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4. Training Models

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6. Decision Trees

Chapter 5. Support Vector Machines

A *Support Vector Machine* (SVM) is a powerful and versatile Machine Learning model, capable of performing linear or nonlinear classification, regression, and even outlier detection. It is one of the most popular models in Machine Learning, and anyone interested in Machine Learning should have it in their toolbox. SVMs are particularly well suited for classification of complex small- or medium-sized datasets.

This chapter will explain the core concepts of SVMs, how to use them, and how they work.

Linear SVM Classification

The fundamental idea behind SVMs is best explained with some pictures. Figure 5-1 shows part of the iris dataset that was introduced at the end of Chapter 4. The two classes can clearly be separated easily with a straight line (they are *linearly separable*). The left plot shows the decision boundaries of three possible linear classifiers. The model whose decision boundary is represented by the dashed line is so bad that it does not even separate the classes properly. The other two models work perfectly on this training set, but their decision boundaries come so close to the instances that these models will probably not perform as well on new instances. In contrast, the solid line in the plot on the right represents the decision boundary of an SVM classifier;

this line not only separates the two classes but also stays as far away from the closest training instances as possible. You can think of an SVM classifier as fitting the widest possible street (represented by the parallel dashed lines) between the classes. This is called *large margin classification*.

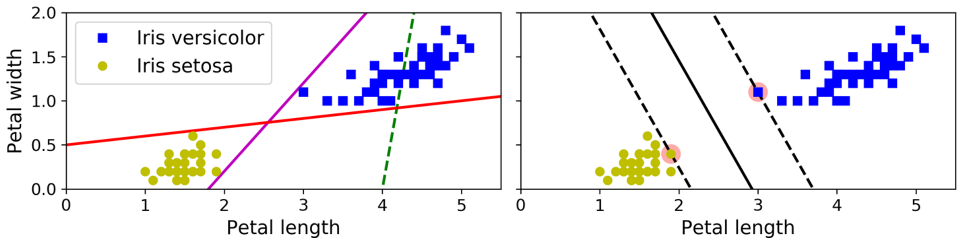

Figure 5-1. Large margin classification

Notice that adding more training instances “off the street” will not affect the decision boundary at all: it is fully determined (or “supported”) by the instances located on the edge of the street. These instances are called the *support vectors* (they are circled in Figure 5-1).

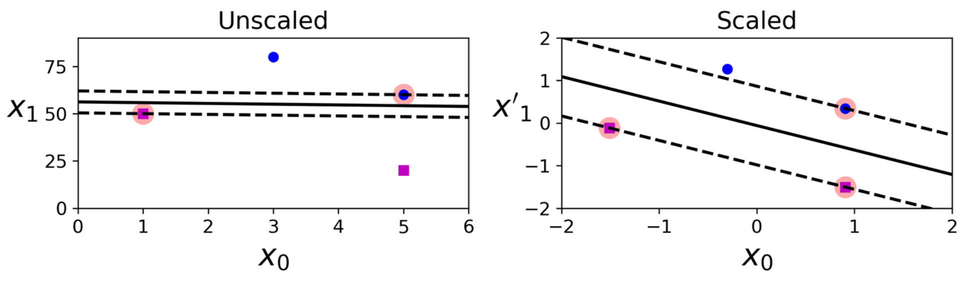

Figure 5-2. Sensitivity to feature scales

WARNING

SVMs are sensitive to the feature scales, as you can see in Figure 5-2: in the left plot, the vertical scale is much larger than the horizontal scale, so the widest possible street is close to horizontal. After feature scaling (e.g., using Scikit-Learn’s `StandardScaler`), the decision boundary in the right plot looks much better.

Soft Margin Classification

If we strictly impose that all instances must be off the street and on the right side, this is called *hard margin classification*. There are two main issues with

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hard margin classification. First, it only works if the data is linearly separable. Second, it is sensitive to outliers. Figure 5-3 shows the iris dataset with just one additional outlier: on the left, it is impossible to find a hard margin; on the right, the decision boundary ends up very different from the one we saw in Figure 5-1 without the outlier, and it will probably not generalize as well.

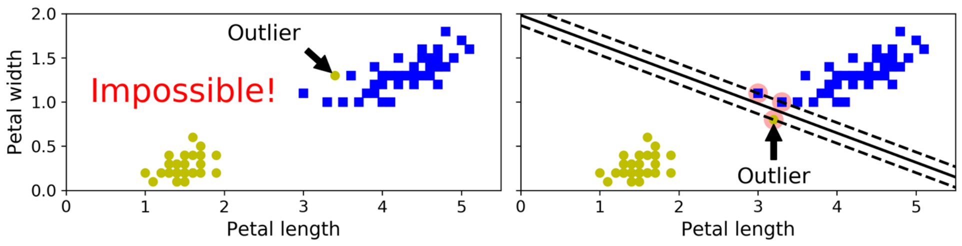

Figure 5-3. Hard margin sensitivity to outliers

To avoid these issues, use a more flexible model. The objective is to find a good balance between keeping the street as large as possible and limiting the *margin violations* (i.e., instances that end up in the middle of the street or even on the wrong side). This is called *soft margin classification*.

When creating an SVM model using Scikit-Learn, we can specify a number of hyperparameters. `C` is one of those hyperparameters. If we set it to a low value, then we end up with the model on the left of Figure 5-4. With a high value, we get the model on the right. Margin violations are bad. It's usually better to have few of them. However, in this case the model on the left has a lot of margin violations but will probably generalize better.

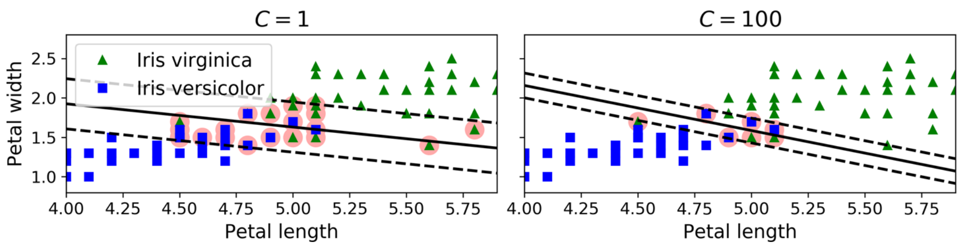

Figure 5-4. Large margin (left) versus fewer margin violations (right)

TIP

If your SVM model is overfitting, you can try regularizing it by reducing `C`.

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The following Scikit-Learn code loads the iris dataset, scales the features, and then trains a linear SVM model (using the `LinearSVC` class with `C=1` and the *hinge loss* function, described shortly) to detect *Iris virginica* flowers:

```
import numpy as np
from sklearn import datasets
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.svm import LinearSVC

iris = datasets.load_iris()
X = iris["data"][:, (2, 3)]  # petal length, petal width
y = (iris["target"] == 2).astype(np.float64)  # Iris virginica

svm_clf = Pipeline([
        ("scaler", StandardScaler()),
        ("linear_svc", LinearSVC(C=1, loss="hinge")),
    ])

svm_clf.fit(X, y)
```

The resulting model is represented on the left in Figure 5-4.

Then, as usual, you can use the model to make predictions:

```
>>> svm_clf.predict([[5.5, 1.7]])
array([1.])
```

NOTE

Unlike Logistic Regression classifiers, SVM classifiers do not output probabilities for each class.

Instead of using the `LinearSVC` class, we could use the `SVC` class with a linear kernel. When creating the SVC model, we would write `SVC(kernel="linear", C=1)`. Or we could use the `SGDClassifier` class, with `SGDClassifier(loss="hinge", alpha=1/(m*C))`. This applies regular Stochastic Gradient Descent (see Chapter 4) to train a linear SVM

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classifier. It does not converge as fast as the `LinearSVC` class, but it can be useful to handle online classification tasks or huge datasets that do not fit in memory (out-of-core training).

TIP

The `LinearSVC` class regularizes the bias term, so you should center the training set first by subtracting its mean. This is automatic if you scale the data using the `StandardScaler`. Also make sure you set the `loss` hyperparameter to `"hinge"`, as it is not the default value. Finally, for better performance, you should set the `dual` hyperparameter to `False`, unless there are more features than training instances (we will discuss duality later in the chapter).

Nonlinear SVM Classification

Although linear SVM classifiers are efficient and work surprisingly well in many cases, many datasets are not even close to being linearly separable. One approach to handling nonlinear datasets is to add more features, such as polynomial features (as you did in Chapter 4); in some cases this can result in a linearly separable dataset. Consider the left plot in Figure 5-5: it represents a simple dataset with just one feature, x_1. This dataset is not linearly separable, as you can see. But if you add a second feature $x_2 = (x_1)^2$, the resulting 2D dataset is perfectly linearly separable.

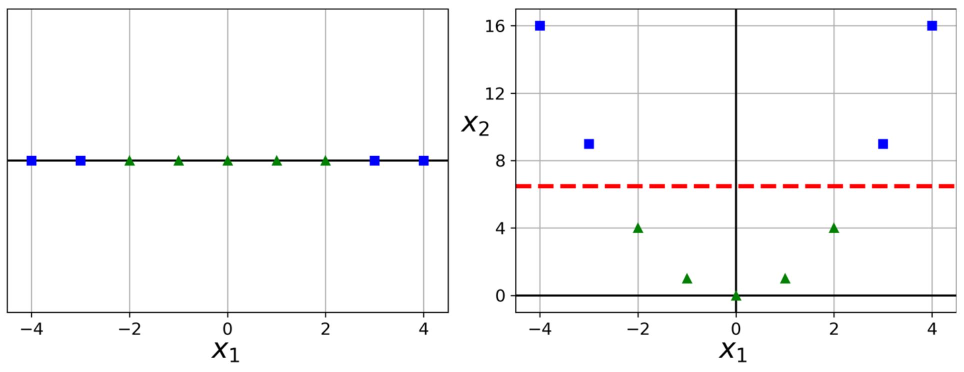

Figure 5-5. Adding features to make a dataset linearly separable

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To implement this idea using Scikit-Learn, create a `Pipeline` containing a `PolynomialFeatures` transformer (discussed in "Polynomial Regression"), followed by a `StandardScaler` and a `LinearSVC`. Let's test this on the moons dataset: this is a toy dataset for binary classification in which the data points are shaped as two interleaving half circles (see Figure 5-6). You can generate this dataset using the `make_moons()` function:

```
from sklearn.datasets import make_moons
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures

X, y = make_moons(n_samples=100, noise=0.15)
polynomial_svm_clf = Pipeline([
        ("poly_features", PolynomialFeatures(degree=3)),
        ("scaler", StandardScaler()),
        ("svm_clf", LinearSVC(C=10, loss="hinge"))
    ])

polynomial_svm_clf.fit(X, y)
```

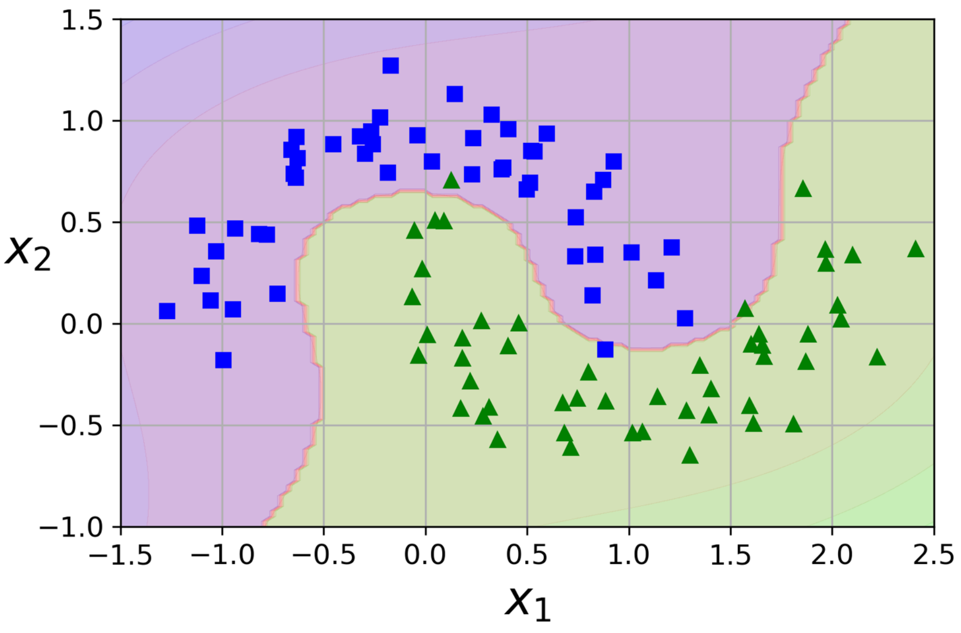

Figure 5-6. Linear SVM classifier using polynomial features

Polynomial Kernel

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Adding polynomial features is simple to implement and can work great with all sorts of Machine Learning algorithms (not just SVMs). That said, at a low polynomial degree, this method cannot deal with very complex datasets, and with a high polynomial degree it creates a huge number of features, making the model too slow.

Fortunately, when using SVMs you can apply an almost miraculous mathematical technique called the *kernel trick* (explained in a moment). The kernel trick makes it possible to get the same result as if you had added many polynomial features, even with very high-degree polynomials, without actually having to add them. So there is no combinatorial explosion of the number of features because you don't actually add any features. This trick is implemented by the `SVC` class. Let's test it on the moons dataset:

```
from sklearn.svm import SVC
poly_kernel_svm_clf = Pipeline([
        ("scaler", StandardScaler()),
        ("svm_clf", SVC(kernel="poly", degree=3, coef0=1, C=5))
    ])
poly_kernel_svm_clf.fit(X, y)
```

This code trains an SVM classifier using a third-degree polynomial kernel. It is represented on the left in Figure 5-7. On the right is another SVM classifier using a 10th-degree polynomial kernel. Obviously, if your model is overfitting, you might want to reduce the polynomial degree. Conversely, if it is underfitting, you can try increasing it. The hyperparameter `coef0` controls how much the model is influenced by high-degree polynomials versus low-degree polynomials.

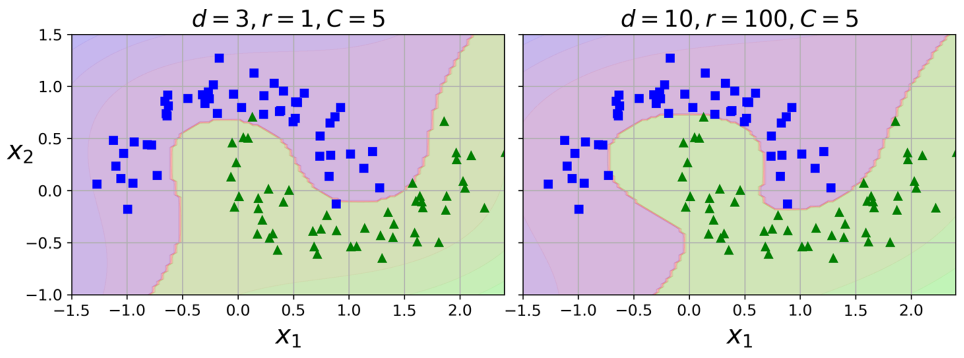

Figure 5-7. SVM classifiers with a polynomial kernel

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TIP

A common approach to finding the right hyperparameter values is to use grid search (see Chapter 2). It is often faster to first do a very coarse grid search, then a finer grid search around the best values found. Having a good sense of what each hyperparameter actually does can also help you search in the right part of the hyperparameter space.

Similarity Features

Another technique to tackle nonlinear problems is to add features computed using a *similarity function*, which measures how much each instance resembles a particular *landmark*. For example, let's take the 1D dataset discussed earlier and add two landmarks to it at $x_1 = –2$ and $x_1 = 1$ (see the left plot in Figure 5-8). Next, let's define the similarity function to be the Gaussian *Radial Basis Function* (RBF) with $\gamma = 0.3$ (see Equation 5-1).

Equation 5-1. Gaussian RBF

$$\phi_\gamma\left(\mathbf{x}, \ell\right) = \exp\left(-\gamma \|\mathbf{x} - \ell\|^2\right)$$

This is a bell-shaped function varying from 0 (very far away from the landmark) to 1 (at the landmark). Now we are ready to compute the new features. For example, let's look at the instance $x_1 = –1$: it is located at a distance of 1 from the first landmark and 2 from the second landmark. Therefore its new features are $x_2 = \exp(–0.3 \times 1^2) \approx 0.74$ and $x_3 = \exp(–0.3 \times 2^2) \approx 0.30$. The plot on the right in Figure 5-8 shows the transformed dataset (dropping the original features). As you can see, it is now linearly separable.

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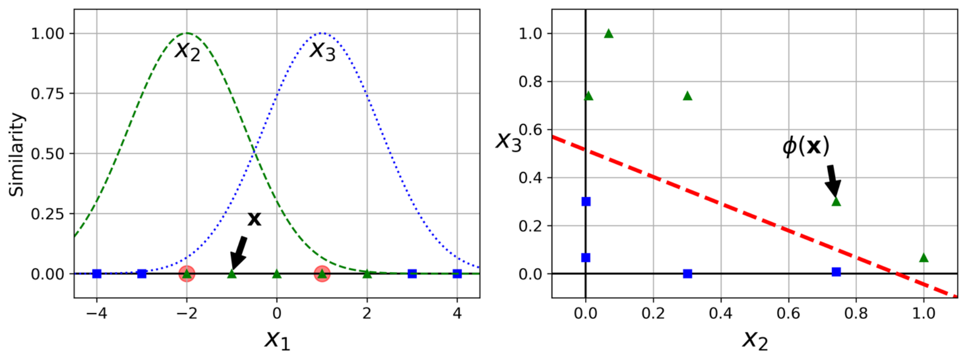

Figure 5-8. Similarity features using the Gaussian RBF

You may wonder how to select the landmarks. The simplest approach is to create a landmark at the location of each and every instance in the dataset. Doing that creates many dimensions and thus increases the chances that the transformed training set will be linearly separable. The downside is that a training set with *m* instances and *n* features gets transformed into a training set with *m* instances and *m* features (assuming you drop the original features). If your training set is very large, you end up with an equally large number of features.

Gaussian RBF Kernel

Just like the polynomial features method, the similarity features method can be useful with any Machine Learning algorithm, but it may be computationally expensive to compute all the additional features, especially on large training sets. Once again the kernel trick does its SVM magic, making it possible to obtain a similar result as if you had added many similarity features. Let's try the `SVC` class with the Gaussian RBF kernel:

```
rbf_kernel_svm_clf = Pipeline([
        ("scaler", StandardScaler()),
        ("svm_clf", SVC(kernel="rbf", gamma=5, C=0.001))
    ])
rbf_kernel_svm_clf.fit(X, y)
```

This model is represented at the bottom left in Figure 5-9. The other plots show models trained with different values of hyperparameters `gamma` (γ) and `C`. Increasing `gamma` makes the bell-shaped curve narrower (see the lefthand plots in Figure 5-8). As a result, each instance's range of influence is smaller:

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the decision boundary ends up being more irregular, wiggling around individual instances. Conversely, a small `gamma` value makes the bell-shaped curve wider: instances have a larger range of influence, and the decision boundary ends up smoother. So γ acts like a regularization hyperparameter: if your model is overfitting, you should reduce it; if it is underfitting, you should increase it (similar to the `C` hyperparameter).

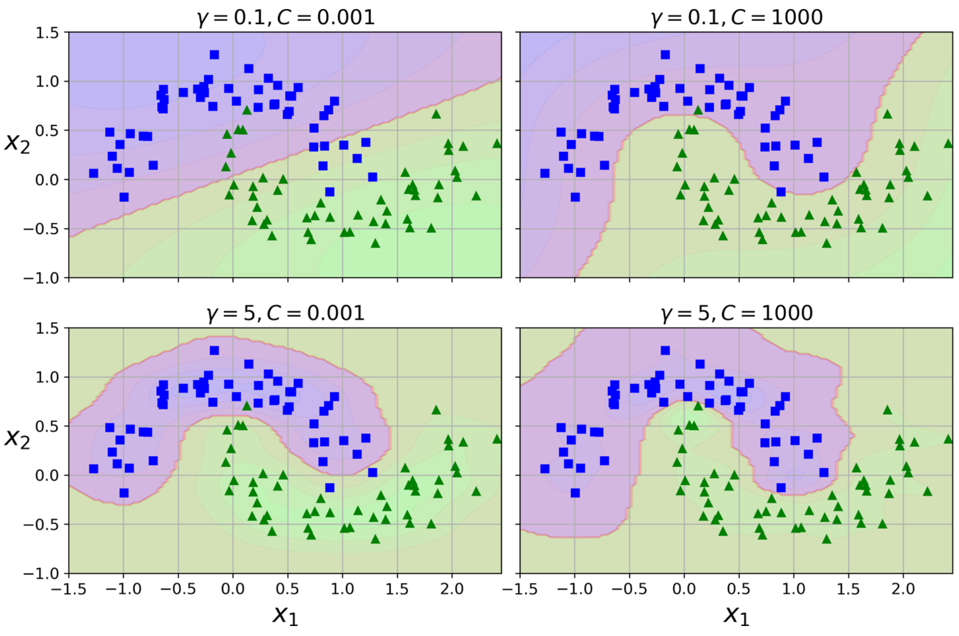

Figure 5-9. SVM classifiers using an RBF kernel

Other kernels exist but are used much more rarely. Some kernels are specialized for specific data structures. *String kernels* are sometimes used when classifying text documents or DNA sequences (e.g., using the *string subsequence kernel* or kernels based on the *Levenshtein distance*).

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TIP

With so many kernels to choose from, how can you decide which one to use? As a rule of thumb, you should always try the linear kernel first (remember that `LinearSVC` is much faster than `SVC(kernel="linear")`), especially if the training set is very large or if it has plenty of features. If the training set is not too large, you should also try the Gaussian RBF kernel; it works well in most cases. Then if you have spare time and computing power, you can experiment with a few other kernels, using cross-validation and grid search. You'd want to experiment like that especially if there are kernels specialized for your training set's data structure.

Computational Complexity

The `LinearSVC` class is based on the `liblinear` library, which implements an optimized algorithm for linear SVMs.[1] It does not support the kernel trick, but it scales almost linearly with the number of training instances and the number of features. Its training time complexity is roughly $O(m \times n)$.

The algorithm takes longer if you require very high precision. This is controlled by the tolerance hyperparameter ϵ (called `tol` in Scikit-Learn). In most classification tasks, the default tolerance is fine.

The `SVC` class is based on the `libsvm` library, which implements an algorithm that supports the kernel trick.[2] The training time complexity is usually between $O(m^2 \times n)$ and $O(m^3 \times n)$. Unfortunately, this means that it gets dreadfully slow when the number of training instances gets large (e.g., hundreds of thousands of instances). This algorithm is perfect for complex small or medium-sized training sets. It scales well with the number of features, especially with *sparse features* (i.e., when each instance has few nonzero features). In this case, the algorithm scales roughly with the average number of nonzero features per instance. Table 5-1 compares Scikit-Learn's SVM classification classes.

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Table 5-1. Comparison of Scikit-Learn classes for SVM classification

Class	Time complexity	Out-of-core support	Scaling required	Kernel trick
`LinearSVC`	$O(m \times n)$	No	Yes	No
`SGDClassifier`	$O(m \times n)$	Yes	Yes	No
`SVC`	$O(m^2 \times n)$ to $O(m^3 \times n)$	No	Yes	Yes

SVM Regression

As mentioned earlier, the SVM algorithm is versatile: not only does it support linear and nonlinear classification, but it also supports linear and nonlinear regression. To use SVMs for regression instead of classification, the trick is to reverse the objective: instead of trying to fit the largest possible street between two classes while limiting margin violations, SVM Regression tries to fit as many instances as possible *on* the street while limiting margin violations (i.e., instances *off* the street). The width of the street is controlled by a hyperparameter, ϵ. Figure 5-10 shows two linear SVM Regression models trained on some random linear data, one with a large margin ($\epsilon = 1.5$) and the other with a small margin ($\epsilon = 0.5$).

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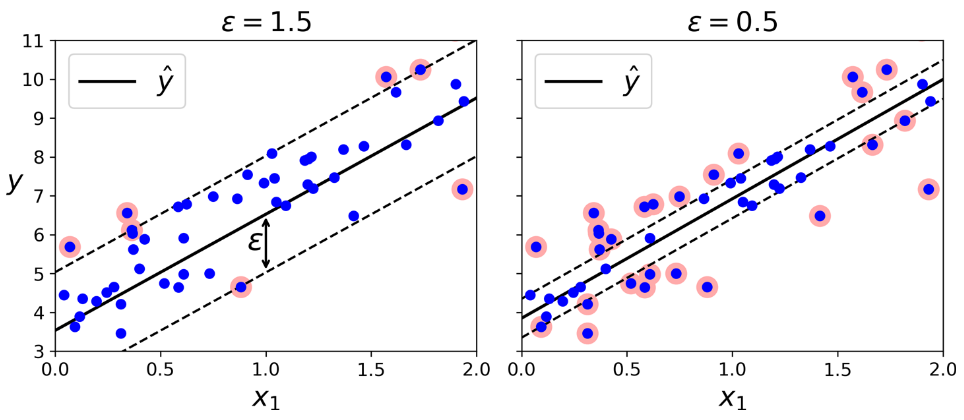

Figure 5-10. SVM Regression

Adding more training instances within the margin does not affect the model's predictions; thus, the model is said to be *ϵ-insensitive*.

You can use Scikit-Learn's `LinearSVR` class to perform linear SVM Regression. The following code produces the model represented on the left in Figure 5-10 (the training data should be scaled and centered first):

```
from sklearn.svm import LinearSVR

svm_reg = LinearSVR(epsilon=1.5)
svm_reg.fit(X, y)
```

To tackle nonlinear regression tasks, you can use a kernelized SVM model. Figure 5-11 shows SVM Regression on a random quadratic training set, using a second-degree polynomial kernel. There is little regularization in the left plot (i.e., a large `C` value), and much more regularization in the right plot (i.e., a small `C` value).

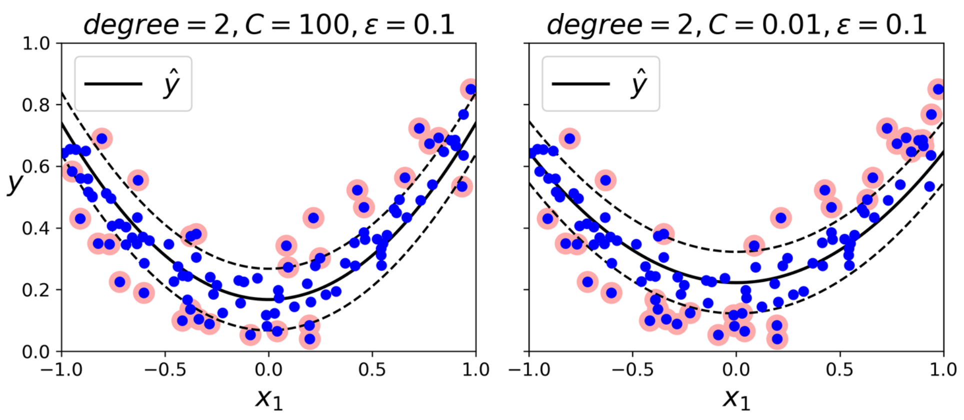

Figure 5-11. SVM Regression using a second-degree polynomial kernel

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The following code uses Scikit-Learn's `SVR` class (which supports the kernel trick) to produce the model represented on the left in Figure 5-11:

```
from sklearn.svm import SVR

svm_poly_reg = SVR(kernel="poly", degree=2, C=100, epsilon=0.1)
svm_poly_reg.fit(X, y)
```

The `SVR` class is the regression equivalent of the `SVC` class, and the `LinearSVR` class is the regression equivalent of the `LinearSVC` class. The `LinearSVR` class scales linearly with the size of the training set (just like the `LinearSVC` class), while the `SVR` class gets much too slow when the training set grows large (just like the `SVC` class).

NOTE

SVMs can also be used for outlier detection; see Scikit-Learn's documentation for more details.

Under the Hood

This section explains how SVMs make predictions and how their training algorithms work, starting with linear SVM classifiers. If you are just getting started with Machine Learning, you can safely skip it and go straight to the exercises at the end of this chapter, and come back later when you want to get a deeper understanding of SVMs.

First, a word about notations. In Chapter 4 we used the convention of putting all the model parameters in one vector $\boldsymbol{\theta}$, including the bias term θ_0 and the input feature weights θ_1 to θ_n, and adding a bias input $x_0 = 1$ to all instances. In this chapter we will use a convention that is more convenient (and more common) when dealing with SVMs: the bias term will be called b, and the feature weights vector will be called $\mathbf{w}$. No bias feature will be added to the input feature vectors.

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Decision Function and Predictions

The linear SVM classifier model predicts the class of a new instance **x** by simply computing the decision function $\mathbf{w}^\top \mathbf{x} + b = w_1 x_1 + \cdots + w_n x_n + b$. If the result is positive, the predicted class $\hat{y}$ is the positive class (1), and otherwise it is the negative class (0); see Equation 5-2.

Equation 5-2. Linear SVM classifier prediction

$$\hat{y} = \begin{cases} 0 & \text{if } \mathbf{w}^\intercal \mathbf{x} + b < 0, \\ 1 & \text{if } \mathbf{w}^\intercal \mathbf{x} + b \geq 0 \end{cases}$$

Figure 5-12 shows the decision function that corresponds to the model in the left in Figure 5-4: it is a 2D plane because this dataset has two features (petal width and petal length). The decision boundary is the set of points where the decision function is equal to 0: it is the intersection of two planes, which is a straight line (represented by the thick solid line).[3]

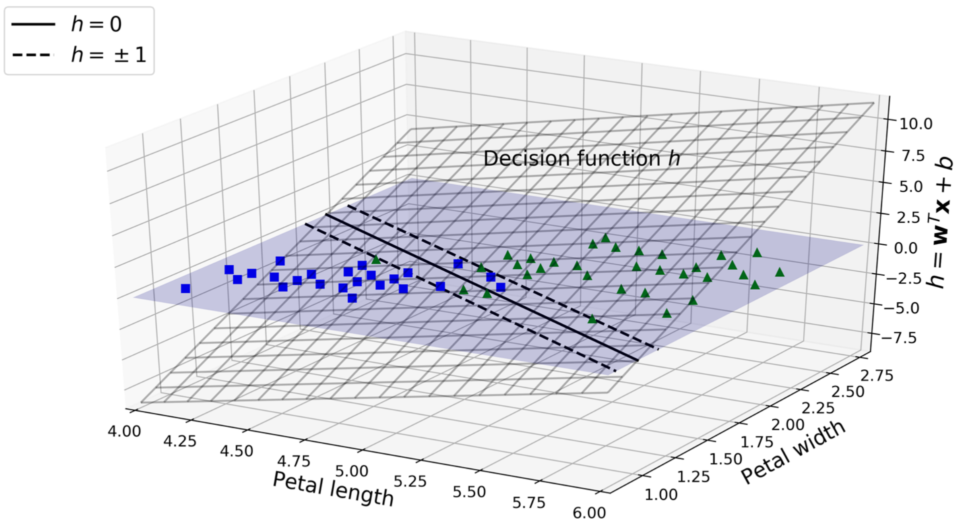

Figure 5-12. Decision function for the iris dataset

The dashed lines represent the points where the decision function is equal to 1 or –1: they are parallel and at equal distance to the decision boundary, and they form a margin around it. Training a linear SVM classifier means finding the values of **w** and *b* that make this margin as wide as possible while avoiding margin violations (hard margin) or limiting them (soft margin).

Training Objective

Consider the slope of the decision function: it is equal to the norm of the weight vector, $\| \mathbf{w} \|$. If we divide this slope by 2, the points where the

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decision function is equal to ±1 are going to be twice as far away from the decision boundary. In other words, dividing the slope by 2 will multiply the margin by 2. This may be easier to visualize in 2D, as shown in Figure 5-13. The smaller the weight vector **w**, the larger the margin.

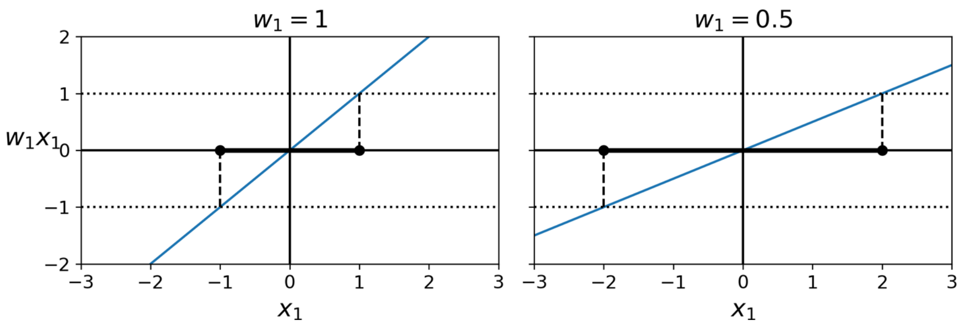

Figure 5-13. A smaller weight vector results in a larger margin

So we want to minimize ‖ **w** ‖ to get a large margin. If we also want to avoid any margin violations (hard margin), then we need the decision function to be greater than 1 for all positive training instances and lower than –1 for negative training instances. If we define $t^{(i)} = -1$ for negative instances (if $y^{(i)} = 0$) and $t^{(i)} = 1$ for positive instances (if $y^{(i)} = 1$), then we can express this constraint as $t^{(i)}(\mathbf{w}^\intercal \mathbf{x}^{(i)} + b) \geq 1$ for all instances.

We can therefore express the hard margin linear SVM classifier objective as the constrained optimization problem in Equation 5-3.

Equation 5-3. Hard margin linear SVM classifier objective

$$\begin{aligned} &\underset{\mathbf{w},b}{\text{minimize}} && \frac{1}{2}\mathbf{w}^\intercal \mathbf{w} \\ &\text{subject to} && t^{(i)}\left(\mathbf{w}^\intercal \mathbf{x}^{(i)} + b\right) \geq 1 \quad \text{for } i = 1, 2, \cdots, m \end{aligned}$$

NOTE

We are minimizing ½ $\mathbf{w}^\intercal \mathbf{w}$, which is equal to ½‖ **w** ‖^2, rather than minimizing ‖ **w** ‖. Indeed, ½‖ **w** ‖^2 has a nice, simple derivative (it is just **w**), while ‖ **w** ‖ is not differentiable at **w** = 0. Optimization algorithms work much better on differentiable functions.

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To get the soft margin objective, we need to introduce a *slack variable* $\zeta^{(i)} \geq 0$ for each instance:[4] $\zeta^{(i)}$ measures how much the i^{th} instance is allowed to violate the margin. We now have two conflicting objectives: make the slack variables as small as possible to reduce the margin violations, and make ½ $\mathbf{w}^\top \mathbf{w}$ as small as possible to increase the margin. This is where the `C` hyperparameter comes in: it allows us to define the tradeoff between these two objectives. This gives us the constrained optimization problem in Equation 5-4.

Equation 5-4. Soft margin linear SVM classifier objective

$$\begin{array}{ll} \underset{\mathbf{w},b,\zeta}{\text{minimize}} & \frac{1}{2}\mathbf{w}^\top\mathbf{w} + C\sum_{i=1}^{m}\zeta^{(i)} \\ \text{subject to} & t^{(i)}\left(\mathbf{w}^\top\mathbf{x}^{(i)} + b\right) \geq 1 - \zeta^{(i)} \quad \text{and} \quad \zeta^{(i)} \geq 0 \quad \text{for } i = 1, 2, \cdot \end{array}$$

Quadratic Programming

The hard margin and soft margin problems are both convex quadratic optimization problems with linear constraints. Such problems are known as *Quadratic Programming* (QP) problems. Many off-the-shelf solvers are available to solve QP problems by using a variety of techniques that are outside the scope of this book.[5]

The general problem formulation is given by Equation 5-5.

Equation 5-5. Quadratic Programming problem

$$\begin{array}{ll} \underset{\mathbf{p}}{\text{Minimize}} & \frac{1}{2}\mathbf{p}^\top\mathbf{H}\mathbf{p} \quad + \quad \mathbf{f}^\top\mathbf{p} \\ \text{subject to} & \mathbf{A}\mathbf{p} \leq \mathbf{b} \\ \text{where} & \left\{ \begin{array}{ll} \mathbf{p} & \text{is an } n_p\text{-dimensional vector } (n_p = \text{number of par} \\ \mathbf{H} & \text{is an } n_p \times n_p \text{ matrix,} \\ \mathbf{f} & \text{is an } n_p\text{-dimensional vector,} \\ \mathbf{A} & \text{is an } n_c \times n_p \text{ matrix } (n_c = \text{number of constraint} \\ \mathbf{b} & \text{is an } n_c\text{-dimensional vector.} \end{array} \right. \end{array}$$

Note that the expression $\mathbf{A}\ \mathbf{p} \leq \mathbf{b}$ defines n_c constraints: $\mathbf{p}^\top\ \mathbf{a}^{(i)} \leq b^{(i)}$ for i = 1, 2, ⋯, n_c, where $\mathbf{a}^{(i)}$ is the vector containing the elements of the i^{th} row of $\mathbf{A}$ and $b^{(i)}$ is the i^{th} element of $\mathbf{b}$.

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You can easily verify that if you set the QP parameters in the following way, you get the hard margin linear SVM classifier objective:

- $n_p = n + 1$, where n is the number of features (the +1 is for the bias term).
- $n_c = m$, where m is the number of training instances.
- **H** is the $n_p \times n_p$ identity matrix, except with a zero in the top-left cell (to ignore the bias term).
- $\mathbf{f} = 0$, an n_p-dimensional vector full of 0s.
- $\mathbf{b} = -1$, an n_c-dimensional vector full of –1s.
- $\mathbf{a}^{(i)} = -t^{(i)}\,\dot{\mathbf{x}}^{(i)}$, where $\dot{\mathbf{x}}^{(i)}$ is equal to $\mathbf{x}^{(i)}$ with an extra bias feature $\dot{\mathbf{x}}_0 = 1$.

One way to train a hard margin linear SVM classifier is to use an off-the-shelf QP solver and pass it the preceding parameters. The resulting vector **p** will contain the bias term $b = p_0$ and the feature weights $w_i = p_i$ for $i = 1, 2, \cdots, n$. Similarly, you can use a QP solver to solve the soft margin problem (see the exercises at the end of the chapter).

To use the kernel trick, we are going to look at a different constrained optimization problem.

The Dual Problem

Given a constrained optimization problem, known as the *primal problem*, it is possible to express a different but closely related problem, called its *dual problem*. The solution to the dual problem typically gives a lower bound to the solution of the primal problem, but under some conditions it can have the same solution as the primal problem. Luckily, the SVM problem happens to meet these conditions,[6] so you can choose to solve the primal problem or the dual problem; both will have the same solution. Equation 5-6 shows the dual form of the linear SVM objective (if you are interested in knowing how to derive the dual problem from the primal problem, see Appendix C).

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Equation 5-6. Dual form of the linear SVM objective

$$\underset{\alpha}{\text{minimize}}\ \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{m}\alpha^{(i)}\alpha^{(j)}t^{(i)}t^{(j)}\mathbf{x}^{(i)\intercal}\mathbf{x}^{(j)} \quad - \quad \sum_{i=1}^{m}\alpha^{(i)}$$
$$\text{subject to} \quad \alpha^{(i)} \geq 0 \quad \text{for } i = 1, 2, \cdots, m$$

Once you find the vector $\widehat{\boldsymbol{\alpha}}$ that minimizes this equation (using a QP solver), use Equation 5-7 to compute $\widehat{\mathbf{w}}$ and $\hat{b}$ that minimize the primal problem.

Equation 5-7. From the dual solution to the primal solution

$$\widehat{\mathbf{w}} = \sum_{i=1}^{m}\widehat{\alpha}^{(i)}t^{(i)}\mathbf{x}^{(i)}$$
$$\hat{b} = \frac{1}{n_s}\sum_{\substack{i=1 \\ \widehat{\alpha}^{(i)}>0}}^{m}\left(t^{(i)} - \widehat{\mathbf{w}}^\intercal\mathbf{x}^{(i)}\right)$$

The dual problem is faster to solve than the primal one when the number of training instances is smaller than the number of features. More importantly, the dual problem makes the kernel trick possible, while the primal does not. So what is this kernel trick, anyway?

Kernelized SVMs

Suppose you want to apply a second-degree polynomial transformation to a two-dimensional training set (such as the moons training set), then train a linear SVM classifier on the transformed training set. Equation 5-8 shows the second-degree polynomial mapping function ϕ that you want to apply.

Equation 5-8. Second-degree polynomial mapping

$$\phi\left(\mathbf{x}\right) = \phi\left(\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right) = \begin{pmatrix} {x_1}^2 \\ \sqrt{2}\,x_1x_2 \\ {x_2}^2 \end{pmatrix}$$

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

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

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 $\phi(\mathbf{a})^\intercal\ \phi(\mathbf{b})$, 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

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

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 $K(\mathbf{a}, \mathbf{b}) = \phi(\mathbf{a})^\top \phi(\mathbf{b})$. 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

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

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

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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

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

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.

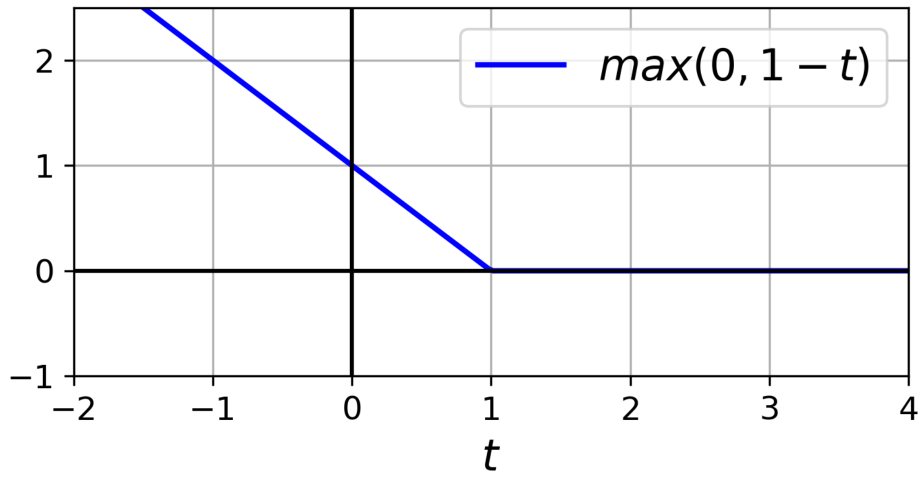
Equation 5-13. Linear SVM classifier cost function

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

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"), 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 implemented 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.

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1 Chih-Jen Lin et al., "A Dual Coordinate Descent Method for Large-Scale Linear SVM," *Proceedings of the 25th International Conference on Machine Learning* (2008): 408–415.

2 John Platt, "Sequential Minimal Optimization: A Fast Algorithm for Training Support Vector Machines" (Microsoft Research technical report, April 21, 1998), *https://www.microsoft.com/en-us/research/wp-content/uploads/2016/02/tr-98-14.pdf*.

3 More generally, when there are *n* features, the decision function is an *n*-dimensional *hyperplane*, and the decision boundary is an (n – 1)-

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dimensional hyperplane.

4 Zeta (ζ) is the sixth letter of the Greek alphabet.

5 To learn more about Quadratic Programming, you can start by reading Stephen Boyd and Lieven Vandenberghe's book *Convex Optimization* (Cambridge University Press, 2004) or watch Richard Brown's series of video lectures.

6 The objective function is convex, and the inequality constraints are continuously differentiable and convex functions.

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.

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.

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