Regression

Decision Trees are also capable of performing regression tasks. Let's build a regression tree using Scikit-Learn's DecisionTreeRegressor class, training it on a noisy quadratic dataset with max_depth=2:

```
from sklearn.tree import DecisionTreeRegressor
tree_reg = DecisionTreeRegressor(max_depth=2)
tree_reg.fit(X, y)
```

The resulting tree is represented on Figure 6-4.

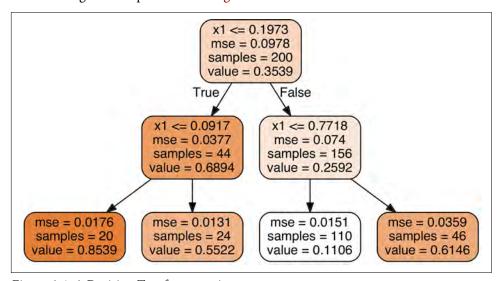


Figure 6-4. A Decision Tree for regression

This tree looks very similar to the classification tree you built earlier. The main difference is that instead of predicting a class in each node, it predicts a value. For example, suppose you want to make a prediction for a new instance with $x_1 = 0.6$. You traverse the tree starting at the root, and you eventually reach the leaf node that predicts value=0.1106. This prediction is simply the average target value of the 110 training instances associated to this leaf node. This prediction results in a Mean Squared Error (MSE) equal to 0.0151 over these 110 instances.

This model's predictions are represented on the left of Figure 6-5. If you set max_depth=3, you get the predictions represented on the right. Notice how the predicted value for each region is always the average target value of the instances in that region. The algorithm splits each region in a way that makes most training instances as close as possible to that predicted value.

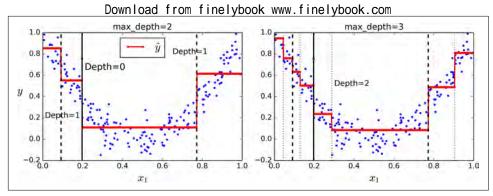


Figure 6-5. Predictions of two Decision Tree regression models

The CART algorithm works mostly the same way as earlier, except that instead of trying to split the training set in a way that minimizes impurity, it now tries to split the training set in a way that minimizes the MSE. Equation 6-4 shows the cost function that the algorithm tries to minimize.

Equation 6-4. CART cost function for regression

$$J(k, t_k) = \frac{m_{\text{left}}}{m} \text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m} \text{MSE}_{\text{right}} \quad \text{where} \begin{cases} \text{MSE}_{\text{node}} = \sum_{i \in \text{node}} \left(\hat{y}_{\text{node}} - y^{(i)}\right)^2 \\ \hat{y}_{\text{node}} = \frac{1}{m_{\text{node}}} \sum_{i \in \text{node}} y^{(i)} \end{cases}$$

Just like for classification tasks, Decision Trees are prone to overfitting when dealing with regression tasks. Without any regularization (i.e., using the default hyperparameters), you get the predictions on the left of Figure 6-6. It is obviously overfitting the training set very badly. Just setting min_samples_leaf=10 results in a much more reasonable model, represented on the right of Figure 6-6.

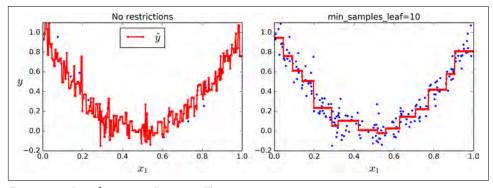


Figure 6-6. Regularizing a Decision Tree regressor

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Instability

Hopefully by now you are convinced that Decision Trees have a lot going for them: they are simple to understand and interpret, easy to use, versatile, and powerful. However they do have a few limitations. First, as you may have noticed, Decision Trees love orthogonal decision boundaries (all splits are perpendicular to an axis), which makes them sensitive to training set rotation. For example, Figure 6-7 shows a simple linearly separable dataset: on the left, a Decision Tree can split it easily, while on the right, after the dataset is rotated by 45°, the decision boundary looks unnecessarily convoluted. Although both Decision Trees fit the training set perfectly, it is very likely that the model on the right will not generalize well. One way to limit this problem is to use PCA (see Chapter 8), which often results in a better orientation of the training data.

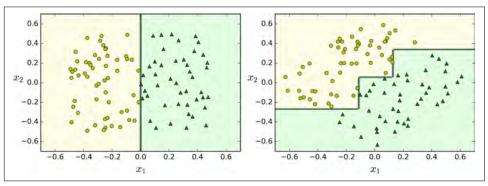


Figure 6-7. Sensitivity to training set rotation

More generally, the main issue with Decision Trees is that they are very sensitive to small variations in the training data. For example, if you just remove the widest Iris-Versicolor from the iris training set (the one with petals 4.8 cm long and 1.8 cm wide) and train a new Decision Tree, you may get the model represented in Figure 6-8. As you can see, it looks very different from the previous Decision Tree (Figure 6-2). Actually, since the training algorithm used by Scikit-Learn is stochastic⁶ you may get very different models even on the same training data (unless you set the random state hyperparameter).

⁶ It randomly selects the set of features to evaluate at each node.