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."

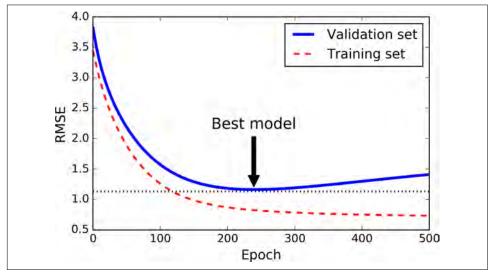


Figure 4-20. Early stopping regularization



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

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)

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

The logistic—also called the *logit*, 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.