov Accelerated Gradient, AdaGrad, RMSProp, and finally Adam and Nadam optimization.

Momentum Optimization

Imagine a bowling ball rolling down a gentle slope on a smooth surface: it will start out slowly, but it will quickly pick up momentum until it eventually reaches terminal velocity (if there is some friction or air resistance). This is the very simple idea behind *momentum optimization*, [proposed by Boris Polyak in 1964](#).¹³ In contrast, regular Gradient Descent will simply take small, regular steps down the slope, so the algorithm will take much more time to reach the bottom.

¹³ Boris T. Polyak, “Some Methods of Speeding Up the Convergence of Iteration Methods,” *USSR Computational Mathematics and Mathematical Physics* 4, no. 5 (1964): 1–17.

Recall that Gradient Descent updates the weights θ by directly subtracting the gradient of the cost function $J(\theta)$ with regard to the weights ($\nabla_{\theta}J(\theta)$) multiplied by the learning rate η . The equation is: $\theta \leftarrow \theta - \eta \nabla_{\theta}J(\theta)$. It does not care about what the earlier gradients were. If the local gradient is tiny, it goes very slowly.

Momentum optimization cares a great deal about what previous gradients were: at each iteration, it subtracts the local gradient from the *momentum vector* \mathbf{m} (multiplied by the learning rate η), and it updates the weights by adding this momentum vector (see [Equation 11-4](#)). In other words, the gradient is used for acceleration, not for speed. To simulate some sort of friction mechanism and prevent the momentum from growing too large, the algorithm introduces a new hyperparameter β , called the *momentum*, which must be set between 0 (high friction) and 1 (no friction). A typical momentum value is 0.9.

Equation 11-4. Momentum algorithm

1. $\mathbf{m} \leftarrow \beta \mathbf{m} - \eta \nabla_{\theta}J(\theta)$
2. $\theta \leftarrow \theta + \mathbf{m}$

You can easily verify that if the gradient remains constant, the terminal velocity (i.e., the maximum size of the weight updates) is equal to that gradient multiplied by the learning rate η multiplied by $1/(1-\beta)$ (ignoring the sign). For example, if $\beta = 0.9$, then the terminal velocity is equal to 10 times the gradient times the learning rate, so momentum optimization ends up going 10 times faster than Gradient Descent! This allows momentum optimization to escape from plateaus much faster than Gradient Descent. We saw in [Chapter 4](#) that when the inputs have very different scales, the cost function will look like an elongated bowl (see [Figure 4-7](#)). Gradient Descent goes down the steep slope quite fast, but then it takes a very long time to go down the valley. In contrast, momentum optimization will roll down the valley faster and faster until it reaches the bottom (the optimum). In deep neural networks that don't use Batch Normalization, the upper layers will often end up having inputs with very different scales, so using momentum optimization helps a lot. It can also help roll past local optima.



Due to the momentum, the optimizer may overshoot a bit, then come back, overshoot again, and oscillate like this many times before stabilizing at the minimum. This is one of the reasons it's good to have a bit of friction in the system: it gets rid of these oscillations and thus speeds up convergence.

Implementing momentum optimization in Keras is a no-brainer: just use the SGD optimizer and set its `momentum` hyperparameter, then lie back and profit!

```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9)
```

The one drawback of momentum optimization is that it adds yet another hyperparameter to tune. However, the momentum value of 0.9 usually works well in practice and almost always goes faster than regular Gradient Descent.

Nesterov Accelerated Gradient

One small variant to momentum optimization, proposed by **Yurii Nesterov in 1983**,¹⁴ is almost always faster than vanilla momentum optimization. The *Nesterov Accelerated Gradient* (NAG) method, also known as *Nesterov momentum optimization*, measures the gradient of the cost function not at the local position θ but slightly ahead in the direction of the momentum, at $\theta + \beta \mathbf{m}$ (see **Equation 11-5**).

Equation 11-5. Nesterov Accelerated Gradient algorithm

1. $\mathbf{m} \leftarrow \beta \mathbf{m} - \eta \nabla_{\theta} J(\theta + \beta \mathbf{m})$
2. $\theta \leftarrow \theta + \mathbf{m}$

This small tweak works because in general the momentum vector will be pointing in the right direction (i.e., toward the optimum), so it will be slightly more accurate to use the gradient measured a bit farther in that direction rather than the gradient at the original position, as you can see in **Figure 11-6** (where ∇_1 represents the gradient of the cost function measured at the starting point θ , and ∇_2 represents the gradient at the point located at $\theta + \beta \mathbf{m}$).

As you can see, the Nesterov update ends up slightly closer to the optimum. After a while, these small improvements add up and NAG ends up being significantly faster than regular momentum optimization. Moreover, note that when the momentum pushes the weights across a valley, ∇_1 continues to push farther across the valley, while ∇_2 pushes back toward the bottom of the valley. This helps reduce oscillations and thus NAG converges faster.

NAG is generally faster than regular momentum optimization. To use it, simply set `nesterov=True` when creating the SGD optimizer:

```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9, nesterov=True)
```

¹⁴ Yurii Nesterov, "A Method for Unconstrained Convex Minimization Problem with the Rate of Convergence $O(1/k^2)$," *Doklady AN USSR* 269 (1983): 543–547.

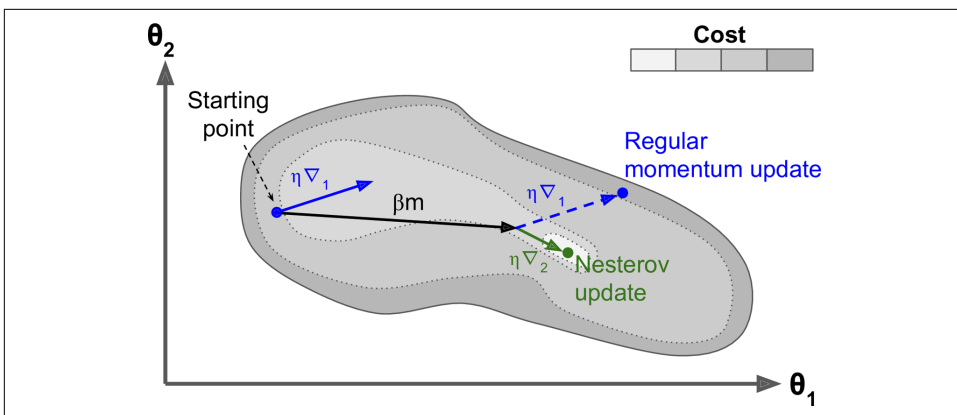


Figure 11-6. Regular versus Nesterov momentum optimization: the former applies the gradients computed before the momentum step, while the latter applies the gradients computed after

AdaGrad

Consider the elongated bowl problem again: Gradient Descent starts by quickly going down the steepest slope, which does not point straight toward the global optimum, then it very slowly goes down to the bottom of the valley. It would be nice if the algorithm could correct its direction earlier to point a bit more toward the global optimum. The *AdaGrad algorithm*¹⁵ achieves this correction by scaling down the gradient vector along the steepest dimensions (see Equation 11-6).

Equation 11-6. AdaGrad algorithm

1. $\mathbf{s} \leftarrow \mathbf{s} + \nabla_{\theta} J(\theta) \otimes \nabla_{\theta} J(\theta)$
2. $\theta \leftarrow \theta - \eta \nabla_{\theta} J(\theta) \oslash \sqrt{\mathbf{s} + \epsilon}$

The first step accumulates the square of the gradients into the vector \mathbf{s} (recall that the \otimes symbol represents the element-wise multiplication). This vectorized form is equivalent to computing $s_i \leftarrow s_i + (\partial J(\theta) / \partial \theta_i)^2$ for each element s_i of the vector \mathbf{s} ; in other words, each s_i accumulates the squares of the partial derivative of the cost function with regard to parameter θ_i . If the cost function is steep along the i^{th} dimension, then s_i will get larger and larger at each iteration.

The second step is almost identical to Gradient Descent, but with one big difference: the gradient vector is scaled down by a factor of $\sqrt{\mathbf{s} + \epsilon}$ (the \oslash symbol represents the

¹⁵ John Duchi et al., “Adaptive Subgradient Methods for Online Learning and Stochastic Optimization,” *Journal of Machine Learning Research* 12 (2011): 2121–2159.

element-wise division, and ε is a smoothing term to avoid division by zero, typically set to 10^{-10}). This vectorized form is equivalent to simultaneously computing $\theta_i \leftarrow \theta_i - \eta \partial J(\boldsymbol{\theta}) / \partial \theta_i / \sqrt{s_i + \varepsilon}$ for all parameters θ_i .

In short, this algorithm decays the learning rate, but it does so faster for steep dimensions than for dimensions with gentler slopes. This is called an *adaptive learning rate*. It helps point the resulting updates more directly toward the global optimum (see [Figure 11-7](#)). One additional benefit is that it requires much less tuning of the learning rate hyperparameter η .

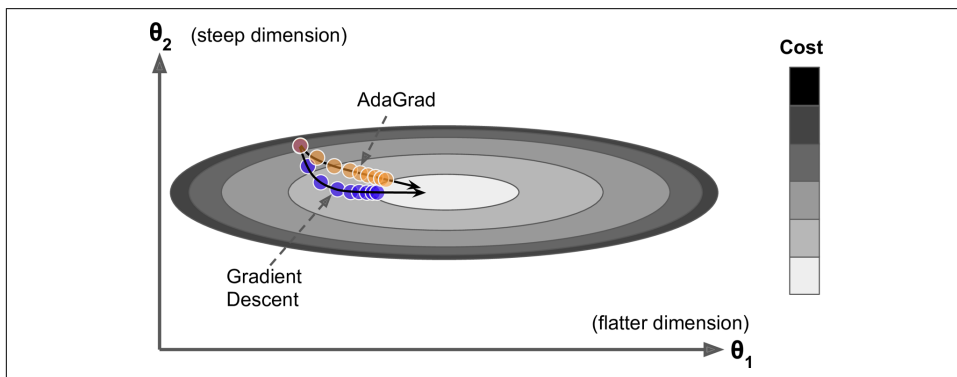


Figure 11-7. *AdaGrad versus Gradient Descent: the former can correct its direction earlier to point to the optimum*

AdaGrad frequently performs well for simple quadratic problems, but it often stops too early when training neural networks. The learning rate gets scaled down so much that the algorithm ends up stopping entirely before reaching the global optimum. So even though Keras has an `Adagrad` optimizer, you should not use it to train deep neural networks (it may be efficient for simpler tasks such as Linear Regression, though). Still, understanding AdaGrad is helpful to grasp the other adaptive learning rate optimizers.

RMSProp

As we’ve seen, AdaGrad runs the risk of slowing down a bit too fast and never converging to the global optimum. The *RMSProp* algorithm¹⁶ fixes this by accumulating only the gradients from the most recent iterations (as opposed to all the gradients

¹⁶ This algorithm was created by Geoffrey Hinton and Tijmen Tieleman in 2012 and presented by Geoffrey Hinton in his Coursera class on neural networks (slides: <https://homl.info/57>; video: <https://homl.info/58>). Amusingly, since the authors did not write a paper to describe the algorithm, researchers often cite “slide 29 in lecture 6” in their papers.

since the beginning of training). It does so by using exponential decay in the first step (see Equation 11-7).

Equation 11-7. RMSProp algorithm

1. $\mathbf{s} \leftarrow \beta \mathbf{s} + (1 - \beta) \nabla_{\theta} J(\theta) \otimes \nabla_{\theta} J(\theta)$
2. $\theta \leftarrow \theta - \eta \nabla_{\theta} J(\theta) \oslash \sqrt{\mathbf{s} + \varepsilon}$

The decay rate β is typically set to 0.9. Yes, it is once again a new hyperparameter, but this default value often works well, so you may not need to tune it at all.

As you might expect, Keras has an RMSprop optimizer:

```
optimizer = keras.optimizers.RMSprop(lr=0.001, rho=0.9)
```

Note that the rho argument corresponds to β in Equation 11-7. Except on very simple problems, this optimizer almost always performs much better than AdaGrad. In fact, it was the preferred optimization algorithm of many researchers until Adam optimization came around.

Adam and Nadam Optimization

Adam,¹⁷ which stands for *adaptive moment estimation*, combines the ideas of momentum optimization and RMSProp: just like momentum optimization, it keeps track of an exponentially decaying average of past gradients; and just like RMSProp, it keeps track of an exponentially decaying average of past squared gradients (see Equation 11-8).¹⁸

Equation 11-8. Adam algorithm

1. $\mathbf{m} \leftarrow \beta_1 \mathbf{m} - (1 - \beta_1) \nabla_{\theta} J(\theta)$
2. $\mathbf{s} \leftarrow \beta_2 \mathbf{s} + (1 - \beta_2) \nabla_{\theta} J(\theta) \otimes \nabla_{\theta} J(\theta)$
3. $\widehat{\mathbf{m}} \leftarrow \frac{\mathbf{m}}{1 - \beta_1^t}$
4. $\widehat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \beta_2^t}$
5. $\theta \leftarrow \theta + \eta \widehat{\mathbf{m}} \oslash \sqrt{\widehat{\mathbf{s}} + \varepsilon}$

17 Diederik P. Kingma and Jimmy Ba, “Adam: A Method for Stochastic Optimization,” arXiv preprint arXiv: 1412.6980 (2014).

18 These are estimations of the mean and (uncentered) variance of the gradients. The mean is often called the *first moment* while the variance is often called the *second moment*, hence the name of the algorithm.

In this equation, t represents the iteration number (starting at 1).

If you just look at steps 1, 2, and 5, you will notice Adam's close similarity to both momentum optimization and RMSProp. The only difference is that step 1 computes an exponentially decaying average rather than an exponentially decaying sum, but these are actually equivalent except for a constant factor (the decaying average is just $1 - \beta_1$ times the decaying sum). Steps 3 and 4 are somewhat of a technical detail: since \mathbf{m} and \mathbf{s} are initialized at 0, they will be biased toward 0 at the beginning of training, so these two steps will help boost \mathbf{m} and \mathbf{s} at the beginning of training.

The momentum decay hyperparameter β_1 is typically initialized to 0.9, while the scaling decay hyperparameter β_2 is often initialized to 0.999. As earlier, the smoothing term ϵ is usually initialized to a tiny number such as 10^{-7} . These are the default values for the Adam class (to be precise, epsilon defaults to None, which tells Keras to use `keras.backend.epsilon()`, which defaults to 10^{-7} ; you can change it using `keras.backend.set_epsilon()`). Here is how to create an Adam optimizer using Keras:

```
optimizer = keras.optimizers.Adam(lr=0.001, beta_1=0.9, beta_2=0.999)
```

Since Adam is an adaptive learning rate algorithm (like AdaGrad and RMSProp), it requires less tuning of the learning rate hyperparameter η . You can often use the default value $\eta = 0.001$, making Adam even easier to use than Gradient Descent.



If you are starting to feel overwhelmed by all these different techniques and are wondering how to choose the right ones for your task, don't worry: some practical guidelines are provided at the end of this chapter.

Finally, two variants of Adam are worth mentioning:

AdaMax

Notice that in step 2 of [Equation 11-8](#), Adam accumulates the squares of the gradients in \mathbf{s} (with a greater weight for more recent gradients). In step 5, if we ignore ϵ and steps 3 and 4 (which are technical details anyway), Adam scales down the parameter updates by the square root of \mathbf{s} . In short, Adam scales down the parameter updates by the ℓ_2 norm of the time-decayed gradients (recall that the ℓ_2 norm is the square root of the sum of squares). AdaMax, introduced in the same paper as Adam, replaces the ℓ_2 norm with the ℓ_∞ norm (a fancy way of saying the max). Specifically, it replaces step 2 in [Equation 11-8](#) with $\mathbf{s} \leftarrow \max(\beta_2 \mathbf{s}, \nabla_\theta J(\boldsymbol{\theta}))$, it drops step 4, and in step 5 it scales down the gradient updates by a factor of \mathbf{s} , which is just the max of the time-decayed gradients. In practice, this can make AdaMax more stable than Adam, but it really depends on the dataset,

and in general Adam performs better. So, this is just one more optimizer you can try if you experience problems with Adam on some task.

Nadam

Nadam optimization is Adam optimization plus the Nesterov trick, so it will often converge slightly faster than Adam. In [his report introducing this technique](#),¹⁹ the researcher Timothy Dozat compares many different optimizers on various tasks and finds that Nadam generally outperforms Adam but is sometimes outperformed by RMSProp.



Adaptive optimization methods (including RMSProp, Adam, and Nadam optimization) are often great, converging fast to a good solution. However, a [2017 paper](#)²⁰ by Ashia C. Wilson et al. showed that they can lead to solutions that generalize poorly on some datasets. So when you are disappointed by your model's performance, try using plain Nesterov Accelerated Gradient instead: your dataset may just be allergic to adaptive gradients. Also check out the latest research, because it's moving fast.

All the optimization techniques discussed so far only rely on the *first-order partial derivatives (Jacobians)*. The optimization literature also contains amazing algorithms based on the *second-order partial derivatives* (the *Hessians*, which are the partial derivatives of the Jacobians). Unfortunately, these algorithms are very hard to apply to deep neural networks because there are n^2 Hessians per output (where n is the number of parameters), as opposed to just n Jacobians per output. Since DNNs typically have tens of thousands of parameters, the second-order optimization algorithms often don't even fit in memory, and even when they do, computing the Hessians is just too slow.

¹⁹ Timothy Dozat, "Incorporating Nesterov Momentum into Adam" (2016).

²⁰ Ashia C. Wilson et al., "The Marginal Value of Adaptive Gradient Methods in Machine Learning," *Advances in Neural Information Processing Systems* 30 (2017): 4148–4158.

Training Sparse Models

All the optimization algorithms just presented produce dense models, meaning that most parameters will be nonzero. If you need a blazingly fast model at runtime, or if you need it to take up less memory, you may prefer to end up with a sparse model instead.

One easy way to achieve this is to train the model as usual, then get rid of the tiny weights (set them to zero). Note that this will typically not lead to a very sparse model, and it may degrade the model's performance.

A better option is to apply strong ℓ_1 regularization during training (we will see how later in this chapter), as it pushes the optimizer to zero out as many weights as it can (as discussed in “[Lasso Regression](#)” on page 137 in [Chapter 4](#)).

If these techniques remain insufficient, check out the [TensorFlow Model Optimization Toolkit \(TF-MOT\)](#), which provides a pruning API capable of iteratively removing connections during training based on their magnitude.

Table 11-2 compares all the optimizers we've discussed so far (* is bad, ** is average, and *** is good).

Table 11-2. Optimizer comparison

Class	Convergence speed	Convergence quality
SGD	*	***
SGD(momentum=...)	**	***
SGD(momentum=..., nesterov=True)	**	***
Adagrad	***	* (stops too early)
RMSprop	***	** or ***
Adam	***	** or ***
Nadam	***	** or ***
AdaMax	***	** or ***

Learning Rate Scheduling

Finding a good learning rate is very important. If you set it much too high, training may diverge (as we discussed in “[Gradient Descent](#)” on page 118). If you set it too low, training will eventually converge to the optimum, but it will take a very long time. If you set it slightly too high, it will make progress very quickly at first, but it will end up dancing around the optimum, never really settling down. If you have a limited computing budget, you may have to interrupt training before it has converged properly, yielding a suboptimal solution (see [Figure 11-8](#)).

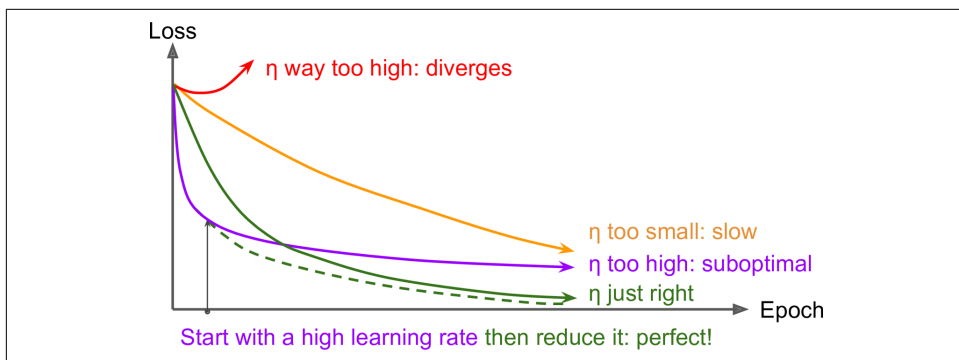


Figure 11-8. Learning curves for various learning rates η

As we discussed in [Chapter 10](#), you can find a good learning rate by training the model for a few hundred iterations, exponentially increasing the learning rate from a very small value to a very large value, and then looking at the learning curve and picking a learning rate slightly lower than the one at which the learning curve starts shooting back up. You can then reinitialize your model and train it with that learning rate.

But you can do better than a constant learning rate: if you start with a large learning rate and then reduce it once training stops making fast progress, you can reach a good solution faster than with the optimal constant learning rate. There are many different strategies to reduce the learning rate during training. It can also be beneficial to start with a low learning rate, increase it, then drop it again. These strategies are called *learning schedules* (we briefly introduced this concept in [Chapter 4](#)). These are the most commonly used learning schedules:

Power scheduling

Set the learning rate to a function of the iteration number t : $\eta(t) = \eta_0 / (1 + t/s)^c$. The initial learning rate η_0 , the power c (typically set to 1), and the steps s are hyperparameters. The learning rate drops at each step. After s steps, it is down to $\eta_0 / 2$. After s more steps, it is down to $\eta_0 / 3$, then it goes down to $\eta_0 / 4$, then $\eta_0 / 5$, and so on. As you can see, this schedule first drops quickly, then more and more slowly. Of course, power scheduling requires tuning η_0 and s (and possibly c).

Exponential scheduling

Set the learning rate to $\eta(t) = \eta_0 \cdot 0.1^{t/s}$. The learning rate will gradually drop by a factor of 10 every s steps. While power scheduling reduces the learning rate more and more slowly, exponential scheduling keeps slashing it by a factor of 10 every s steps.

Piecewise constant scheduling

Use a constant learning rate for a number of epochs (e.g., $\eta_0 = 0.1$ for 5 epochs), then a smaller learning rate for another number of epochs (e.g., $\eta_1 = 0.001$ for 50 epochs), and so on. Although this solution can work very well, it requires fiddling around to figure out the right sequence of learning rates and how long to use each of them.

Performance scheduling

Measure the validation error every N steps (just like for early stopping), and reduce the learning rate by a factor of λ when the error stops dropping.

1cycle scheduling

Contrary to the other approaches, *1cycle* (introduced in a [2018 paper](#)²¹ by Leslie Smith) starts by increasing the initial learning rate η_0 , growing linearly up to η_1 halfway through training. Then it decreases the learning rate linearly down to η_0 again during the second half of training, finishing the last few epochs by dropping the rate down by several orders of magnitude (still linearly). The maximum learning rate η_1 is chosen using the same approach we used to find the optimal learning rate, and the initial learning rate η_0 is chosen to be roughly 10 times lower. When using a momentum, we start with a high momentum first (e.g., 0.95), then drop it down to a lower momentum during the first half of training (e.g., down to 0.85, linearly), and then bring it back up to the maximum value (e.g., 0.95) during the second half of training, finishing the last few epochs with that maximum value. Smith did many experiments showing that this approach was often able to speed up training considerably and reach better performance. For example, on the popular CIFAR10 image dataset, this approach reached 91.9% validation accuracy in just 100 epochs, instead of 90.3% accuracy in 800 epochs through a standard approach (with the same neural network architecture).

A [2013 paper](#)²² by Andrew Senior et al. compared the performance of some of the most popular learning schedules when using momentum optimization to train deep neural networks for speech recognition. The authors concluded that, in this setting, both performance scheduling and exponential scheduling performed well. They favored exponential scheduling because it was easy to tune and it converged slightly faster to the optimal solution (they also mentioned that it was easier to implement

21 Leslie N. Smith, “A Disciplined Approach to Neural Network Hyper-Parameters: Part 1—Learning Rate, Batch Size, Momentum, and Weight Decay,” arXiv preprint arXiv:1803.09820 (2018).

22 Andrew Senior et al., “An Empirical Study of Learning Rates in Deep Neural Networks for Speech Recognition,” *Proceedings of the IEEE International Conference on Acoustics, Speech, and Signal Processing* (2013): 6724–6728.

than performance scheduling, but in Keras both options are easy). That said, the 1cycle approach seems to perform even better.

Implementing power scheduling in Keras is the easiest option: just set the decay hyperparameter when creating an optimizer:

```
optimizer = keras.optimizers.SGD(lr=0.01, decay=1e-4)
```

The decay is the inverse of s (the number of steps it takes to divide the learning rate by one more unit), and Keras assumes that c is equal to 1.

Exponential scheduling and piecewise scheduling are quite simple too. You first need to define a function that takes the current epoch and returns the learning rate. For example, let's implement exponential scheduling:

```
def exponential_decay_fn(epoch):  
    return 0.01 * 0.1**(epoch / 20)
```

If you do not want to hardcode η_0 and s , you can create a function that returns a configured function:

```
def exponential_decay(lr0, s):  
    def exponential_decay_fn(epoch):  
        return lr0 * 0.1**(epoch / s)  
    return exponential_decay_fn
```

```
exponential_decay_fn = exponential_decay(lr0=0.01, s=20)
```

Next, create a `LearningRateScheduler` callback, giving it the schedule function, and pass this callback to the `fit()` method:

```
lr_scheduler = keras.callbacks.LearningRateScheduler(exponential_decay_fn)  
history = model.fit(X_train_scaled, y_train, [...], callbacks=[lr_scheduler])
```

The `LearningRateScheduler` will update the optimizer's `learning_rate` attribute at the beginning of each epoch. Updating the learning rate once per epoch is usually enough, but if you want it to be updated more often, for example at every step, you can always write your own callback (see the “Exponential Scheduling” section of the notebook for an example). Updating the learning rate at every step makes sense if there are many steps per epoch. Alternatively, you can use the `keras.optimizers.schedules` approach, described shortly.

The schedule function can optionally take the current learning rate as a second argument. For example, the following schedule function multiplies the previous learning rate by $0.1^{1/20}$, which results in the same exponential decay (except the decay now starts at the beginning of epoch 0 instead of 1):

```
def exponential_decay_fn(epoch, lr):  
    return lr * 0.1**(1 / 20)
```

This implementation relies on the optimizer’s initial learning rate (contrary to the previous implementation), so make sure to set it appropriately.

When you save a model, the optimizer and its learning rate get saved along with it. This means that with this new schedule function, you could just load a trained model and continue training where it left off, no problem. Things are not so simple if your schedule function uses the epoch argument, however: the epoch does not get saved, and it gets reset to 0 every time you call the `fit()` method. If you were to continue training a model where it left off, this could lead to a very large learning rate, which would likely damage your model’s weights. One solution is to manually set the `fit()` method’s `initial_epoch` argument so the epoch starts at the right value.

For piecewise constant scheduling, you can use a schedule function like the following one (as earlier, you can define a more general function if you want; see the “Piecewise Constant Scheduling” section of the notebook for an example), then create a `LearningRateScheduler` callback with this function and pass it to the `fit()` method, just like we did for exponential scheduling:

```
def piecewise_constant_fn(epoch):  
    if epoch < 5:  
        return 0.01  
    elif epoch < 15:  
        return 0.005  
    else:  
        return 0.001
```

For performance scheduling, use the `ReduceLRonPlateau` callback. For example, if you pass the following callback to the `fit()` method, it will multiply the learning rate by 0.5 whenever the best validation loss does not improve for five consecutive epochs (other options are available; please check the documentation for more details):

```
lr_scheduler = keras.callbacks.ReduceLRonPlateau(factor=0.5, patience=5)
```

Lastly, `tf.keras` offers an alternative way to implement learning rate scheduling: define the learning rate using one of the schedules available in `keras.optimizers.schedules`, then pass this learning rate to any optimizer. This approach updates the learning rate at each step rather than at each epoch. For example, here is how to implement the same exponential schedule as the `exponential_decay_fn()` function we defined earlier:

```
s = 20 * len(X_train) // 32 # number of steps in 20 epochs (batch size = 32)  
learning_rate = keras.optimizers.schedules.ExponentialDecay(0.01, s, 0.1)  
optimizer = keras.optimizers.SGD(learning_rate)
```

This is nice and simple, plus when you save the model, the learning rate and its schedule (including its state) get saved as well. This approach, however, is not part of the Keras API; it is specific to `tf.keras`.

As for the 1cycle approach, the implementation poses no particular difficulty: just create a custom callback that modifies the learning rate at each iteration (you can update the optimizer's learning rate by changing `self.model.optimizer.lr`). See the “1Cycle scheduling” section of the notebook for an example.

To sum up, exponential decay, performance scheduling, and 1cycle can considerably speed up convergence, so give them a try!

Avoiding Overfitting Through Regularization

With four parameters I can fit an elephant and with five I can make him wiggle his trunk.

—John von Neumann, cited by Enrico Fermi in *Nature* 427

With thousands of parameters, you can fit the whole zoo. Deep neural networks typically have tens of thousands of parameters, sometimes even millions. This gives them an incredible amount of freedom and means they can fit a huge variety of complex datasets. But this great flexibility also makes the network prone to overfitting the training set. We need regularization.

We already implemented one of the best regularization techniques in [Chapter 10](#): early stopping. Moreover, even though Batch Normalization was designed to solve the unstable gradients problems, it also acts like a pretty good regularizer. In this section we will examine other popular regularization techniques for neural networks: ℓ_1 and ℓ_2 regularization, dropout, and max-norm regularization.

ℓ_1 and ℓ_2 Regularization

Just like you did in [Chapter 4](#) for simple linear models, you can use ℓ_2 regularization to constrain a neural network's connection weights, and/or ℓ_1 regularization if you want a sparse model (with many weights equal to 0). Here is how to apply ℓ_2 regularization to a Keras layer's connection weights, using a regularization factor of 0.01:

```
layer = keras.layers.Dense(100, activation="elu",
                             kernel_initializer="he_normal",
                             kernel_regularizer=keras.regularizers.l2(0.01))
```

The `l2()` function returns a regularizer that will be called at each step during training to compute the regularization loss. This is then added to the final loss. As you might expect, you can just use `keras.regularizers.l1()` if you want ℓ_1 regularization; if you want both ℓ_1 and ℓ_2 regularization, use `keras.regularizers.l1_l2()` (specifying both regularization factors).

Since you will typically want to apply the same regularizer to all layers in your network, as well as using the same activation function and the same initialization strategy in all hidden layers, you may find yourself repeating the same arguments. This

makes the code ugly and error-prone. To avoid this, you can try refactoring your code to use loops. Another option is to use Python's `functools.partial()` function, which lets you create a thin wrapper for any callable, with some default argument values:

```
from functools import partial

RegularizedDense = partial(keras.layers.Dense,
                           activation="elu",
                           kernel_initializer="he_normal",
                           kernel_regularizer=keras.regularizers.l2(0.01))

model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    RegularizedDense(300),
    RegularizedDense(100),
    RegularizedDense(10, activation="softmax",
                     kernel_initializer="glorot_uniform")
])
```

Dropout

Dropout is one of the most popular regularization techniques for deep neural networks. It was **proposed in a paper**²³ by Geoffrey Hinton in 2012 and further detailed in a **2014 paper**²⁴ by Nitish Srivastava et al., and it has proven to be highly successful: even the state-of-the-art neural networks get a 1–2% accuracy boost simply by adding dropout. This may not sound like a lot, but when a model already has 95% accuracy, getting a 2% accuracy boost means dropping the error rate by almost 40% (going from 5% error to roughly 3%).

It is a fairly simple algorithm: at every training step, every neuron (including the input neurons, but always excluding the output neurons) has a probability p of being temporarily “dropped out,” meaning it will be entirely ignored during this training step, but it may be active during the next step (see **Figure 11-9**). The hyperparameter p is called the *dropout rate*, and it is typically set between 10% and 50%: closer to 20–30% in recurrent neural nets (see **Chapter 15**), and closer to 40–50% in convolutional neural networks (see **Chapter 14**). After training, neurons don’t get dropped anymore. And that’s all (except for a technical detail we will discuss momentarily).

23 Geoffrey E. Hinton et al., “Improving Neural Networks by Preventing Co-Adaptation of Feature Detectors,” arXiv preprint arXiv:1207.0580 (2012).

24 Nitish Srivastava et al., “Dropout: A Simple Way to Prevent Neural Networks from Overfitting,” *Journal of Machine Learning Research* 15 (2014): 1929–1958.

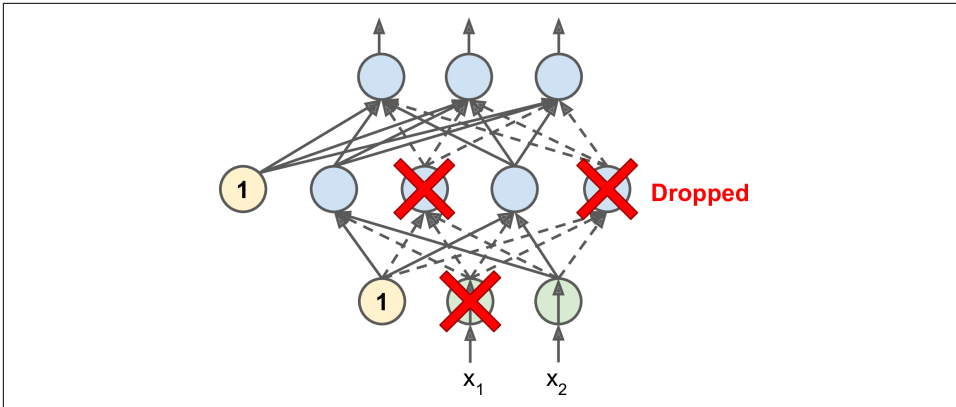


Figure 11-9. With dropout regularization, at each training iteration a random subset of all neurons in one or more layers—except the output layer—are “dropped out”; these neurons output 0 at this iteration (represented by the dashed arrows)

It’s surprising at first that this destructive technique works at all. Would a company perform better if its employees were told to toss a coin every morning to decide whether or not to go to work? Well, who knows; perhaps it would! The company would be forced to adapt its organization; it could not rely on any single person to work the coffee machine or perform any other critical tasks, so this expertise would have to be spread across several people. Employees would have to learn to cooperate with many of their coworkers, not just a handful of them. The company would become much more resilient. If one person quit, it wouldn’t make much of a difference. It’s unclear whether this idea would actually work for companies, but it certainly does for neural networks. Neurons trained with dropout cannot co-adapt with their neighboring neurons; they have to be as useful as possible on their own. They also cannot rely excessively on just a few input neurons; they must pay attention to each of their input neurons. They end up being less sensitive to slight changes in the inputs. In the end, you get a more robust network that generalizes better.

Another way to understand the power of dropout is to realize that a unique neural network is generated at each training step. Since each neuron can be either present or absent, there are a total of 2^N possible networks (where N is the total number of drop-pable neurons). This is such a huge number that it is virtually impossible for the same neural network to be sampled twice. Once you have run 10,000 training steps, you have essentially trained 10,000 different neural networks (each with just one training instance). These neural networks are obviously not independent because they share many of their weights, but they are nevertheless all different. The resulting neural network can be seen as an averaging ensemble of all these smaller neural networks.



In practice, you can usually apply dropout only to the neurons in the top one to three layers (excluding the output layer).

There is one small but important technical detail. Suppose $p = 50\%$, in which case during testing a neuron would be connected to twice as many input neurons as it would be (on average) during training. To compensate for this fact, we need to multiply each neuron's input connection weights by 0.5 after training. If we don't, each neuron will get a total input signal roughly twice as large as what the network was trained on and will be unlikely to perform well. More generally, we need to multiply each input connection weight by the *keep probability* ($1 - p$) after training. Alternatively, we can divide each neuron's output by the keep probability during training (these alternatives are not perfectly equivalent, but they work equally well).

To implement dropout using Keras, you can use the `keras.layers.Dropout` layer. During training, it randomly drops some inputs (setting them to 0) and divides the remaining inputs by the keep probability. After training, it does nothing at all; it just passes the inputs to the next layer. The following code applies dropout regularization before every Dense layer, using a dropout rate of 0.2:

```
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dropout(rate=0.2),
    keras.layers.Dense(300, activation="elu", kernel_initializer="he_normal"),
    keras.layers.Dropout(rate=0.2),
    keras.layers.Dense(100, activation="elu", kernel_initializer="he_normal"),
    keras.layers.Dropout(rate=0.2),
    keras.layers.Dense(10, activation="softmax")
])
```



Since dropout is only active during training, comparing the training loss and the validation loss can be misleading. In particular, a model may be overfitting the training set and yet have similar training and validation losses. So make sure to evaluate the training loss without dropout (e.g., after training).

If you observe that the model is overfitting, you can increase the dropout rate. Conversely, you should try decreasing the dropout rate if the model underfits the training set. It can also help to increase the dropout rate for large layers, and reduce it for small ones. Moreover, many state-of-the-art architectures only use dropout after the last hidden layer, so you may want to try this if full dropout is too strong.

Dropout does tend to significantly slow down convergence, but it usually results in a much better model when tuned properly. So, it is generally well worth the extra time and effort.



If you want to regularize a self-normalizing network based on the SELU activation function (as discussed earlier), you should use *alpha dropout*: this is a variant of dropout that preserves the mean and standard deviation of its inputs (it was introduced in the same paper as SELU, as regular dropout would break self-normalization).

Monte Carlo (MC) Dropout

In 2016, a [paper](#)²⁵ by Yarin Gal and Zoubin Ghahramani added a few more good reasons to use dropout:

- First, the paper established a profound connection between dropout networks (i.e., neural networks containing a Dropout layer before every weight layer) and approximate Bayesian inference,²⁶ giving dropout a solid mathematical justification.
- Second, the authors introduced a powerful technique called *MC Dropout*, which can boost the performance of any trained dropout model without having to retrain it or even modify it at all, provides a much better measure of the model's uncertainty, and is also amazingly simple to implement.

If this all sounds like a “one weird trick” advertisement, then take a look at the following code. It is the full implementation of *MC Dropout*, boosting the dropout model we trained earlier without retraining it:

```
y_probas = np.stack([model(X_test_scaled, training=True)
                     for sample in range(100)])
y_proba = y_probas.mean(axis=0)
```

We just make 100 predictions over the test set, setting `training=True` to ensure that the Dropout layer is active, and stack the predictions. Since dropout is active, all the predictions will be different. Recall that `predict()` returns a matrix with one row per instance and one column per class. Because there are 10,000 instances in the test set and 10 classes, this is a matrix of shape [10000, 10]. We stack 100 such matrices, so `y_probas` is an array of shape [100, 10000, 10]. Once we average over the first

25 Yarin Gal and Zoubin Ghahramani, “Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning,” *Proceedings of the 33rd International Conference on Machine Learning* (2016): 1050–1059.

26 Specifically, they show that training a dropout network is mathematically equivalent to approximate Bayesian inference in a specific type of probabilistic model called a *Deep Gaussian Process*.

dimension (`axis=0`), we get `y_proba`, an array of shape `[10000, 10]`, like we would get with a single prediction. That's all! Averaging over multiple predictions with dropout on gives us a Monte Carlo estimate that is generally more reliable than the result of a single prediction with dropout off. For example, let's look at the model's prediction for the first instance in the Fashion MNIST test set, with dropout off:

```
>>> np.round(model.predict(X_test_scaled[:1]), 2)
array([[0. , 0. , 0. , 0. , 0. , 0. , 0. , 0.01, 0. , 0.99]],
      dtype=float32)
```

The model seems almost certain that this image belongs to class 9 (ankle boot). Should you trust it? Is there really so little room for doubt? Compare this with the predictions made when dropout is activated:

```
>>> np.round(y_probas[:, :1], 2)
array([[0. , 0. , 0. , 0. , 0. , 0.14, 0. , 0.17, 0. , 0.68]],
      [[0. , 0. , 0. , 0. , 0. , 0.16, 0. , 0.2 , 0. , 0.64]],
      [[0. , 0. , 0. , 0. , 0. , 0.02, 0. , 0.01, 0. , 0.97]],
      [...])
```

This tells a very different story: apparently, when we activate dropout, the model is not sure anymore. It still seems to prefer class 9, but sometimes it hesitates with classes 5 (sandal) and 7 (sneaker), which makes sense given they're all footwear. Once we average over the first dimension, we get the following MC Dropout predictions:

```
>>> np.round(y_proba[:1], 2)
array([[0. , 0. , 0. , 0. , 0. , 0.22, 0. , 0.16, 0. , 0.62]],
      dtype=float32)
```

The model still thinks this image belongs to class 9, but only with a 62% confidence, which seems much more reasonable than 99%. Plus it's useful to know exactly which other classes it thinks are likely. And you can also take a look at the **standard deviation of the probability estimates**:

```
>>> y_std = y_probas.std(axis=0)
>>> np.round(y_std[:1], 2)
array([[0. , 0. , 0. , 0. , 0. , 0.28, 0. , 0.21, 0.02, 0.32]],
      dtype=float32)
```

Apparently there's quite a lot of variance in the probability estimates: if you were building a risk-sensitive system (e.g., a medical or financial system), you should probably treat such an uncertain prediction with extreme caution. You definitely would not treat it like a 99% confident prediction. Moreover, the model's accuracy got a small boost from 86.8 to 86.9:

```
>>> accuracy = np.sum(y_pred == y_test) / len(y_test)
>>> accuracy
0.8694
```



The number of Monte Carlo samples you use (100 in this example) is a hyperparameter you can tweak. The higher it is, the more accurate the predictions and their uncertainty estimates will be. However, if you double it, inference time will also be doubled. Moreover, above a certain number of samples, you will notice little improvement. So your job is to find the right trade-off between latency and accuracy, depending on your application.

If your model contains other layers that behave in a special way during training (such as `BatchNormalization` layers), then you should not force training mode like we just did. Instead, you should replace the `Dropout` layers with the following `MCDropout` class:²⁷

```
class MCDropout(keras.layers.Dropout):
    def call(self, inputs):
        return super().call(inputs, training=True)
```

Here, we just subclass the `Dropout` layer and override the `call()` method to force its `training` argument to `True` (see [Chapter 12](#)). Similarly, you could define an `MCAphaDropout` class by subclassing `AlphaDropout` instead. If you are creating a model from scratch, it's just a matter of using `MCDropout` rather than `Dropout`. But if you have a model that was already trained using `Dropout`, you need to create a new model that's identical to the existing model except that it replaces the `Dropout` layers with `MCDropout`, then copy the existing model's weights to your new model.

In short, MC Dropout is a fantastic technique that boosts dropout models and provides better uncertainty estimates. And of course, since it is just regular dropout during training, it also acts like a regularizer.

Max-Norm Regularization

Another regularization technique that is popular for neural networks is called *max-norm regularization*: for each neuron, it constrains the weights \mathbf{w} of the incoming connections such that $\|\mathbf{w}\|_2 \leq r$, where r is the max-norm hyperparameter and $\|\cdot\|_2$ is the ℓ_2 norm.

Max-norm regularization does not add a regularization loss term to the overall loss function. Instead, it is typically implemented by computing $\|\mathbf{w}\|_2$ after each training step and rescaling \mathbf{w} if needed ($\mathbf{w} \leftarrow \mathbf{w} r / \|\mathbf{w}\|_2$).

²⁷ This `MCDropout` class will work with all Keras APIs, including the Sequential API. If you only care about the Functional API or the Subclassing API, you do not have to create an `MCDropout` class; you can create a regular `Dropout` layer and call it with `training=True`.

Reducing r increases the amount of regularization and helps reduce overfitting. Max-norm regularization can also help alleviate the unstable gradients problems (if you are not using Batch Normalization).

To implement max-norm regularization in Keras, set the `kernel_constraint` argument of each hidden layer to a `max_norm()` constraint with the appropriate max value, like this:

```
keras.layers.Dense(100, activation="elu", kernel_initializer="he_normal",  
                    kernel_constraint=keras.constraints.max_norm(1.))
```

After each training iteration, the model's `fit()` method will call the object returned by `max_norm()`, passing it the layer's weights and getting rescaled weights in return, which then replace the layer's weights. As you'll see in [Chapter 12](#), you can define your own custom constraint function if necessary and use it as the `kernel_constraint`. You can also constrain the bias terms by setting the `bias_constraint` argument.

The `max_norm()` function has an `axis` argument that defaults to 0. A Dense layer usually has weights of shape *[number of inputs, number of neurons]*, so using `axis=0` means that the max-norm constraint will apply independently to each neuron's weight vector. If you want to use max-norm with convolutional layers (see [Chapter 14](#)), make sure to set the `max_norm()` constraint's `axis` argument appropriately (usually `axis=[0, 1, 2]`).

Summary and Practical Guidelines

In this chapter we have covered a wide range of techniques, and you may be wondering which ones you should use. This depends on the task, and there is no clear consensus yet, but I have found the configuration in [Table 11-3](#) to work fine in most cases, without requiring much hyperparameter tuning. That said, please do not consider these defaults as hard rules!

Table 11-3. Default DNN configuration

Hyperparameter	Default value
Kernel initializer	He initialization
Activation function	ELU
Normalization	None if shallow; Batch Norm if deep
Regularization	Early stopping (+ ℓ_2 reg. if needed)
Optimizer	Momentum optimization (or RMSProp or Nadam)
Learning rate schedule	1cycle

If the network is a simple stack of dense layers, then it can self-normalize, and you should use the configuration in [Table 11-4](#) instead.

Table 11-4. DNN configuration for a self-normalizing net

Hyperparameter	Default value
Kernel initializer	LeCun initialization
Activation function	SELU
Normalization	None (self-normalization)
Regularization	Alpha dropout if needed
Optimizer	Momentum optimization (or RMSProp or Nadam)
Learning rate schedule	1cycle

Don't forget to normalize the input features! You should also try to reuse parts of a pretrained neural network if you can find one that solves a similar problem, or use unsupervised pretraining if you have a lot of unlabeled data, or use pretraining on an auxiliary task if you have a lot of labeled data for a similar task.

While the previous guidelines should cover most cases, here are some exceptions:

- If you need a sparse model, you can use ℓ_1 regularization (and optionally zero out the tiny weights after training). If you need an even sparser model, you can use the TensorFlow Model Optimization Toolkit. This will break self-normalization, so you should use the default configuration in this case.
- If you need a low-latency model (one that performs lightning-fast predictions), you may need to use fewer layers, fold the Batch Normalization layers into the previous layers, and possibly use a faster activation function such as leaky ReLU or just ReLU. Having a sparse model will also help. Finally, you may want to reduce the float precision from 32 bits to 16 or even 8 bits (see [“Deploying a Model to a Mobile or Embedded Device” on page 685](#)). Again, check out TF-MOT.
- If you are building a risk-sensitive application, or inference latency is not very important in your application, you can use MC Dropout to boost performance and get more reliable probability estimates, along with uncertainty estimates.

With these guidelines, you are now ready to train very deep nets! I hope you are now convinced that you can go quite a long way using just Keras. There may come a time, however, when you need to have even more control; for example, to write a custom loss function or to tweak the training algorithm. For such cases you will need to use TensorFlow's lower-level API, as you will see in the next chapter.

Exercises

1. Is it OK to initialize all the weights to the same value as long as that value is selected randomly using He initialization?
2. Is it OK to initialize the bias terms to 0?
3. Name three advantages of the SELU activation function over ReLU.
4. In which cases would you want to use each of the following activation functions: SELU, leaky ReLU (and its variants), ReLU, tanh, logistic, and softmax?
5. What may happen if you set the momentum hyperparameter too close to 1 (e.g., 0.99999) when using an SGD optimizer?
6. Name three ways you can produce a sparse model.
7. Does dropout slow down training? Does it slow down inference (i.e., making predictions on new instances)? What about MC Dropout?
8. Practice training a deep neural network on the CIFAR10 image dataset:
 - a. Build a DNN with 20 hidden layers of 100 neurons each (that's too many, but it's the point of this exercise). Use He initialization and the ELU activation function.
 - b. Using Nadam optimization and early stopping, train the network on the CIFAR10 dataset. You can load it with `keras.datasets.cifar10.load_data()`. The dataset is composed of 60,000 32×32 -pixel color images (50,000 for training, 10,000 for testing) with 10 classes, so you'll need a softmax output layer with 10 neurons. Remember to search for the right learning rate each time you change the model's architecture or hyperparameters.
 - c. Now try adding Batch Normalization and compare the learning curves: Is it converging faster than before? Does it produce a better model? How does it affect training speed?
 - d. Try replacing Batch Normalization with SELU, and make the necessary adjustments to ensure the network self-normalizes (i.e., standardize the input features, use LeCun normal initialization, make sure the DNN contains only a sequence of dense layers, etc.).
 - e. Try regularizing the model with alpha dropout. Then, without retraining your model, see if you can achieve better accuracy using MC Dropout.
 - f. Retrain your model using 1cycle scheduling and see if it improves training speed and model accuracy.

Solutions to these exercises are available in [Appendix A](#).

Custom Models and Training with TensorFlow

Up until now, we've used only TensorFlow's high-level API, `tf.keras`, but it already got us pretty far: we built various neural network architectures, including regression and classification nets, Wide & Deep nets, and self-normalizing nets, using all sorts of techniques, such as Batch Normalization, dropout, and learning rate schedules. In fact, 95% of the use cases you will encounter will not require anything other than `tf.keras` (and `tf.data`; see [Chapter 13](#)). But now it's time to dive deeper into TensorFlow and take a look at its lower-level [Python API](#). This will be useful when you need extra control to write custom loss functions, custom metrics, layers, models, initializers, regularizers, weight constraints, and more. You may even need to fully control the training loop itself, for example to apply special transformations or constraints to the gradients (beyond just clipping them) or to use multiple optimizers for different parts of the network. We will cover all these cases in this chapter, and we will also look at how you can boost your custom models and training algorithms using TensorFlow's automatic graph generation feature. But first, let's take a quick tour of TensorFlow.



TensorFlow 2.0 (beta) was released in June 2019, making TensorFlow much easier to use. The first edition of this book used TF 1, while this edition uses TF 2.