```
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

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

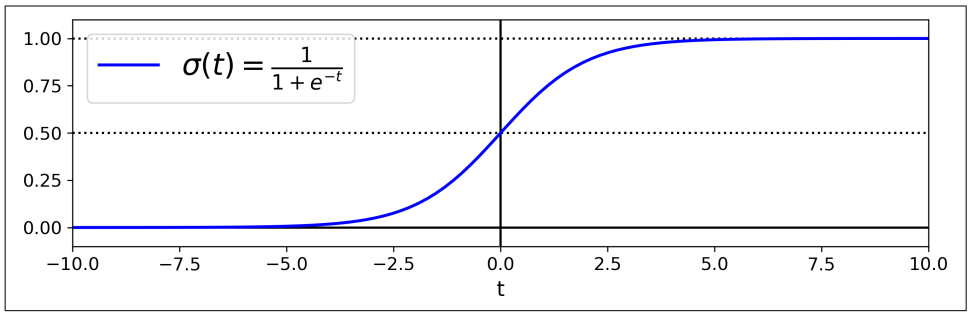

Figure 4-21. Logistic function

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

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

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

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

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).

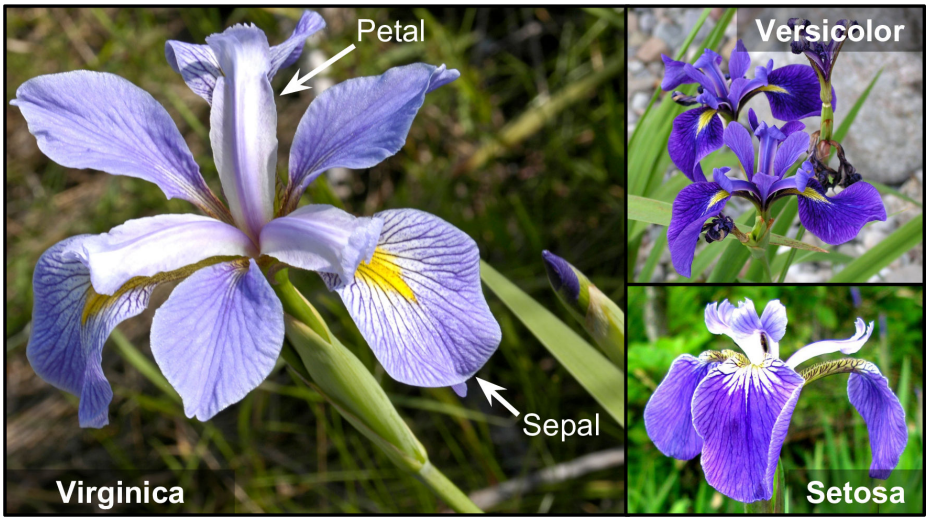

Figure 4-22. Flowers of three iris plant species[16]

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")
```

16 Photos reproduced from the corresponding Wikipedia pages. Iris-Virginica photo by Frank Mayfield (Creative Commons BY-SA 2.0), Iris-Versicolor photo by D. Gordon E. Robertson (Creative Commons BY-SA 3.0), and Iris-Setosa photo is public domain.

17 NumPy's `reshape()` function allows one dimension to be –1, which means "unspecified": the value is inferred from the length of the array and the remaining dimensions.

```
plt.plot(X_new, y_proba[:, 0], "b--", label="Not Iris-Virginica")
# + more Matplotlib code to make the image look pretty
```

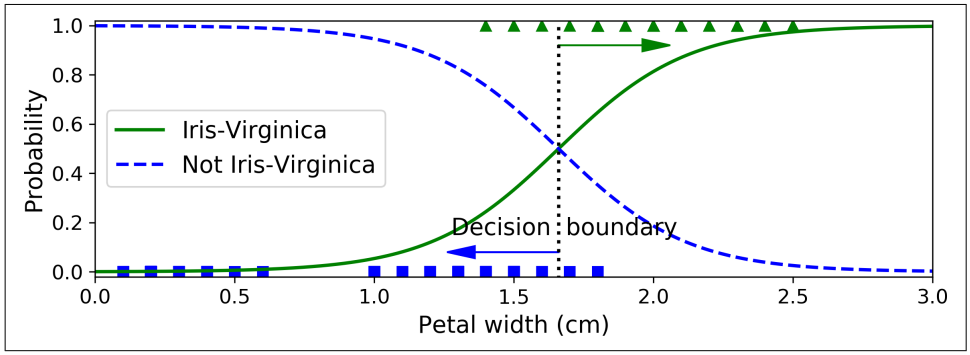

Figure 4-23. Estimated probabilities and decision boundary

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.

18 It is the the set of points $\mathbf{x}$ such that $\theta_0 + \theta_1 x_1 + \theta_2 x_2 = 0$, which defines a straight line.

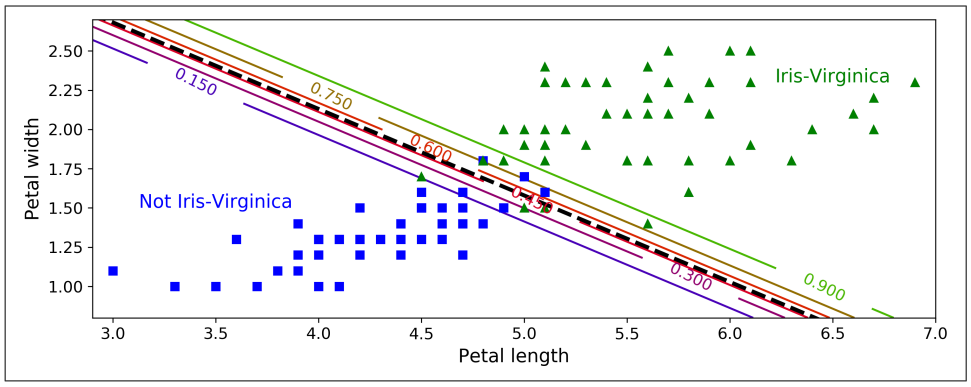

Figure 4-24. Linear decision boundary

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,