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Estimating Class Probabilities

A Decision Tree can also estimate the probability that an instance belongs to a particular class k: first it traverses the tree to find the leaf node for this instance, and then it returns the ratio of training instances of class k in this node. For example, suppose you have found a flower whose petals are 5 cm long and 1.5 cm wide. The corresponding leaf node is the depth-2 left node, so the Decision Tree should output the following probabilities: 0% for Iris-Setosa (0/54), 90.7% for Iris-Versicolor (49/54), and 9.3% for Iris-Virginica (5/54). And of course if you ask it to predict the class, it should output Iris-Versicolor (class 1) since it has the highest probability. Let's check this:

```
>>> tree_clf.predict_proba([[5, 1.5]])
array([[ 0. , 0.90740741, 0.09259259]])
>>> tree_clf.predict([[5, 1.5]])
array([1])
```

Perfect! Notice that the estimated probabilities would be identical anywhere else in the bottom-right rectangle of Figure 6-2—for example, if the petals were 6 cm long and 1.5 cm wide (even though it seems obvious that it would most likely be an Iris-Virginica in this case).

The CART Training Algorithm

Scikit-Learn uses the Classification And Regression Tree (CART) algorithm to train Decision Trees (also called "growing" trees). The idea is really quite simple: the algorithm first splits the training set in two subsets using a single feature k and a threshold t_k (e.g., "petal length ≤ 2.45 cm"). How does it choose k and t_k ? It searches for the pair (k, t_k) that produces the purest subsets (weighted by their size). The cost function that the algorithm tries to minimize is given by Equation 6-2.

Equation 6-2. CART cost function for classification

$$\begin{split} J(k,t_k) &= \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}} \\ \text{where} &\begin{cases} G_{\text{left/right}} \text{ measures the impurity of the left/right subset,} \\ m_{\text{left/right}} \text{ is the number of instances in the left/right subset.} \end{cases} \end{split}$$

Once it has successfully split the training set in two, it splits the subsets using the same logic, then the sub-subsets and so on, recursively. It stops recursing once it reaches the maximum depth (defined by the max_depth hyperparameter), or if it cannot find a split that will reduce impurity. A few other hyperparameters (described in a