Lecture 3: 31 January, 2022

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Data Mining and Machine Learning
January–May 2022

Supervised learning

- A set of items
  - Each item is characterized by attributes $(a_1, a_2, \ldots, a_k)$ — columns in a table
  - Each item is assigned a class or category c
- Given a set of examples, predict c for a new item with attributes $(a'_1, a'_2, \ldots, a'_k)$

Supervised learning

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- Examples provided are called training data
- Aim is to learn a mathematical model that generalizes the training data
  - Model built from training data should extend to previously unseen inputs

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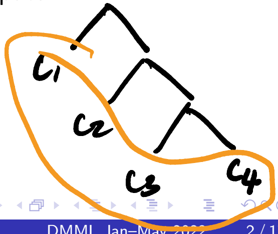
- Classification problem
  - Usually assumed to binary — two classes

Simulate multiway by a cascading choice



Example: Loan application data set

boolean

ID	Age	Has_job	Own_house	Credit_rating	Class
1	young	false	false	fair	No
2	young	false	false	good	No
3	young	true	false	good	Yes
4	young	true	true	fair	Yes
5	young	false	false	fair	No
6	middle	false	false	fair	No
7	middle	false	false	good	No
8	middle	true	true	good	Yes
9	middle	false	true	excellent	Yes
10	middle	false	true	excellent	Yes
11	old	false	true	excellent	Yes
12	old	false	true	good	Yes
13	old	true	false	good	Yes
14	old	true	false	excellent	Yes
15	old	false	false	fair	No

old true true fair

Class label

15 rows

9 Yes
6 No

≥ 50%

Basic assumptions

Fundamental assumption of machine learning

- Distribution of training examples is identical to distribution of unseen data

training

prediction

Basic assumptions

Fundamental assumption of machine learning

- Distribution of training examples is identical to distribution of unseen data

What does it mean to learn from the data?

- Build a model that does better than random guessing
  - In the loan data set, always saying Yes would be correct about $9/15$ of the time
- Performance should ideally improve with more training data

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How do we evaluate the performance of a model?

- Model is optimized for the training data. How well does it work for unseen data?
- Don't know the correct answers in advance to compare — different from normal software verification

The road ahead

Many different models

- Decision trees
- Probabilistic models — naïve Bayes classifiers
- Models based on geometric separators
  - Support vector machines (SVM)
  - Neural networks

The road ahead

Trivial model

Lookup table

Many different models

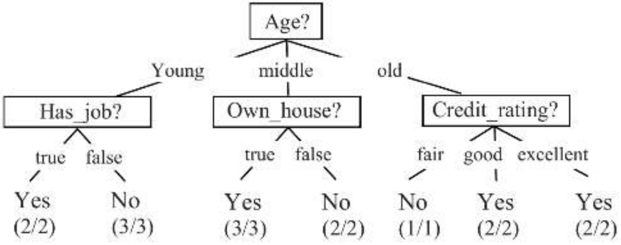
- Decision trees
- Probabilistic models — naïve Bayes classifiers
- Models based on geometric separators
  - Support vector machines (SVM)
  - Neural networks

Important issues related to supervised learning

- Evaluating models
- Ensuring that models generalize well to unseen data
  - A theoretical framework to provide some guarantees
- Strategies to deal with the training data bottleneck

Decision trees

- Play "20 Questions" with the training data



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Decision trees

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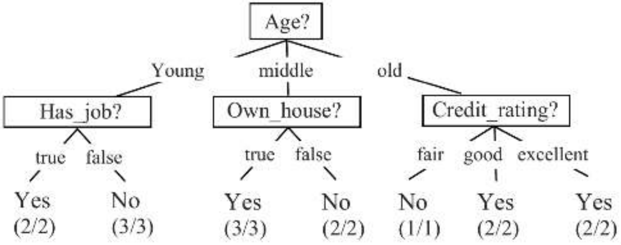
- Query an attribute
  - Partition the training data based on the answer



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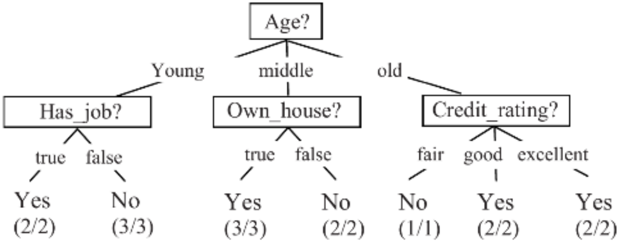

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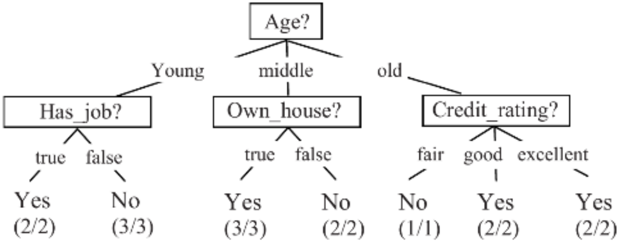
Decision trees

- Play "20 Questions" with the training data
- Query an attribute
  - Partition the training data based on the answer
- Repeat until you reach a partition with a uniform category
- Queries are adaptive
  - Different along each path, depends on history



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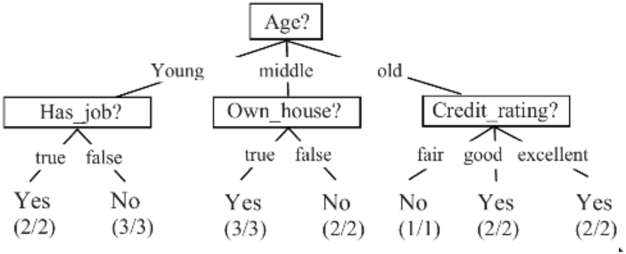
Decision tree algorithm

A : current set of attributes



Decision tree algorithm

A : current set of attributes

Pick $a \in A$, create children corresponding to resulting partition with attributes $A \setminus \{a\}$

Stopping criterion:

- Current node has uniform class label
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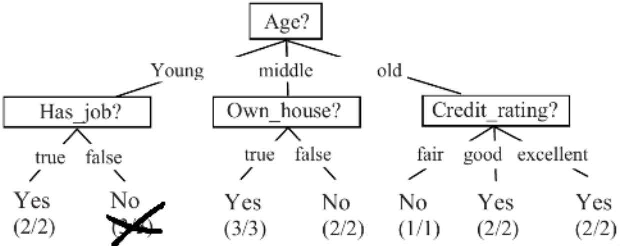

2/3

How many questions can I ask along a path?

At most no. of columns

1/2

$x_1 \quad x_2 \quad x_3 \quad x_4 \quad$ Yes

$x_1 \quad x_2 \quad x_3 \quad x_4 \quad$ No

$a_1 = x_1 \rightarrow a_2 = x_2 \rightarrow a_3 = x_3 \rightarrow a_4 = x_4$

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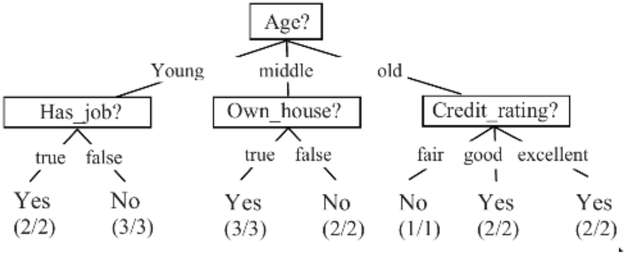

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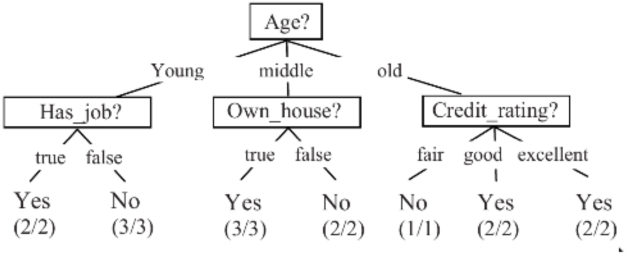

- Non-uniform leaf node — identical combination of attributes, but different classes

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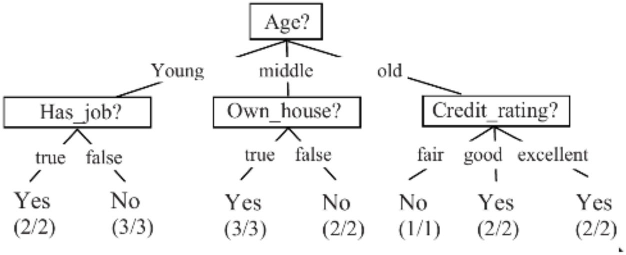
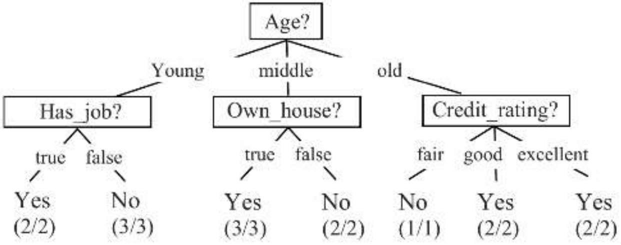
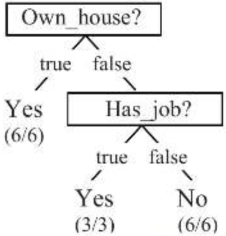


- Non-uniform leaf node — identical combination of attributes, but different classes
- Attributes do not capture all criteria used for classification

Decision trees

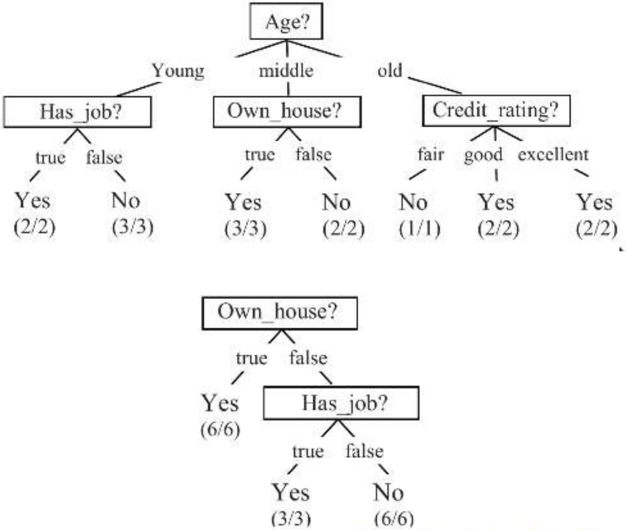
- Tree is not unique





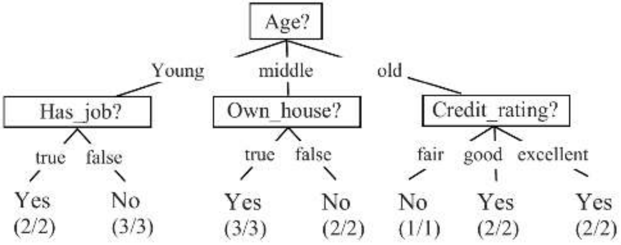
Decision trees

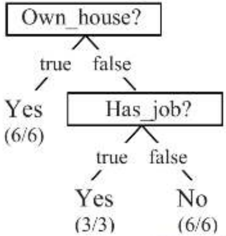
- Tree is not unique
- Which tree is better?



Decision trees

- Tree is not unique
- Which tree is better?
- Prefer small trees





Decision trees

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- Which tree is better?
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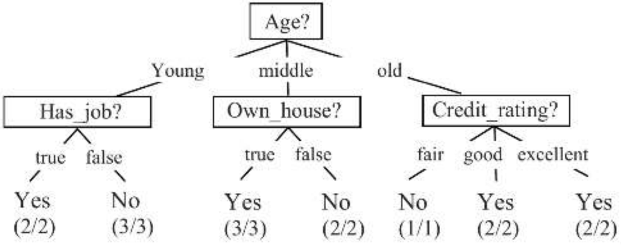
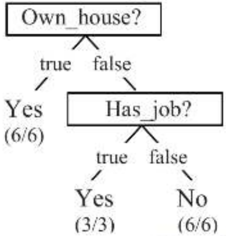
  - Explainability





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- Which tree is better?
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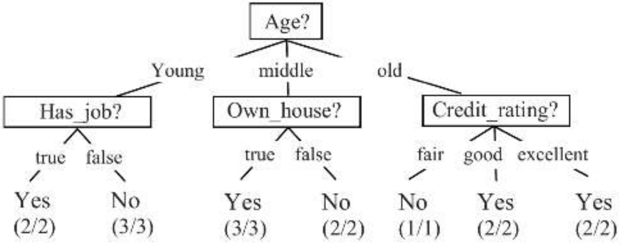
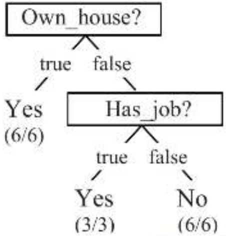
  - Generalize better (see later)





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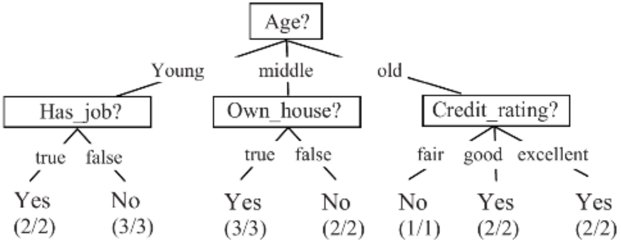
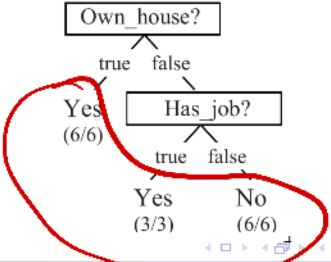
Unfortunately

- Finding smallest tree is NP-complete — for any definition of "smallest"

Exhaustive search





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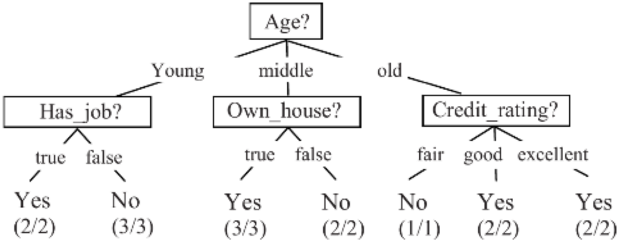
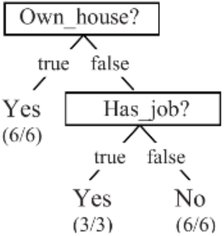
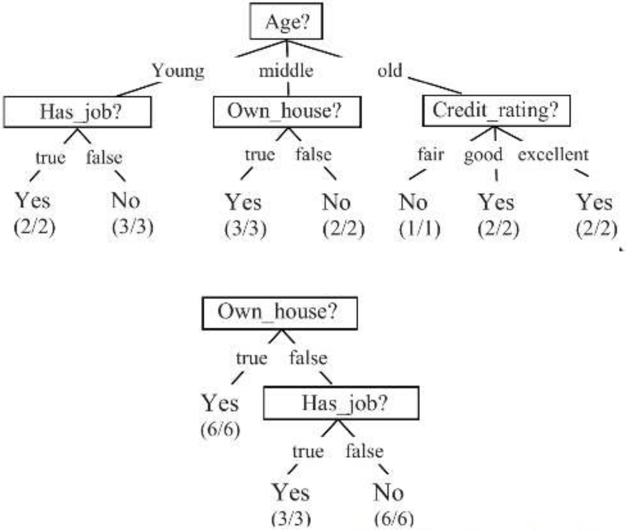
- Instead, greedy heuristic





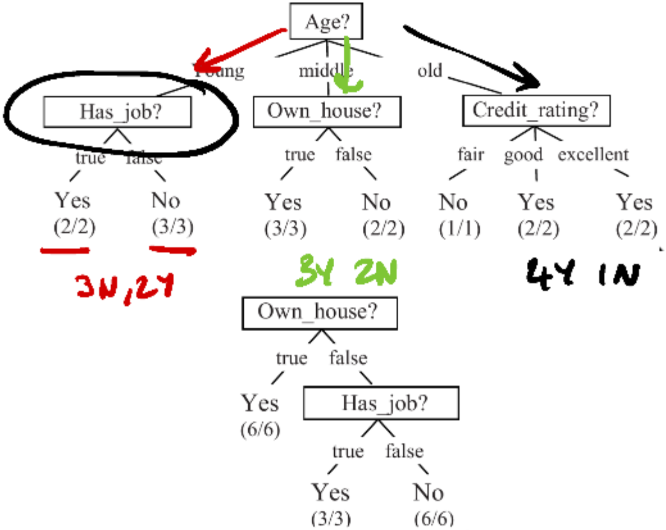
Greedy heuristic

- Goal: partition with uniform category — pure leaf



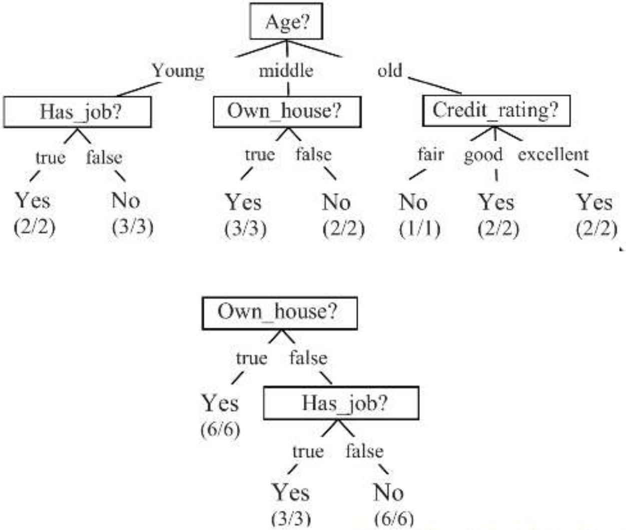
Greedy heuristic

- Goal: partition with uniform category — pure leaf
- Impure node — best prediction is majority value



Greedy heuristic

- Goal: partition with uniform category — pure leaf
- Impure node — best prediction is majority value
- Minority ratio is impurity



Greedy heuristic

- Goal: partition with uniform category — pure leaf
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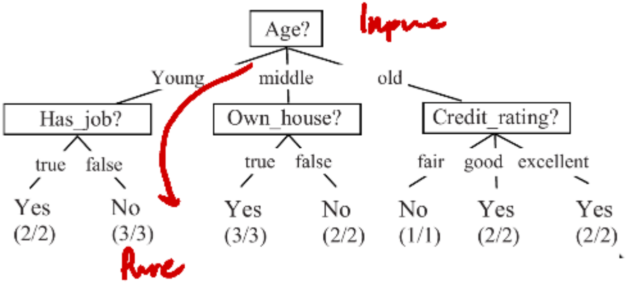
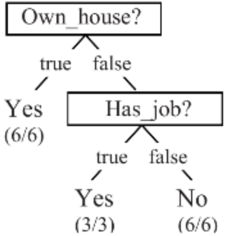
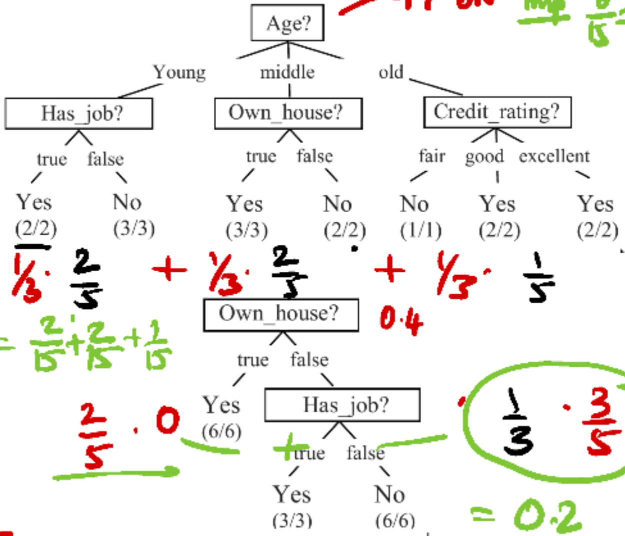
- Minority ratio is impurity
- Heuristic: reduce impurity as much as possible





- Goal: partition with uniform category — pure leaf
- Impure node — best prediction is majority value
- Minority ratio is impurity
- Heuristic: reduce impurity as much as possible
- For each attribute, compute weighted average impurity of children



9Y 6N Imp $\frac{6}{15} = 0.4$

$\frac{1}{3} \cdot \frac{2}{5} + \frac{1}{3} \cdot \frac{2}{5} + \frac{1}{3} \cdot \frac{1}{5}$

0.4

$\frac{5}{15} = \frac{2}{15} + \frac{2}{15} + \frac{1}{15} = \frac{1}{3} = 0.33$

$\frac{2}{5} \cdot 0 + \frac{1}{3} \cdot \frac{3}{5} = 0.2$

Age?

2Y, 3N   3Y, 2N   4Y, 1N

Wt avg

House?

6Y   3Y, 6N

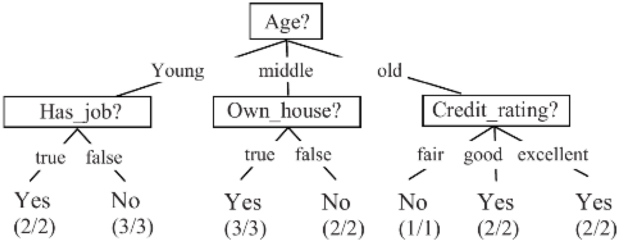
Wt avg

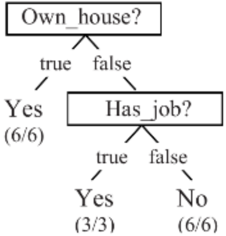
Job?

Credit Rank

Greedy heuristic

- Goal: partition with uniform category — pure leaf
- Impure node — best prediction is majority value
- Minority ratio is impurity
- Heuristic: reduce impurity as much as possible
- For each attribute, compute weighted average impurity of children
- Choose the minimum





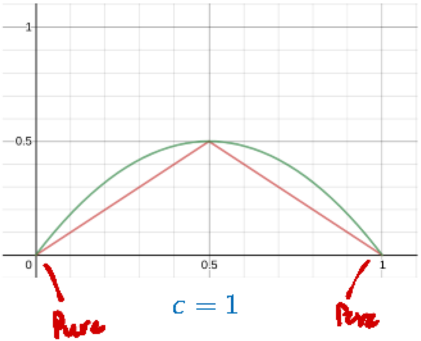
A better impurity function

- Misclassification rate is linear

$c = 1$

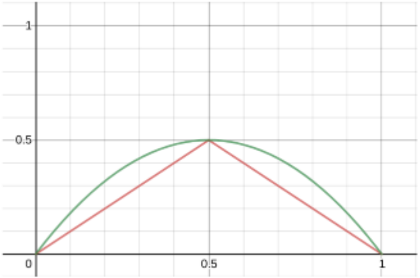
fraction of $c = 'ke'$
$= 1$

- Misclassification rate is linear
- Impurity measure that increases more sharply performs better, empirically



A better impurity function

- Misclassification rate is linear
- Impurity measure that increases more sharply performs better, empirically
- Entropy — [Quinlan]



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A better impurity function

- Misclassification rate is linear
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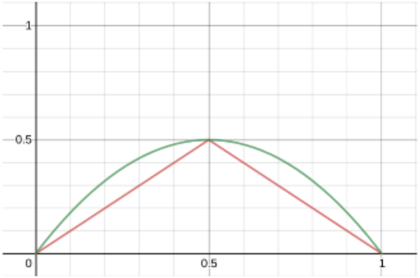
- Entropy — [Quinlan]
- Gini index — [Breiman]



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Entropy

- Information theoretic measure of randomness
- Minimum number of bits to transmit a message — [Shannon]

Entropy

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- Minimum number of bits to transmit a message — [Shannon]
- n data items
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$

$n = n_0 + n_1$

Entropy

- Information theoretic measure of randomness
- Minimum number of bits to transmit a message — [Shannon]
- n data items
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
- Entropy
  $E = -(p_0 \log_2 p_0 + p_1 \log_2 p_1)$

2^{-k}

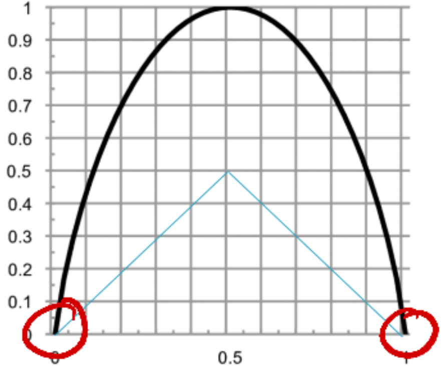
$\frac{1}{2^k}$ $2^0 = 1$

$p_0, p_1 < 1$

$\log p_0, \log p_1 < 0$

Entropy

- Information theoretic measure of randomness
- Minimum number of bits to transmit a message — [Shannon]
- n data items
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
- Entropy
  $E = -(p_0 \log_2 p_0 + p_1 \log_2 p_1)$
- Minimum when $p_0 = 1, p_1 = 0$ or vice versa — note, declare $0 \log_2 0$ to be 0
- Maximum when $p_0 = p_1 = 0.5$



$c = 1$

Gini Index

- Measure of unequal distribution of wealth
- Economics — [Corrado Gini]
- As before, n data items
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- Gini Index $G = 1 - (p_0^2 + p_1^2)$

$$\frac{1}{2} \quad \frac{1}{2}$$

$$1 - \left(\frac{1}{4} + \frac{1}{4}\right) = \frac{1}{2}$$

Gini Index

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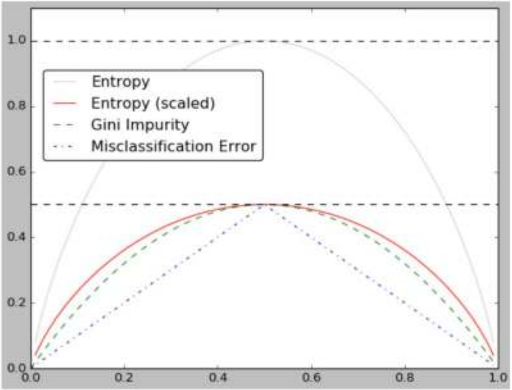
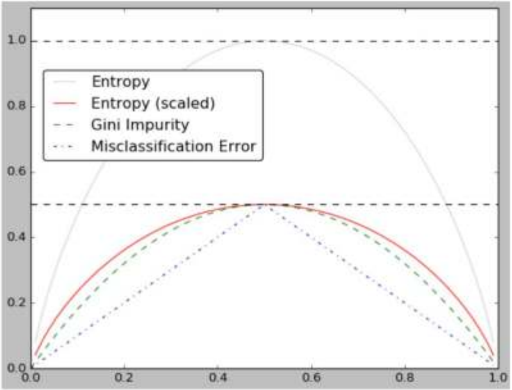
- As before, n data items
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
- Gini Index $G = 1 - (p_0^2 + p_1^2)$
- $G = 0$ when $p_0 = 0$, $p_1 = 0$ or v.v.
  $G = 0.5$ when $p_0 = p_1 = 0.5$



$c = 1$

Gini Index

- Measure of unequal distribution of wealth
- Economics — [Corrado Gini]
- As before, n data items
  - n_0 with $c = 0$, $p_0 = n_0/n$
  - n_1 with $c = 1$, $p_1 = n_1/n$
- Gini Index $G = 1 - (p_0^2 + p_1^2)$
- $G = 0$ when $p_0 = 0$, $p_1 = 0$ or v.v.
  $G = 0.5$ when $p_0 = p_1 = 0.5$
- Entropy curve is slightly steeper, but Gini index is easier to compute



$c = 1$

Gini Index

- Measure of unequal distribution of wealth
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  - n_0 with $c = 0$, $p_0 = n_0/n$
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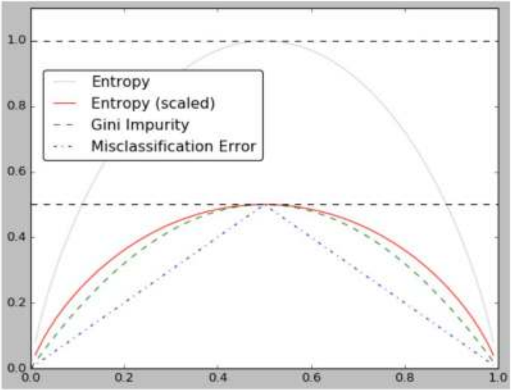
- Gini Index $G = 1 - (p_0^2 + p_1^2)$
- $G = 0$ when $p_0 = 0$, $p_1 = 0$ or v.v.
  $G = 0.5$ when $p_0 = p_1 = 0.5$
- Entropy curve is slightly steeper, but Gini index is easier to compute
- Decision tree libraries usually use Gini index



$c = 1$