Data Mining 2025
Classification Trees (1)

Ad Feelders

Universiteit Utrecht

Classification

Predict the class of an object on the basis of some of its attributes.
For example, predict:

- Good/bad credit for loan applicants, using
  - income
  - age
  - ...
- Spam/no spam for e-mail messages, using
  - % of words matching a given word (e.g. "free")
  - use of CAPITAL LETTERS
  - ...
- Music Genre (Rock, Techno, Death Metal, ...) based on audio
  文藝作品的類型
  features and lyrics.

Building a classification model

The basic idea is to build a classification model using a set of training examples. Each training example contains attribute 屬性 values and the corresponding class label.

There are many techniques to do that:

- Statistical Techniques
  - Discriminant 判別 Analysis
  - Logistic Regression
- Data Mining/Machine Learning
  - Classification Trees
  - Bayesian Network Classifiers
  - Neural Networks
  - Support Vector Machines
  - ...

Strong and Weak Points of Classification Trees

Strong points:

- Are easy to interpret (if not too large).
- Select relevant attributes automatically.
- Can handle both numeric and categorical attributes.

Weak point:

- Single trees are usually not among the top performers.

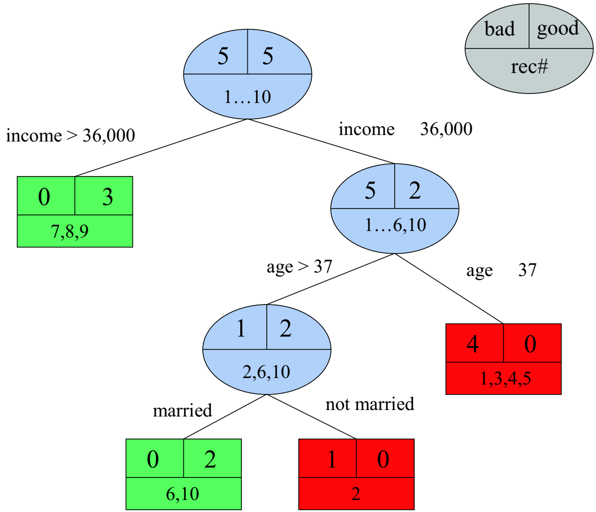
However:

- Averaging multiple trees (bagging, boosting, random forests) can bring them back to the top!
- But ease of interpretation suffers as a consequence.

Example: Loan Data

Record	age	married?	own house	income	gender	class
1	22	no	no	28,000	male	bad
2	46	no	yes	32,000	female	bad
3	24	yes	yes	24,000	male	bad
4	25	no	no	27,000	male	bad
5	29	yes	yes	32,000	female	bad
6	45	yes	yes	30,000	female	good
7	63	yes	yes	58,000	male	good
8	36	yes	no	52,000	male	good
9	23	no	yes	40,000	female	good
10	50	yes	yes	28,000	female	good

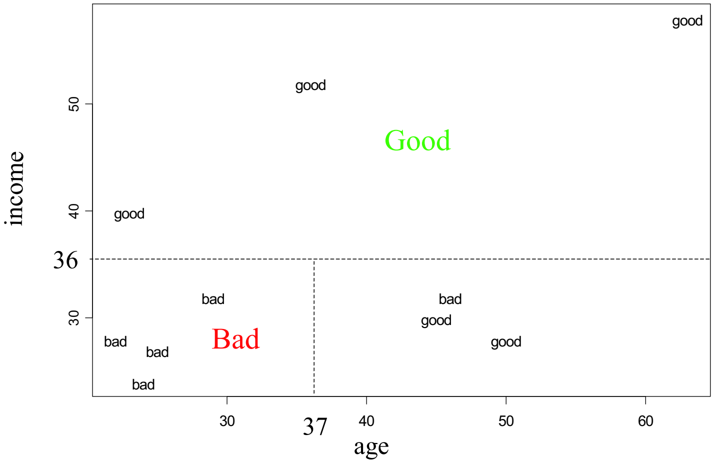
Credit Scoring Tree



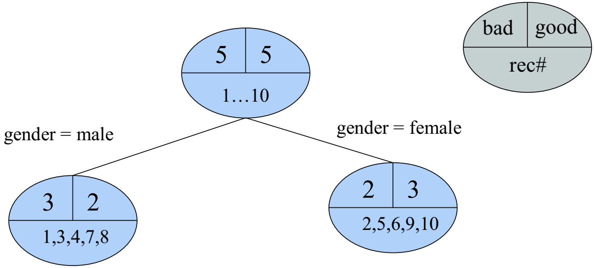
Cases with income $> 36,000$

Record	age	married?	own house	income	gender	class
1	22	no	no	28,000	male	bad
2	46	no	yes	32,000	female	bad
3	24	yes	yes	24,000	male	bad
4	25	no	no	27,000	male	bad
5	29	yes	yes	32,000	female	bad
6	45	yes	yes	30,000	female	good
7	63	yes	yes	58,000	male	good
8	36	yes	no	52,000	male	good
9	23	no	yes	40,000	female	good
10	50	yes	yes	28,000	female	good

Partitioning the attribute space



Why not split on gender in the root node?



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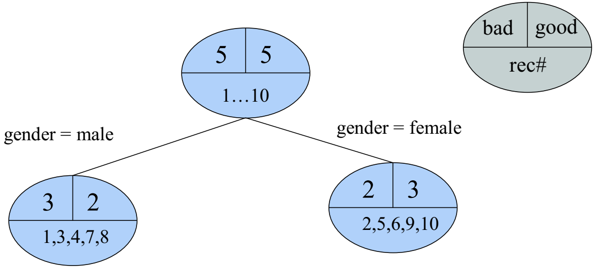


Intuitively: learning the value of gender doesn't provide much information about the class label.

Impurity of a node
不純

- We strive towards nodes that are *pure* in the sense that they only contain observations of a single class.
- We need a measure that indicates "how far" a node is removed from this ideal. 節點有多不純
- We call such a measure an *impurity* measure.

Impurity function

The impurity $i(t)$ of a node t is a function of the relative frequencies of the classes in that node:

$$i(t) = \phi(p_1, p_2, \ldots, p_J)$$ φ：表示某個函式

where the $p_j (j = 1, \ldots, J)$ are the relative frequencies of the J different classes in node t.

Sensible requirements of any quantification of impurity:

1. Should be at a maximum when the observations are distributed evenly over all classes.
2. Should be at a minimum when all observations belong to a single class.
3. Should be a symmetric function of $p_1, \ldots, p_J$.

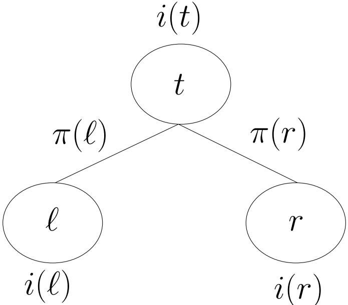
Quality of a split (test)

We define the quality of binary split s in node t as the *reduction* of impurity that it achieves

i (t) : impurity

$$\boxed{\Delta i(s,t) = i(t) - \{\pi(\ell)i(\ell) + \pi(r)i(r)\}}$$

where ℓ is the left child of t, r is the right child of t, $\pi(\ell)$ is the proportion of cases sent to the left, and $\pi(r)$ the proportion of cases sent to the right.



Well known impurity functions

Impurity functions we consider:

- Resubstitution error 替代誤差
- Gini-index
- Entropy

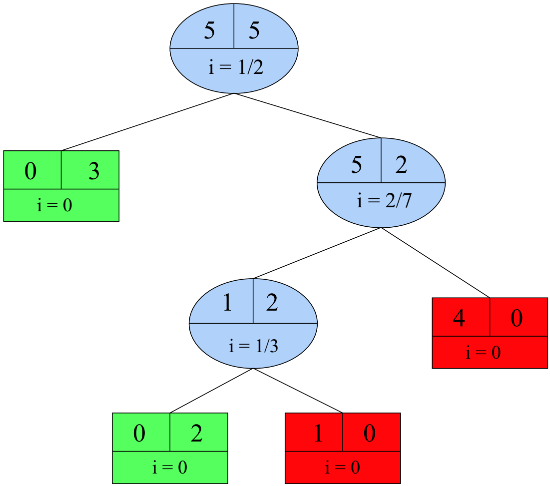
Resubstitution error

Measures the fraction 碎片；片段 of cases that is classified incorrectly if we assign every case in node t to the majority class in that node. That is

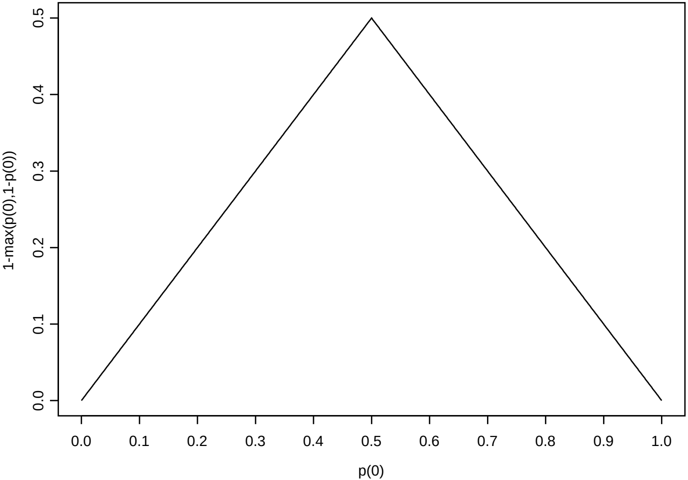
$$\boxed{i(t) = 1 - \max_j p(j|t)}$$

where $p(j|t)$ is the relative frequency of class j in node t.

Resubstitution error: credit scoring tree



Graph of resubstitution error for two-class case



Resubstitution error

Questions:

- Does resubstitution error meet the sensible requirements?

合理的

Sensible Requirements:

1. Should be at a maximum when the observations are distributed evenly over all classes
2. Should be at a minimum when all observations belong to a single class.
3. Should be a symmetric function of p1,...,pJ.

Resubstitution error

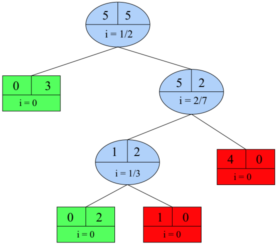
Questions:

- Does resubstitution error meet the sensible requirements?
- What is the impurity reduction of the second split in the credit scoring tree if we use resubstitution error as impurity measure?

Impurity Reduction: $\Delta i(s,t) = i(t) - \{\pi(\ell)i(\ell) + \pi(r)i(r)\}$

Resubstitution Error: $i(t) = 1 - \max_j p(j|t)$

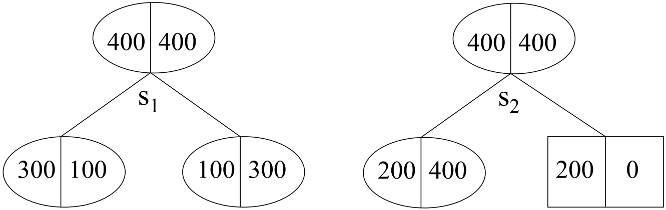
Impurity Reduction



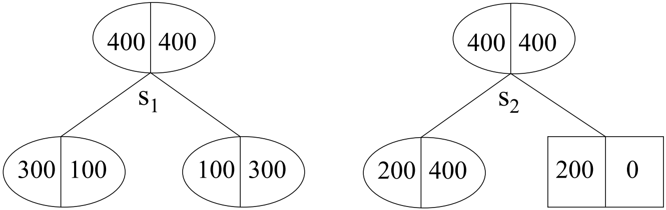
Impurity reduction of second split (using resubstitution error):

$$\begin{aligned}\Delta i(s,t) &= i(t) - \{\pi(\ell)i(\ell) + \pi(r)i(r)\} \\ &= \frac{2}{7} - \left(\frac{3}{7} \times \frac{1}{3} + \frac{4}{7} \times 0\right) \\ &= \frac{2}{7} - \frac{1}{7} = \frac{1}{7}\end{aligned}$$

Which split is better?



Which split is better?



These splits have the same resubstitution error, but s_2 is commonly preferred because it creates a leaf node.

Class of suitable impurity functions

- Problem: resubstitution error only decreases at a *constant* rate as the node becomes purer.
- We need an impurity measure which gives greater rewards to purer nodes. Impurity should decrease at an *increasing* rate as the node becomes purer.
- Hence, impurity should be a strictly *concave* function of $p(0)$.

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We define the class $\mathcal{F}$ of impurity functions (for two-class problems) that has this property:

1. $\phi(0) = \phi(1) = 0$ (minimum at $p(0) = 0$ and $p(0) = 1$)
2. $\phi(p(0)) = \phi(1 - p(0))$ (symmetric)
3. $\phi''(p(0)) < 0, 0 < p(0) < 1$ (strictly concave)

假設節點中有兩個類別：0 和 1。
p(0) = 節點中類別 0 的相對頻率 = 「類別 0 的樣本數 ÷ 總樣本數」
p(1)=1−p(0) = 類別 1 的相對頻率

Impurity function: Gini index

唸書：Bernoulli random variable
唸書：Note 那句話

For the two-class case the Gini index is

$$\boxed{i(t) = p(0|t)p(1|t) = p(0|t)(1 - p(0|t))}$$

Question 1: Check that the Gini index is belongs to $\mathcal{F}$.

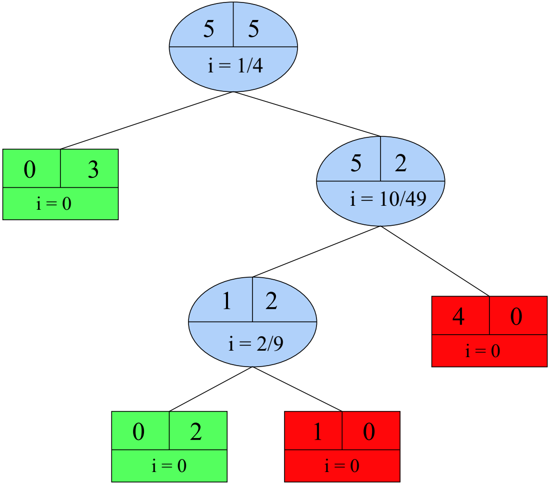
計算二階導數：ϕ''(p(0)) <0,0 <p(0) <1 (strictly concave)

Question 2: Check that if we use the Gini index, split s_2 is indeed preferred.

split s2 指的是 信用評分樹 (credit scoring tree) 中的第二個分裂（second split）
計算例子中的impurity reduction (不純度下降)

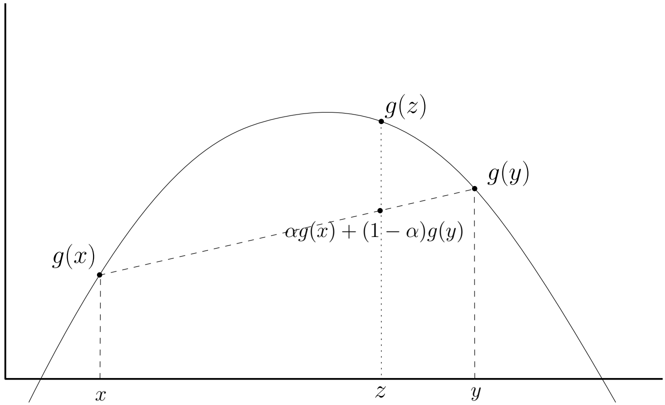
Note: The variance of a Bernoulli random variable with probability of success p is $p(1-p)$. Hence we are attempting to minimize the variance of the class distribution.

Gini index: credit scoring tree



Can impurity increase?

推導公式：z = αx + (1−α)y



A concave function g. For any x and y, the line segment connecting $g(x)$ and $g(y)$ is below the graph of g. $z = \alpha x + (1-\alpha)y$.

$$g(\alpha x + (1-\alpha)y) \geq \alpha g(x) + (1-\alpha)g(y)$$

Can impurity increase?

Is it possible that a split makes things worse, i.e. $\Delta i(s, t) < 0$?

Not if $\phi \in \mathcal{F}$. Because ϕ is a concave function, we have

$$\phi(p(0|\ell)\pi(\ell) + p(0|r)\pi(r)) \geq \pi(\ell)\phi(p(0|\ell)) + \pi(r)\phi(p(0|r))$$

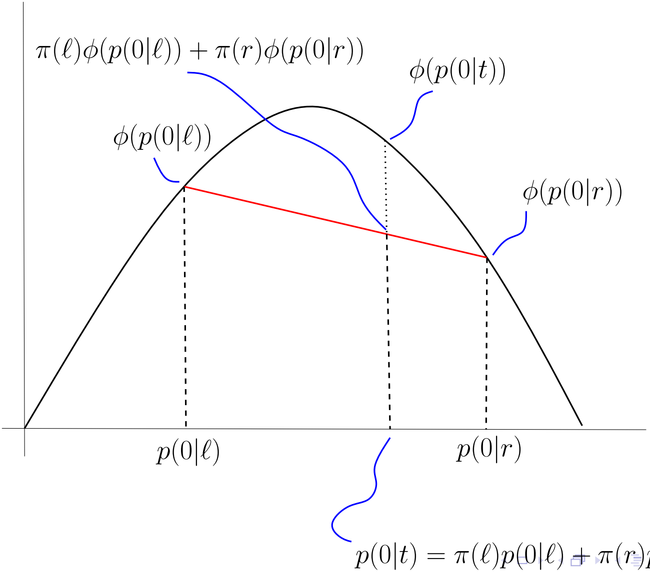
Since

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

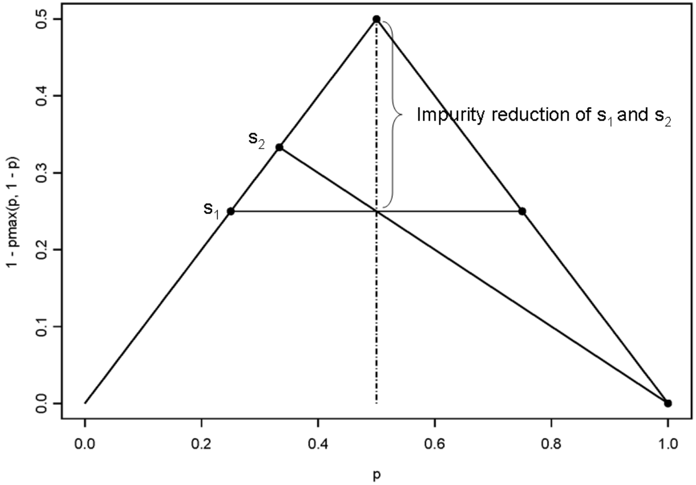
it follows that

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

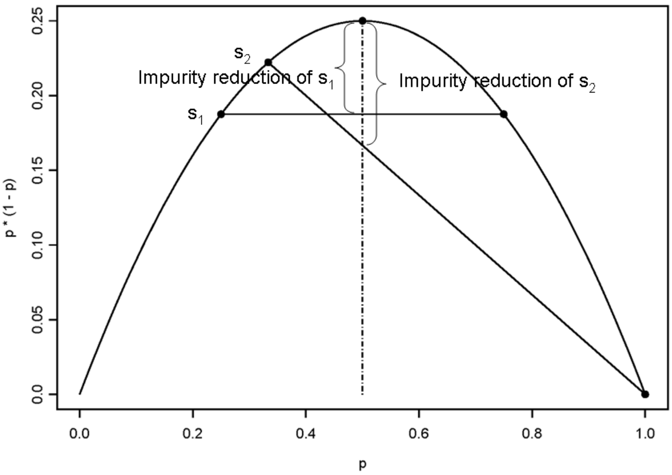
Can impurity increase? Not if ϕ is concave.



Split s_1 and s_2 with resubstitution error



Split s_1 and s_2 with Gini



Impurity function: Entropy

For the two-class case the entropy is

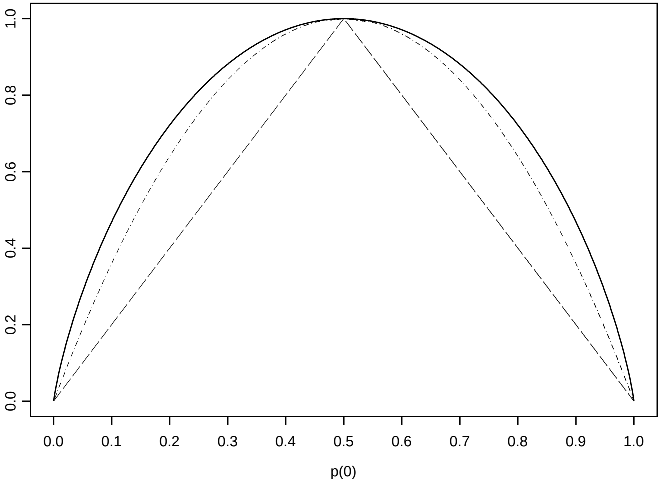
$$\boxed{i(t) = -p(0|t)\log p(0|t) - p(1|t)\log p(1|t)}$$

t : node

Question: Check that entropy impurity belongs to $\mathcal{F}$.

Remark: this is the average amount of information generated by drawing 抽籤 (with replacement 有放回) an example at random from this node, and observing its class.

Three (rescaled) impurity measures



Entropy (solid), Gini (dot-dash) and resubstitution (dash) impurity.

The set of splits considered

1. Each split depends on the value of only a *single* attribute. 屬性
2. If attribute x is numeric, we consider all splits of type $x \leq c$ where c is (halfway) between two consecutive 連續不斷的 values of x in their sorted order.
3. If attribute x is categorical, taking values in $\{b_1, b_2, \ldots, b_L\}$, we consider all splits of type $x \in S$, where S is any non-empty proper 非空且不是全集的子集合 subset of $\{b_1, b_2, \ldots, b_L\}$.

Splits on numeric attributes

There is only a finite number of distinct splits, because there are at most n distinct values of a numeric attribute in the training sample (where n is the number of examples in the training sample).

Example: possible splits on income in the root for the loan data

Income	Class	Quality (split after) 0.25−
24	B	$0.1(1)(0)+0.9(4/9)(5/9) = 0.03$
27	B	$0.2(1)(0) + 0.8\,(3/8)(5/8) = 0.06$
28	B,G	$0.4(3/4)(1/4) + 0.6(2/6)(4/6) = 0.04$
30	G	$0.5(3/5)(2/5) + 0.5(2/5)(3/5) = 0.01$
32	B,B	$0.7(5/7)(2/7) + 0.3(0)(1) = 0.11$
40	G	$0.8(5/8)(3/8) + 0.2(0)(1) = 0.06$
52	G	$0.9(5/9)(4/9) + 0.1(0)(1) = 0.03$
58	G	

Splits on a categorical attribute

For a categorical attribute with L distinct values there are $2^{L-1} - 1$ distinct splits to consider. Why?

Splits on a categorical attribute

For a categorical attribute with L distinct values there are $2^{L-1} - 1$ distinct splits to consider. Why?

There are $2^L - 2$ non-empty proper subsets of $\{b_1, b_2, \ldots, b_L\}$.

But a subset and the complement 補集 of that subset result in the same split, so we should divide this number by 2.

Splitting on categorical attributes: shortcut

L : distinct values
b1, b2, ...bL : 一個屬性的各種不同類別值

For two-class problems, and $\phi \in \mathcal{F}$, we don't have to check all $2^{L-1} - 1$ possible splits. Sort the $p(0|x = b_\ell)$, that is,

當屬性 x 取值為 bl 時，樣本屬於「類別 0」的機率。

$$p(0|x = b_{\ell_1}) \leq p(0|x = b_{\ell_2}) \leq \ldots \leq p(0|x = b_{\ell_L})$$

Then one of the $L - 1$ subsets

$$\{b_{\ell_1}, \ldots, b_{\ell_h}\}, \quad h = 1, \ldots, L - 1,$$

is the optimal split. Thus the search is reduced from computing $2^{L-1} - 1$ splits to computing only $L - 1$ splits.

Splitting on categorical attributes: example

Let x be a categorical attribute with possible values a, b, c, d. Suppose

$$p(0|x = a) = 0.6, p(0|x = b) = 0.4, p(0|x = c) = 0.2, p(0|x = d) = 0.8$$

Sort the values of x according to probability of class 0

$$c \qquad b \qquad a \qquad d$$

We only have to consider the splits: $\{c\}, \{c, b\}$, and $\{c, b, a\}$.

Intuition: put values with low probability of class 0 in one group, and values with high probability of class 0 in the other.

Splitting on numerical attributes: shortcut

分裂品質 (quality) 是根據 impurity reduction (純度降低) 來計算的。
每個候選切點，都會把資料分成「左子節點」和「右子節點」
再根據左右節點的樣本比例 & 類別分布，計算 impurity。

捷徑 (shortcut) 規則
最佳分裂點只可能出現在「類別分布改變的地方」
換句話說：
如果排序後的數值樣本中，連續幾筆資料的類別標籤一樣，那麼在它們之間切開沒有意義。
只有當左右兩邊的類別組成不同時，這個切點才可能成為最佳分裂。

B: Bad
G: Good

Income	Class	Quality (split after) 0.25−
24	B	$0.1(1)(0)+0.9(4/9)(5/9) = 0.03$
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Optimal split can only occur between consecutive values with *different* class distributions.

連續的

Splitting on numerical attributes

Income	Class	Quality (split after)
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58	G	

Optimal split can only occur between consecutive values with *different* class distributions.

Segment borders: numeric example

A segment is a block of consecutive values of the split attribute for which the class distribution is identical. Optimal splits can only occur at segment borders.

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

x	8	8	12	12	14	16	16	18	20	20
y	A	B	A	B	A	A	A	A	A	B

The class probabilities (relative frequencies) are:

x	8	12	14	16	18	20
$P(A)$	0.5	0.5	1	1	1	0.5
$P(B)$	0.5	0.5	0	0	0	0.5

So we obtain the segments: $(8, 12)$, $(14, 16, 18)$ and (20).
Only consider the splits: $x \leq 13$ and $x \leq 19$
Ignore: $x \leq 10$, $x \leq 15$ and $x \leq 17$

Basic Tree Construction Algorithm (control flow)

Construct tree

nodelist $\leftarrow$ {{training data}}
Repeat
current node $\leftarrow$ select node from nodelist 從 nodelist 中選一個節點當作 current node（目前處理的節點）
nodelist $\leftarrow$ nodelist $-$ current node 將這個節點從列表中移除（表示正在處理）
if impurity(current node) > 0
then
S $\leftarrow$ set of candidate splits in current node S：節點可以選擇的所有分裂方式（例如對不同特徵做切分）
s* $\leftarrow$ arg $\max_{s \in S}$ impurity reduction(s,current node) s*：選擇使不純度下降最多的分裂（impurity reduction 最大的分裂）
child nodes $\leftarrow$ apply(s*,current node) 對 current node 套用最佳分裂 s*，產生子節點
nodelist $\leftarrow$ nodelist $\cup$ child nodes 將子節點加入 nodelist，後續還會處理這些節點
fi
Until nodelist $= \varnothing$ 當 nodelist 變空（所有節點都處理完，或都是純節點）時，演算法結束