Training Models

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as he or she writes—so you can take advantage of these technologies long before the official release of these titles. The following will be Chapter 4 in the final release of the book.

So far we have treated Machine Learning models and their training algorithms mostly like black boxes. If you went through some of the exercises in the previous chapters, you may have been surprised by how much you can get done without knowing anything about what's under the hood: you optimized a regression system, you improved a digit image classifier, and you even built a spam classifier from scratch—all this without knowing how they actually work. Indeed, in many situations you don't really need to know the implementation details.

However, having a good understanding of how things work can help you quickly home in on the appropriate model, the right training algorithm to use, and a good set of hyperparameters for your task. Understanding what's under the hood will also help you debug issues and perform error analysis more efficiently. Lastly, most of the topics discussed in this chapter will be essential in understanding, building, and training neural networks (discussed in Part II of this book).

In this chapter, we will start by looking at the Linear Regression model, one of the simplest models there is. We will discuss two very different ways to train it:

- Using a direct "closed-form" equation that directly computes the model parameters that best fit the model to the training set (i.e., the model parameters that minimize the cost function over the training set).

- Using an iterative optimization approach, called Gradient Descent (GD), that gradually tweaks the model parameters to minimize the cost function over the training set, eventually converging to the same set of parameters as the first method. We will look at a few variants of Gradient Descent that we will use again and again when we study neural networks in Part II: Batch GD, Mini-batch GD, and Stochastic GD.

Next we will look at Polynomial Regression, a more complex model that can fit nonlinear datasets. Since this model has more parameters than Linear Regression, it is more prone to overfitting the training data, so we will look at how to detect whether or not this is the case, using learning curves, and then we will look at several regularization techniques that can reduce the risk of overfitting the training set.

Finally, we will look at two more models that are commonly used for classification tasks: Logistic Regression and Softmax Regression.

There will be quite a few math equations in this chapter, using basic notions of linear algebra and calculus. To understand these equations, you will need to know what vectors and matrices are, how to transpose them, multiply them, and inverse them, and what partial derivatives are. If you are unfamiliar with these concepts, please go through the linear algebra and calculus introductory tutorials available as Jupyter notebooks in the online supplemental material. For those who are truly allergic to mathematics, you should still go through this chapter and simply skip the equations; hopefully, the text will be sufficient to help you understand most of the concepts.

Linear Regression

In Chapter 1, we looked at a simple regression model of life satisfaction: $life\_satisfaction = \theta_0 + \theta_1 \times GDP\_per\_capita$.

This model is just a linear function of the input feature `GDP_per_capita`. θ_0 and θ_1 are the model's parameters.

More generally, a linear model makes a prediction by simply computing a weighted sum of the input features, plus a constant called the *bias term* (also called the *intercept term*), as shown in Equation 4-1.

Equation 4-1. Linear Regression model prediction

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$$

- $\hat{y}$ is the predicted value.

- n is the number of features.
- x_i is the ith feature value.
- θ_j is the jth model parameter (including the bias term θ_0 and the feature weights $\theta_1, \theta_2, \cdots, \theta_n$).

This can be written much more concisely using a vectorized form, as shown in Equation 4-2.

Equation 4-2. Linear Regression model prediction (vectorized form)

$$\hat{y} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta} \cdot \mathbf{x}$$

- $\boldsymbol{\theta}$ is the model's *parameter vector*, containing the bias term θ_0 and the feature weights θ_1 to θ_n.
- $\mathbf{x}$ is the instance's *feature vector*, containing x_0 to x_n, with x_0 always equal to 1.
- $\boldsymbol{\theta} \cdot \mathbf{x}$ is the dot product of the vectors $\boldsymbol{\theta}$ and $\mathbf{x}$, which is of course equal to $\theta_0 x_0 + \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_n x_n$.
- $h_{\boldsymbol{\theta}}$ is the hypothesis function, using the model parameters $\boldsymbol{\theta}$.

In Machine Learning, vectors are often represented as *column vectors*, which are 2D arrays with a single column. If $\boldsymbol{\theta}$ and $\mathbf{x}$ are column vectors, then the prediction is: $\hat{y} = \boldsymbol{\theta}^{\mathbf{T}}\mathbf{x}$, where $\boldsymbol{\theta}^{\mathbf{T}}$ is the *transpose* of $\boldsymbol{\theta}$ (a row vector instead of a column vector) and $\boldsymbol{\theta}^{\mathbf{T}}\mathbf{x}$ is the matrix multiplication of $\boldsymbol{\theta}^{\mathbf{T}}$ and $\mathbf{x}$. It is of course the same prediction, except it is now represented as a single cell matrix rather than a scalar value. In this book we will use this notation to avoid switching between dot products and matrix multiplications.

Okay, that's the Linear Regression model, so now how do we train it? Well, recall that training a model means setting its parameters so that the model best fits the training set. For this purpose, we first need a measure of how well (or poorly) the model fits the training data. In Chapter 2 we saw that the most common performance measure of a regression model is the Root Mean Square Error (RMSE) (Equation 2-1). Therefore, to train a Linear Regression model, you need to find the value of $\boldsymbol{\theta}$ that minimizes the RMSE. In practice, it is simpler to minimize the Mean Square Error (MSE) than the RMSE, and it leads to the same result (because the value that minimizes a function also minimizes its square root).[1]

The MSE of a Linear Regression hypothesis $h_{\boldsymbol{\theta}}$ on a training set $\mathbf{X}$ is calculated using Equation 4-3.

Equation 4-3. MSE cost function for a Linear Regression model

$$\text{MSE}\left(\mathbf{X}, h_{\boldsymbol{\theta}}\right) = \frac{1}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}\right)^2$$

Most of these notations were presented in Chapter 2 (see "Notations" on page 43). The only difference is that we write $h_{\boldsymbol{\theta}}$ instead of just h in order to make it clear that the model is parametrized by the vector $\boldsymbol{\theta}$. To simplify notations, we will just write MSE($\boldsymbol{\theta}$) instead of MSE($\mathbf{X}$, $h_{\boldsymbol{\theta}}$).

The Normal Equation

To find the value of $\boldsymbol{\theta}$ that minimizes the cost function, there is a *closed-form solution* —in other words, a mathematical equation that gives the result directly. This is called the *Normal Equation* (Equation 4-4).[2]

Equation 4-4. Normal Equation

$$\widehat{\boldsymbol{\theta}} = \left(\mathbf{X}^T \mathbf{X}\right)^{-1} \quad \mathbf{X}^T \quad \mathbf{y}$$

- $\widehat{\boldsymbol{\theta}}$ is the value of $\boldsymbol{\theta}$ that minimizes the cost function.
- $\mathbf{y}$ is the vector of target values containing $y^{(1)}$ to $y^{(m)}$.

Let's generate some linear-looking data to test this equation on (Figure 4-1):

```
import numpy as np

X = 2 * np.random.rand(100, 1)
y = 4 + 3 * X + np.random.randn(100, 1)
```

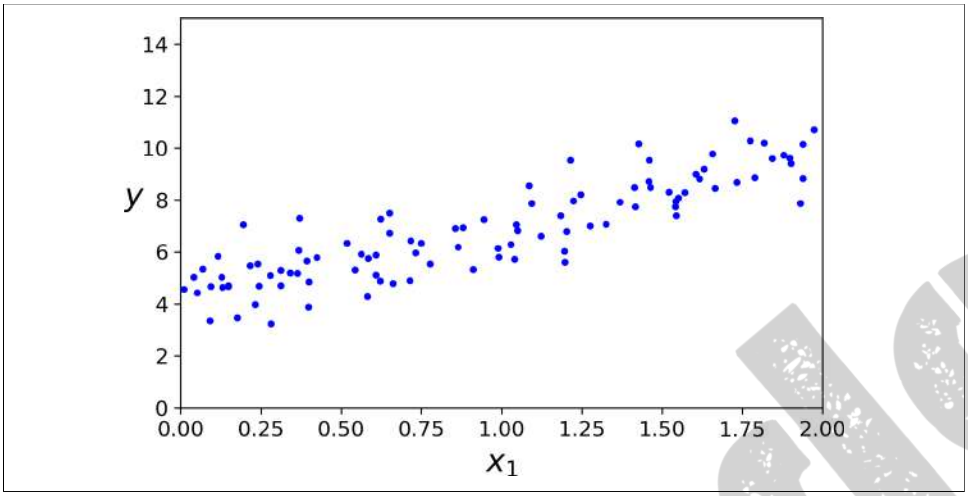


Figure 4-1. Randomly generated linear dataset

Now let's compute $\hat{\boldsymbol{\theta}}$ using the Normal Equation. We will use the `inv()` function from NumPy's Linear Algebra module (`np.linalg`) to compute the inverse of a matrix, and the `dot()` method for matrix multiplication:

```
X_b = np.c_[np.ones((100, 1)), X]  # add x0 = 1 to each instance
theta_best = np.linalg.inv(X_b.T.dot(X_b)).dot(X_b.T).dot(y)
```

The actual function that we used to generate the data is $y = 4 + 3x_1$ + Gaussian noise. Let's see what the equation found:

```
>>> theta_best
array([[4.21509616],
       [2.77011339]])
```

We would have hoped for $\theta_0 = 4$ and $\theta_1 = 3$ instead of $\theta_0 = 4.215$ and $\theta_1 = 2.770$. Close enough, but the noise made it impossible to recover the exact parameters of the original function.

Now you can make predictions using $\hat{\boldsymbol{\theta}}$:

```
>>> X_new = np.array([[0], [2]])
>>> X_new_b = np.c_[np.ones((2, 1)), X_new] # add x0 = 1 to each instance
>>> y_predict = X_new_b.dot(theta_best)
>>> y_predict
array([[4.21509616],
       [9.75532293]])
```

Let's plot this model's predictions (Figure 4-2):

```
plt.plot(X_new, y_predict, "r-")
plt.plot(X, y, "b.")
```

```
    plt.axis([0, 2, 0, 15])
    plt.show()
```

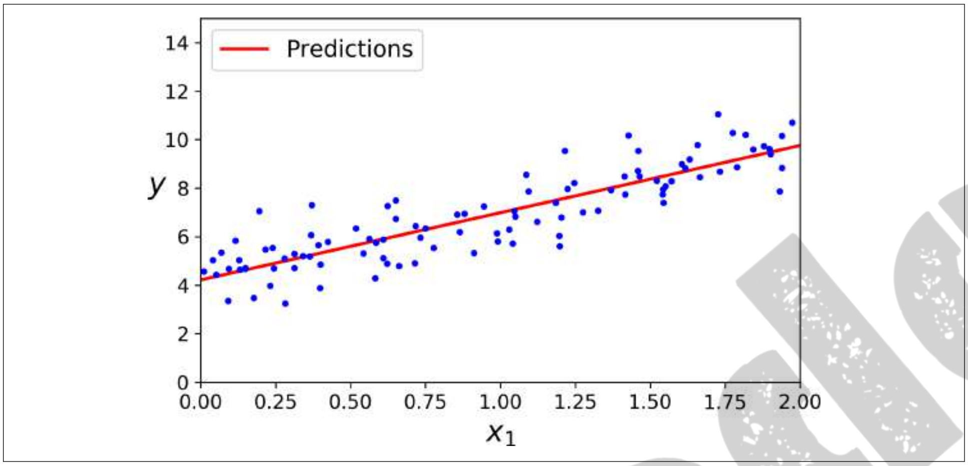


Figure 4-2. Linear Regression model predictions

Performing linear regression using Scikit-Learn is quite simple:[3]

```
>>> from sklearn.linear_model import LinearRegression
>>> lin_reg = LinearRegression()
>>> lin_reg.fit(X, y)
>>> lin_reg.intercept_, lin_reg.coef_
(array([4.21509616]), array([[2.77011339]]))
>>> lin_reg.predict(X_new)
array([[4.21509616],
       [9.75532293]])
```

The `LinearRegression` class is based on the `scipy.linalg.lstsq()` function (the name stands for "least squares"), which you could call directly:

```
>>> theta_best_svd, residuals, rank, s = np.linalg.lstsq(X_b, y, rcond=1e-6)
>>> theta_best_svd
array([[4.21509616],
       [2.77011339]])
```

This function computes $\hat{\boldsymbol{\theta}} = \mathbf{X}^{+}\mathbf{y}$, where $\mathbf{X}^{+}$ is the *pseudoinverse* of $\mathbf{X}$ (specifically the Moore-Penrose inverse). You can use `np.linalg.pinv()` to compute the pseudoinverse directly:

```
>>> np.linalg.pinv(X_b).dot(y)
array([[4.21509616],
       [2.77011339]])
```

The pseudoinverse itself is computed using 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 $\mathbf{U}\ \mathbf{\Sigma}\ \mathbf{V}^T$ (see `numpy.linalg.svd()`). The pseudoinverse is computed as $\mathbf{X}^+ = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^T$. To compute the matrix $\mathbf{\Sigma}^+$, the algorithm takes $\mathbf{\Sigma}$ and sets to zero all values smaller than a tiny threshold value, then it replaces all the non-zero values with their inverse, and finally it transposes the resulting matrix. This approach is more efficient than computing the Normal Equation, plus it handles edge cases nicely: indeed, the Normal Equation may not work if the matrix $\mathbf{X}^T\mathbf{X}$ is not invertible (i.e., singular), such as if $m < n$ or if some features are redundant, but the pseudoinverse is always defined.

Computational Complexity

The Normal Equation computes the inverse of $\mathbf{X}^T\ \mathbf{X}$, which is an $(n + 1) \times (n + 1)$ matrix (where n is the number of features). The *computational complexity* of inverting such a matrix is typically about $O(n^{2.4})$ to $O(n^3)$ (depending on the implementation). In other words, if you double the number of features, you multiply the computation time by roughly $2^{2.4} = 5.3$ to $2^3 = 8$.

The SVD approach used by Scikit-Learn's `LinearRegression` class is about $O(n^2)$. If you double the number of features, you multiply the computation time by roughly 4.

Both the Normal Equation and the SVD approach get very slow when the number of features grows large (e.g., 100,000). On the positive side, both are linear with regards to the number of instances in the training set (they are $O(m)$), so they handle large training sets efficiently, provided they can fit in memory.

Also, once you have trained your Linear Regression model (using the Normal Equation or any other algorithm), predictions are very fast: the computational complexity is linear with regards to both the number of instances you want to make predictions on and the number of features. In other words, making predictions on twice as many instances (or twice as many features) will just take roughly twice as much time.

Now we will look at very different ways to train a Linear Regression model, better suited for cases where there are a large number of features, or too many training instances to fit in memory.

Gradient Descent

Gradient Descent is a very generic optimization algorithm capable of finding optimal solutions to a wide range of problems. The general idea of Gradient Descent is to tweak parameters iteratively in order to minimize a cost function.

Suppose you are lost in the mountains in a dense fog; you can only feel the slope of the ground below your feet. A good strategy to get to the bottom of the valley quickly is to go downhill in the direction of the steepest slope. This is exactly what Gradient Descent does: it measures the local gradient of the error function with regards to the parameter vector **θ**, and it goes in the direction of descending gradient. Once the gradient is zero, you have reached a minimum!

Concretely, you start by filling **θ** with random values (this is called *random initialization*), and then you improve it gradually, taking one baby step at a time, each step attempting to decrease the cost function (e.g., the MSE), until the algorithm *converges* to a minimum (see Figure 4-3).

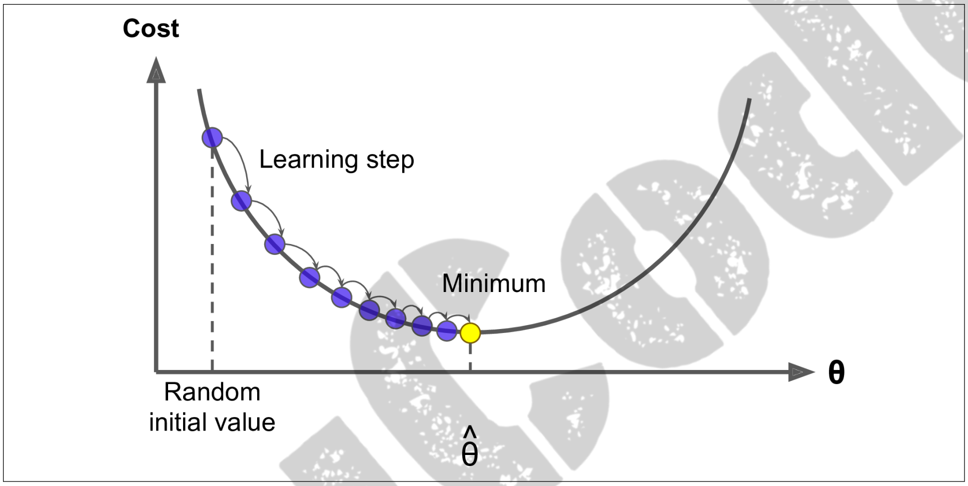


Figure 4-3. Gradient Descent

An important parameter in Gradient Descent is the size of the steps, determined by the *learning rate* hyperparameter. If the learning rate is too small, then the algorithm will have to go through many iterations to converge, which will take a long time (see Figure 4-4).

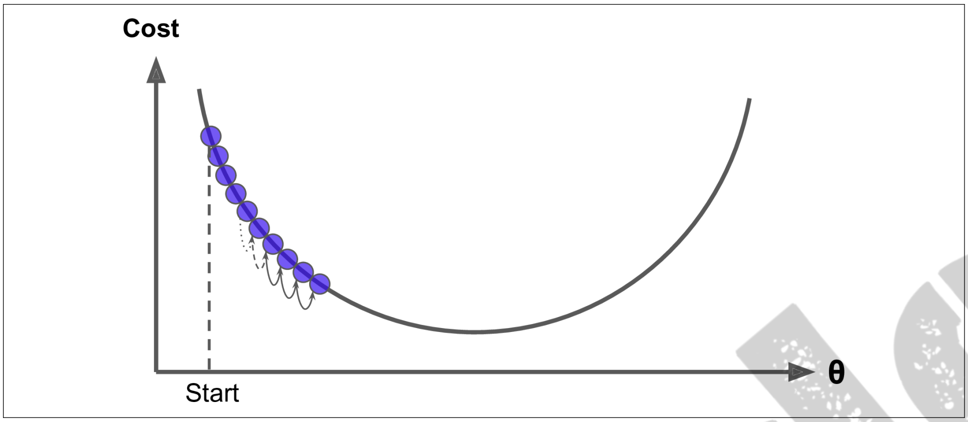


Figure 4-4. Learning rate too small

On the other hand, if the learning rate is too high, you might jump across the valley and end up on the other side, possibly even higher up than you were before. This might make the algorithm diverge, with larger and larger values, failing to find a good solution (see Figure 4-5).

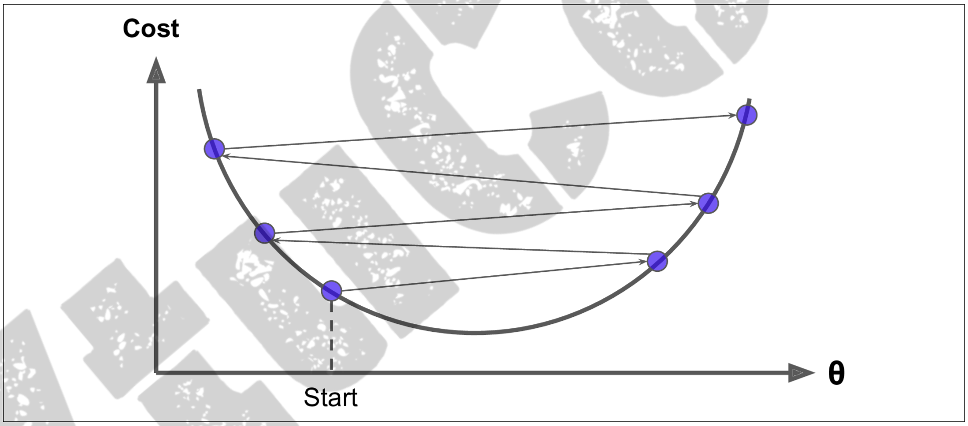


Figure 4-5. Learning rate too large

Finally, not all cost functions look like nice regular bowls. There may be holes, ridges, plateaus, and all sorts of irregular terrains, making convergence to the minimum very difficult. Figure 4-6 shows the two main challenges with Gradient Descent: if the random initialization starts the algorithm on the left, then it will converge to a *local minimum*, which is not as good as the *global minimum*. If it starts on the right, then it will take a very long time to cross the plateau, and if you stop too early you will never reach the global minimum.

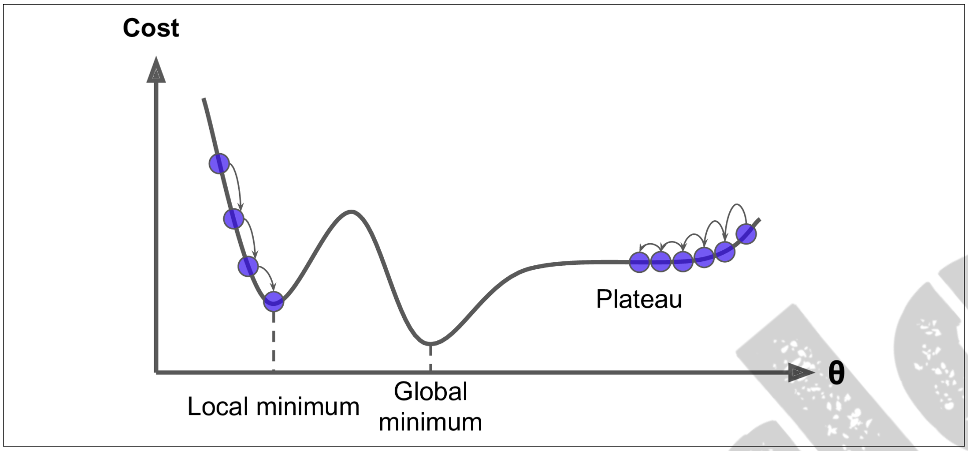


Figure 4-6. Gradient Descent pitfalls

Fortunately, the MSE cost function for a Linear Regression model happens to be a *convex function*, which means that if you pick any two points on the curve, the line segment joining them never crosses the curve. This implies that there are no local minima, just one global minimum. It is also a continuous function with a slope that never changes abruptly.[4] These two facts have a great consequence: Gradient Descent is guaranteed to approach arbitrarily close the global minimum (if you wait long enough and if the learning rate is not too high).

In fact, the cost function has the shape of a bowl, but it can be an elongated bowl if the features have very different scales. Figure 4-7 shows Gradient Descent on a training set where features 1 and 2 have the same scale (on the left), and on a training set where feature 1 has much smaller values than feature 2 (on the right).[5]

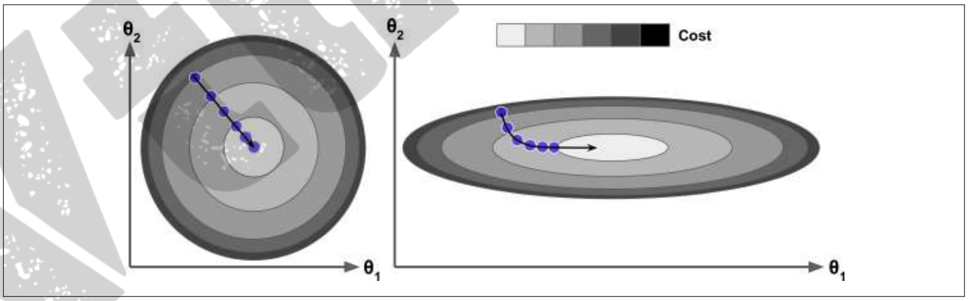


Figure 4-7. Gradient Descent with and without feature scaling

As you can see, on the left the Gradient Descent algorithm goes straight toward the minimum, thereby reaching it quickly, whereas on the right it first goes in a direction almost orthogonal to the direction of the global minimum, and it ends with a long march down an almost flat valley. It will eventually reach the minimum, but it will take a long time.

When using Gradient Descent, you should ensure that all features have a similar scale (e.g., using Scikit-Learn's `StandardScaler` class), or else it will take much longer to converge.

This diagram also illustrates the fact that training a model means searching for a combination of model parameters that minimizes a cost function (over the training set). It is a search in the model's *parameter space*: the more parameters a model has, the more dimensions this space has, and the harder the search is: searching for a needle in a 300-dimensional haystack is much trickier than in three dimensions. Fortunately, since the cost function is convex in the case of Linear Regression, the needle is simply at the bottom of the bowl.

Batch Gradient Descent

To implement Gradient Descent, you need to compute the gradient of the cost function with regards to each model parameter θ_j. In other words, you need to calculate how much the cost function will change if you change θ_j just a little bit. This is called a *partial derivative*. It is like asking "what is the slope of the mountain under my feet if I face east?" and then asking the same question facing north (and so on for all other dimensions, if you can imagine a universe with more than three dimensions). Equation 4-5 computes the partial derivative of the cost function with regards to parameter θ_j, noted $\frac{\partial}{\partial \theta_j} \text{MSE}(\boldsymbol{\theta})$.

Equation 4-5. Partial derivatives of the cost function

$$\frac{\partial}{\partial \theta_j} \text{MSE}(\boldsymbol{\theta}) = \frac{2}{m} \sum_{i=1}^{m} \left(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)} \right) x_j^{(i)}$$

Instead of computing these partial derivatives individually, you can use Equation 4-6 to compute them all in one go. The gradient vector, noted $\nabla_{\boldsymbol{\theta}} \text{MSE}(\boldsymbol{\theta})$, contains all the partial derivatives of the cost function (one for each model parameter).

Equation 4-6. Gradient vector of the cost function

$$\nabla_{\boldsymbol{\theta}}\,\text{MSE}(\boldsymbol{\theta}) = \begin{pmatrix} \frac{\partial}{\partial \theta_0}\text{MSE}(\boldsymbol{\theta}) \\ \frac{\partial}{\partial \theta_1}\text{MSE}(\boldsymbol{\theta}) \\ \vdots \\ \frac{\partial}{\partial \theta_n}\text{MSE}(\boldsymbol{\theta}) \end{pmatrix} = \frac{2}{m}\mathbf{X}^T(\mathbf{X}\boldsymbol{\theta} - \mathbf{y})$$

Notice that this formula involves calculations over the full training set **X**, at each Gradient Descent step! This is why the algorithm is called *Batch Gradient Descent*: it uses the whole batch of training data at every step (actually, *Full Gradient Descent* would probably be a better name). As a result it is terribly slow on very large training sets (but we will see much faster Gradient Descent algorithms shortly). However, Gradient Descent scales well with the number of features; training a Linear Regression model when there are hundreds of thousands of features is much faster using Gradient Descent than using the Normal Equation or SVD decomposition.

Once you have the gradient vector, which points uphill, just go in the opposite direction to go downhill. This means subtracting $\nabla_{\boldsymbol{\theta}}\text{MSE}(\boldsymbol{\theta})$ from $\boldsymbol{\theta}$. This is where the learning rate η comes into play:[6] multiply the gradient vector by η to determine the size of the downhill step (Equation 4-7).

Equation 4-7. Gradient Descent step

$$\boldsymbol{\theta}^{(\text{next step})} = \boldsymbol{\theta} - \eta\nabla_{\boldsymbol{\theta}}\,\text{MSE}(\boldsymbol{\theta})$$

Let's look at a quick implementation of this algorithm:

```
eta = 0.1  # learning rate
n_iterations = 1000
m = 100

theta = np.random.randn(2,1)  # random initialization

for iteration in range(n_iterations):
    gradients = 2/m * X_b.T.dot(X_b.dot(theta) - y)
    theta = theta - eta * gradients
```

That wasn't too hard! Let's look at the resulting `theta`:

```
>>> theta
array([[4.21509616],
       [2.77011339]])
```

Hey, that's exactly what the Normal Equation found! Gradient Descent worked perfectly. But what if you had used a different learning rate `eta`? Figure 4-8 shows the first 10 steps of Gradient Descent using three different learning rates (the dashed line represents the starting point).

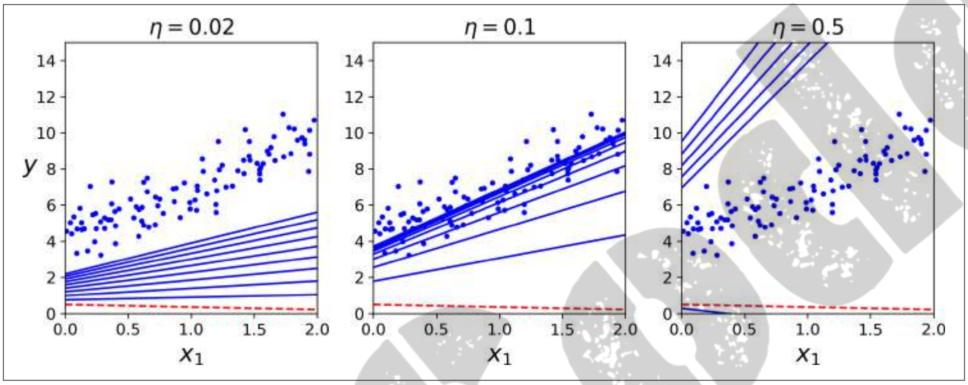


Figure 4-8. Gradient Descent with various learning rates

On the left, the learning rate is too low: the algorithm will eventually reach the solution, but it will take a long time. In the middle, the learning rate looks pretty good: in just a few iterations, it has already converged to the solution. On the right, the learning rate is too high: the algorithm diverges, jumping all over the place and actually getting further and further away from the solution at every step.

To find a good learning rate, you can use grid search (see Chapter 2). However, you may want to limit the number of iterations so that grid search can eliminate models that take too long to converge.

You may wonder how to set the number of iterations. If it is too low, you will still be far away from the optimal solution when the algorithm stops, but if it is too high, you will waste time while the model parameters do not change anymore. A simple solution is to set a very large number of iterations but to interrupt the algorithm when the gradient vector becomes tiny—that is, when its norm becomes smaller than a tiny number ϵ (called the *tolerance*)—because this happens when Gradient Descent has (almost) reached the minimum.

Convergence Rate

When the cost function is convex and its slope does not change abruptly (as is the case for the MSE cost function), Batch Gradient Descent with a fixed learning rate will eventually converge to the optimal solution, but you may have to wait a while: it can take $O(1/\epsilon)$ iterations to reach the optimum within a range of ϵ depending on the shape of the cost function. If you divide the tolerance by 10 to have a more precise solution, then the algorithm may have to run about 10 times longer.

Stochastic Gradient Descent

The main problem with Batch Gradient Descent is the fact that it uses the whole training set to compute the gradients at every step, which makes it very slow when the training set is large. At the opposite extreme, *Stochastic Gradient Descent* just picks a random instance in the training set at every step and computes the gradients based only on that single instance. Obviously this makes the algorithm much faster since it has very little data to manipulate at every iteration. It also makes it possible to train on huge training sets, since only one instance needs to be in memory at each iteration (SGD can be implemented as an out-of-core algorithm.[7])

On the other hand, due to its stochastic (i.e., random) nature, this algorithm is much less regular than Batch Gradient Descent: instead of gently decreasing until it reaches the minimum, the cost function will bounce up and down, decreasing only on average. Over time it will end up very close to the minimum, but once it gets there it will continue to bounce around, never settling down (see Figure 4-9). So once the algorithm stops, the final parameter values are good, but not optimal.

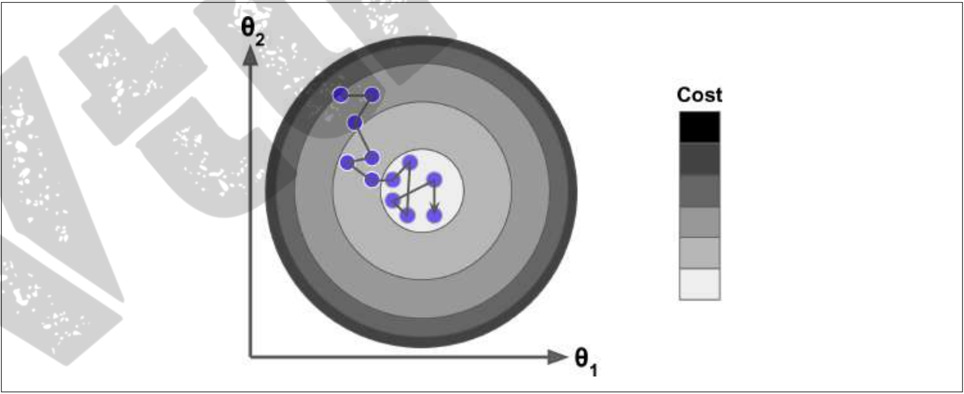


Figure 4-9. Stochastic Gradient Descent

When the cost function is very irregular (as in Figure 4-6), this can actually help the algorithm jump out of local minima, so Stochastic Gradient Descent has a better chance of finding the global minimum than Batch Gradient Descent does.

Therefore randomness is good to escape from local optima, but bad because it means that the algorithm can never settle at the minimum. One solution to this dilemma is to gradually reduce the learning rate. The steps start out large (which helps make quick progress and escape local minima), then get smaller and smaller, allowing the algorithm to settle at the global minimum. This process is akin to *simulated annealing*, an algorithm inspired from the process of annealing in metallurgy where molten metal is slowly cooled down. The function that determines the learning rate at each iteration is called the *learning schedule*. If the learning rate is reduced too quickly, you may get stuck in a local minimum, or even end up frozen halfway to the minimum. If the learning rate is reduced too slowly, you may jump around the minimum for a long time and end up with a suboptimal solution if you halt training too early.

This code implements Stochastic Gradient Descent using a simple learning schedule:

```
n_epochs = 50
t0, t1 = 5, 50  # learning schedule hyperparameters

def learning_schedule(t):
    return t0 / (t + t1)

theta = np.random.randn(2,1)  # random initialization

for epoch in range(n_epochs):
    for i in range(m):
        random_index = np.random.randint(m)
        xi = X_b[random_index:random_index+1]
        yi = y[random_index:random_index+1]
        gradients = 2 * xi.T.dot(xi.dot(theta) - yi)
        eta = learning_schedule(epoch * m + i)
        theta = theta - eta * gradients
```

By convention we iterate by rounds of m iterations; each round is called an *epoch*. While the Batch Gradient Descent code iterated 1,000 times through the whole training set, this code goes through the training set only 50 times and reaches a fairly good solution:

```
>>> theta
array([[4.21076011],
       [2.74856079]])
```

Figure 4-10 shows the first 20 steps of training (notice how irregular the steps are).

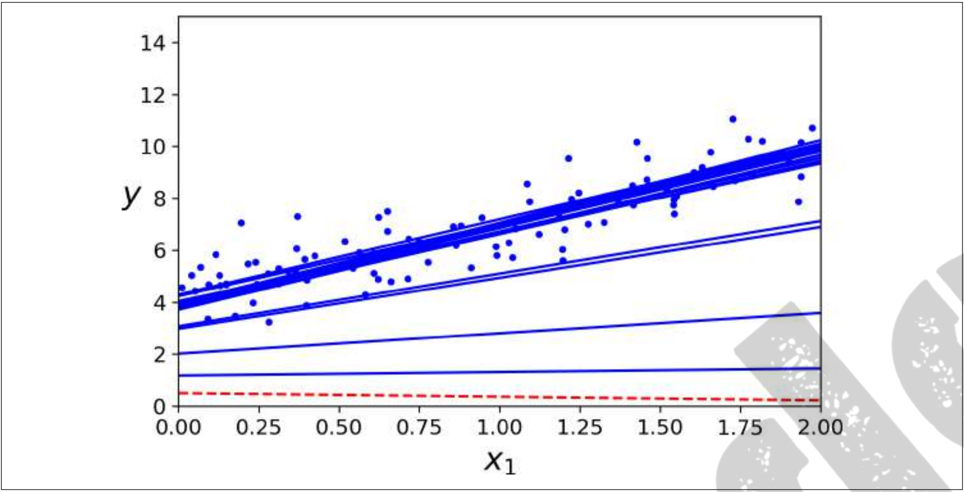


Figure 4-10. Stochastic Gradient Descent first 20 steps

Note that since instances are picked randomly, some instances may be picked several times per epoch while others may not be picked at all. If you want to be sure that the algorithm goes through every instance at each epoch, another approach is to shuffle the training set (making sure to shuffle the input features and the labels jointly), then go through it instance by instance, then shuffle it again, and so on. However, this generally converges more slowly.

When using Stochastic Gradient Descent, the training instances must be independent and identically distributed (IID), to ensure that the parameters get pulled towards the global optimum, on average. A simple way to ensure this is to shuffle the instances during training (e.g., pick each instance randomly, or shuffle the training set at the beginning of each epoch). If you do not do this, for example if the instances are sorted by label, then SGD will start by optimizing for one label, then the next, and so on, and it will not settle close to the global minimum.

To perform Linear Regression using SGD with Scikit-Learn, you can use the `SGDRegressor` class, which defaults to optimizing the squared error cost function. The following code runs for maximum 1000 epochs (`max_iter=1000`) or until the loss drops by less than 1e-3 during one epoch (`tol=1e-3`), starting with a learning rate of 0.1 (`eta0=0.1`), using the default learning schedule (different from the preceding one), and it does not use any regularization (`penalty=None`; more details on this shortly):

```
from sklearn.linear_model import SGDRegressor
sgd_reg = SGDRegressor(max_iter=1000, tol=1e-3, penalty=None, eta0=0.1)
sgd_reg.fit(X, y.ravel())
```

Once again, you find a solution quite close to the one returned by the Normal Equation:

```
>>> sgd_reg.intercept_, sgd_reg.coef_
(array([4.24365286]), array([2.8250878]))
```

Mini-batch Gradient Descent

The last Gradient Descent algorithm we will look at is called *Mini-batch Gradient Descent*. It is quite simple to understand once you know Batch and Stochastic Gradient Descent: at each step, instead of computing the gradients based on the full training set (as in Batch GD) or based on just one instance (as in Stochastic GD), Mini-batch GD computes the gradients on small random sets of instances called *mini-batches*. The main advantage of Mini-batch GD over Stochastic GD is that you can get a performance boost from hardware optimization of matrix operations, especially when using GPUs.

The algorithm's progress in parameter space is less erratic than with SGD, especially with fairly large mini-batches. As a result, Mini-batch GD will end up walking around a bit closer to the minimum than SGD. But, on the other hand, it may be harder for it to escape from local minima (in the case of problems that suffer from local minima, unlike Linear Regression as we saw earlier). Figure 4-11 shows the paths taken by the three Gradient Descent algorithms in parameter space during training. They all end up near the minimum, but Batch GD's path actually stops at the minimum, while both Stochastic GD and Mini-batch GD continue to walk around. However, don't forget that Batch GD takes a lot of time to take each step, and Stochastic GD and Mini-batch GD would also reach the minimum if you used a good learning schedule.

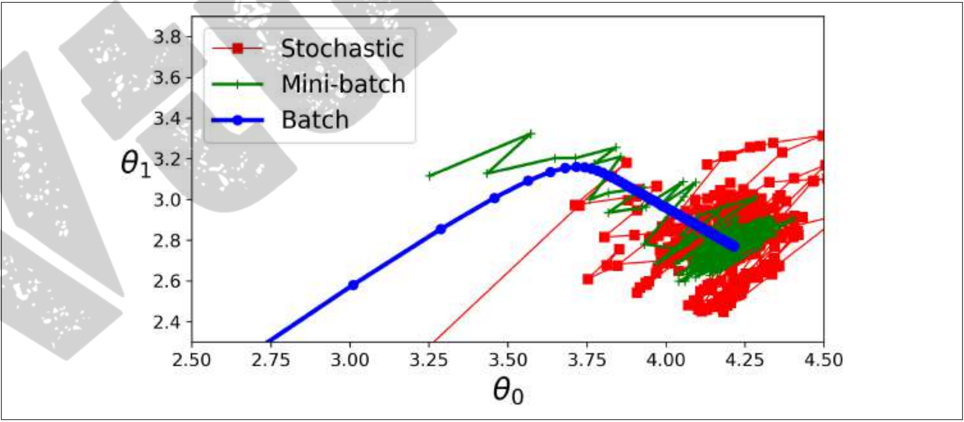


Figure 4-11. Gradient Descent paths in parameter space

Let's compare the algorithms we've discussed so far for Linear Regression[8] (recall that m is the number of training instances and n is the number of features); see Table 4-1.

Table 4-1. Comparison of algorithms for Linear Regression

Algorithm	Large m	Out-of-core support	Large n	Hyperparams	Scaling required	Scikit-Learn
Normal Equation	Fast	No	Slow	0	No	n/a
SVD	Fast	No	Slow	0	No	`LinearRegression`
Batch GD	Slow	No	Fast	2	Yes	`SGDRegressor`
Stochastic GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`
Mini-batch GD	Fast	Yes	Fast	≥2	Yes	`SGDRegressor`

There is almost no difference after training: all these algorithms end up with very similar models and make predictions in exactly the same way.

Polynomial Regression

What if your data is actually more complex than a simple straight line? Surprisingly, you can actually use a linear model to fit nonlinear data. A simple way to do this is to add powers of each feature as new features, then train a linear model on this extended set of features. This technique is called *Polynomial Regression*.

Let's look at an example. First, let's generate some nonlinear data, based on a simple *quadratic equation*[9] (plus some noise; see Figure 4-12):

```
m = 100
X = 6 * np.random.rand(m, 1) - 3
y = 0.5 * X**2 + X + 2 + np.random.randn(m, 1)
```

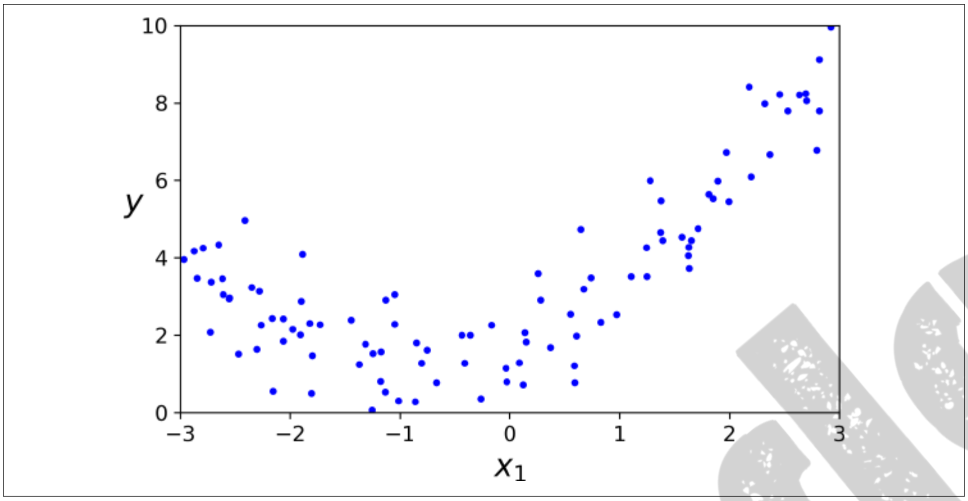


Figure 4-12. Generated nonlinear and noisy dataset

Clearly, a straight line will never fit this data properly. So let's use Scikit-Learn's `PolynomialFeatures` class to transform our training data, adding the square (2nd-degree polynomial) of each feature in the training set as new features (in this case there is just one feature):

```
>>> from sklearn.preprocessing import PolynomialFeatures
>>> poly_features = PolynomialFeatures(degree=2, include_bias=False)
>>> X_poly = poly_features.fit_transform(X)
>>> X[0]
array([-0.75275929])
>>> X_poly[0]
array([-0.75275929, 0.56664654])
```

`X_poly` now contains the original feature of `X` plus the square of this feature. Now you can fit a `LinearRegression` model to this extended training data (Figure 4-13):

```
>>> lin_reg = LinearRegression()
>>> lin_reg.fit(X_poly, y)
>>> lin_reg.intercept_, lin_reg.coef_
(array([1.78134581]), array([[0.93366893, 0.56456263]]))
```

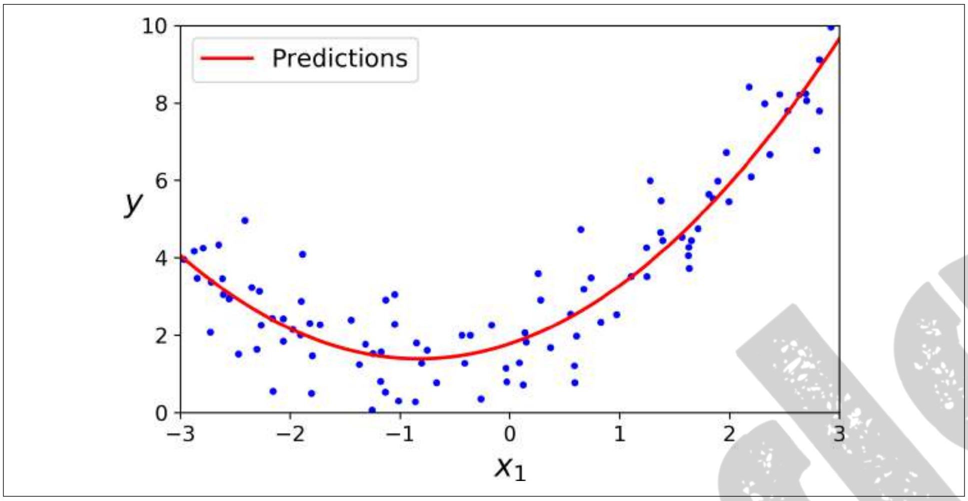


Figure 4-13. Polynomial Regression model predictions

Not bad: the model estimates $\hat{y} = 0.56x_1^2 + 0.93x_1 + 1.78$ when in fact the original function was $y = 0.5x_1^2 + 1.0x_1 + 2.0 + \text{Gaussian noise}$.

Note that when there are multiple features, Polynomial Regression is capable of finding relationships between features (which is something a plain Linear Regression model cannot do). This is made possible by the fact that `PolynomialFeatures` also adds all combinations of features up to the given degree. For example, if there were two features *a* and *b*, `PolynomialFeatures` with `degree=3` would not only add the features a^2, a^3, b^2, and b^3, but also the combinations ab, a^2b, and ab^2.

`PolynomialFeatures(degree=d)` transforms an array containing *n* features into an array containing $\frac{(n+d)!}{d!\,n!}$ features, where *n*! is the *factorial* of *n*, equal to $1 \times 2 \times 3 \times \cdots \times n$. Beware of the combinatorial explosion of the number of features!

Learning Curves

If you perform high-degree Polynomial Regression, you will likely fit the training data much better than with plain Linear Regression. For example, Figure 4-14 applies a 300-degree polynomial model to the preceding training data, and compares the result with a pure linear model and a quadratic model (2nd-degree polynomial). Notice how the 300-degree polynomial model wiggles around to get as close as possible to the training instances.

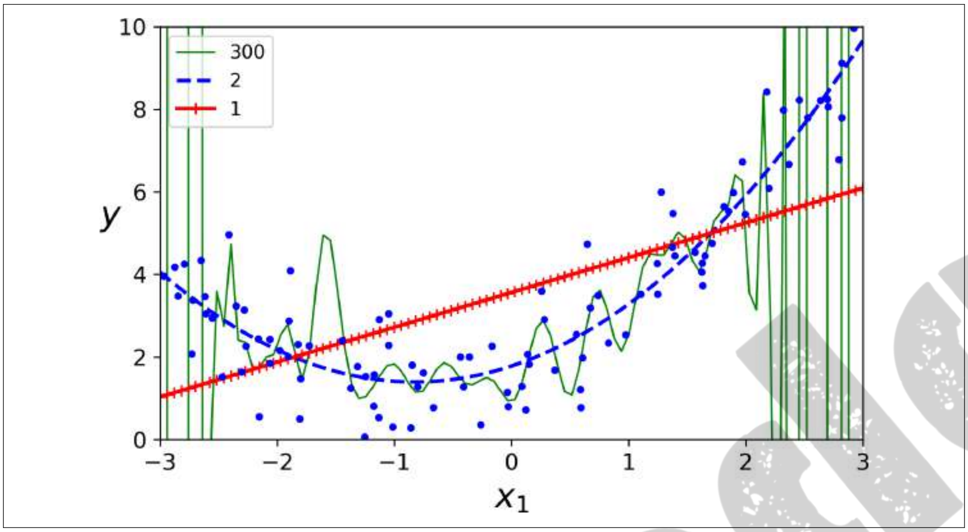


Figure 4-14. High-degree Polynomial Regression

Of course, this high-degree Polynomial Regression model is severely overfitting the training data, while the linear model is underfitting it. The model that will generalize best in this case is the quadratic model. It makes sense since the data was generated using a quadratic model, but in general you won't know what function generated the data, so how can you decide how complex your model should be? How can you tell that your model is overfitting or underfitting the data?

In Chapter 2 you used cross-validation to get an estimate of a model's generalization performance. If a model performs well on the training data but generalizes poorly according to the cross-validation metrics, then your model is overfitting. If it performs poorly on both, then it is underfitting. This is one way to tell when a model is too simple or too complex.

Another way is to look at the *learning curves*: these are plots of the model's performance on the training set and the validation set as a function of the training set size (or the training iteration). To generate the plots, simply train the model several times on different sized subsets of the training set. The following code defines a function that plots the learning curves of a model given some training data:

```
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import train_test_split

def plot_learning_curves(model, X, y):
    X_train, X_val, y_train, y_val = train_test_split(X, y, test_size=0.2)
    train_errors, val_errors = [], []
    for m in range(1, len(X_train)):
        model.fit(X_train[:m], y_train[:m])
        y_train_predict = model.predict(X_train[:m])
```

```
            y_val_predict = model.predict(X_val)
            train_errors.append(mean_squared_error(y_train[:m], y_train_predict))
            val_errors.append(mean_squared_error(y_val, y_val_predict))
        plt.plot(np.sqrt(train_errors), "r-+", linewidth=2, label="train")
        plt.plot(np.sqrt(val_errors), "b-", linewidth=3, label="val")
```

Let's look at the learning curves of the plain Linear Regression model (a straight line; Figure 4-15):

```
    lin_reg = LinearRegression()
    plot_learning_curves(lin_reg, X, y)
```

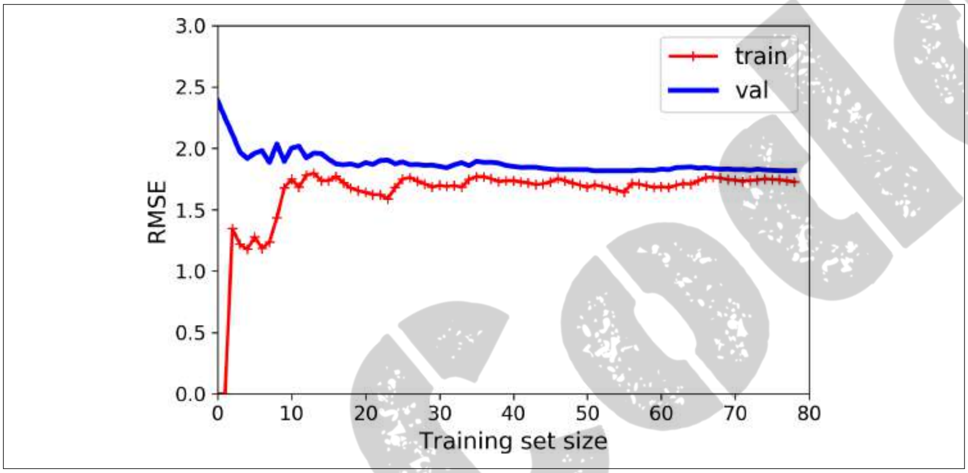


Figure 4-15. Learning curves

This deserves a bit of explanation. First, let's look at the performance on the training data: when there are just one or two instances in the training set, the model can fit them perfectly, which is why the curve starts at zero. But as new instances are added to the training set, it becomes impossible for the model to fit the training data perfectly, both because the data is noisy and because it is not linear at all. So the error on the training data goes up until it reaches a plateau, at which point adding new instances to the training set doesn't make the average error much better or worse. Now let's look at the performance of the model on the validation data. When the model is trained on very few training instances, it is incapable of generalizing properly, which is why the validation error is initially quite big. Then as the model is shown more training examples, it learns and thus the validation error slowly goes down. However, once again a straight line cannot do a good job modeling the data, so the error ends up at a plateau, very close to the other curve.

These learning curves are typical of an underfitting model. Both curves have reached a plateau; they are close and fairly high.

If your model is underfitting the training data, adding more training examples will not help. You need to use a more complex model or come up with better features.

Now let's look at the learning curves of a 10th-degree polynomial model on the same data (Figure 4-16):

```
from sklearn.pipeline import Pipeline

polynomial_regression = Pipeline([
        ("poly_features", PolynomialFeatures(degree=10, include_bias=False)),
        ("lin_reg", LinearRegression()),
    ])

plot_learning_curves(polynomial_regression, X, y)
```

These learning curves look a bit like the previous ones, but there are two very important differences:

- The error on the training data is much lower than with the Linear Regression model.
- There is a gap between the curves. This means that the model performs significantly better on the training data than on the validation data, which is the hallmark of an overfitting model. However, if you used a much larger training set, the two curves would continue to get closer.

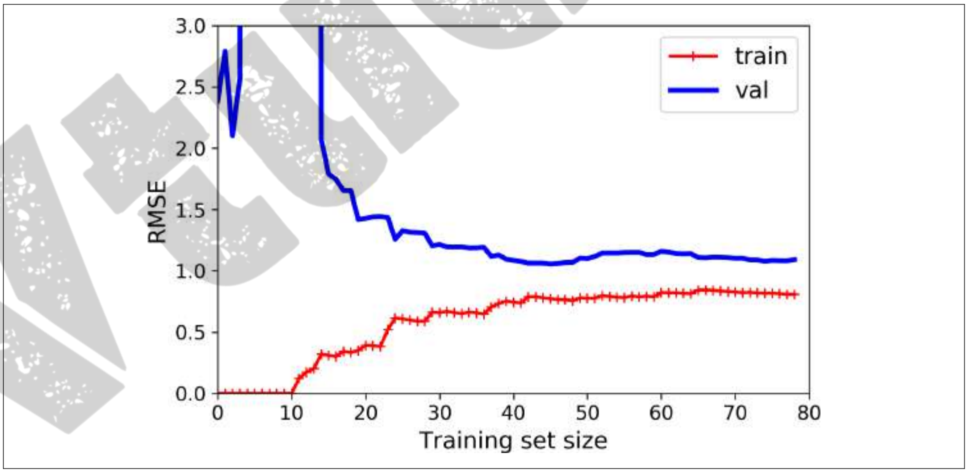


Figure 4-16. Learning curves for the polynomial model

One way to improve an overfitting model is to feed it more training data until the validation error reaches the training error.

The Bias/Variance Tradeoff

An important theoretical result of statistics and Machine Learning is the fact that a model's generalization error can be expressed as the sum of three very different errors:

Bias
: This part of the generalization error is due to wrong assumptions, such as assuming that the data is linear when it is actually quadratic. A high-bias model is most likely to underfit the training data.[10]

Variance
: This part is due to the model's excessive sensitivity to small variations in the training data. A model with many degrees of freedom (such as a high-degree polynomial model) is likely to have high variance, and thus to overfit the training data.

Irreducible error
: This part is due to the noisiness of the data itself. The only way to reduce this part of the error is to clean up the data (e.g., fix the data sources, such as broken sensors, or detect and remove outliers).

Increasing a model's complexity will typically increase its variance and reduce its bias. Conversely, reducing a model's complexity increases its bias and reduces its variance. This is why it is called a tradeoff.

Regularized Linear Models

As we saw in Chapters 1 and 2, a good way to reduce overfitting is to regularize the model (i.e., to constrain it): the fewer degrees of freedom it has, the harder it will be for it to overfit the data. For example, a simple way to regularize a polynomial model is to reduce the number of polynomial degrees.

For a linear model, regularization is typically achieved by constraining the weights of the model. We will now look at Ridge Regression, Lasso Regression, and Elastic Net, which implement three different ways to constrain the weights.

Ridge Regression

Ridge Regression (also called *Tikhonov regularization*) is a regularized version of Linear Regression: a *regularization term* equal to $\alpha \sum_{i=1}^{n} \theta_i^2$ is added to the cost function. This forces the learning algorithm to not only fit the data but also keep the model weights as small as possible. Note that the regularization term should only be added to the cost function during training. Once the model is trained, you want to evaluate the model's performance using the unregularized performance measure.

It is quite common for the cost function used during training to be different from the performance measure used for testing. Apart from regularization, another reason why they might be different is that a good training cost function should have optimization-friendly derivatives, while the performance measure used for testing should be as close as possible to the final objective. A good example of this is a classifier trained using a cost function such as the log loss (discussed in a moment) but evaluated using precision/recall.

The hyperparameter α controls how much you want to regularize the model. If $\alpha = 0$ then Ridge Regression is just Linear Regression. If α is very large, then all weights end up very close to zero and the result is a flat line going through the data's mean. Equation 4-8 presents the Ridge Regression cost function.[11]

Equation 4-8. Ridge Regression cost function

$$J(\boldsymbol{\theta}) = \text{MSE}(\boldsymbol{\theta}) + \alpha \frac{1}{2} \sum_{i=1}^{n} \theta_i^2$$

Note that the bias term θ_0 is not regularized (the sum starts at $i = 1$, not 0). If we define $\mathbf{w}$ as the vector of feature weights (θ_1 to θ_n), then the regularization term is simply equal to $\frac{1}{2}(\| \mathbf{w} \|_2)^2$, where $\| \mathbf{w} \|_2$ represents the ℓ_2 norm of the weight vector.[12] For Gradient Descent, just add $\alpha\mathbf{w}$ to the MSE gradient vector (Equation 4-6).

It is important to scale the data (e.g., using a `StandardScaler`) before performing Ridge Regression, as it is sensitive to the scale of the input features. This is true of most regularized models.

Figure 4-17 shows several Ridge models trained on some linear data using different α value. On the left, plain Ridge models are used, leading to linear predictions. On the right, the data is first expanded using `PolynomialFeatures(degree=10)`, then it is scaled using a `StandardScaler`, and finally the Ridge models are applied to the resulting features: this is Polynomial Regression with Ridge regularization. Note how increasing α leads to flatter (i.e., less extreme, more reasonable) predictions; this reduces the model's variance but increases its bias.

As with Linear Regression, we can perform Ridge Regression either by computing a closed-form equation or by performing Gradient Descent. The pros and cons are the same. Equation 4-9 shows the closed-form solution (where **A** is the $(n + 1) \times (n + 1)$ *identity matrix*[13] except with a 0 in the top-left cell, corresponding to the bias term).

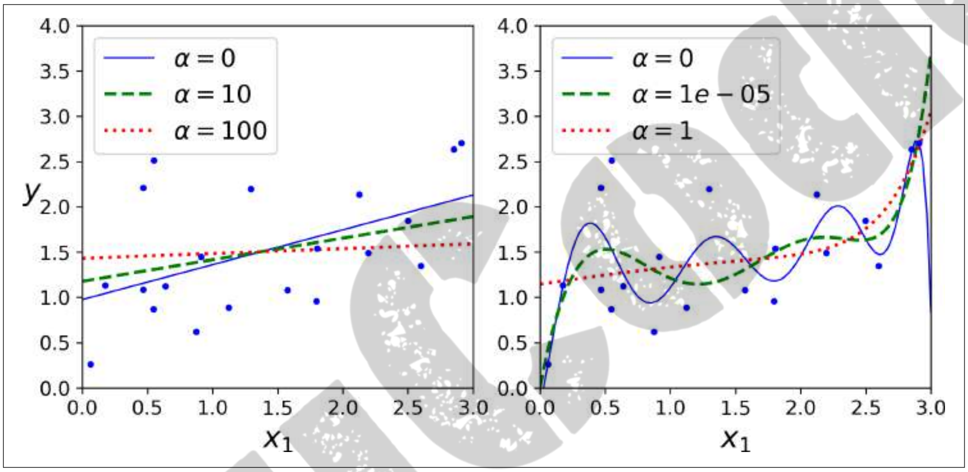


Figure 4-17. Ridge Regression

Equation 4-9. Ridge Regression closed-form solution

$$\hat{\boldsymbol{\theta}} = \left(\mathbf{X}^T\mathbf{X} + \alpha\mathbf{A}\right)^{-1} \quad \mathbf{X}^T \quad \mathbf{y}$$

Here is how to perform Ridge Regression with Scikit-Learn using a closed-form solution (a variant of Equation 4-9 using a matrix factorization technique by André-Louis Cholesky):

```
>>> from sklearn.linear_model import Ridge
>>> ridge_reg = Ridge(alpha=1, solver="cholesky")
>>> ridge_reg.fit(X, y)
>>> ridge_reg.predict([[1.5]])
array([[1.55071465]])
```

And using Stochastic Gradient Descent:[14]

```
>>> sgd_reg = SGDRegressor(penalty="l2")
>>> sgd_reg.fit(X, y.ravel())
>>> sgd_reg.predict([[1.5]])
array([1.47012588])
```

The `penalty` hyperparameter sets the type of regularization term to use. Specifying `"l2"` indicates that you want SGD to add a regularization term to the cost function equal to half the square of the ℓ_2 norm of the weight vector: this is simply Ridge Regression.

Lasso Regression

Least Absolute Shrinkage and Selection Operator Regression (simply called *Lasso Regression*) is another regularized version of Linear Regression: just like Ridge Regression, it adds a regularization term to the cost function, but it uses the ℓ_1 norm of the weight vector instead of half the square of the ℓ_2 norm (see Equation 4-10).

Equation 4-10. Lasso Regression cost function

$$J(\boldsymbol{\theta}) = \text{MSE}(\boldsymbol{\theta}) + \alpha \sum_{i=1}^{n} \left| \theta_i \right|$$

Figure 4-18 shows the same thing as Figure 4-17 but replaces Ridge models with Lasso models and uses smaller α values.

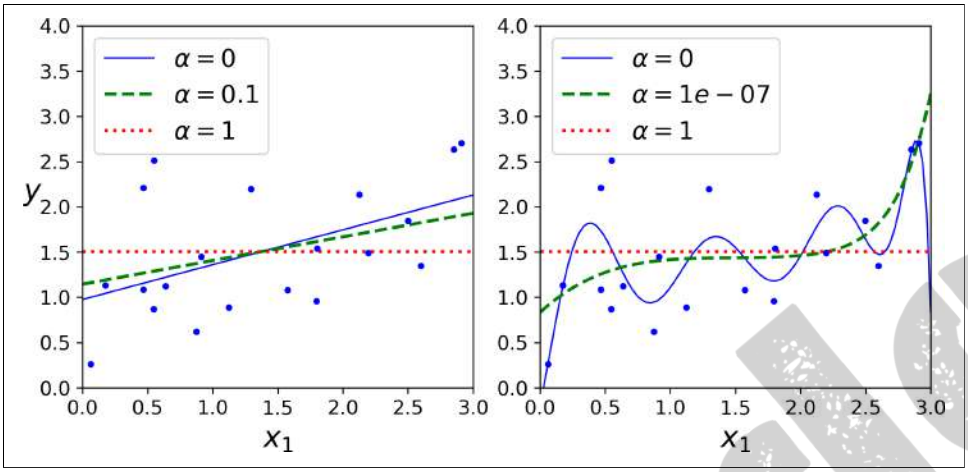


Figure 4-18. Lasso Regression

An important characteristic of Lasso Regression is that it tends to completely eliminate the weights of the least important features (i.e., set them to zero). For example, the dashed line in the right plot on Figure 4-18 (with $\alpha = 10^{-7}$) looks quadratic, almost linear: all the weights for the high-degree polynomial features are equal to zero. In other words, Lasso Regression automatically performs feature selection and outputs a *sparse model* (i.e., with few nonzero feature weights).

You can get a sense of why this is the case by looking at Figure 4-19: on the top-left plot, the background contours (ellipses) represent an unregularized MSE cost function ($\alpha = 0$), and the white circles show the Batch Gradient Descent path with that cost function. The foreground contours (diamonds) represent the ℓ_1 penalty, and the triangles show the BGD path for this penalty only ($\alpha \to \infty$). Notice how the path first reaches $\theta_1 = 0$, then rolls down a gutter until it reaches $\theta_2 = 0$. On the top-right plot, the contours represent the same cost function plus an ℓ_1 penalty with $\alpha = 0.5$. The global minimum is on the $\theta_2 = 0$ axis. BGD first reaches $\theta_2 = 0$, then rolls down the gutter until it reaches the global minimum. The two bottom plots show the same thing but uses an ℓ_2 penalty instead. The regularized minimum is closer to $\boldsymbol{\theta} = \mathbf{0}$ than the unregularized minimum, but the weights do not get fully eliminated.

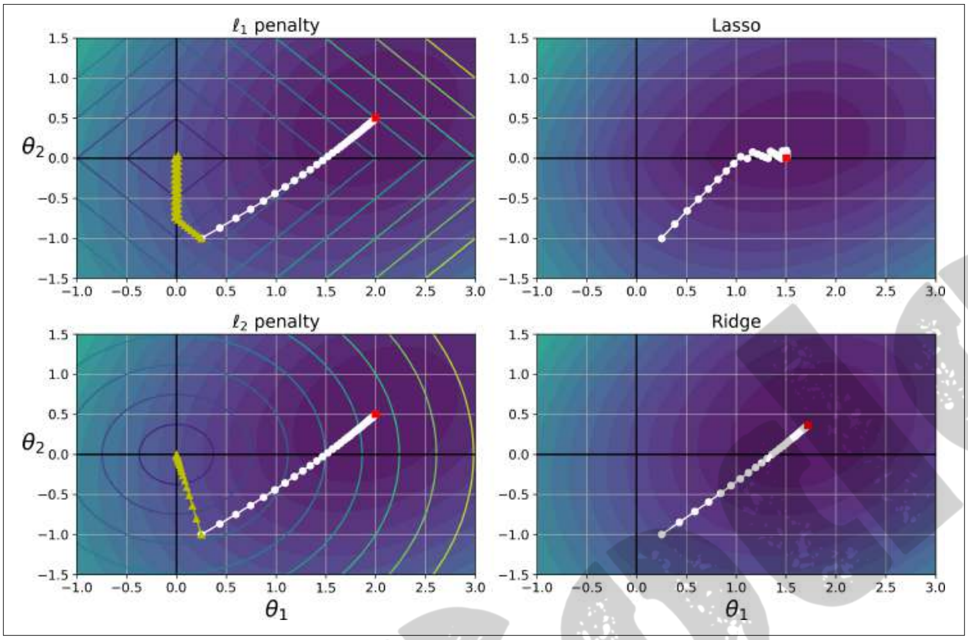


Figure 4-19. Lasso versus Ridge regularization

On the Lasso cost function, the BGD path tends to bounce across the gutter toward the end. This is because the slope changes abruptly at $\theta_2 = 0$. You need to gradually reduce the learning rate in order to actually converge to the global minimum.

The Lasso cost function is not differentiable at $\theta_i = 0$ (for $i = 1, 2, \cdots, n$), but Gradient Descent still works fine if you use a *subgradient vector* **g**[15] instead when any $\theta_i = 0$. Equation 4-11 shows a subgradient vector equation you can use for Gradient Descent with the Lasso cost function.

Equation 4-11. Lasso Regression subgradient vector

$$g(\boldsymbol{\theta}, J) = \nabla_{\boldsymbol{\theta}}\,\text{MSE}(\boldsymbol{\theta}) + \alpha \begin{pmatrix} \text{sign}\,(\theta_1) \\ \text{sign}\,(\theta_2) \\ \vdots \\ \text{sign}\,(\theta_n) \end{pmatrix} \quad \text{where} \ \ \text{sign}\,(\theta_i) = \begin{cases} -1 & \text{if } \theta_i < 0 \\ 0 & \text{if } \theta_i = 0 \\ +1 & \text{if } \theta_i > 0 \end{cases}$$

Here is a small Scikit-Learn example using the `Lasso` class. Note that you could instead use an `SGDRegressor(penalty="l1")`.

```
>>> from sklearn.linear_model import Lasso
>>> lasso_reg = Lasso(alpha=0.1)
>>> lasso_reg.fit(X, y)
>>> lasso_reg.predict([[1.5]])
array([1.53788174])
```

Elastic Net

Elastic Net is a middle ground between Ridge Regression and Lasso Regression. The regularization term is a simple mix of both Ridge and Lasso's regularization terms, and you can control the mix ratio r. When $r = 0$, Elastic Net is equivalent to Ridge Regression, and when $r = 1$, it is equivalent to Lasso Regression (see Equation 4-12).

Equation 4-12. Elastic Net cost function

$$J(\boldsymbol{\theta}) = \text{MSE}(\boldsymbol{\theta}) + r\alpha\Sigma_{i=1}^{n}\left|\theta_i\right| + \frac{1-r}{2}\alpha\Sigma_{i=1}^{n}\theta_i^{\ 2}$$

So when should you use plain Linear Regression (i.e., without any regularization), Ridge, Lasso, or Elastic Net? It is almost always preferable to have at least a little bit of regularization, so generally you should avoid plain Linear Regression. Ridge is a good default, but if you suspect that only a few features are actually useful, you should prefer Lasso or Elastic Net since they tend to reduce the useless features' weights down to zero as we have discussed. In general, Elastic Net is preferred over Lasso since Lasso may behave erratically when the number of features is greater than the number of training instances or when several features are strongly correlated.

Here is a short example using Scikit-Learn's `ElasticNet` (`l1_ratio` corresponds to the mix ratio r):

```
>>> from sklearn.linear_model import ElasticNet
>>> elastic_net = ElasticNet(alpha=0.1, l1_ratio=0.5)
>>> elastic_net.fit(X, y)
>>> elastic_net.predict([[1.5]])
array([1.54333232])
```

Early Stopping

A very different way to regularize iterative learning algorithms such as Gradient Descent is to stop training as soon as the validation error reaches a minimum. This is called *early stopping*. Figure 4-20 shows a complex model (in this case a high-degree Polynomial Regression model) being trained using Batch Gradient Descent. As the epochs go by, the algorithm learns and its prediction error (RMSE) on the training set naturally goes down, and so does its prediction error on the validation set. However, after a while the validation error stops decreasing and actually starts to go back up. This indicates that the model has started to overfit the training data. With early stopping you just stop training as soon as the validation error reaches the minimum. It is such a simple and efficient regularization technique that Geoffrey Hinton called it a "beautiful free lunch."

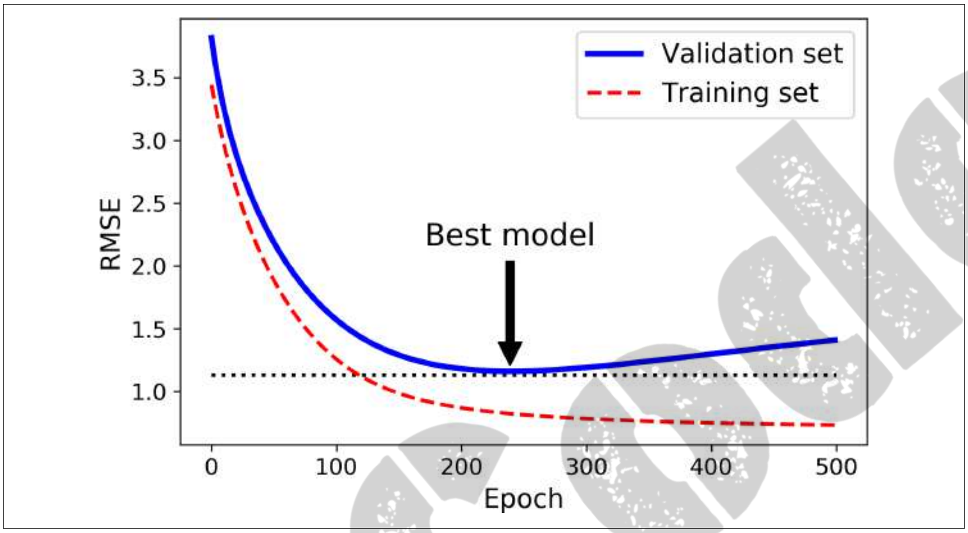


Figure 4-20. Early stopping regularization

With Stochastic and Mini-batch Gradient Descent, the curves are not so smooth, and it may be hard to know whether you have reached the minimum or not. One solution is to stop only after the validation error has been above the minimum for some time (when you are confident that the model will not do any better), then roll back the model parameters to the point where the validation error was at a minimum.

Here is a basic implementation of early stopping:

```
from sklearn.base import clone

# prepare the data
poly_scaler = Pipeline([
        ("poly_features", PolynomialFeatures(degree=90, include_bias=False)),
        ("std_scaler", StandardScaler())
    ])
X_train_poly_scaled = poly_scaler.fit_transform(X_train)
X_val_poly_scaled = poly_scaler.transform(X_val)

sgd_reg = SGDRegressor(max_iter=1, tol=-np.infty, warm_start=True,
                       penalty=None, learning_rate="constant", eta0=0.0005)
```

```
minimum_val_error = float("inf")
best_epoch = None
best_model = None
for epoch in range(1000):
    sgd_reg.fit(X_train_poly_scaled, y_train)  # continues where it left off
    y_val_predict = sgd_reg.predict(X_val_poly_scaled)
    val_error = mean_squared_error(y_val, y_val_predict)
    if val_error < minimum_val_error:
        minimum_val_error = val_error
        best_epoch = epoch
        best_model = clone(sgd_reg)
```

Note that with `warm_start=True`, when the `fit()` method is called, it just continues training where it left off instead of restarting from scratch.

Logistic Regression

As we discussed in Chapter 1, some regression algorithms can be used for classification as well (and vice versa). *Logistic Regression* (also called *Logit Regression*) is commonly used to estimate the probability that an instance belongs to a particular class (e.g., what is the probability that this email is spam?). If the estimated probability is greater than 50%, then the model predicts that the instance belongs to that class (called the positive class, labeled "1"), or else it predicts that it does not (i.e., it belongs to the negative class, labeled "0"). This makes it a binary classifier.

Estimating Probabilities

So how does it work? Just like a Linear Regression model, a Logistic Regression model computes a weighted sum of the input features (plus a bias term), but instead of outputting the result directly like the Linear Regression model does, it outputs the *logistic* of this result (see Equation 4-13).

Equation 4-13. Logistic Regression model estimated probability (vectorized form)

$$\hat{p} = h_{\boldsymbol{\theta}}(\mathbf{x}) = \sigma\left(\mathbf{x}^T \boldsymbol{\theta}\right)$$

The logistic—noted $\sigma(\cdot)$—is a *sigmoid function* (i.e., *S*-shaped) that outputs a number between 0 and 1. It is defined as shown in Equation 4-14 and Figure 4-21.

Equation 4-14. Logistic function

$$\sigma(t) = \frac{1}{1 + \exp(-t)}$$

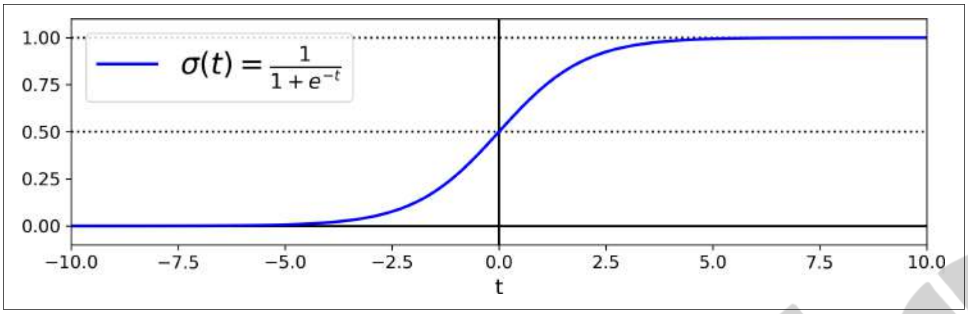


Figure 4-21. Logistic function

Once the Logistic Regression model has estimated the probability $\hat{p} = h_{\boldsymbol{\theta}}(\mathbf{x})$ that an instance $\mathbf{x}$ belongs to the positive class, it can make its prediction $\hat{y}$ easily (see Equation 4-15).

Equation 4-15. Logistic Regression model prediction

$$\hat{y} = \begin{cases} 0 & \text{if } \hat{p} < 0.5 \\ 1 & \text{if } \hat{p} \geq 0.5 \end{cases}$$

Notice that $\sigma(t) < 0.5$ when $t < 0$, and $\sigma(t) \geq 0.5$ when $t \geq 0$, so a Logistic Regression model predicts 1 if $\mathbf{x}^T \boldsymbol{\theta}$ is positive, and 0 if it is negative.

The score t is often called the *logit*: this name comes from the fact that the logit function, defined as logit(p) = log(p / (1 - p)), is the inverse of the logistic function. Indeed, if you compute the logit of the estimated probability p, you will find that the result is t. The logit is also called the *log-odds*, since it is the log of the ratio between the estimated probability for the positive class and the estimated probability for the negative class.

Training and Cost Function

Good, now you know how a Logistic Regression model estimates probabilities and makes predictions. But how is it trained? The objective of training is to set the parameter vector $\boldsymbol{\theta}$ so that the model estimates high probabilities for positive instances (y = 1) and low probabilities for negative instances (y = 0). This idea is captured by the cost function shown in Equation 4-16 for a single training instance $\mathbf{x}$.

Equation 4-16. Cost function of a single training instance

$$c(\boldsymbol{\theta}) = \begin{cases} -\log(\hat{p}) & \text{if } y = 1 \\ -\log(1 - \hat{p}) & \text{if } y = 0 \end{cases}$$

This cost function makes sense because $-\log(t)$ grows very large when t approaches 0, so the cost will be large if the model estimates a probability close to 0 for a positive instance, and it will also be very large if the model estimates a probability close to 1 for a negative instance. On the other hand, $-\log(t)$ is close to 0 when t is close to 1, so the cost will be close to 0 if the estimated probability is close to 0 for a negative instance or close to 1 for a positive instance, which is precisely what we want.

The cost function over the whole training set is simply the average cost over all training instances. It can be written in a single expression (as you can verify easily), called the *log loss*, shown in Equation 4-17.

Equation 4-17. Logistic Regression cost function (log loss)

$$J(\boldsymbol{\theta}) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}log\left(\hat{p}^{(i)}\right) + \left(1 - y^{(i)}\right)log\left(1 - \hat{p}^{(i)}\right)\right]$$

The bad news is that there is no known closed-form equation to compute the value of $\boldsymbol{\theta}$ that minimizes this cost function (there is no equivalent of the Normal Equation). But the good news is that this cost function is convex, so Gradient Descent (or any other optimization algorithm) is guaranteed to find the global minimum (if the learning rate is not too large and you wait long enough). The partial derivatives of the cost function with regards to the jth model parameter θ_j is given by Equation 4-18.

Equation 4-18. Logistic cost function partial derivatives

$$\frac{\partial}{\partial\theta_j}\text{J}(\boldsymbol{\theta}) = \frac{1}{m}\sum_{i=1}^{m}\left(\sigma\left(\boldsymbol{\theta}^T\mathbf{x}^{(i)}\right) - y^{(i)}\right)x_j^{(i)}$$

This equation looks very much like Equation 4-5: for each instance it computes the prediction error and multiplies it by the jth feature value, and then it computes the average over all training instances. Once you have the gradient vector containing all the partial derivatives you can use it in the Batch Gradient Descent algorithm. That's it: you now know how to train a Logistic Regression model. For Stochastic GD you would of course just take one instance at a time, and for Mini-batch GD you would use a mini-batch at a time.

Decision Boundaries

Let's use the iris dataset to illustrate Logistic Regression. This is a famous dataset that contains the sepal and petal length and width of 150 iris flowers of three different species: Iris-Setosa, Iris-Versicolor, and Iris-Virginica (see Figure 4-22).

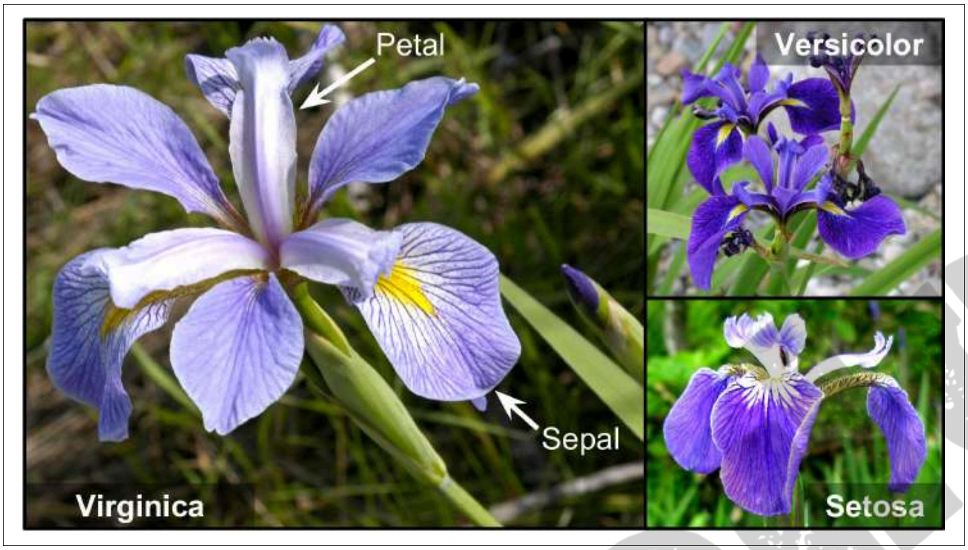


Figure 4-22. Flowers of three iris plant species[16]

Let's try to build a classifier to detect the Iris-Virginica type based only on the petal width feature. First let's load the data:

```
>>> from sklearn import datasets
>>> iris = datasets.load_iris()
>>> list(iris.keys())
['data', 'target', 'target_names', 'DESCR', 'feature_names', 'filename']
>>> X = iris["data"][:, 3:]  # petal width
>>> y = (iris["target"] == 2).astype(np.int)  # 1 if Iris-Virginica, else 0
```

Now let's train a Logistic Regression model:

```
from sklearn.linear_model import LogisticRegression

log_reg = LogisticRegression()
log_reg.fit(X, y)
```

Let's look at the model's estimated probabilities for flowers with petal widths varying from 0 to 3 cm (Figure 4-23)[17]:

```
X_new = np.linspace(0, 3, 1000).reshape(-1, 1)
y_proba = log_reg.predict_proba(X_new)
plt.plot(X_new, y_proba[:, 1], "g-", label="Iris-Virginica")
plt.plot(X_new, y_proba[:, 0], "b--", label="Not Iris-Virginica")
# + more Matplotlib code to make the image look pretty
```

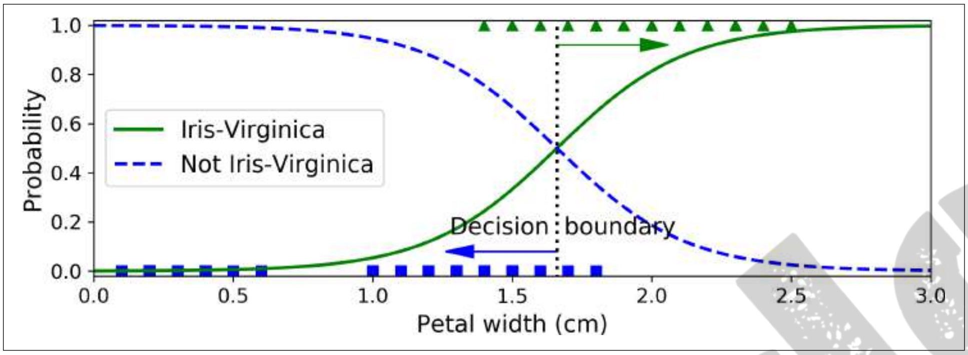


Figure 4-23. Estimated probabilities and decision boundary

The petal width of Iris-Virginica flowers (represented by triangles) ranges from 1.4 cm to 2.5 cm, while the other iris flowers (represented by squares) generally have a smaller petal width, ranging from 0.1 cm to 1.8 cm. Notice that there is a bit of overlap. Above about 2 cm the classifier is highly confident that the flower is an Iris-Virginica (it outputs a high probability to that class), while below 1 cm it is highly confident that it is not an Iris-Virginica (high probability for the "Not Iris-Virginica" class). In between these extremes, the classifier is unsure. However, if you ask it to predict the class (using the `predict()` method rather than the `predict_proba()` method), it will return whichever class is the most likely. Therefore, there is a *decision boundary* at around 1.6 cm where both probabilities are equal to 50%: if the petal width is higher than 1.6 cm, the classifier will predict that the flower is an Iris-Virginica, or else it will predict that it is not (even if it is not very confident):

```
>>> log_reg.predict([[1.7], [1.5]])
array([1, 0])
```

Figure 4-24 shows the same dataset but this time displaying two features: petal width and length. Once trained, the Logistic Regression classifier can estimate the probability that a new flower is an Iris-Virginica based on these two features. The dashed line represents the points where the model estimates a 50% probability: this is the model's decision boundary. Note that it is a linear boundary.[18] Each parallel line represents the points where the model outputs a specific probability, from 15% (bottom left) to 90% (top right). All the flowers beyond the top-right line have an over 90% chance of being Iris-Virginica according to the model.

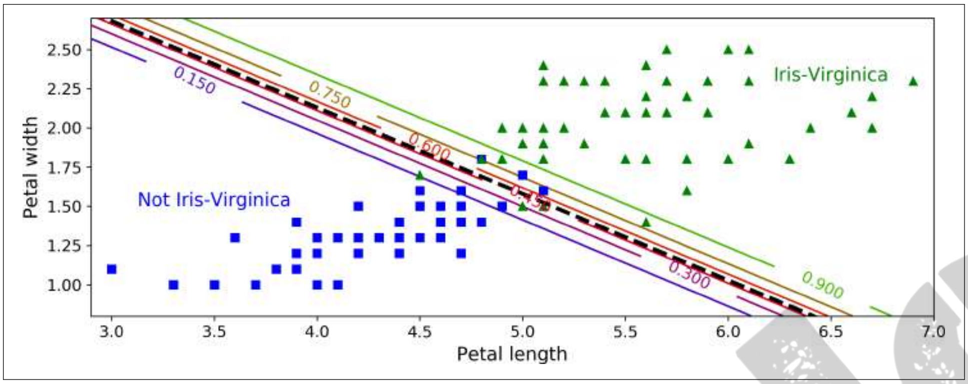


Figure 4-24. Linear decision boundary

Just like the other linear models, Logistic Regression models can be regularized using ℓ_1 or ℓ_2 penalties. Scitkit-Learn actually adds an ℓ_2 penalty by default.

The hyperparameter controlling the regularization strength of a Scikit-Learn `LogisticRegression` model is not `alpha` (as in other linear models), but its inverse: `C`. The higher the value of `C`, the *less* the model is regularized.

Softmax Regression

The Logistic Regression model can be generalized to support multiple classes directly, without having to train and combine multiple binary classifiers (as discussed in Chapter 3). This is called *Softmax Regression*, or *Multinomial Logistic Regression*.

The idea is quite simple: when given an instance $\mathbf{x}$, the Softmax Regression model first computes a score $s_k(\mathbf{x})$ for each class k, then estimates the probability of each class by applying the *softmax function* (also called the *normalized exponential*) to the scores. The equation to compute $s_k(\mathbf{x})$ should look familiar, as it is just like the equation for Linear Regression prediction (see Equation 4-19).

Equation 4-19. Softmax score for class k

$$s_k(\mathbf{x}) = \mathbf{x}^T \boldsymbol{\theta}^{(k)}$$

Note that each class has its own dedicated parameter vector $\boldsymbol{\theta}^{(k)}$. All these vectors are typically stored as rows in a *parameter matrix* $\boldsymbol{\Theta}$.

Once you have computed the score of every class for the instance $\mathbf{x}$, you can estimate the probability $\hat{p}_k$ that the instance belongs to class k by running the scores through the softmax function (Equation 4-20): it computes the exponential of every score, then normalizes them (dividing by the sum of all the exponentials). The scores are generally called logits or log-odds (although they are actually unnormalized log-odds).

Equation 4-20. Softmax function

$$\hat{p}_k = \sigma(\mathbf{s}(\mathbf{x}))_k = \frac{\exp\left(s_k(\mathbf{x})\right)}{\sum_{j=1}^{K} \exp\left(s_j(\mathbf{x})\right)}$$

- K is the number of classes.
- $\mathbf{s}(\mathbf{x})$ is a vector containing the scores of each class for the instance $\mathbf{x}$.
- $\sigma(\mathbf{s}(\mathbf{x}))_k$ is the estimated probability that the instance $\mathbf{x}$ belongs to class k given the scores of each class for that instance.

Just like the Logistic Regression classifier, the Softmax Regression classifier predicts the class with the highest estimated probability (which is simply the class with the highest score), as shown in Equation 4-21.

Equation 4-21. Softmax Regression classifier prediction

$$\hat{y} = \underset{k}{\operatorname{argmax}}\ \sigma(\mathbf{s}(\mathbf{x}))_k = \underset{k}{\operatorname{argmax}}\ s_k(\mathbf{x}) = \underset{k}{\operatorname{argmax}}\ \left(\left(\boldsymbol{\theta}^{(k)}\right)^T \mathbf{x}\right)$$

- The *argmax* operator returns the value of a variable that maximizes a function. In this equation, it returns the value of k that maximizes the estimated probability $\sigma(\mathbf{s}(\mathbf{x}))_k$.

The Softmax Regression classifier predicts only one class at a time (i.e., it is multiclass, not multioutput) so it should be used only with mutually exclusive classes such as different types of plants. You cannot use it to recognize multiple people in one picture.

Now that you know how the model estimates probabilities and makes predictions, let's take a look at training. The objective is to have a model that estimates a high probability for the target class (and consequently a low probability for the other classes). Minimizing the cost function shown in Equation 4-22, called the *cross entropy*, should lead to this objective because it penalizes the model when it estimates a low probability for a target class. Cross entropy is frequently used to measure how well a set of estimated class probabilities match the target classes (we will use it again several times in the following chapters).

Equation 4-22. Cross entropy cost function

$$J(\boldsymbol{\Theta}) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)}\log\left(\hat{p}_k^{(i)}\right)$$

- $y_k^{(i)}$ is the target probability that the ith instance belongs to class k. In general, it is either equal to 1 or 0, depending on whether the instance belongs to the class or not.

Notice that when there are just two classes ($K = 2$), this cost function is equivalent to the Logistic Regression's cost function (log loss; see Equation 4-17).

Cross Entropy

Cross entropy originated from information theory. Suppose you want to efficiently transmit information about the weather every day. If there are eight options (sunny, rainy, etc.), you could encode each option using 3 bits since $2^3 = 8$. However, if you think it will be sunny almost every day, it would be much more efficient to code "sunny" on just one bit (0) and the other seven options on 4 bits (starting with a 1). Cross entropy measures the average number of bits you actually send per option. If your assumption about the weather is perfect, cross entropy will just be equal to the entropy of the weather itself (i.e., its intrinsic unpredictability). But if your assumptions are wrong (e.g., if it rains often), cross entropy will be greater by an amount called the *Kullback–Leibler divergence*.

The cross entropy between two probability distributions p and q is defined as $H(p,q) = -\sum_x p(x)\log q(x)$ (at least when the distributions are discrete). For more details, check out this video.

The gradient vector of this cost function with regards to $\boldsymbol{\theta}^{(k)}$ is given by Equation 4-23:

Equation 4-23. Cross entropy gradient vector for class k

$$\nabla_{\boldsymbol{\theta}^{(k)}} J(\boldsymbol{\Theta}) = \frac{1}{m}\sum_{i=1}^{m}\left(\hat{p}_k^{(i)} - y_k^{(i)}\right)\mathbf{x}^{(i)}$$

Now you can compute the gradient vector for every class, then use Gradient Descent (or any other optimization algorithm) to find the parameter matrix $\boldsymbol{\Theta}$ that minimizes the cost function.

Let's use Softmax Regression to classify the iris flowers into all three classes. Scikit-Learn's `LogisticRegression` uses one-versus-all by default when you train it on more than two classes, but you can set the `multi_class` hyperparameter to `"multinomial"` to switch it to Softmax Regression instead. You must also specify a solver that supports Softmax Regression, such as the `"lbfgs"` solver (see Scikit-Learn's documentation for more details). It also applies ℓ_2 regularization by default, which you can control using the hyperparameter `C`.

```
X = iris["data"][:, (2, 3)]  # petal length, petal width
y = iris["target"]

softmax_reg = LogisticRegression(multi_class="multinomial",solver="lbfgs", C=10)
softmax_reg.fit(X, y)
```

So the next time you find an iris with 5 cm long and 2 cm wide petals, you can ask your model to tell you what type of iris it is, and it will answer Iris-Virginica (class 2) with 94.2% probability (or Iris-Versicolor with 5.8% probability):

```
>>> softmax_reg.predict([[5, 2]])
array([2])
>>> softmax_reg.predict_proba([[5, 2]])
array([[6.38014896e-07, 5.74929995e-02, 9.42506362e-01]])
```

Figure 4-25 shows the resulting decision boundaries, represented by the background colors. Notice that the decision boundaries between any two classes are linear. The figure also shows the probabilities for the Iris-Versicolor class, represented by the curved lines (e.g., the line labeled with 0.450 represents the 45% probability boundary). Notice that the model can predict a class that has an estimated probability below 50%. For example, at the point where all decision boundaries meet, all classes have an equal estimated probability of 33%.

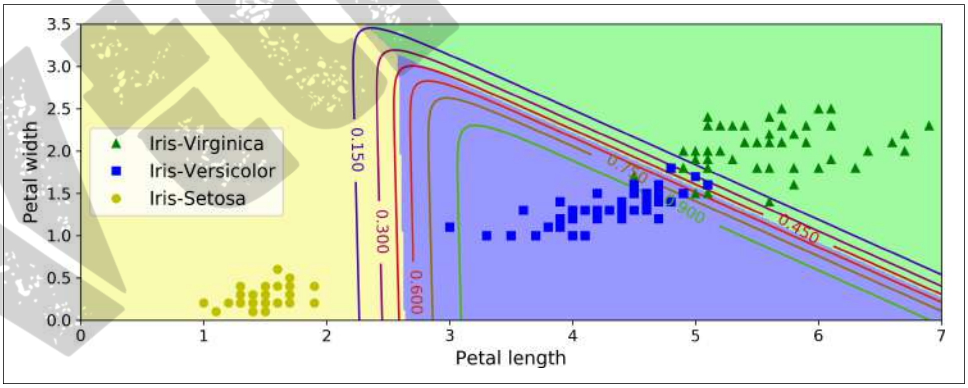


Figure 4-25. Softmax Regression decision boundaries

Support Vector Machines

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as he or she writes—so you can take advantage of these technologies long before the official release of these titles. The following will be Chapter 5 in the final release of the book.

A *Support Vector Machine* (SVM) is a very 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 but 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*.

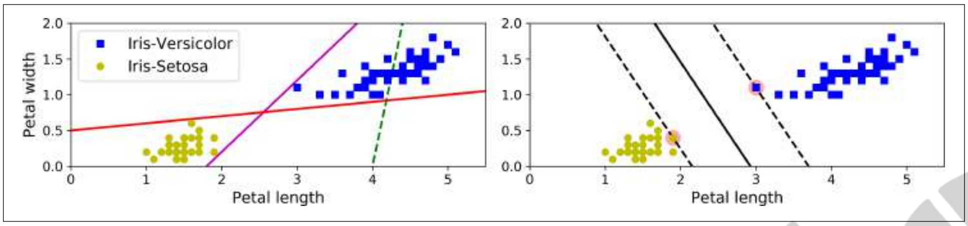


Figure 5-1. Large margin classification

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).

SVMs are sensitive to the feature scales, as you can see in Figure 5-2: on 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 looks much better (on the right plot).

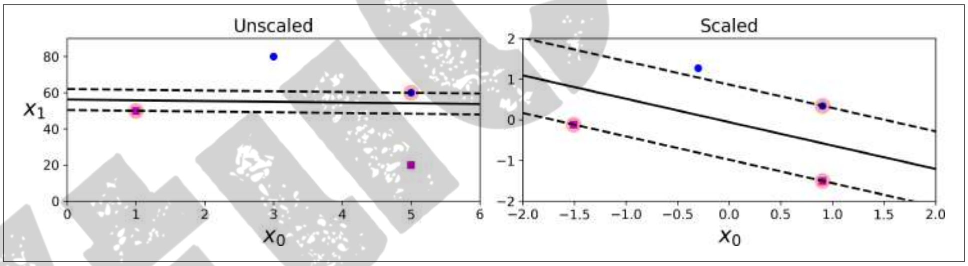


Figure 5-2. Sensitivity to feature scales

Soft Margin Classification

If we strictly impose that all instances be off the street and on the right side, this is called *hard margin classification*. There are two main issues with hard margin classification. First, it only works if the data is linearly separable, and second it is quite 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, and 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.

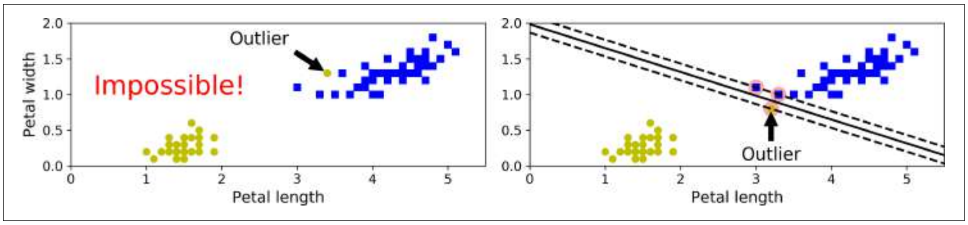


Figure 5-3. Hard margin sensitivity to outliers

To avoid these issues it is preferable to 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*.

In Scikit-Learn's SVM classes, you can control this balance using the `C` hyperparameter: a smaller `C` value leads to a wider street but more margin violations. Figure 5-4 shows the decision boundaries and margins of two soft margin SVM classifiers on a nonlinearly separable dataset. On the left, using a low `C` value the margin is quite large, but many instances end up on the street. On the right, using a high `C` value the classifier makes fewer margin violations but ends up with a smaller margin. However, it seems likely that the first classifier will generalize better: in fact even on this training set it makes fewer prediction errors, since most of the margin violations are actually on the correct side of the decision boundary.

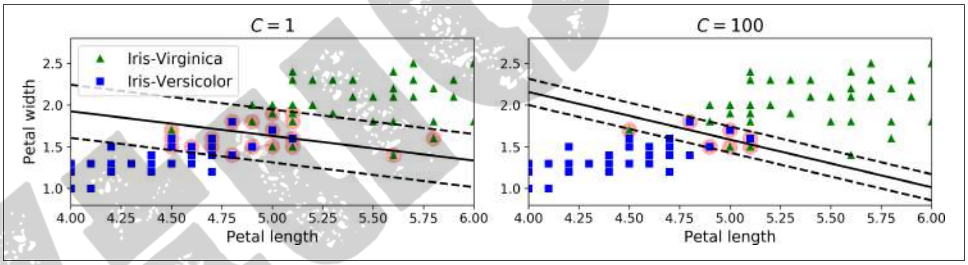


Figure 5-4. Large margin (left) versus fewer margin violations (right)

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

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

```
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)
```

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

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

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

Alternatively, you could use the SVC class, using SVC(kernel="linear", C=1), but it is much slower, especially with large training sets, so it is not recommended. Another option is to 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 classifier. It does not converge as fast as the LinearSVC class, but it can be useful to handle huge datasets that do not fit in memory (out-of-core training), or to handle online classification tasks.

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. Moreover, 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.

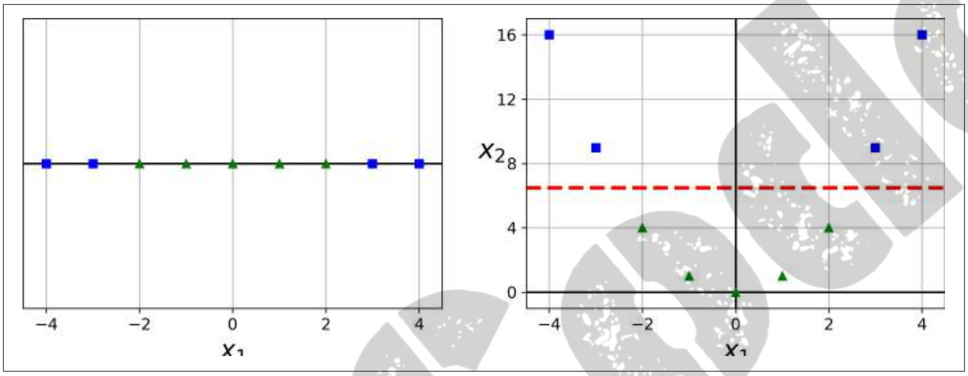


Figure 5-5. Adding features to make a dataset linearly separable

To implement this idea using Scikit-Learn, you can create a `Pipeline` containing a `PolynomialFeatures` transformer (discussed in "Polynomial Regression" on page 130), 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:

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

polynomial_svm_clf = Pipeline([
        ("poly_features", PolynomialFeatures(degree=3)),
        ("scaler", StandardScaler()),
        ("svm_clf", LinearSVC(C=10, loss="hinge"))
    ])

polynomial_svm_clf.fit(X, y)
```

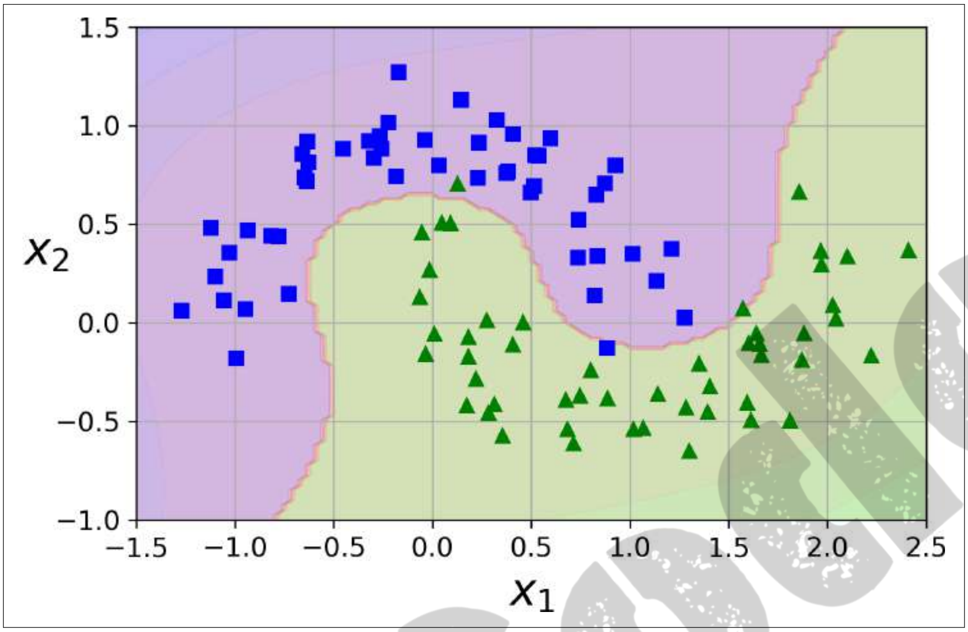


Figure 5-6. Linear SVM classifier using polynomial features

Polynomial Kernel

Adding polynomial features is simple to implement and can work great with all sorts of Machine Learning algorithms (not just SVMs), but at a low polynomial degree it 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* (it is explained in a moment). It makes it possible to get the same result as if you 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 since 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 3rd-degree polynomial kernel. It is represented on the left of 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.

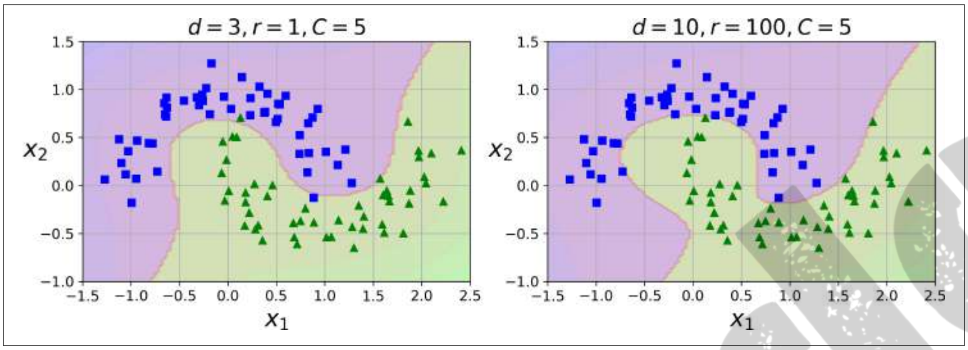


Figure 5-7. SVM classifiers with a polynomial kernel

A common approach to find 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.

Adding Similarity Features

Another technique to tackle nonlinear problems is to add features computed using a *similarity function* that measures how much each instance resembles a particular *landmark*. For example, let's take the one-dimensional 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

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

It 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 of Figure 5-8 shows the transformed dataset (dropping the original features). As you can see, it is now linearly separable.

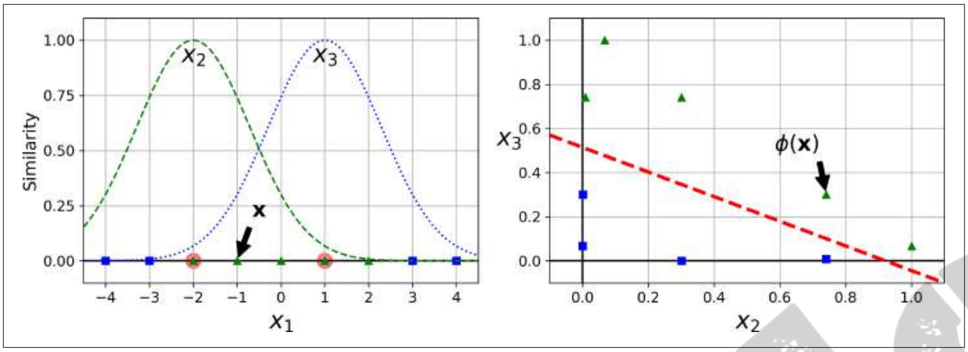


Figure 5-8. Similarity features using the Gaussian RBF

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. This 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. However, once again the kernel trick does its SVM magic: it makes it possible to obtain a similar result as if you had added many similarity features, without actually having to add them. Let's try the Gaussian RBF kernel using the SVC class:

```
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 on the bottom left of Figure 5-9. The other plots show models trained with different values of hyperparameters gamma (γ) and *C*. Increasing gamma makes the bell-shape curve narrower (see the left plot of Figure 5-8), and as a result each instance's range of influence is smaller: the decision boundary ends up being more irregular, wiggling around individual instances. Conversely, a small gamma value makes the bell-shaped curve wider, so 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, and if it is underfitting, you should increase it (similar to the C hyperparameter).

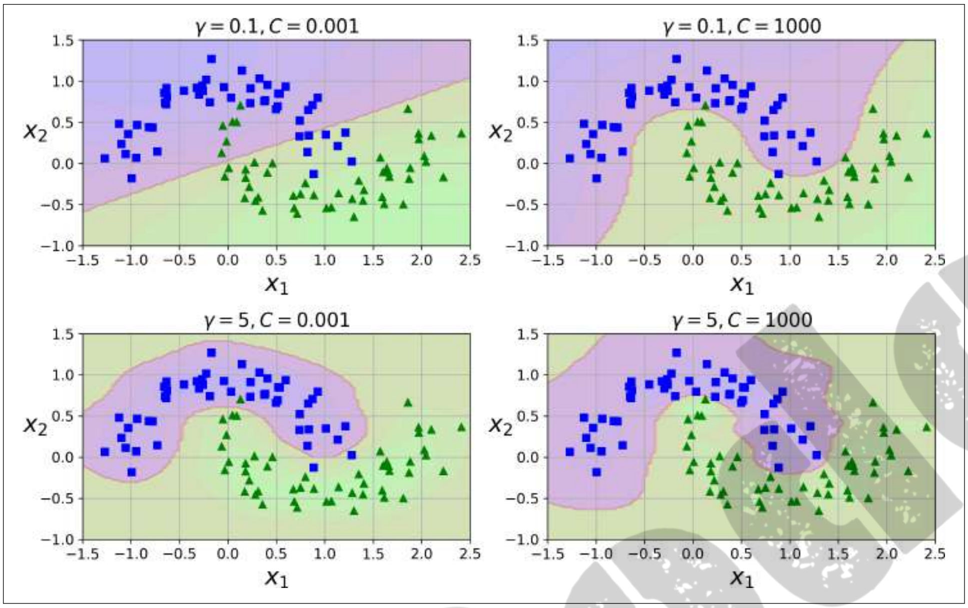


Figure 5-9. SVM classifiers using an RBF kernel

Other kernels exist but are used much more rarely. For example, 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*).

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 try the Gaussian RBF kernel as well; it works well in most cases. Then if you have spare time and computing power, you can also experiment with a few other kernels using cross-validation and grid search, 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 a 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 but small or medium training sets. However, 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.

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 we mentioned earlier, the SVM algorithm is quite versatile: not only does it support linear and nonlinear classification, but it also supports linear and nonlinear regression. 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 ($\epsilon = 0.5$).

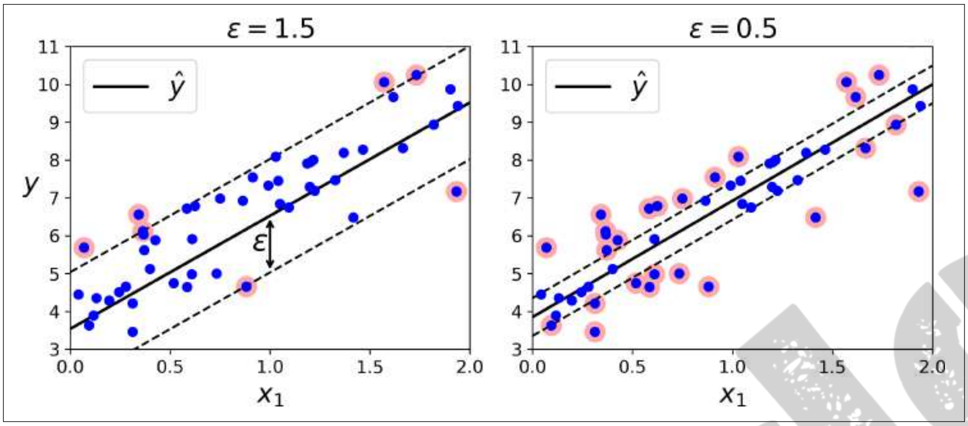


Figure 5-10. SVM Regression

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 of 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. For example, Figure 5-11 shows SVM Regression on a random quadratic training set, using a 2nd-degree polynomial kernel. There is little regularization on the left plot (i.e., a large `C` value), and much more regularization on the right plot (i.e., a small `C` value).

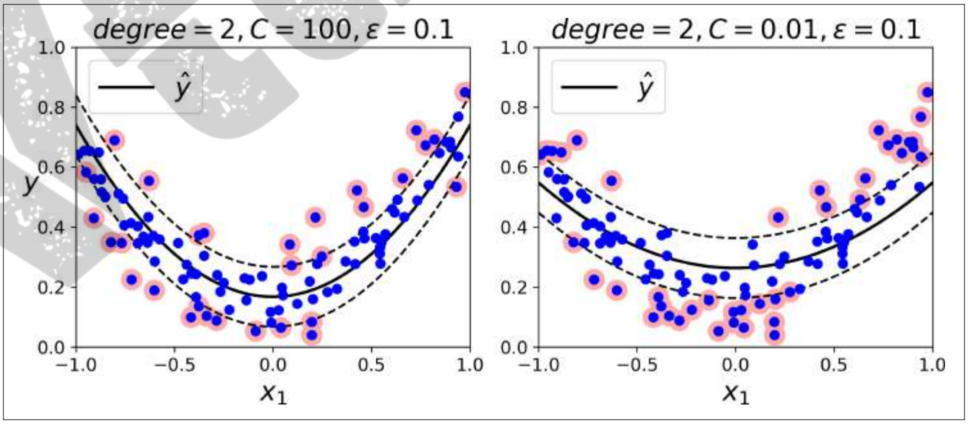


Figure 5-11. SVM regression using a 2nd-degree polynomial kernel

The following code produces the model represented on the left of Figure 5-11 using Scikit-Learn's `SVR` class (which supports the kernel trick). 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).

```
from sklearn.svm import SVR

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

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. You can safely skip it and go straight to the exercises at the end of this chapter if you are just getting started with Machine Learning, 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 different convention, which is more convenient (and more common) when you are 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.

Decision Function and Predictions

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

Equation 5-2. Linear SVM classifier prediction

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

Figure 5-12 shows the decision function that corresponds to the model on the left of Figure 5-4: it is a two-dimensional plane since 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]

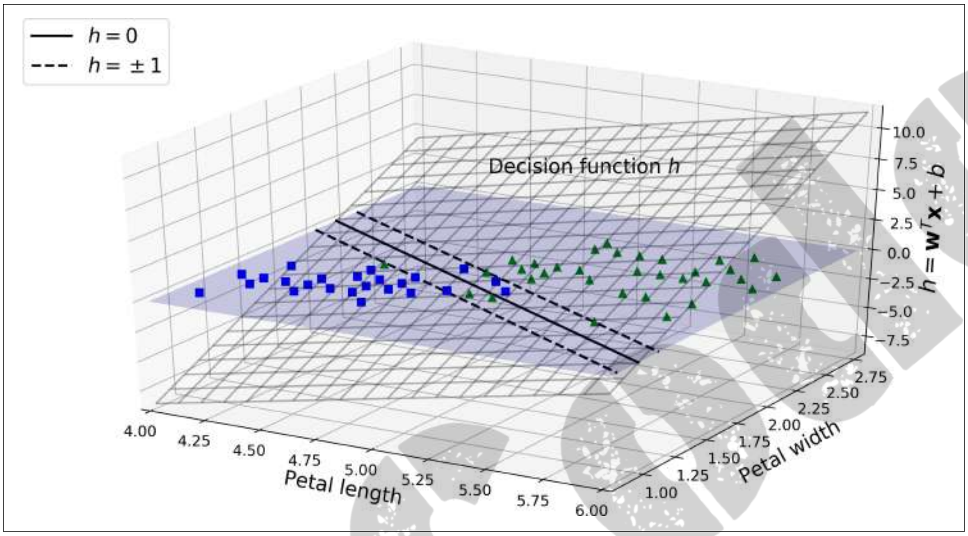


Figure 5-12. Decision function for the iris dataset

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, forming a margin around it. Training a linear SVM classifier means finding the value 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 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. Perhaps this is easier to visualize in 2D in Figure 5-13. The smaller the weight vector **w**, the larger the margin.

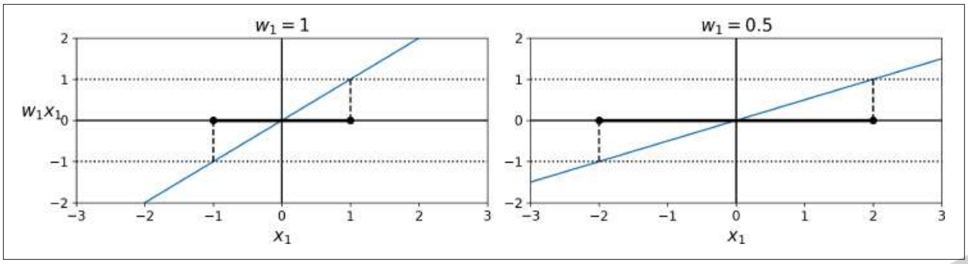


Figure 5-13. A smaller weight vector results in a larger margin

So we want to minimize $\| \mathbf{w} \|$ to get a large margin. However, if we also want to avoid any margin violation (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 $t^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b) \geq 1$ 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

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

We are minimizing $\frac{1}{2}\mathbf{w}^T \mathbf{w}$, which is equal to $\frac{1}{2}\| \mathbf{w} \|^2$, rather than minimizing $\| \mathbf{w} \|$. Indeed, $\frac{1}{2}\| \mathbf{w} \|^2$ has a nice and simple derivative (it is just $\mathbf{w}$) while $\| \mathbf{w} \|$ is not differentiable at $\mathbf{w} = \mathbf{0}$. Optimization algorithms work much better on differentiable functions.

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 ith instance is allowed to violate the margin. We now have two conflicting objectives: making the slack variables as small as possible to reduce the margin violations, and making $\frac{1}{2}\mathbf{w}^T \mathbf{w}$ 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

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

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 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

$$\begin{aligned} &\underset{\mathbf{p}}{\text{Minimize}} \quad \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} \quad + \quad \mathbf{f}^T\mathbf{p} \\ &\text{subject to} \quad \mathbf{A}\mathbf{p} \leq \mathbf{b} \\ &\text{where} \quad \begin{cases} \mathbf{p} & \text{is an } n_p\text{-dimensional vector } (n_p = \text{number of parameters}), \\ \mathbf{H} & \text{is an } n_p \times n_p \text{ matrix}, \\ \mathbf{f} & \text{is an } n_p\text{-dimensional vector}, \\ \mathbf{A} & \text{is an } n_c \times n_p \text{ matrix } (n_c = \text{number of constraints}), \\ \mathbf{b} & \text{is an } n_c\text{-dimensional vector}. \end{cases} \end{aligned}$$

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

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.
- $\mathbf{H}$ is the $n_p \times n_p$ identity matrix, except with a zero in the top-left cell (to ignore the bias term).
- $\mathbf{f} = \mathbf{0}$, an n_p-dimensional vector full of 0s.
- $\mathbf{b} = -\mathbf{1}$, 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 $\dot{\mathbf{x}}_0 = 1$.

So one way to train a hard margin linear SVM classifier is just to use an off-the-shelf QP solver by passing 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).

However, 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 even have the same solutions 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 ???).

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

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

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

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

$$\hat{\mathbf{w}} = \sum_{i=1}^{m} \hat{\alpha}^{(i)} t^{(i)} \mathbf{x}^{(i)}$$

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

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

Kernelized SVM

Suppose you want to apply a 2nd-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 2nd-degree polynomial mapping function ϕ that you want to apply.

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 three-dimensional instead of two-dimensional. Now let's look at what happens to a couple of two-dimensional vectors, **a** and **b**, if we apply this 2nd-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 2nd-degree polynomial mapping

$$\begin{aligned}
\phi(\mathbf{a})^T\phi(\mathbf{b}) &= \begin{pmatrix} {a_1}^2 \\ \sqrt{2}\,a_1a_2 \\ {a_2}^2 \end{pmatrix}^T \begin{pmatrix} {b_1}^2 \\ \sqrt{2}\,b_1b_2 \\ {b_2}^2 \end{pmatrix} = {a_1}^2{b_1}^2 + 2a_1b_1a_2b_2 + {a_2}^2{b_2}^2 \\
&= \left(a_1b_1 + a_2b_2\right)^2 = \left(\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}^T \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}\right)^2 = \left(\mathbf{a}^T\mathbf{b}\right)^2
\end{aligned}$$

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

Now 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 $\phi(\mathbf{x}^{(i)})^T$ $\phi(\mathbf{x}^{(j)})$. But if ϕ is the 2nd-degree polynomial transformation defined in Equation 5-8, then you can replace this dot product of transformed vectors simply by $\left({\mathbf{x}^{(i)}}^T\mathbf{x}^{(j)}\right)^2$. So you don't actually 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 went through the trouble of actually transforming the training set then fitting a linear SVM algorithm, but this trick makes the whole process much more computationally efficient. This is the essence of the kernel trick.

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

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

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* (K must be continuous, symmetric in its arguments so $K(\mathbf{a}, \mathbf{b}) = K(\mathbf{b}, \mathbf{a})$, etc.), then there exists a function ϕ that maps $\mathbf{a}$ and $\mathbf{b}$ into another space (possibly with much higher dimensions) such that $K(\mathbf{a}, \mathbf{b}) = \phi(\mathbf{a})^T \phi(\mathbf{b})$. So you can use K as a kernel since 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 actually 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. 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 in 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, once again (Equation 5-11).

Equation 5-11. Making predictions with a kernelized SVM

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

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 also need to compute the bias term $\hat{b}$, using the same trick (Equation 5-12).

Equation 5-12. Computing the bias term using the kernel trick

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

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 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 it converges much more slowly than the methods based on QP.

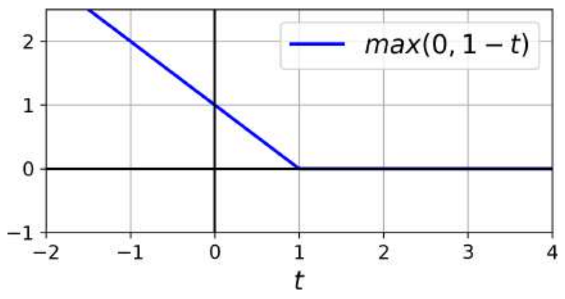
Equation 5-13. Linear SVM classifier cost function

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

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 (represented below). 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 139) 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—for example, using "Incremental and Decremental SVM Learning"[8] or "Fast Kernel Classifiers with Online and Active Learning."[9] However, these are implemented in Matlab and C++. For large-scale nonlinear problems, you may want to consider using neural networks instead (see Part II).