# Machine Learning Using Python

Lesson 5: Decision Trees and Random Forests

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## Lesson 5: Decision Trees and Random Forests

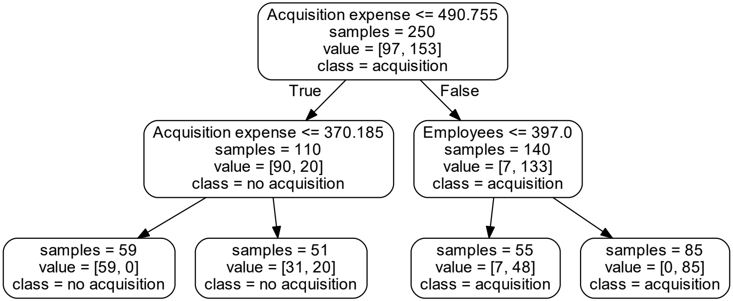
1. Regression trees
2. Classification trees
3. Bagging
4. Random forests

## Decision trees

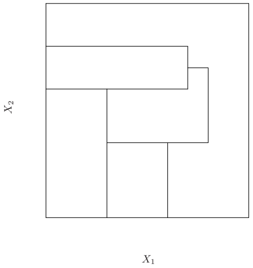
- Tree-based methods for regression and classification partition the predictor space into a set of rectangles, and fit a simple model such as a constant in each one.

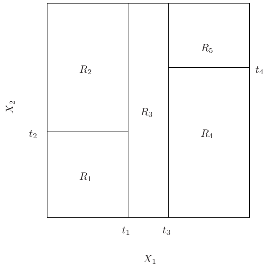
- The partitions are based on *recursive binary splitting*, enabling an interpretable visualisation of the prediction rule as a decision tree.

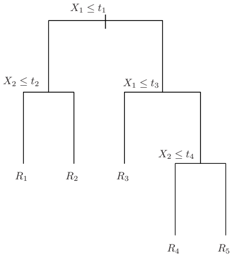
## Example (classification tree): Customer Acquisition

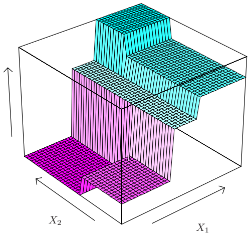


## Rectangular partitions and trees









## Regression trees

## Regression trees (key concept)

We predict with a **regression tree** as follows:

1. Divide the predictor space – that is, the set of possible values for $X_1, X_2, \ldots, X_p$ – into $M$ distinct and non-overlapping regions, $R_1, R_2, \ldots, R_M$.

2. We then model the response $Y$ as a constant $c_m$ in each region. We make the same prediction $c_m$ for each observation that falls in the region,

$$f(\boldsymbol{x}) = \sum_{m=1}^{M} c_m I(\boldsymbol{x} \in R_m).$$

## Regression trees

Regression tree:

$$f(\boldsymbol{x}) = \sum_{m=1}^{M} c_m I(\boldsymbol{x} \in R_m).$$

To fit a tree, we therefore need to construct the regions $R_1, R_2, \ldots, R_M$ and choose constants $c_1, c_2, \ldots, c_M$ for each of them.

## Fitting a regression tree

If we adopt the sum of squared errors as the criterion for fitting the model, the estimated constant $\widehat{c}_m$ is the sample average of the response values $y_i$ in region $m$:

$$\widehat{c}_m = \frac{1}{N_m} \sum_{i:\, \boldsymbol{x}_i \in R_m} y_i,$$

where $N_m$ in the number of samples in region $m$,

$$N_m = \sum_{i=1}^{N} I(\boldsymbol{x}_i \in R_m).$$

## Fitting a regression tree

To find the best rectangular partition of the predictor space, our goal is to select regions $R_1, R_2, \ldots, R_M$ that minimise the RSS, given by

$$\begin{aligned}\mathsf{RSS} &= \sum_{i=1}^{N} \left( y_i - \sum_{m=1}^{M} \widehat{c}_m \, I(\boldsymbol{x}_i \in R_m) \right)^2 \\ &= \sum_{m=1}^{M} \sum_{i:\, \boldsymbol{x}_i \in R_m} \left( y_i - \widehat{c}_m \right)^2 .\end{aligned}$$

## Fitting a regression tree

Fitting a regression tree:

$$\min_{R_1,\ldots,R_M} \sum_{m=1}^{M} \sum_{i:\, \boldsymbol{x}_i \in R_m} (y_i - \widehat{c}_m)^2$$

Solving this problem is generally computationally infeasible. We proceed with a greedy algorithm known as **recursive binary splitting**.

## Growing a tree by binary splitting (key concept)

Starting with all of the data, consider a splitting variable $j$ and a split point $s$, and define the regions

$$R_1(j,s) = \{X|X_j \leq s\} \text{ and } R_2(j,s) = \{X|X_j > s\}.$$

We then seek a splitting variable $j$ and split point $s$ that solve

$$\min_{j,s} \left\{ \left( \sum_{i:\, \boldsymbol{x}_i \in R_1(j,s)} (y_i - \widehat{c}_1)^2 \right) + \left( \sum_{i:\, \boldsymbol{x}_i \in R_2(j,s)} (y_i - \widehat{c}_2)^2 \right) \right\}.$$

## Growing a tree by binary splitting

$$\min_{j,s}\left\{\left(\sum_{i:\,\boldsymbol{x}_i\in R_1(j,s)}(y_i-\widehat{c}_1)^2\right)+\left(\sum_{i:\,\boldsymbol{x}_i\in R_2(j,s)}(y_i-\widehat{c}_2)^2\right)\right\}.$$

- We can find $j$ and $s$ very quickly by scanning through all the predictors, especially if $p$ is not large.
- Having found the best split, we partition the data into the two resulting regions, and repeat the splitting process on each of them.
- We repeat this process until we reach a minimum node size (say, 5).

## Tree size

How large should we grow the tree?

- A large tree will clearly overfit the data, with the small number of samples in each region leading to high variance estimators of the the constants $c_m$.
- A small tree may fail to capture important structure in the data.
- The tree size is therefore a tuning parameter governing the complexity of the model, and we should select it adaptively from the data.

## Classification trees

## Classification tree

A **classification tree** is very similar to a regression tree, except that we predict a qualitative response instead of quantitative one.

We split the predictor space in non-overlapping regions $R_1, R_2, \ldots, R_M$, and estimate the class probabilities within each region. We then classify the observations according to the estimated probabilities.

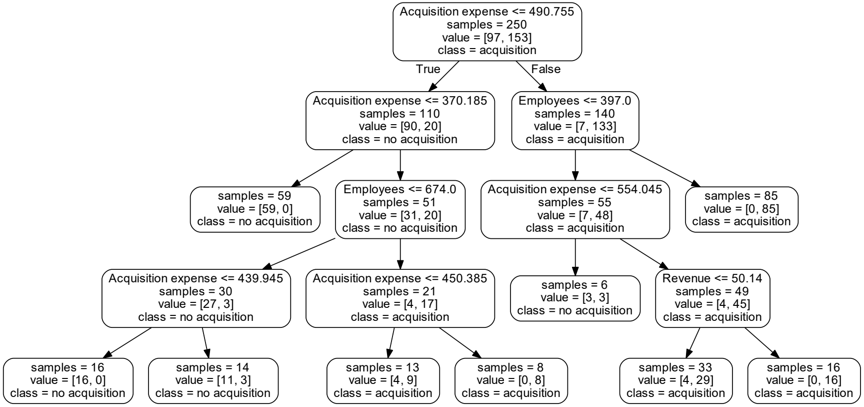
## Classification trees

Let the response take values $y \in \{1, \ldots, C\}$. In a node $m$ representing region $R_m$ with $N_m$ observations, we compute

$$\widehat{p}_{mc} = \frac{1}{N_m} \sum_{\boldsymbol{x}_i \in R_M} I(y_i = c)$$

the proportion of class $c$ observations in node $m$.

## Example: Customer Acquisition



## Growing a classification tree

We need an appropriate criterion for growing a classification tree by binary splitting (the role of the residual sum of squares in a regression tree).

The **node impurity measures** for classification include the misclassification error, Gini index, cross-entropy.

## Node impurity measures

The **misclassification error** is

$$1 - \widehat{p}_{mc'},$$

where $c' = \widehat{y}_m$ and $\widehat{p}_{mc'}$ is the proportion of training observations in node $m$ that are correctly classified.

## Gini index

- The **Gini index** is

$$\sum_{c=1}^{C} \widehat{p}_{mc}(1 - \widehat{p}_{mc}) = \sum_{c=1}^{C} \sum_{j \neq c} \widehat{p}_{mc}\, \widehat{p}_{mj},$$

  which measures the total variance across the classes.

- For example, when $C = 2$ the Gini index is $2\,\widehat{p}\,(1 - \widehat{p})$, where $\widehat{p}$ is the proportion in the second class.

- The Gini index takes on a small value if all the probabilities are close to zero or one (that is, when the node is pure).

## Cross-entropy

- The **cross-entropy** or **deviance** is
$$-\sum_{c=1}^{C} \widehat{p}_{mc} \log(\widehat{p}_{mc}),$$
which corresponds to negative multinoulli log-likelihood for the training observations in node $m$ evaluated at $\widehat{p}_{m1}, \ldots, \widehat{p}_{mC}$.

- When $C = 2$ the cross-entropy is $-\widehat{p}\log(\widehat{p}) - (1-\widehat{p})\log(1-\widehat{p})$, where $\widehat{p}$ is the proportion in the second class.

- Like the Gini index, the cross-entropy takes on a small value if all the probabilities are close to zero or one (that is, when the node is pure).

## Node impurity measures

In the two class case (the cross-entropy is scaled for visualisation):

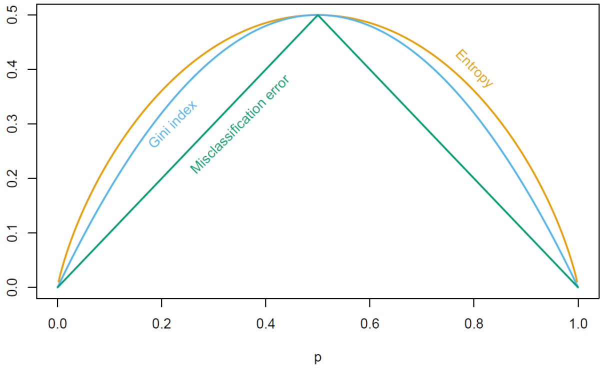


Figure from ESL.

## Node impurity measures

- The Gini index and the cross entropy are more sensitive to changes in the node probabilities than the misclassification error, so that we prefer these measures when growing the tree.
- These two measures also have the advantage of being differentiable, which makes them more amenable to numerical optimisation.
- We can use any of the measures (including the misclassification error) to prune the tree.

## Advantages of trees

- Trees are simple.
- Trees lead to interpretable prediction rules.
- Trees can easily handle categorical and ordinal features without the need to create dummy variables.
- Trees can approximate complex nonlinearities, including interactions.
- Trees are the basic component of powerful prediction methods such as random forests and boosting.

## Disadvantages of trees

- Instability: due to their hierarchical nature, trees are inherently unstable and have high variance. Small changes in the data can lead to a very different sequence of splits, compromising interpretability if the objective is to describe the population.
- Lack of smoothness: trees lead to non-smooth prediction functions, which can degrade performance specially in regression settings.
- Trees have difficulty in capturing additive structure.
- Therefore, decision trees tend to have low predictive accuracy.

## Trees versus linear models

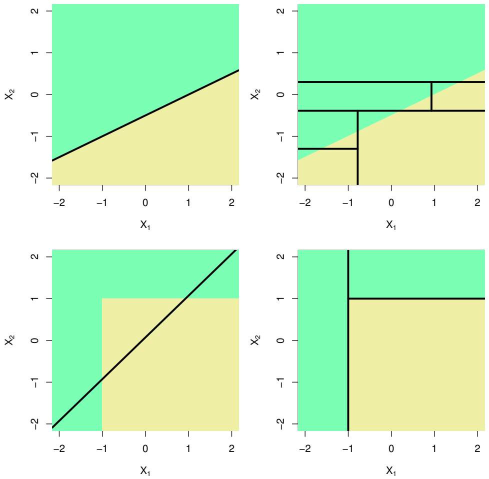


Figure from ISL.

## Bagging

## Bagging

The idea of **bootstrap aggregation** or **bagging** is to average many noisy but approximately unbiased models, therefore reducing variance.

Decision trees are ideal candidates for bagging, since they capture complex interaction structures in the data, and if grown deeply, have relatively low bias, but high variance.

## Bagging (key concept)

Suppose that we fit a regression model to the training data $\mathcal{D}$ to obtain the prediction $\widehat{f}(\boldsymbol{x})$ for an input point $\boldsymbol{x}$. Bagging averages this prediction over a collection of bootstrap samples (resampled versions of the training data), thereby reducing its variance.

For each bootstrap sample $\mathcal{D}_b^*$, $b = 1, \ldots, B$, we fit the model to obtain a prediction $\widehat{f}_b^*(\boldsymbol{x})$. The bagging prediction is:

$$\widehat{f}_{\text{bag}}(\boldsymbol{x}) = \frac{1}{B} \sum_{b=1}^{B} \widehat{f}_b^*(\boldsymbol{x}).$$

## Bootstrap: graphical illustration

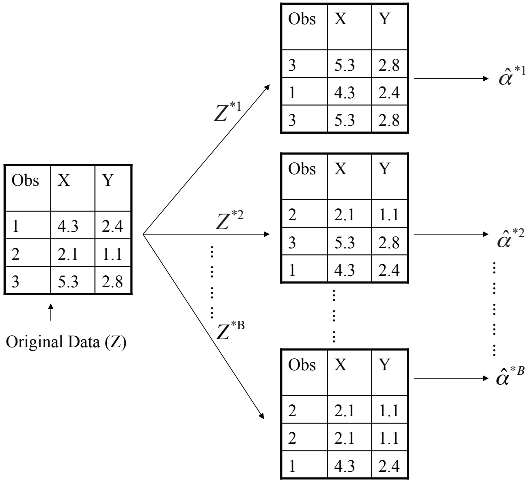


Figure from ISL

## Bagging

- The bagged estimate will differ from the original prediction ($B \to \infty$) only when the estimator $\widehat{f}(\cdot)$ is a nonlinear or adaptive function of the data (due to the linearity of expectations).
- Therefore, bagging does not improve the prediction from linear models.
- Trees in turn are highly nonlinear estimators, and may benefit greatly from averaging.
- Increasing $B$ does not overfit. The higher the $B$, the more stable the average.

## Bagging classifiers (key concept)

In the classification setting, we obtain a prediction $\widehat{y}_b^*(\boldsymbol{x})$ for each bootstrap $\mathcal{D}_b^*$, $b = 1, \ldots, B$. The bagged classifier selects the class with the most "votes" from the $B$ trees,

$$\widehat{y}_{\mathsf{bag}}(\boldsymbol{x}) = \underset{c}{\operatorname{argmax}} \sum_{b=1}^{B} I(\widehat{y}_b^*(\boldsymbol{x}) = c).$$

If we require a class probability estimate $\widehat{p}(\boldsymbol{x})$, the bagged probability estimate is

$$\widehat{p}_{\mathsf{bag}}(\boldsymbol{x}) = \frac{1}{B} \sum_{b=1}^{B} \widehat{p}_b^*(\boldsymbol{x}),$$

where $\widehat{p}_b^*(\boldsymbol{x})$ is the estimated probability according to the model fitted to the bootstrap sample $b$.

## Random forests

## Random forests (key concept)

**Random forests** improve over bagging by adding a tweak that decorrelates the trees: before each binary split, we select a *random sample* of only $k \leq p$ predictors as split candidates.

## Random forest (key concept)

**Algorithm** Random forest

```
1: for $b = 1$ to $B$ do
2:     Sample $N$ observations with replacement from the training data $\mathcal{D}$
       to obtain the bootstrap sample $\mathcal{D}_b^*$.
3:     Grow a random forest tree $T_b$ to $\mathcal{D}_b^*$ by repeating the following
       steps for each terminal node of the tree, until the minimum node
       size $n_{\text{min}}$ is reached:
4:     (i) Select $k$ variables at random from the $p$ variables.
5:     (ii) Pick the best variable and split point among the $k$ candidates.
6:     (iii) Split the node into two daughter nodes.
7: end for
8: Output the ensemble of trees $\{T_b\}_1^B$.
```

## Random forest: implementation details

The tuning parameters in a random forest are $k$ (the number of split variables) and the minimum node size for each tree.

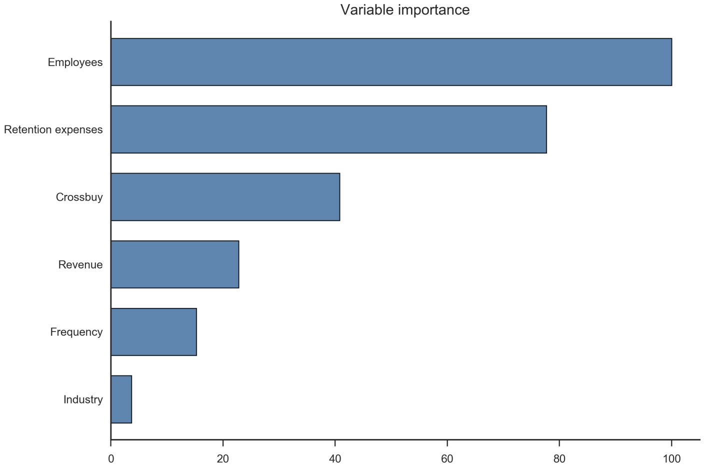
- For classification the default value for $k$ is $\lfloor \sqrt{p} \rfloor$ and the minimum node size is one.
- For regression, the default value for $k$ is $\lfloor p/3 \rfloor$ and the minimum node size is five.

In practice the best values depend on the problem, and we can use cross validation to select them. Using a small $k$ will typically be helpful when there is a large number of correlated predictors.

## Variable importance measures

- Random forests (including bagging as a special case) improve prediction at the expense of the simple interpretability of the prediction generated by a single tree.
- We can obtain an overall summary of the importance of a predictor in a random forest by using the RSS (regressor) or the Gini index/cross-entropy (classifier).
- We measure the importance of each variable by adding up the total decrease in the split criterion due to splits over a single predictor, averaged over all $B$ trees.

## Example: Customer Churn



## Why do random forests work?

- When there is a small subset of strong predictors, these variables will tend to dominate the top splits of the trees over the bootstrap samples, making the bagged trees quite similar to each other. Since the trees are similar, the bagged trees will be highly correlated.
- Averaging over highly correlated variables does not lead to a large reduction in variance.
- Random forests overcome this problem by giving a higher chance to other predictors, leading to decorrelation (at the expense of some bias).