Data Mining 2018
Classification Trees (1)

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Modeling: Data Mining Tasks

- Classification / Regression
- Dependency Modeling (Graphical Models; Bayesian Networks)
- Frequent Patterns Mining (Association Rules)
- Subgroup Discovery (Rule Induction; *Bump-hunting*)
- Clustering
- Ranking

Classification

The prediction of 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 features and lyrics.

Building a classification model

The basic idea is to build a classification model using a set of training examples. There are many techniques to do that:

- Statistical Techniques
  - discriminant 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.

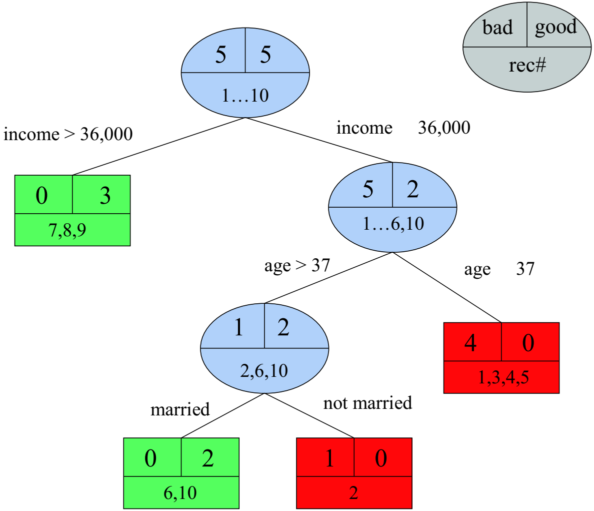
However:

- Averaging multiple trees (bagging, random forests) can bring them back to the top!

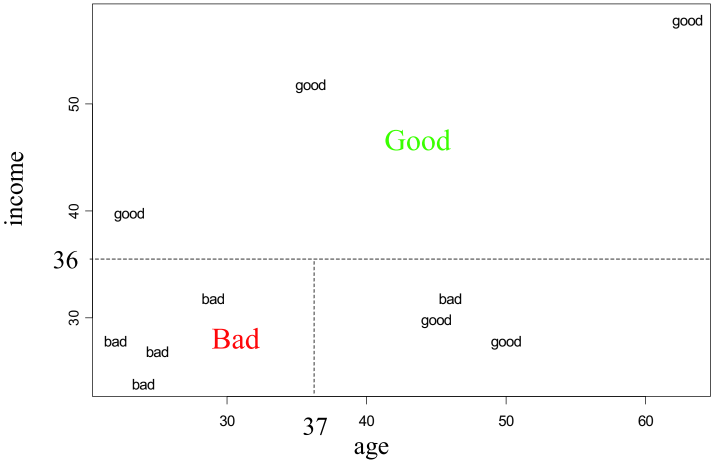
Example: Loan Data

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

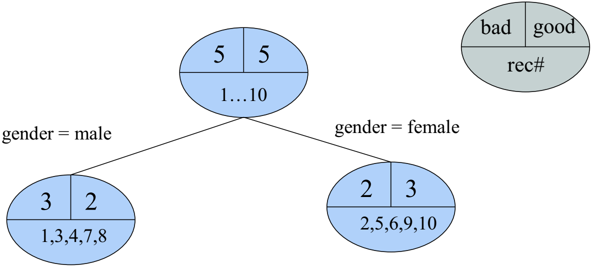
Credit Scoring Tree



Partitioning the attribute space



Why not split on gender in top node?



Impurity of a node

- 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.
- 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:

$$i(t) = \phi(p_1, p_2, \ldots, p_J)$$

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:

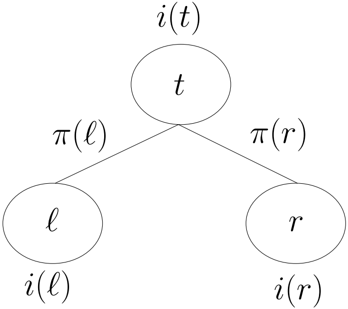
1. Should be at a maximum when the observations are distributed evenly over all classes.
2. Should be at a minimum when all observations belong to a single class.
3. Should be a symmetric function of $p_1, \ldots, p_J$.

Quality of a split (test)

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

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

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
- Gini-index (CART, Rpart)
- Entropy (C4.5, Rpart)

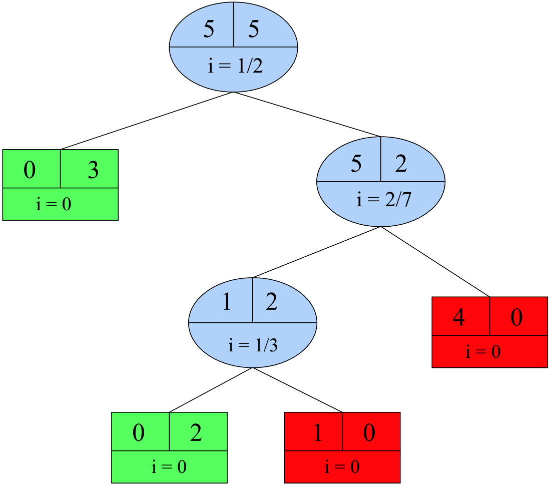
Resubstitution error

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

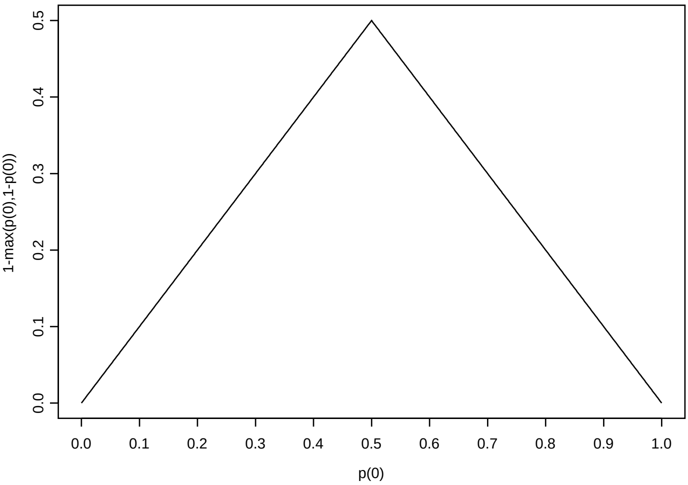
$$i(t) = 1 - \max_j p(j|t)$$

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?

Resubstitution error

Questions:

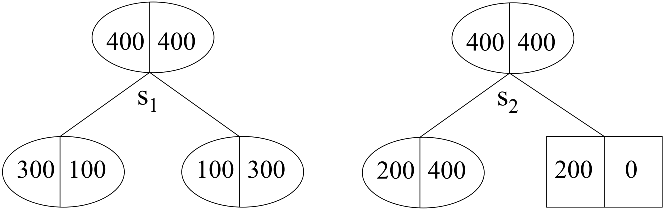
- Does resubstitution error meet the sensible requirements?
- What is the impurity reduction of the second split in the credit scoring tree if we use resubstitution error as impurity measure?

Impurity Reduction

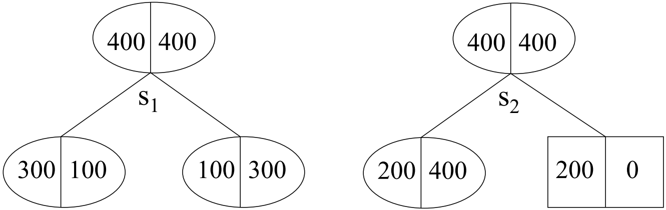
Impurity reduction of second split (using resubstitution error):

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

Which split is better?



Which split is better?



These splits have the same resubstitution error, but s_2 is 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 $p(0)$.

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)

Impurity function: Gini index

For the two-class case the Gini index is

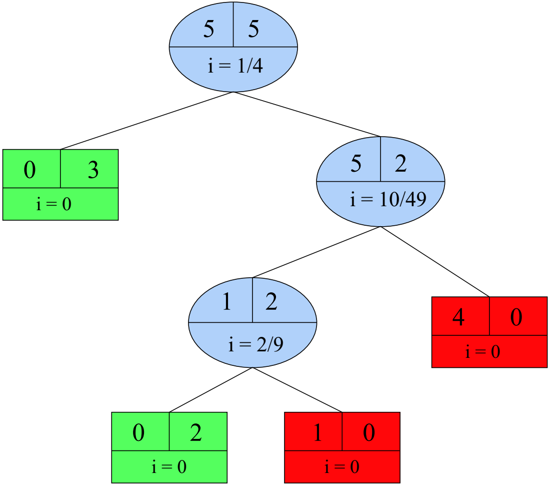
$$i(t) = p(0|t)p(1|t) = p(0|t)(1 - p(0|t))$$

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

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

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?

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

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

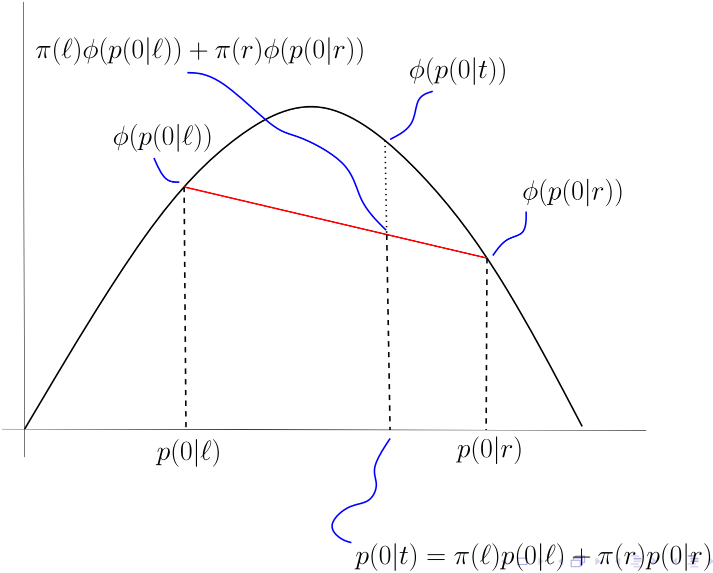
Since

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

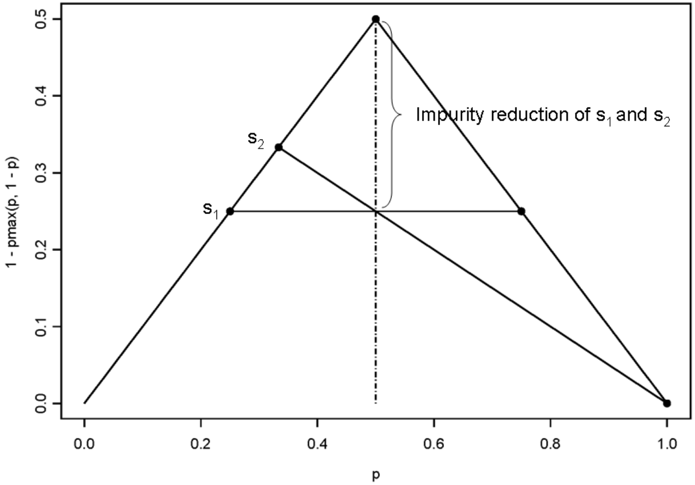
it follows that

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

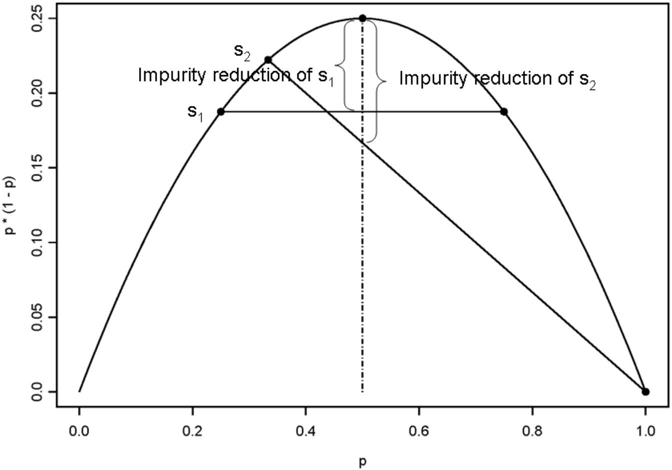
Can impurity increase? Not if ϕ is concave.


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

Split s_1 and s_2 with resubstitution error



Split s_1 and s_2 with Gini



Impurity function: Entropy

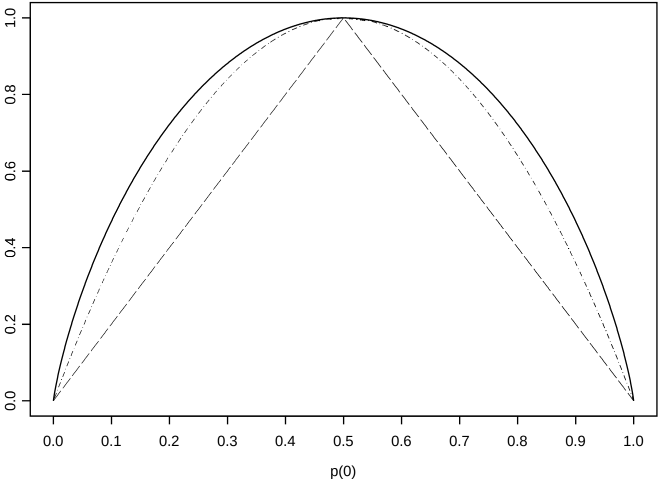
For the two-class case the entropy is

$$\begin{aligned} i(t) &= -p(0|t)\log p(0|t) - p(1|t)\log p(1|t) \\ &= -p(0|t)\log p(0|t) - (1-p(0|t))\log(1-p(0|t)) \end{aligned}$$

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

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

Three 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.
2. If attribute x is numeric, we consider all splits of type $x \leq c$ where c is (halfway) between two consecutive values of x.
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 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?

Splitting on categorical attributes

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,

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

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

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.

Splitting on numerical attributes

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24	B	
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40	G	
52	G	
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 $x \leq 17$

Optimal splits of gini index

Theorem

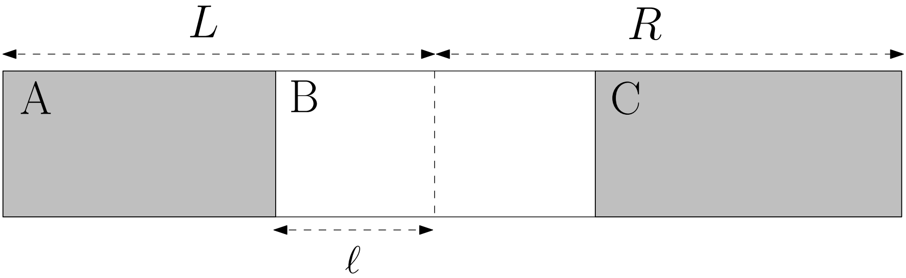
The gini index optimal splits can only occur on segment borders.

Consider the two-class case and binary splits. Let B be a segment, and let A be everything to the left of B, and C everything to the right of B.

We show that the optimal split cannot occur inside B. Define:

- a: the number of cases in part A.
- a_1: the number of cases in part A belonging to class 1.
- b: the number of cases in segment B.
- p_1: the relative frequency of class 1 in segment B.
- ℓ: the number of cases from segment B sent to the left by the split. $\ell \in [0, b]$.

Optimal splits of gini index



- We perform a binary split into a left part L and a right part R.
- ℓ denotes the number of cases of segment B that goes to the left.
- Wherever we split inside B, the class distribution of the part of B that goes to the left (right) is the same, and has probability of class 1 equal to p_1.

Optimal splits of gini index

Note that the probability of class 1 in the left part is given by

$$p_L = \frac{a_1 + \ell p_1}{a + \ell}$$

So the impurity of the left group as a function of ℓ is given by

$$i(L) = p_L(1 - p_L) = p_L - p_L^2 = \frac{a_1 + \ell p_1}{a + \ell} - \left(\frac{a_1 + \ell p_1}{a + \ell}\right)^2$$

The weighted average of the gini index of the child nodes is given by:

$$\frac{N_L}{N} i(L) + \frac{N_R}{N} i(R),$$

where N_L is the number of cases sent to the left, etc.

Note that we want to *minimize* this weighted average.

Optimal splits of gini index

The contribution of the left part is (ignore constant $\frac{1}{N}$):

$$f(\ell) = N_L \times i(L) = (a+\ell)\left(\frac{a_1+\ell p_1}{a+\ell} - \frac{(a_1+\ell p_1)^2}{(a+\ell)^2}\right)$$
$$= (a_1+\ell p_1) - \frac{(a_1+\ell p_1)^2}{a+\ell}$$

We show that this is a concave function of ℓ, which implies that the minimum is attained either for $\ell = 0$, or $\ell = b$.

The second derivative with respect to ℓ is given by

$$f''(\ell) = -2\,\frac{(ap_1 - a_1)^2}{(a+\ell)^3} \leq 0$$

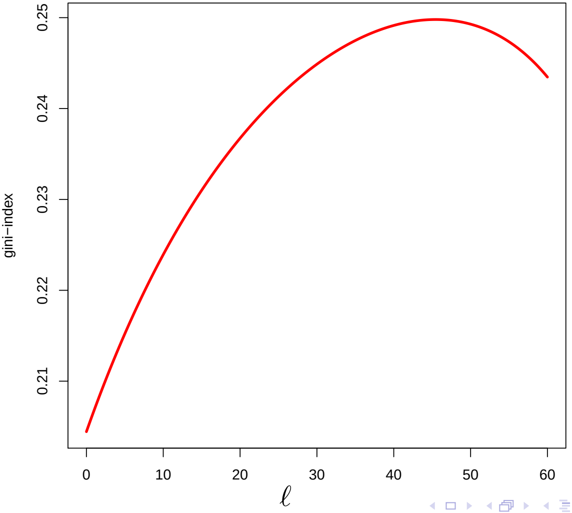
The second derivative is negative everywhere, so the function is indeed concave.

Optimal splits of gini index

1. By symmetry, the contribution of the right child to the weighted average is also a concave function of ℓ, and therefore the average gini index as a whole is a concave function of ℓ.
2. Hence, it attains its minimum for $\ell = 0$, or $\ell = b$ (i.e. at the segment borders), so the optimal split can never occur inside segment B.
3. This result is true for arbitrary concave impurity measures (e.g. entropy) and generalizes to arbitrary number of classes.

Weighted average of gini index

Numeric example with $a = 50$, $a_1 = 10$, $b = 60$, $p_1 = 0.8, c = 30, c_1 = 10$.



Basic Tree Construction Algorithm (control flow)

Construct tree

```
    nodelist ← {{training sample}}
    Repeat
        current node ← select node from nodelist
        nodelist ← nodelist − current node
        if impurity(current node) $> 0$
        then
            S ← candidate splits in current node
            s* ← $\arg\max_{s \in S}$ impurity reduction(s,current node)
            child nodes ← apply(s*,current node)
            nodelist ← nodelist ∪ child nodes
        fi
    Until nodelist = ∅
```