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As you can see, the CART algorithm is a *greedy algorithm*: it greedily searches for an optimum split at the top level, then repeats the process at each level. It does not check whether or not the split will lead to the lowest possible impurity several levels down. A greedy algorithm often produces a reasonably good solution, but it is not guaranteed to be the optimal solution.

Unfortunately, finding the optimal tree is known to be an *NP-Complete* problem:<sup>2</sup> it requires  $O(\exp(m))$  time, making the problem intractable even for fairly small training sets. This is why we must settle for a “reasonably good” solution.

## Computational Complexity

Making predictions requires traversing the Decision Tree from the root to a leaf. Decision Trees are generally approximately balanced, so traversing the Decision Tree requires going through roughly  $O(\log_2(m))$  nodes.<sup>3</sup> Since each node only requires checking the value of one feature, the overall prediction complexity is just  $O(\log_2(m))$ , independent of the number of features. So predictions are very fast, even when dealing with large training sets.

However, the training algorithm compares all features (or less if `max_features` is set) on all samples at each node. This results in a training complexity of  $O(n \times m \log(m))$ . For small training sets (less than a few thousand instances), Scikit-Learn can speed up training by presorting the data (set `presort=True`), but this slows down training considerably for larger training sets.

## Gini Impurity or Entropy?

By default, the Gini impurity measure is used, but you can select the *entropy* impurity measure instead by setting the `criterion` hyperparameter to “entropy”. The concept of entropy originated in thermodynamics as a measure of molecular disorder: entropy approaches zero when molecules are still and well ordered. It later spread to a wide variety of domains, including Shannon’s *information theory*, where it measures

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<sup>2</sup> P is the set of problems that can be solved in polynomial time. NP is the set of problems whose solutions can be verified in polynomial time. An NP-Hard problem is a problem to which any NP problem can be reduced in polynomial time. An NP-Complete problem is both NP and NP-Hard. A major open mathematical question is whether or not  $P = NP$ . If  $P \neq NP$  (which seems likely), then no polynomial algorithm will ever be found for any NP-Complete problem (except perhaps on a quantum computer).

<sup>3</sup>  $\log_2$  is the binary logarithm. It is equal to  $\log_2(m) = \log(m) / \log(2)$ .