because increasing the number of hidden units increases the capacity of the model. For some hyperparameters, overfitting occurs when the value of the hyperparameter is small. For example, the smallest allowable weight decay coefficient of zero corresponds to the greatest effective capacity of the learning algorithm.

Not every hyperparameter will be able to explore the entire U-shaped curve. Many hyperparameters are discrete, such as the number of units in a layer or the number of linear pieces in a maxout unit, so it is only possible to visit a few points along the curve. Some hyperparameters are binary. Usually these hyperparameters are switches that specify whether or not to use some optional component of the learning algorithm, such as a preprocessing step that normalizes the input features by subtracting their mean and dividing by their standard deviation. These hyperparameters can only explore two points on the curve. Other hyperparameters have some minimum or maximum value that prevents them from exploring some part of the curve. For example, the minimum weight decay coefficient is zero. This means that if the model is underfitting when weight decay is zero, we can not enter the overfitting region by modifying the weight decay coefficient. In other words, some hyperparameters can only subtract capacity.

The learning rate is perhaps the most important hyperparameter. If you have time to tune only one hyperparameter, tune the learning rate. It controls the effective capacity of the model in a more complicated way than other hyperparameters—the effective capacity of the model is highest when the learning rate is correct for the optimization problem, not when the learning rate is especially large or especially small. The learning rate has a U-shaped curve for training error, illustrated in figure 11.1. When the learning rate is too large, gradient descent can inadvertently increase rather than decrease the training error. In the idealized quadratic case, this occurs if the learning rate is at least twice as large as its optimal value (LeCun et al., 1998a). When the learning rate is too small, training is not only slower, but may become permanently stuck with a high training error. This effect is poorly understood (it would not happen for a convex loss function).

Tuning the parameters other than the learning rate requires monitoring both training and test error to diagnose whether your model is overfitting or underfitting, then adjusting its capacity appropriately.

If your error on the training set is higher than your target error rate, you have no choice but to increase capacity. If you are not using regularization and you are confident that your optimization algorithm is performing correctly, then you must add more layers to your network or add more hidden units. Unfortunately, this increases the computational costs associated with the model.

If your error on the test set is higher than than your target error rate, you can