Equation 5-8. Second-degree polynomial mapping

$$\phi(\mathbf{x}) = \phi\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right) = \begin{pmatrix} {x_1}^2 \\ \sqrt{2}\, x_1 x_2 \\ {x_2}^2 \end{pmatrix}$$

Notice that the transformed vector is 3D instead of 2D. Now let's look at what happens to a couple of 2D vectors, **a** and **b**, if we apply this second-degree polynomial mapping and then compute the dot product[7] of the transformed vectors (See Equation 5-9).

Equation 5-9. Kernel trick for a second-degree polynomial mapping

$$\begin{aligned} \phi(\mathbf{a})^\intercal \phi(\mathbf{b}) &= \begin{pmatrix} {a_1}^2 \\ \sqrt{2}\, a_1 a_2 \\ {a_2}^2 \end{pmatrix}^\intercal \begin{pmatrix} {b_1}^2 \\ \sqrt{2}\, b_1 b_2 \\ {b_2}^2 \end{pmatrix} = {a_1}^2 {b_1}^2 + 2 a_1 b_1 a_2 b_2 + {a_2}^2 {b_2}^2 \\ &= (a_1 b_1 + a_2 b_2)^2 = \left(\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}^\intercal \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}\right)^2 = (\mathbf{a}^\intercal \mathbf{b})^2 \end{aligned}$$

How about that? The dot product of the transformed vectors is equal to the square of the dot product of the original vectors: $\phi(\mathbf{a})^\intercal\, \phi(\mathbf{b}) = (\mathbf{a}^\intercal\, \mathbf{b})^2$.

Here is the key insight: if you apply the transformation ϕ to all training instances, then the dual problem (see Equation 5-6) will contain the dot product $\phi(\mathbf{x}^{(i)})^\intercal\, \phi(\mathbf{x}^{(j)})$. But if ϕ is the second-degree polynomial transformation defined in Equation 5-8, then you can replace this dot product of transformed vectors simply by $\left(\mathbf{x}^{(i)\intercal} \mathbf{x}^{(j)}\right)^2$. So, you don't need to transform the training instances at all; just replace the dot product by its square in Equation 5-6. The result will be strictly the same as if you had gone through the trouble of transforming the training set then fitting a linear SVM algorithm, but this trick makes the whole process much more computationally efficient.

The function $K(\mathbf{a}, \mathbf{b}) = (\mathbf{a}^\intercal\, \mathbf{b})^2$ is a second-degree polynomial kernel. In Machine Learning, a *kernel* is a function capable of computing the dot product $\phi(\mathbf{a})^\intercal\, \phi(\mathbf{b})$,

7 As explained in Chapter 4, the dot product of two vectors **a** and **b** is normally noted $\mathbf{a} \cdot \mathbf{b}$. However, in Machine Learning, vectors are frequently represented as column vectors (i.e., single-column matrices), so the dot product is achieved by computing $\mathbf{a}^\intercal \mathbf{b}$. To remain consistent with the rest of the book, we will use this notation here, ignoring the fact that this technically results in a single-cell matrix rather than a scalar value.

based only on the original vectors **a** and **b**, without having to compute (or even to know about) the transformation ϕ. Equation 5-10 lists some of the most commonly used kernels.

Equation 5-10. Common kernels

$$\begin{aligned}
\text{Linear:} \quad & K(\mathbf{a}, \mathbf{b}) = \mathbf{a}^\intercal \mathbf{b} \\
\text{Polynomial:} \quad & K(\mathbf{a}, \mathbf{b}) = (\gamma \mathbf{a}^\intercal \mathbf{b} + r)^d \\
\text{Gaussian RBF:} \quad & K(\mathbf{a}, \mathbf{b}) = \exp\left(-\gamma \| \mathbf{a} - \mathbf{b} \|^2\right) \\
\text{Sigmoid:} \quad & K(\mathbf{a}, \mathbf{b}) = \tanh(\gamma \mathbf{a}^\intercal \mathbf{b} + r)
\end{aligned}$$

Mercer's Theorem

According to *Mercer's theorem*, if a function $K(\mathbf{a}, \mathbf{b})$ respects a few mathematical conditions called *Mercer's conditions* (e.g., K must be continuous and symmetric in its arguments so that $K(\mathbf{a}, \mathbf{b}) = K(\mathbf{b}, \mathbf{a})$, etc.), then there exists a function ϕ that maps **a** and **b** into another space (possibly with much higher dimensions) such that $K(\mathbf{a}, \mathbf{b}) = \phi(\mathbf{a})^\intercal \phi(\mathbf{b})$. You can use K as a kernel because you know ϕ exists, even if you don't know what ϕ is. In the case of the Gaussian RBF kernel, it can be shown that ϕ maps each training instance to an infinite-dimensional space, so it's a good thing you don't need to actually perform the mapping!

Note that some frequently used kernels (such as the sigmoid kernel) don't respect all of Mercer's conditions, yet they generally work well in practice.

There is still one loose end we must tie up. Equation 5-7 shows how to go from the dual solution to the primal solution in the case of a linear SVM classifier. But if you apply the kernel trick, you end up with equations that include $\phi(x^{(i)})$. In fact, $\widehat{\mathbf{w}}$ must have the same number of dimensions as $\phi(x^{(i)})$, which may be huge or even infinite, so you can't compute it. But how can you make predictions without knowing $\widehat{\mathbf{w}}$? Well, the good news is that you can plug the formula for $\widehat{\mathbf{w}}$ from Equation 5-7 into the decision function for a new instance $\mathbf{x}^{(n)}$, and you get an equation with only dot products between input vectors. This makes it possible to use the kernel trick (Equation 5-11).

Equation 5-11. Making predictions with a kernelized SVM

$$
\begin{aligned}
h_{\hat{\mathbf{w}}, \hat{b}}\left(\phi\left(\mathbf{x}^{(n)}\right)\right) &= \hat{\mathbf{w}}^{\top}\phi\left(\mathbf{x}^{(n)}\right) + \hat{b} = \left(\sum_{i=1}^{m} \hat{\alpha}^{(i)} t^{(i)} \phi\left(\mathbf{x}^{(i)}\right)\right)^{\top} \phi\left(\mathbf{x}^{(n)}\right) + \hat{b} \\
&= \sum_{i=1}^{m} \hat{\alpha}^{(i)} t^{(i)} \left(\phi\left(\mathbf{x}^{(i)}\right)^{\top} \phi\left(\mathbf{x}^{(n)}\right)\right) + \hat{b} \\
&= \sum_{\substack{i=1 \\ \hat{\alpha}^{(i)} > 0}}^{m} \hat{\alpha}^{(i)} t^{(i)} K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(n)}\right) + \hat{b}
\end{aligned}
$$

Note that since $\alpha^{(i)} \neq 0$ only for support vectors, making predictions involves computing the dot product of the new input vector $\mathbf{x}^{(n)}$ with only the support vectors, not all the training instances. Of course, you need to use the same trick to compute the bias term $\hat{b}$ (Equation 5-12).

Equation 5-12. Using the kernel trick to compute the bias term

$$
\begin{aligned}
\hat{b} &= \frac{1}{n_s} \sum_{\substack{i=1 \\ \hat{\alpha}^{(i)} > 0}}^{m} \left(t^{(i)} - \hat{\mathbf{w}}^{\top}\phi\left(\mathbf{x}^{(i)}\right)\right) = \frac{1}{n_s} \sum_{\substack{i=1 \\ \hat{\alpha}^{(i)} > 0}}^{m} \left(t^{(i)} - \left(\sum_{j=1}^{m} \hat{\alpha}^{(j)} t^{(j)} \phi\left(\mathbf{x}^{(j)}\right)\right)^{\top} \phi\left(\mathbf{x}^{(i)}\right)\right) \\
&= \frac{1}{n_s} \sum_{\substack{i=1 \\ \hat{\alpha}^{(i)} > 0}}^{m} \left(t^{(i)} - \sum_{\substack{j=1 \\ \hat{\alpha}^{(j)} > 0}}^{m} \hat{\alpha}^{(j)} t^{(j)} K\left(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}\right)\right)
\end{aligned}
$$

If you are starting to get a headache, it's perfectly normal: it's an unfortunate side effect of the kernel trick.

Online SVMs

Before concluding this chapter, let's take a quick look at online SVM classifiers (recall that online learning means learning incrementally, typically as new instances arrive).

For linear SVM classifiers, one method for implementing an online SVM classifier is to use Gradient Descent (e.g., using `SGDClassifier`) to minimize the cost function in Equation 5-13, which is derived from the primal problem. Unfortunately, Gradient Descent converges much more slowly than the methods based on QP.

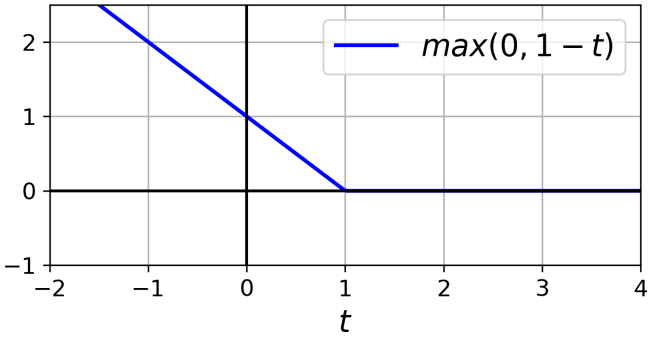
Equation 5-13. Linear SVM classifier cost function

$$J(\mathbf{w}, b) = \frac{1}{2}\mathbf{w}^\intercal\mathbf{w} \quad + \quad C\sum_{i=1}^{m} max\left(0, 1 - t^{(i)}\left(\mathbf{w}^\intercal\mathbf{x}^{(i)} + b\right)\right)$$

The first sum in the cost function will push the model to have a small weight vector **w**, leading to a larger margin. The second sum computes the total of all margin violations. An instance's margin violation is equal to 0 if it is located off the street and on the correct side, or else it is proportional to the distance to the correct side of the street. Minimizing this term ensures that the model makes the margin violations as small and as few as possible.

Hinge Loss

The function $max(0, 1 - t)$ is called the *hinge loss* function (see the following image). It is equal to 0 when $t \geq 1$. Its derivative (slope) is equal to –1 if $t < 1$ and 0 if $t > 1$. It is not differentiable at $t = 1$, but just like for Lasso Regression (see "Lasso Regression" on page 137), you can still use Gradient Descent using any *subderivative* at $t = 1$ (i.e., any value between –1 and 0).



It is also possible to implement online kernelized SVMs, as described in the papers "Incremental and Decremental Support Vector Machine Learning"[8] and "Fast Kernel Classifiers with Online and Active Learning".[9] These kernelized SVMs are imple-

8 Gert Cauwenberghs and Tomaso Poggio, "Incremental and Decremental Support Vector Machine Learning," *Proceedings of the 13th International Conference on Neural Information Processing Systems* (2000): 388–394.

9 Antoine Bordes et al., "Fast Kernel Classifiers with Online and Active Learning," *Journal of Machine Learning Research* 6 (2005): 1579–1619.

mented in Matlab and C++. For large-scale nonlinear problems, you may want to consider using neural networks instead (see Part II).

Exercises

1. What is the fundamental idea behind Support Vector Machines?
2. What is a support vector?
3. Why is it important to scale the inputs when using SVMs?
4. Can an SVM classifier output a confidence score when it classifies an instance? What about a probability?
5. Should you use the primal or the dual form of the SVM problem to train a model on a training set with millions of instances and hundreds of features?
6. Say you've trained an SVM classifier with an RBF kernel, but it seems to underfit the training set. Should you increase or decrease γ (`gamma`)? What about `C`?
7. How should you set the QP parameters (**H**, **f**, **A**, and **b**) to solve the soft margin linear SVM classifier problem using an off-the-shelf QP solver?
8. Train a `LinearSVC` on a linearly separable dataset. Then train an `SVC` and a `SGDClassifier` on the same dataset. See if you can get them to produce roughly the same model.
9. Train an SVM classifier on the MNIST dataset. Since SVM classifiers are binary classifiers, you will need to use one-versus-the-rest to classify all 10 digits. You may want to tune the hyperparameters using small validation sets to speed up the process. What accuracy can you reach?
10. Train an SVM regressor on the California housing dataset.

Solutions to these exercises are available in Appendix A.

CHAPTER 6
Decision Trees

Like SVMs, *Decision Trees* are versatile Machine Learning algorithms that can perform both classification and regression tasks, and even multioutput tasks. They are powerful algorithms, capable of fitting complex datasets. For example, in Chapter 2 you trained a `DecisionTreeRegressor` model on the California housing dataset, fitting it perfectly (actually, overfitting it).

Decision Trees are also the fundamental components of Random Forests (see Chapter 7), which are among the most powerful Machine Learning algorithms available today.

In this chapter we will start by discussing how to train, visualize, and make predictions with Decision Trees. Then we will go through the CART training algorithm used by Scikit-Learn, and we will discuss how to regularize trees and use them for regression tasks. Finally, we will discuss some of the limitations of Decision Trees.

Training and Visualizing a Decision Tree

To understand Decision Trees, let's build one and take a look at how it makes predictions. The following code trains a `DecisionTreeClassifier` on the iris dataset (see Chapter 4):

```
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier

iris = load_iris()
X = iris.data[:, 2:] # petal length and width
y = iris.target

tree_clf = DecisionTreeClassifier(max_depth=2)
tree_clf.fit(X, y)
```

You can visualize the trained Decision Tree by first using the `export_graphviz()` method to output a graph definition file called *iris_tree.dot*:

```
from sklearn.tree import export_graphviz

export_graphviz(
        tree_clf,
        out_file=image_path("iris_tree.dot"),
        feature_names=iris.feature_names[2:],
        class_names=iris.target_names,
        rounded=True,
        filled=True
    )
```

Then you can use the `dot` command-line tool from the Graphviz package to convert this *.dot* file to a variety of formats, such as PDF or PNG.[1] This command line converts the *.dot* file to a *.png* image file:

```
$ dot -Tpng iris_tree.dot -o iris_tree.png
```

Your first Decision Tree looks like Figure 6-1.

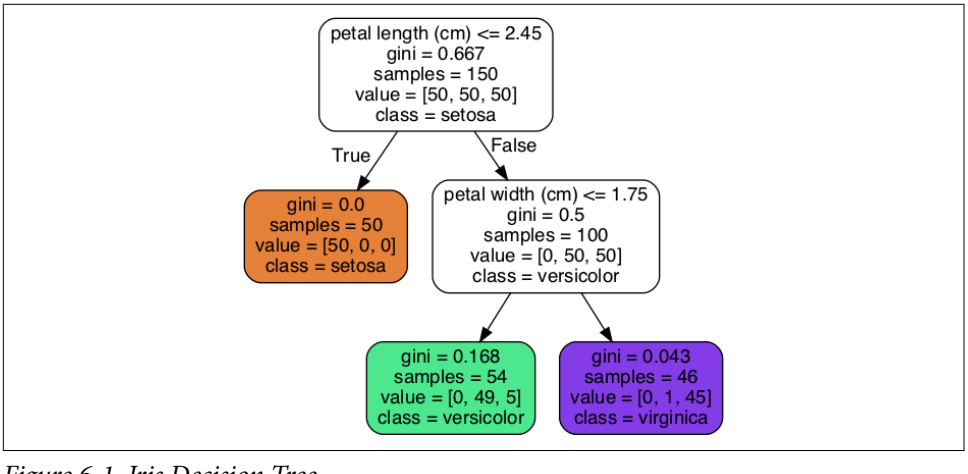


Figure 6-1. Iris Decision Tree

Making Predictions

Let's see how the tree represented in Figure 6-1 makes predictions. Suppose you find an iris flower and you want to classify it. You start at the *root node* (depth 0, at the top): this node asks whether the flower's petal length is smaller than 2.45 cm. If it is, then you move down to the root's left child node (depth 1, left). In this case, it is a *leaf*

1 Graphviz is an open source graph visualization software package, available at *http://www.graphviz.org/*.

node (i.e., it does not have any child nodes), so it does not ask any questions: simply look at the predicted class for that node, and the Decision Tree predicts that your flower is an *Iris setosa* (`class=setosa`).

Now suppose you find another flower, and this time the petal length is greater than 2.45 cm. You must move down to the root's right child node (depth 1, right), which is not a leaf node, so the node asks another question: is the petal width smaller than 1.75 cm? If it is, then your flower is most likely an *Iris versicolor* (depth 2, left). If not, it is likely an *Iris virginica* (depth 2, right). It's really that simple.

One of the many qualities of Decision Trees is that they require very little data preparation. In fact, they don't require feature scaling or centering at all.

A node's `samples` attribute counts how many training instances it applies to. For example, 100 training instances have a petal length greater than 2.45 cm (depth 1, right), and of those 100, 54 have a petal width smaller than 1.75 cm (depth 2, left). A node's `value` attribute tells you how many training instances of each class this node applies to: for example, the bottom-right node applies to 0 *Iris setosa*, 1 *Iris versicolor*, and 45 *Iris virginica*. Finally, a node's `gini` attribute measures its *impurity*: a node is "pure" (`gini=0`) if all training instances it applies to belong to the same class. For example, since the depth-1 left node applies only to *Iris setosa* training instances, it is pure and its `gini` score is 0. Equation 6-1 shows how the training algorithm computes the `gini` score G_i of the i^{th} node. The depth-2 left node has a `gini` score equal to $1 - (0/54)^2 - (49/54)^2 - (5/54)^2 \approx 0.168$.

Equation 6-1. Gini impurity

$$G_i = 1 - \sum_{k=1}^{n} {p_{i,k}}^2$$

In this equation:

- $p_{i,k}$ is the ratio of class k instances among the training instances in the i^{th} node.

Scikit-Learn uses the CART algorithm, which produces only *binary trees*: nonleaf nodes always have two children (i.e., questions only have yes/no answers). However, other algorithms such as ID3 can produce Decision Trees with nodes that have more than two children.

Figure 6-2 shows this Decision Tree's decision boundaries. The thick vertical line represents the decision boundary of the root node (depth 0): petal length = 2.45 cm. Since the lefthand area is pure (only *Iris setosa*), it cannot be split any further. However, the righthand area is impure, so the depth-1 right node splits it at petal width = 1.75 cm (represented by the dashed line). Since `max_depth` was set to 2, the Decision Tree stops right there. If you set `max_depth` to 3, then the two depth-2 nodes would each add another decision boundary (represented by the dotted lines).

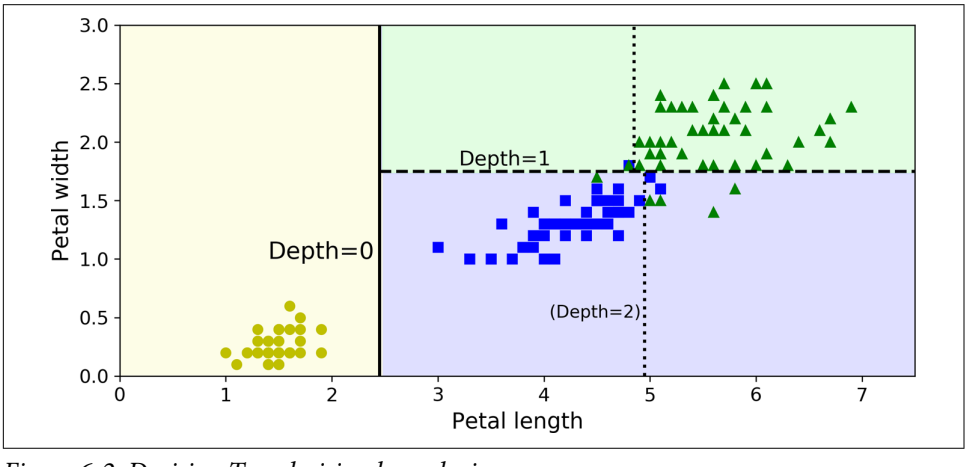


Figure 6-2. Decision Tree decision boundaries

Model Interpretation: White Box Versus Black Box

Decision Trees are intuitive, and their decisions are easy to interpret. Such models are often called *white box models*. In contrast, as we will see, Random Forests or neural networks are generally considered *black box models*. They make great predictions, and you can easily check the calculations that they performed to make these predictions; nevertheless, it is usually hard to explain in simple terms why the predictions were made. For example, if a neural network says that a particular person appears on a picture, it is hard to know what contributed to this prediction: did the model recognize that person's eyes? Their mouth? Their nose? Their shoes? Or even the couch that they were sitting on? Conversely, Decision Trees provide nice, simple classification rules that can even be applied manually if need be (e.g., for flower classification).

Estimating Class Probabilities

A Decision Tree can also estimate the probability that an instance belongs to a particular class *k*. First it traverses the tree to find the leaf node for this instance, and then it returns the ratio of training instances of class *k* in this node. For example, suppose you have found a flower whose petals are 5 cm long and 1.5 cm wide. The

corresponding leaf node is the depth-2 left node, so the Decision Tree should output the following probabilities: 0% for *Iris setosa* (0/54), 90.7% for *Iris versicolor* (49/54), and 9.3% for *Iris virginica* (5/54). And if you ask it to predict the class, it should output *Iris versicolor* (class 1) because it has the highest probability. Let's check this:

```
>>> tree_clf.predict_proba([[5, 1.5]])
array([[0.        , 0.90740741, 0.09259259]])
>>> tree_clf.predict([[5, 1.5]])
array([1])
```

Perfect! Notice that the estimated probabilities would be identical anywhere else in the bottom-right rectangle of Figure 6-2—for example, if the petals were 6 cm long and 1.5 cm wide (even though it seems obvious that it would most likely be an *Iris virginica* in this case).

The CART Training Algorithm

Scikit-Learn uses the *Classification and Regression Tree* (CART) algorithm to train Decision Trees (also called "growing" trees). The algorithm works by first splitting the training set into two subsets using a single feature k and a threshold t_k (e.g., "petal length ≤ 2.45 cm"). How does it choose k and t_k? It searches for the pair (k, t_k) that produces the purest subsets (weighted by their size). Equation 6-2 gives the cost function that the algorithm tries to minimize.

Equation 6-2. CART cost function for classification

$$J(k, t_k) = \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}}$$

$$\text{where} \begin{cases} G_{\text{left/right}} \text{ measures the impurity of the left/right subset,} \\ m_{\text{left/right}} \text{ is the number of instances in the left/right subset.} \end{cases}$$

Once the CART algorithm has successfully split the training set in two, it splits the subsets using the same logic, then the sub-subsets, and so on, recursively. It stops recursing once it reaches the maximum depth (defined by the `max_depth` hyperparameter), or if it cannot find a split that will reduce impurity. A few other hyperparameters (described in a moment) control additional stopping conditions (`min_samples_split`, `min_samples_leaf`, `min_weight_fraction_leaf`, and `max_leaf_nodes`).

As you can see, the CART algorithm is a *greedy algorithm*: it greedily searches for an optimum split at the top level, then repeats the process at each subsequent level. It does not check whether or not the split will lead to the lowest possible impurity several levels down. A greedy algorithm often produces a solution that's reasonably good but not guaranteed to be optimal.

Unfortunately, finding the optimal tree is known to be an *NP-Complete* problem:[2] it requires $O(\exp(m))$ time, making the problem intractable even for small training sets. This is why we must settle for a "reasonably good" solution.

Computational Complexity

Making predictions requires traversing the Decision Tree from the root to a leaf. Decision Trees generally are approximately balanced, so traversing the Decision Tree requires going through roughly $O(\log_2(m))$ nodes.[3] Since each node only requires checking the value of one feature, the overall prediction complexity is $O(\log_2(m))$, independent of the number of features. So predictions are very fast, even when dealing with large training sets.

The training algorithm compares all features (or less if `max_features` is set) on all samples at each node. Comparing all features on all samples at each node results in a training complexity of $O(n \times m \log_2(m))$. For small training sets (less than a few thousand instances), Scikit-Learn can speed up training by presorting the data (set `presort=True`), but doing that slows down training considerably for larger training sets.

Gini Impurity or Entropy?

By default, the Gini impurity measure is used, but you can select the *entropy* impurity measure instead by setting the `criterion` hyperparameter to `"entropy"`. The concept of entropy originated in thermodynamics as a measure of molecular disorder: entropy approaches zero when molecules are still and well ordered. Entropy later spread to a wide variety of domains, including Shannon's *information theory*, where it measures the average information content of a message:[4] entropy is zero when all messages are identical. In Machine Learning, entropy is frequently used as an

2 P is the set of problems that can be solved in polynomial time. NP is the set of problems whose solutions can be verified in polynomial time. An NP-Hard problem is a problem to which any NP problem can be reduced in polynomial time. An NP-Complete problem is both NP and NP-Hard. A major open mathematical question is whether or not P = NP. If P ≠ NP (which seems likely), then no polynomial algorithm will ever be found for any NP-Complete problem (except perhaps on a quantum computer).

3 $\log_2$ is the binary logarithm. It is equal to $\log_2(m) = \log(m) / \log(2)$.

4 A reduction of entropy is often called an *information gain*.

impurity measure: a set's entropy is zero when it contains instances of only one class. Equation 6-3 shows the definition of the entropy of the i^{th} node. For example, the depth-2 left node in Figure 6-1 has an entropy equal to $-(49/54) \log_2 (49/54) - (5/54) \log_2 (5/54) \approx 0.445$.

Equation 6-3. Entropy

$$H_i = - \sum_{\substack{k=1 \\ p_{i,k} \neq 0}}^{n} p_{i,k} \log_2 \left(p_{i,k} \right)$$

So, should you use Gini impurity or entropy? The truth is, most of the time it does not make a big difference: they lead to similar trees. Gini impurity is slightly faster to compute, so it is a good default. However, when they differ, Gini impurity tends to isolate the most frequent class in its own branch of the tree, while entropy tends to produce slightly more balanced trees.[5]

Regularization Hyperparameters

Decision Trees make very few assumptions about the training data (as opposed to linear models, which assume that the data is linear, for example). If left unconstrained, the tree structure will adapt itself to the training data, fitting it very closely—indeed, most likely overfitting it. Such a model is often called a *nonparametric model*, not because it does not have any parameters (it often has a lot) but because the number of parameters is not determined prior to training, so the model structure is free to stick closely to the data. In contrast, a *parametric model*, such as a linear model, has a predetermined number of parameters, so its degree of freedom is limited, reducing the risk of overfitting (but increasing the risk of underfitting).

To avoid overfitting the training data, you need to restrict the Decision Tree's freedom during training. As you know by now, this is called regularization. The regularization hyperparameters depend on the algorithm used, but generally you can at least restrict the maximum depth of the Decision Tree. In Scikit-Learn, this is controlled by the `max_depth` hyperparameter (the default value is `None`, which means unlimited). Reducing `max_depth` will regularize the model and thus reduce the risk of overfitting.

The `DecisionTreeClassifier` class has a few other parameters that similarly restrict the shape of the Decision Tree: `min_samples_split` (the minimum number of samples a node must have before it can be split), `min_samples_leaf` (the minimum number of samples a leaf node must have), `min_weight_fraction_leaf` (same as

5 See Sebastian Raschka's interesting analysis for more details.

`min_samples_leaf` but expressed as a fraction of the total number of weighted instances), `max_leaf_nodes` (the maximum number of leaf nodes), and `max_features` (the maximum number of features that are evaluated for splitting at each node). Increasing `min_*` hyperparameters or reducing `max_*` hyperparameters will regularize the model.

Other algorithms work by first training the Decision Tree without restrictions, then *pruning* (deleting) unnecessary nodes. A node whose children are all leaf nodes is considered unnecessary if the purity improvement it provides is not statistically significant. Standard statistical tests, such as the χ^2 *test* (chi-squared test), are used to estimate the probability that the improvement is purely the result of chance (which is called the *null hypothesis*). If this probability, called the *p-value*, is higher than a given threshold (typically 5%, controlled by a hyperparameter), then the node is considered unnecessary and its children are deleted. The pruning continues until all unnecessary nodes have been pruned.

Figure 6-3 shows two Decision Trees trained on the moons dataset (introduced in Chapter 5). On the left the Decision Tree is trained with the default hyperparameters (i.e., no restrictions), and on the right it's trained with `min_samples_leaf=4`. It is quite obvious that the model on the left is overfitting, and the model on the right will probably generalize better.

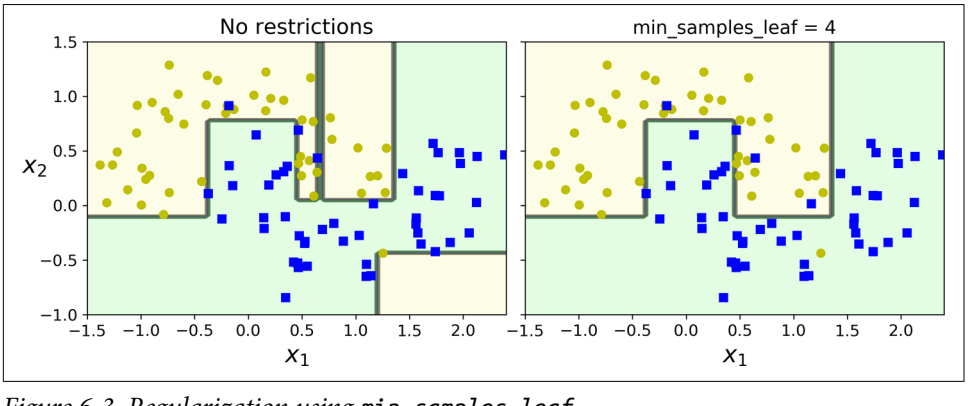


Figure 6-3. Regularization using `min_samples_leaf`

Regression

Decision Trees are also capable of performing regression tasks. Let's build a regression tree using Scikit-Learn's `DecisionTreeRegressor` class, training it on a noisy quadratic dataset with `max_depth=2`:

```
from sklearn.tree import DecisionTreeRegressor

tree_reg = DecisionTreeRegressor(max_depth=2)
tree_reg.fit(X, y)
```

The resulting tree is represented in Figure 6-4.

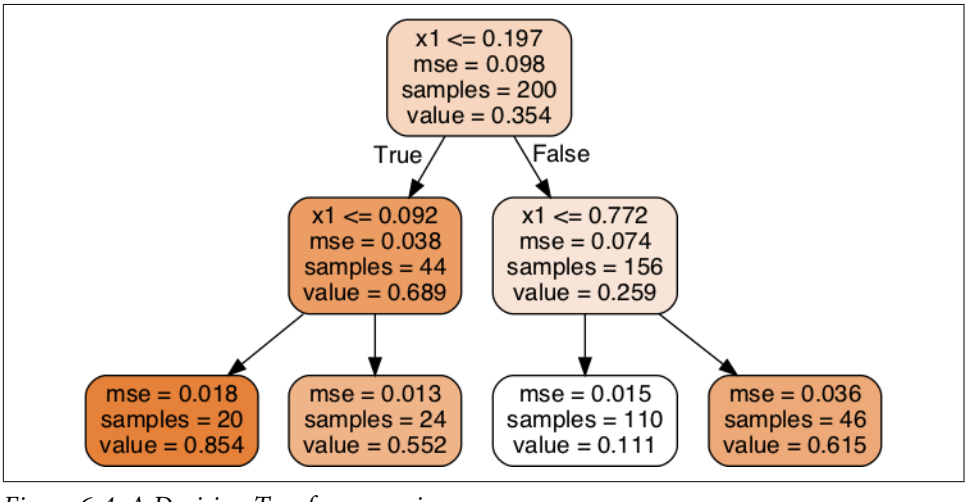


Figure 6-4. A Decision Tree for regression

This tree looks very similar to the classification tree you built earlier. The main difference is that instead of predicting a class in each node, it predicts a value. For example, suppose you want to make a prediction for a new instance with $x_1 = 0.6$. You traverse the tree starting at the root, and you eventually reach the leaf node that predicts `value=0.111`. This prediction is the average target value of the 110 training instances associated with this leaf node, and it results in a mean squared error equal to 0.015 over these 110 instances.

This model's predictions are represented on the left in Figure 6-5. If you set `max_depth=3`, you get the predictions represented on the right. Notice how the predicted value for each region is always the average target value of the instances in that region. The algorithm splits each region in a way that makes most training instances as close as possible to that predicted value.

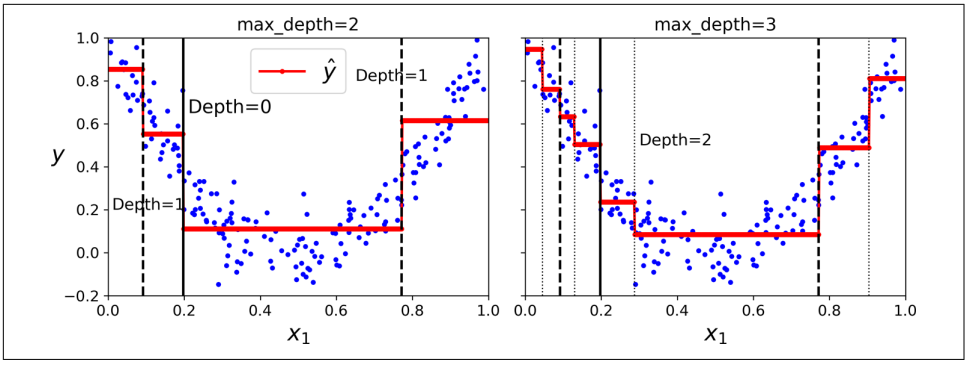


Figure 6-5. Predictions of two Decision Tree regression models

The CART algorithm works mostly the same way as earlier, except that instead of trying to split the training set in a way that minimizes impurity, it now tries to split the training set in a way that minimizes the MSE. Equation 6-4 shows the cost function that the algorithm tries to minimize.

Equation 6-4. CART cost function for regression

$$J(k, t_k) = \frac{m_{\text{left}}}{m}\text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m}\text{MSE}_{\text{right}} \quad \text{where} \begin{cases} \text{MSE}_{\text{node}} = \sum_{i \in \text{node}} \left(\hat{y}_{\text{node}} - y^{(i)}\right)^2 \\ \hat{y}_{\text{node}} = \frac{1}{m_{\text{node}}} \sum_{i \in \text{node}} y^{(i)} \end{cases}$$

Just like for classification tasks, Decision Trees are prone to overfitting when dealing with regression tasks. Without any regularization (i.e., using the default hyperparameters), you get the predictions on the left in Figure 6-6. These predictions are obviously overfitting the training set very badly. Just setting `min_samples_leaf=10` results in a much more reasonable model, represented on the right in Figure 6-6.

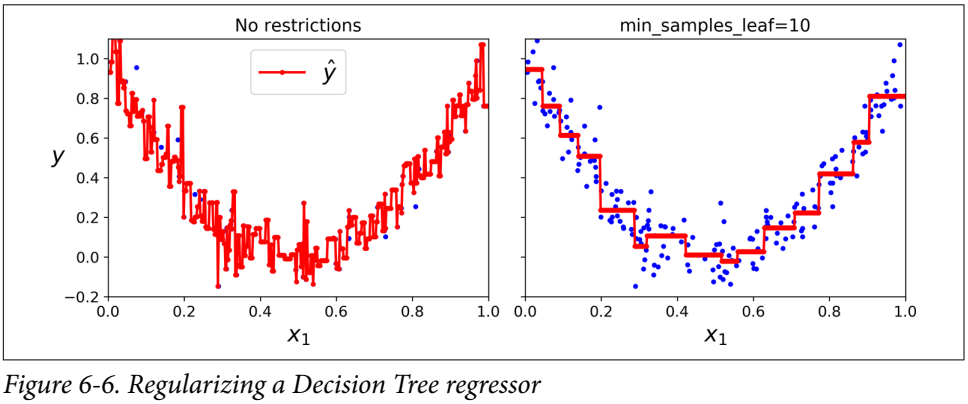


Figure 6-6. Regularizing a Decision Tree regressor

Instability

Hopefully by now you are convinced that Decision Trees have a lot going for them: they are simple to understand and interpret, easy to use, versatile, and powerful. However, they do have a few limitations. First, as you may have noticed, Decision Trees love orthogonal decision boundaries (all splits are perpendicular to an axis), which makes them sensitive to training set rotation. For example, Figure 6-7 shows a simple linearly separable dataset: on the left, a Decision Tree can split it easily, while on the right, after the dataset is rotated by 45°, the decision boundary looks unnecessarily convoluted. Although both Decision Trees fit the training set perfectly, it is very likely that the model on the right will not generalize well. One way to limit this problem is to use Principal Component Analysis (see Chapter 8), which often results in a better orientation of the training data.

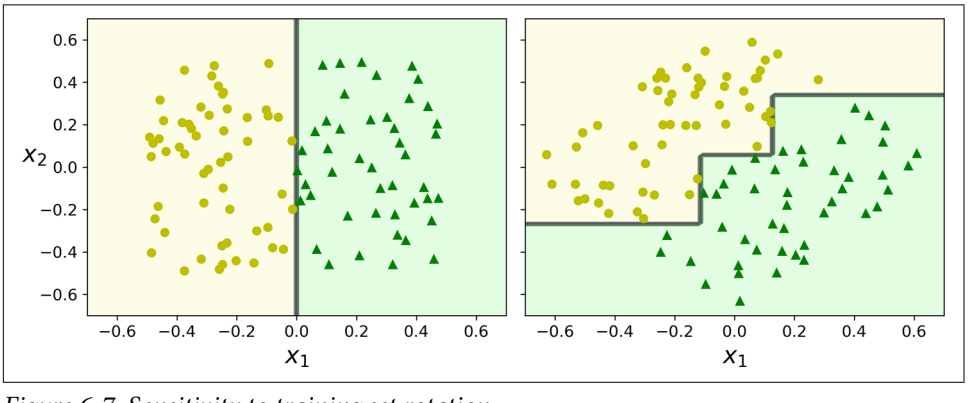


Figure 6-7. Sensitivity to training set rotation

More generally, the main issue with Decision Trees is that they are very sensitive to small variations in the training data. For example, if you just remove the widest *Iris versicolor* from the iris training set (the one with petals 4.8 cm long and 1.8 cm wide) and train a new Decision Tree, you may get the model represented in Figure 6-8. As you can see, it looks very different from the previous Decision Tree (Figure 6-2). Actually, since the training algorithm used by Scikit-Learn is stochastic,[6] you may get very different models even on the same training data (unless you set the `random_state` hyperparameter).

6 It randomly selects the set of features to evaluate at each node.

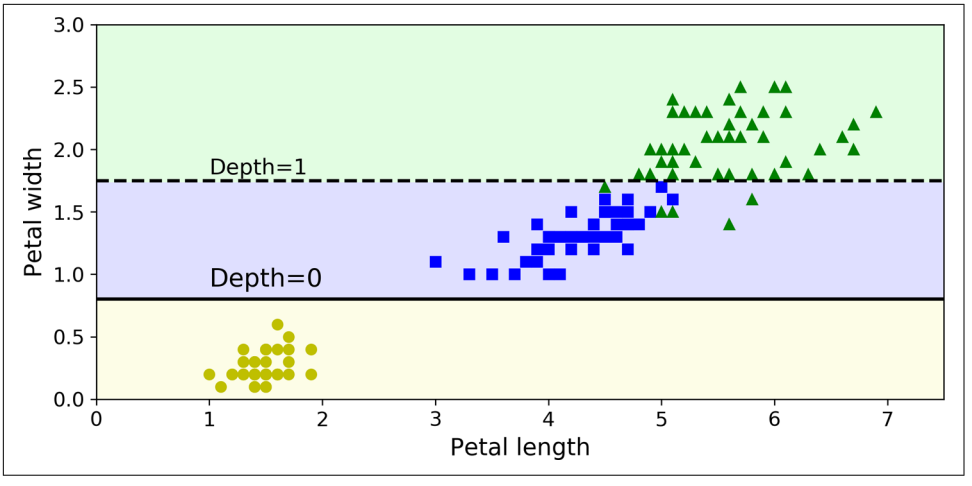


Figure 6-8. Sensitivity to training set details

Random Forests can limit this instability by averaging predictions over many trees, as we will see in the next chapter.

Exercises

1. What is the approximate depth of a Decision Tree trained (without restrictions) on a training set with one million instances?
2. Is a node's Gini impurity generally lower or greater than its parent's? Is it *generally* lower/greater, or *always* lower/greater?
3. If a Decision Tree is overfitting the training set, is it a good idea to try decreasing `max_depth`?
4. If a Decision Tree is underfitting the training set, is it a good idea to try scaling the input features?
5. If it takes one hour to train a Decision Tree on a training set containing 1 million instances, roughly how much time will it take to train another Decision Tree on a training set containing 10 million instances?
6. If your training set contains 100,000 instances, will setting `presort=True` speed up training?
7. Train and fine-tune a Decision Tree for the moons dataset by following these steps:
   a. Use `make_moons(n_samples=10000, noise=0.4)` to generate a moons dataset.
   b. Use `train_test_split()` to split the dataset into a training set and a test set.

c. Use grid search with cross-validation (with the help of the `GridSearchCV` class) to find good hyperparameter values for a `DecisionTreeClassifier`. Hint: try various values for `max_leaf_nodes`.

d. Train it on the full training set using these hyperparameters, and measure your model's performance on the test set. You should get roughly 85% to 87% accuracy.

8. Grow a forest by following these steps:

a. Continuing the previous exercise, generate 1,000 subsets of the training set, each containing 100 instances selected randomly. Hint: you can use Scikit-Learn's `ShuffleSplit` class for this.

b. Train one Decision Tree on each subset, using the best hyperparameter values found in the previous exercise. Evaluate these 1,000 Decision Trees on the test set. Since they were trained on smaller sets, these Decision Trees will likely perform worse than the first Decision Tree, achieving only about 80% accuracy.

c. Now comes the magic. For each test set instance, generate the predictions of the 1,000 Decision Trees, and keep only the most frequent prediction (you can use SciPy's `mode()` function for this). This approach gives you *majority-vote predictions* over the test set.

d. Evaluate these predictions on the test set: you should obtain a slightly higher accuracy than your first model (about 0.5 to 1.5% higher). Congratulations, you have trained a Random Forest classifier!

Solutions to these exercises are available in Appendix A.

CHAPTER 7

Ensemble Learning and Random Forests

Suppose you pose a complex question to thousands of random people, then aggregate their answers. In many cases you will find that this aggregated answer is better than an expert's answer. This is called the *wisdom of the crowd*. Similarly, if you aggregate the predictions of a group of predictors (such as classifiers or regressors), you will often get better predictions than with the best individual predictor. A group of predictors is called an *ensemble*; thus, this technique is called *Ensemble Learning*, and an Ensemble Learning algorithm is called an *Ensemble method*.

As an example of an Ensemble method, you can train a group of Decision Tree classifiers, each on a different random subset of the training set. To make predictions, you obtain the predictions of all the individual trees, then predict the class that gets the most votes (see the last exercise in Chapter 6). Such an ensemble of Decision Trees is called a *Random Forest*, and despite its simplicity, this is one of the most powerful Machine Learning algorithms available today.

As discussed in Chapter 2, you will often use Ensemble methods near the end of a project, once you have already built a few good predictors, to combine them into an even better predictor. In fact, the winning solutions in Machine Learning competitions often involve several Ensemble methods (most famously in the Netflix Prize competition).

In this chapter we will discuss the most popular Ensemble methods, including *bagging*, *boosting*, and *stacking*. We will also explore Random Forests.

Voting Classifiers

Suppose you have trained a few classifiers, each one achieving about 80% accuracy. You may have a Logistic Regression classifier, an SVM classifier, a Random Forest classifier, a K-Nearest Neighbors classifier, and perhaps a few more (see Figure 7-1).

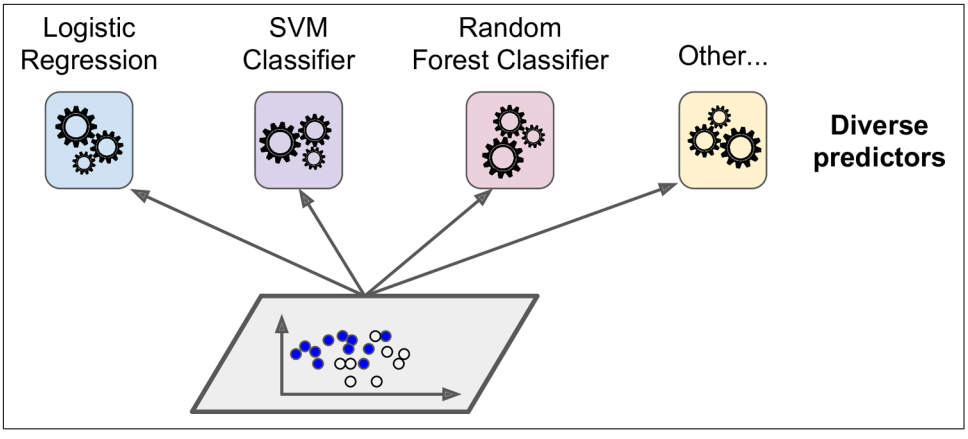


Figure 7-1. Training diverse classifiers

A very simple way to create an even better classifier is to aggregate the predictions of each classifier and predict the class that gets the most votes. This majority-vote classifier is called a *hard voting* classifier (see Figure 7-2).

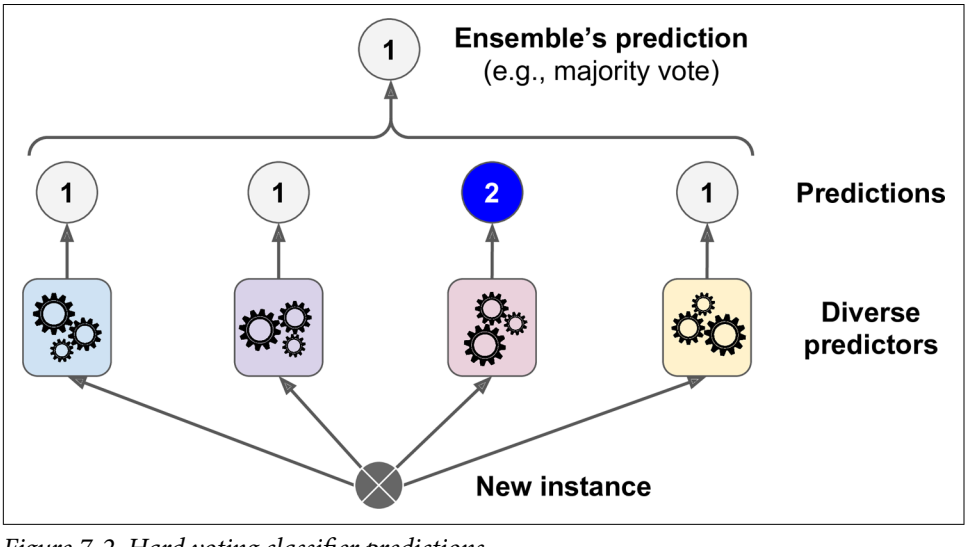


Figure 7-2. Hard voting classifier predictions

Somewhat surprisingly, this voting classifier often achieves a higher accuracy than the best classifier in the ensemble. In fact, even if each classifier is a *weak learner* (meaning it does only slightly better than random guessing), the ensemble can still be a *strong learner* (achieving high accuracy), provided there are a sufficient number of weak learners and they are sufficiently diverse.

How is this possible? The following analogy can help shed some light on this mystery. Suppose you have a slightly biased coin that has a 51% chance of coming up heads and 49% chance of coming up tails. If you toss it 1,000 times, you will generally get more or less 510 heads and 490 tails, and hence a majority of heads. If you do the math, you will find that the probability of obtaining a majority of heads after 1,000 tosses is close to 75%. The more you toss the coin, the higher the probability (e.g., with 10,000 tosses, the probability climbs over 97%). This is due to the *law of large numbers*: as you keep tossing the coin, the ratio of heads gets closer and closer to the probability of heads (51%). Figure 7-3 shows 10 series of biased coin tosses. You can see that as the number of tosses increases, the ratio of heads approaches 51%. Eventually all 10 series end up so close to 51% that they are consistently above 50%.

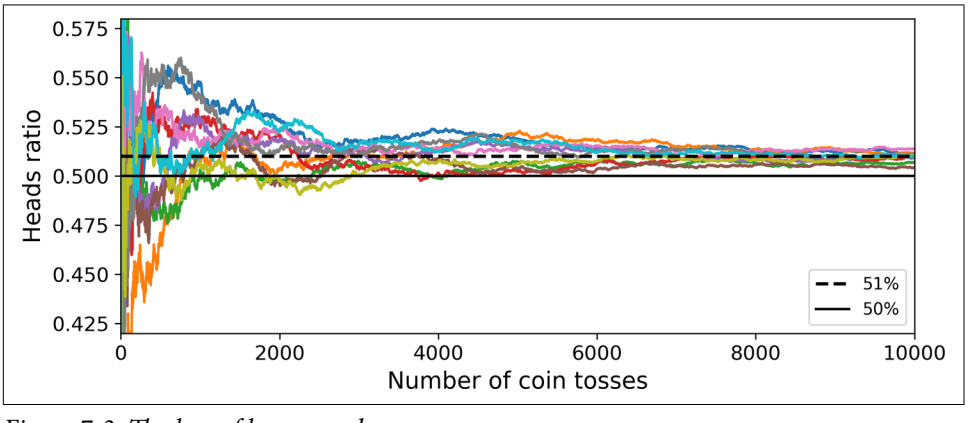


Figure 7-3. The law of large numbers

Similarly, suppose you build an ensemble containing 1,000 classifiers that are individually correct only 51% of the time (barely better than random guessing). If you predict the majority voted class, you can hope for up to 75% accuracy! However, this is only true if all classifiers are perfectly independent, making uncorrelated errors, which is clearly not the case because they are trained on the same data. They are likely to make the same types of errors, so there will be many majority votes for the wrong class, reducing the ensemble's accuracy.

Ensemble methods work best when the predictors are as independent from one another as possible. One way to get diverse classifiers is to train them using very different algorithms. This increases the chance that they will make very different types of errors, improving the ensemble's accuracy.

The following code creates and trains a voting classifier in Scikit-Learn, composed of three diverse classifiers (the training set is the moons dataset, introduced in Chapter 5):

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import VotingClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC

log_clf = LogisticRegression()
rnd_clf = RandomForestClassifier()
svm_clf = SVC()

voting_clf = VotingClassifier(
    estimators=[('lr', log_clf), ('rf', rnd_clf), ('svc', svm_clf)],
    voting='hard')
voting_clf.fit(X_train, y_train)
```

Let's look at each classifier's accuracy on the test set:

```
>>> from sklearn.metrics import accuracy_score
>>> for clf in (log_clf, rnd_clf, svm_clf, voting_clf):
...     clf.fit(X_train, y_train)
...     y_pred = clf.predict(X_test)
...     print(clf.__class__.__name__, accuracy_score(y_test, y_pred))
...
LogisticRegression 0.864
RandomForestClassifier 0.896
SVC 0.888
VotingClassifier 0.904
```

There you have it! The voting classifier slightly outperforms all the individual classifiers.

If all classifiers are able to estimate class probabilities (i.e., they all have a `predict_proba()` method), then you can tell Scikit-Learn to predict the class with the highest class probability, averaged over all the individual classifiers. This is called *soft voting*. It often achieves higher performance than hard voting because it gives more weight to highly confident votes. All you need to do is replace `voting="hard"` with `voting="soft"` and ensure that all classifiers can estimate class probabilities. This is not the case for the `SVC` class by default, so you need to set its `probability` hyperparameter to `True` (this will make the `SVC` class use cross-validation to estimate class probabilities, slowing down training, and it will add a `predict_proba()` method). If you modify the preceding code to use soft voting, you will find that the voting classifier achieves over 91.2% accuracy!

Bagging and Pasting

One way to get a diverse set of classifiers is to use very different training algorithms, as just discussed. Another approach is to use the same training algorithm for every predictor and train them on different random subsets of the training set. When sam-

pling is performed *with* replacement, this method is called *bagging*[1] (short for *bootstrap aggregating*[2]). When sampling is performed *without* replacement, it is called *pasting*.[3]

In other words, both bagging and pasting allow training instances to be sampled several times across multiple predictors, but only bagging allows training instances to be sampled several times for the same predictor. This sampling and training process is represented in Figure 7-4.

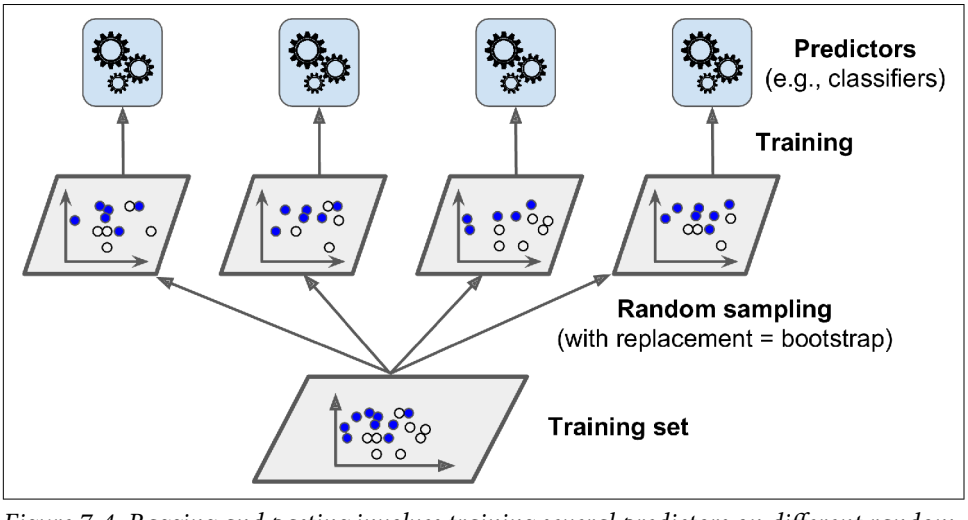


Figure 7-4. Bagging and pasting involves training several predictors on different random samples of the training set

Once all predictors are trained, the ensemble can make a prediction for a new instance by simply aggregating the predictions of all predictors. The aggregation function is typically the *statistical mode* (i.e., the most frequent prediction, just like a hard voting classifier) for classification, or the average for regression. Each individual predictor has a higher bias than if it were trained on the original training set, but aggregation reduces both bias and variance.[4] Generally, the net result is that the ensemble has a similar bias but a lower variance than a single predictor trained on the original training set.

1 Leo Breiman, "Bagging Predictors," *Machine Learning* 24, no. 2 (1996): 123–140.

2 In statistics, resampling with replacement is called *bootstrapping*.

3 Leo Breiman, "Pasting Small Votes for Classification in Large Databases and On-Line," *Machine Learning* 36, no. 1–2 (1999): 85–103.

4 Bias and variance were introduced in Chapter 4.

As you can see in Figure 7-4, predictors can all be trained in parallel, via different CPU cores or even different servers. Similarly, predictions can be made in parallel. This is one of the reasons bagging and pasting are such popular methods: they scale very well.

Bagging and Pasting in Scikit-Learn

Scikit-Learn offers a simple API for both bagging and pasting with the `BaggingClassifier` class (or `BaggingRegressor` for regression). The following code trains an ensemble of 500 Decision Tree classifiers:[5] each is trained on 100 training instances randomly sampled from the training set with replacement (this is an example of bagging, but if you want to use pasting instead, just set `bootstrap=False`). The `n_jobs` parameter tells Scikit-Learn the number of CPU cores to use for training and predictions (`-1` tells Scikit-Learn to use all available cores):

```
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier

bag_clf = BaggingClassifier(
    DecisionTreeClassifier(), n_estimators=500,
    max_samples=100, bootstrap=True, n_jobs=-1)
bag_clf.fit(X_train, y_train)
y_pred = bag_clf.predict(X_test)
```

The `BaggingClassifier` automatically performs soft voting instead of hard voting if the base classifier can estimate class probabilities (i.e., if it has a `predict_proba()` method), which is the case with Decision Tree classifiers.

Figure 7-5 compares the decision boundary of a single Decision Tree with the decision boundary of a bagging ensemble of 500 trees (from the preceding code), both trained on the moons dataset. As you can see, the ensemble's predictions will likely generalize much better than the single Decision Tree's predictions: the ensemble has a comparable bias but a smaller variance (it makes roughly the same number of errors on the training set, but the decision boundary is less irregular).

5 `max_samples` can alternatively be set to a float between 0.0 and 1.0, in which case the max number of instances to sample is equal to the size of the training set times `max_samples`.

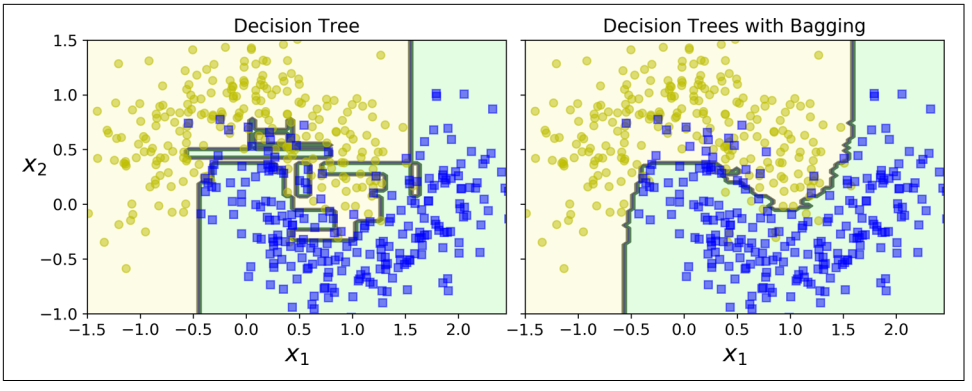


Figure 7-5. A single Decision Tree (left) versus a bagging ensemble of 500 trees (right)

Bootstrapping introduces a bit more diversity in the subsets that each predictor is trained on, so bagging ends up with a slightly higher bias than pasting; but the extra diversity also means that the predictors end up being less correlated, so the ensemble's variance is reduced. Overall, bagging often results in better models, which explains why it is generally preferred. However, if you have spare time and CPU power, you can use cross-validation to evaluate both bagging and pasting and select the one that works best.

Out-of-Bag Evaluation

With bagging, some instances may be sampled several times for any given predictor, while others may not be sampled at all. By default a `BaggingClassifier` samples m training instances with replacement (`bootstrap=True`), where m is the size of the training set. This means that only about 63% of the training instances are sampled on average for each predictor.[6] The remaining 37% of the training instances that are not sampled are called *out-of-bag* (oob) instances. Note that they are not the same 37% for all predictors.

Since a predictor never sees the oob instances during training, it can be evaluated on these instances, without the need for a separate validation set. You can evaluate the ensemble itself by averaging out the oob evaluations of each predictor.

In Scikit-Learn, you can set `oob_score=True` when creating a `BaggingClassifier` to request an automatic oob evaluation after training. The following code demonstrates this. The resulting evaluation score is available through the `oob_score_` variable:

6 As m grows, this ratio approaches $1 - \exp(-1) \approx 63.212\%$.

```
>>> bag_clf = BaggingClassifier(
...     DecisionTreeClassifier(), n_estimators=500,
...     bootstrap=True, n_jobs=-1, oob_score=True)
...
>>> bag_clf.fit(X_train, y_train)
>>> bag_clf.oob_score_
0.90133333333333332
```

According to this oob evaluation, this `BaggingClassifier` is likely to achieve about 90.1% accuracy on the test set. Let's verify this:

```
>>> from sklearn.metrics import accuracy_score
>>> y_pred = bag_clf.predict(X_test)
>>> accuracy_score(y_test, y_pred)
0.91200000000000003
```

We get 91.2% accuracy on the test set—close enough!

The oob decision function for each training instance is also available through the `oob_decision_function_` variable. In this case (since the base estimator has a `predict_proba()` method), the decision function returns the class probabilities for each training instance. For example, the oob evaluation estimates that the first training instance has a 68.25% probability of belonging to the positive class (and 31.75% of belonging to the negative class):

```
>>> bag_clf.oob_decision_function_
array([[0.31746032, 0.68253968],
       [0.34117647, 0.65882353],
       [1.        , 0.        ],
       ...
       [1.        , 0.        ],
       [0.03108808, 0.96891192],
       [0.57291667, 0.42708333]])
```

Random Patches and Random Subspaces

The `BaggingClassifier` class supports sampling the features as well. Sampling is controlled by two hyperparameters: `max_features` and `bootstrap_features`. They work the same way as `max_samples` and `bootstrap`, but for feature sampling instead of instance sampling. Thus, each predictor will be trained on a random subset of the input features.

This technique is particularly useful when you are dealing with high-dimensional inputs (such as images). Sampling both training instances and features is called the *Random Patches* method.[7] Keeping all training instances (by setting `bootstrap=False`

7 Gilles Louppe and Pierre Geurts, "Ensembles on Random Patches," *Lecture Notes in Computer Science* 7523 (2012): 346–361.

and `max_samples=1.0`) but sampling features (by setting `bootstrap_features` to `True` and/or `max_features` to a value smaller than `1.0`) is called the *Random Subspaces* method.[8]

Sampling features results in even more predictor diversity, trading a bit more bias for a lower variance.

Random Forests

As we have discussed, a Random Forest[9] is an ensemble of Decision Trees, generally trained via the bagging method (or sometimes pasting), typically with `max_samples` set to the size of the training set. Instead of building a `BaggingClassifier` and passing it a `DecisionTreeClassifier`, you can instead use the `RandomForestClassifier` class, which is more convenient and optimized for Decision Trees[10] (similarly, there is a `RandomForestRegressor` class for regression tasks). The following code uses all available CPU cores to train a Random Forest classifier with 500 trees (each limited to maximum 16 nodes):

```
from sklearn.ensemble import RandomForestClassifier

rnd_clf = RandomForestClassifier(n_estimators=500, max_leaf_nodes=16, n_jobs=-1)
rnd_clf.fit(X_train, y_train)

y_pred_rf = rnd_clf.predict(X_test)
```

With a few exceptions, a `RandomForestClassifier` has all the hyperparameters of a `DecisionTreeClassifier` (to control how trees are grown), plus all the hyperparameters of a `BaggingClassifier` to control the ensemble itself.[11]

The Random Forest algorithm introduces extra randomness when growing trees; instead of searching for the very best feature when splitting a node (see Chapter 6), it searches for the best feature among a random subset of features. The algorithm results in greater tree diversity, which (again) trades a higher bias for a lower variance, generally yielding an overall better model. The following `BaggingClassifier` is roughly equivalent to the previous `RandomForestClassifier`:

8 Tin Kam Ho, "The Random Subspace Method for Constructing Decision Forests," *IEEE Transactions on Pattern Analysis and Machine Intelligence* 20, no. 8 (1998): 832–844.

9 Tin Kam Ho, "Random Decision Forests," *Proceedings of the Third International Conference on Document Analysis and Recognition* 1 (1995): 278.

10 The `BaggingClassifier` class remains useful if you want a bag of something other than Decision Trees.

11 There are a few notable exceptions: `splitter` is absent (forced to `"random"`), `presort` is absent (forced to `False`), `max_samples` is absent (forced to `1.0`), and `base_estimator` is absent (forced to `DecisionTreeClassifier` with the provided hyperparameters).

```
bag_clf = BaggingClassifier(
    DecisionTreeClassifier(splitter="random", max_leaf_nodes=16),
    n_estimators=500, max_samples=1.0, bootstrap=True, n_jobs=-1)
```

Extra-Trees

When you are growing a tree in a Random Forest, at each node only a random subset of the features is considered for splitting (as discussed earlier). It is possible to make trees even more random by also using random thresholds for each feature rather than searching for the best possible thresholds (like regular Decision Trees do).

A forest of such extremely random trees is called an *Extremely Randomized Trees* ensemble[12] (or *Extra-Trees* for short). Once again, this technique trades more bias for a lower variance. It also makes Extra-Trees much faster to train than regular Random Forests, because finding the best possible threshold for each feature at every node is one of the most time-consuming tasks of growing a tree.

You can create an Extra-Trees classifier using Scikit-Learn's `ExtraTreesClassifier` class. Its API is identical to the `RandomForestClassifier` class. Similarly, the `ExtraTreesRegressor` class has the same API as the `RandomForestRegressor` class.

It is hard to tell in advance whether a `RandomForestClassifier` will perform better or worse than an `ExtraTreesClassifier`. Generally, the only way to know is to try both and compare them using cross-validation (tuning the hyperparameters using grid search).

Feature Importance

Yet another great quality of Random Forests is that they make it easy to measure the relative importance of each feature. Scikit-Learn measures a feature's importance by looking at how much the tree nodes that use that feature reduce impurity on average (across all trees in the forest). More precisely, it is a weighted average, where each node's weight is equal to the number of training samples that are associated with it (see Chapter 6).

Scikit-Learn computes this score automatically for each feature after training, then it scales the results so that the sum of all importances is equal to 1. You can access the result using the `feature_importances_` variable. For example, the following code trains a `RandomForestClassifier` on the iris dataset (introduced in Chapter 4) and outputs each feature's importance. It seems that the most important features are the petal length (44%) and width (42%), while sepal length and width are rather unimportant in comparison (11% and 2%, respectively):

12 Pierre Geurts et al., "Extremely Randomized Trees," *Machine Learning* 63, no. 1 (2006): 3–42.

```
>>> from sklearn.datasets import load_iris
>>> iris = load_iris()
>>> rnd_clf = RandomForestClassifier(n_estimators=500, n_jobs=-1)
>>> rnd_clf.fit(iris["data"], iris["target"])
>>> for name, score in zip(iris["feature_names"], rnd_clf.feature_importances_):
...     print(name, score)
...
sepal length (cm) 0.112492250999
sepal width (cm) 0.0231192882825
petal length (cm) 0.441030464364
petal width (cm) 0.423357996355
```

Similarly, if you train a Random Forest classifier on the MNIST dataset (introduced in Chapter 3) and plot each pixel's importance, you get the image represented in Figure 7-6.

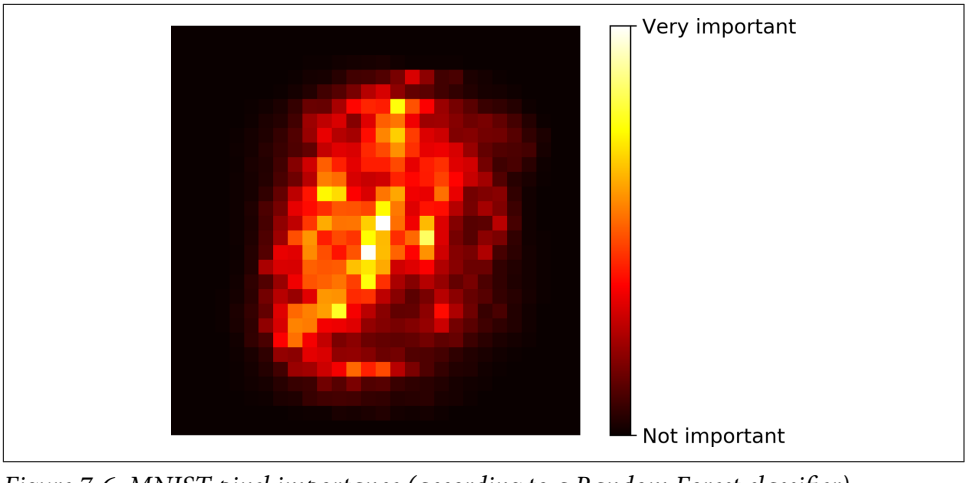


Figure 7-6. MNIST pixel importance (according to a Random Forest classifier)

Random Forests are very handy to get a quick understanding of what features actually matter, in particular if you need to perform feature selection.

Boosting

Boosting (originally called *hypothesis boosting*) refers to any Ensemble method that can combine several weak learners into a strong learner. The general idea of most boosting methods is to train predictors sequentially, each trying to correct its predecessor. There are many boosting methods available, but by far the most popular are

AdaBoost[13] (short for *Adaptive Boosting*) and *Gradient Boosting*. Let's start with AdaBoost.

AdaBoost

One way for a new predictor to correct its predecessor is to pay a bit more attention to the training instances that the predecessor underfitted. This results in new predictors focusing more and more on the hard cases. This is the technique used by AdaBoost.

For example, when training an AdaBoost classifier, the algorithm first trains a base classifier (such as a Decision Tree) and uses it to make predictions on the training set. The algorithm then increases the relative weight of misclassified training instances. Then it trains a second classifier, using the updated weights, and again makes predictions on the training set, updates the instance weights, and so on (see Figure 7-7).

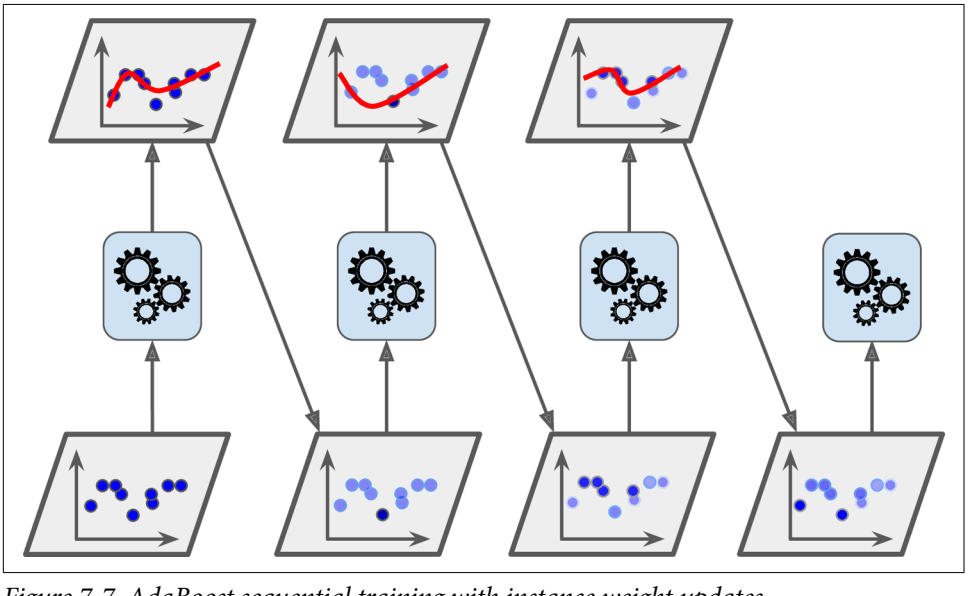


Figure 7-7. AdaBoost sequential training with instance weight updates

Figure 7-8 shows the decision boundaries of five consecutive predictors on the moons dataset (in this example, each predictor is a highly regularized SVM classifier with an RBF kernel[14]). The first classifier gets many instances wrong, so their weights

13 Yoav Freund and Robert E. Schapire, "A Decision-Theoretic Generalization of On-Line Learning and an Application to Boosting," *Journal of Computer and System Sciences* 55, no. 1 (1997): 119–139.

14 This is just for illustrative purposes. SVMs are generally not good base predictors for AdaBoost; they are slow and tend to be unstable with it.

get boosted. The second classifier therefore does a better job on these instances, and so on. The plot on the right represents the same sequence of predictors, except that the learning rate is halved (i.e., the misclassified instance weights are boosted half as much at every iteration). As you can see, this sequential learning technique has some similarities with Gradient Descent, except that instead of tweaking a single predictor's parameters to minimize a cost function, AdaBoost adds predictors to the ensemble, gradually making it better.

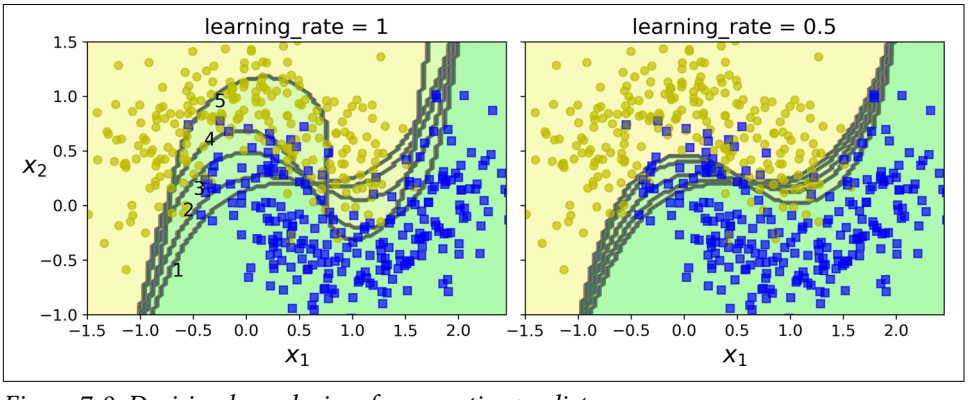


Figure 7-8. Decision boundaries of consecutive predictors

Once all predictors are trained, the ensemble makes predictions very much like bagging or pasting, except that predictors have different weights depending on their overall accuracy on the weighted training set.

There is one important drawback to this sequential learning technique: it cannot be parallelized (or only partially), since each predictor can only be trained after the previous predictor has been trained and evaluated. As a result, it does not scale as well as bagging or pasting.

Let's take a closer look at the AdaBoost algorithm. Each instance weight $w^{(i)}$ is initially set to $1/m$. A first predictor is trained, and its weighted error rate r_1 is computed on the training set; see Equation 7-1.

Equation 7-1. Weighted error rate of the j^{th} predictor

$$r_j = \frac{\sum_{\substack{i=1 \\ \hat{y}_j^{(i)} \neq y^{(i)}}}^{m} w^{(i)}}{\sum_{i=1}^{m} w^{(i)}}$$

where $\hat{y}_j^{(i)}$ is the j^{th} predictor's prediction for the i^{th} instance.

The predictor's weight α_j is then computed using Equation 7-2, where η is the learning rate hyperparameter (defaults to 1).[15] The more accurate the predictor is, the higher its weight will be. If it is just guessing randomly, then its weight will be close to zero. However, if it is most often wrong (i.e., less accurate than random guessing), then its weight will be negative.

Equation 7-2. Predictor weight

$$\alpha_j = \eta \log \frac{1 - r_j}{r_j}$$

Next, the AdaBoost algorithm updates the instance weights, using Equation 7-3, which boosts the weights of the misclassified instances.

Equation 7-3. Weight update rule

$$\text{for } i = 1, 2, \cdots, m$$
$$w^{(i)} \leftarrow \begin{cases} w^{(i)} & \text{if } \widehat{y}_j^{(i)} = y^{(i)} \\ w^{(i)} \exp\left(\alpha_j\right) & \text{if } \widehat{y}_j^{(i)} \neq y^{(i)} \end{cases}$$

Then all the instance weights are normalized (i.e., divided by $\sum_{i=1}^{m} w^{(i)}$).

Finally, a new predictor is trained using the updated weights, and the whole process is repeated (the new predictor's weight is computed, the instance weights are updated, then another predictor is trained, and so on). The algorithm stops when the desired number of predictors is reached, or when a perfect predictor is found.

To make predictions, AdaBoost simply computes the predictions of all the predictors and weighs them using the predictor weights α_j. The predicted class is the one that receives the majority of weighted votes (see Equation 7-4).

Equation 7-4. AdaBoost predictions

$$\hat{y}(\mathbf{x}) = \underset{k}{\operatorname{argmax}} \sum_{\substack{j=1 \\ \hat{y}_j(\mathbf{x}) = k}}^{N} \alpha_j \quad \text{where } N \text{ is the number of predictors.}$$

15 The original AdaBoost algorithm does not use a learning rate hyperparameter.

Scikit-Learn uses a multiclass version of AdaBoost called *SAMME*[16] (which stands for *Stagewise Additive Modeling using a Multiclass Exponential loss function*). When there are just two classes, SAMME is equivalent to AdaBoost. If the predictors can estimate class probabilities (i.e., if they have a `predict_proba()` method), Scikit-Learn can use a variant of SAMME called *SAMME.R* (the *R* stands for "Real"), which relies on class probabilities rather than predictions and generally performs better.

The following code trains an AdaBoost classifier based on 200 *Decision Stumps* using Scikit-Learn's `AdaBoostClassifier` class (as you might expect, there is also an `AdaBoostRegressor` class). A Decision Stump is a Decision Tree with `max_depth=1`—in other words, a tree composed of a single decision node plus two leaf nodes. This is the default base estimator for the `AdaBoostClassifier` class:

```
from sklearn.ensemble import AdaBoostClassifier

ada_clf = AdaBoostClassifier(
    DecisionTreeClassifier(max_depth=1), n_estimators=200,
    algorithm="SAMME.R", learning_rate=0.5)
ada_clf.fit(X_train, y_train)
```

If your AdaBoost ensemble is overfitting the training set, you can try reducing the number of estimators or more strongly regularizing the base estimator.

Gradient Boosting

Another very popular boosting algorithm is *Gradient Boosting*.[17] Just like AdaBoost, Gradient Boosting works by sequentially adding predictors to an ensemble, each one correcting its predecessor. However, instead of tweaking the instance weights at every iteration like AdaBoost does, this method tries to fit the new predictor to the *residual errors* made by the previous predictor.

Let's go through a simple regression example, using Decision Trees as the base predictors (of course, Gradient Boosting also works great with regression tasks). This is called *Gradient Tree Boosting*, or *Gradient Boosted Regression Trees* (GBRT). First, let's fit a `DecisionTreeRegressor` to the training set (for example, a noisy quadratic training set):

16 For more details, see Ji Zhu et al., "Multi-Class AdaBoost," *Statistics and Its Interface* 2, no. 3 (2009): 349–360.

17 Gradient Boosting was first introduced in Leo Breiman's 1997 paper "Arcing the Edge" and was further developed in the 1999 paper "Greedy Function Approximation: A Gradient Boosting Machine" by Jerome H. Friedman.

```
from sklearn.tree import DecisionTreeRegressor

tree_reg1 = DecisionTreeRegressor(max_depth=2)
tree_reg1.fit(X, y)
```

Next, we'll train a second `DecisionTreeRegressor` on the residual errors made by the first predictor:

```
y2 = y - tree_reg1.predict(X)
tree_reg2 = DecisionTreeRegressor(max_depth=2)
tree_reg2.fit(X, y2)
```

Then we train a third regressor on the residual errors made by the second predictor:

```
y3 = y2 - tree_reg2.predict(X)
tree_reg3 = DecisionTreeRegressor(max_depth=2)
tree_reg3.fit(X, y3)
```

Now we have an ensemble containing three trees. It can make predictions on a new instance simply by adding up the predictions of all the trees:

```
y_pred = sum(tree.predict(X_new) for tree in (tree_reg1, tree_reg2, tree_reg3))
```

Figure 7-9 represents the predictions of these three trees in the left column, and the ensemble's predictions in the right column. In the first row, the ensemble has just one tree, so its predictions are exactly the same as the first tree's predictions. In the second row, a new tree is trained on the residual errors of the first tree. On the right you can see that the ensemble's predictions are equal to the sum of the predictions of the first two trees. Similarly, in the third row another tree is trained on the residual errors of the second tree. You can see that the ensemble's predictions gradually get better as trees are added to the ensemble.

A simpler way to train GBRT ensembles is to use Scikit-Learn's `GradientBoostingRegressor` class. Much like the `RandomForestRegressor` class, it has hyperparameters to control the growth of Decision Trees (e.g., `max_depth`, `min_samples_leaf`), as well as hyperparameters to control the ensemble training, such as the number of trees (`n_estimators`). The following code creates the same ensemble as the previous one:

```
from sklearn.ensemble import GradientBoostingRegressor

gbrt = GradientBoostingRegressor(max_depth=2, n_estimators=3, learning_rate=1.0)
gbrt.fit(X, y)
```

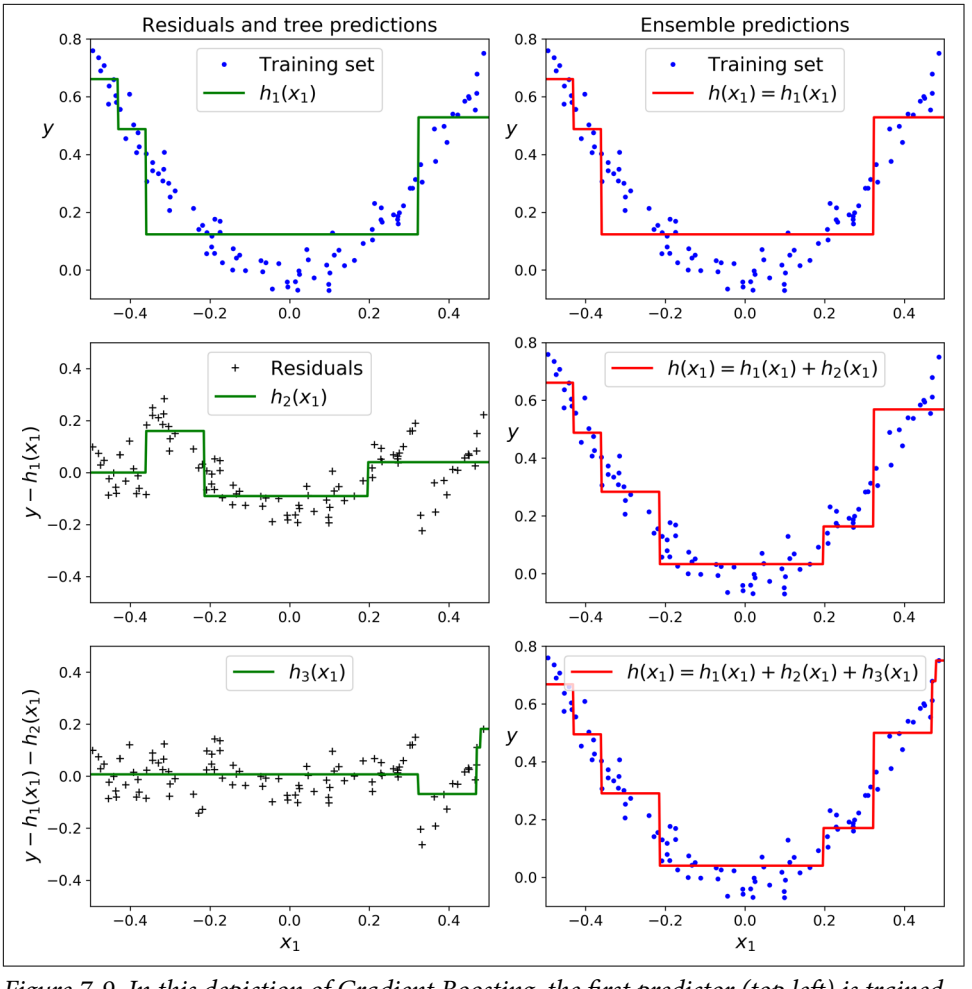


Figure 7-9. In this depiction of Gradient Boosting, the first predictor (top left) is trained normally, then each consecutive predictor (middle left and lower left) is trained on the previous predictor's residuals; the right column shows the resulting ensemble's predictions

The `learning_rate` hyperparameter scales the contribution of each tree. If you set it to a low value, such as `0.1`, you will need more trees in the ensemble to fit the training set, but the predictions will usually generalize better. This is a regularization technique called *shrinkage*. Figure 7-10 shows two GBRT ensembles trained with a low learning rate: the one on the left does not have enough trees to fit the training set, while the one on the right has too many trees and overfits the training set.

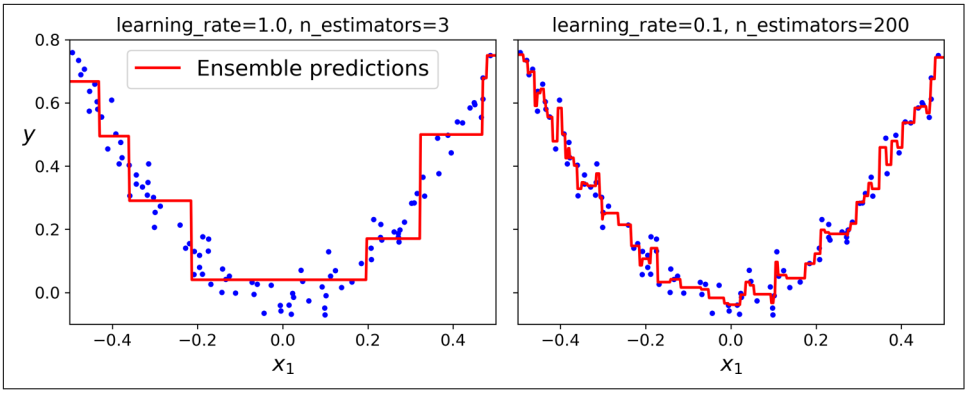


Figure 7-10. GBRT ensembles with not enough predictors (left) and too many (right)

In order to find the optimal number of trees, you can use early stopping (see Chapter 4). A simple way to implement this is to use the `staged_predict()` method: it returns an iterator over the predictions made by the ensemble at each stage of training (with one tree, two trees, etc.). The following code trains a GBRT ensemble with 120 trees, then measures the validation error at each stage of training to find the optimal number of trees, and finally trains another GBRT ensemble using the optimal number of trees:

```
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error

X_train, X_val, y_train, y_val = train_test_split(X, y)

gbrt = GradientBoostingRegressor(max_depth=2, n_estimators=120)
gbrt.fit(X_train, y_train)

errors = [mean_squared_error(y_val, y_pred)
          for y_pred in gbrt.staged_predict(X_val)]
bst_n_estimators = np.argmin(errors) + 1

gbrt_best = GradientBoostingRegressor(max_depth=2,n_estimators=bst_n_estimators)
gbrt_best.fit(X_train, y_train)
```

The validation errors are represented on the left of Figure 7-11, and the best model's predictions are represented on the right.

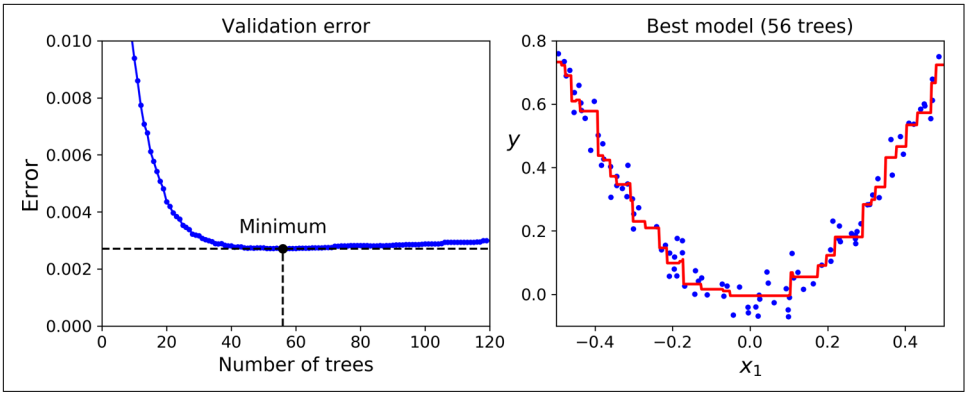


Figure 7-11. Tuning the number of trees using early stopping

It is also possible to implement early stopping by actually stopping training early (instead of training a large number of trees first and then looking back to find the optimal number). You can do so by setting `warm_start=True`, which makes Scikit-Learn keep existing trees when the `fit()` method is called, allowing incremental training. The following code stops training when the validation error does not improve for five iterations in a row:

```
gbrt = GradientBoostingRegressor(max_depth=2, warm_start=True)

min_val_error = float("inf")
error_going_up = 0
for n_estimators in range(1, 120):
    gbrt.n_estimators = n_estimators
    gbrt.fit(X_train, y_train)
    y_pred = gbrt.predict(X_val)
    val_error = mean_squared_error(y_val, y_pred)
    if val_error < min_val_error:
        min_val_error = val_error
        error_going_up = 0
    else:
        error_going_up += 1
        if error_going_up == 5:
            break  # early stopping
```

The `GradientBoostingRegressor` class also supports a `subsample` hyperparameter, which specifies the fraction of training instances to be used for training each tree. For example, if `subsample=0.25`, then each tree is trained on 25% of the training instances, selected randomly. As you can probably guess by now, this technique trades a higher bias for a lower variance. It also speeds up training considerably. This is called *Stochastic Gradient Boosting*.

It is possible to use Gradient Boosting with other cost functions. This is controlled by the `loss` hyperparameter (see Scikit-Learn's documentation for more details).

It is worth noting that an optimized implementation of Gradient Boosting is available in the popular Python library XGBoost, which stands for Extreme Gradient Boosting. This package was initially developed by Tianqi Chen as part of the Distributed (Deep) Machine Learning Community (DMLC), and it aims to be extremely fast, scalable, and portable. In fact, XGBoost is often an important component of the winning entries in ML competitions. XGBoost's API is quite similar to Scikit-Learn's:

```
import xgboost

xgb_reg = xgboost.XGBRegressor()
xgb_reg.fit(X_train, y_train)
y_pred = xgb_reg.predict(X_val)
```

XGBoost also offers several nice features, such as automatically taking care of early stopping:

```
xgb_reg.fit(X_train, y_train,
            eval_set=[(X_val, y_val)], early_stopping_rounds=2)
y_pred = xgb_reg.predict(X_val)
```

You should definitely check it out!

Stacking

The last Ensemble method we will discuss in this chapter is called *stacking* (short for *stacked generalization*).[18] It is based on a simple idea: instead of using trivial functions (such as hard voting) to aggregate the predictions of all predictors in an ensemble, why don't we train a model to perform this aggregation? Figure 7-12 shows such an ensemble performing a regression task on a new instance. Each of the bottom three predictors predicts a different value (3.1, 2.7, and 2.9), and then the final predictor (called a *blender*, or a *meta learner*) takes these predictions as inputs and makes the final prediction (3.0).

18 David H. Wolpert, "Stacked Generalization," *Neural Networks* 5, no. 2 (1992): 241–259.

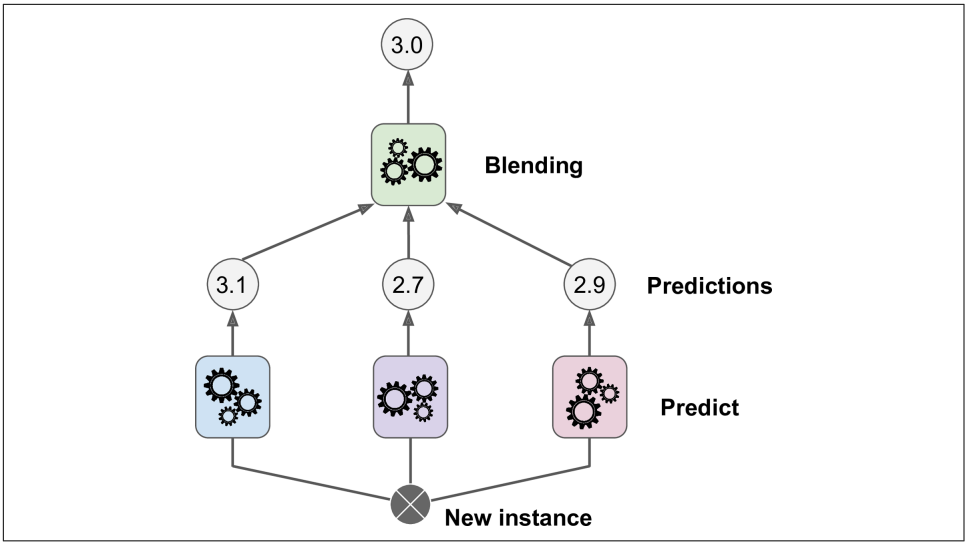


Figure 7-12. Aggregating predictions using a blending predictor

To train the blender, a common approach is to use a hold-out set.[19] Let's see how it works. First, the training set is split into two subsets. The first subset is used to train the predictors in the first layer (see Figure 7-13).

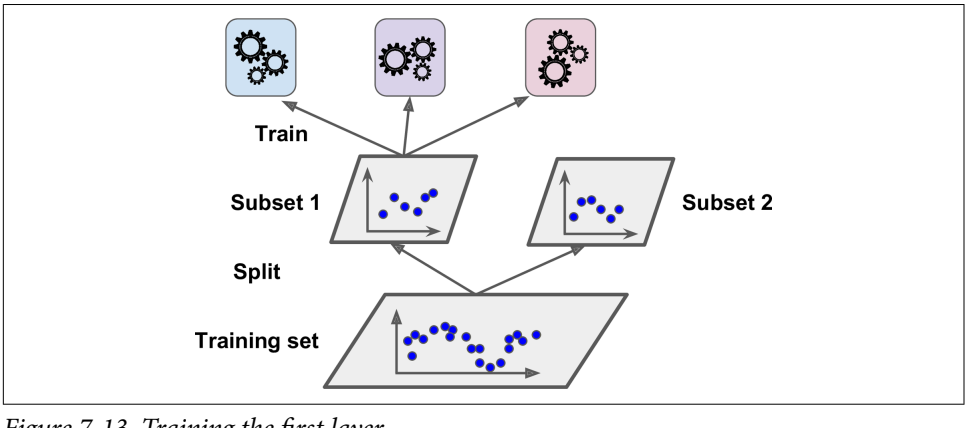


Figure 7-13. Training the first layer

Next, the first layer's predictors are used to make predictions on the second (held-out) set (see Figure 7-14). This ensures that the predictions are "clean," since the predictors never saw these instances during training. For each instance in the hold-out

19 Alternatively, it is possible to use out-of-fold predictions. In some contexts this is called *stacking*, while using a hold-out set is called *blending*. For many people these terms are synonymous.

set, there are three predicted values. We can create a new training set using these predicted values as input features (which makes this new training set 3D), and keeping the target values. The blender is trained on this new training set, so it learns to predict the target value, given the first layer's predictions.

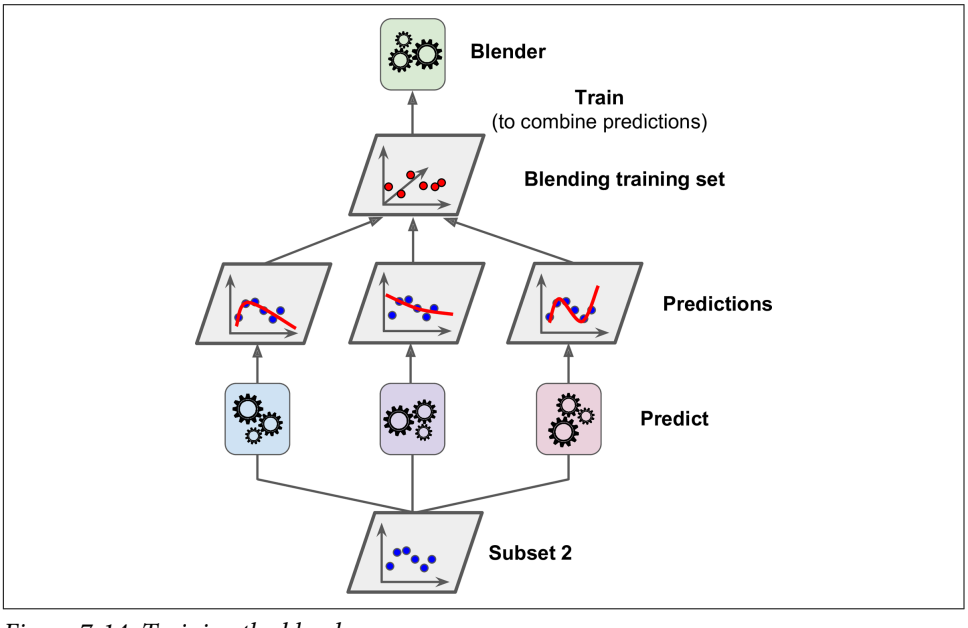


Figure 7-14. Training the blender

It is actually possible to train several different blenders this way (e.g., one using Linear Regression, another using Random Forest Regression), to get a whole layer of blenders. The trick is to split the training set into three subsets: the first one is used to train the first layer, the second one is used to create the training set used to train the second layer (using predictions made by the predictors of the first layer), and the third one is used to create the training set to train the third layer (using predictions made by the predictors of the second layer). Once this is done, we can make a prediction for a new instance by going through each layer sequentially, as shown in Figure 7-15.

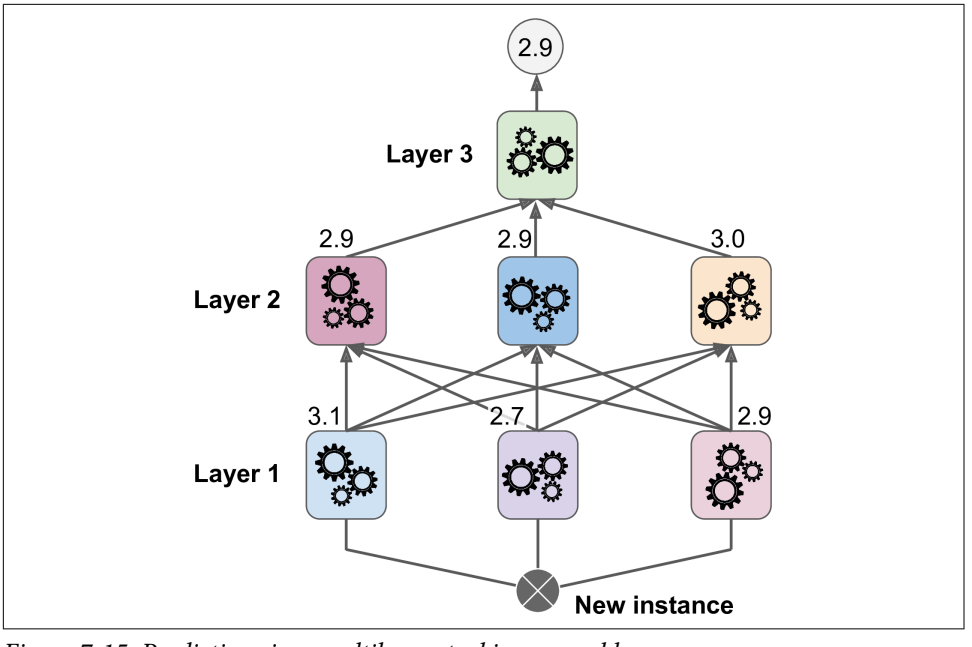


Figure 7-15. Predictions in a multilayer stacking ensemble

Unfortunately, Scikit-Learn does not support stacking directly, but it is not too hard to roll out your own implementation (see the following exercises). Alternatively, you can use an open source implementation such as `DESlib`.

Exercises

1. If you have trained five different models on the exact same training data, and they all achieve 95% precision, is there any chance that you can combine these models to get better results? If so, how? If not, why?
2. What is the difference between hard and soft voting classifiers?
3. Is it possible to speed up training of a bagging ensemble by distributing it across multiple servers? What about pasting ensembles, boosting ensembles, Random Forests, or stacking ensembles?
4. What is the benefit of out-of-bag evaluation?
5. What makes Extra-Trees more random than regular Random Forests? How can this extra randomness help? Are Extra-Trees slower or faster than regular Random Forests?
6. If your AdaBoost ensemble underfits the training data, which hyperparameters should you tweak and how?

7. If your Gradient Boosting ensemble overfits the training set, should you increase or decrease the learning rate?
8. Load the MNIST data (introduced in Chapter 3), and split it into a training set, a validation set, and a test set (e.g., use 50,000 instances for training, 10,000 for validation, and 10,000 for testing). Then train various classifiers, such as a Random Forest classifier, an Extra-Trees classifier, and an SVM classifier. Next, try to combine them into an ensemble that outperforms each individual classifier on the validation set, using soft or hard voting. Once you have found one, try it on the test set. How much better does it perform compared to the individual classifiers?
9. Run the individual classifiers from the previous exercise to make predictions on the validation set, and create a new training set with the resulting predictions: each training instance is a vector containing the set of predictions from all your classifiers for an image, and the target is the image's class. Train a classifier on this new training set. Congratulations, you have just trained a blender, and together with the classifiers it forms a stacking ensemble! Now evaluate the ensemble on the test set. For each image in the test set, make predictions with all your classifiers, then feed the predictions to the blender to get the ensemble's predictions. How does it compare to the voting classifier you trained earlier?

Solutions to these exercises are available in Appendix A.

CHAPTER 8
Dimensionality Reduction

Many Machine Learning problems involve thousands or even millions of features for each training instance. Not only do all these features make training extremely slow, but they can also make it much harder to find a good solution, as we will see. This problem is often referred to as the *curse of dimensionality*.

Fortunately, in real-world problems, it is often possible to reduce the number of features considerably, turning an intractable problem into a tractable one. For example, consider the MNIST images (introduced in Chapter 3): the pixels on the image borders are almost always white, so you could completely drop these pixels from the training set without losing much information. Figure 7-6 confirms that these pixels are utterly unimportant for the classification task. Additionally, two neighboring pixels are often highly correlated: if you merge them into a single pixel (e.g., by taking the mean of the two pixel intensities), you will not lose much information.

Reducing dimensionality does cause some information loss (just like compressing an image to JPEG can degrade its quality), so even though it will speed up training, it may make your system perform slightly worse. It also makes your pipelines a bit more complex and thus harder to maintain. So, if training is too slow, you should first try to train your system with the original data before considering using dimensionality reduction. In some cases, reducing the dimensionality of the training data may filter out some noise and unnecessary details and thus result in higher performance, but in general it won't; it will just speed up training.

Apart from speeding up training, dimensionality reduction is also extremely useful for data visualization (or *DataViz*). Reducing the number of dimensions down to two (or three) makes it possible to plot a condensed view of a high-dimensional training

set on a graph and often gain some important insights by visually detecting patterns, such as clusters. Moreover, DataViz is essential to communicate your conclusions to people who are not data scientists—in particular, decision makers who will use your results.

In this chapter we will discuss the curse of dimensionality and get a sense of what goes on in high-dimensional space. Then, we will consider the two main approaches to dimensionality reduction (projection and Manifold Learning), and we will go through three of the most popular dimensionality reduction techniques: PCA, Kernel PCA, and LLE.

The Curse of Dimensionality

We are so used to living in three dimensions[1] that our intuition fails us when we try to imagine a high-dimensional space. Even a basic 4D hypercube is incredibly hard to picture in our minds (see Figure 8-1), let alone a 200-dimensional ellipsoid bent in a 1,000-dimensional space.

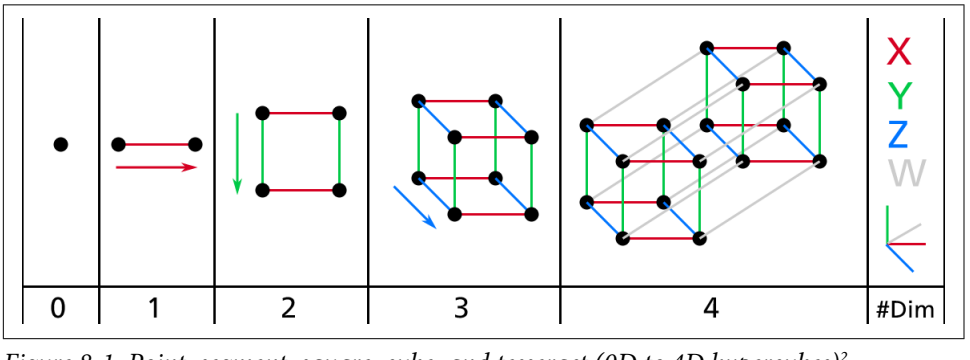


Figure 8-1. Point, segment, square, cube, and tesseract (0D to 4D hypercubes)[2]

It turns out that many things behave very differently in high-dimensional space. For example, if you pick a random point in a unit square (a 1 × 1 square), it will have only about a 0.4% chance of being located less than 0.001 from a border (in other words, it is very unlikely that a random point will be "extreme" along any dimension). But in a 10,000-dimensional unit hypercube, this probability is greater than 99.999999%. Most points in a high-dimensional hypercube are very close to the border.[3]

1 Well, four dimensions if you count time, and a few more if you are a string theorist.

2 Watch a rotating tesseract projected into 3D space at *https://homl.info/30*. Image by Wikipedia user Nerd-Boy1392 (Creative Commons BY-SA 3.0). Reproduced from *https://en.wikipedia.org/wiki/Tesseract*.

3 Fun fact: anyone you know is probably an extremist in at least one dimension (e.g., how much sugar they put in their coffee), if you consider enough dimensions.

Here is a more troublesome difference: if you pick two points randomly in a unit square, the distance between these two points will be, on average, roughly 0.52. If you pick two random points in a unit 3D cube, the average distance will be roughly 0.66. But what about two points picked randomly in a 1,000,000-dimensional hypercube? The average distance, believe it or not, will be about 408.25 (roughly $\sqrt{1,000,000/6}$)! This is counterintuitive: how can two points be so far apart when they both lie within the same unit hypercube? Well, there's just plenty of space in high dimensions. As a result, high-dimensional datasets are at risk of being very sparse: most training instances are likely to be far away from each other. This also means that a new instance will likely be far away from any training instance, making predictions much less reliable than in lower dimensions, since they will be based on much larger extrapolations. In short, the more dimensions the training set has, the greater the risk of overfitting it.

In theory, one solution to the curse of dimensionality could be to increase the size of the training set to reach a sufficient density of training instances. Unfortunately, in practice, the number of training instances required to reach a given density grows exponentially with the number of dimensions. With just 100 features (significantly fewer than in the MNIST problem), you would need more training instances than atoms in the observable universe in order for training instances to be within 0.1 of each other on average, assuming they were spread out uniformly across all dimensions.

Main Approaches for Dimensionality Reduction

Before we dive into specific dimensionality reduction algorithms, let's take a look at the two main approaches to reducing dimensionality: projection and Manifold Learning.

Projection

In most real-world problems, training instances are *not* spread out uniformly across all dimensions. Many features are almost constant, while others are highly correlated (as discussed earlier for MNIST). As a result, all training instances lie within (or close to) a much lower-dimensional *subspace* of the high-dimensional space. This sounds very abstract, so let's look at an example. In Figure 8-2 you can see a 3D dataset represented by circles.

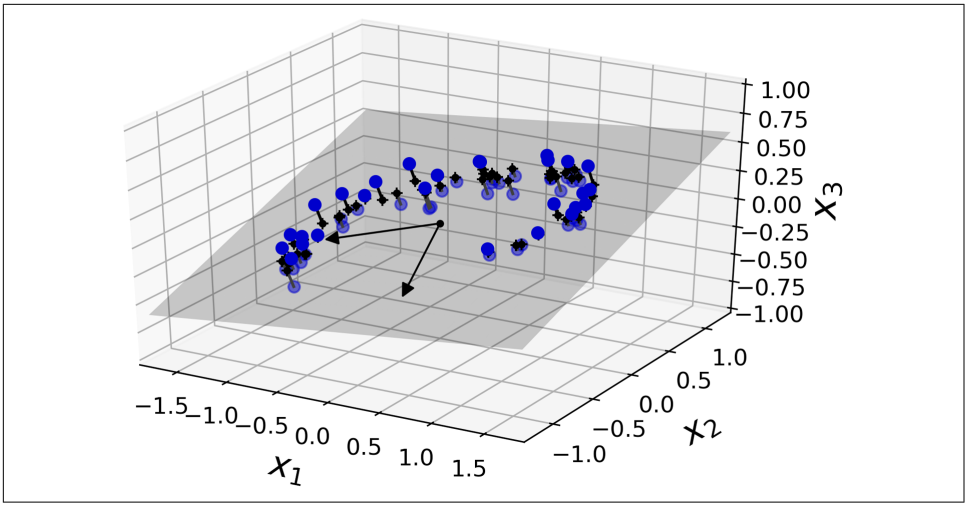


Figure 8-2. A 3D dataset lying close to a 2D subspace

Notice that all training instances lie close to a plane: this is a lower-dimensional (2D) subspace of the high-dimensional (3D) space. If we project every training instance perpendicularly onto this subspace (as represented by the short lines connecting the instances to the plane), we get the new 2D dataset shown in Figure 8-3. Ta-da! We have just reduced the dataset's dimensionality from 3D to 2D. Note that the axes correspond to new features z_1 and z_2 (the coordinates of the projections on the plane).

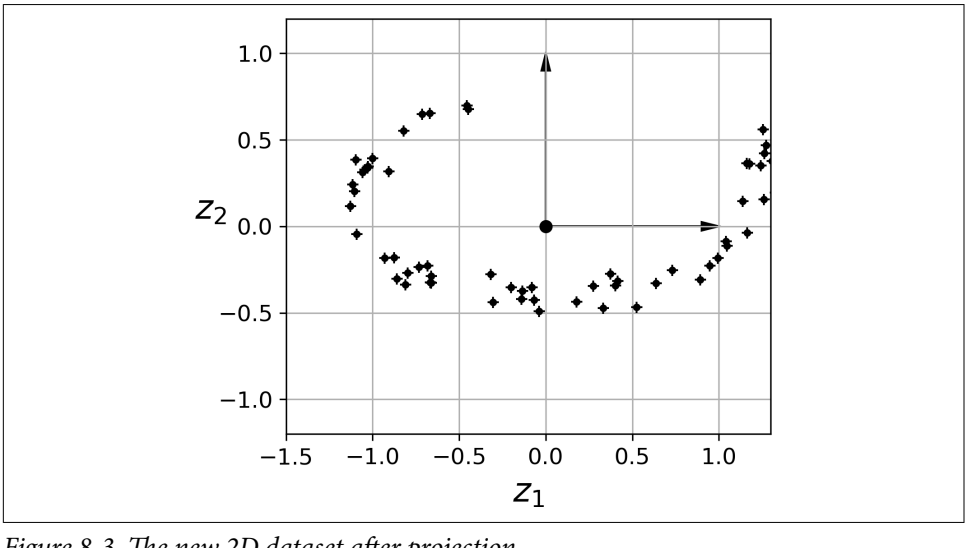


Figure 8-3. The new 2D dataset after projection

However, projection is not always the best approach to dimensionality reduction. In many cases the subspace may twist and turn, such as in the famous *Swiss roll* toy dataset represented in Figure 8-4.

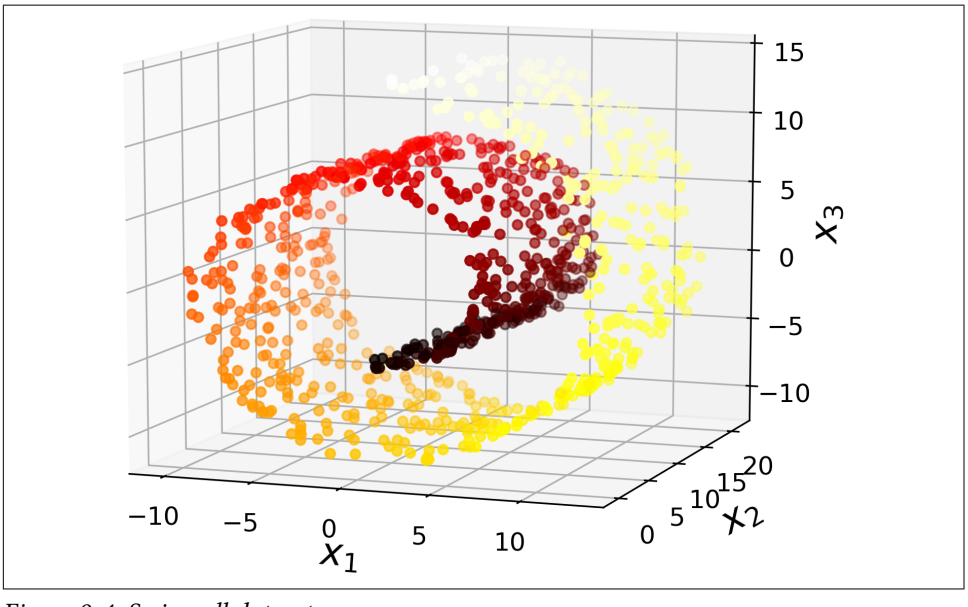


Figure 8-4. Swiss roll dataset

Simply projecting onto a plane (e.g., by dropping x_3) would squash different layers of the Swiss roll together, as shown on the left side of Figure 8-5. What you really want is to unroll the Swiss roll to obtain the 2D dataset on the right side of Figure 8-5.

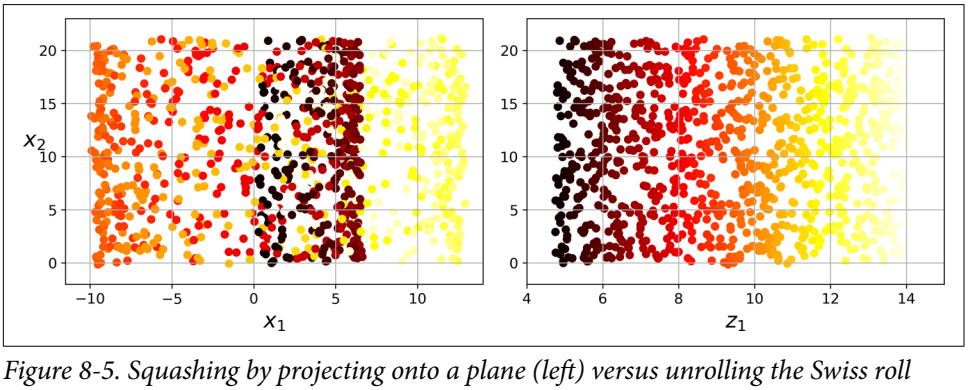


Figure 8-5. Squashing by projecting onto a plane (left) versus unrolling the Swiss roll (right)

Manifold Learning

The Swiss roll is an example of a 2D *manifold*. Put simply, a 2D manifold is a 2D shape that can be bent and twisted in a higher-dimensional space. More generally, a d-dimensional manifold is a part of an n-dimensional space (where $d < n$) that locally resembles a d-dimensional hyperplane. In the case of the Swiss roll, $d = 2$ and $n = 3$: it locally resembles a 2D plane, but it is rolled in the third dimension.

Many dimensionality reduction algorithms work by modeling the manifold on which the training instances lie; this is called *Manifold Learning*. It relies on the *manifold assumption*, also called the *manifold hypothesis*, which holds that most real-world high-dimensional datasets lie close to a much lower-dimensional manifold. This assumption is very often empirically observed.

Once again, think about the MNIST dataset: all handwritten digit images have some similarities. They are made of connected lines, the borders are white, and they are more or less centered. If you randomly generated images, only a ridiculously tiny fraction of them would look like handwritten digits. In other words, the degrees of freedom available to you if you try to create a digit image are dramatically lower than the degrees of freedom you would have if you were allowed to generate any image you wanted. These constraints tend to squeeze the dataset into a lower-dimensional manifold.

The manifold assumption is often accompanied by another implicit assumption: that the task at hand (e.g., classification or regression) will be simpler if expressed in the lower-dimensional space of the manifold. For example, in the top row of Figure 8-6 the Swiss roll is split into two classes: in the 3D space (on the left), the decision boundary would be fairly complex, but in the 2D unrolled manifold space (on the right), the decision boundary is a straight line.

However, this implicit assumption does not always hold. For example, in the bottom row of Figure 8-6, the decision boundary is located at $x_1 = 5$. This decision boundary looks very simple in the original 3D space (a vertical plane), but it looks more complex in the unrolled manifold (a collection of four independent line segments).

In short, reducing the dimensionality of your training set before training a model will usually speed up training, but it may not always lead to a better or simpler solution; it all depends on the dataset.

Hopefully you now have a good sense of what the curse of dimensionality is and how dimensionality reduction algorithms can fight it, especially when the manifold assumption holds. The rest of this chapter will go through some of the most popular algorithms.

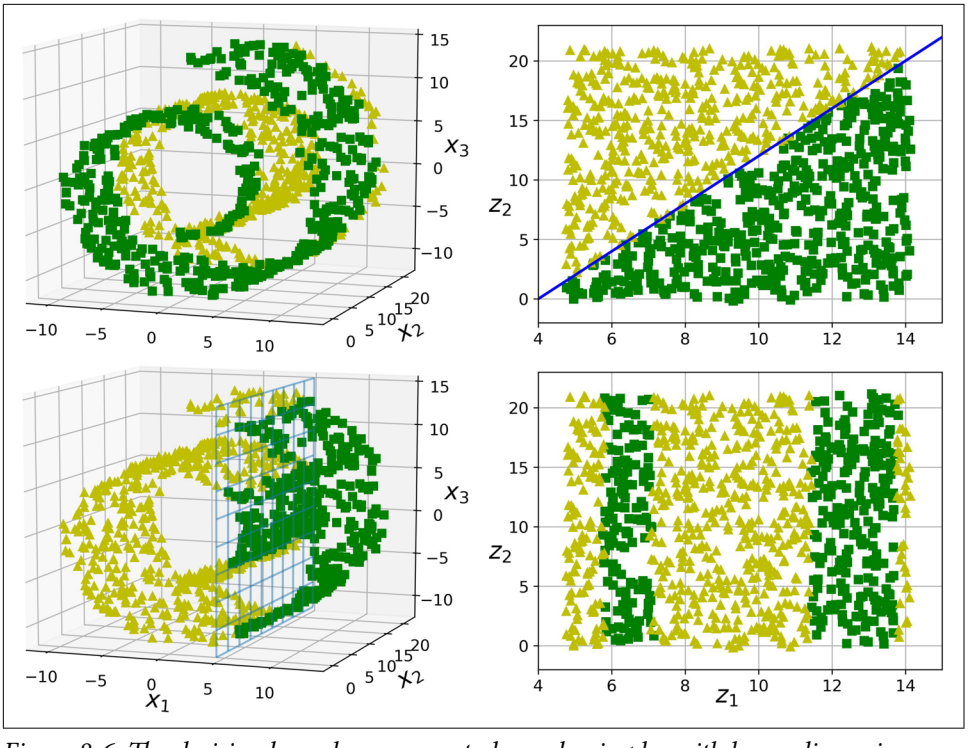


Figure 8-6. The decision boundary may not always be simpler with lower dimensions

PCA

Principal Component Analysis (PCA) is by far the most popular dimensionality reduction algorithm. First it identifies the hyperplane that lies closest to the data, and then it projects the data onto it, just like in Figure 8-2.

Preserving the Variance

Before you can project the training set onto a lower-dimensional hyperplane, you first need to choose the right hyperplane. For example, a simple 2D dataset is represented on the left in Figure 8-7, along with three different axes (i.e., 1D hyperplanes). On the right is the result of the projection of the dataset onto each of these axes. As you can see, the projection onto the solid line preserves the maximum variance, while the projection onto the dotted line preserves very little variance and the projection onto the dashed line preserves an intermediate amount of variance.

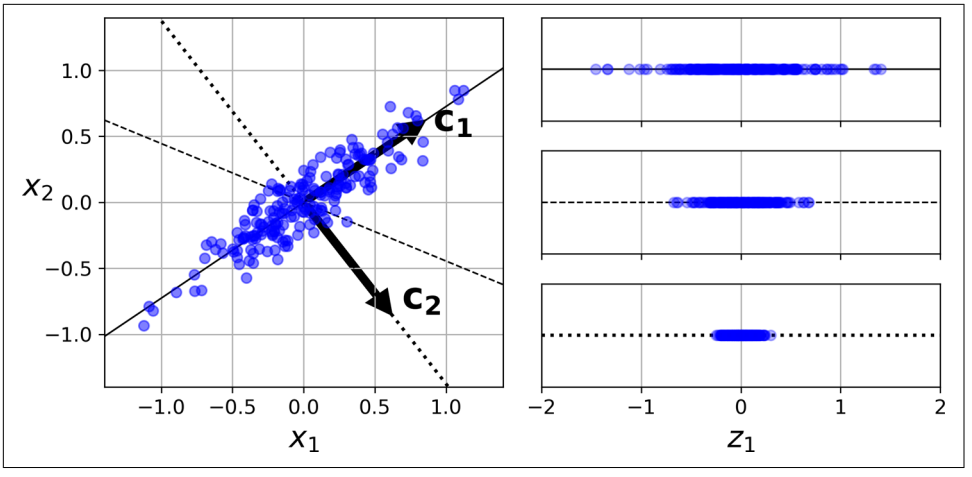


Figure 8-7. Selecting the subspace to project on

It seems reasonable to select the axis that preserves the maximum amount of variance, as it will most likely lose less information than the other projections. Another way to justify this choice is that it is the axis that minimizes the mean squared distance between the original dataset and its projection onto that axis. This is the rather simple idea behind PCA.[4]

Principal Components

PCA identifies the axis that accounts for the largest amount of variance in the training set. In Figure 8-7, it is the solid line. It also finds a second axis, orthogonal to the first one, that accounts for the largest amount of remaining variance. In this 2D example there is no choice: it is the dotted line. If it were a higher-dimensional dataset, PCA would also find a third axis, orthogonal to both previous axes, and a fourth, a fifth, and so on—as many axes as the number of dimensions in the dataset.

The i^{th} axis is called the i^{th} *principal component* (PC) of the data. In Figure 8-7, the first PC is the axis on which vector $\mathbf{c}_1$ lies, and the second PC is the axis on which vector $\mathbf{c}_2$ lies. In Figure 8-2 the first two PCs are the orthogonal axes on which the two arrows lie, on the plane, and the third PC is the axis orthogonal to that plane.

4 Karl Pearson, "On Lines and Planes of Closest Fit to Systems of Points in Space," *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 2, no. 11 (1901): 559-572, *https://homl.info/pca*.

For each principal component, PCA finds a zero-centered unit vector pointing in the direction of the PC. Since two opposing unit vectors lie on the same axis, the direction of the unit vectors returned by PCA is not stable: if you perturb the training set slightly and run PCA again, the unit vectors may point in the opposite direction as the original vectors. However, they will generally still lie on the same axes. In some cases, a pair of unit vectors may even rotate or swap (if the variances along these two axes are close), but the plane they define will generally remain the same.

So how can you find the principal components of a training set? Luckily, there is a standard matrix factorization technique called *Singular Value Decomposition* (SVD) that can decompose the training set matrix $\mathbf{X}$ into the matrix multiplication of three matrices $\mathbf{U}\ \mathbf{\Sigma}\ \mathbf{V}^{\intercal}$, where $\mathbf{V}$ contains the unit vectors that define all the principal components that we are looking for, as shown in Equation 8-1.

Equation 8-1. Principal components matrix

$$\mathbf{V} = \begin{pmatrix} | & | & & | \\ \mathbf{c}_1 & \mathbf{c}_2 & \cdots & \mathbf{c}_n \\ | & | & & | \end{pmatrix}$$

The following Python code uses NumPy's `svd()` function to obtain all the principal components of the training set, then extracts the two unit vectors that define the first two PCs:

```
X_centered = X - X.mean(axis=0)
U, s, Vt = np.linalg.svd(X_centered)
c1 = Vt.T[:, 0]
c2 = Vt.T[:, 1]
```

PCA assumes that the dataset is centered around the origin. As we will see, Scikit-Learn's PCA classes take care of centering the data for you. If you implement PCA yourself (as in the preceding example), or if you use other libraries, don't forget to center the data first.

Projecting Down to d Dimensions

Once you have identified all the principal components, you can reduce the dimensionality of the dataset down to d dimensions by projecting it onto the hyperplane defined by the first d principal components. Selecting this hyperplane ensures that the projection will preserve as much variance as possible. For example, in Figure 8-2 the 3D dataset is projected down to the 2D plane defined by the first two principal

components, preserving a large part of the dataset's variance. As a result, the 2D projection looks very much like the original 3D dataset.

To project the training set onto the hyperplane and obtain a reduced dataset $\mathbf{X}_{d\text{-proj}}$ of dimensionality d, compute the matrix multiplication of the training set matrix $\mathbf{X}$ by the matrix $\mathbf{W}_d$, defined as the matrix containing the first d columns of $\mathbf{V}$, as shown in Equation 8-2.

Equation 8-2. Projecting the training set down to d dimensions

$$\mathbf{X}_{d\text{-proj}} = \mathbf{X}\mathbf{W}_d$$

The following Python code projects the training set onto the plane defined by the first two principal components:

```
W2 = Vt.T[:, :2]
X2D = X_centered.dot(W2)
```

There you have it! You now know how to reduce the dimensionality of any dataset down to any number of dimensions, while preserving as much variance as possible.

Using Scikit-Learn

Scikit-Learn's `PCA` class uses SVD decomposition to implement PCA, just like we did earlier in this chapter. The following code applies PCA to reduce the dimensionality of the dataset down to two dimensions (note that it automatically takes care of centering the data):

```
from sklearn.decomposition import PCA

pca = PCA(n_components = 2)
X2D = pca.fit_transform(X)
```

After fitting the `PCA` transformer to the dataset, its `components_` attribute holds the transpose of $\mathbf{W}_d$ (e.g., the unit vector that defines the first principal component is equal to `pca.components_.T[:, 0]`).

Explained Variance Ratio

Another useful piece of information is the *explained variance ratio* of each principal component, available via the `explained_variance_ratio_` variable. The ratio indicates the proportion of the dataset's variance that lies along each principal component. For example, let's look at the explained variance ratios of the first two components of the 3D dataset represented in Figure 8-2:

```
>>> pca.explained_variance_ratio_
array([0.84248607, 0.14631839])
```

This output tells you that 84.2% of the dataset's variance lies along the first PC, and 14.6% lies along the second PC. This leaves less than 1.2% for the third PC, so it is reasonable to assume that the third PC probably carries little information.

Choosing the Right Number of Dimensions

Instead of arbitrarily choosing the number of dimensions to reduce down to, it is simpler to choose the number of dimensions that add up to a sufficiently large portion of the variance (e.g., 95%). Unless, of course, you are reducing dimensionality for data visualization—in that case you will want to reduce the dimensionality down to 2 or 3.

The following code performs PCA without reducing dimensionality, then computes the minimum number of dimensions required to preserve 95% of the training set's variance:

```
pca = PCA()
pca.fit(X_train)
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.95) + 1
```

You could then set `n_components=d` and run PCA again. But there is a much better option: instead of specifying the number of principal components you want to preserve, you can set `n_components` to be a float between 0.0 and 1.0, indicating the ratio of variance you wish to preserve:

```
pca = PCA(n_components=0.95)
X_reduced = pca.fit_transform(X_train)
```

Yet another option is to plot the explained variance as a function of the number of dimensions (simply plot `cumsum`; see Figure 8-8). There will usually be an elbow in the curve, where the explained variance stops growing fast. In this case, you can see that reducing the dimensionality down to about 100 dimensions wouldn't lose too much explained variance.

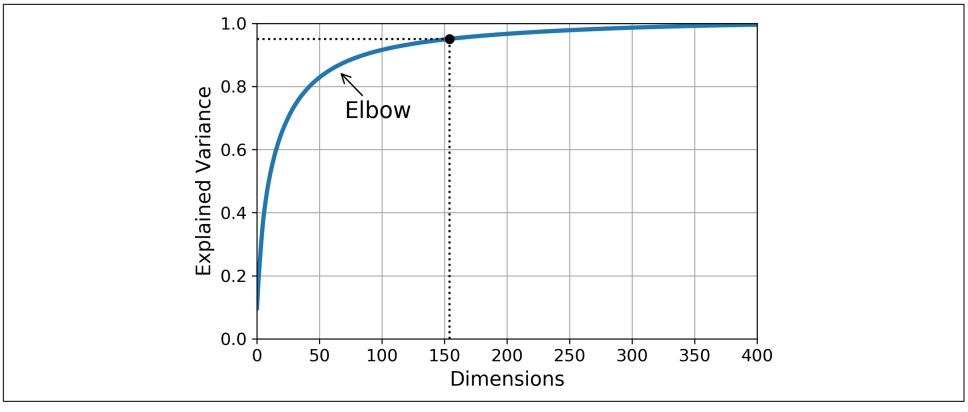


Figure 8-8. Explained variance as a function of the number of dimensions

PCA for Compression

After dimensionality reduction, the training set takes up much less space. As an example, try applying PCA to the MNIST dataset while preserving 95% of its variance. You should find that each instance will have just over 150 features, instead of the original 784 features. So, while most of the variance is preserved, the dataset is now less than 20% of its original size! This is a reasonable compression ratio, and you can see how this size reduction can speed up a classification algorithm (such as an SVM classifier) tremendously.

It is also possible to decompress the reduced dataset back to 784 dimensions by applying the inverse transformation of the PCA projection. This won't give you back the original data, since the projection lost a bit of information (within the 5% variance that was dropped), but it will likely be close to the original data. The mean squared distance between the original data and the reconstructed data (compressed and then decompressed) is called the *reconstruction error*.

The following code compresses the MNIST dataset down to 154 dimensions, then uses the `inverse_transform()` method to decompress it back to 784 dimensions:

```
pca = PCA(n_components = 154)
X_reduced = pca.fit_transform(X_train)
X_recovered = pca.inverse_transform(X_reduced)
```

Figure 8-9 shows a few digits from the original training set (on the left), and the corresponding digits after compression and decompression. You can see that there is a slight image quality loss, but the digits are still mostly intact.

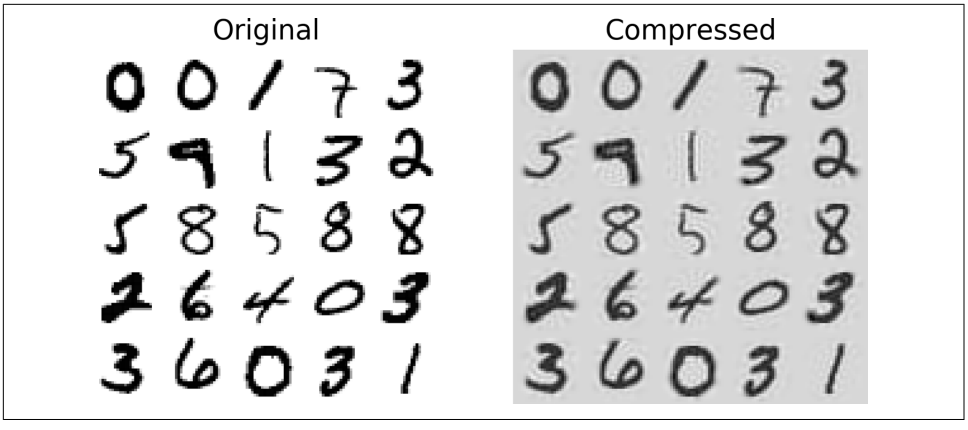


Figure 8-9. MNIST compression that preserves 95% of the variance

The equation of the inverse transformation is shown in Equation 8-3.

> *Equation 8-3. PCA inverse transformation, back to the original number of dimensions*
>
> $$\mathbf{X}_{\text{recovered}} = \mathbf{X}_{d\text{-proj}}\mathbf{W}_d^{\mathsf{T}}$$

Randomized PCA

If you set the `svd_solver` hyperparameter to `"randomized"`, Scikit-Learn uses a stochastic algorithm called *Randomized PCA* that quickly finds an approximation of the first d principal components. Its computational complexity is $O(m \times d^2) + O(d^3)$, instead of $O(m \times n^2) + O(n^3)$ for the full SVD approach, so it is dramatically faster than full SVD when d is much smaller than n:

```
rnd_pca = PCA(n_components=154, svd_solver="randomized")
X_reduced = rnd_pca.fit_transform(X_train)
```

By default, `svd_solver` is actually set to `"auto"`: Scikit-Learn automatically uses the randomized PCA algorithm if m or n is greater than 500 and d is less than 80% of m or n, or else it uses the full SVD approach. If you want to force Scikit-Learn to use full SVD, you can set the `svd_solver` hyperparameter to `"full"`.

Incremental PCA

One problem with the preceding implementations of PCA is that they require the whole training set to fit in memory in order for the algorithm to run. Fortunately, *Incremental PCA* (IPCA) algorithms have been developed. They allow you to split the training set into mini-batches and feed an IPCA algorithm one mini-batch at a time.

This is useful for large training sets and for applying PCA online (i.e., on the fly, as new instances arrive).

The following code splits the MNIST dataset into 100 mini-batches (using NumPy's `array_split()` function) and feeds them to Scikit-Learn's `IncrementalPCA` class[5] to reduce the dimensionality of the MNIST dataset down to 154 dimensions (just like before). Note that you must call the `partial_fit()` method with each mini-batch, rather than the `fit()` method with the whole training set:

```
from sklearn.decomposition import IncrementalPCA

n_batches = 100
inc_pca = IncrementalPCA(n_components=154)
for X_batch in np.array_split(X_train, n_batches):
    inc_pca.partial_fit(X_batch)

X_reduced = inc_pca.transform(X_train)
```

Alternatively, you can use NumPy's `memmap` class, which allows you to manipulate a large array stored in a binary file on disk as if it were entirely in memory; the class loads only the data it needs in memory, when it needs it. Since the `IncrementalPCA` class uses only a small part of the array at any given time, the memory usage remains under control. This makes it possible to call the usual `fit()` method, as you can see in the following code:

```
X_mm = np.memmap(filename, dtype="float32", mode="readonly", shape=(m, n))

batch_size = m // n_batches
inc_pca = IncrementalPCA(n_components=154, batch_size=batch_size)
inc_pca.fit(X_mm)
```

Kernel PCA

In Chapter 5 we discussed the kernel trick, a mathematical technique that implicitly maps instances into a very high-dimensional space (called the *feature space*), enabling nonlinear classification and regression with Support Vector Machines. Recall that a linear decision boundary in the high-dimensional feature space corresponds to a complex nonlinear decision boundary in the *original space*.

It turns out that the same trick can be applied to PCA, making it possible to perform complex nonlinear projections for dimensionality reduction. This is called *Kernel*

5 Scikit-Learn uses the algorithm described in David A. Ross et al., "Incremental Learning for Robust Visual Tracking," *International Journal of Computer Vision* 77, no. 1–3 (2008): 125–141.

PCA (kPCA).[6] It is often good at preserving clusters of instances after projection, or sometimes even unrolling datasets that lie close to a twisted manifold.

The following code uses Scikit-Learn's `KernelPCA` class to perform kPCA with an RBF kernel (see Chapter 5 for more details about the RBF kernel and other kernels):

```
from sklearn.decomposition import KernelPCA

rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.04)
X_reduced = rbf_pca.fit_transform(X)
```

Figure 8-10 shows the Swiss roll, reduced to two dimensions using a linear kernel (equivalent to simply using the `PCA` class), an RBF kernel, and a sigmoid kernel.

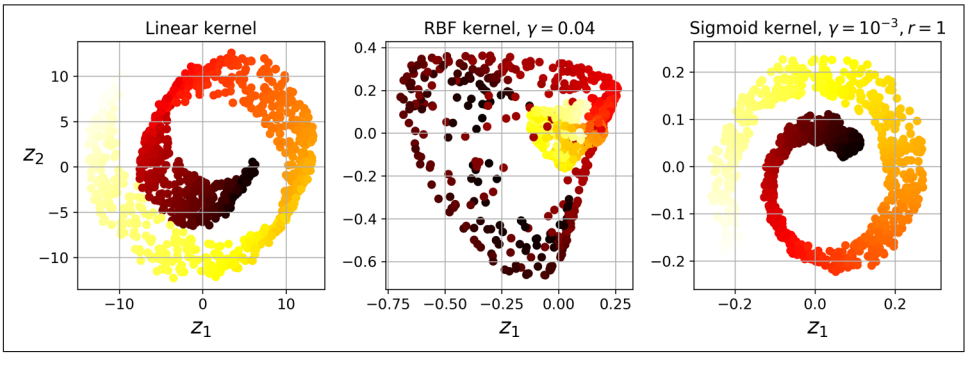


Figure 8-10. Swiss roll reduced to 2D using kPCA with various kernels

Selecting a Kernel and Tuning Hyperparameters

As kPCA is an unsupervised learning algorithm, there is no obvious performance measure to help you select the best kernel and hyperparameter values. That said, dimensionality reduction is often a preparation step for a supervised learning task (e.g., classification), so you can use grid search to select the kernel and hyperparameters that lead to the best performance on that task. The following code creates a two-step pipeline, first reducing dimensionality to two dimensions using kPCA, then applying Logistic Regression for classification. Then it uses `GridSearchCV` to find the best kernel and `gamma` value for kPCA in order to get the best classification accuracy at the end of the pipeline:

```
from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline
```

6 Bernhard Schölkopf et al., "Kernel Principal Component Analysis," in *Lecture Notes in Computer Science* 1327 (Berlin: Springer, 1997): 583–588.

```
clf = Pipeline([
        ("kpca", KernelPCA(n_components=2)),
        ("log_reg", LogisticRegression())
    ])

param_grid = [{
        "kpca__gamma": np.linspace(0.03, 0.05, 10),
        "kpca__kernel": ["rbf", "sigmoid"]
    }]

grid_search = GridSearchCV(clf, param_grid, cv=3)
grid_search.fit(X, y)
```

The best kernel and hyperparameters are then available through the `best_params_` variable:

```
>>> print(grid_search.best_params_)
{'kpca__gamma': 0.043333333333333335, 'kpca__kernel': 'rbf'}
```

Another approach, this time entirely unsupervised, is to select the kernel and hyperparameters that yield the lowest reconstruction error. Note that reconstruction is not as easy as with linear PCA. Here's why. Figure 8-11 shows the original Swiss roll 3D dataset (top left) and the resulting 2D dataset after kPCA is applied using an RBF kernel (top right). Thanks to the kernel trick, this transformation is mathematically equivalent to using the *feature map* φ to map the training set to an infinite-dimensional feature space (bottom right), then projecting the transformed training set down to 2D using linear PCA.

Notice that if we could invert the linear PCA step for a given instance in the reduced space, the reconstructed point would lie in feature space, not in the original space (e.g., like the one represented by an X in the diagram). Since the feature space is infinite-dimensional, we cannot compute the reconstructed point, and therefore we cannot compute the true reconstruction error. Fortunately, it is possible to find a point in the original space that would map close to the reconstructed point. This point is called the reconstruction *pre-image*. Once you have this pre-image, you can measure its squared distance to the original instance. You can then select the kernel and hyperparameters that minimize this reconstruction pre-image error.

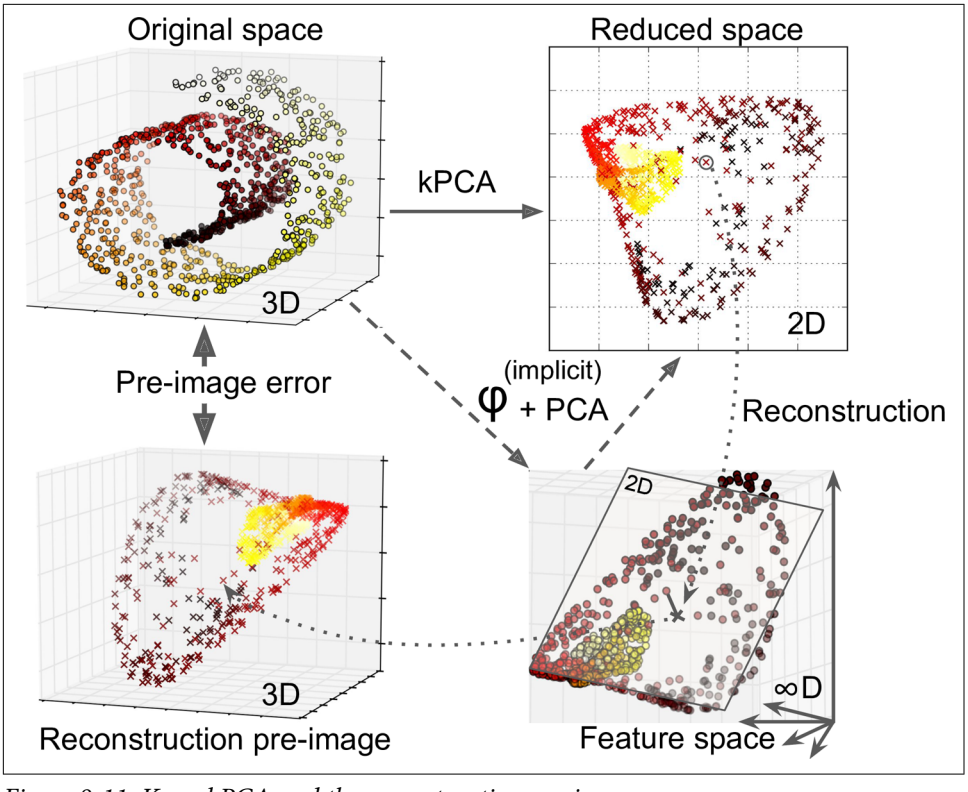


Figure 8-11. Kernel PCA and the reconstruction pre-image error

You may be wondering how to perform this reconstruction. One solution is to train a supervised regression model, with the projected instances as the training set and the original instances as the targets. Scikit-Learn will do this automatically if you set `fit_inverse_transform=True`, as shown in the following code:[7]

```
rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.0433,
                    fit_inverse_transform=True)
X_reduced = rbf_pca.fit_transform(X)
X_preimage = rbf_pca.inverse_transform(X_reduced)
```

By default, `fit_inverse_transform=False` and `KernelPCA` has no `inverse_transform()` method. This method only gets created when you set `fit_inverse_transform=True`.

7 If you set `fit_inverse_transform=True`, Scikit-Learn will use the algorithm (based on Kernel Ridge Regression) described in Gokhan H. Bakır et al., "Learning to Find Pre-Images", *Proceedings of the 16th International Conference on Neural Information Processing Systems* (2004): 449–456.

You can then compute the reconstruction pre-image error:

```
>>> from sklearn.metrics import mean_squared_error
>>> mean_squared_error(X, X_preimage)
32.786308795766132
```

Now you can use grid search with cross-validation to find the kernel and hyperparameters that minimize this error.

LLE

Locally Linear Embedding (LLE)[8] is another powerful *nonlinear dimensionality reduction* (NLDR) technique. It is a Manifold Learning technique that does not rely on projections, like the previous algorithms do. In a nutshell, LLE works by first measuring how each training instance linearly relates to its closest neighbors (c.n.), and then looking for a low-dimensional representation of the training set where these local relationships are best preserved (more details shortly). This approach makes it particularly good at unrolling twisted manifolds, especially when there is not too much noise.

The following code uses Scikit-Learn's `LocallyLinearEmbedding` class to unroll the Swiss roll:

```
from sklearn.manifold import LocallyLinearEmbedding

lle = LocallyLinearEmbedding(n_components=2, n_neighbors=10)
X_reduced = lle.fit_transform(X)
```

The resulting 2D dataset is shown in Figure 8-12. As you can see, the Swiss roll is completely unrolled, and the distances between instances are locally well preserved. However, distances are not preserved on a larger scale: the left part of the unrolled Swiss roll is stretched, while the right part is squeezed. Nevertheless, LLE did a pretty good job at modeling the manifold.

8 Sam T. Roweis and Lawrence K. Saul, "Nonlinear Dimensionality Reduction by Locally Linear Embedding," *Science* 290, no. 5500 (2000): 2323–2326.

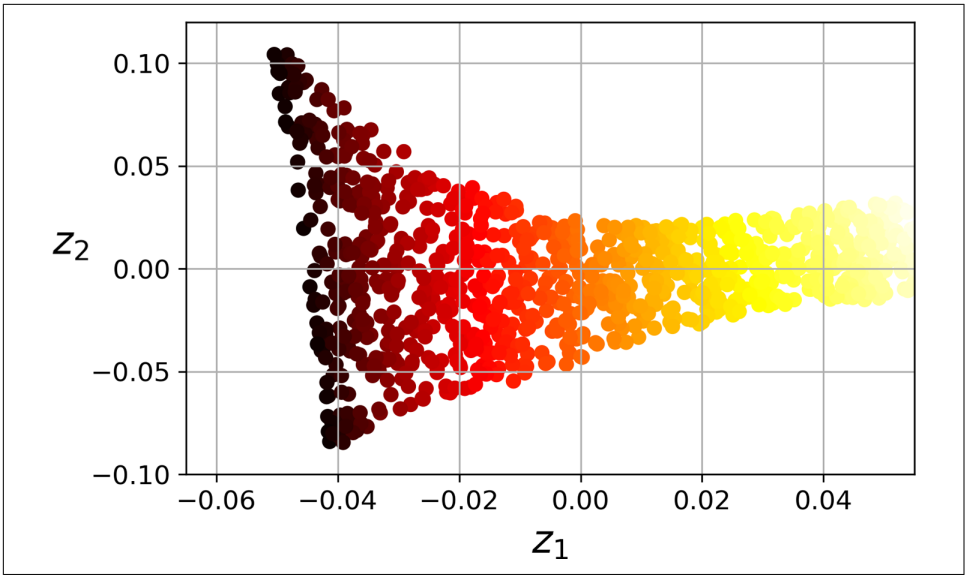


Figure 8-12. Unrolled Swiss roll using LLE

Here's how LLE works: for each training instance $\mathbf{x}^{(i)}$, the algorithm identifies its k closest neighbors (in the preceding code $k = 10$), then tries to reconstruct $\mathbf{x}^{(i)}$ as a linear function of these neighbors. More specifically, it finds the weights $w_{i,j}$ such that the squared distance between $\mathbf{x}^{(i)}$ and $\sum_{j=1}^{m} w_{i,j}\mathbf{x}^{(j)}$ is as small as possible, assuming $w_{i,j} = 0$ if $\mathbf{x}^{(j)}$ is not one of the k closest neighbors of $\mathbf{x}^{(i)}$. Thus the first step of LLE is the constrained optimization problem described in Equation 8-4, where $\mathbf{W}$ is the weight matrix containing all the weights $w_{i,j}$. The second constraint simply normalizes the weights for each training instance $\mathbf{x}^{(i)}$.

Equation 8-4. LLE step one: linearly modeling local relationships

$$\widehat{\mathbf{W}} = \underset{\mathbf{W}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{x}^{(i)} - \sum_{j=1}^{m} w_{i,j}\mathbf{x}^{(j)} \right)^2$$

$$\text{subject to} \begin{cases} w_{i,j} = 0 & \text{if } \mathbf{x}^{(j)} \text{ is not one of the } k \text{ c.n. of } \mathbf{x}^{(i)} \\ \sum_{j=1}^{m} w_{i,j} = 1 & \text{for } i = 1, 2, \cdots, m \end{cases}$$

After this step, the weight matrix $\widehat{\mathbf{W}}$ (containing the weights $\widehat{w}_{i,j}$) encodes the local linear relationships between the training instances. The second step is to map the training instances into a d-dimensional space (where $d < n$) while preserving these local relationships as much as possible. If $\mathbf{z}^{(i)}$ is the image of $\mathbf{x}^{(i)}$ in this d-dimensional

space, then we want the squared distance between $\mathbf{z}^{(i)}$ and $\sum_{j=1}^{m} \widehat{w}_{i,j}\mathbf{z}^{(j)}$ to be as small as possible. This idea leads to the unconstrained optimization problem described in Equation 8-5. It looks very similar to the first step, but instead of keeping the instances fixed and finding the optimal weights, we are doing the reverse: keeping the weights fixed and finding the optimal position of the instances' images in the low-dimensional space. Note that $\mathbf{Z}$ is the matrix containing all $\mathbf{z}^{(i)}$.

Equation 8-5. LLE step two: reducing dimensionality while preserving relationships

$$\widehat{\mathbf{Z}} = \underset{\mathbf{Z}}{\operatorname{argmin}} \sum_{i=1}^{m} \left(\mathbf{z}^{(i)} - \sum_{j=1}^{m} \widehat{w}_{i,j}\mathbf{z}^{(j)} \right)^2$$

Scikit-Learn's LLE implementation has the following computational complexity: $O(m \log(m)n \log(k))$ for finding the k nearest neighbors, $O(mnk^3)$ for optimizing the weights, and $O(dm^2)$ for constructing the low-dimensional representations. Unfortunately, the m^2 in the last term makes this algorithm scale poorly to very large datasets.

Other Dimensionality Reduction Techniques

There are many other dimensionality reduction techniques, several of which are available in Scikit-Learn. Here are some of the most popular ones:

Random Projections
: As its name suggests, projects the data to a lower-dimensional space using a random linear projection. This may sound crazy, but it turns out that such a random projection is actually very likely to preserve distances well, as was demonstrated mathematically by William B. Johnson and Joram Lindenstrauss in a famous lemma. The quality of the dimensionality reduction depends on the number of instances and the target dimensionality, but surprisingly not on the initial dimensionality. Check out the documentation for the `sklearn.random_projection` package for more details.

Multidimensional Scaling (MDS)
: Reduces dimensionality while trying to preserve the distances between the instances.

Isomap
: Creates a graph by connecting each instance to its nearest neighbors, then reduces dimensionality while trying to preserve the *geodesic distances*[9] between the instances.

t-Distributed Stochastic Neighbor Embedding (t-SNE)
: Reduces dimensionality while trying to keep similar instances close and dissimilar instances apart. It is mostly used for visualization, in particular to visualize clusters of instances in high-dimensional space (e.g., to visualize the MNIST images in 2D).

Linear Discriminant Analysis (LDA)
: Is a classification algorithm, but during training it learns the most discriminative axes between the classes, and these axes can then be used to define a hyperplane onto which to project the data. The benefit of this approach is that the projection will keep classes as far apart as possible, so LDA is a good technique to reduce dimensionality before running another classification algorithm such as an SVM classifier.

Figure 8-13 shows the results of a few of these techniques.

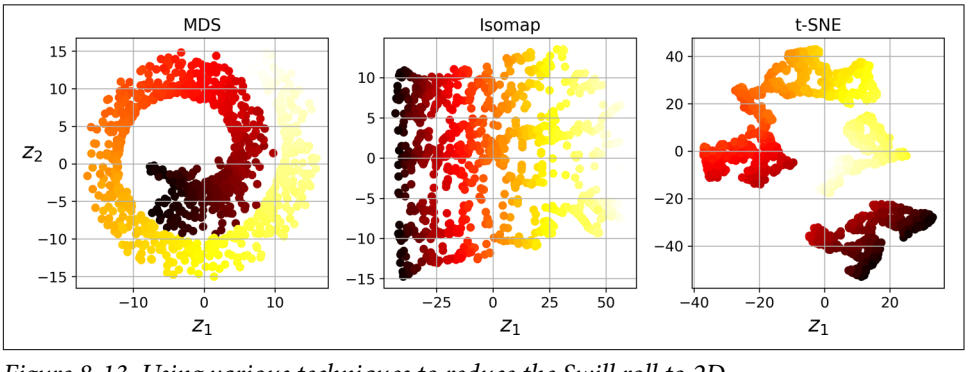


Figure 8-13. Using various techniques to reduce the Swill roll to 2D

Exercises

1. What are the main motivations for reducing a dataset's dimensionality? What are the main drawbacks?
2. What is the curse of dimensionality?

9 The geodesic distance between two nodes in a graph is the number of nodes on the shortest path between these nodes.

3. Once a dataset's dimensionality has been reduced, is it possible to reverse the operation? If so, how? If not, why?
4. Can PCA be used to reduce the dimensionality of a highly nonlinear dataset?
5. Suppose you perform PCA on a 1,000-dimensional dataset, setting the explained variance ratio to 95%. How many dimensions will the resulting dataset have?
6. In what cases would you use vanilla PCA, Incremental PCA, Randomized PCA, or Kernel PCA?
7. How can you evaluate the performance of a dimensionality reduction algorithm on your dataset?
8. Does it make any sense to chain two different dimensionality reduction algorithms?
9. Load the MNIST dataset (introduced in Chapter 3) and split it into a training set and a test set (take the first 60,000 instances for training, and the remaining 10,000 for testing). Train a Random Forest classifier on the dataset and time how long it takes, then evaluate the resulting model on the test set. Next, use PCA to reduce the dataset's dimensionality, with an explained variance ratio of 95%. Train a new Random Forest classifier on the reduced dataset and see how long it takes. Was training much faster? Next, evaluate the classifier on the test set. How does it compare to the previous classifier?
10. Use t-SNE to reduce the MNIST dataset down to two dimensions and plot the result using Matplotlib. You can use a scatterplot using 10 different colors to represent each image's target class. Alternatively, you can replace each dot in the scatterplot with the corresponding instance's class (a digit from 0 to 9), or even plot scaled-down versions of the digit images themselves (if you plot all digits, the visualization will be too cluttered, so you should either draw a random sample or plot an instance only if no other instance has already been plotted at a close distance). You should get a nice visualization with well-separated clusters of digits. Try using other dimensionality reduction algorithms such as PCA, LLE, or MDS and compare the resulting visualizations.

Solutions to these exercises are available in Appendix A.

CHAPTER 9
Unsupervised Learning Techniques

Although most of the applications of Machine Learning today are based on supervised learning (and as a result, this is where most of the investments go to), the vast majority of the available data is unlabeled: we have the input features **X**, but we do not have the labels **y**. The computer scientist Yann LeCun famously said that "if intelligence was a cake, unsupervised learning would be the cake, supervised learning would be the icing on the cake, and reinforcement learning would be the cherry on the cake." In other words, there is a huge potential in unsupervised learning that we have only barely started to sink our teeth into.

Say you want to create a system that will take a few pictures of each item on a manufacturing production line and detect which items are defective. You can fairly easily create a system that will take pictures automatically, and this might give you thousands of pictures every day. You can then build a reasonably large dataset in just a few weeks. But wait, there are no labels! If you want to train a regular binary classifier that will predict whether an item is defective or not, you will need to label every single picture as "defective" or "normal." This will generally require human experts to sit down and manually go through all the pictures. This is a long, costly, and tedious task, so it will usually only be done on a small subset of the available pictures. As a result, the labeled dataset will be quite small, and the classifier's performance will be disappointing. Moreover, every time the company makes any change to its products, the whole process will need to be started over from scratch. Wouldn't it be great if the algorithm could just exploit the unlabeled data without needing humans to label every picture? Enter unsupervised learning.

In Chapter 8 we looked at the most common unsupervised learning task: dimensionality reduction. In this chapter we will look at a few more unsupervised learning tasks and algorithms:

Clustering
: The goal is to group similar instances together into *clusters*. Clustering is a great tool for data analysis, customer segmentation, recommender systems, search engines, image segmentation, semi-supervised learning, dimensionality reduction, and more.

Anomaly detection
: The objective is to learn what "normal" data looks like, and then use that to detect abnormal instances, such as defective items on a production line or a new trend in a time series.

Density estimation
: This is the task of estimating the *probability density function* (PDF) of the random process that generated the dataset. Density estimation is commonly used for anomaly detection: instances located in very low-density regions are likely to be anomalies. It is also useful for data analysis and visualization.

Ready for some cake? We will start with clustering, using K-Means and DBSCAN, and then we will discuss Gaussian mixture models and see how they can be used for density estimation, clustering, and anomaly detection.

Clustering

As you enjoy a hike in the mountains, you stumble upon a plant you have never seen before. You look around and you notice a few more. They are not identical, yet they are sufficiently similar for you to know that they most likely belong to the same species (or at least the same genus). You may need a botanist to tell you what species that is, but you certainly don't need an expert to identify groups of similar-looking objects. This is called *clustering*: it is the task of identifying similar instances and assigning them to *clusters*, or groups of similar instances.

Just like in classification, each instance gets assigned to a group. However, unlike classification, clustering is an unsupervised task. Consider Figure 9-1: on the left is the iris dataset (introduced in Chapter 4), where each instance's species (i.e., its class) is represented with a different marker. It is a labeled dataset, for which classification algorithms such as Logistic Regression, SVMs, or Random Forest classifiers are well suited. On the right is the same dataset, but without the labels, so you cannot use a classification algorithm anymore. This is where clustering algorithms step in: many of them can easily detect the lower-left cluster. It is also quite easy to see with our own eyes, but it is not so obvious that the upper-right cluster is composed of two distinct sub-clusters. That said, the dataset has two additional features (sepal length and width), not represented here, and clustering algorithms can make good use of all features, so in fact they identify the three clusters fairly well (e.g., using a Gaussian mixture model, only 5 instances out of 150 are assigned to the wrong cluster).

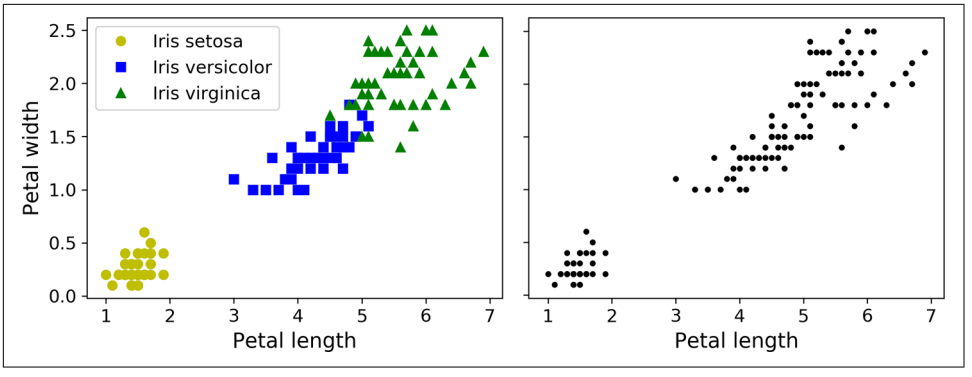


Figure 9-1. Classification (left) versus clustering (right)

Clustering is used in a wide variety of applications, including these:

For customer segmentation
: You can cluster your customers based on their purchases and their activity on your website. This is useful to understand who your customers are and what they need, so you can adapt your products and marketing campaigns to each segment. For example, customer segmentation can be useful in *recommender systems* to suggest content that other users in the same cluster enjoyed.

For data analysis
: When you analyze a new dataset, it can be helpful to run a clustering algorithm, and then analyze each cluster separately.

As a dimensionality reduction technique
: Once a dataset has been clustered, it is usually possible to measure each instance's *affinity* with each cluster (affinity is any measure of how well an instance fits into a cluster). Each instance's feature vector $\mathbf{x}$ can then be replaced with the vector of its cluster affinities. If there are k clusters, then this vector is k-dimensional. This vector is typically much lower-dimensional than the original feature vector, but it can preserve enough information for further processing.

For anomaly detection (also called outlier detection)
: Any instance that has a low affinity to all the clusters is likely to be an anomaly. For example, if you have clustered the users of your website based on their behavior, you can detect users with unusual behavior, such as an unusual number of requests per second. Anomaly detection is particularly useful in detecting defects in manufacturing, or for *fraud detection*.

For semi-supervised learning
: If you only have a few labels, you could perform clustering and propagate the labels to all the instances in the same cluster. This technique can greatly increase

the number of labels available for a subsequent supervised learning algorithm, and thus improve its performance.

For search engines
: Some search engines let you search for images that are similar to a reference image. To build such a system, you would first apply a clustering algorithm to all the images in your database; similar images would end up in the same cluster. Then when a user provides a reference image, all you need to do is use the trained clustering model to find this image's cluster, and you can then simply return all the images from this cluster.

To segment an image
: By clustering pixels according to their color, then replacing each pixel's color with the mean color of its cluster, it is possible to considerably reduce the number of different colors in the image. Image segmentation is used in many object detection and tracking systems, as it makes it easier to detect the contour of each object.

There is no universal definition of what a cluster is: it really depends on the context, and different algorithms will capture different kinds of clusters. Some algorithms look for instances centered around a particular point, called a *centroid*. Others look for continuous regions of densely packed instances: these clusters can take on any shape. Some algorithms are hierarchical, looking for clusters of clusters. And the list goes on.

In this section, we will look at two popular clustering algorithms, K-Means and DBSCAN, and explore some of their applications, such as nonlinear dimensionality reduction, semi-supervised learning, and anomaly detection.

K-Means

Consider the unlabeled dataset represented in Figure 9-2: you can clearly see five blobs of instances. The K-Means algorithm is a simple algorithm capable of clustering this kind of dataset very quickly and efficiently, often in just a few iterations. It was proposed by Stuart Lloyd at Bell Labs in 1957 as a technique for pulse-code modulation, but it was only published outside of the company in 1982.[1] In 1965, Edward W. Forgy had published virtually the same algorithm, so K-Means is sometimes referred to as Lloyd–Forgy.

1 Stuart P. Lloyd, "Least Squares Quantization in PCM," *IEEE Transactions on Information Theory* 28, no. 2 (1982): 129–137.

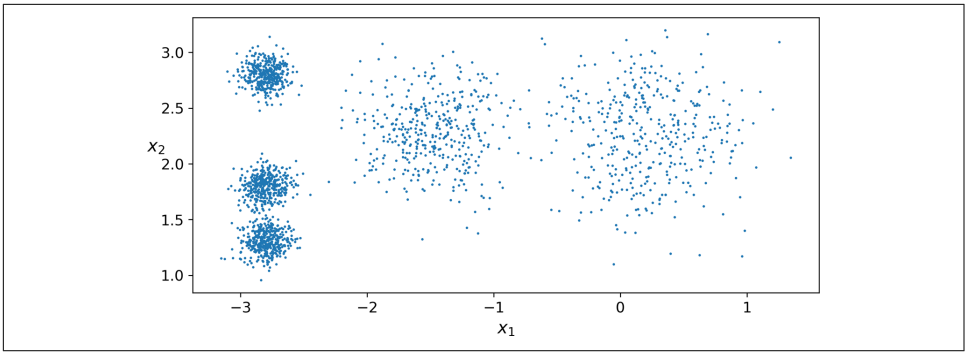


Figure 9-2. An unlabeled dataset composed of five blobs of instances

Let's train a K-Means clusterer on this dataset. It will try to find each blob's center and assign each instance to the closest blob:

```
from sklearn.cluster import KMeans
k = 5
kmeans = KMeans(n_clusters=k)
y_pred = kmeans.fit_predict(X)
```

Note that you have to specify the number of clusters k that the algorithm must find. In this example, it is pretty obvious from looking at the data that k should be set to 5, but in general it is not that easy. We will discuss this shortly.

Each instance was assigned to one of the five clusters. In the context of clustering, an instance's *label* is the index of the cluster that this instance gets assigned to by the algorithm: this is not to be confused with the class labels in classification (remember that clustering is an unsupervised learning task). The `KMeans` instance preserves a copy of the labels of the instances it was trained on, available via the `labels_` instance variable:

```
>>> y_pred
array([4, 0, 1, ..., 2, 1, 0], dtype=int32)
>>> y_pred is kmeans.labels_
True
```

We can also take a look at the five centroids that the algorithm found:

```
>>> kmeans.cluster_centers_
array([[-2.80389616,  1.80117999],
       [ 0.20876306,  2.25551336],
       [-2.79290307,  2.79641063],
       [-1.46679593,  2.28585348],
       [-2.80037642,  1.30082566]])
```

You can easily assign new instances to the cluster whose centroid is closest:

```
>>> X_new = np.array([[0, 2], [3, 2], [-3, 3], [-3, 2.5]])
>>> kmeans.predict(X_new)
array([1, 1, 2, 2], dtype=int32)
```

If you plot the cluster's decision boundaries, you get a Voronoi tessellation (see Figure 9-3, where each centroid is represented with an X).

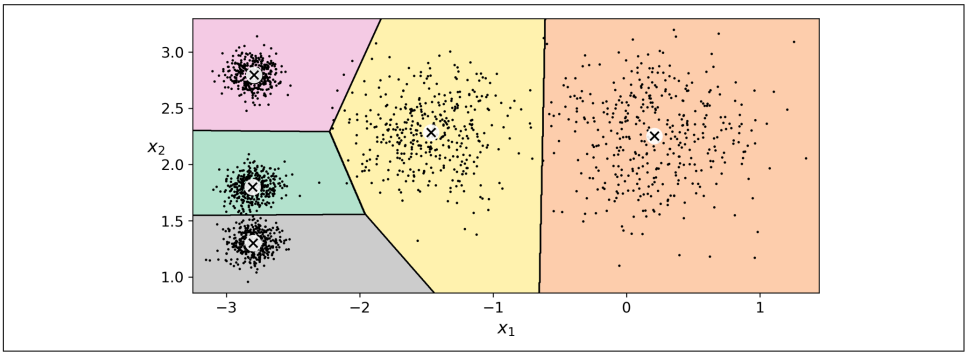


Figure 9-3. K-Means decision boundaries (Voronoi tessellation)

The vast majority of the instances were clearly assigned to the appropriate cluster, but a few instances were probably mislabeled (especially near the boundary between the top-left cluster and the central cluster). Indeed, the K-Means algorithm does not behave very well when the blobs have very different diameters because all it cares about when assigning an instance to a cluster is the distance to the centroid.

Instead of assigning each instance to a single cluster, which is called *hard clustering*, it can be useful to give each instance a score per cluster, which is called *soft clustering*. The score can be the distance between the instance and the centroid; conversely, it can be a similarity score (or affinity), such as the Gaussian Radial Basis Function (introduced in Chapter 5). In the `KMeans` class, the `transform()` method measures the distance from each instance to every centroid:

```
>>> kmeans.transform(X_new)
array([[2.81093633, 0.32995317, 2.9042344 , 1.49439034, 2.88633901],
       [5.80730058, 2.80290755, 5.84739223, 4.4759332 , 5.84236351],
       [1.21475352, 3.29399768, 0.29040966, 1.69136631, 1.71086031],
       [0.72581411, 3.21806371, 0.36159148, 1.54808703, 1.21567622]])
```

In this example, the first instance in `X_new` is located at a distance of 2.81 from the first centroid, 0.33 from the second centroid, 2.90 from the third centroid, 1.49 from the fourth centroid, and 2.89 from the fifth centroid. If you have a high-dimensional dataset and you transform it this way, you end up with a k-dimensional dataset: this transformation can be a very efficient nonlinear dimensionality reduction technique.

The K-Means algorithm

So, how does the algorithm work? Well, suppose you were given the centroids. You could easily label all the instances in the dataset by assigning each of them to the cluster whose centroid is closest. Conversely, if you were given all the instance labels, you could easily locate all the centroids by computing the mean of the instances for each cluster. But you are given neither the labels nor the centroids, so how can you proceed? Well, just start by placing the centroids randomly (e.g., by picking *k* instances at random and using their locations as centroids). Then label the instances, update the centroids, label the instances, update the centroids, and so on until the centroids stop moving. The algorithm is guaranteed to converge in a finite number of steps (usually quite small); it will not oscillate forever.[2]

You can see the algorithm in action in Figure 9-4: the centroids are initialized randomly (top left), then the instances are labeled (top right), then the centroids are updated (center left), the instances are relabeled (center right), and so on. As you can see, in just three iterations, the algorithm has reached a clustering that seems close to optimal.

The computational complexity of the algorithm is generally linear with regard to the number of instances *m*, the number of clusters *k*, and the number of dimensions *n*. However, this is only true when the data has a clustering structure. If it does not, then in the worst-case scenario the complexity can increase exponentially with the number of instances. In practice, this rarely happens, and K-Means is generally one of the fastest clustering algorithms.

2 That's because the mean squared distance between the instances and their closest centroid can only go down at each step.

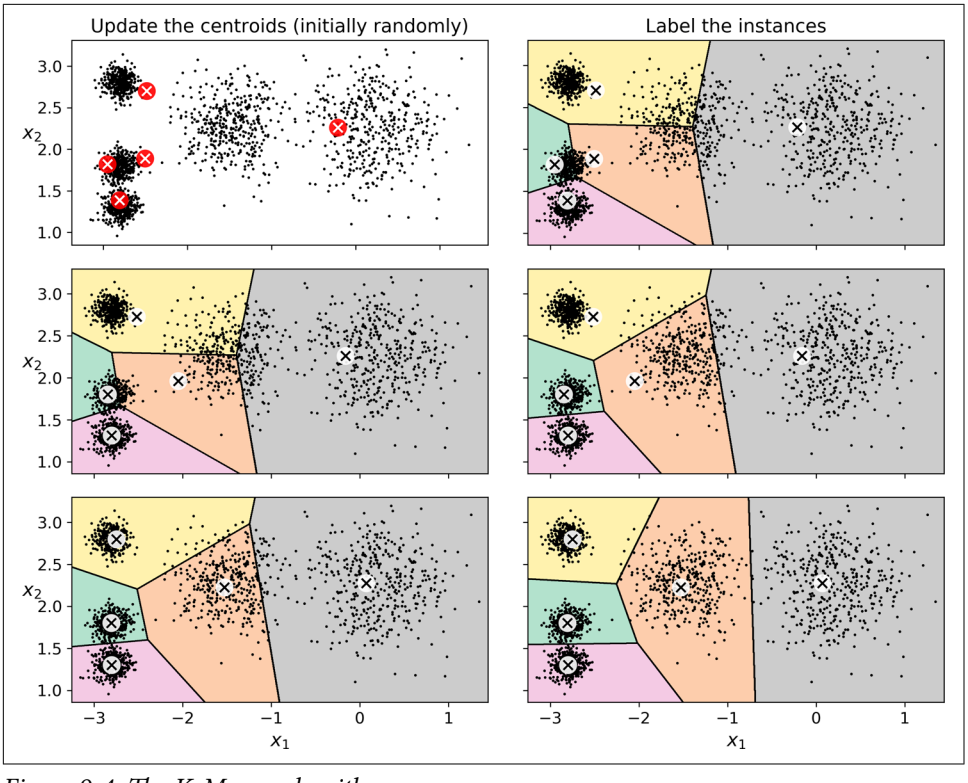


Figure 9-4. The K-Means algorithm

Although the algorithm is guaranteed to converge, it may not converge to the right solution (i.e., it may converge to a local optimum): whether it does or not depends on the centroid initialization. Figure 9-5 shows two suboptimal solutions that the algorithm can converge to if you are not lucky with the random initialization step.

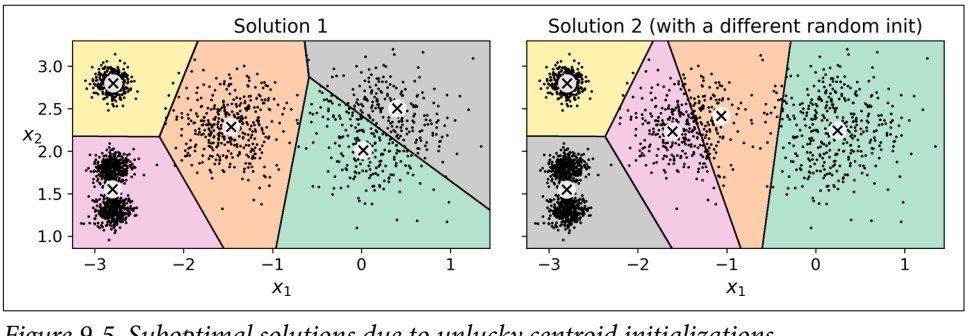


Figure 9-5. Suboptimal solutions due to unlucky centroid initializations

Let's look at a few ways you can mitigate this risk by improving the centroid initialization.

Centroid initialization methods

If you happen to know approximately where the centroids should be (e.g., if you ran another clustering algorithm earlier), then you can set the `init` hyperparameter to a NumPy array containing the list of centroids, and set `n_init` to `1`:

```
good_init = np.array([[-3, 3], [-3, 2], [-3, 1], [-1, 2], [0, 2]])
kmeans = KMeans(n_clusters=5, init=good_init, n_init=1)
```

Another solution is to run the algorithm multiple times with different random initializations and keep the best solution. The number of random initializations is controlled by the `n_init` hyperparameter: by default, it is equal to `10`, which means that the whole algorithm described earlier runs 10 times when you call `fit()`, and Scikit-Learn keeps the best solution. But how exactly does it know which solution is the best? It uses a performance metric! That metric is called the model's *inertia*, which is the mean squared distance between each instance and its closest centroid. It is roughly equal to 223.3 for the model on the left in Figure 9-5, 237.5 for the model on the right in Figure 9-5, and 211.6 for the model in Figure 9-3. The `KMeans` class runs the algorithm `n_init` times and keeps the model with the lowest inertia. In this example, the model in Figure 9-3 will be selected (unless we are very unlucky with `n_init` consecutive random initializations). If you are curious, a model's inertia is accessible via the `inertia_` instance variable:

```
>>> kmeans.inertia_
211.59853725816856
```

The `score()` method returns the negative inertia. Why negative? Because a predictor's `score()` method must always respect Scikit-Learn's "greater is better" rule: if a predictor is better than another, its `score()` method should return a greater score.

```
>>> kmeans.score(X)
-211.59853725816856
```

An important improvement to the K-Means algorithm, *K-Means++*, was proposed in a 2006 paper by David Arthur and Sergei Vassilvitskii.[3] They introduced a smarter initialization step that tends to select centroids that are distant from one another, and this improvement makes the K-Means algorithm much less likely to converge to a suboptimal solution. They showed that the additional computation required for the smarter initialization step is well worth it because it makes it possible to drastically reduce the number of times the algorithm needs to be run to find the optimal solution. Here is the K-Means++ initialization algorithm:

1. Take one centroid $\mathbf{c}^{(1)}$, chosen uniformly at random from the dataset.

3 David Arthur and Sergei Vassilvitskii, "k-Means++: The Advantages of Careful Seeding," *Proceedings of the 18th Annual ACM-SIAM Symposium on Discrete Algorithms* (2007): 1027–1035.

2. Take a new centroid $\mathbf{c}^{(i)}$, choosing an instance $\mathbf{x}^{(i)}$ with probability $D\left(\mathbf{x}^{(i)}\right)^2 / \sum_{j=1}^{m} D\left(\mathbf{x}^{(j)}\right)^2$, where $D(\mathbf{x}^{(i)})$ is the distance between the instance $\mathbf{x}^{(i)}$ and the closest centroid that was already chosen. This probability distribution ensures that instances farther away from already chosen centroids are much more likely be selected as centroids.
3. Repeat the previous step until all k centroids have been chosen.

The `KMeans` class uses this initialization method by default. If you want to force it to use the original method (i.e., picking k instances randomly to define the initial centroids), then you can set the `init` hyperparameter to `"random"`. You will rarely need to do this.

Accelerated K-Means and mini-batch K-Means

Another important improvement to the K-Means algorithm was proposed in a 2003 paper by Charles Elkan.[4] It considerably accelerates the algorithm by avoiding many unnecessary distance calculations. Elkan achieved this by exploiting the triangle inequality (i.e., that a straight line is always the shortest distance between two points[5]) and by keeping track of lower and upper bounds for distances between instances and centroids. This is the algorithm the `KMeans` class uses by default (you can force it to use the original algorithm by setting the `algorithm` hyperparameter to `"full"`, although you probably will never need to).

Yet another important variant of the K-Means algorithm was proposed in a 2010 paper by David Sculley.[6] Instead of using the full dataset at each iteration, the algorithm is capable of using mini-batches, moving the centroids just slightly at each iteration. This speeds up the algorithm typically by a factor of three or four and makes it possible to cluster huge datasets that do not fit in memory. Scikit-Learn implements this algorithm in the `MiniBatchKMeans` class. You can just use this class like the `KMeans` class:

```
from sklearn.cluster import MiniBatchKMeans

minibatch_kmeans = MiniBatchKMeans(n_clusters=5)
minibatch_kmeans.fit(X)
```

4 Charles Elkan, "Using the Triangle Inequality to Accelerate k-Means," *Proceedings of the 20th International Conference on Machine Learning* (2003): 147–153.

5 The triangle inequality is AC ≤ AB + BC where A, B and C are three points and AB, AC, and BC are the distances between these points.

6 David Sculley, "Web-Scale K-Means Clustering," *Proceedings of the 19th International Conference on World Wide Web* (2010): 1177–1178.

If the dataset does not fit in memory, the simplest option is to use the `memmap` class, as we did for incremental PCA in Chapter 8. Alternatively, you can pass one mini-batch at a time to the `partial_fit()` method, but this will require much more work, since you will need to perform multiple initializations and select the best one yourself (see the mini-batch K-Means section of the notebook for an example).

Although the Mini-batch K-Means algorithm is much faster than the regular K-Means algorithm, its inertia is generally slightly worse, especially as the number of clusters increases. You can see this in Figure 9-6: the plot on the left compares the inertias of Mini-batch K-Means and regular K-Means models trained on the previous dataset using various numbers of clusters *k*. The difference between the two curves remains fairly constant, but this difference becomes more and more significant as *k* increases, since the inertia becomes smaller and smaller. In the plot on the right, you can see that Mini-batch K-Means is much faster than regular K-Means, and this difference increases with *k*.

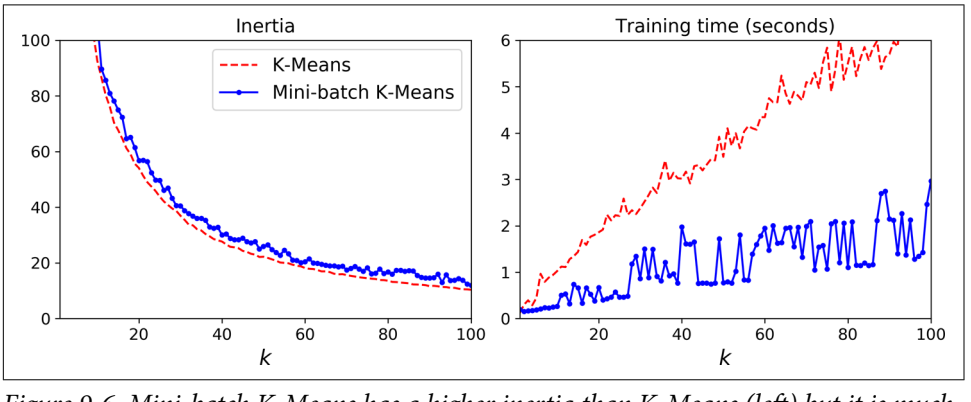


Figure 9-6. Mini-batch K-Means has a higher inertia than K-Means (left) but it is much faster (right), especially as k increases

Finding the optimal number of clusters

So far, we have set the number of clusters *k* to 5 because it was obvious by looking at the data that this was the correct number of clusters. But in general, it will not be so easy to know how to set *k*, and the result might be quite bad if you set it to the wrong value. As you can see in Figure 9-7, setting *k* to 3 or 8 results in fairly bad models.

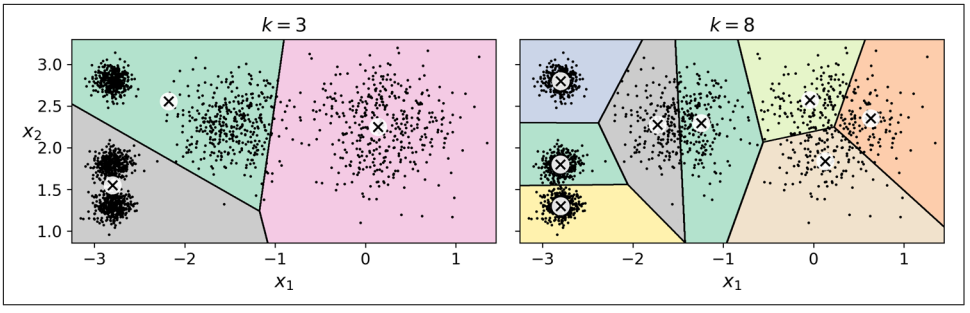


Figure 9-7. Bad choices for the number of clusters: when k is too small, separate clusters get merged (left), and when k is too large, some clusters get chopped into multiple pieces (right)

You might be thinking that we could just pick the model with the lowest inertia, right? Unfortunately, it is not that simple. The inertia for k=3 is 653.2, which is much higher than for k=5 (which was 211.6). But with k=8, the inertia is just 119.1. The inertia is not a good performance metric when trying to choose k because it keeps getting lower as we increase k. Indeed, the more clusters there are, the closer each instance will be to its closest centroid, and therefore the lower the inertia will be. Let's plot the inertia as a function of k (see Figure 9-8).

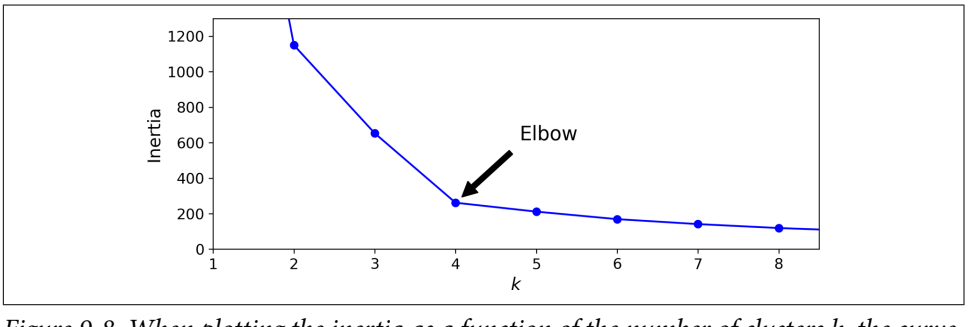


Figure 9-8. When plotting the inertia as a function of the number of clusters k, the curve often contains an inflexion point called the "elbow"

As you can see, the inertia drops very quickly as we increase k up to 4, but then it decreases much more slowly as we keep increasing k. This curve has roughly the shape of an arm, and there is an "elbow" at k = 4. So, if we did not know better, 4 would be a good choice: any lower value would be dramatic, while any higher value would not help much, and we might just be splitting perfectly good clusters in half for no good reason.

This technique for choosing the best value for the number of clusters is rather coarse. A more precise approach (but also more computationally expensive) is to use the *silhouette score*, which is the mean *silhouette coefficient* over all the instances. An

instance's silhouette coefficient is equal to $(b - a) / \max(a, b)$, where a is the mean distance to the other instances in the same cluster (i.e., the mean intra-cluster distance) and b is the mean nearest-cluster distance (i.e., the mean distance to the instances of the next closest cluster, defined as the one that minimizes b, excluding the instance's own cluster). The silhouette coefficient can vary between –1 and +1. A coefficient close to +1 means that the instance is well inside its own cluster and far from other clusters, while a coefficient close to 0 means that it is close to a cluster boundary, and finally a coefficient close to –1 means that the instance may have been assigned to the wrong cluster.

To compute the silhouette score, you can use Scikit-Learn's `silhouette_score()` function, giving it all the instances in the dataset and the labels they were assigned:

```
>>> from sklearn.metrics import silhouette_score
>>> silhouette_score(X, kmeans.labels_)
0.655517642572828
```

Let's compare the silhouette scores for different numbers of clusters (see Figure 9-9).

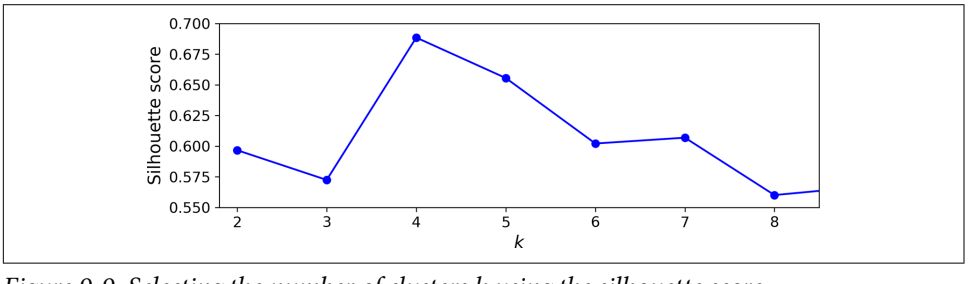


Figure 9-9. Selecting the number of clusters k using the silhouette score

As you can see, this visualization is much richer than the previous one: although it confirms that $k = 4$ is a very good choice, it also underlines the fact that $k = 5$ is quite good as well, and much better than $k = 6$ or 7. This was not visible when comparing inertias.

An even more informative visualization is obtained when you plot every instance's silhouette coefficient, sorted by the cluster they are assigned to and by the value of the coefficient. This is called a *silhouette diagram* (see Figure 9-10). Each diagram contains one knife shape per cluster. The shape's height indicates the number of instances the cluster contains, and its width represents the sorted silhouette coefficients of the instances in the cluster (wider is better). The dashed line indicates the mean silhouette coefficient.

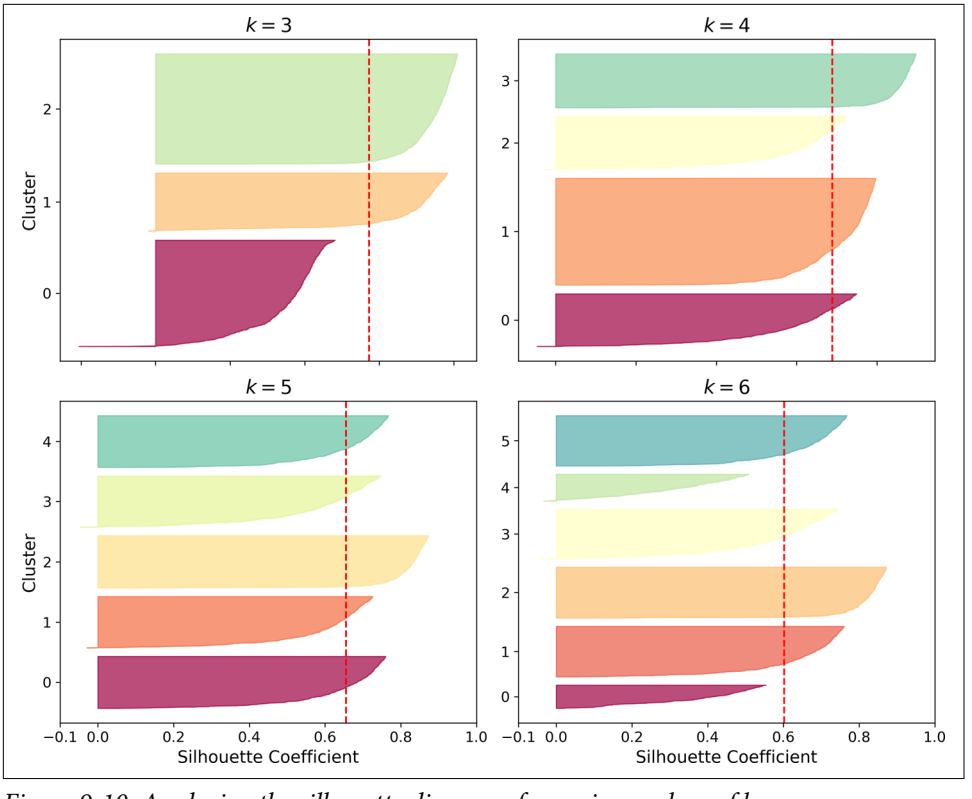


Figure 9-10. Analyzing the silhouette diagrams for various values of k

The vertical dashed lines represent the silhouette score for each number of clusters. When most of the instances in a cluster have a lower coefficient than this score (i.e., if many of the instances stop short of the dashed line, ending to the left of it), then the cluster is rather bad since this means its instances are much too close to other clusters. We can see that when $k = 3$ and when $k = 6$, we get bad clusters. But when $k = 4$ or $k = 5$, the clusters look pretty good: most instances extend beyond the dashed line, to the right and closer to 1.0. When $k = 4$, the cluster at index 1 (the third from the top) is rather big. When $k = 5$, all clusters have similar sizes. So, even though the overall silhouette score from $k = 4$ is slightly greater than for $k = 5$, it seems like a good idea to use $k = 5$ to get clusters of similar sizes.

Limits of K-Means

Despite its many merits, most notably being fast and scalable, K-Means is not perfect. As we saw, it is necessary to run the algorithm several times to avoid suboptimal solutions, plus you need to specify the number of clusters, which can be quite a hassle. Moreover, K-Means does not behave very well when the clusters have varying sizes,

different densities, or nonspherical shapes. For example, Figure 9-11 shows how K-Means clusters a dataset containing three ellipsoidal clusters of different dimensions, densities, and orientations.

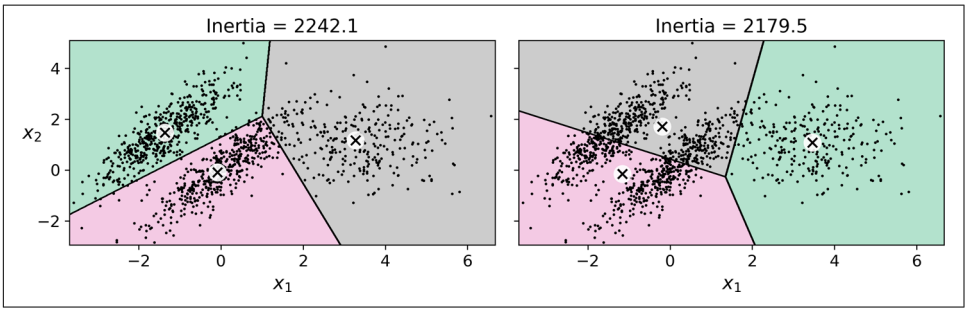


Figure 9-11. K-Means fails to cluster these ellipsoidal blobs properly

As you can see, neither of these solutions is any good. The solution on the left is better, but it still chops off 25% of the middle cluster and assigns it to the cluster on the right. The solution on the right is just terrible, even though its inertia is lower. So, depending on the data, different clustering algorithms may perform better. On these types of elliptical clusters, Gaussian mixture models work great.

It is important to scale the input features before you run K-Means, or the clusters may be very stretched and K-Means will perform poorly. Scaling the features does not guarantee that all the clusters will be nice and spherical, but it generally improves things.

Now let's look at a few ways we can benefit from clustering. We will use K-Means, but feel free to experiment with other clustering algorithms.

Using Clustering for Image Segmentation

Image segmentation is the task of partitioning an image into multiple segments. In *semantic segmentation*, all pixels that are part of the same object type get assigned to the same segment. For example, in a self-driving car's vision system, all pixels that are part of a pedestrian's image might be assigned to the "pedestrian" segment (there would be one segment containing all the pedestrians). In *instance segmentation*, all pixels that are part of the same individual object are assigned to the same segment. In this case there would be a different segment for each pedestrian. The state of the art in semantic or instance segmentation today is achieved using complex architectures based on convolutional neural networks (see Chapter 14). Here, we are going to do something much simpler: *color segmentation*. We will simply assign pixels to the same segment if they have a similar color. In some applications, this may be sufficient. For

example, if you want to analyze satellite images to measure how much total forest area there is in a region, color segmentation may be just fine.

First, use Matplotlib's `imread()` function to load the image (see the upper-left image in Figure 9-12):

```
>>> from matplotlib.image import imread  # or `from imageio import imread`
>>> image = imread(os.path.join("images","unsupervised_learning","ladybug.png"))
>>> image.shape
(533, 800, 3)
```

The image is represented as a 3D array. The first dimension's size is the height; the second is the width; and the third is the number of color channels, in this case red, green, and blue (RGB). In other words, for each pixel there is a 3D vector containing the intensities of red, green, and blue, each between 0.0 and 1.0 (or between 0 and 255, if you use `imageio.imread()`). Some images may have fewer channels, such as grayscale images (one channel). And some images may have more channels, such as images with an additional *alpha channel* for transparency or satellite images, which often contain channels for many light frequencies (e.g., infrared). The following code reshapes the array to get a long list of RGB colors, then it clusters these colors using K-Means:

```
X = image.reshape(-1, 3)
kmeans = KMeans(n_clusters=8).fit(X)
segmented_img = kmeans.cluster_centers_[kmeans.labels_]
segmented_img = segmented_img.reshape(image.shape)
```

For example, it may identify a color cluster for all shades of green. Next, for each color (e.g., dark green), it looks for the mean color of the pixel's color cluster. For example, all shades of green may be replaced with the same light green color (assuming the mean color of the green cluster is light green). Finally, it reshapes this long list of colors to get the same shape as the original image. And we're done!

This outputs the image shown in the upper right of Figure 9-12. You can experiment with various numbers of clusters, as shown in the figure. When you use fewer than eight clusters, notice that the ladybug's flashy red color fails to get a cluster of its own: it gets merged with colors from the environment. This is because K-Means prefers clusters of similar sizes. The ladybug is small—much smaller than the rest of the image—so even though its color is flashy, K-Means fails to dedicate a cluster to it.

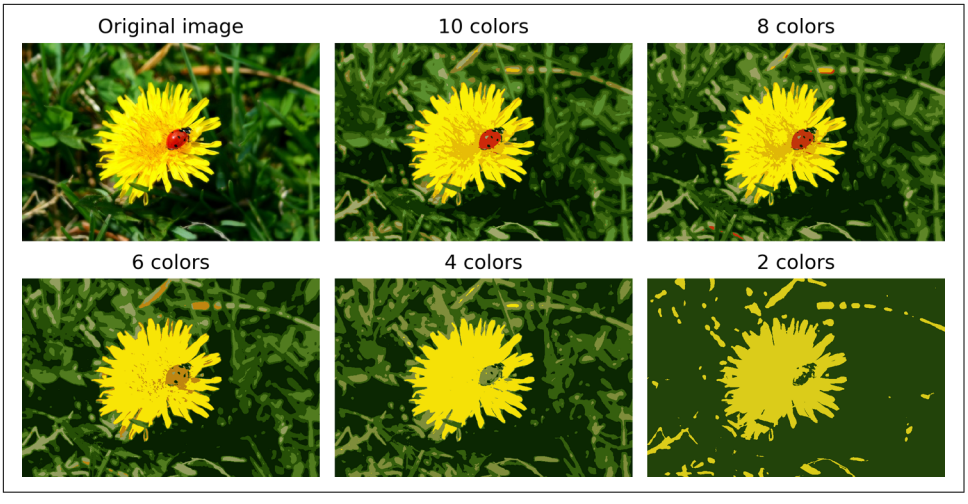


Figure 9-12. Image segmentation using K-Means with various numbers of color clusters

That wasn't too hard, was it? Now let's look at another application of clustering: preprocessing.

Using Clustering for Preprocessing

Clustering can be an efficient approach to dimensionality reduction, in particular as a preprocessing step before a supervised learning algorithm. As an example of using clustering for dimensionality reduction, let's tackle the digits dataset, which is a simple MNIST-like dataset containing 1,797 grayscale 8 × 8 images representing the digits 0 to 9. First, load the dataset:

```
from sklearn.datasets import load_digits

X_digits, y_digits = load_digits(return_X_y=True)
```

Now, split it into a training set and a test set:

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X_digits, y_digits)
```

Next, fit a Logistic Regression model:

```
from sklearn.linear_model import LogisticRegression

log_reg = LogisticRegression()
log_reg.fit(X_train, y_train)
```

Let's evaluate its accuracy on the test set:

```
>>> log_reg.score(X_test, y_test)
0.9688888888888889
```

OK, that's our baseline: 96.9% accuracy. Let's see if we can do better by using K-Means as a preprocessing step. We will create a pipeline that will first cluster the training set into 50 clusters and replace the images with their distances to these 50 clusters, then apply a Logistic Regression model:

```
from sklearn.pipeline import Pipeline

pipeline = Pipeline([
    ("kmeans", KMeans(n_clusters=50)),
    ("log_reg", LogisticRegression()),
])
pipeline.fit(X_train, y_train)
```

Since there are 10 different digits, it is tempting to set the number of clusters to 10. However, each digit can be written several different ways, so it is preferable to use a larger number of clusters, such as 50.

Now let's evaluate this classification pipeline:

```
>>> pipeline.score(X_test, y_test)
0.9777777777777777
```

How about that? We reduced the error rate by almost 30% (from about 3.1% to about 2.2%)!

But we chose the number of clusters k arbitrarily; we can surely do better. Since K-Means is just a preprocessing step in a classification pipeline, finding a good value for k is much simpler than earlier. There's no need to perform silhouette analysis or minimize the inertia; the best value of k is simply the one that results in the best classification performance during cross-validation. We can use `GridSearchCV` to find the optimal number of clusters:

```
from sklearn.model_selection import GridSearchCV

param_grid = dict(kmeans__n_clusters=range(2, 100))
grid_clf = GridSearchCV(pipeline, param_grid, cv=3, verbose=2)
grid_clf.fit(X_train, y_train)
```

Let's look at the best value for k and the performance of the resulting pipeline:

```
>>> grid_clf.best_params_
{'kmeans__n_clusters': 99}
>>> grid_clf.score(X_test, y_test)
0.9822222222222222
```

With $k = 99$ clusters, we get a significant accuracy boost, reaching 98.22% accuracy on the test set. Cool! You may want to keep exploring higher values for k, since 99 was the largest value in the range we explored.

Using Clustering for Semi-Supervised Learning

Another use case for clustering is in semi-supervised learning, when we have plenty of unlabeled instances and very few labeled instances. Let's train a Logistic Regression model on a sample of 50 labeled instances from the digits dataset:

```
n_labeled = 50
log_reg = LogisticRegression()
log_reg.fit(X_train[:n_labeled], y_train[:n_labeled])
```

What is the performance of this model on the test set?

```
>>> log_reg.score(X_test, y_test)
0.8333333333333334
```

The accuracy is just 83.3%. It should come as no surprise that this is much lower than earlier, when we trained the model on the full training set. Let's see how we can do better. First, let's cluster the training set into 50 clusters. Then for each cluster, let's find the image closest to the centroid. We will call these images the *representative images*:

```
k = 50
kmeans = KMeans(n_clusters=k)
X_digits_dist = kmeans.fit_transform(X_train)
representative_digit_idx = np.argmin(X_digits_dist, axis=0)
X_representative_digits = X_train[representative_digit_idx]
```

Figure 9-13 shows these 50 representative images.

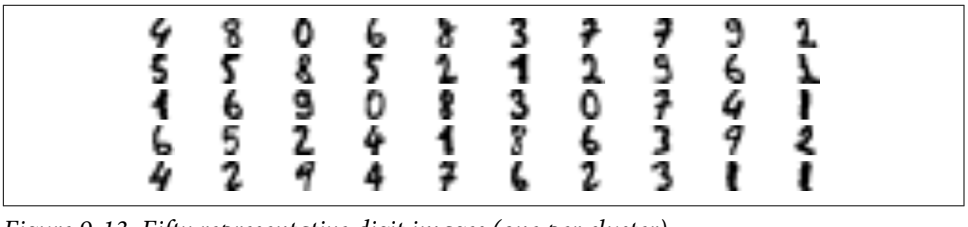


Figure 9-13. Fifty representative digit images (one per cluster)

Let's look at each image and manually label it:

```
y_representative_digits = np.array([4, 8, 0, 6, 8, 3, ..., 7, 6, 2, 3, 1, 1])
```

Now we have a dataset with just 50 labeled instances, but instead of being random instances, each of them is a representative image of its cluster. Let's see if the performance is any better:

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_representative_digits, y_representative_digits)
>>> log_reg.score(X_test, y_test)
0.9222222222222223
```

Wow! We jumped from 83.3% accuracy to 92.2%, although we are still only training the model on 50 instances. Since it is often costly and painful to label instances, especially when it has to be done manually by experts, it is a good idea to label representative instances rather than just random instances.

But perhaps we can go one step further: what if we propagated the labels to all the other instances in the same cluster? This is called *label propagation*:

```
y_train_propagated = np.empty(len(X_train), dtype=np.int32)
for i in range(k):
    y_train_propagated[kmeans.labels_==i] = y_representative_digits[i]
```

Now let's train the model again and look at its performance:

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_train, y_train_propagated)
>>> log_reg.score(X_test, y_test)
0.9333333333333333
```

We got a reasonable accuracy boost, but nothing absolutely astounding. The problem is that we propagated each representative instance's label to all the instances in the same cluster, including the instances located close to the cluster boundaries, which are more likely to be mislabeled. Let's see what happens if we only propagate the labels to the 20% of the instances that are closest to the centroids:

```
percentile_closest = 20

X_cluster_dist = X_digits_dist[np.arange(len(X_train)), kmeans.labels_]
for i in range(k):
    in_cluster = (kmeans.labels_ == i)
    cluster_dist = X_cluster_dist[in_cluster]
    cutoff_distance = np.percentile(cluster_dist, percentile_closest)
    above_cutoff = (X_cluster_dist > cutoff_distance)
    X_cluster_dist[in_cluster & above_cutoff] = -1

partially_propagated = (X_cluster_dist != -1)
X_train_partially_propagated = X_train[partially_propagated]
y_train_partially_propagated = y_train_propagated[partially_propagated]
```

Now let's train the model again on this partially propagated dataset:

```
>>> log_reg = LogisticRegression()
>>> log_reg.fit(X_train_partially_propagated, y_train_partially_propagated)
>>> log_reg.score(X_test, y_test)
0.94
```

Nice! With just 50 labeled instances (only 5 examples per class on average!), we got 94.0% accuracy, which is pretty close to the performance of Logistic Regression on the fully labeled digits dataset (which was 96.9%). This good performance is due to the fact that the propagated labels are actually pretty good—their accuracy is very close to 99%, as the following code shows:

```
>>> np.mean(y_train_partially_propagated == y_train[partially_propagated])
0.9896907216494846
```

Active Learning

To continue improving your model and your training set, the next step could be to do a few rounds of *active learning*, which is when a human expert interacts with the learning algorithm, providing labels for specific instances when the algorithm requests them. There are many different strategies for active learning, but one of the most common ones is called *uncertainty sampling*. Here is how it works:

1. The model is trained on the labeled instances gathered so far, and this model is used to make predictions on all the unlabeled instances.
2. The instances for which the model is most uncertain (i.e., when its estimated probability is lowest) are given to the expert to be labeled.
3. You iterate this process until the performance improvement stops being worth the labeling effort.

Other strategies include labeling the instances that would result in the largest model change, or the largest drop in the model's validation error, or the instances that different models disagree on (e.g., an SVM or a Random Forest).

Before we move on to Gaussian mixture models, let's take a look at DBSCAN, another popular clustering algorithm that illustrates a very different approach based on local density estimation. This approach allows the algorithm to identify clusters of arbitrary shapes.

DBSCAN

This algorithm defines clusters as continuous regions of high density. Here is how it works:

- For each instance, the algorithm counts how many instances are located within a small distance ε (epsilon) from it. This region is called the instance's *ε-neighborhood*.
- If an instance has at least `min_samples` instances in its ε-neighborhood (including itself), then it is considered a *core instance*. In other words, core instances are those that are located in dense regions.
- All instances in the neighborhood of a core instance belong to the same cluster. This neighborhood may include other core instances; therefore, a long sequence of neighboring core instances forms a single cluster.

- Any instance that is not a core instance and does not have one in its neighborhood is considered an anomaly.

This algorithm works well if all the clusters are dense enough and if they are well separated by low-density regions. The `DBSCAN` class in Scikit-Learn is as simple to use as you might expect. Let's test it on the moons dataset, introduced in Chapter 5:

```
from sklearn.cluster import DBSCAN
from sklearn.datasets import make_moons

X, y = make_moons(n_samples=1000, noise=0.05)
dbscan = DBSCAN(eps=0.05, min_samples=5)
dbscan.fit(X)
```

The labels of all the instances are now available in the `labels_` instance variable:

```
>>> dbscan.labels_
array([ 0,  2, -1, -1,  1,  0,  0,  0, ...,  3,  2,  3,  3,  4,  2,  6,  3])
```

Notice that some instances have a cluster index equal to –1, which means that they are considered as anomalies by the algorithm. The indices of the core instances are available in the `core_sample_indices_` instance variable, and the core instances themselves are available in the `components_` instance variable:

```
>>> len(dbscan.core_sample_indices_)
808
>>> dbscan.core_sample_indices_
array([ 0,  4,  5,  6,  7,  8, 10, 11, ..., 992, 993, 995, 997, 998, 999])
>>> dbscan.components_
array([[-0.02137124,  0.40618608],
       [-0.84192557,  0.53058695],
                  ...
       [-0.94355873,  0.3278936 ],
       [ 0.79419406,  0.60777171]])
```

This clustering is represented in the lefthand plot of Figure 9-14. As you can see, it identified quite a lot of anomalies, plus seven different clusters. How disappointing! Fortunately, if we widen each instance's neighborhood by increasing `eps` to 0.2, we get the clustering on the right, which looks perfect. Let's continue with this model.

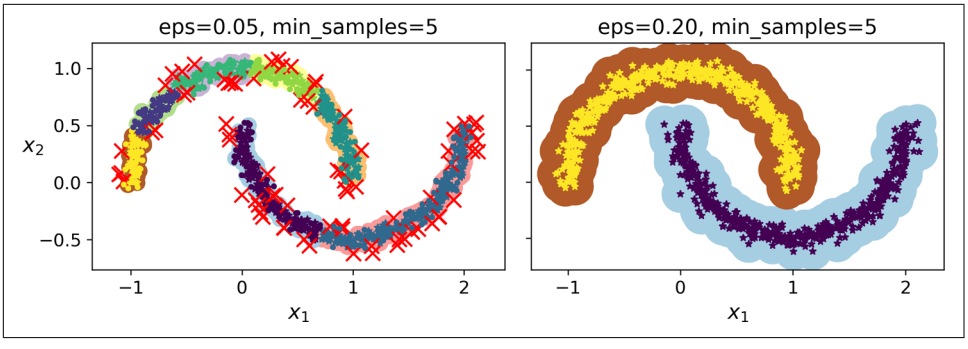


Figure 9-14. DBSCAN clustering using two different neighborhood radiuses

Somewhat surprisingly, the `DBSCAN` class does not have a `predict()` method, although it has a `fit_predict()` method. In other words, it cannot predict which cluster a new instance belongs to. This implementation decision was made because different classification algorithms can be better for different tasks, so the authors decided to let the user choose which one to use. Moreover, it's not hard to implement. For example, let's train a `KNeighborsClassifier`:

```
from sklearn.neighbors import KNeighborsClassifier

knn = KNeighborsClassifier(n_neighbors=50)
knn.fit(dbscan.components_, dbscan.labels_[dbscan.core_sample_indices_])
```

Now, given a few new instances, we can predict which cluster they most likely belong to and even estimate a probability for each cluster:

```
>>> X_new = np.array([[-0.5, 0], [0, 0.5], [1, -0.1], [2, 1]])
>>> knn.predict(X_new)
array([1, 0, 1, 0])
>>> knn.predict_proba(X_new)
array([[0.18, 0.82],
       [1.  , 0.  ],
       [0.12, 0.88],
       [1.  , 0.  ]])
```

Note that we only trained the classifier on the core instances, but we could also have chosen to train it on all the instances, or all but the anomalies: this choice depends on the final task.

The decision boundary is represented in Figure 9-15 (the crosses represent the four instances in `X_new`). Notice that since there is no anomaly in the training set, the classifier always chooses a cluster, even when that cluster is far away. It is fairly straightforward to introduce a maximum distance, in which case the two instances that are far away from both clusters are classified as anomalies. To do this, use the `kneighbors()` method of the `KNeighborsClassifier`. Given a set of instances, it returns the

distances and the indices of the k nearest neighbors in the training set (two matrices, each with k columns):

```
>>> y_dist, y_pred_idx = knn.kneighbors(X_new, n_neighbors=1)
>>> y_pred = dbscan.labels_[dbscan.core_sample_indices_][y_pred_idx]
>>> y_pred[y_dist > 0.2] = -1
>>> y_pred.ravel()
array([-1,  0,  1, -1])
```

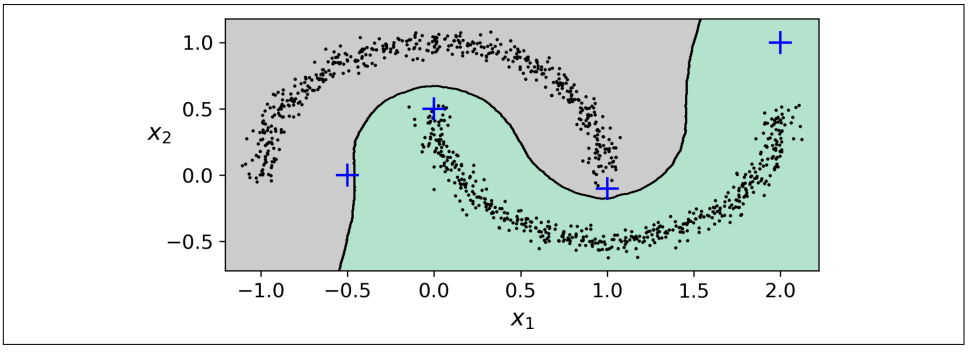


Figure 9-15. Decision boundary between two clusters

In short, DBSCAN is a very simple yet powerful algorithm capable of identifying any number of clusters of any shape. It is robust to outliers, and it has just two hyperparameters (`eps` and `min_samples`). If the density varies significantly across the clusters, however, it can be impossible for it to capture all the clusters properly. Its computational complexity is roughly $O(m \log m)$, making it pretty close to linear with regard to the number of instances, but Scikit-Learn's implementation can require up to $O(m^2)$ memory if `eps` is large.

You may also want to try *Hierarchical DBSCAN* (HDBSCAN), which is implemented in the scikit-learn-contrib project.

Other Clustering Algorithms

Scikit-Learn implements several more clustering algorithms that you should take a look at. We cannot cover them all in detail here, but here is a brief overview:

Agglomerative clustering
: A hierarchy of clusters is built from the bottom up. Think of many tiny bubbles floating on water and gradually attaching to each other until there's one big group of bubbles. Similarly, at each iteration, agglomerative clustering connects the nearest pair of clusters (starting with individual instances). If you drew a tree

with a branch for every pair of clusters that merged, you would get a binary tree of clusters, where the leaves are the individual instances. This approach scales very well to large numbers of instances or clusters. It can capture clusters of various shapes, it produces a flexible and informative cluster tree instead of forcing you to choose a particular cluster scale, and it can be used with any pairwise distance. It can scale nicely to large numbers of instances if you provide a connectivity matrix, which is a sparse $m \times m$ matrix that indicates which pairs of instances are neighbors (e.g., returned by `sklearn.neighbors.kneighbors_graph()`). Without a connectivity matrix, the algorithm does not scale well to large datasets.

BIRCH
: The BIRCH (Balanced Iterative Reducing and Clustering using Hierarchies) algorithm was designed specifically for very large datasets, and it can be faster than batch K-Means, with similar results, as long as the number of features is not too large (<20). During training, it builds a tree structure containing just enough information to quickly assign each new instance to a cluster, without having to store all the instances in the tree: this approach allows it to use limited memory, while handling huge datasets.

Mean-Shift
: This algorithm starts by placing a circle centered on each instance; then for each circle it computes the mean of all the instances located within it, and it shifts the circle so that it is centered on the mean. Next, it iterates this mean-shifting step until all the circles stop moving (i.e., until each of them is centered on the mean of the instances it contains). Mean-Shift shifts the circles in the direction of higher density, until each of them has found a local density maximum. Finally, all the instances whose circles have settled in the same place (or close enough) are assigned to the same cluster. Mean-Shift has some of the same features as DBSCAN, like how it can find any number of clusters of any shape, it has very few hyperparameters (just one—the radius of the circles, called the *bandwidth*), and it relies on local density estimation. But unlike DBSCAN, Mean-Shift tends to chop clusters into pieces when they have internal density variations. Unfortunately, its computational complexity is $O(m^2)$, so it is not suited for large datasets.

Affinity propagation
: This algorithm uses a voting system, where instances vote for similar instances to be their representatives, and once the algorithm converges, each representative and its voters form a cluster. Affinity propagation can detect any number of clusters of different sizes. Unfortunately, this algorithm has a computational complexity of $O(m^2)$, so it too is not suited for large datasets.

Spectral clustering
: This algorithm takes a similarity matrix between the instances and creates a low-dimensional embedding from it (i.e., it reduces its dimensionality), then it uses

another clustering algorithm in this low-dimensional space (Scikit-Learn's implementation uses K-Means.) Spectral clustering can capture complex cluster structures, and it can also be used to cut graphs (e.g., to identify clusters of friends on a social network). It does not scale well to large numbers of instances, and it does not behave well when the clusters have very different sizes.

Now let's dive into Gaussian mixture models, which can be used for density estimation, clustering, and anomaly detection.

Gaussian Mixtures

A *Gaussian mixture model* (GMM) is a probabilistic model that assumes that the instances were generated from a mixture of several Gaussian distributions whose parameters are unknown. All the instances generated from a single Gaussian distribution form a cluster that typically looks like an ellipsoid. Each cluster can have a different ellipsoidal shape, size, density, and orientation, just like in Figure 9-11. When you observe an instance, you know it was generated from one of the Gaussian distributions, but you are not told which one, and you do not know what the parameters of these distributions are.

There are several GMM variants. In the simplest variant, implemented in the `GaussianMixture` class, you must know in advance the number k of Gaussian distributions. The dataset $\mathbf{X}$ is assumed to have been generated through the following probabilistic process:

- For each instance, a cluster is picked randomly from among k clusters. The probability of choosing the j^{th} cluster is defined by the cluster's weight, $\phi^{(j)}$.[7] The index of the cluster chosen for the i^{th} instance is noted $z^{(i)}$.
- If $z^{(i)}=j$, meaning the i^{th} instance has been assigned to the j^{th} cluster, the location $\mathbf{x}^{(i)}$ of this instance is sampled randomly from the Gaussian distribution with mean $\boldsymbol{\mu}^{(j)}$ and covariance matrix $\boldsymbol{\Sigma}^{(j)}$. This is noted $\mathbf{x}^{(i)} \sim \mathcal{N}\left(\boldsymbol{\mu}^{(j)}, \boldsymbol{\Sigma}^{(j)}\right)$.

This generative process can be represented as a graphical model. Figure 9-16 represents the structure of the conditional dependencies between random variables.

7 Phi (ϕ or φ) is the 21st letter of the Greek alphabet.

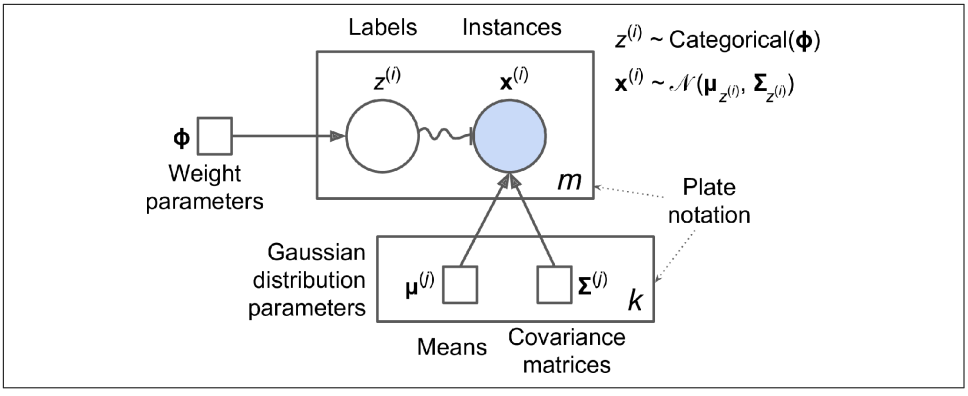


Figure 9-16. A graphical representation of a Gaussian mixture model, including its parameters (squares), random variables (circles), and their conditional dependencies (solid arrows)

Here is how to interpret the figure:[8]

- The circles represent random variables.
- The squares represent fixed values (i.e., parameters of the model).
- The large rectangles are called *plates*. They indicate that their content is repeated several times.
- The number at the bottom right of each plate indicates how many times its content is repeated. So, there are m random variables $z^{(i)}$ (from $z^{(1)}$ to $z^{(m)}$) and m random variables $\mathbf{x}^{(i)}$. There are also k means $\boldsymbol{\mu}^{(j)}$ and k covariance matrices $\boldsymbol{\Sigma}^{(j)}$. Lastly, there is just one weight vector $\boldsymbol{\phi}$ (containing all the weights $\phi^{(1)}$ to $\phi^{(k)}$).
- Each variable $z^{(i)}$ is drawn from the *categorical distribution* with weights $\boldsymbol{\phi}$. Each variable $\mathbf{x}^{(i)}$ is drawn from the normal distribution, with the mean and covariance matrix defined by its cluster $z^{(i)}$.
- The solid arrows represent conditional dependencies. For example, the probability distribution for each random variable $z^{(i)}$ depends on the weight vector $\boldsymbol{\phi}$. Note that when an arrow crosses a plate boundary, it means that it applies to all the repetitions of that plate. For example, the weight vector $\boldsymbol{\phi}$ conditions the probability distributions of all the random variables $\mathbf{x}^{(1)}$ to $\mathbf{x}^{(m)}$.
- The squiggly arrow from $z^{(i)}$ to $\mathbf{x}^{(i)}$ represents a switch: depending on the value of $z^{(i)}$, the instance $\mathbf{x}^{(i)}$ will be sampled from a different Gaussian distribution. For example, if $z^{(i)}=j$, then $\mathbf{x}^{(i)} \sim \mathcal{N}\left(\boldsymbol{\mu}^{(j)}, \boldsymbol{\Sigma}^{(j)}\right)$.

8 Most of these notations are standard, but a few additional notations were taken from the Wikipedia article on plate notation.

- Shaded nodes indicate that the value is known. So, in this case, only the random variables $\mathbf{x}^{(i)}$ have known values: they are called *observed variables*. The unknown random variables $z^{(i)}$ are called *latent variables*.

So, what can you do with such a model? Well, given the dataset $\mathbf{X}$, you typically want to start by estimating the weights $\boldsymbol{\phi}$ and all the distribution parameters $\boldsymbol{\mu}^{(1)}$ to $\boldsymbol{\mu}^{(k)}$ and $\boldsymbol{\Sigma}^{(1)}$ to $\boldsymbol{\Sigma}^{(k)}$. Scikit-Learn's `GaussianMixture` class makes this super easy:

```
from sklearn.mixture import GaussianMixture

gm = GaussianMixture(n_components=3, n_init=10)
gm.fit(X)
```

Let's look at the parameters that the algorithm estimated:

```
>>> gm.weights_
array([0.20965228, 0.4000662 , 0.39028152])
>>> gm.means_
array([[ 3.39909717,  1.05933727],
       [-1.40763984,  1.42710194],
       [ 0.05135313,  0.07524095]])
>>> gm.covariances_
array([[[ 1.14807234, -0.03270354],
        [-0.03270354,  0.95496237]],

       [[ 0.63478101,  0.72969804],
        [ 0.72969804,  1.1609872 ]],

       [[ 0.68809572,  0.79608475],
        [ 0.79608475,  1.21234145]]])
```

Great, it worked fine! Indeed, the weights that were used to generate the data were 0.2, 0.4, and 0.4; and similarly, the means and covariance matrices were very close to those found by the algorithm. But how? This class relies on the *Expectation-Maximization* (EM) algorithm, which has many similarities with the K-Means algorithm: it also initializes the cluster parameters randomly, then it repeats two steps until convergence, first assigning instances to clusters (this is called the *expectation step*) and then updating the clusters (this is called the *maximization step*). Sounds familiar, right? In the context of clustering, you can think of EM as a generalization of K-Means that not only finds the cluster centers ($\boldsymbol{\mu}^{(1)}$ to $\boldsymbol{\mu}^{(k)}$), but also their size, shape, and orientation ($\boldsymbol{\Sigma}^{(1)}$ to $\boldsymbol{\Sigma}^{(k)}$), as well as their relative weights ($\phi^{(1)}$ to $\phi^{(k)}$). Unlike K-Means, though, EM uses soft cluster assignments, not hard assignments. For each instance, during the expectation step, the algorithm estimates the probability that it belongs to each cluster (based on the current cluster parameters). Then, during the maximization step, each cluster is updated using *all* the instances in the dataset, with each instance weighted by the estimated probability that it belongs to that cluster. These probabilities are called the *responsibilities* of the clusters for the instances.

During the maximization step, each cluster's update will mostly be impacted by the instances it is most responsible for.

Unfortunately, just like K-Means, EM can end up converging to poor solutions, so it needs to be run several times, keeping only the best solution. This is why we set `n_init` to `10`. Be careful: by default `n_init` is set to `1`.

You can check whether or not the algorithm converged and how many iterations it took:

```
>>> gm.converged_
True
>>> gm.n_iter_
3
```

Now that you have an estimate of the location, size, shape, orientation, and relative weight of each cluster, the model can easily assign each instance to the most likely cluster (hard clustering) or estimate the probability that it belongs to a particular cluster (soft clustering). Just use the `predict()` method for hard clustering, or the `predict_proba()` method for soft clustering:

```
>>> gm.predict(X)
array([2, 2, 1, ..., 0, 0, 0])
>>> gm.predict_proba(X)
array([[2.32389467e-02, 6.77397850e-07, 9.76760376e-01],
       [1.64685609e-02, 6.75361303e-04, 9.82856078e-01],
       [2.01535333e-06, 9.99923053e-01, 7.49319577e-05],
       ...,
       [9.99999571e-01, 2.13946075e-26, 4.28788333e-07],
       [1.00000000e+00, 1.46454409e-41, 5.12459171e-16],
       [1.00000000e+00, 8.02006365e-41, 2.27626238e-15]])
```

A Gaussian mixture model is a *generative model*, meaning you can sample new instances from it (note that they are ordered by cluster index):

```
>>> X_new, y_new = gm.sample(6)
>>> X_new
array([[ 2.95400315,  2.63680992],
       [-1.16654575,  1.62792705],
       [-1.39477712, -1.48511338],
       [ 0.27221525,  0.690366  ],
       [ 0.54095936,  0.48591934],
       [ 0.38064009, -0.56240465]])

>>> y_new
array([0, 1, 2, 2, 2, 2])
```

It is also possible to estimate the density of the model at any given location. This is achieved using the `score_samples()` method: for each instance it is given, this

method estimates the log of the *probability density function* (PDF) at that location. The greater the score, the higher the density:

```
>>> gm.score_samples(X)
array([-2.60782346, -3.57106041, -3.33003479, ..., -3.51352783,
       -4.39802535, -3.80743859])
```

If you compute the exponential of these scores, you get the value of the PDF at the location of the given instances. These are not probabilities, but probability *densities*: they can take on any positive value, not just a value between 0 and 1. To estimate the probability that an instance will fall within a particular region, you would have to integrate the PDF over that region (if you do so over the entire space of possible instance locations, the result will be 1).

Figure 9-17 shows the cluster means, the decision boundaries (dashed lines), and the density contours of this model.

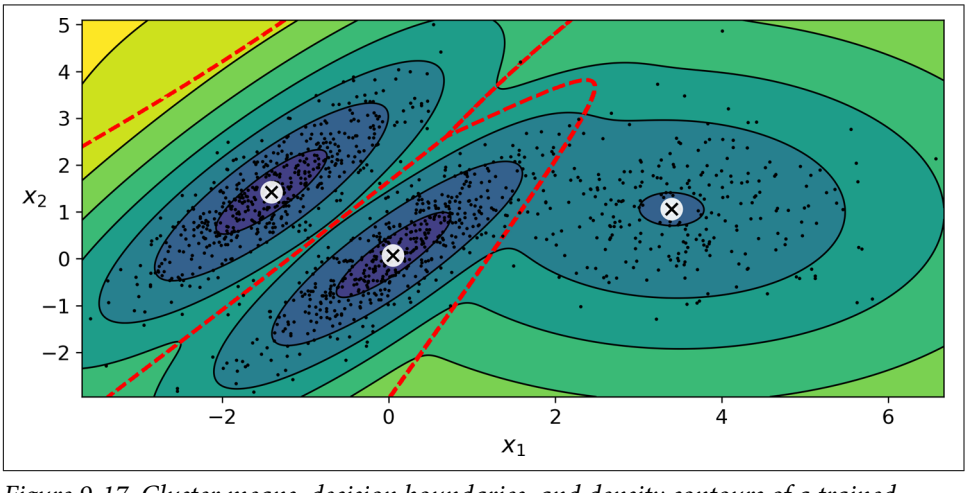


Figure 9-17. Cluster means, decision boundaries, and density contours of a trained Gaussian mixture model

Nice! The algorithm clearly found an excellent solution. Of course, we made its task easy by generating the data using a set of 2D Gaussian distributions (unfortunately, real-life data is not always so Gaussian and low-dimensional). We also gave the algorithm the correct number of clusters. When there are many dimensions, or many clusters, or few instances, EM can struggle to converge to the optimal solution. You might need to reduce the difficulty of the task by limiting the number of parameters that the algorithm has to learn. One way to do this is to limit the range of shapes and orientations that the clusters can have. This can be achieved by imposing constraints on the covariance matrices. To do this, set the `covariance_type` hyperparameter to one of the following values:

`"spherical"`
: All clusters must be spherical, but they can have different diameters (i.e., different variances).

`"diag"`
: Clusters can take on any ellipsoidal shape of any size, but the ellipsoid's axes must be parallel to the coordinate axes (i.e., the covariance matrices must be diagonal).

`"tied"`
: All clusters must have the same ellipsoidal shape, size, and orientation (i.e., all clusters share the same covariance matrix).

By default, `covariance_type` is equal to `"full"`, which means that each cluster can take on any shape, size, and orientation (it has its own unconstrained covariance matrix). Figure 9-18 plots the solutions found by the EM algorithm when `covariance_type` is set to `"tied"` or `"spherical"`.

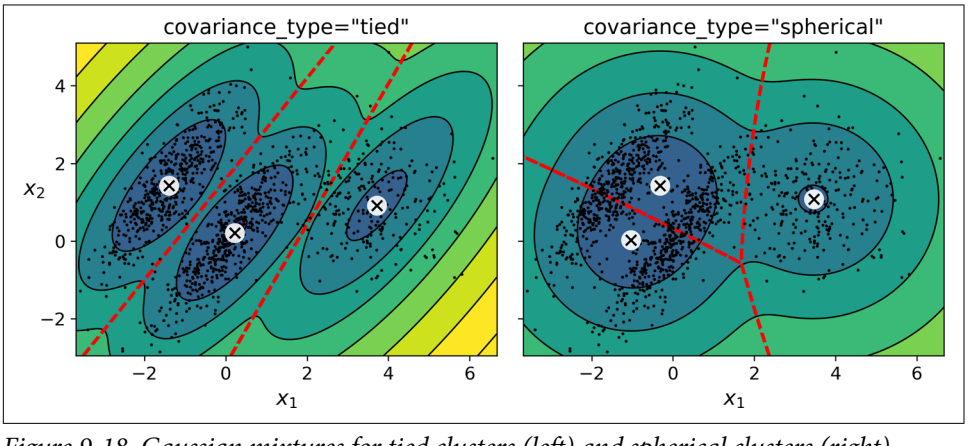


Figure 9-18. Gaussian mixtures for tied clusters (left) and spherical clusters (right)

The computational complexity of training a `GaussianMixture` model depends on the number of instances m, the number of dimensions n, the number of clusters k, and the constraints on the covariance matrices. If `covariance_type` is `"spherical"` or `"diag"`, it is $O(kmn)$, assuming the data has a clustering structure. If `covariance_type` is `"tied"` or `"full"`, it is $O(kmn^2 + kn^3)$, so it will not scale to large numbers of features.

Gaussian mixture models can also be used for anomaly detection. Let's see how.

Anomaly Detection Using Gaussian Mixtures

Anomaly detection (also called *outlier detection*) is the task of detecting instances that deviate strongly from the norm. These instances are called *anomalies*, or *outliers*, while the normal instances are called *inliers*. Anomaly detection is useful in a wide variety of applications, such as fraud detection, detecting defective products in manufacturing, or removing outliers from a dataset before training another model (which can significantly improve the performance of the resulting model).

Using a Gaussian mixture model for anomaly detection is quite simple: any instance located in a low-density region can be considered an anomaly. You must define what density threshold you want to use. For example, in a manufacturing company that tries to detect defective products, the ratio of defective products is usually well known. Say it is equal to 4%. You then set the density threshold to be the value that results in having 4% of the instances located in areas below that threshold density. If you notice that you get too many false positives (i.e., perfectly good products that are flagged as defective), you can lower the threshold. Conversely, if you have too many false negatives (i.e., defective products that the system does not flag as defective), you can increase the threshold. This is the usual precision/recall trade-off (see Chapter 3). Here is how you would identify the outliers using the fourth percentile lowest density as the threshold (i.e., approximately 4% of the instances will be flagged as anomalies):

```
densities = gm.score_samples(X)
density_threshold = np.percentile(densities, 4)
anomalies = X[densities < density_threshold]
```

Figure 9-19 represents these anomalies as stars.

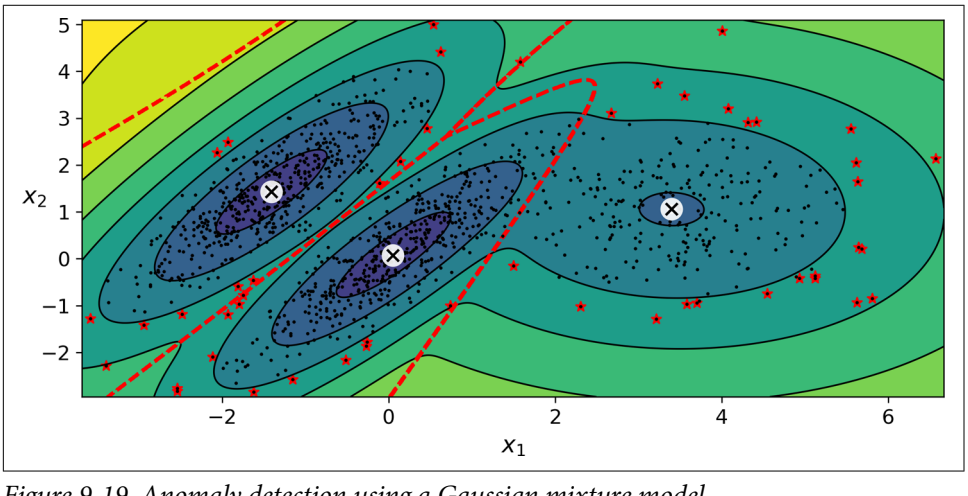


Figure 9-19. Anomaly detection using a Gaussian mixture model

A closely related task is *novelty detection*: it differs from anomaly detection in that the algorithm is assumed to be trained on a "clean" dataset, uncontaminated by outliers, whereas anomaly detection does not make this assumption. Indeed, outlier detection is often used to clean up a dataset.

Gaussian mixture models try to fit all the data, including the outliers, so if you have too many of them, this will bias the model's view of "normality," and some outliers may wrongly be considered as normal. If this happens, you can try to fit the model once, use it to detect and remove the most extreme outliers, then fit the model again on the cleaned-up dataset. Another approach is to use robust covariance estimation methods (see the `EllipticEnvelope` class).

Just like K-Means, the `GaussianMixture` algorithm requires you to specify the number of clusters. So, how can you find it?

Selecting the Number of Clusters

With K-Means, you could use the inertia or the silhouette score to select the appropriate number of clusters. But with Gaussian mixtures, it is not possible to use these metrics because they are not reliable when the clusters are not spherical or have different sizes. Instead, you can try to find the model that minimizes a *theoretical information criterion*, such as the *Bayesian information criterion* (BIC) or the *Akaike information criterion* (AIC), defined in Equation 9-1.

Equation 9-1. Bayesian information criterion (BIC) and Akaike information criterion (AIC)

$$BIC = \log(m)p - 2\log\left(\hat{L}\right)$$

$$AIC = 2p - 2\log\left(\hat{L}\right)$$

In these equations:

- m is the number of instances, as always.
- p is the number of parameters learned by the model.
- $\hat{L}$ is the maximized value of the *likelihood function* of the model.

Both the BIC and the AIC penalize models that have more parameters to learn (e.g., more clusters) and reward models that fit the data well. They often end up selecting the same model. When they differ, the model selected by the BIC tends to be simpler

(fewer parameters) than the one selected by the AIC, but tends to not fit the data quite as well (this is especially true for larger datasets).

Likelihood Function

The terms "probability" and "likelihood" are often used interchangeably in the English language, but they have very different meanings in statistics. Given a statistical model with some parameters **θ**, the word "probability" is used to describe how plausible a future outcome **x** is (knowing the parameter values **θ**), while the word "likelihood" is used to describe how plausible a particular set of parameter values **θ** are, after the outcome **x** is known.

Consider a 1D mixture model of two Gaussian distributions centered at –4 and +1. For simplicity, this toy model has a single parameter θ that controls the standard deviations of both distributions. The top-left contour plot in Figure 9-20 shows the entire model $f(x; \theta)$ as a function of both x and θ. To estimate the probability distribution of a future outcome x, you need to set the model parameter θ. For example, if you set θ to 1.3 (the horizontal line), you get the probability density function $f(x; \theta{=}1.3)$ shown in the lower-left plot. Say you want to estimate the probability that x will fall between –2 and +2. You must calculate the integral of the PDF on this range (i.e., the surface of the shaded region). But what if you don't know θ, and instead if you have observed a single instance $x{=}2.5$ (the vertical line in the upper-left plot)? In this case, you get the likelihood function $\mathcal{L}(\theta|x{=}2.5){=}f(x{=}2.5; \theta)$, represented in the upper-right plot.

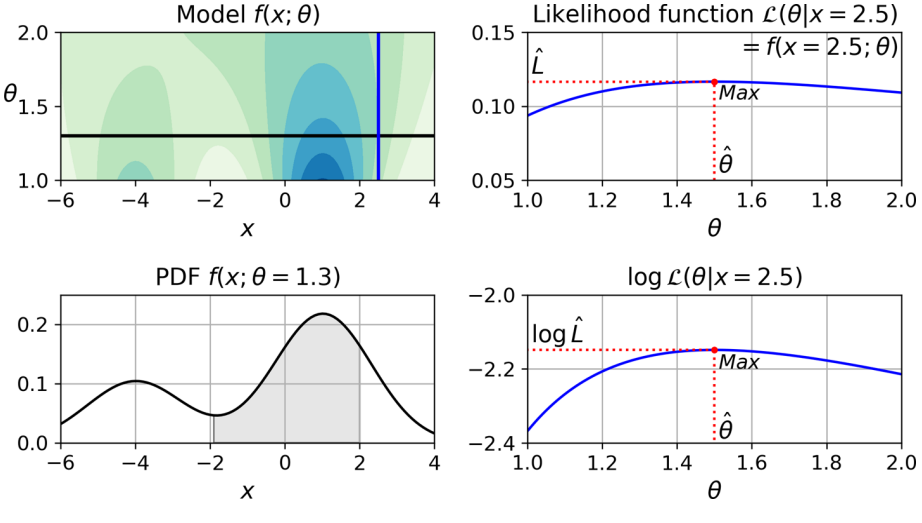


Figure 9-20. A model's parametric function (top left), and some derived functions: a PDF (lower left), a likelihood function (top right), and a log likelihood function (lower right)

In short, the PDF is a function of x (with θ fixed), while the likelihood function is a function of θ (with x fixed). It is important to understand that the likelihood function is *not* a probability distribution: if you integrate a probability distribution over all possible values of x, you always get 1; but if you integrate the likelihood function over all possible values of θ, the result can be any positive value.

Given a dataset **X**, a common task is to try to estimate the most likely values for the model parameters. To do this, you must find the values that maximize the likelihood function, given **X**. In this example, if you have observed a single instance x=2.5, the *maximum likelihood estimate* (MLE) of θ is $\hat{\theta}$=1.5. If a prior probability distribution g over θ exists, it is possible to take it into account by maximizing $\mathscr{L}(\theta|x)g(\theta)$ rather than just maximizing $\mathscr{L}(\theta|x)$. This is called *maximum a-posteriori* (MAP) estimation. Since MAP constrains the parameter values, you can think of it as a regularized version of MLE.

Notice that maximizing the likelihood function is equivalent to maximizing its logarithm (represented in the lower-righthand plot in Figure 9-20). Indeed the logarithm is a strictly increasing function, so if θ maximizes the log likelihood, it also maximizes the likelihood. It turns out that it is generally easier to maximize the log likelihood. For example, if you observed several independent instances $x^{(1)}$ to $x^{(m)}$, you would need to find the value of θ that maximizes the product of the individual likelihood functions. But it is equivalent, and much simpler, to maximize the sum (not the product) of the log likelihood functions, thanks to the magic of the logarithm which converts products into sums: $\log(ab)=\log(a)+\log(b)$.

Once you have estimated $\hat{\theta}$, the value of θ that maximizes the likelihood function, then you are ready to compute $\hat{L} = \mathscr{L}\left(\hat{\theta}, \mathbf{X}\right)$, which is the value used to compute the AIC and BIC; you can think of it as a measure of how well the model fits the data.

To compute the BIC and AIC, call the `bic()` and `aic()` methods:

```
>>> gm.bic(X)
8189.74345832983
>>> gm.aic(X)
8102.518178214792
```

Figure 9-21 shows the BIC for different numbers of clusters k. As you can see, both the BIC and the AIC are lowest when k=3, so it is most likely the best choice. Note that we could also search for the best value for the `covariance_type` hyperparameter. For example, if it is `"spherical"` rather than `"full"`, then the model has significantly fewer parameters to learn, but it does not fit the data as well.

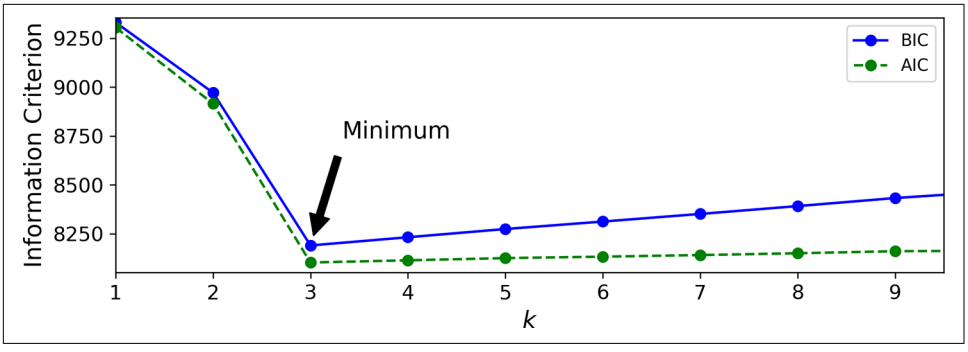


Figure 9-21. AIC and BIC for different numbers of clusters k

Bayesian Gaussian Mixture Models

Rather than manually searching for the optimal number of clusters, you can use the `BayesianGaussianMixture` class, which is capable of giving weights equal (or close) to zero to unnecessary clusters. Set the number of clusters `n_components` to a value that you have good reason to believe is greater than the optimal number of clusters (this assumes some minimal knowledge about the problem at hand), and the algorithm will eliminate the unnecessary clusters automatically. For example, let's set the number of clusters to 10 and see what happens:

```
>>> from sklearn.mixture import BayesianGaussianMixture
>>> bgm = BayesianGaussianMixture(n_components=10, n_init=10)
>>> bgm.fit(X)
>>> np.round(bgm.weights_, 2)
array([0.4 , 0.21, 0.4 , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  ])
```

Perfect: the algorithm automatically detected that only three clusters are needed, and the resulting clusters are almost identical to the ones in Figure 9-17.

In this model, the cluster parameters (including the weights, means, and covariance matrices) are not treated as fixed model parameters anymore, but as latent random variables, like the cluster assignments (see Figure 9-22). So $\mathbf{z}$ now includes both the cluster parameters and the cluster assignments.

The Beta distribution is commonly used to model random variables whose values lie within a fixed range. In this case, the range is from 0 to 1. The Stick-Breaking Process (SBP) is best explained through an example: suppose Φ=[0.3, 0.6, 0.5,…], then 30% of the instances will be assigned to cluster 0, then 60% of the remaining instances will be assigned to cluster 1, then 50% of the remaining instances will be assigned to cluster 2, and so on. This process is a good model for datasets where new instances are more likely to join large clusters than small clusters (e.g., people are more likely to move to larger cities). If the concentration α is high, then Φ values will likely be close to 0, and the SBP generate many clusters. Conversely, if the concentration is low, then Φ values

will likely be close to 1, and there will be few clusters. Finally, the Wishart distribution is used to sample covariance matrices: the parameters d and V control the distribution of cluster shapes.

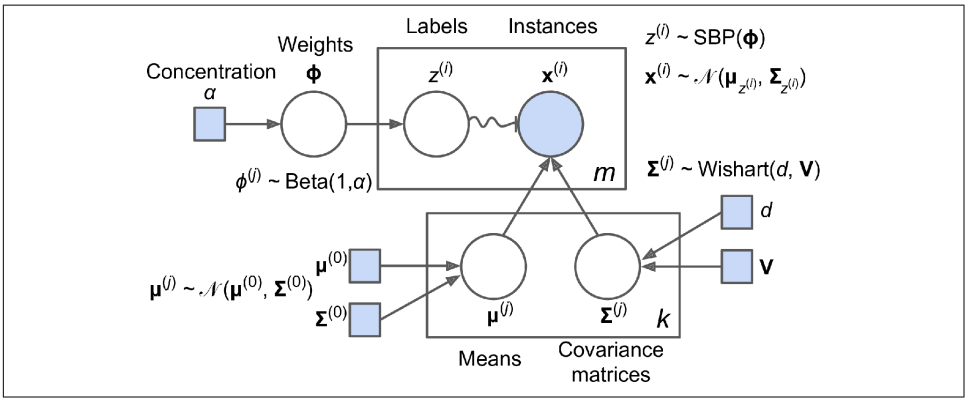


Figure 9-22. Bayesian Gaussian mixture model

Prior knowledge about the latent variables **z** can be encoded in a probability distribution $p(\mathbf{z})$ called the *prior*. For example, we may have a prior belief that the clusters are likely to be few (low concentration), or conversely, that they are likely to be plentiful (high concentration). This prior belief about the number of clusters can be adjusted using the `weight_concentration_prior` hyperparameter. Setting it to 0.01 or 10,000 gives very different clusterings (see Figure 9-23). The more data we have, however, the less the priors matter. In fact, to plot diagrams with such large differences, you must use very strong priors and little data.

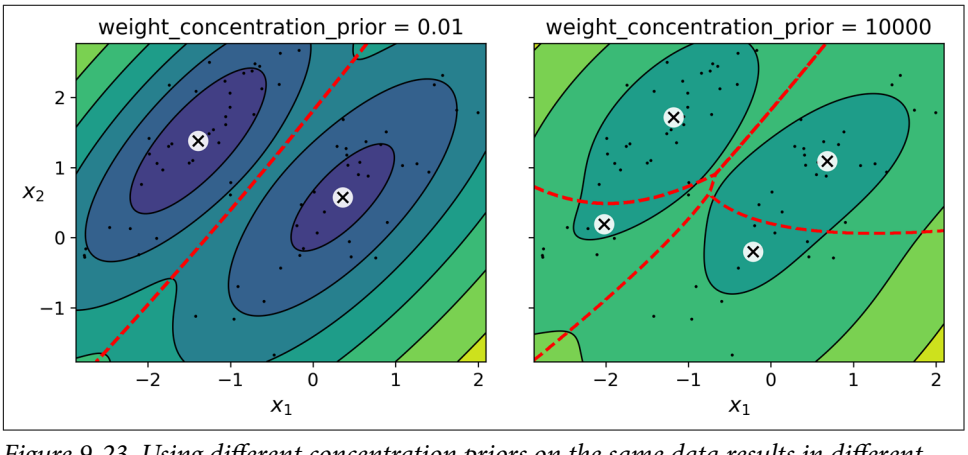


Figure 9-23. Using different concentration priors on the same data results in different numbers of clusters

Bayes' theorem (Equation 9-2) tells us how to update the probability distribution over the latent variables after we observe some data **X**. It computes the *posterior* distribution $p(\mathbf{z}|\mathbf{X})$, which is the conditional probability of **z** given **X**.

Equation 9-2. Bayes' theorem

$$p(\mathbf{z}|\mathbf{X}) = \text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{evidence}} = \frac{p(\mathbf{X}|\mathbf{z})\,p(\mathbf{z})}{p(\mathbf{X})}$$

Unfortunately, in a Gaussian mixture model (and many other problems), the denominator $p(\mathbf{x})$ is intractable, as it requires integrating over all the possible values of **z** (Equation 9-3), which would require considering all possible combinations of cluster parameters and cluster assignments.

Equation 9-3. The evidence $p(\mathbf{X})$ is often intractable

$$p\left(\mathbf{X}\right) = \int p(\mathbf{X}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$

This intractability is one of the central problems in Bayesian statistics, and there are several approaches to solving it. One of them is *variational inference*, which picks a family of distributions $q(\mathbf{z}; \boldsymbol{\lambda})$ with its own *variational parameters* $\boldsymbol{\lambda}$ (lambda), then optimizes these parameters to make $q(\mathbf{z})$ a good approximation of $p(\mathbf{z}|\mathbf{X})$. This is achieved by finding the value of $\boldsymbol{\lambda}$ that minimizes the KL divergence from $q(\mathbf{z})$ to $p(\mathbf{z}|\mathbf{X})$, noted $D_{\text{KL}}(q\|p)$. The KL divergence equation is shown in Equation 9-4, and it can be rewritten as the log of the evidence ($\log p(\mathbf{X})$) minus the *evidence lower bound* (ELBO). Since the log of the evidence does not depend on q, it is a constant term, so minimizing the KL divergence just requires maximizing the ELBO.

Equation 9-4. KL divergence from $q(\mathbf{z})$ to $p(\mathbf{z}|\mathbf{X})$

$$\begin{aligned}
D_{KL}(q \parallel p) &= \mathbb{E}_q\left[\log \frac{q(\mathbf{z})}{p(\mathbf{z} \mid \mathbf{X})}\right] \\
&= \mathbb{E}_q[\log q(\mathbf{z}) - \log p(\mathbf{z} \mid \mathbf{X})] \\
&= \mathbb{E}_q\left[\log q(\mathbf{z}) - \log \frac{p(\mathbf{z}, \mathbf{X})}{p(\mathbf{X})}\right] \\
&= \mathbb{E}_q[\log q(\mathbf{z}) - \log p(\mathbf{z}, \mathbf{X}) + \log p(\mathbf{X})] \\
&= \mathbb{E}_q[\log q(\mathbf{z})] - \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{X})] + \mathbb{E}_q[\log p(\mathbf{X})] \\
&= \mathbb{E}_q[\log p(\mathbf{X})] - \left(\mathbb{E}_q[\log p(\mathbf{z}, \mathbf{X})] - \mathbb{E}_q[\log q(\mathbf{z})]\right) \\
&= \log p(\mathbf{X}) - \text{ELBO} \\
&\quad \text{where ELBO} = \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{X})] - \mathbb{E}_q[\log q(\mathbf{z})]
\end{aligned}$$

In practice, there are different techniques to maximize the ELBO. In *mean field variational inference*, it is necessary to pick the family of distributions $q(\mathbf{z}; \boldsymbol{\lambda})$ and the prior $p(z)$ very carefully to ensure that the equation for the ELBO simplifies to a form that can be computed. Unfortunately, there is no general way to do this. Picking the right family of distributions and the right prior depends on the task and requires some mathematical skills. For example, the distributions and lower-bound equations used in Scikit-Learn's `BayesianGaussianMixture` class are presented in the documentation. From these equations it is possible to derive update equations for the cluster parameters and assignment variables: these are then used very much like in the Expectation-Maximization algorithm. In fact, the computational complexity of the `BayesianGaussianMixture` class is similar to that of the `GaussianMixture` class (but generally significantly slower). A simpler approach to maximizing the ELBO is called *black box stochastic variational inference* (BBSVI): at each iteration, a few samples are drawn from q, and they are used to estimate the gradients of the ELBO with regard to the variational parameters $\boldsymbol{\lambda}$, which are then used in a gradient ascent step. This approach makes it possible to use Bayesian inference with any kind of model (provided it is differentiable), even deep neural networks; using Bayesian inference with deep neural networks is called Bayesian Deep Learning.

If you want to dive deeper into Bayesian statistics, check out the book *Bayesian Data Analysis* by Andrew Gelman et al. (Chapman & Hall).

Gaussian mixture models work great on clusters with ellipsoidal shapes, but if you try to fit a dataset with different shapes, you may have bad surprises. For example, let's see what happens if we use a Bayesian Gaussian mixture model to cluster the moons dataset (see Figure 9-24).

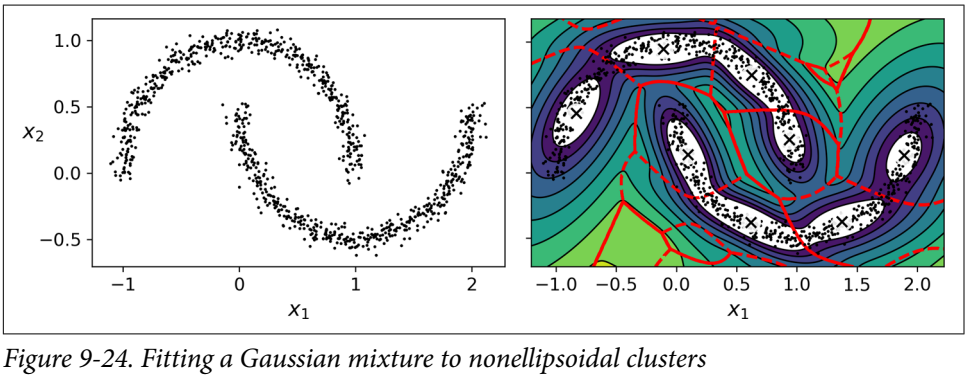


Figure 9-24. Fitting a Gaussian mixture to nonellipsoidal clusters

Oops! The algorithm desperately searched for ellipsoids, so it found eight different clusters instead of two. The density estimation is not too bad, so this model could perhaps be used for anomaly detection, but it failed to identify the two moons. Let's now look at a few clustering algorithms capable of dealing with arbitrarily shaped clusters.

Other Algorithms for Anomaly and Novelty Detection

Scikit-Learn implements other algorithms dedicated to anomaly detection or novelty detection:

PCA (and other dimensionality reduction techniques with an `inverse_transform()` method)
: If you compare the reconstruction error of a normal instance with the reconstruction error of an anomaly, the latter will usually be much larger. This is a simple and often quite efficient anomaly detection approach (see this chapter's exercises for an application of this approach).

Fast-MCD (minimum covariance determinant)
: Implemented by the `EllipticEnvelope` class, this algorithm is useful for outlier detection, in particular to clean up a dataset. It assumes that the normal instances (inliers) are generated from a single Gaussian distribution (not a mixture). It also assumes that the dataset is contaminated with outliers that were not generated from this Gaussian distribution. When the algorithm estimates the parameters of the Gaussian distribution (i.e., the shape of the elliptic envelope around the inliers), it is careful to ignore the instances that are most likely outliers. This technique gives a better estimation of the elliptic envelope and thus makes the algorithm better at identifying the outliers.

Isolation Forest
: This is an efficient algorithm for outlier detection, especially in high-dimensional datasets. The algorithm builds a Random Forest in which each Decision Tree is grown randomly: at each node, it picks a feature randomly, then it picks a random threshold value (between the min and max values) to split the dataset in two. The dataset gradually gets chopped into pieces this way, until all instances end up isolated from the other instances. Anomalies are usually far from other instances, so on average (across all the Decision Trees) they tend to get isolated in fewer steps than normal instances.

Local Outlier Factor (LOF)
: This algorithm is also good for outlier detection. It compares the density of instances around a given instance to the density around its neighbors. An anomaly is often more isolated than its k nearest neighbors.

One-class SVM

This algorithm is better suited for novelty detection. Recall that a kernelized SVM classifier separates two classes by first (implicitly) mapping all the instances to a high-dimensional space, then separating the two classes using a linear SVM classifier within this high-dimensional space (see Chapter 5). Since we just have one class of instances, the one-class SVM algorithm instead tries to separate the instances in high-dimensional space from the origin. In the original space, this will correspond to finding a small region that encompasses all the instances. If a new instance does not fall within this region, it is an anomaly. There are a few hyperparameters to tweak: the usual ones for a kernelized SVM, plus a margin hyperparameter that corresponds to the probability of a new instance being mistakenly considered as novel when it is in fact normal. It works great, especially with high-dimensional datasets, but like all SVMs it does not scale to large datasets.

Exercises

1. How would you define clustering? Can you name a few clustering algorithms?
2. What are some of the main applications of clustering algorithms?
3. Describe two techniques to select the right number of clusters when using K-Means.
4. What is label propagation? Why would you implement it, and how?
5. Can you name two clustering algorithms that can scale to large datasets? And two that look for regions of high density?
6. Can you think of a use case where active learning would be useful? How would you implement it?
7. What is the difference between anomaly detection and novelty detection?
8. What is a Gaussian mixture? What tasks can you use it for?
9. Can you name two techniques to find the right number of clusters when using a Gaussian mixture model?
10. The classic Olivetti faces dataset contains 400 grayscale 64 × 64–pixel images of faces. Each image is flattened to a 1D vector of size 4,096. 40 different people were photographed (10 times each), and the usual task is to train a model that can predict which person is represented in each picture. Load the dataset using the `sklearn.datasets.fetch_olivetti_faces()` function, then split it into a training set, a validation set, and a test set (note that the dataset is already scaled between 0 and 1). Since the dataset is quite small, you probably want to use stratified sampling to ensure that there are the same number of images per person in each set. Next, cluster the images using K-Means, and ensure that you have a

good number of clusters (using one of the techniques discussed in this chapter). Visualize the clusters: do you see similar faces in each cluster?

11. Continuing with the Olivetti faces dataset, train a classifier to predict which person is represented in each picture, and evaluate it on the validation set. Next, use K-Means as a dimensionality reduction tool, and train a classifier on the reduced set. Search for the number of clusters that allows the classifier to get the best performance: what performance can you reach? What if you append the features from the reduced set to the original features (again, searching for the best number of clusters)?
12. Train a Gaussian mixture model on the Olivetti faces dataset. To speed up the algorithm, you should probably reduce the dataset's dimensionality (e.g., use PCA, preserving 99% of the variance). Use the model to generate some new faces (using the `sample()` method), and visualize them (if you used PCA, you will need to use its `inverse_transform()` method). Try to modify some images (e.g., rotate, flip, darken) and see if the model can detect the anomalies (i.e., compare the output of the `score_samples()` method for normal images and for anomalies).
13. Some dimensionality reduction techniques can also be used for anomaly detection. For example, take the Olivetti faces dataset and reduce it with PCA, preserving 99% of the variance. Then compute the reconstruction error for each image. Next, take some of the modified images you built in the previous exercise, and look at their reconstruction error: notice how much larger the reconstruction error is. If you plot a reconstructed image, you will see why: it tries to reconstruct a normal face.

Solutions to these exercises are available in Appendix A.

PART II

Neural Networks and Deep Learning

CHAPTER 10

Introduction to Artificial Neural Networks with Keras

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

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

The first part of this chapter introduces artificial neural networks, starting with a quick tour of the very first ANN architectures and leading up to *Multilayer Perceptrons* (MLPs), which are heavily used today (other architectures will be explored in the next chapters). In the second part, we will look at how to implement neural networks using the popular Keras API. This is a beautifully designed and simple high-

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

level API for building, training, evaluating, and running neural networks. But don't be fooled by its simplicity: it is expressive and flexible enough to let you build a wide variety of neural network architectures. In fact, it will probably be sufficient for most of your use cases. And should you ever need extra flexibility, you can always write custom Keras components using its lower-level API, as we will see in Chapter 12.

But first, let's go back in time to see how artificial neural networks came to be!

From Biological to Artificial Neurons

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

The early successes of ANNs led to the widespread belief that we would soon be conversing with truly intelligent machines. When it became clear in the 1960s that this promise would go unfulfilled (at least for quite a while), funding flew elsewhere, and ANNs entered a long winter. In the early 1980s, new architectures were invented and better training techniques were developed, sparking a revival of interest in *connectionism* (the study of neural networks). But progress was slow, and by the 1990s other powerful Machine Learning techniques were invented, such as Support Vector Machines (see Chapter 5). These techniques seemed to offer better results and stronger theoretical foundations than ANNs, so once again the study of neural networks was put on hold.

We are now witnessing yet another wave of interest in ANNs. Will this wave die out like the previous ones did? Well, here are a few good reasons to believe that this time is different and that the renewed interest in ANNs will have a much more profound impact on our lives:

- There is now a huge quantity of data available to train neural networks, and ANNs frequently outperform other ML techniques on very large and complex problems.
- The tremendous increase in computing power since the 1990s now makes it possible to train large neural networks in a reasonable amount of time. This is in part due to Moore's law (the number of components in integrated circuits has

2 Warren S. McCulloch and Walter Pitts, "A Logical Calculus of the Ideas Immanent in Nervous Activity," *The Bulletin of Mathematical Biology* 5, no. 4 (1943): 115–113.

doubled about every 2 years over the last 50 years), but also thanks to the gaming industry, which has stimulated the production of powerful GPU cards by the millions. Moreover, cloud platforms have made this power accessible to everyone.

- The training algorithms have been improved. To be fair they are only slightly different from the ones used in the 1990s, but these relatively small tweaks have had a huge positive impact.
- Some theoretical limitations of ANNs have turned out to be benign in practice. For example, many people thought that ANN training algorithms were doomed because they were likely to get stuck in local optima, but it turns out that this is rather rare in practice (and when it is the case, they are usually fairly close to the global optimum).
- ANNs seem to have entered a virtuous circle of funding and progress. Amazing products based on ANNs regularly make the headline news, which pulls more and more attention and funding toward them, resulting in more and more progress and even more amazing products.

Biological Neurons

Before we discuss artificial neurons, let's take a quick look at a biological neuron (represented in Figure 10-1). It is an unusual-looking cell mostly found in animal brains. It's composed of a *cell body* containing the nucleus and most of the cell's complex components, many branching extensions called *dendrites*, plus one very long extension called the *axon*. The axon's length may be just a few times longer than the cell body, or up to tens of thousands of times longer. Near its extremity the axon splits off into many branches called *telodendria*, and at the tip of these branches are minuscule structures called *synaptic terminals* (or simply *synapses*), which are connected to the dendrites or cell bodies of other neurons.[3] Biological neurons produce short electrical impulses called *action potentials* (APs, or just *signals*) which travel along the axons and make the synapses release chemical signals called *neurotransmitters*. When a neuron receives a sufficient amount of these neurotransmitters within a few milliseconds, it fires its own electrical impulses (actually, it depends on the neurotransmitters, as some of them inhibit the neuron from firing).

3 They are not actually attached, just so close that they can very quickly exchange chemical signals.

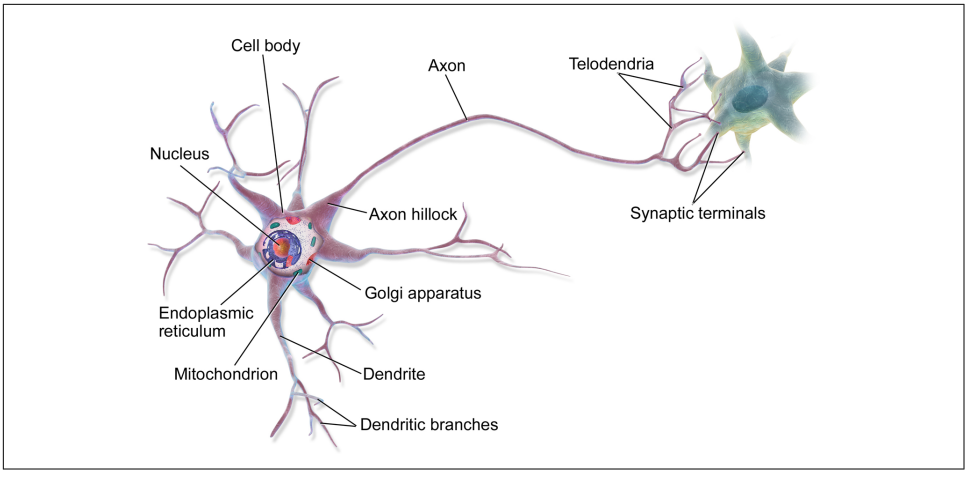


Figure 10-1. Biological neuron[4]

Thus, individual biological neurons seem to behave in a rather simple way, but they are organized in a vast network of billions, with each neuron typically connected to thousands of other neurons. Highly complex computations can be performed by a network of fairly simple neurons, much like a complex anthill can emerge from the combined efforts of simple ants. The architecture of biological neural networks (BNNs)[5] is still the subject of active research, but some parts of the brain have been mapped, and it seems that neurons are often organized in consecutive layers, especially in the cerebral cortex (i.e., the outer layer of your brain), as shown in Figure 10-2.

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

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

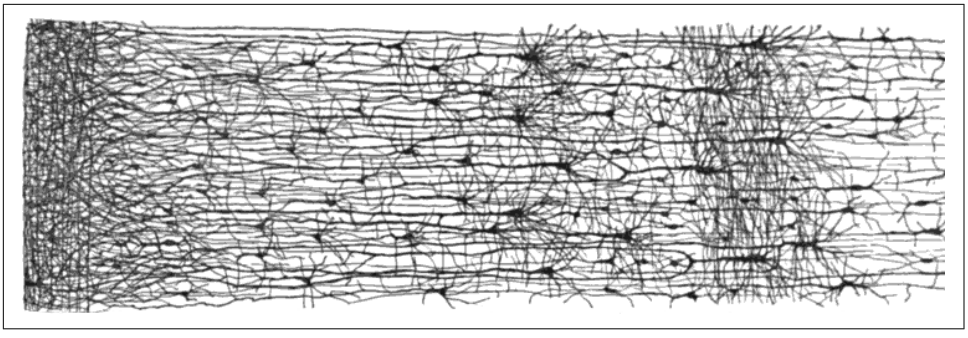


Figure 10-2. Multiple layers in a biological neural network (human cortex)[6]

Logical Computations with Neurons

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

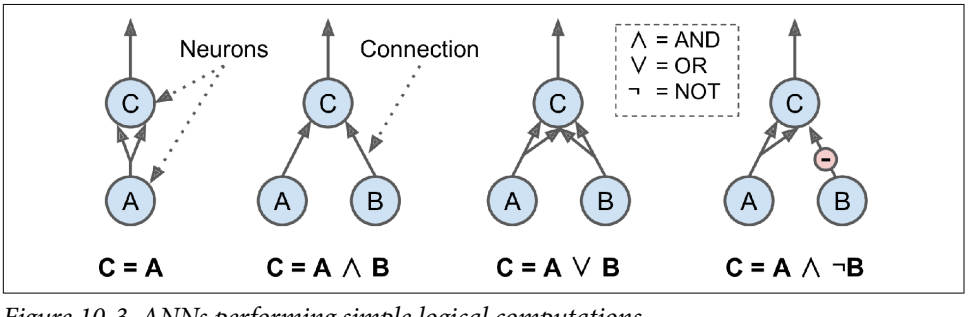


Figure 10-3. ANNs performing simple logical computations

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

Let's see what these networks do:

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

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

The Perceptron

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

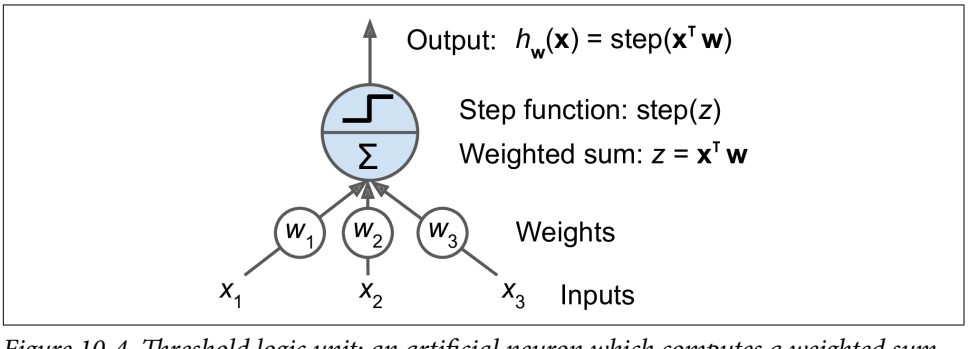


Figure 10-4. Threshold logic unit: an artificial neuron which computes a weighted sum of its inputs then applies a step function

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

Equation 10-1. Common step functions used in Perceptrons (assuming threshold = 0)

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

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

A Perceptron is simply composed of a single layer of TLUs,[7] with each TLU connected to all the inputs. When all the neurons in a layer are connected to every neuron in the previous layer (i.e., its input neurons), the layer is called a *fully connected layer*, or a *dense layer*. The inputs of the Perceptron are fed to special passthrough neurons called *input neurons*: they output whatever input they are fed. All the input neurons form the *input layer*. Moreover, an extra bias feature is generally added ($x_0 = 1$): it is typically represented using a special type of neuron called a *bias neuron*, which outputs 1 all the time. A Perceptron with two inputs and three outputs is represented in Figure 10-5. This Perceptron can classify instances simultaneously into three different binary classes, which makes it a multioutput classifier.

7 The name *Perceptron* is sometimes used to mean a tiny network with a single TLU.

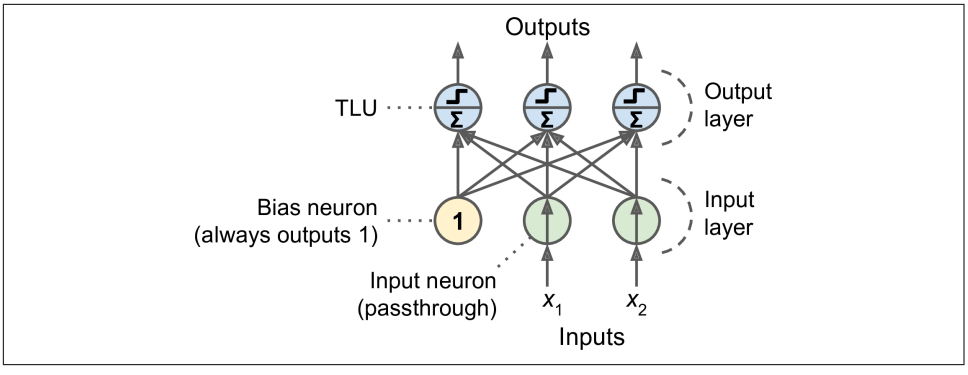


Figure 10-5. Architecture of a Perceptron with two input neurons, one bias neuron, and three output neurons

Thanks to the magic of linear algebra, Equation 10-2 makes it possible to efficiently compute the outputs of a layer of artificial neurons for several instances at once.

Equation 10-2. Computing the outputs of a fully connected layer

$$h_{\mathbf{W},\mathbf{b}}(\mathbf{X}) = \phi(\mathbf{X}\mathbf{W} + \mathbf{b})$$

In this equation:

- As always, **X** represents the matrix of input features. It has one row per instance and one column per feature.
- The weight matrix **W** contains all the connection weights except for the ones from the bias neuron. It has one row per input neuron and one column per artificial neuron in the layer.
- The bias vector **b** contains all the connection weights between the bias neuron and the artificial neurons. It has one bias term per artificial neuron.
- The function ϕ is called the *activation function*: when the artificial neurons are TLUs, it is a step function (but we will discuss other activation functions shortly).

So, how is a Perceptron trained? The Perceptron training algorithm proposed by Rosenblatt was largely inspired by *Hebb's rule*. In his 1949 book *The Organization of Behavior* (Wiley), Donald Hebb suggested that when a biological neuron triggers another neuron often, the connection between these two neurons grows stronger. Siegrid Löwel later summarized Hebb's idea in the catchy phrase, "Cells that fire together, wire together"; that is, the connection weight between two neurons tends to increase when they fire simultaneously. This rule later became known as Hebb's rule (or *Hebbian learning*). Perceptrons are trained using a variant of this rule that takes into account the error made by the network when it makes a prediction; the

Perceptron learning rule reinforces connections that help reduce the error. More specifically, the Perceptron is fed one training instance at a time, and for each instance it makes its predictions. For every output neuron that produced a wrong prediction, it reinforces the connection weights from the inputs that would have contributed to the correct prediction. The rule is shown in Equation 10-3.

Equation 10-3. Perceptron learning rule (weight update)

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

In this equation:

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

The decision boundary of each output neuron is linear, so Perceptrons are incapable of learning complex patterns (just like Logistic Regression classifiers). However, if the training instances are linearly separable, Rosenblatt demonstrated that this algorithm would converge to a solution.[8] This is called the *Perceptron convergence theorem*.

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

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

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

per_clf = Perceptron()
per_clf.fit(X, y)

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

8 Note that this solution is not unique: when data points are linearly separable, there is an infinity of hyperplanes that can separate them.

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

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

In their 1969 monograph *Perceptrons*, Marvin Minsky and Seymour Papert highlighted a number of serious weaknesses of Perceptrons—in particular, the fact that they are incapable of solving some trivial problems (e.g., the *Exclusive OR* (XOR) classification problem; see the left side of Figure 10-6). This is true of any other linear classification model (such as Logistic Regression classifiers), but researchers had expected much more from Perceptrons, and some were so disappointed that they dropped neural networks altogether in favor of higher-level problems such as logic, problem solving, and search.

It turns out that some of the limitations of Perceptrons can be eliminated by stacking multiple Perceptrons. The resulting ANN is called a *Multilayer Perceptron* (MLP). An MLP can solve the XOR problem, as you can verify by computing the output of the MLP represented on the right side of Figure 10-6: with inputs (0, 0) or (1, 1), the network outputs 0, and with inputs (0, 1) or (1, 0) it outputs 1. All connections have a weight equal to 1, except the four connections where the weight is shown. Try verifying that this network indeed solves the XOR problem!

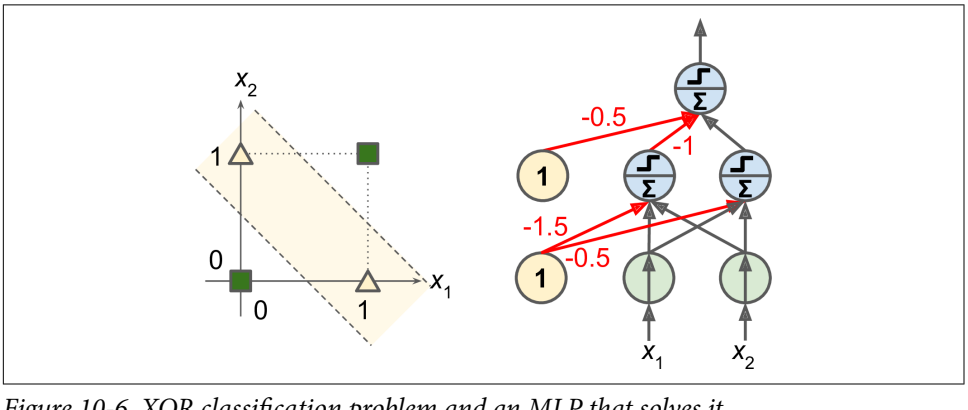


Figure 10-6. XOR classification problem and an MLP that solves it

The Multilayer Perceptron and Backpropagation

An MLP is composed of one (passthrough) *input layer*, one or more layers of TLUs, called *hidden layers*, and one final layer of TLUs called the *output layer* (see Figure 10-7). The layers close to the input layer are usually called the *lower layers*, and the ones close to the outputs are usually called the *upper layers*. Every layer except the output layer includes a bias neuron and is fully connected to the next layer.

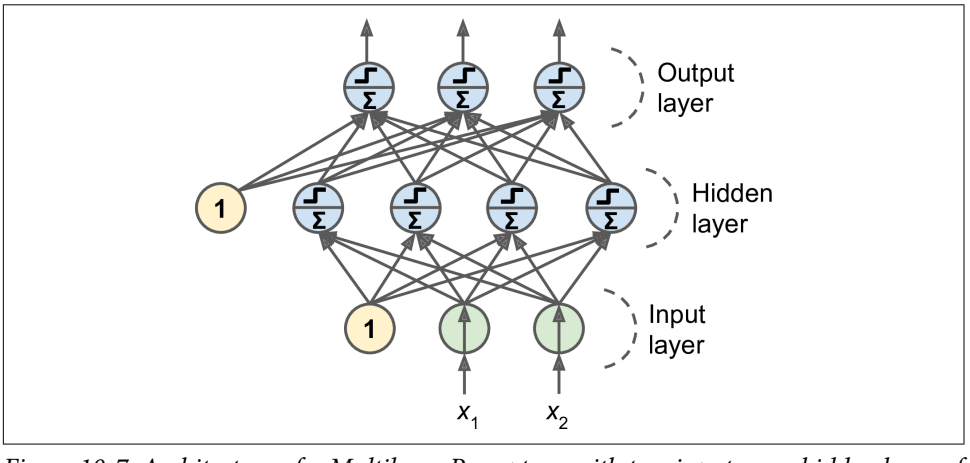


Figure 10-7. Architecture of a Multilayer Perceptron with two inputs, one hidden layer of four neurons, and three output neurons (the bias neurons are shown here, but usually they are implicit)

The signal flows only in one direction (from the inputs to the outputs), so this architecture is an example of a *feedforward neural network* (FNN).

When an ANN contains a deep stack of hidden layers,[9] it is called a *deep neural network* (DNN). The field of Deep Learning studies DNNs, and more generally models containing deep stacks of computations. Even so, many people talk about Deep Learning whenever neural networks are involved (even shallow ones).

For many years researchers struggled to find a way to train MLPs, without success. But in 1986, David Rumelhart, Geoffrey Hinton, and Ronald Williams published a

9 In the 1990s, an ANN with more than two hidden layers was considered deep. Nowadays, it is common to see ANNs with dozens of layers, or even hundreds, so the definition of "deep" is quite fuzzy.

groundbreaking paper[10] that introduced the *backpropagation* training algorithm, which is still used today. In short, it is Gradient Descent (introduced in Chapter 4) using an efficient technique for computing the gradients automatically:[11] in just two passes through the network (one forward, one backward), the backpropagation algorithm is able to compute the gradient of the network's error with regard to every single model parameter. In other words, it can find out how each connection weight and each bias term should be tweaked in order to reduce the error. Once it has these gradients, it just performs a regular Gradient Descent step, and the whole process is repeated until the network converges to the solution.

Automatically computing gradients is called *automatic differentiation*, or *autodiff*. There are various autodiff techniques, with different pros and cons. The one used by backpropagation is called *reverse-mode autodiff*. It is fast and precise, and is well suited when the function to differentiate has many variables (e.g., connection weights) and few outputs (e.g., one loss). If you want to learn more about autodiff, check out Appendix D.

Let's run through this algorithm in a bit more detail:

- It handles one mini-batch at a time (for example, containing 32 instances each), and it goes through the full training set multiple times. Each pass is called an *epoch*.
- Each mini-batch is passed to the network's input layer, which sends it to the first hidden layer. The algorithm then computes the output of all the neurons in this layer (for every instance in the mini-batch). The result is passed on to the next layer, its output is computed and passed to the next layer, and so on until we get the output of the last layer, the output layer. This is the *forward pass*: it is exactly like making predictions, except all intermediate results are preserved since they are needed for the backward pass.
- Next, the algorithm measures the network's output error (i.e., it uses a loss function that compares the desired output and the actual output of the network, and returns some measure of the error).
- Then it computes how much each output connection contributed to the error. This is done analytically by applying the *chain rule* (perhaps the most fundamental rule in calculus), which makes this step fast and precise.

10 David Rumelhart et al. "Learning Internal Representations by Error Propagation," (Defense Technical Information Center technical report, September 1985).

11 This technique was actually independently invented several times by various researchers in different fields, starting with Paul Werbos in 1974.

- The algorithm then measures how much of these error contributions came from each connection in the layer below, again using the chain rule, working backward until the algorithm reaches the input layer. As explained earlier, this reverse pass efficiently measures the error gradient across all the connection weights in the network by propagating the error gradient backward through the network (hence the name of the algorithm).
- Finally, the algorithm performs a Gradient Descent step to tweak all the connection weights in the network, using the error gradients it just computed.

This algorithm is so important that it's worth summarizing it again: for each training instance, the backpropagation algorithm first makes a prediction (forward pass) and measures the error, then goes through each layer in reverse to measure the error contribution from each connection (reverse pass), and finally tweaks the connection weights to reduce the error (Gradient Descent step).

It is important to initialize all the hidden layers' connection weights randomly, or else training will fail. For example, if you initialize all weights and biases to zero, then all neurons in a given layer will be perfectly identical, and thus backpropagation will affect them in exactly the same way, so they will remain identical. In other words, despite having hundreds of neurons per layer, your model will act as if it had only one neuron per layer: it won't be too smart. If instead you randomly initialize the weights, you *break the symmetry* and allow backpropagation to train a diverse team of neurons.

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

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

The Rectified Linear Unit function: ReLU(z) = max(0, z)

The ReLU function is continuous but unfortunately not differentiable at $z = 0$ (the slope changes abruptly, which can make Gradient Descent bounce around), and its derivative is 0 for $z < 0$. In practice, however, it works very well and has the advantage of being fast to compute, so it has become the default.[12] Most importantly, the fact that it does not have a maximum output value helps reduce some issues during Gradient Descent (we will come back to this in Chapter 11).

These popular activation functions and their derivatives are represented in Figure 10-8. But wait! Why do we need activation functions in the first place? Well, if you chain several linear transformations, all you get is a linear transformation. For example, if $f(x) = 2x + 3$ and $g(x) = 5x - 1$, then chaining these two linear functions gives you another linear function: $f(g(x)) = 2(5x - 1) + 3 = 10x + 1$. So if you don't have some nonlinearity between layers, then even a deep stack of layers is equivalent to a single layer, and you can't solve very complex problems with that. Conversely, a large enough DNN with nonlinear activations can theoretically approximate any continuous function.

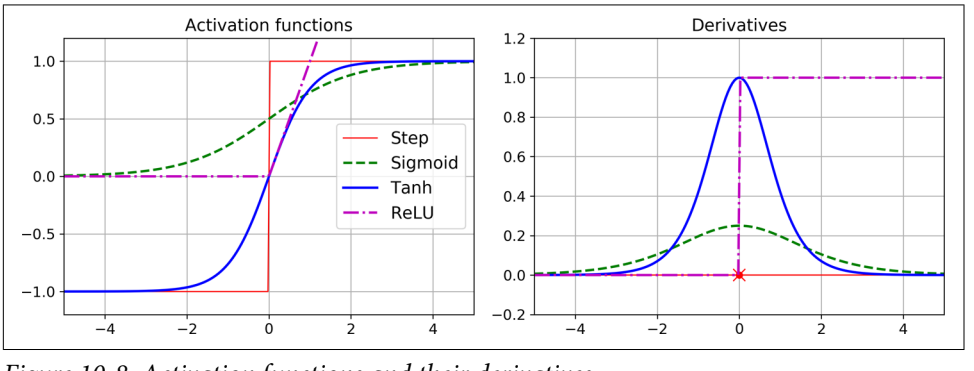


Figure 10-8. Activation functions and their derivatives

OK! You know where neural nets came from, what their architecture is, and how to compute their outputs. You've also learned about the backpropagation algorithm. But what exactly can you do with them?

Regression MLPs

First, MLPs can be used for regression tasks. If you want to predict a single value (e.g., the price of a house, given many of its features), then you just need a single output neuron: its output is the predicted value. For multivariate regression (i.e., to predict

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

multiple values at once), you need one output neuron per output dimension. For example, to locate the center of an object in an image, you need to predict 2D coordinates, so you need two output neurons. If you also want to place a bounding box around the object, then you need two more numbers: the width and the height of the object. So, you end up with four output neurons.

In general, when building an MLP for regression, you do not want to use any activation function for the output neurons, so they are free to output any range of values. If you want to guarantee that the output will always be positive, then you can use the ReLU activation function in the output layer. Alternatively, you can use the *softplus* activation function, which is a smooth variant of ReLU: $\text{softplus}(z) = \log(1 + \exp(z))$. It is close to 0 when z is negative, and close to z when z is positive. Finally, if you want to guarantee that the predictions will fall within a given range of values, then you can use the logistic function or the hyperbolic tangent, and then scale the labels to the appropriate range: 0 to 1 for the logistic function and –1 to 1 for the hyperbolic tangent.

The loss function to use during training is typically the mean squared error, but if you have a lot of outliers in the training set, you may prefer to use the mean absolute error instead. Alternatively, you can use the Huber loss, which is a combination of both.

The Huber loss is quadratic when the error is smaller than a threshold δ (typically 1) but linear when the error is larger than δ. The linear part makes it less sensitive to outliers than the mean squared error, and the quadratic part allows it to converge faster and be more precise than the mean absolute error.

Table 10-1 summarizes the typical architecture of a regression MLP.

Table 10-1. Typical regression MLP architecture

Hyperparameter	Typical value
# input neurons	One per input feature (e.g., 28 x 28 = 784 for MNIST)
# hidden layers	Depends on the problem, but typically 1 to 5
# neurons per hidden layer	Depends on the problem, but typically 10 to 100
# output neurons	1 per prediction dimension
Hidden activation	ReLU (or SELU, see Chapter 11)
Output activation	None, or ReLU/softplus (if positive outputs) or logistic/tanh (if bounded outputs)
Loss function	MSE or MAE/Huber (if outliers)

Classification MLPs

MLPs can also be used for classification tasks. For a binary classification problem, you just need a single output neuron using the logistic activation function: the output will be a number between 0 and 1, which you can interpret as the estimated probability of the positive class. The estimated probability of the negative class is equal to one minus that number.

MLPs can also easily handle multilabel binary classification tasks (see Chapter 3). For example, you could have an email classification system that predicts whether each incoming email is ham or spam, and simultaneously predicts whether it is an urgent or nonurgent email. In this case, you would need two output neurons, both using the logistic activation function: the first would output the probability that the email is spam, and the second would output the probability that it is urgent. More generally, you would dedicate one output neuron for each positive class. Note that the output probabilities do not necessarily add up to 1. This lets the model output any combination of labels: you can have nonurgent ham, urgent ham, nonurgent spam, and perhaps even urgent spam (although that would probably be an error).

If each instance can belong only to a single class, out of three or more possible classes (e.g., classes 0 through 9 for digit image classification), then you need to have one output neuron per class, and you should use the softmax activation function for the whole output layer (see Figure 10-9). The softmax function (introduced in Chapter 4) will ensure that all the estimated probabilities are between 0 and 1 and that they add up to 1 (which is required if the classes are exclusive). This is called multiclass classification.

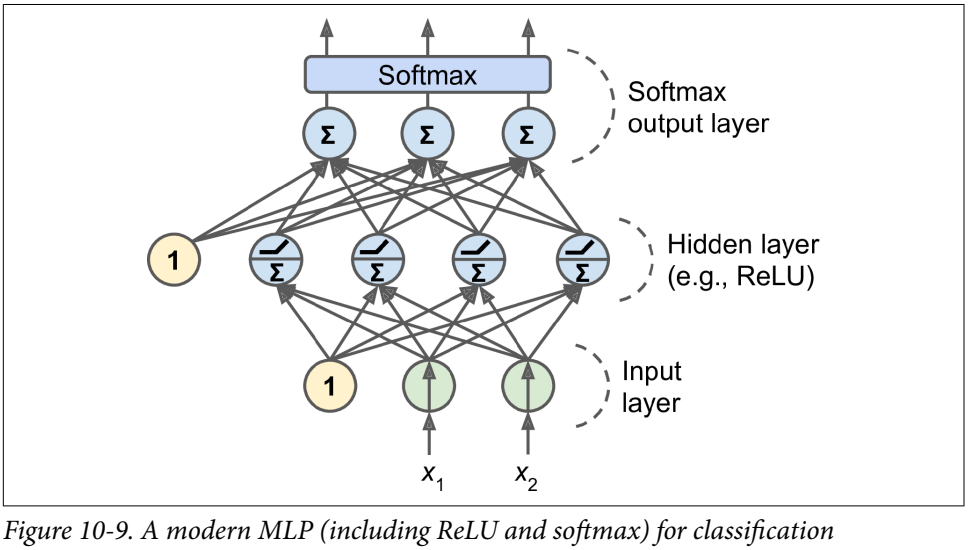


Figure 10-9. A modern MLP (including ReLU and softmax) for classification

Regarding the loss function, since we are predicting probability distributions, the cross-entropy loss (also called the log loss, see Chapter 4) is generally a good choice.

Table 10-2 summarizes the typical architecture of a classification MLP.

Table 10-2. Typical classification MLP architecture

Hyperparameter	Binary classification	Multilabel binary classification	Multiclass classification
Input and hidden layers	Same as regression	Same as regression	Same as regression
# output neurons	1	1 per label	1 per class
Output layer activation	Logistic	Logistic	Softmax
Loss function	Cross entropy	Cross entropy	Cross entropy

Before we go on, I recommend you go through exercise 1 at the end of this chapter. You will play with various neural network architectures and visualize their outputs using the *TensorFlow Playground*. This will be very useful to better understand MLPs, including the effects of all the hyperparameters (number of layers and neurons, activation functions, and more).

Now you have all the concepts you need to start implementing MLPs with Keras!

Implementing MLPs with Keras

Keras is a high-level Deep Learning API that allows you to easily build, train, evaluate, and execute all sorts of neural networks. Its documentation (or specification) is available at *https://keras.io/*. The reference implementation, also called Keras, was developed by François Chollet as part of a research project[13] and was released as an open source project in March 2015. It quickly gained popularity, owing to its ease of use, flexibility, and beautiful design. To perform the heavy computations required by neural networks, this reference implementation relies on a computation backend. At present, you can choose from three popular open source Deep Learning libraries: TensorFlow, Microsoft Cognitive Toolkit (CNTK), and Theano. Therefore, to avoid any confusion, we will refer to this reference implementation as *multibackend Keras*.

Since late 2016, other implementations have been released. You can now run Keras on Apache MXNet, Apple's Core ML, JavaScript or TypeScript (to run Keras code in a web browser), and PlaidML (which can run on all sorts of GPU devices, not just Nvidia). Moreover, TensorFlow itself now comes bundled with its own Keras implementation, tf.keras. It only supports TensorFlow as the backend, but it has the advantage of offering some very useful extra features (see Figure 10-10): for example, it supports

13 Project ONEIROS (Open-ended Neuro-Electronic Intelligent Robot Operating System).

TensorFlow's Data API, which makes it easy to load and preprocess data efficiently. For this reason, we will use tf.keras in this book. However, in this chapter we will not use any of the TensorFlow-specific features, so the code should run fine on other Keras implementations as well (at least in Python), with only minor modifications, such as changing the imports.

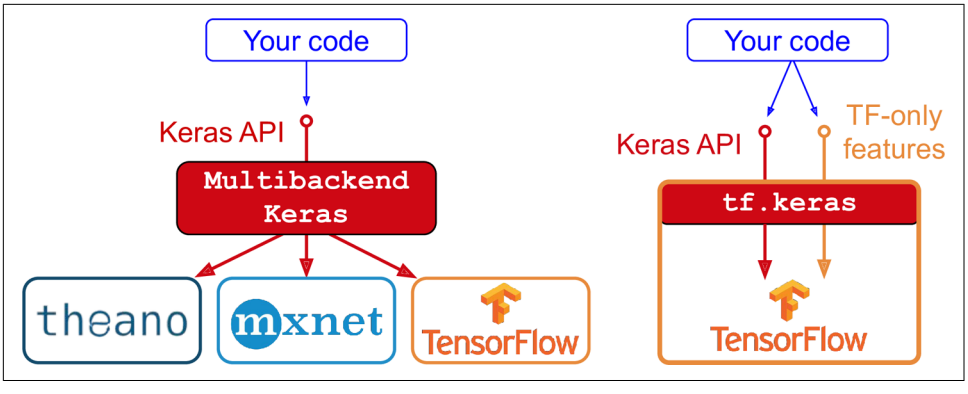


Figure 10-10. Two implementations of the Keras API: multibackend Keras (left) and tf.keras (right)

The most popular Deep Learning library, after Keras and TensorFlow, is Facebook's PyTorch library. The good news is that its API is quite similar to Keras's (in part because both APIs were inspired by Scikit-Learn and Chainer), so once you know Keras, it is not difficult to switch to PyTorch, if you ever want to. PyTorch's popularity grew exponentially in 2018, largely thanks to its simplicity and excellent documentation, which were not TensorFlow 1.x's main strengths. However, TensorFlow 2 is arguably just as simple as PyTorch, as it has adopted Keras as its official high-level API and its developers have greatly simplified and cleaned up the rest of the API. The documentation has also been completely reorganized, and it is much easier to find what you need now. Similarly, PyTorch's main weaknesses (e.g., limited portability and no computation graph analysis) have been largely addressed in PyTorch 1.0. Healthy competition is beneficial to everyone.

All right, it's time to code! As tf.keras is bundled with TensorFlow, let's start by installing TensorFlow.

Installing TensorFlow 2

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

```
$ cd $ML_PATH                # Your ML working directory (e.g., $HOME/ml)
$ source my_env/bin/activate # on Linux or macOS
$ .\my_env\Scripts\activate  # on Windows
```

Next, install TensorFlow 2 (if you are not using a virtualenv, you will need administrator rights, or to add the `--user` option):

```
$ python3 -m pip install -U tensorflow
```

For GPU support, at the time of this writing you need to install `tensorflow-gpu` instead of `tensorflow`, but the TensorFlow team is working on having a single library that will support both CPU-only and GPU-equipped systems. You will still need to install extra libraries for GPU support (see *https://tensorflow.org/install* for more details). We will look at GPUs in more depth in Chapter 19.

To test your installation, open a Python shell or a Jupyter notebook, then import TensorFlow and tf.keras and print their versions:

```
>>> import tensorflow as tf
>>> from tensorflow import keras
>>> tf.__version__
'2.0.0'
>>> keras.__version__
'2.2.4-tf'
```

The second version is the version of the Keras API implemented by tf.keras. Note that it ends with `-tf`, highlighting the fact that tf.keras implements the Keras API, plus some extra TensorFlow-specific features.

Now let's use tf.keras! We'll start by building a simple image classifier.

Building an Image Classifier Using the Sequential API

First, we need to load a dataset. In this chapter we will tackle Fashion MNIST, which is a drop-in replacement of MNIST (introduced in Chapter 3). It has the exact same format as MNIST (70,000 grayscale images of 28 × 28 pixels each, with 10 classes), but the images represent fashion items rather than handwritten digits, so each class is more diverse, and the problem turns out to be significantly more challenging than MNIST. For example, a simple linear model reaches about 92% accuracy on MNIST, but only about 83% on Fashion MNIST.

Using Keras to load the dataset

Keras provides some utility functions to fetch and load common datasets, including MNIST, Fashion MNIST, and the California housing dataset we used in Chapter 2. Let's load Fashion MNIST:

```
fashion_mnist = keras.datasets.fashion_mnist
(X_train_full, y_train_full), (X_test, y_test) = fashion_mnist.load_data()
```

When loading MNIST or Fashion MNIST using Keras rather than Scikit-Learn, one important difference is that every image is represented as a 28 × 28 array rather than a 1D array of size 784. Moreover, the pixel intensities are represented as integers (from 0 to 255) rather than floats (from 0.0 to 255.0). Let's take a look at the shape and data type of the training set:

```
>>> X_train_full.shape
(60000, 28, 28)
>>> X_train_full.dtype
dtype('uint8')
```

Note that the dataset is already split into a training set and a test set, but there is no validation set, so we'll create one now. Additionally, since we are going to train the neural network using Gradient Descent, we must scale the input features. For simplicity, we'll scale the pixel intensities down to the 0–1 range by dividing them by 255.0 (this also converts them to floats):

```
X_valid, X_train = X_train_full[:5000] / 255.0, X_train_full[5000:] / 255.0
y_valid, y_train = y_train_full[:5000], y_train_full[5000:]
```

With MNIST, when the label is equal to 5, it means that the image represents the handwritten digit 5. Easy. For Fashion MNIST, however, we need the list of class names to know what we are dealing with:

```
class_names = ["T-shirt/top", "Trouser", "Pullover", "Dress", "Coat",
               "Sandal", "Shirt", "Sneaker", "Bag", "Ankle boot"]
```

For example, the first image in the training set represents a coat:

```
>>> class_names[y_train[0]]
'Coat'
```

Figure 10-11 shows some samples from the Fashion MNIST dataset.

Figure 10-11. Samples from Fashion MNIST

Creating the model using the Sequential API

Now let's build the neural network! Here is a classification MLP with two hidden layers:

```
model = keras.models.Sequential()
model.add(keras.layers.Flatten(input_shape=[28, 28]))
model.add(keras.layers.Dense(300, activation="relu"))
model.add(keras.layers.Dense(100, activation="relu"))
model.add(keras.layers.Dense(10, activation="softmax"))
```

Let's go through this code line by line:

- The first line creates a `Sequential` model. This is the simplest kind of Keras model for neural networks that are just composed of a single stack of layers connected sequentially. This is called the Sequential API.
- Next, we build the first layer and add it to the model. It is a `Flatten` layer whose role is to convert each input image into a 1D array: if it receives input data `X`, it computes `X.reshape(-1, 1)`. This layer does not have any parameters; it is just there to do some simple preprocessing. Since it is the first layer in the model, you should specify the `input_shape`, which doesn't include the batch size, only the shape of the instances. Alternatively, you could add a `keras.layers.InputLayer` as the first layer, setting `input_shape=[28,28]`.
- Next we add a `Dense` hidden layer with 300 neurons. It will use the ReLU activation function. Each `Dense` layer manages its own weight matrix, containing all the connection weights between the neurons and their inputs. It also manages a vector of bias terms (one per neuron). When it receives some input data, it computes Equation 10-2.
- Then we add a second `Dense` hidden layer with 100 neurons, also using the ReLU activation function.
- Finally, we add a `Dense` output layer with 10 neurons (one per class), using the softmax activation function (because the classes are exclusive).

Specifying `activation="relu"` is equivalent to specifying `activation=keras.activations.relu`. Other activation functions are available in the `keras.activations` package, we will use many of them in this book. See *https://keras.io/activations/* for the full list.

Instead of adding the layers one by one as we just did, you can pass a list of layers when creating the `Sequential` model:

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

Using Code Examples from keras.io

Code examples documented on keras.io will work fine with tf.keras, but you need to change the imports. For example, consider this keras.io code:

```
from keras.layers import Dense
output_layer = Dense(10)
```

You must change the imports like this:

```
from tensorflow.keras.layers import Dense
output_layer = Dense(10)
```

Or simply use full paths, if you prefer:

```
from tensorflow import keras
output_layer = keras.layers.Dense(10)
```

This approach is more verbose, but I use it in this book so you can easily see which packages to use, and to avoid confusion between standard classes and custom classes. In production code, I prefer the previous approach. Many people also use `from tensorflow.keras import layers` followed by `layers.Dense(10)`.

The model's `summary()` method displays all the model's layers,[14] including each layer's name (which is automatically generated unless you set it when creating the layer), its output shape (`None` means the batch size can be anything), and its number of parameters. The summary ends with the total number of parameters, including trainable and non-trainable parameters. Here we only have trainable parameters (we will see examples of non-trainable parameters in Chapter 11):

```
>>> model.summary()
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
flatten (Flatten)            (None, 784)               0
_________________________________________________________________
dense (Dense)                (None, 300)               235500
_________________________________________________________________
```

14 You can use `keras.utils.plot_model()` to generate an image of your model.

```
dense_1 (Dense)              (None, 100)               30100
_________________________________________________________________
dense_2 (Dense)              (None, 10)                1010
=================================================================
Total params: 266,610
Trainable params: 266,610
Non-trainable params: 0
_________________________________________________________________
```

Note that `Dense` layers often have a *lot* of parameters. For example, the first hidden layer has 784 × 300 connection weights, plus 300 bias terms, which adds up to 235,500 parameters! This gives the model quite a lot of flexibility to fit the training data, but it also means that the model runs the risk of overfitting, especially when you do not have a lot of training data. We will come back to this later.

You can easily get a model's list of layers, to fetch a layer by its index, or you can fetch it by name:

```
>>> model.layers
[<tensorflow.python.keras.layers.core.Flatten at 0x132414e48>,
 <tensorflow.python.keras.layers.core.Dense at 0x1324149b0>,
 <tensorflow.python.keras.layers.core.Dense at 0x1356ba8d0>,
 <tensorflow.python.keras.layers.core.Dense at 0x13240d240>]
>>> hidden1 = model.layers[1]
>>> hidden1.name
'dense'
>>> model.get_layer('dense') is hidden1
True
```

All the parameters of a layer can be accessed using its `get_weights()` and `set_weights()` methods. For a `Dense` layer, this includes both the connection weights and the bias terms:

```
>>> weights, biases = hidden1.get_weights()
>>> weights
array([[ 0.02448617, -0.00877795, -0.02189048, ..., -0.02766046,
         0.03859074, -0.06889391],
       ...,
       [-0.06022581,  0.01577859, -0.02585464, ..., -0.00527829,
         0.00272203, -0.06793761]], dtype=float32)
>>> weights.shape
(784, 300)
>>> biases
array([0., 0., 0., 0., 0., 0., 0., 0., 0., ...,  0., 0., 0.], dtype=float32)
>>> biases.shape
(300,)
```

Notice that the `Dense` layer initialized the connection weights randomly (which is needed to break symmetry, as we discussed earlier), and the biases were initialized to zeros, which is fine. If you ever want to use a different initialization method, you can set `kernel_initializer` (*kernel* is another name for the matrix of connection

weights) or `bias_initializer` when creating the layer. We will discuss initializers further in Chapter 11, but if you want the full list, see *https://keras.io/initializers/*.

The shape of the weight matrix depends on the number of inputs. This is why it is recommended to specify the `input_shape` when creating the first layer in a `Sequential` model. However, if you do not specify the input shape, it's OK: Keras will simply wait until it knows the input shape before it actually builds the model. This will happen either when you feed it actual data (e.g., during training), or when you call its `build()` method. Until the model is really built, the layers will not have any weights, and you will not be able to do certain things (such as print the model summary or save the model). So, if you know the input shape when creating the model, it is best to specify it.

Compiling the model

After a model is created, you must call its `compile()` method to specify the loss function and the optimizer to use. Optionally, you can specify a list of extra metrics to compute during training and evaluation:

```
model.compile(loss="sparse_categorical_crossentropy",
              optimizer="sgd",
              metrics=["accuracy"])
```

Using `loss="sparse_categorical_crossentropy"` is equivalent to using `loss=keras.losses.sparse_categorical_crossentropy`. Similarly, specifying `optimizer="sgd"` is equivalent to specifying `optimizer=keras.optimizers.SGD()`, and `metrics=["accuracy"]` is equivalent to `metrics=[keras.metrics.sparse_categorical_accuracy]` (when using this loss). We will use many other losses, optimizers, and metrics in this book; for the full lists, see *https://keras.io/losses*, *https://keras.io/optimizers*, and *https://keras.io/metrics*.

This code requires some explanation. First, we use the `"sparse_categorical_crossentropy"` loss because we have sparse labels (i.e., for each instance, there is just a target class index, from 0 to 9 in this case), and the classes are exclusive. If instead we had one target probability per class for each instance (such as one-hot vectors, e.g. `[0., 0., 0., 1., 0., 0., 0., 0., 0., 0.]` to represent class 3), then we would need to use the `"categorical_crossentropy"` loss instead. If we were doing binary classification (with one or more binary labels), then we would use the `"sigmoid"` (i.e., logistic) activation function in the output layer instead of the `"softmax"` activation function, and we would use the `"binary_crossentropy"` loss.

If you want to convert sparse labels (i.e., class indices) to one-hot vector labels, use the `keras.utils.to_categorical()` function. To go the other way round, use the `np.argmax()` function with `axis=1`.

Regarding the optimizer, `"sgd"` means that we will train the model using simple Stochastic Gradient Descent. In other words, Keras will perform the backpropagation algorithm described earlier (i.e., reverse-mode autodiff plus Gradient Descent). We will discuss more efficient optimizers in Chapter 11 (they improve the Gradient Descent part, not the autodiff).

When using the `SGD` optimizer, it is important to tune the learning rate. So, you will generally want to use `optimizer=keras.optimizers.SGD(lr=???)` to set the learning rate, rather than `optimizer="sgd"`, which defaults to `lr=0.01`.

Finally, since this is a classifier, it's useful to measure its `"accuracy"` during training and evaluation.

Training and evaluating the model

Now the model is ready to be trained. For this we simply need to call its `fit()` method:

```
>>> history = model.fit(X_train, y_train, epochs=30,
...                     validation_data=(X_valid, y_valid))
...
Train on 55000 samples, validate on 5000 samples
Epoch 1/30
55000/55000 [======] - 3s 49us/sample - loss: 0.7218     - accuracy: 0.7660
                                       - val_loss: 0.4973 - val_accuracy: 0.8366
Epoch 2/30
55000/55000 [======] - 2s 45us/sample - loss: 0.4840     - accuracy: 0.8327
                                       - val_loss: 0.4456 - val_accuracy: 0.8480
[...]
Epoch 30/30
55000/55000 [======] - 3s 53us/sample - loss: 0.2252     - accuracy: 0.9192
                                       - val_loss: 0.2999 - val_accuracy: 0.8926
```

We pass it the input features (`X_train`) and the target classes (`y_train`), as well as the number of epochs to train (or else it would default to just 1, which would definitely not be enough to converge to a good solution). We also pass a validation set (this is optional). Keras will measure the loss and the extra metrics on this set at the end of each epoch, which is very useful to see how well the model really performs. If the performance on the training set is much better than on the validation set, your model is

probably overfitting the training set (or there is a bug, such as a data mismatch between the training set and the validation set).

And that's it! The neural network is trained.[15] At each epoch during training, Keras displays the number of instances processed so far (along with a progress bar), the mean training time per sample, and the loss and accuracy (or any other extra metrics you asked for) on both the training set and the validation set. You can see that the training loss went down, which is a good sign, and the validation accuracy reached 89.26% after 30 epochs. That's not too far from the training accuracy, so there does not seem to be much overfitting going on.

Instead of passing a validation set using the `validation_data` argument, you could set `validation_split` to the ratio of the training set that you want Keras to use for validation. For example, `validation_split=0.1` tells Keras to use the last 10% of the data (before shuffling) for validation.

If the training set was very skewed, with some classes being overrepresented and others underrepresented, it would be useful to set the `class_weight` argument when calling the `fit()` method, which would give a larger weight to underrepresented classes and a lower weight to overrepresented classes. These weights would be used by Keras when computing the loss. If you need per-instance weights, set the `sample_weight` argument (if both `class_weight` and `sample_weight` are provided, Keras multiplies them). Per-instance weights could be useful if some instances were labeled by experts while others were labeled using a crowdsourcing platform: you might want to give more weight to the former. You can also provide sample weights (but not class weights) for the validation set by adding them as a third item in the `validation_data` tuple.

The `fit()` method returns a `History` object containing the training parameters (`history.params`), the list of epochs it went through (`history.epoch`), and most importantly a dictionary (`history.history`) containing the loss and extra metrics it measured at the end of each epoch on the training set and on the validation set (if any). If you use this dictionary to create a pandas DataFrame and call its `plot()` method, you get the learning curves shown in Figure 10-12:

15 If your training or validation data does not match the expected shape, you will get an exception. This is perhaps the most common error, so you should get familiar with the error message. The message is actually quite clear: for example, if you try to train this model with an array containing flattened images (`X_train.reshape(-1, 784)`), then you will get the following exception: "ValueError: Error when checking input: expected flatten_input to have 3 dimensions, but got array with shape (60000, 784)."

```
import pandas as pd
import matplotlib.pyplot as plt

pd.DataFrame(history.history).plot(figsize=(8, 5))
plt.grid(True)
plt.gca().set_ylim(0, 1) # set the vertical range to [0-1]
plt.show()
```

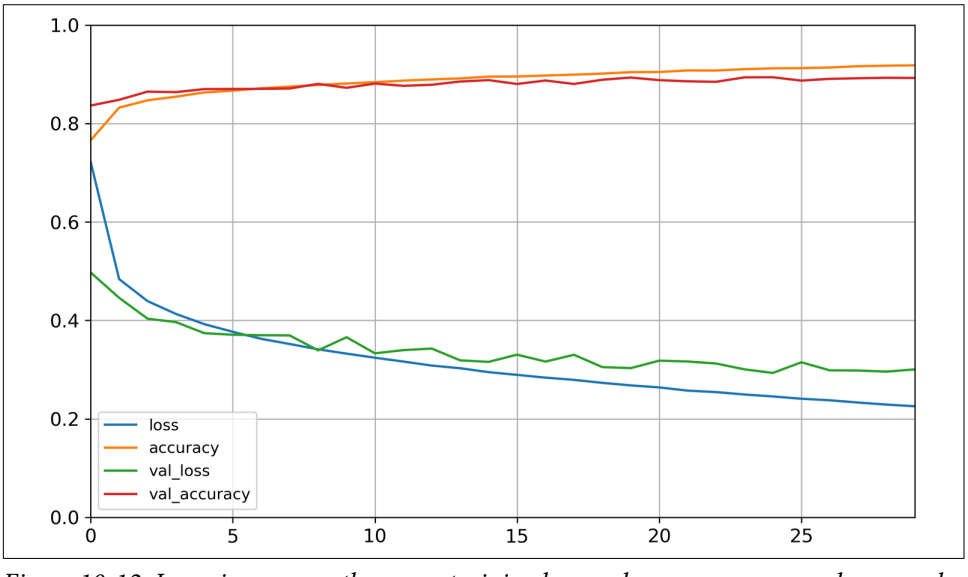


Figure 10-12. Learning curves: the mean training loss and accuracy measured over each epoch, and the mean validation loss and accuracy measured at the end of each epoch

You can see that both the training accuracy and the validation accuracy steadily increase during training, while the training loss and the validation loss decrease. Good! Moreover, the validation curves are close to the training curves, which means that there is not too much overfitting. In this particular case, the model looks like it performed better on the validation set than on the training set at the beginning of training. But that's not the case: indeed, the validation error is computed at the *end* of each epoch, while the training error is computed using a running mean *during* each epoch. So the training curve should be shifted by half an epoch to the left. If you do that, you will see that the training and validation curves overlap almost perfectly at the beginning of training.

When plotting the training curve, it should be shifted by half an epoch to the left.

The training set performance ends up beating the validation performance, as is generally the case when you train for long enough. You can tell that the model has not quite converged yet, as the validation loss is still going down, so you should probably continue training. It's as simple as calling the `fit()` method again, since Keras just continues training where it left off (you should be able to reach close to 89% validation accuracy).

If you are not satisfied with the performance of your model, you should go back and tune the hyperparameters. The first one to check is the learning rate. If that doesn't help, try another optimizer (and always retune the learning rate after changing any hyperparameter). If the performance is still not great, then try tuning model hyperparameters such as the number of layers, the number of neurons per layer, and the types of activation functions to use for each hidden layer. You can also try tuning other hyperparameters, such as the batch size (it can be set in the `fit()` method using the `batch_size` argument, which defaults to 32). We will get back to hyperparameter tuning at the end of this chapter. Once you are satisfied with your model's validation accuracy, you should evaluate it on the test set to estimate the generalization error before you deploy the model to production. You can easily do this using the `evaluate()` method (it also supports several other arguments, such as `batch_size` and `sample_weight`; please check the documentation for more details):

```
>>> model.evaluate(X_test, y_test)
10000/10000 [==========] - 0s 29us/sample - loss: 0.3340 - accuracy: 0.8851
[0.3339798209667206, 0.8851]
```

As we saw in Chapter 2, it is common to get slightly lower performance on the test set than on the validation set, because the hyperparameters are tuned on the validation set, not the test set (however, in this example, we did not do any hyperparameter tuning, so the lower accuracy is just bad luck). Remember to resist the temptation to tweak the hyperparameters on the test set, or else your estimate of the generalization error will be too optimistic.

Using the model to make predictions

Next, we can use the model's `predict()` method to make predictions on new instances. Since we don't have actual new instances, we will just use the first three instances of the test set:

```
>>> X_new = X_test[:3]
>>> y_proba = model.predict(X_new)
>>> y_proba.round(2)
array([[0.  , 0.  , 0.  , 0.  , 0.  , 0.03, 0.  , 0.01, 0.  , 0.96],
       [0.  , 0.  , 0.98, 0.  , 0.02, 0.  , 0.  , 0.  , 0.  , 0.  ],
       [0.  , 1.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  , 0.  ]],
      dtype=float32)
```

As you can see, for each instance the model estimates one probability per class, from class 0 to class 9. For example, for the first image it estimates that the probability of class 9 (ankle boot) is 96%, the probability of class 5 (sandal) is 3%, the probability of class 7 (sneaker) is 1%, and the probabilities of the other classes are negligible. In other words, it "believes" the first image is footwear, most likely ankle boots but possibly sandals or sneakers. If you only care about the class with the highest estimated probability (even if that probability is quite low), then you can use the `predict_classes()` method instead:

```
>>> y_pred = model.predict_classes(X_new)
>>> y_pred
array([9, 2, 1])
>>> np.array(class_names)[y_pred]
array(['Ankle boot', 'Pullover', 'Trouser'], dtype='<U11')
```

Here, the classifier actually classified all three images correctly (these images are shown in Figure 10-13):

```
>>> y_new = y_test[:3]
>>> y_new
array([9, 2, 1])
```

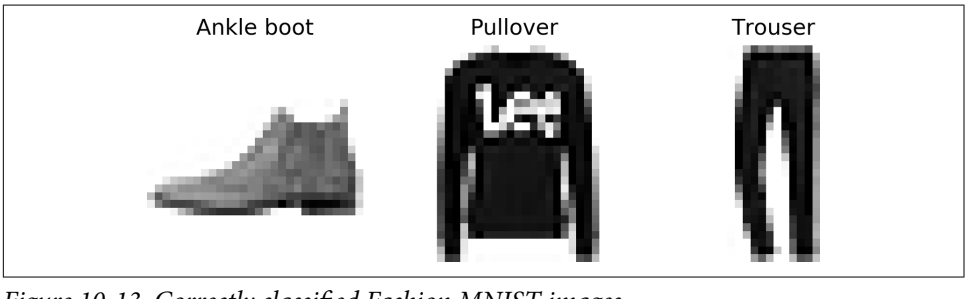


Figure 10-13. Correctly classified Fashion MNIST images

Now you know how to use the Sequential API to build, train, evaluate, and use a classification MLP. But what about regression?

Building a Regression MLP Using the Sequential API

Let's switch to the California housing problem and tackle it using a regression neural network. For simplicity, we will use Scikit-Learn's `fetch_california_housing()` function to load the data. This dataset is simpler than the one we used in Chapter 2, since it contains only numerical features (there is no `ocean_proximity` feature), and there is no missing value. After loading the data, we split it into a training set, a validation set, and a test set, and we scale all the features:

```
from sklearn.datasets import fetch_california_housing
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
```

```
housing = fetch_california_housing()

X_train_full, X_test, y_train_full, y_test = train_test_split(
    housing.data, housing.target)
X_train, X_valid, y_train, y_valid = train_test_split(
    X_train_full, y_train_full)

scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_valid = scaler.transform(X_valid)
X_test = scaler.transform(X_test)
```

Using the Sequential API to build, train, evaluate, and use a regression MLP to make predictions is quite similar to what we did for classification. The main differences are the fact that the output layer has a single neuron (since we only want to predict a single value) and uses no activation function, and the loss function is the mean squared error. Since the dataset is quite noisy, we just use a single hidden layer with fewer neurons than before, to avoid overfitting:

```
model = keras.models.Sequential([
    keras.layers.Dense(30, activation="relu", input_shape=X_train.shape[1:]),
    keras.layers.Dense(1)
])
model.compile(loss="mean_squared_error", optimizer="sgd")
history = model.fit(X_train, y_train, epochs=20,
                    validation_data=(X_valid, y_valid))
mse_test = model.evaluate(X_test, y_test)
X_new = X_test[:3] # pretend these are new instances
y_pred = model.predict(X_new)
```

As you can see, the Sequential API is quite easy to use. However, although `Sequential` models are extremely common, it is sometimes useful to build neural networks with more complex topologies, or with multiple inputs or outputs. For this purpose, Keras offers the Functional API.

Building Complex Models Using the Functional API

One example of a nonsequential neural network is a *Wide & Deep* neural network. This neural network architecture was introduced in a 2016 paper by Heng-Tze Cheng et al.[16] It connects all or part of the inputs directly to the output layer, as shown in Figure 10-14. This architecture makes it possible for the neural network to learn both deep patterns (using the deep path) and simple rules (through the short path).[17] In contrast, a regular MLP forces all the data to flow through the full stack of layers;

16 Heng-Tze Cheng et al., "Wide & Deep Learning for Recommender Systems," *Proceedings of the First Workshop on Deep Learning for Recommender Systems* (2016): 7–10.

17 The short path can also be used to provide manually engineered features to the neural network.

thus, simple patterns in the data may end up being distorted by this sequence of transformations.

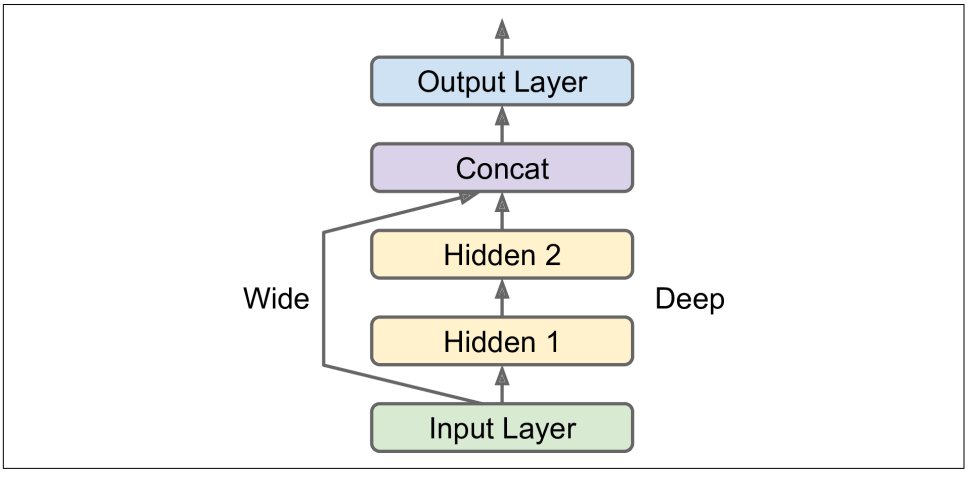


Figure 10-14. Wide & Deep neural network

Let's build such a neural network to tackle the California housing problem:

```
input_ = keras.layers.Input(shape=X_train.shape[1:])
hidden1 = keras.layers.Dense(30, activation="relu")(input_)
hidden2 = keras.layers.Dense(30, activation="relu")(hidden1)
concat = keras.layers.Concatenate()([input_, hidden2])
output = keras.layers.Dense(1)(concat)
model = keras.Model(inputs=[input_], outputs=[output])
```

Let's go through each line of this code:

- First, we need to create an `Input` object.[18] This is a specification of the kind of input the model will get, including its `shape` and `dtype`. A model may actually have multiple inputs, as we will see shortly.
- Next, we create a `Dense` layer with 30 neurons, using the ReLU activation function. As soon as it is created, notice that we call it like a function, passing it the input. This is why this is called the Functional API. Note that we are just telling Keras how it should connect the layers together; no actual data is being processed yet.
- We then create a second hidden layer, and again we use it as a function. Note that we pass it the output of the first hidden layer.

18 The name `input_` is used to avoid overshadowing Python's built-in `input()` function.

- Next, we create a `Concatenate` layer, and once again we immediately use it like a function, to concatenate the input and the output of the second hidden layer. You may prefer the `keras.layers.concatenate()` function, which creates a `Concatenate` layer and immediately calls it with the given inputs.
- Then we create the output layer, with a single neuron and no activation function, and we call it like a function, passing it the result of the concatenation.
- Lastly, we create a Keras `Model`, specifying which inputs and outputs to use.

Once you have built the Keras model, everything is exactly like earlier, so there's no need to repeat it here: you must compile the model, train it, evaluate it, and use it to make predictions.

But what if you want to send a subset of the features through the wide path and a different subset (possibly overlapping) through the deep path (see Figure 10-15)? In this case, one solution is to use multiple inputs. For example, suppose we want to send five features through the wide path (features 0 to 4), and six features through the deep path (features 2 to 7):

```
input_A = keras.layers.Input(shape=[5], name="wide_input")
input_B = keras.layers.Input(shape=[6], name="deep_input")
hidden1 = keras.layers.Dense(30, activation="relu")(input_B)
hidden2 = keras.layers.Dense(30, activation="relu")(hidden1)
concat = keras.layers.concatenate([input_A, hidden2])
output = keras.layers.Dense(1, name="output")(concat)
model = keras.Model(inputs=[input_A, input_B], outputs=[output])
```

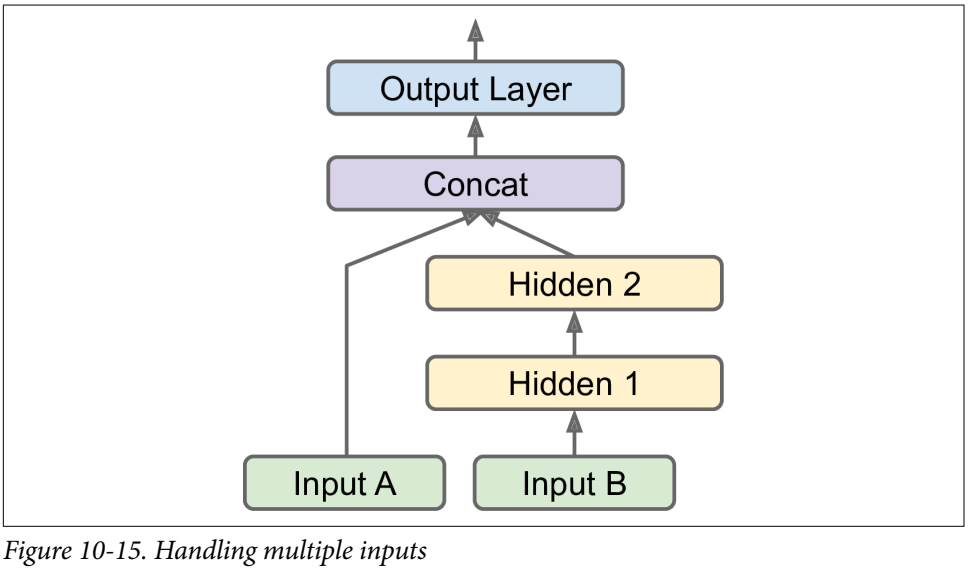


Figure 10-15. Handling multiple inputs

The code is self-explanatory. You should name at least the most important layers, especially when the model gets a bit complex like this. Note that we specified `inputs=[input_A, input_B]` when creating the model. Now we can compile the model as usual, but when we call the `fit()` method, instead of passing a single input matrix `X_train`, we must pass a pair of matrices `(X_train_A, X_train_B)`: one per input.[19] The same is true for `X_valid`, and also for `X_test` and `X_new` when you call `evaluate()` or `predict()`:

```
model.compile(loss="mse", optimizer=keras.optimizers.SGD(lr=1e-3))

X_train_A, X_train_B = X_train[:, :5], X_train[:, 2:]
X_valid_A, X_valid_B = X_valid[:, :5], X_valid[:, 2:]
X_test_A, X_test_B = X_test[:, :5], X_test[:, 2:]
X_new_A, X_new_B = X_test_A[:3], X_test_B[:3]

history = model.fit((X_train_A, X_train_B), y_train, epochs=20,
                    validation_data=((X_valid_A, X_valid_B), y_valid))
mse_test = model.evaluate((X_test_A, X_test_B), y_test)
y_pred = model.predict((X_new_A, X_new_B))
```

There are many use cases in which you may want to have multiple outputs:

- The task may demand it. For instance, you may want to locate and classify the main object in a picture. This is both a regression task (finding the coordinates of the object's center, as well as its width and height) and a classification task.
- Similarly, you may have multiple independent tasks based on the same data. Sure, you could train one neural network per task, but in many cases you will get better results on all tasks by training a single neural network with one output per task. This is because the neural network can learn features in the data that are useful across tasks. For example, you could perform *multitask classification* on pictures of faces, using one output to classify the person's facial expression (smiling, surprised, etc.) and another output to identify whether they are wearing glasses or not.
- Another use case is as a regularization technique (i.e., a training constraint whose objective is to reduce overfitting and thus improve the model's ability to generalize). For example, you may want to add some auxiliary outputs in a neural network architecture (see Figure 10-16) to ensure that the underlying part of the network learns something useful on its own, without relying on the rest of the network.

19 Alternatively, you can pass a dictionary mapping the input names to the input values, like `{"wide_input": X_train_A, "deep_input": X_train_B}`. This is especially useful when there are many inputs, to avoid getting the order wrong.

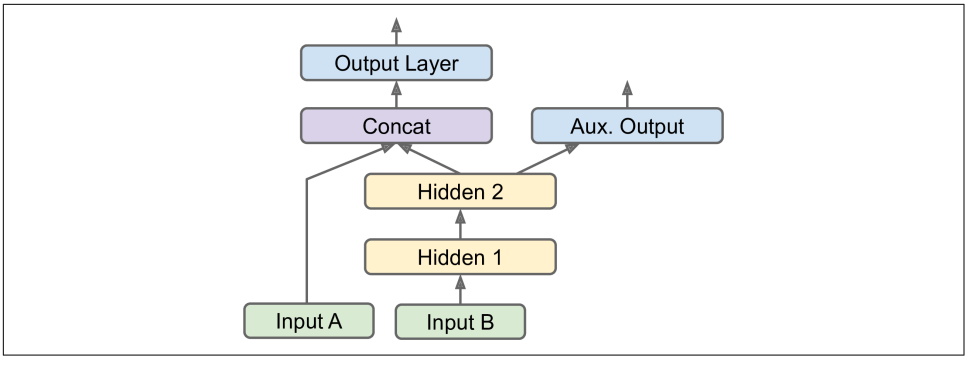


Figure 10-16. Handling multiple outputs, in this example to add an auxiliary output for regularization

Adding extra outputs is quite easy: just connect them to the appropriate layers and add them to your model's list of outputs. For example, the following code builds the network represented in Figure 10-16:

```
[...] # Same as above, up to the main output layer
output = keras.layers.Dense(1, name="main_output")(concat)
aux_output = keras.layers.Dense(1, name="aux_output")(hidden2)
model = keras.Model(inputs=[input_A, input_B], outputs=[output, aux_output])
```

Each output will need its own loss function. Therefore, when we compile the model, we should pass a list of losses[20] (if we pass a single loss, Keras will assume that the same loss must be used for all outputs). By default, Keras will compute all these losses and simply add them up to get the final loss used for training. We care much more about the main output than about the auxiliary output (as it is just used for regularization), so we want to give the main output's loss a much greater weight. Fortunately, it is possible to set all the loss weights when compiling the model:

```
model.compile(loss=["mse", "mse"], loss_weights=[0.9, 0.1], optimizer="sgd")
```

Now when we train the model, we need to provide labels for each output. In this example, the main output and the auxiliary output should try to predict the same thing, so they should use the same labels. So instead of passing `y_train`, we need to pass `(y_train, y_train)` (and the same goes for `y_valid` and `y_test`):

```
history = model.fit(
    [X_train_A, X_train_B], [y_train, y_train], epochs=20,
    validation_data=([X_valid_A, X_valid_B], [y_valid, y_valid]))
```

20 Alternatively, you can pass a dictionary that maps each output name to the corresponding loss. Just like for the inputs, this is useful when there are multiple outputs, to avoid getting the order wrong. The loss weights and metrics (discussed shortly) can also be set using dictionaries.

When we evaluate the model, Keras will return the total loss, as well as all the individual losses:

```
total_loss, main_loss, aux_loss = model.evaluate(
    [X_test_A, X_test_B], [y_test, y_test])
```

Similarly, the `predict()` method will return predictions for each output:

```
y_pred_main, y_pred_aux = model.predict([X_new_A, X_new_B])
```

As you can see, you can build any sort of architecture you want quite easily with the Functional API. Let's look at one last way you can build Keras models.

Using the Subclassing API to Build Dynamic Models

Both the Sequential API and the Functional API are declarative: you start by declaring which layers you want to use and how they should be connected, and only then can you start feeding the model some data for training or inference. This has many advantages: the model can easily be saved, cloned, and shared; its structure can be displayed and analyzed; the framework can infer shapes and check types, so errors can be caught early (i.e., before any data ever goes through the model). It's also fairly easy to debug, since the whole model is a static graph of layers. But the flip side is just that: it's static. Some models involve loops, varying shapes, conditional branching, and other dynamic behaviors. For such cases, or simply if you prefer a more imperative programming style, the Subclassing API is for you.

Simply subclass the `Model` class, create the layers you need in the constructor, and use them to perform the computations you want in the `call()` method. For example, creating an instance of the following `WideAndDeepModel` class gives us an equivalent model to the one we just built with the Functional API. You can then compile it, evaluate it, and use it to make predictions, exactly like we just did:

```
class WideAndDeepModel(keras.Model):
    def __init__(self, units=30, activation="relu", **kwargs):
        super().__init__(**kwargs) # handles standard args (e.g., name)
        self.hidden1 = keras.layers.Dense(units, activation=activation)
        self.hidden2 = keras.layers.Dense(units, activation=activation)
        self.main_output = keras.layers.Dense(1)
        self.aux_output = keras.layers.Dense(1)

    def call(self, inputs):
        input_A, input_B = inputs
        hidden1 = self.hidden1(input_B)
        hidden2 = self.hidden2(hidden1)
        concat = keras.layers.concatenate([input_A, hidden2])
        main_output = self.main_output(concat)
        aux_output = self.aux_output(hidden2)
        return main_output, aux_output

model = WideAndDeepModel()
```

This example looks very much like the Functional API, except we do not need to create the inputs; we just use the `input` argument to the `call()` method, and we separate the creation of the layers[21] in the constructor from their usage in the `call()` method. The big difference is that you can do pretty much anything you want in the `call()` method: `for` loops, `if` statements, low-level TensorFlow operations—your imagination is the limit (see Chapter 12)! This makes it a great API for researchers experimenting with new ideas.

This extra flexibility does come at a cost: your model's architecture is hidden within the `call()` method, so Keras cannot easily inspect it; it cannot save or clone it; and when you call the `summary()` method, you only get a list of layers, without any information on how they are connected to each other. Moreover, Keras cannot check types and shapes ahead of time, and it is easier to make mistakes. So unless you really need that extra flexibility, you should probably stick to the Sequential API or the Functional API.

Keras models can be used just like regular layers, so you can easily combine them to build complex architectures.

Now that you know how to build and train neural nets using Keras, you will want to save them!

Saving and Restoring a Model

When using the Sequential API or the Functional API, saving a trained Keras model is as simple as it gets:

```
model = keras.models.Sequential([...]) # or keras.Model([...])
model.compile([...])
model.fit([...])
model.save("my_keras_model.h5")
```

Keras will use the HDF5 format to save both the model's architecture (including every layer's hyperparameters) and the values of all the model parameters for every layer (e.g., connection weights and biases). It also saves the optimizer (including its hyperparameters and any state it may have). In Chapter 19, we will see how to save a tf.keras model using TensorFlow's SavedModel format instead.

21 Keras models have an `output` attribute, so we cannot use that name for the main output layer, which is why we renamed it to `main_output`.

You will typically have a script that trains a model and saves it, and one or more scripts (or web services) that load the model and use it to make predictions. Loading the model is just as easy:

```
model = keras.models.load_model("my_keras_model.h5")
```

This will work when using the Sequential API or the Functional API, but unfortunately not when using model subclassing. You can use `save_weights()` and `load_weights()` to at least save and restore the model parameters, but you will need to save and restore everything else yourself.

But what if training lasts several hours? This is quite common, especially when training on large datasets. In this case, you should not only save your model at the end of training, but also save checkpoints at regular intervals during training, to avoid losing everything if your computer crashes. But how can you tell the `fit()` method to save checkpoints? Use callbacks.

Using Callbacks

The `fit()` method accepts a `callbacks` argument that lets you specify a list of objects that Keras will call at the start and end of training, at the start and end of each epoch, and even before and after processing each batch. For example, the `ModelCheckpoint` callback saves checkpoints of your model at regular intervals during training, by default at the end of each epoch:

```
[...] # build and compile the model
checkpoint_cb = keras.callbacks.ModelCheckpoint("my_keras_model.h5")
history = model.fit(X_train, y_train, epochs=10, callbacks=[checkpoint_cb])
```

Moreover, if you use a validation set during training, you can set `save_best_only=True` when creating the `ModelCheckpoint`. In this case, it will only save your model when its performance on the validation set is the best so far. This way, you do not need to worry about training for too long and overfitting the training set: simply restore the last model saved after training, and this will be the best model on the validation set. The following code is a simple way to implement early stopping (introduced in Chapter 4):

```
checkpoint_cb = keras.callbacks.ModelCheckpoint("my_keras_model.h5",
                                                save_best_only=True)
history = model.fit(X_train, y_train, epochs=10,
                    validation_data=(X_valid, y_valid),
                    callbacks=[checkpoint_cb])
model = keras.models.load_model("my_keras_model.h5") # roll back to best model
```

Another way to implement early stopping is to simply use the `EarlyStopping` callback. It will interrupt training when it measures no progress on the validation set for

a number of epochs (defined by the `patience` argument), and it will optionally roll back to the best model. You can combine both callbacks to save checkpoints of your model (in case your computer crashes) and interrupt training early when there is no more progress (to avoid wasting time and resources):

```
early_stopping_cb = keras.callbacks.EarlyStopping(patience=10,
                                                  restore_best_weights=True)
history = model.fit(X_train, y_train, epochs=100,
                    validation_data=(X_valid, y_valid),
                    callbacks=[checkpoint_cb, early_stopping_cb])
```

The number of epochs can be set to a large value since training will stop automatically when there is no more progress. In this case, there is no need to restore the best model saved because the `EarlyStopping` callback will keep track of the best weights and restore them for you at the end of training.

There are many other callbacks available in the `keras.callbacks` package.

If you need extra control, you can easily write your own custom callbacks. As an example of how to do that, the following custom callback will display the ratio between the validation loss and the training loss during training (e.g., to detect overfitting):

```
class PrintValTrainRatioCallback(keras.callbacks.Callback):
    def on_epoch_end(self, epoch, logs):
        print("\nval/train: {:.2f}".format(logs["val_loss"] / logs["loss"]))
```

As you might expect, you can implement `on_train_begin()`, `on_train_end()`, `on_epoch_begin()`, `on_epoch_end()`, `on_batch_begin()`, and `on_batch_end()`. Callbacks can also be used during evaluation and predictions, should you ever need them (e.g., for debugging). For evaluation, you should implement `on_test_begin()`, `on_test_end()`, `on_test_batch_begin()`, or `on_test_batch_end()` (called by `evaluate()`), and for prediction you should implement `on_predict_begin()`, `on_predict_end()`, `on_predict_batch_begin()`, or `on_predict_batch_end()` (called by `predict()`).

Now let's take a look at one more tool you should definitely have in your toolbox when using tf.keras: TensorBoard.

Using TensorBoard for Visualization

TensorBoard is a great interactive visualization tool that you can use to view the learning curves during training, compare learning curves between multiple runs, visualize the computation graph, analyze training statistics, view images generated by your model, visualize complex multidimensional data projected down to 3D and automatically clustered for you, and more! This tool is installed automatically when you install TensorFlow, so you already have it.

To use it, you must modify your program so that it outputs the data you want to visualize to special binary log files called *event files*. Each binary data record is called a *summary*. The TensorBoard server will monitor the log directory, and it will automatically pick up the changes and update the visualizations: this allows you to visualize live data (with a short delay), such as the learning curves during training. In general, you want to point the TensorBoard server to a root log directory and configure your program so that it writes to a different subdirectory every time it runs. This way, the same TensorBoard server instance will allow you to visualize and compare data from multiple runs of your program, without getting everything mixed up.

Let's start by defining the root log directory we will use for our TensorBoard logs, plus a small function that will generate a subdirectory path based on the current date and time so that it's different at every run. You may want to include extra information in the log directory name, such as hyperparameter values that you are testing, to make it easier to know what you are looking at in TensorBoard:

```
import os
root_logdir = os.path.join(os.curdir, "my_logs")

def get_run_logdir():
    import time
    run_id = time.strftime("run_%Y_%m_%d-%H_%M_%S")
    return os.path.join(root_logdir, run_id)

run_logdir = get_run_logdir() # e.g., './my_logs/run_2019_06_07-15_15_22'
```

The good news is that Keras provides a nice `TensorBoard()` callback:

```
[...] # Build and compile your model
tensorboard_cb = keras.callbacks.TensorBoard(run_logdir)
history = model.fit(X_train, y_train, epochs=30,
                    validation_data=(X_valid, y_valid),
                    callbacks=[tensorboard_cb])
```

And that's all there is to it! It could hardly be easier to use. If you run this code, the `TensorBoard()` callback will take care of creating the log directory for you (along with its parent directories if needed), and during training it will create event files and write summaries to them. After running the program a second time (perhaps

changing some hyperparameter value), you will end up with a directory structure similar to this one:

```
my_logs/
├── run_2019_06_07-15_15_22
│   ├── train
│   │   ├── events.out.tfevents.1559891732.mycomputer.local.38511.694049.v2
│   │   ├── events.out.tfevents.1559891732.mycomputer.local.profile-empty
│   │   └── plugins/profile/2019-06-07_15-15-32
│   │       └── local.trace
│   └── validation
│       └── events.out.tfevents.1559891733.mycomputer.local.38511.696430.v2
└── run_2019_06_07-15_15_49
    └── [...]
```

There's one directory per run, each containing one subdirectory for training logs and one for validation logs. Both contain event files, but the training logs also include profiling traces: this allows TensorBoard to show you exactly how much time the model spent on each part of your model, across all your devices, which is great for locating performance bottlenecks.

Next you need to start the TensorBoard server. One way to do this is by running a command in a terminal. If you installed TensorFlow within a virtualenv, you should activate it. Next, run the following command at the root of the project (or from anywhere else, as long as you point to the appropriate log directory):

```
$ tensorboard --logdir=./my_logs --port=6006
TensorBoard 2.0.0 at http://mycomputer.local:6006/ (Press CTRL+C to quit)
```

If your shell cannot find the *tensorboard* script, then you must update your `PATH` environment variable so that it contains the directory in which the script was installed (alternatively, you can just replace `tensorboard` in the command line with `python3 -m tensorboard.main`). Once the server is up, you can open a web browser and go to *http://localhost:6006*.

Alternatively, you can use TensorBoard directly within Jupyter, by running the following commands. The first line loads the TensorBoard extension, and the second line starts a TensorBoard server on port 6006 (unless it is already started) and connects to it:

```
%load_ext tensorboard
%tensorboard --logdir=./my_logs --port=6006
```

Either way, you should see TensorBoard's web interface. Click the SCALARS tab to view the learning curves (see Figure 10-17). At the bottom left, select the logs you want to visualize (e.g., the training logs from the first and second run), and click the `epoch_loss` scalar. Notice that the training loss went down nicely during both runs, but the second run went down much faster. Indeed, we used a learning rate of 0.05 (`optimizer=keras.optimizers.SGD(lr=0.05)`) instead of 0.001.

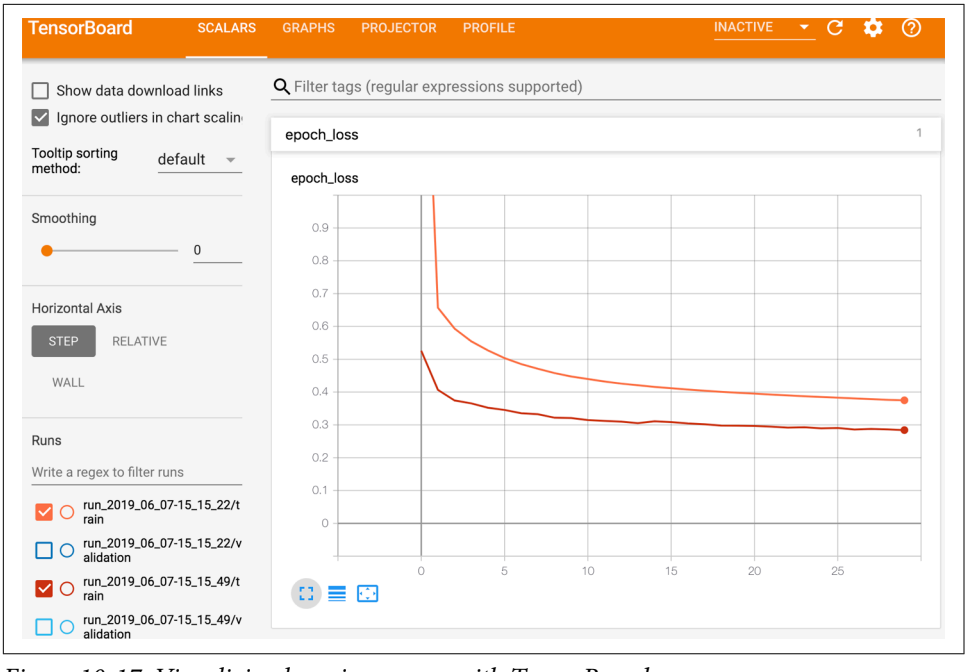


Figure 10-17. Visualizing learning curves with TensorBoard

You can also visualize the whole graph, the learned weights (projected to 3D), or the profiling traces. The `TensorBoard()` callback has options to log extra data too, such as embeddings (see Chapter 13).

Additionally, TensorFlow offers a lower-level API in the `tf.summary` package. The following code creates a `SummaryWriter` using the `create_file_writer()` function, and it uses this writer as a context to log scalars, histograms, images, audio, and text, all of which can then be visualized using TensorBoard (give it a try!):

```
test_logdir = get_run_logdir()
writer = tf.summary.create_file_writer(test_logdir)
with writer.as_default():
    for step in range(1, 1000 + 1):
        tf.summary.scalar("my_scalar", np.sin(step / 10), step=step)
        data = (np.random.randn(100) + 2) * step / 100 # some random data
        tf.summary.histogram("my_hist", data, buckets=50, step=step)
        images = np.random.rand(2, 32, 32, 3) # random 32×32 RGB images
        tf.summary.image("my_images", images * step / 1000, step=step)
        texts = ["The step is " + str(step), "Its square is " + str(step**2)]
        tf.summary.text("my_text", texts, step=step)
        sine_wave = tf.math.sin(tf.range(12000) / 48000 * 2 * np.pi * step)
        audio = tf.reshape(tf.cast(sine_wave, tf.float32), [1, -1, 1])
        tf.summary.audio("my_audio", audio, sample_rate=48000, step=step)
```

This is actually a useful visualization tool to have, even beyond TensorFlow or Deep Learning.

Let's summarize what you've learned so far in this chapter: we saw where neural nets came from, what an MLP is and how you can use it for classification and regression, how to use tf.keras's Sequential API to build MLPs, and how to use the Functional API or the Subclassing API to build more complex model architectures. You learned how to save and restore a model and how to use callbacks for checkpointing, early stopping, and more. Finally, you learned how to use TensorBoard for visualization. You can already go ahead and use neural networks to tackle many problems! However, you may wonder how to choose the number of hidden layers, the number of neurons in the network, and all the other hyperparameters. Let's look at this now.

Fine-Tuning Neural Network Hyperparameters

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

One option is to simply try many combinations of hyperparameters and see which one works best on the validation set (or use K-fold cross-validation). For example, we can use `GridSearchCV` or `RandomizedSearchCV` to explore the hyperparameter space, as we did in Chapter 2. To do this, we need to wrap our Keras models in objects that mimic regular Scikit-Learn regressors. The first step is to create a function that will build and compile a Keras model, given a set of hyperparameters:

```
def build_model(n_hidden=1, n_neurons=30, learning_rate=3e-3, input_shape=[8]):
    model = keras.models.Sequential()
    model.add(keras.layers.InputLayer(input_shape=input_shape))
    for layer in range(n_hidden):
        model.add(keras.layers.Dense(n_neurons, activation="relu"))
    model.add(keras.layers.Dense(1))
    optimizer = keras.optimizers.SGD(lr=learning_rate)
    model.compile(loss="mse", optimizer=optimizer)
    return model
```

This function creates a simple `Sequential` model for univariate regression (only one output neuron), with the given input shape and the given number of hidden layers and neurons, and it compiles it using an `SGD` optimizer configured with the specified learning rate. It is good practice to provide reasonable defaults to as many hyperparameters as you can, as Scikit-Learn does.

Next, let's create a `KerasRegressor` based on this `build_model()` function:

```
keras_reg = keras.wrappers.scikit_learn.KerasRegressor(build_model)
```

The `KerasRegressor` object is a thin wrapper around the Keras model built using `build_model()`. Since we did not specify any hyperparameters when creating it, it will use the default hyperparameters we defined in `build_model()`. Now we can use this object like a regular Scikit-Learn regressor: we can train it using its `fit()` method, then evaluate it using its `score()` method, and use it to make predictions using its `predict()` method, as you can see in the following code:

```
keras_reg.fit(X_train, y_train, epochs=100,
              validation_data=(X_valid, y_valid),
              callbacks=[keras.callbacks.EarlyStopping(patience=10)])
mse_test = keras_reg.score(X_test, y_test)
y_pred = keras_reg.predict(X_new)
```

Note that any extra parameter you pass to the `fit()` method will get passed to the underlying Keras model. Also note that the score will be the opposite of the MSE because Scikit-Learn wants scores, not losses (i.e., higher should be better).

We don't want to train and evaluate a single model like this, though we want to train hundreds of variants and see which one performs best on the validation set. Since there are many hyperparameters, it is preferable to use a randomized search rather than grid search (as we discussed in Chapter 2). Let's try to explore the number of hidden layers, the number of neurons, and the learning rate:

```
from scipy.stats import reciprocal
from sklearn.model_selection import RandomizedSearchCV

param_distribs = {
    "n_hidden": [0, 1, 2, 3],
    "n_neurons": np.arange(1, 100),
    "learning_rate": reciprocal(3e-4, 3e-2),
}

rnd_search_cv = RandomizedSearchCV(keras_reg, param_distribs, n_iter=10, cv=3)
rnd_search_cv.fit(X_train, y_train, epochs=100,
                  validation_data=(X_valid, y_valid),
                  callbacks=[keras.callbacks.EarlyStopping(patience=10)])
```

This is identical to what we did in Chapter 2, except here we pass extra parameters to the `fit()` method, and they get relayed to the underlying Keras models. Note that `RandomizedSearchCV` uses K-fold cross-validation, so it does not use `X_valid` and `y_valid`, which are only used for early stopping.

The exploration may last many hours, depending on the hardware, the size of the dataset, the complexity of the model, and the values of `n_iter` and `cv`. When it's over, you can access the best parameters found, the best score, and the trained Keras model like this:

```
>>> rnd_search_cv.best_params_
{'learning_rate': 0.0033625641252688094, 'n_hidden': 2, 'n_neurons': 42}
>>> rnd_search_cv.best_score_
-0.3189529188278931
>>> model = rnd_search_cv.best_estimator_.model
```

You can now save this model, evaluate it on the test set, and, if you are satisfied with its performance, deploy it to production. Using randomized search is not too hard, and it works well for many fairly simple problems. When training is slow, however (e.g., for more complex problems with larger datasets), this approach will only explore a tiny portion of the hyperparameter space. You can partially alleviate this problem by assisting the search process manually: first run a quick random search using wide ranges of hyperparameter values, then run another search using smaller ranges of values centered on the best ones found during the first run, and so on. This approach will hopefully zoom in on a good set of hyperparameters. However, it's very time consuming, and probably not the best use of your time.

Fortunately, there are many techniques to explore a search space much more efficiently than randomly. Their core idea is simple: when a region of the space turns out to be good, it should be explored more. Such techniques take care of the "zooming" process for you and lead to much better solutions in much less time. Here are some Python libraries you can use to optimize hyperparameters:

Hyperopt
: A popular library for optimizing over all sorts of complex search spaces (including real values, such as the learning rate, and discrete values, such as the number of layers).

Hyperas, kopt, or Talos
: Useful libraries for optimizing hyperparameters for Keras models (the first two are based on Hyperopt).

Keras Tuner
: An easy-to-use hyperparameter optimization library by Google for Keras models, with a hosted service for visualization and analysis.

Scikit-Optimize (`skopt`)
: A general-purpose optimization library. The `BayesSearchCV` class performs Bayesian optimization using an interface similar to `GridSearchCV`.

Spearmint
: A Bayesian optimization library.

Hyperband
: A fast hyperparameter tuning library based on the recent Hyperband paper[22] by Lisha Li et al.

Sklearn-Deap
: A hyperparameter optimization library based on evolutionary algorithms, with a `GridSearchCV`-like interface.

Moreover, many companies offer services for hyperparameter optimization. We'll discuss Google Cloud AI Platform's hyperparameter tuning service in Chapter 19. Other options include services by Arimo and SigOpt, and CallDesk's Oscar.

Hyperparameter tuning is still an active area of research, and evolutionary algorithms are making a comeback. For example, check out DeepMind's excellent 2017 paper,[23] where the authors jointly optimize a population of models and their hyperparameters. Google has also used an evolutionary approach, not just to search for hyperparameters but also to look for the best neural network architecture for the problem; their AutoML suite is already available as a cloud service. Perhaps the days of building neural networks manually will soon be over? Check out Google's post on this topic. In fact, evolutionary algorithms have been used successfully to train individual neural networks, replacing the ubiquitous Gradient Descent! For an example, see the 2017 post by Uber where the authors introduce their *Deep Neuroevolution* technique.

But despite all this exciting progress and all these tools and services, it still helps to have an idea of what values are reasonable for each hyperparameter so that you can build a quick prototype and restrict the search space. The following sections provide guidelines for choosing the number of hidden layers and neurons in an MLP and for selecting good values for some of the main hyperparameters.

Number of Hidden Layers

For many problems, you can begin with a single hidden layer and get reasonable results. An MLP with just one hidden layer can theoretically model even the most complex functions, provided it has enough neurons. But for complex problems, deep networks have a much higher *parameter efficiency* than shallow ones: they can model complex functions using exponentially fewer neurons than shallow nets, allowing them to reach much better performance with the same amount of training data.

To understand why, suppose you are asked to draw a forest using some drawing software, but you are forbidden to copy and paste anything. It would take an enormous

22 Lisha Li et al., "Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization," *Journal of Machine Learning Research* 18 (April 2018): 1–52.

23 Max Jaderberg et al., "Population Based Training of Neural Networks," arXiv preprint arXiv:1711.09846 (2017).

amount of time: you would have to draw each tree individually, branch by branch, leaf by leaf. If you could instead draw one leaf, copy and paste it to draw a branch, then copy and paste that branch to create a tree, and finally copy and paste this tree to make a forest, you would be finished in no time. Real-world data is often structured in such a hierarchical way, and deep neural networks automatically take advantage of this fact: lower hidden layers model low-level structures (e.g., line segments of various shapes and orientations), intermediate hidden layers combine these low-level structures to model intermediate-level structures (e.g., squares, circles), and the highest hidden layers and the output layer combine these intermediate structures to model high-level structures (e.g., faces).

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

In summary, for many problems you can start with just one or two hidden layers and the neural network will work just fine. For instance, you can easily reach above 97% accuracy on the MNIST dataset using just one hidden layer with a few hundred neurons, and above 98% accuracy using two hidden layers with the same total number of neurons, in roughly the same amount of training time. For more complex problems, you can ramp up the number of hidden layers until you start overfitting the training set. Very complex tasks, such as large image classification or speech recognition, typically require networks with dozens of layers (or even hundreds, but not fully connected ones, as we will see in Chapter 14), and they need a huge amount of training data. You will rarely have to train such networks from scratch: it is much more common to reuse parts of a pretrained state-of-the-art network that performs a similar task. Training will then be a lot faster and require much less data (we will discuss this in Chapter 11).

Number of Neurons per Hidden Layer

The number of neurons in the input and output layers is determined by the type of input and output your task requires. For example, the MNIST task requires $28 \times 28 = 784$ input neurons and 10 output neurons.

As for the hidden layers, it used to be common to size them to form a pyramid, with fewer and fewer neurons at each layer—the rationale being that many low-level fea-

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.

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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 **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 **Y**?
    - Write the equation that computes the network's output matrix **Y** as a function of **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.

CHAPTER 11
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.

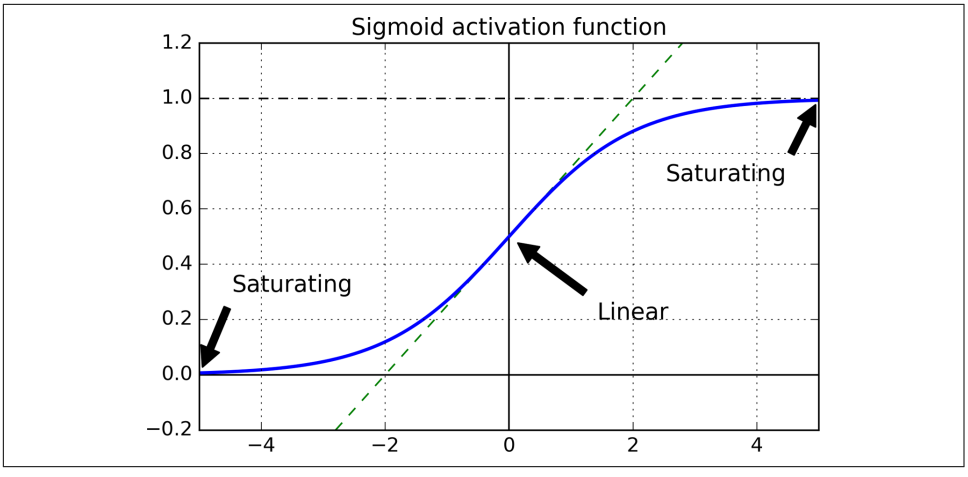

Figure 11-1. Logistic activation function saturation

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 $fan_{avg} = (fan_{in} + fan_{out})/2$. 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 papers[3] 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.

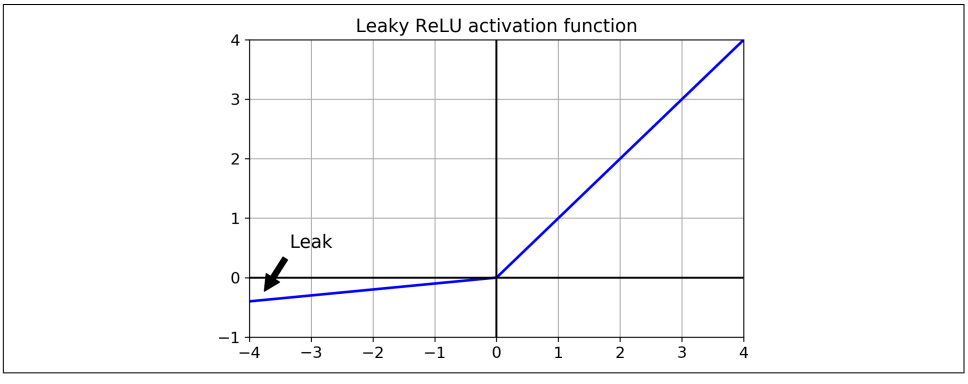

Figure 11-2. Leaky ReLU: like ReLU, but with a small slope for negative values

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

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

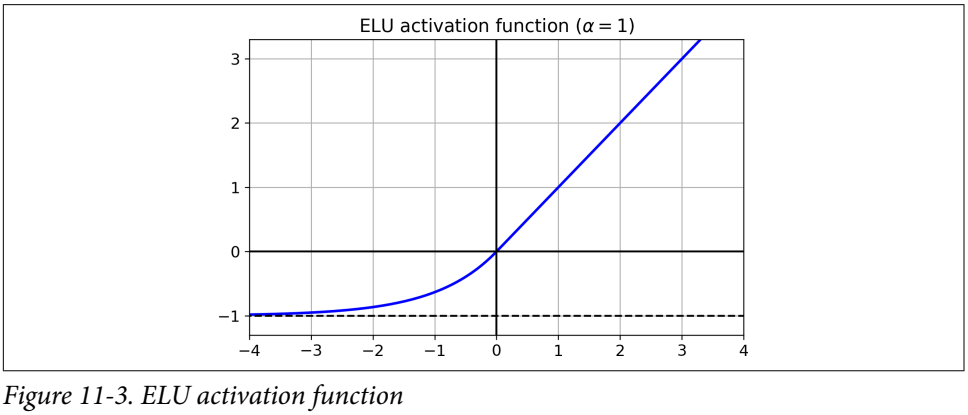

Figure 11-3. ELU activation function

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 SELU > ELU > leaky ReLU (and its variants) > ReLU > tanh > 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

1. $\mathbf{\mu}_B = \frac{1}{m_B} \sum_{i=1}^{m_B} \mathbf{x}^{(i)}$
2. $\mathbf{\sigma}_B^2 = \frac{1}{m_B} \sum_{i=1}^{m_B} \left(\mathbf{x}^{(i)} - \mathbf{\mu}_B\right)^2$
3. $\widehat{\mathbf{x}}^{(i)} = \frac{\mathbf{x}^{(i)} - \mathbf{\mu}_B}{\sqrt{\mathbf{\sigma}_B^2 + \varepsilon}}$
4. $\mathbf{z}^{(i)} = \mathbf{\gamma} \otimes \widehat{\mathbf{x}}^{(i)} + \mathbf{\beta}$

In this algorithm:

- $\mathbf{\mu}_B$ is the vector of input means, evaluated over the whole mini-batch B (it contains one mean per input).
- $\mathbf{\sigma}_B$ 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.
- $\widehat{\mathbf{x}}^{(i)}$ 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.

- $\boldsymbol{\gamma}$ 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).
- $\boldsymbol{\beta}$ 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: $\boldsymbol{\gamma}$ (the output scale vector) and $\boldsymbol{\beta}$ (the output offset vector) are learned through regular backpropagation, and $\boldsymbol{\mu}$ (the final input mean vector) and $\boldsymbol{\sigma}$ (the final input standard deviation vector) are estimated using an exponential moving average. Note that $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$ 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 $\boldsymbol{\gamma} \otimes (\mathbf{XW} + \mathbf{b} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \boldsymbol{\beta}$ (ignoring the smoothing term ε in the denominator). If we define $\mathbf{W}' = \boldsymbol{\gamma} \otimes \mathbf{W} / \boldsymbol{\sigma}$ and $\mathbf{b}' = \boldsymbol{\gamma} \otimes (\mathbf{b} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \boldsymbol{\beta}$, 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 (Batc (None, 784)               3136
_________________________________________________________________
dense_50 (Dense)             (None, 300)               235500
_________________________________________________________________
batch_normalization_v2_1 (Ba (None, 300)               1200
_________________________________________________________________
dense_51 (Dense)             (None, 100)               30100
_________________________________________________________________
batch_normalization_v2_2 (Ba (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: $\boldsymbol{\gamma}$, $\boldsymbol{\beta}$, $\boldsymbol{\mu}$, and $\boldsymbol{\sigma}$ (for example, the first BN layer adds 3,136 parameters, which is 4×784). The last two parameters, $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$, 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 to 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 compute[10] (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).

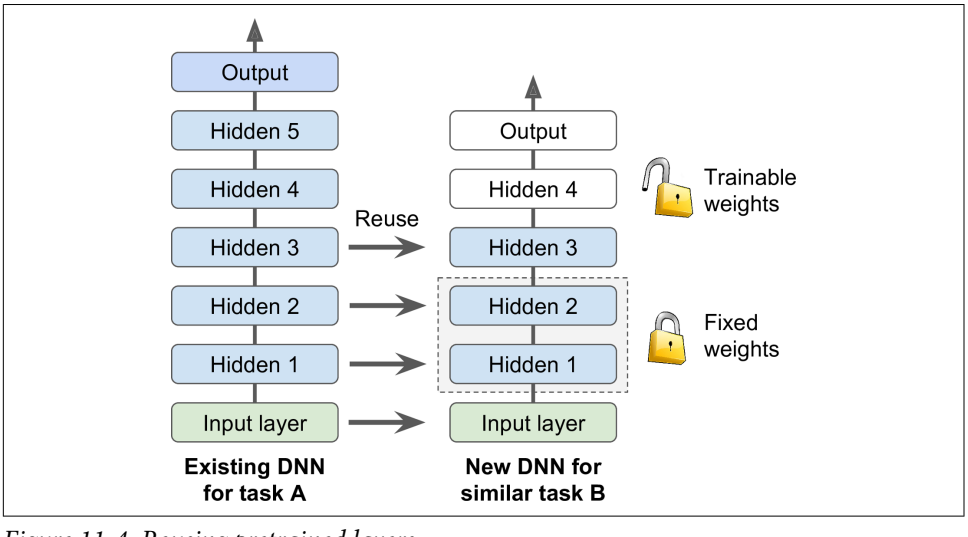

Figure 11-4. Reusing pretrained layers

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.

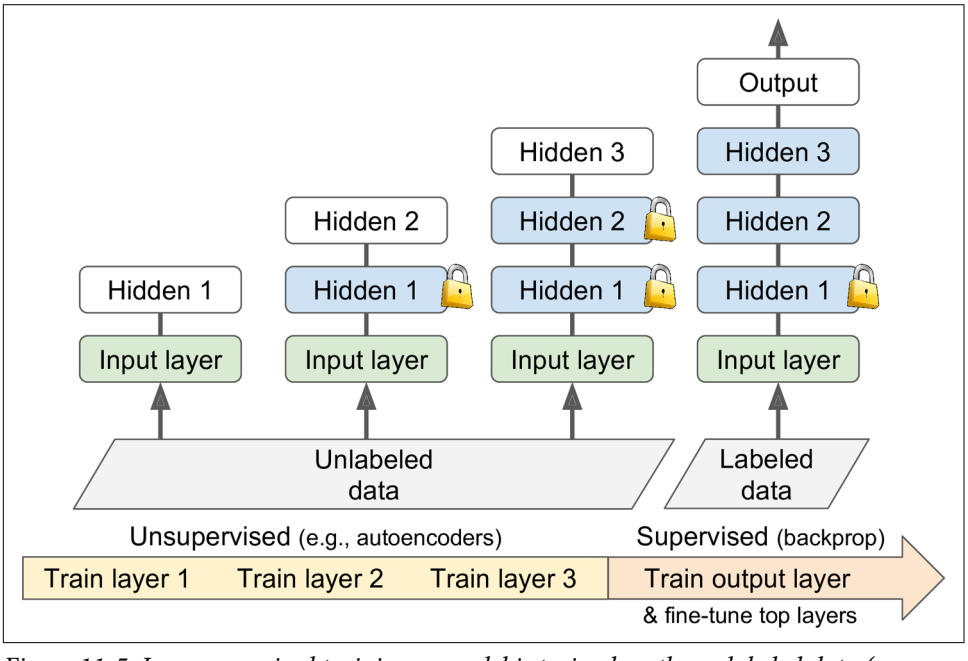

Figure 11-5. In unsupervised training, a model is trained on the unlabeled data (or on all the data) using an unsupervised learning technique, then it is fine-tuned for the final task on the labeled data using a supervised learning technique; the unsupervised part may train one layer at a time as shown 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 $\boldsymbol{\theta}$ by directly subtracting the gradient of the cost function $J(\boldsymbol{\theta})$ with regard to the weights ($\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$) multiplied by the learning rate η. The equation is: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$. 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. $\mathbf{m} \leftarrow \beta\mathbf{m} - \eta \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
2. $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mathbf{m}$

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 $\boldsymbol{\theta}$ but slightly ahead in the direction of the momentum, at $\boldsymbol{\theta} + \beta\mathbf{m}$ (see Equation 11-5).

Equation 11-5. Nesterov Accelerated Gradient algorithm

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

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 $\boldsymbol{\theta}$, and ∇_2 represents the gradient at the point located at $\boldsymbol{\theta} + \beta\mathbf{m}$).

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.

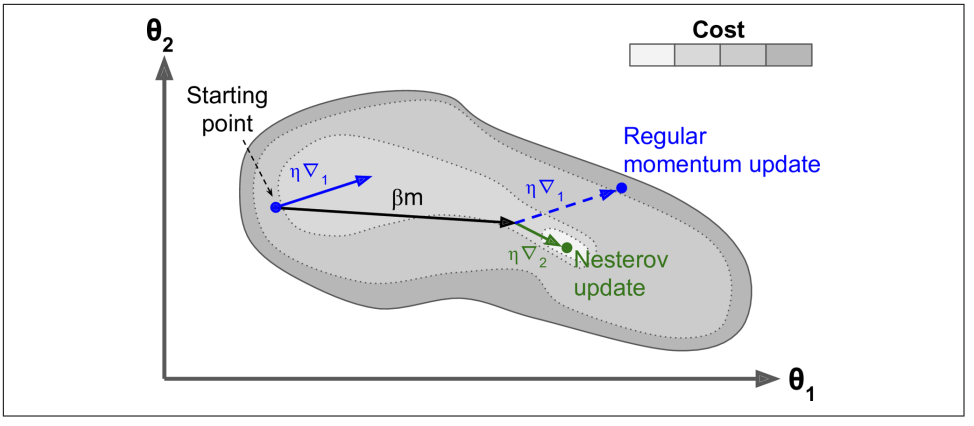

Figure 11-6. Regular versus Nesterov momentum optimization: the former applies the gradients computed before the momentum step, while the latter applies the gradients computed after

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

The first step accumulates the square of the gradients into the vector **s** (recall that the $\otimes$ symbol represents the element-wise multiplication). This vectorized form is equivalent to computing $s_i \leftarrow s_i + (\partial J(\boldsymbol{\theta}) / \partial \theta_i)^2$ for each element s_i of the vector **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 $\sqrt{\mathbf{s} + \varepsilon}$ (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.

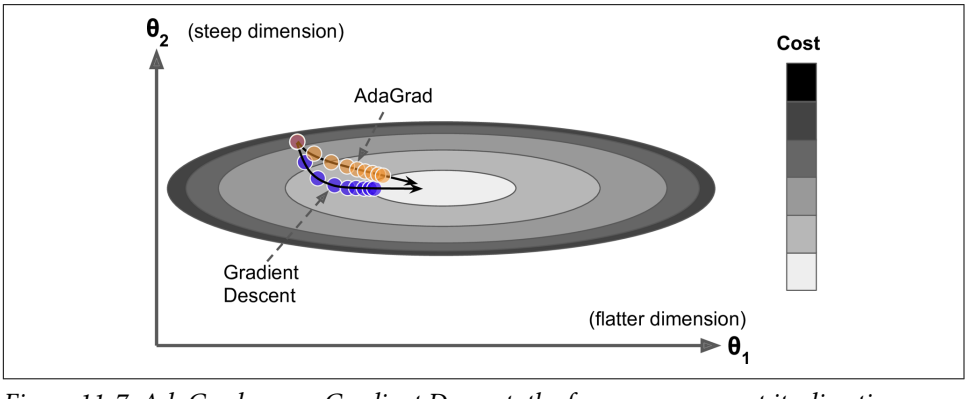

Figure 11-7. AdaGrad versus Gradient Descent: the former can correct its direction earlier to point to the optimum

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* algorithm[16] 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. $\mathbf{s} \leftarrow \beta\mathbf{s} + (1-\beta)\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \otimes \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
2. $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta\, \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) \oslash \sqrt{\mathbf{s} + \varepsilon}$

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

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 **m** and **s** are initialized at 0, they will be biased toward 0 at the beginning of training, so these two steps will help boost **m** and **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 **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 **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 **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).

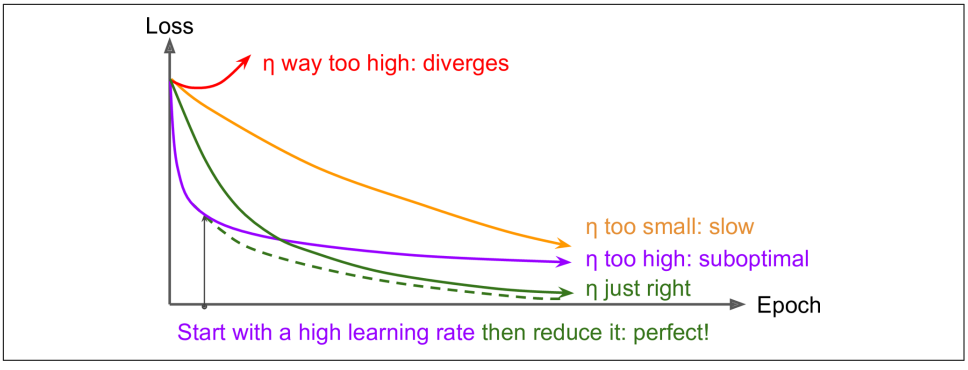

Figure 11-8. Learning curves for various learning rates η

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 $\eta(t) = \eta_0 \, 0.1^{t/s}$. 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.

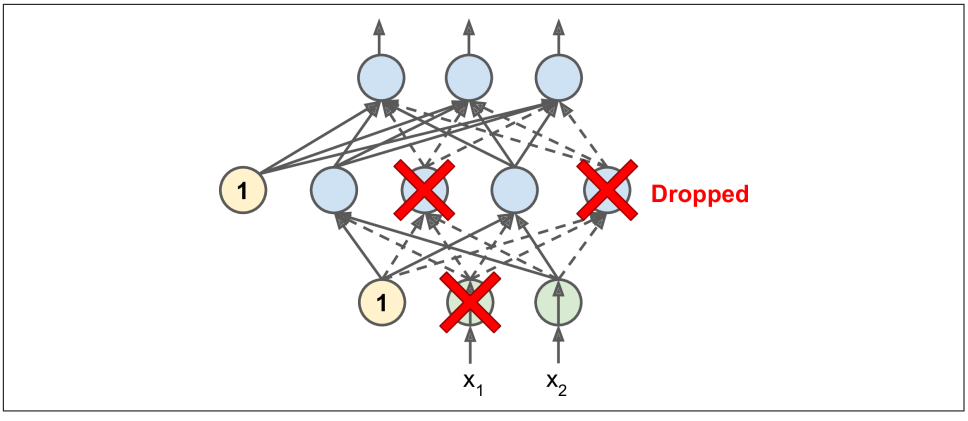

Figure 11-9. With dropout regularization, at each training iteration a random subset of all neurons in one or more layers—except the output layer—are "dropped out"; these neurons output 0 at this iteration (represented by the dashed arrows)

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 droppable 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 `MCAlphaDropout` 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`.