

Chapter ML:VI

VI. Decision Trees

- ❑ Decision Trees Basics
- ❑ Impurity Functions
- ❑ Decision Tree Algorithms
- ❑ Decision Tree Pruning

Impurity Functions

Splitting

Let t be a leaf node of an incomplete decision tree, and let $D(t)$ be the subset of the example set D that is represented by t . [\[illustration\]](#)

Possible criteria for a splitting of $X(t)$:

1. Size of $D(t)$.
2. Purity of $D(t)$.
3. Impurity reduction of $D(t)$.

Impurity Functions

Splitting

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Possible criteria for a splitting of $X(t)$:

1. Size of $D(t)$.

$D(t)$ is not split if $|D(t)|$ is below a threshold.

2. Purity of $D(t)$.

$D(t)$ is not split if all examples in $D(t)$ are members of the same class.

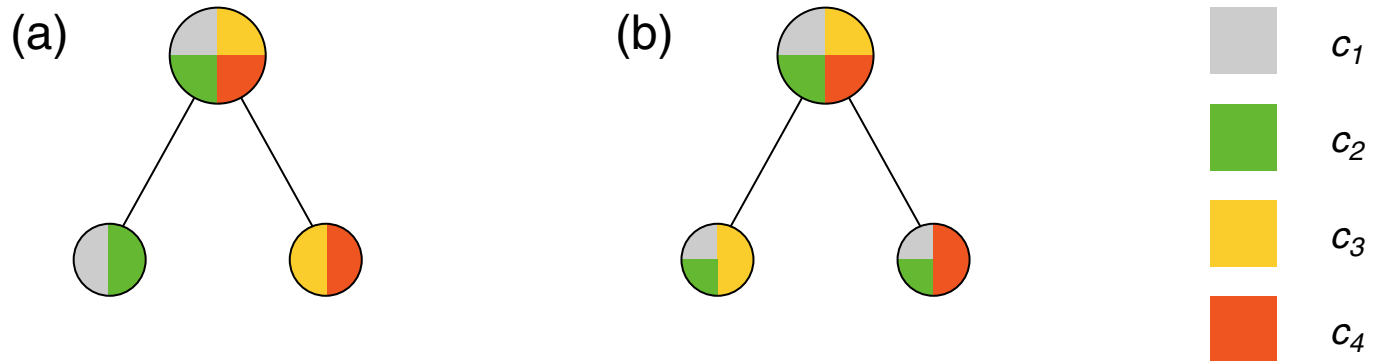
3. Impurity reduction of $D(t)$.

$D(t)$ is not split if its impurity reduction, Δ_{ι} , is below a threshold.

Impurity Functions

Splitting (continued)

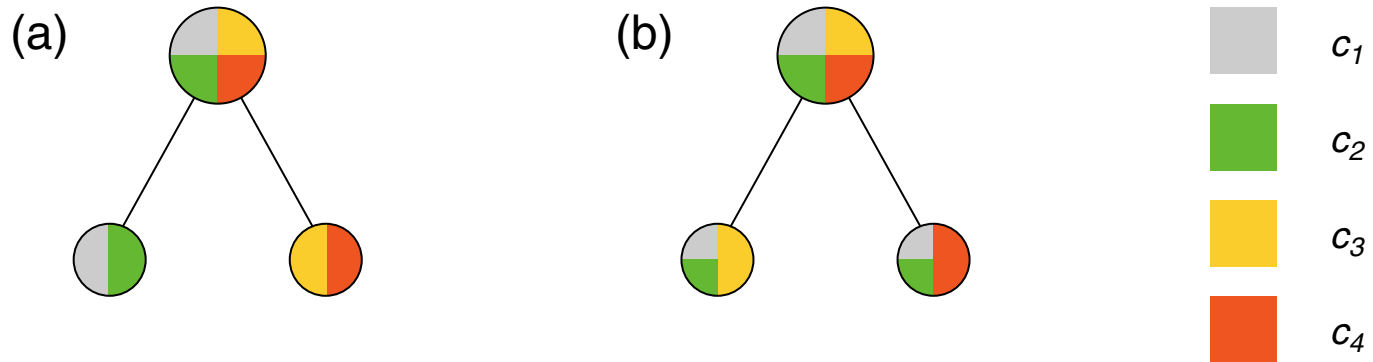
Let X be a multiset of feature vectors, $D \subseteq X$ a multiset of examples, and $C = \{c_1, c_2, c_3, c_4\}$ a set of classes. Distribution of D for two splittings of X :



Impurity Functions

Splitting (continued)

Let X be a multiset of feature vectors, $D \subseteq X$ a multiset of examples, and $C = \{c_1, c_2, c_3, c_4\}$ a set of classes. Distribution of D for two splittings of X :



- ❑ Splitting (a) minimizes the *impurity* of the subsets of D in the leaf nodes and should be preferred over splitting (b). This argument presumes that the misclassification costs are independent of the classes.
- ❑ The impurity is a function defined on $\mathcal{P}(D)$, the set of all subsets of an example set D .

Impurity Functions

Definition 4 (Impurity Function ι)

Let $k \in \mathbb{N}$. An impurity function $\iota : [0; 1]^k \rightarrow \mathbb{R}$ is a function defined on the standard $k-1$ -simplex, denoted Δ^{k-1} , for which the following properties hold:

- (a) ι becomes minimum at points $(1, 0, \dots, 0), (0, 1, \dots, 0), \dots, (0, \dots, 0, 1)$.
- (b) ι is symmetric with regard to its arguments, p_1, \dots, p_k .
- (c) ι becomes maximum at point $(1/k, \dots, 1/k)$.

Impurity Functions

Definition 5 (Impurity of an Example Set $\iota(D)$)

Let X be a multiset of feature vectors, $C = \{c_1, \dots, c_k\}$ a set of classes and $D \subseteq X \times C$ a multiset of examples. Moreover, let $\iota : [0; 1]^k \rightarrow \mathbb{R}$ be an impurity function. Then, the impurity of D , denoted as $\iota(D)$, is defined as follows:

$$\iota(D) = \iota \left(\frac{|\{(\mathbf{x}, c_1) \in D\}|}{|D|}, \dots, \frac{|\{(\mathbf{x}, c_k) \in D\}|}{|D|} \right)$$

Impurity Functions

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Definition 6 (Impurity Reduction $\Delta\iota$)

Let D_1, \dots, D_m be a splitting of an example set D , which is induced by a splitting of X . Then, the resulting impurity reduction, denoted as $\Delta\iota(D, \{D_1, \dots, D_m\})$, is defined as follows:

$$\Delta\iota(D, \{D_1, \dots, D_m\}) = \iota(D) - \sum_{l=1}^m \frac{|D_l|}{|D|} \cdot \iota(D_l)$$

Remarks:

- Δ^{k-1} denotes the standard $k-1$ -simplex, which contains all k -tuples with non-negative elements that sum to 1:

$$\Delta^{k-1} = \left\{ (p_1, \dots, p_k) \in \mathbf{R}^k : \sum_{i=1}^k p_i = 1 \text{ and } p_i \geq 0 \text{ for all } i \right\}$$

- Observe the different domains of the impurity function ι in the definitions for ι and $\iota(D)$, namely, $[0; 1]^k$ and D . The domains correspond to each other: the set of examples, D , defines via its class ratios an element from $[0; 1]^k$ and vice versa.
- The properties in the definition of the impurity function ι suggest to minimize the external path length of T with respect to D in order to minimize the overall impurity characteristics of T .
- Within the DT-construct algorithm usually a greedy strategy (local optimization) is employed to minimize the overall impurity characteristics of a decision tree T .

Impurity Functions

Impurity Functions Based on the Misclassification Rate

Definition for two classes [impurity function] :

$$\iota_{misclass}(p_1, p_2) = 1 - \max\{p_1, p_2\} = \begin{cases} p_1 & \text{if } 0 \leq p_1 \leq 0.5 \\ 1 - p_1 & \text{otherwise} \end{cases}$$

Impurity Functions

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$$\iota_{misclass}(D) = 1 - \max \left\{ \frac{|\{(\mathbf{x}, c_1) \in D\}|}{|D|}, \frac{|\{(\mathbf{x}, c_2) \in D\}|}{|D|} \right\}$$

Impurity Functions

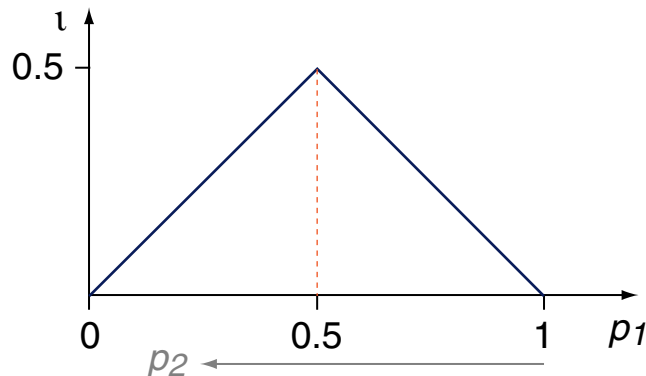
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Graph of the function $\iota_{\text{misclass}}(p_1, 1 - p_1)$, i.e., for two classes:



[Graphs: misclassification, [entropy](#), [Gini](#)]

Impurity Functions

Impurity Functions Based on the Misclassification Rate (continued)

Definition for k classes:

$$\iota_{\text{misclass}}(p_1, \dots, p_k) = 1 - \max_{i=1, \dots, k} p_i$$

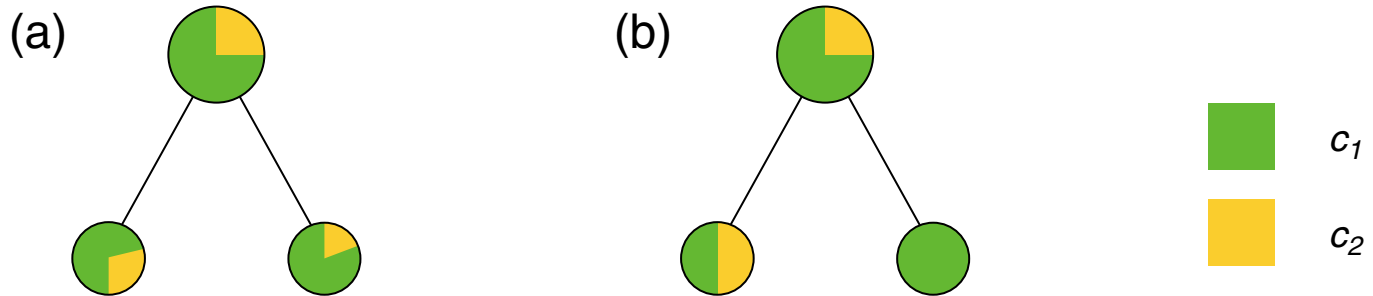
$$\iota_{\text{misclass}}(D) = 1 - \max_{c \in C} \frac{|\{(\mathbf{x}, c) \in D\}|}{|D|}$$

Impurity Functions

Impurity Functions Based on the Misclassification Rate (continued)

Problems:

- $\Delta \ell_{\text{misclass}} = 0$ may hold for all possible splittings.
- The impurity function that is induced by the misclassification rate underestimates pure nodes.

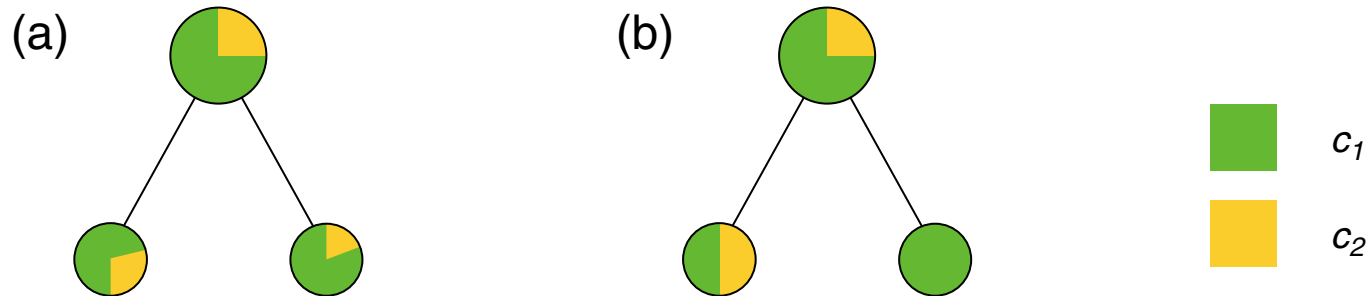


Impurity Functions

Impurity Functions Based on the Misclassification Rate (continued)

Problems:

- $\Delta \iota_{misclass} = 0$ may hold for all possible splittings.
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$$\Delta \iota_{misclass} = \iota_{misclass}(D) - \left(\frac{|D_1|}{|D|} \cdot \iota_{misclass}(D_1) + \frac{|D_2|}{|D|} \cdot \iota_{misclass}(D_2) \right)$$

left splitting: $\Delta \iota_{misclass} = \frac{1}{4} - \left(\frac{1}{2} \cdot \frac{3}{10} + \frac{1}{2} \cdot \frac{2}{10} \right) = 0$

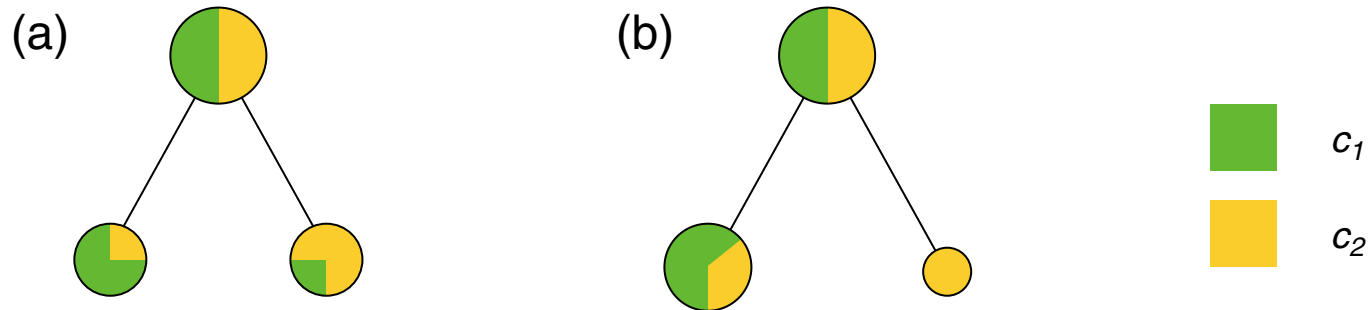
right splitting: $\Delta \iota_{misclass} = \frac{1}{4} - \left(\frac{1}{2} \cdot \frac{1}{2} + \frac{1}{2} \cdot 0 \right) = 0$

Impurity Functions

Impurity Functions Based on the Misclassification Rate (continued)

Problems:

- $\Delta \ell_{\text{misclass}} = 0$ may hold for all possible splittings.
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Impurity Functions

Definition 7 (Strict Impurity Function)

Let $\iota : [0; 1]^k \rightarrow \mathbb{R}$ be an impurity function and let $\mathbf{p}, \mathbf{p}' \in \Delta^{k-1}$. Then ι is called strict, if it is strictly concave:

$$(c) \rightarrow (c') \quad \iota(\lambda \mathbf{p} + (1-\lambda) \mathbf{p}') > \lambda \iota(\mathbf{p}) + (1-\lambda) \iota(\mathbf{p}'), \quad 0 < \lambda < 1, \mathbf{p} \neq \mathbf{p}'$$

Impurity Functions

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Lemma 8

Let ι be a *strict* impurity function and let D_1, \dots, D_m be a splitting of an example set D , which is induced by a splitting of X . Then the following inequality holds:

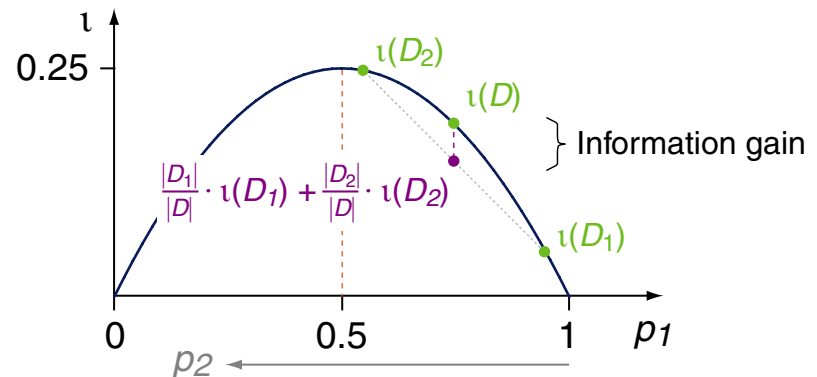
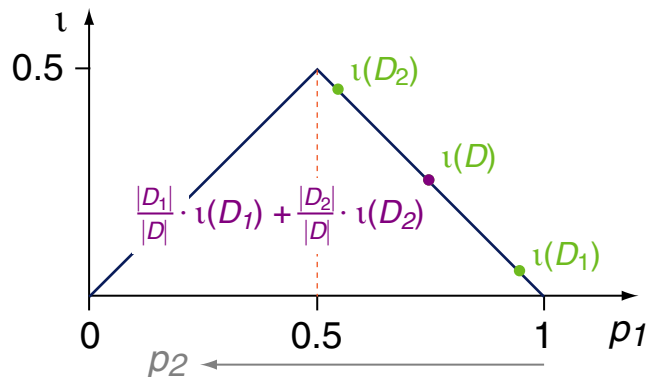
$$\Delta \iota(D, \{D_1, \dots, D_m\}) \geq 0$$

The equality is given iff for all $i \in \{1, \dots, k\}$ and $l \in \{1, \dots, m\}$ holds:

$$\frac{|\{(\mathbf{x}, c_i) \in D\}|}{|D|} = \frac{|\{(\mathbf{x}, c_i) \in D_l\}|}{|D_l|}$$

Remarks:

- ❑ The equality means that the splitting of D resembles exactly the class distribution of D .
- ❑ Strict concavity entails Property (c) of the [impurity function](#) definition.
- ❑ For two classes, strict concavity means $\iota(p_1, 1 - p_1) > 0$, where $0 < p_1 < 1$.
- ❑ If ι is a twice differentiable function, strict concavity is equivalent with a negative definite Hessian of ι .
- ❑ With properly chosen coefficients, polynomials of second degree fulfill the Properties (a) and (b) of the [impurity function](#) definition as well as strict concavity. See impurity functions based on the [Gini index](#) in this regard.
- ❑ The proof of Lemma 8 exploits the strict concavity property of ι .
- ❑ The impurity function induced by the error rate is concave, but not strictly concave, so that the weighted average of a splitting can be a point on the curve and equal the parent's impurity:



Impurity Functions

Impurity Functions Based on Entropy

Definition 9 (Entropy)

Let A denote an event and let $P(A)$ denote the occurrence probability of A . Then the entropy (self-information, information content) of A is defined as $-\log_2(P(A))$.

Let \mathcal{A} be an experiment with the exclusive outcomes (events) A_1, \dots, A_k . Then the mean information content of \mathcal{A} , denoted as $H(\mathcal{A})$, is called Shannon entropy or entropy of experiment \mathcal{A} and is defined as follows:

$$H(\mathcal{A}) = - \sum_{i=1}^k P(A_i) \cdot \log_2(P(A_i))$$

Remarks:

- ❑ The smaller the occurrence probability of an event, the larger is its entropy. An event that is certain has zero entropy.
- ❑ The Shannon entropy combines the entropies of all outcomes of an experiment, using the outcome probabilities as weights.
- ❑ In the entropy definition we stipulate the identity $0 \cdot \log_2(0) = 0$.
- ❑ Related. Entropy encoding methods such as Huffman coding. [\[Wikipedia\]](#)
- ❑ Related. The perplexity of a discrete probability distribution p is defined as $2^{H(p)}$. [\[Wikipedia\]](#)

Impurity Functions

Impurity Functions Based on Entropy (continued)

Definition 10 (Conditional Entropy, Information Gain)

Let \mathcal{A} be an experiment with the exclusive outcomes (events) A_1, \dots, A_k , and let \mathcal{B} be another experiment with the exclusive outcomes (events) B_1, \dots, B_m . Then the conditional entropy of the conditional experiment $\mathcal{A} \mid \mathcal{B}$, i.e., “the entropy of \mathcal{A} if the outcome of \mathcal{B} is known”, is defined as follows:

$$H(\mathcal{A} \mid \mathcal{B}) = \sum_{l=1}^m P(B_l) \cdot H(\mathcal{A} \mid B_l),$$

where $H(\mathcal{A} \mid B_l) = - \sum_{i=1}^k P(A_i \mid B_l) \cdot \log_2(P(A_i \mid B_l))$

Impurity Functions

Impurity Functions Based on Entropy (continued)

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$$\text{where } H(\mathcal{A} \mid B_l) = - \sum_{i=1}^k P(A_i \mid B_l) \cdot \log_2(P(A_i \mid B_l))$$

The information **gain** owed to experiment \mathcal{B} is defined as follows:

$$H(\mathcal{A}) - H(\mathcal{A} \mid \mathcal{B}) = H(\mathcal{A}) - \sum_{l=1}^m P(B_l) \cdot H(\mathcal{A} \mid B_l)$$

Remarks [\[Bayes for classification\]](#) :

- Information gain is defined as reduction in entropy.
- In the context of decision trees, experiment \mathcal{A} corresponds to classifying feature vector \mathbf{x} with regard to the target concept. A question, whose answer will inform us about which of the events in $A \in \mathcal{A}$ occurred, is the following:
 - “Does \mathbf{x} belong to class c ?” or
 - “ $C=c$?” (random variable C has realization c)

Likewise, experiment \mathcal{B} corresponds to evaluating feature j of feature vector \mathbf{x} . A question, whose answer will inform us about which of the events in $B \in \mathcal{B}$ occurred, is the following:

- “Does \mathbf{x} have value a for feature j ?” or
 - “ $X_j=a$?” (random variable X_j has realization a)
- Rationale: Typically, the events “ \mathbf{x} belongs to class c ” and “ \mathbf{x} has value a for feature j ” are statistically dependent. Hence, the entropy of the event “ \mathbf{x} belongs to class c ” will become smaller if we learn about the value of feature j of \mathbf{x} (recall that the class of \mathbf{x} is unknown). We experience an information gain with regard to the outcome of experiment \mathcal{A} , which is rooted in our information about the outcome of experiment \mathcal{B} . Under no circumstances the information gain will be negative; the information gain is zero if the involved events are *conditionally independent*:

$$P(A_i) = P(A_i \mid B_l), \quad i \in \{1, \dots, k\}, \quad l \in \{1, \dots, m\},$$

which leads to a split as specified as the special case in Lemma 8.

Remarks: (continued)

- Since $H(\mathcal{A})$ is constant, the feature that provides the maximum information gain (= the maximally informative feature) is given by the minimization of $H(\mathcal{A} \mid \mathcal{B})$.
- The expanded form of $H(\mathcal{A} \mid \mathcal{B})$ reads as follows:

$$H(\mathcal{A} \mid \mathcal{B}) = - \sum_{l=1}^m P(B_l) \cdot \sum_{i=1}^k P(A_i \mid B_l) \cdot \log_2(P(A_i \mid B_l))$$

Impurity Functions

Impurity Functions Based on Entropy (continued)

Definition for two classes [impurity function] :

$$\iota_{entropy}(p_1, p_2) = -(p_1 \cdot \log_2(p_1) + p_2 \cdot \log_2(p_2))$$

Impurity Functions

Impurity Functions Based on Entropy (continued)

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$$\iota_{entropy}(D) = - \left(\frac{|\{(\mathbf{x}, c_1) \in D\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c_1) \in D\}|}{|D|} + \frac{|\{(\mathbf{x}, c_2) \in D\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c_2) \in D\}|}{|D|} \right)$$

Impurity Functions

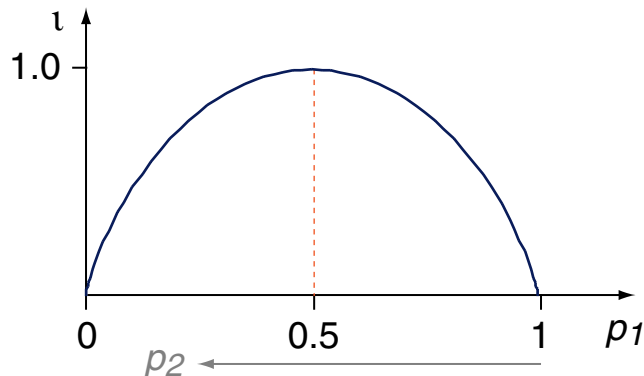
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Graph of the function $\iota_{entropy}(p_1, 1 - p_1)$, i.e., for two classes:

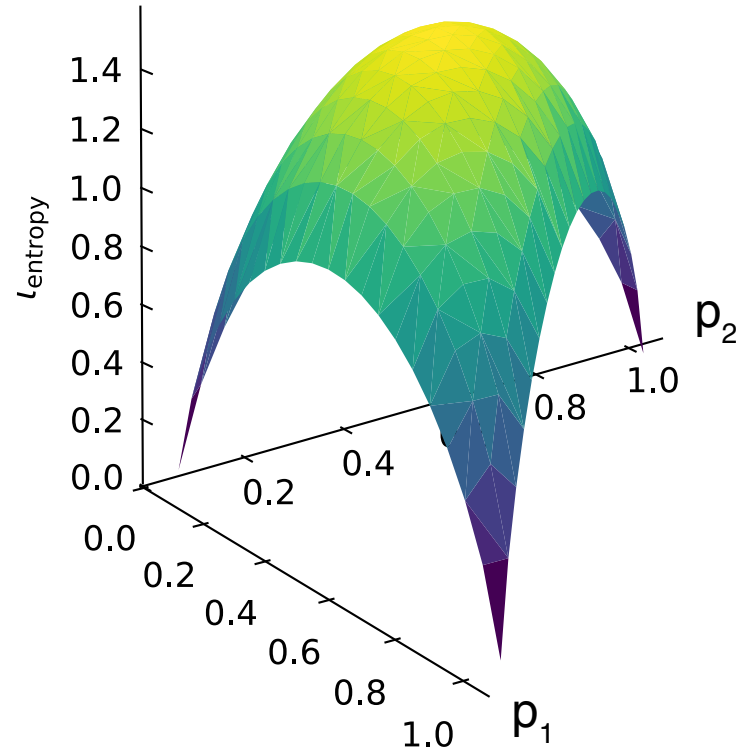
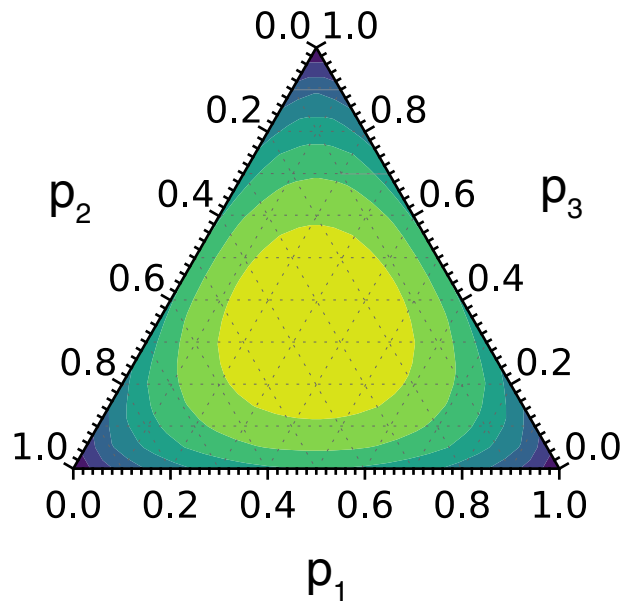


[Graphs: [misclassification](#), entropy, [Gini](#)]

Impurity Functions

Impurity Functions Based on Entropy (continued)

Graph of the function $\iota_{entropy}(p_1, p_2, 1 - p_1 - p_2)$, i.e., for three classes:



Impurity Functions

Impurity Functions Based on Entropy (continued)

Definition for k classes:

$$\iota_{entropy}(p_1, \dots, p_k) = - \sum_{i=1}^k p_i \cdot \log_2(p_i)$$

$$\iota_{entropy}(D) = - \sum_{i=1}^k \frac{|\{(\mathbf{x}, c_i) \in D\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c_i) \in D\}|}{|D|}$$

Impurity Functions

Impurity Functions Based on Entropy (continued)

$\Delta \iota_{entropy}$ corresponds to the information gain $H(\mathcal{A}) - H(\mathcal{A} \mid \mathcal{B})$:

$$\Delta \iota_{entropy} = \underbrace{\iota_{entropy}(D)}_{H(\mathcal{A})} - \underbrace{\sum_{l=1}^m \frac{|D_l|}{|D|} \cdot \iota_{entropy}(D_l)}_{H(\mathcal{A} \mid \mathcal{B})}$$

Impurity Functions

Impurity Functions Based on Entropy (continued)

$\Delta \iota_{\text{entropy}}$ corresponds to the information gain $H(\mathcal{A}) - H(\mathcal{A} \mid \mathcal{B})$:

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Mapping:

- A_i , $i = 1, \dots, k$, denotes the event that $\mathbf{x} \in X(t)$ belongs to class c_i .
The experiment \mathcal{A} corresponds to the classification $c : X(t) \rightarrow C$.
- B_l , $l = 1, \dots, m$, denotes the event that $\mathbf{x} \in X(t)$ has value a_l for feature j .
The experiment \mathcal{B} corresponds to evaluating feature A and entails the following splitting:

$$X(t) = X(t_1) \cup \dots \cup X(t_m) = \{\mathbf{x} \in X(t) : \mathbf{x}|_j = a_1\} \cup \dots \cup \{\mathbf{x} \in X(t) : \mathbf{x}|_j = a_m\}$$

- $\iota_{\text{entropy}}(D) = \iota_{\text{entropy}}(P(A_1), \dots, P(A_k)) = -\sum_{i=1}^k P(A_i) \cdot \log_2(P(A_i)) = H(\mathcal{A})$
- $\frac{|D_l|}{|D|} \cdot \iota_{\text{entropy}}(D_l) = P(B_l) \cdot \iota_{\text{entropy}}(P(A_1 \mid B_l), \dots, P(A_k \mid B_l)) = H(\mathcal{A} \mid B_l)$, $l = 1, \dots, m$
- $P(A_i)$, $P(B_l)$, $P(A_i \mid B_l)$ are estimated as relative frequencies based on D .

Impurity Functions

Impurity Functions Based on the Gini Index

Definition for two classes [[impurity function](#)] :

$$\iota_{Gini}(p_1, p_2) = 1 - (p_1^2 + p_2^2) = 2 \cdot p_1 \cdot p_2$$

Impurity Functions

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Impurity Functions

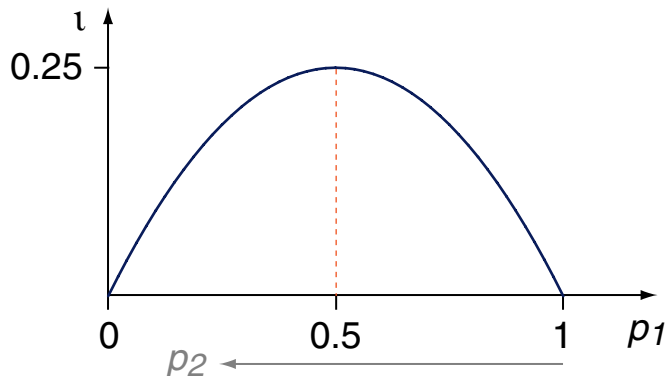
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Graph of the function $\iota_{Gini}(p_1, 1 - p_1)$, i.e., for two classes:



[Graphs: [misclassification](#), [entropy](#), Gini]

Impurity Functions

Impurity Functions Based on the Gini Index (continued)

Definition for k classes:

$$\iota_{Gini}(p_1, \dots, p_k) = 1 - \sum_{i=1}^k (p_i)^2$$

$$\begin{aligned}\iota_{Gini}(D) &= \left(\sum_{i=1}^k \frac{|\{(\mathbf{x}, c_i) \in D\}|}{|D|} \right)^2 - \sum_{i=1}^k \left(\frac{|\{(\mathbf{x}, c_i) \in D\}|}{|D|} \right)^2 \\ &= 1 - \sum_{i=1}^k \left(\frac{|\{(\mathbf{x}, c_i) \in D\}|}{|D|} \right)^2\end{aligned}$$