Data Mining 2025
Exercises Classification Trees

Exercise 1: Computing Splits

We want to determine the optimal split in a node that contains the following data:

x_1	c	b	b	a	a	b	e	e	d	e
x_2	28	31	35	40	40	45	45	52	52	60
y	B	B	B	A	B	A	B	A	A	A

Here x_1 is a categorical attribute with possible values {a,b,c,d,e}, x_2 is a numerical attribute, and y is a binary class label with possible values A and B. We use the gini-index as impurity measure. The best split is the one that maximizes the impurity reduction.

(a) How many possible binary splits are there on x_1?

(b) How many splits on x_1 do we have to evaluate to determine the best one? List them.

(c) How many possible binary splits are there on x_2?

(d) How many splits on x_2 do we have to evaluate to determine the best one? List them. (Use the fact that the best split can not occur inside a segment.)

(e) Give the impurity reduction of the best split on x_2.

Exercise 2: More On Computing Splits

Consider the following data on numeric attribute x and class label y. The class label can take on three different values, coded as A, B and C.

x	6	8	12	12	12	14	14	14	18	20
y	A	A	A	A	B	A	A	B	C	C

We use the gini-index as impurity measure. The formula for the gini-index for an arbitrary number of class labels is given by

$$i(t) = 1 - \sum_{j=1}^{C} p(j|t)^2,$$

where C denotes the number of class labels, and $p(j|t)$ denotes the relative frequency of class j in node t.

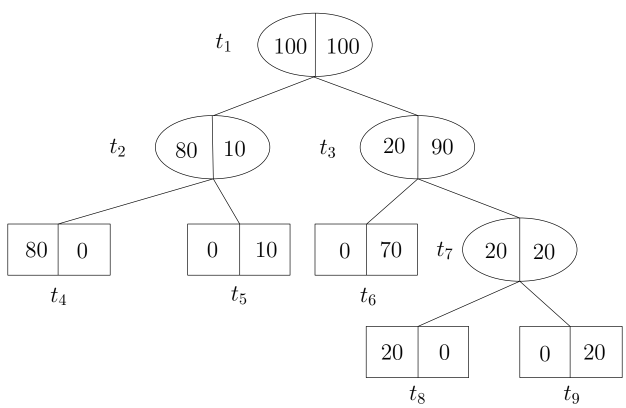
(a) Which candidate split(s) do we have to evaluate to determine the best one? (don't list any more than strictly necessary)

(b) What is the best split on x, and what is the impurity reduction of that split?

(c) Suppose we have the constraint `min_samples_leaf=3`, that is, you are not allowed to create a child node with less than 3 data points. Give the best split on x that satisfies this constraint. Is it on the border of a segment?

Exercise 3: Cost-Complexity Pruning

The tree $T_{\max}$ given below has been grown on the training sample.



In each node the number of observations with class A is given in the left part, and the number of observations with class B in the right part. The leaf nodes have been drawn as rectangles. The total cost of a tree T is defined as:

$$C_\alpha(T) = R(T) + \alpha|\tilde{T}| \tag{1}$$

It can be written as the sum of the contribution of each leaf node to total cost:

$$C_\alpha(T) = \sum_{t \in \tilde{T}} (R(t) + \alpha), \tag{2}$$

where $R(t)$ is the number of classification errors made in node t, divided by the total number of observations in the training set. For $T_{\max}$ as given above, this is:

$$C_\alpha(T_{\max}) = (R(t_4) + \alpha) + (R(t_5) + \alpha) + (R(t_6) + \alpha) + (R(t_8) + \alpha) + (R(t_9) + \alpha) \tag{3}$$

(a) As was done for $T_{\max}$ in equation (3), give an expression for the total cost of $T_{\max} - T_{t_3}$, the tree obtained by pruning $T_{\max}$ in t_3.

(b) Which terms are present in the expression for total cost of $T_{\max}$ but not $T_{\max} - T_{t_3}$? Which terms are present in the expression for total cost of $T_{\max} - T_{t_3}$ but not $T_{\max}$?

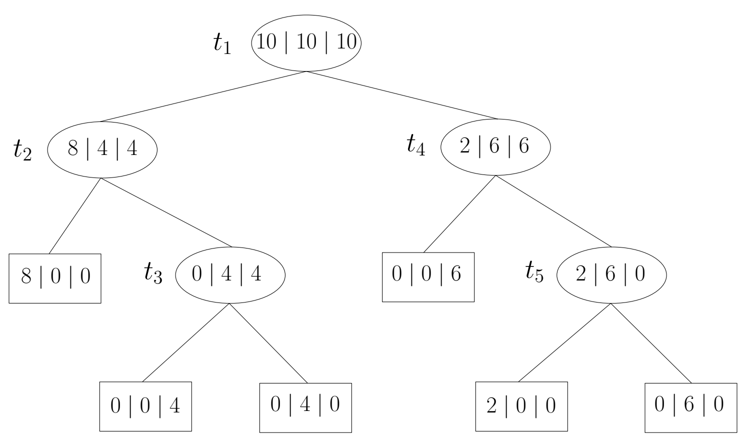
(c) For what value of α is the total cost of $T_{\max}$ and $T_{\max} - T_{t_3}$ the same? Which tree is preferred in that case?

(d) Give $T_1 = T(\alpha = 0)$: the smallest minimizing subtree of $T_{\max}$ for $\alpha = 0$.

(e) Compute the cost-complexity sequence $T_1 > T_2 > \ldots > \{t_1\}$. Also give the corresponding sequence of α values.

Exercise 4: Cost-Complexity Pruning

The tree given below, denoted by $T_{\max}$, has been constructed on the training sample:



In each node, the number of observations with class A is given in the left part, the number of observations with class B is given in the middle part, and the number of observations with class C is given in the right part. The leaf nodes have been drawn as rectangles.

Compute the cost-complexity pruning sequence $T_1 > T_2 > \ldots > \{t_1\}$, where T_1 is the smallest minimizing subtree for $\alpha = 0$. Also give the corresponding sequence of α values.

Exercise 5: An Alternative Pruning Procedure

In their seminal work *Classification and Regression Trees*, Breiman et al. (Chapman & Hall, 1984) consider the following pruning procedure before they describe cost-complexity pruning. Suppose that $T_{\max}$ has L terminal nodes. Construct a sequence of smaller and smaller trees

$$T_{\max}, T_1, T_2, \ldots, \{t_1\}$$

as follows: For every value of H, $1 \leq H \leq L$, consider the class $\mathcal{T}_H$ of all subtrees of $T_{\max}$ having $L - H$ leaf nodes. Select T_H as the subtree in $\mathcal{T}_H$ which minimizes $R(T)$; that is,

$$R(T_H) = \min_{T \in \mathcal{T}_H} R(T).$$

Put another way, T_H is the minimal resubstitution error pruned subtree of $T_{\max}$ having $L - H$ leaf nodes.

(a) Give the sequence

$$T_{\max}, T_1, T_2, \ldots, \{t_1\}$$

obtained when you apply this pruning method to the tree $T_{\max}$ given in exercise 3.

(b) Does the sequence you obtained under (a) have the desirable property that the sequence is nested, i.e., do we have

$$T_{\max} > T_1 > T_2 > \ldots > \{t_1\}?$$

(c) Is the sequence of minimal cost-complexity trees a subsequence of the sequence of subtrees as defined above? In other words, if $T(\alpha)$ has m leaf nodes, can there be another subtree T having m leaf nodes with $R(T) \leq R(T(\alpha))$?

Exercise 6: The Gini index

We have defined the gini index for binary classification as

$$i(t) = p(0|t)p(1|t) = p(0|t)(1 - p(0|t)), \tag{4}$$

where the class values are coded as 0 and 1, and $p(j|t)$ denotes the relative frequency of class j in node t. The generalization to an arbitrary number of classes is given by:

$$i(t) = \sum_{j=1}^{C} p(j|t)(1 - p(j|t)), \tag{5}$$

where C denotes the number of classes.

(a) If we apply equation (5) to the binary case, we should get the same results as when we apply equation (4). Is this indeed the case?

(b) Show that equation (5) can alternatively be written as

$$i(t) = 1 - \sum_{j=1}^{C} p(j|t)^2.$$

Exercise 7: More about the Gini index

The expected value (mean) of a discrete random variable X is defined as

$$\mathbb{E}[X] = \sum_x x \times P(X = x),$$

where the sum is over all possible values x of X. Furthermore,

$$\mathbb{E}[f(X)] = \sum_x f(x) \times P(X = x).$$

The variance of X is defined as its expected squared deviation from the mean:

$$\mathbb{V}[X] = \mathbb{E}[(X - \mathbb{E}[X])^2]$$

Let $X \in \{0, 1\}$ be a binary random variable with $P(X = 1) = p$, and $P(X = 0) = 1 - p$. We also say that X has a Bernoulli distribution. Show that:

(a) $\mathbb{E}[X] = p$, and

(b) $\mathbb{V}[X] = p(1 - p)$.

(c) Gini impurity is defined as $\phi(p) = p(1 - p)$ for $0 \leq p \leq 1$. Use calculus to show that this function achieves its maximum for $p = \frac{1}{2}$.

(d) Use calculus to show that the Gini index is strictly concave.

Exercise 8: The distribution of a sample proportion

Let Y denote the proportion of *ones* in n independent Bernoulli trials:

$$Y = \frac{1}{n} \sum_{i=1}^{n} X_i$$

where $X_1, \ldots, X_n$ are independent Bernoulli random variables, with $P(X_i = 1) = p$, for $i = 1, \ldots, n$.

(a) Show that

$$\mathbb{E}[Y] = p.$$

(b) Show that

$$\mathbb{V}[Y] = \frac{p(1 - p)}{n}.$$

Exercise 9: Splitting can not increase impurity

In lecture 37A we argued that the impurity reduction of a split cannot become negative for concave impurity measures such as the Gini index and entropy. In the proof we made use of the fact that the probability of class 0 in the parent node is a convex combination of the class 0 probabilities in the child nodes:

簡單來說：凸組合convex combination就是「加權平均」

$$p(0|t) = \pi(\ell)p(0|\ell) + \pi(r)p(0|r)$$

Prove that this is indeed the case.

Some Useful Properties of Expectation and Variance

1. $\mathbb{E}(c) = c$ for constant c. "The expected value of a constant is the constant itself".
2. $\mathbb{E}(cX) = c\mathbb{E}(X)$.
3. $\mathbb{E}(X \pm Y) = \mathbb{E}(X) \pm \mathbb{E}(Y)$.
4. $\mathbb{V}(c) = 0$ for constant c. "The variance of a constant is zero".
5. $\mathbb{V}(cX) = c^2\,\mathbb{V}(X)$. "The variance of a constant times a random variable is equal to the square of the constant times the variance of the random variable".
6. $\mathbb{V}(X \pm Y) = \mathbb{V}(X) + \mathbb{V}(Y)$ if X and Y are independent.

More generally, let $Z = c_0 + \sum_{i=1}^{n} c_i X_i$. Then

1. $\mathbb{E}(Z) = \mathbb{E}\left(c_0 + \sum_{i=1}^{n} c_i X_i\right) = c_0 + \sum_{i=1}^{n} c_i \mathbb{E}(X_i)$
2. $\mathbb{V}(Z) = \mathbb{V}\left(c_0 + \sum_{i=1}^{n} c_i X_i\right) = \sum_{i=1}^{n} c_i^2\,\mathbb{V}(X_i)$, provided that the X_i are mutually independent.