

manually requires understanding what the hyperparameters do and how machine learning models achieve good generalization. Automatic hyperparameter selection algorithms greatly reduce the need to understand these ideas, but they are often much more computationally costly.

11.4.1 Manual Hyperparameter Tuning

To set hyperparameters manually, one must understand the relationship between hyperparameters, training error, generalization error and computational resources (memory and runtime). This means establishing a solid foundation on the fundamental ideas concerning the effective capacity of a learning algorithm from chapter 5.

The goal of manual hyperparameter search is usually to find the lowest generalization error subject to some runtime and memory budget. We do not discuss how to determine the runtime and memory impact of various hyperparameters here because this is highly platform-dependent.

The primary goal of manual hyperparameter search is to adjust the effective capacity of the model to match the complexity of the task. Effective capacity is constrained by three factors: the representational capacity of the model, the ability of the learning algorithm to successfully minimize the cost function used to train the model, and the degree to which the cost function and training procedure regularize the model. A model with more layers and more hidden units per layer has higher representational capacity—it is capable of representing more complicated functions. It can not necessarily actually learn all of these functions though, if the training algorithm cannot discover that certain functions do a good job of minimizing the training cost, or if regularization terms such as weight decay forbid some of these functions.

The generalization error typically follows a U-shaped curve when plotted as a function of one of the hyperparameters, as in figure 5.3. At one extreme, the hyperparameter value corresponds to low capacity, and generalization error is high because training error is high. This is the underfitting regime. At the other extreme, the hyperparameter value corresponds to high capacity, and the generalization error is high because the gap between training and test error is high. Somewhere in the middle lies the optimal model capacity, which achieves the lowest possible generalization error, by adding a medium generalization gap to a medium amount of training error.

For some hyperparameters, overfitting occurs when the value of the hyperparameter is large. The number of hidden units in a layer is one such example,