Unlike in the case of a grid search, one *should not discretize* or bin the values of the hyperparameters. This allows one to explore a larger set of values, and does not incur additional computational cost. In fact, as illustrated in figure 11.2, a random search can be exponentially more efficient than a grid search, when there are several hyperparameters that do not strongly affect the performance measure. This is studied at length in Bergstra and Bengio (2012), who found that random search reduces the validation set error much faster than grid search, in terms of the number of trials run by each method.

As with grid search, one may often want to run repeated versions of random search, to refine the search based on the results of the first run.

The main reason why random search finds good solutions faster than grid search is that there are no wasted experimental runs, unlike in the case of grid search, when two values of a hyperparameter (given values of the other hyperparameters) would give the same result. In the case of grid search, the other hyperparameters would have the same values for these two runs, whereas with random search, they would usually have different values. Hence if the change between these two values does not marginally make much difference in terms of validation set error, grid search will unnecessarily repeat two equivalent experiments while random search will still give two independent explorations of the other hyperparameters.

11.4.5 Model-Based Hyperparameter Optimization

The search for good hyperparameters can be cast as an optimization problem. The decision variables are the hyperparameters. The cost to be optimized is the validation set error that results from training using these hyperparameters. In simplified settings where it is feasible to compute the gradient of some differentiable error measure on the validation set with respect to the hyperparameters, we can simply follow this gradient (Bengio et al., 1999; Bengio, 2000; Maclaurin et al., 2015). Unfortunately, in most practical settings, this gradient is unavailable, either due to its high computation and memory cost, or due to hyperparameters having intrinsically non-differentiable interactions with the validation set error, as in the case of discrete-valued hyperparameters.

To compensate for this lack of a gradient, we can build a model of the validation set error, then propose new hyperparameter guesses by performing optimization within this model. Most model-based algorithms for hyperparameter search use a Bayesian regression model to estimate both the expected value of the validation set error for each hyperparameter and the uncertainty around this expectation. Optimization thus involves a tradeoff between exploration (proposing hyperparameters