Lecture 3: 16 January, 2024

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Data Mining and Machine Learning
January–April 2024

Supervised learning

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

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- Classification problem
  - Usually assumed to binary — two classes

Example: Loan application data set

ID	Age a_1	Has_job a_2	Own_house a_3	Credit_rating a_4	Class c
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

6N
9Y

Basic assumptions

Fundamental assumption of machine learning

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

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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

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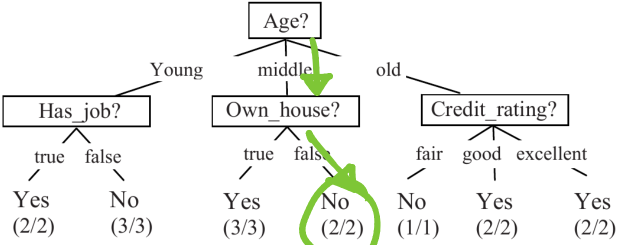
Important issues related to supervised learning

- 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

- Play "20 Questions" with the training data

Age Job Home Credit

(middle, true, false, fair)



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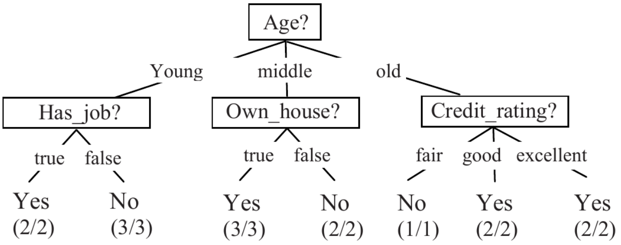
- Play "20 Questions" with the training data
- Query an attribute
  - Partition the training data based on the answer



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Decision trees

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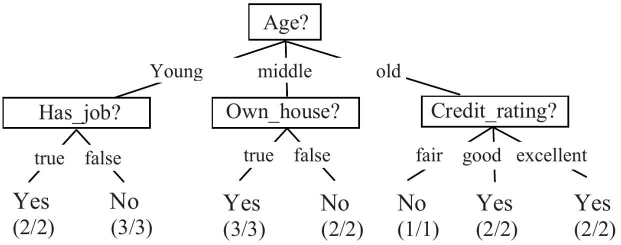

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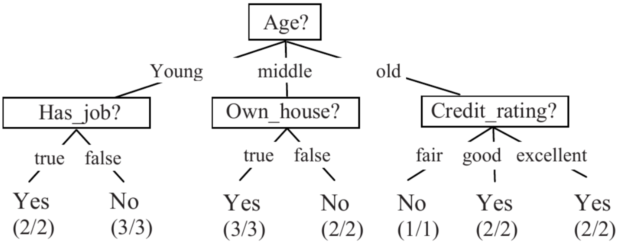
Decision trees

- 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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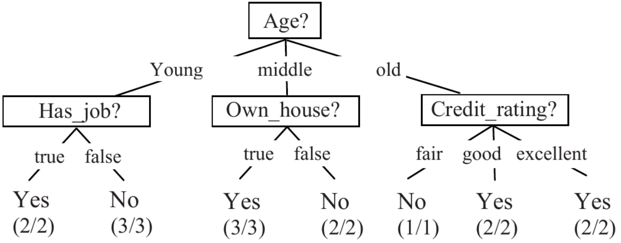
Decision tree algorithm

A : current set of attributes



Decision tree algorithm

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Stopping criterion:

- Current node has uniform class label
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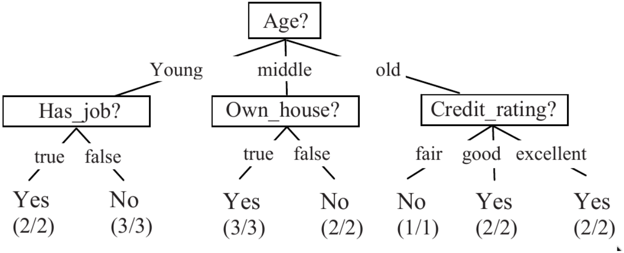

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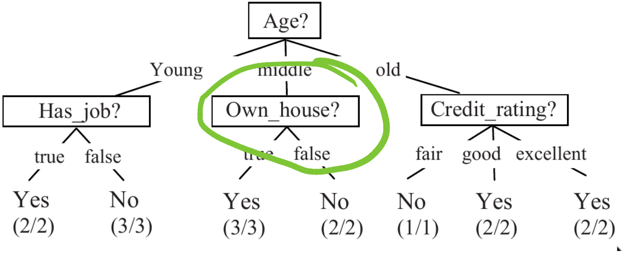

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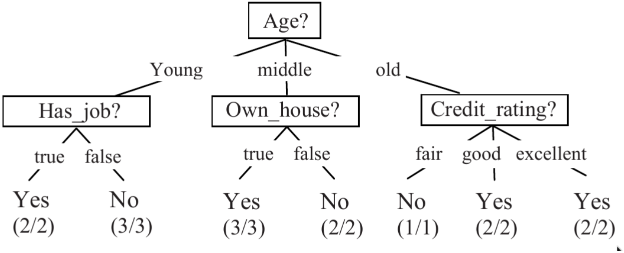

- Non-uniform leaf node — identical combination of attributes, but different classes

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How?

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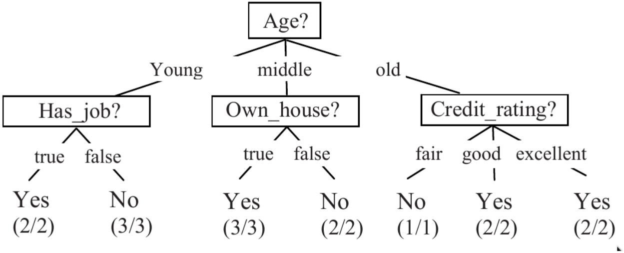
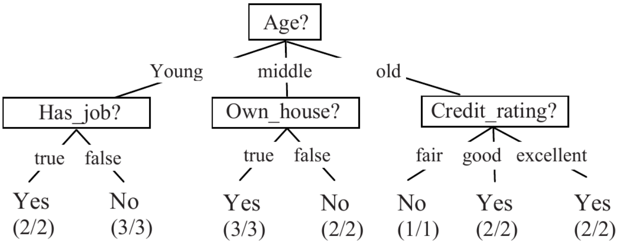
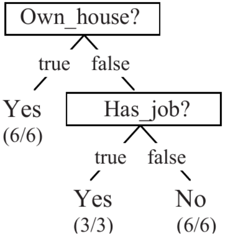


- Non-uniform leaf node — identical combination of attributes, but different classes
- Attributes do not capture all criteria used for classification

Decision trees

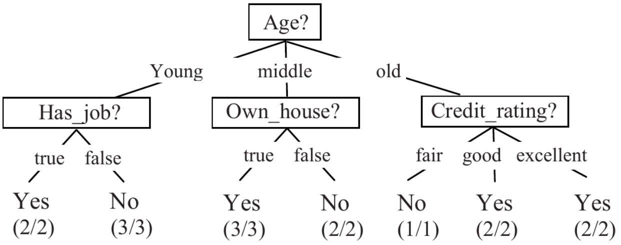
- Tree is not unique

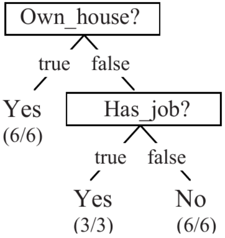




Decision trees

- Tree is not unique
- Which tree is better?

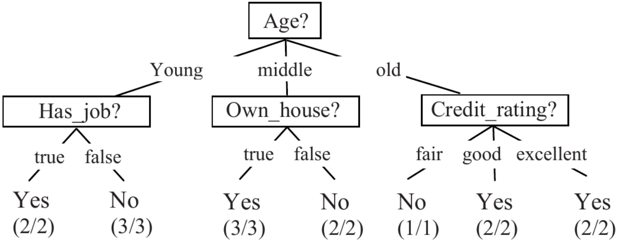


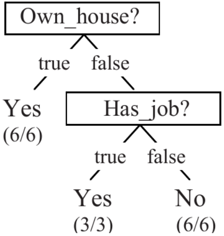


Decision trees

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

Occam's Razor





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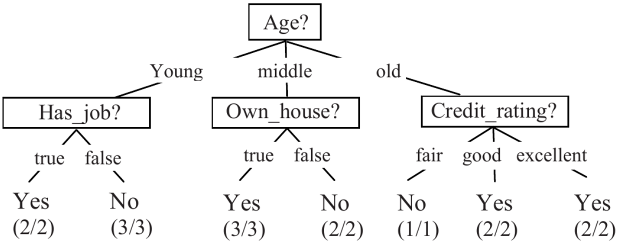
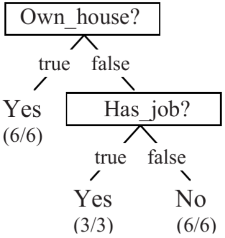
  - Explainability





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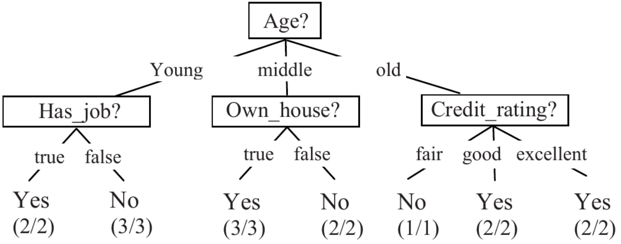
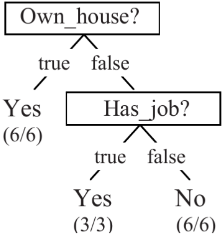
  - Generalize better (see later)





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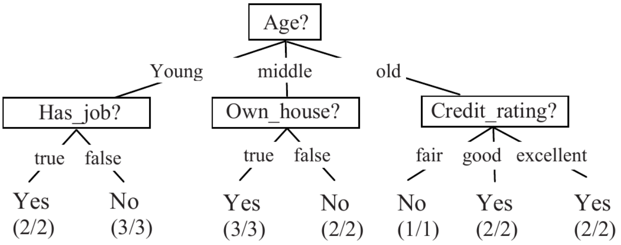
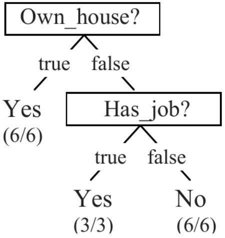
- Finding smallest tree is NP-complete — for any definition of "smallest"





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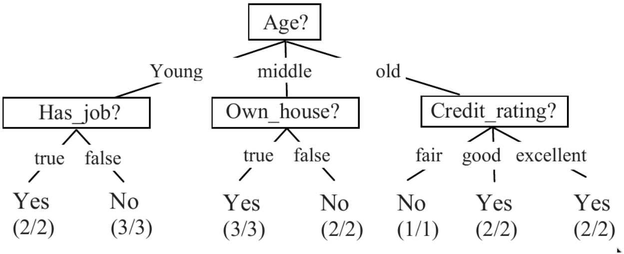
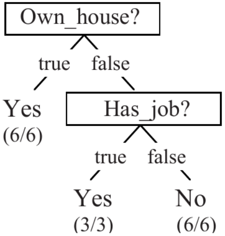
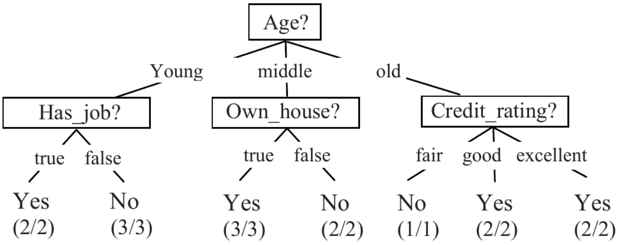
- Instead, greedy heuristic

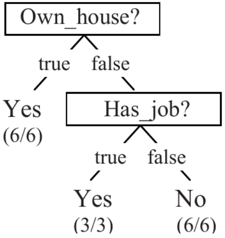




Greedy heuristic

- Goal: partition with uniform category — pure leaf





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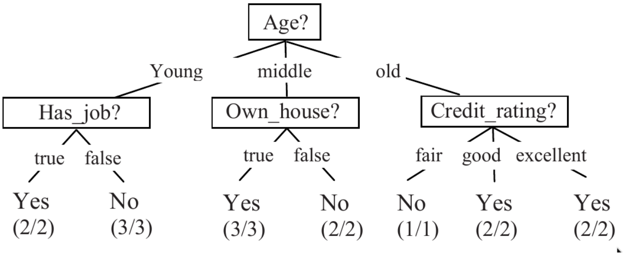

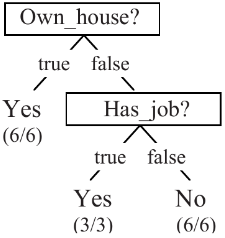

Greedy heuristic

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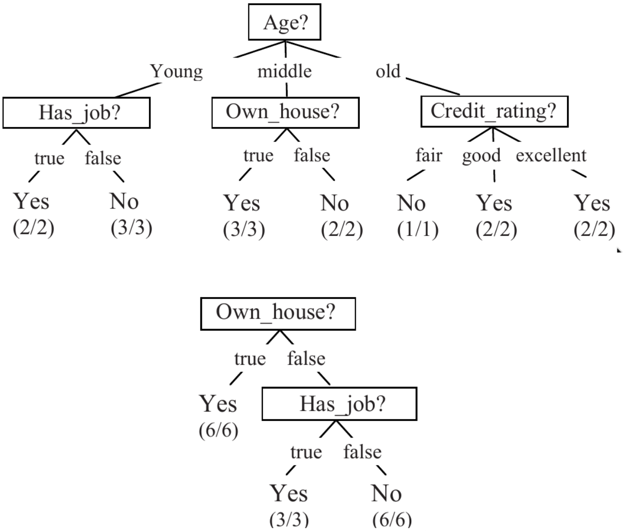
- Impure node — best prediction is majority value
- Minority ratio is impurity



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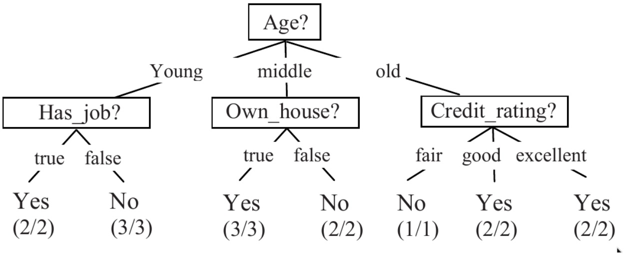
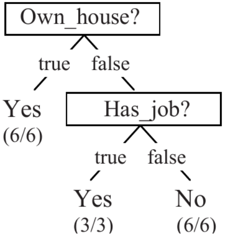
- Heuristic: reduce impurity as much as possible





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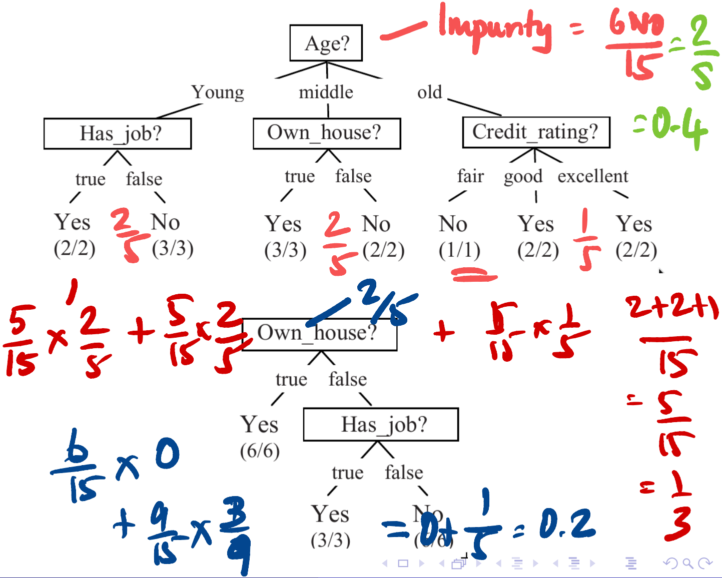

Greedy heuristic

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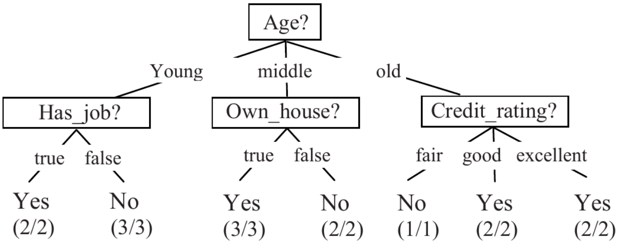
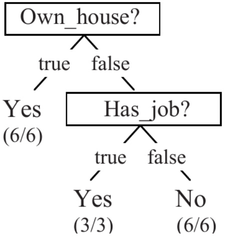
- Heuristic: reduce impurity as much as possible
- For each attribute, compute weighted average impurity of children
- Choose the minimum

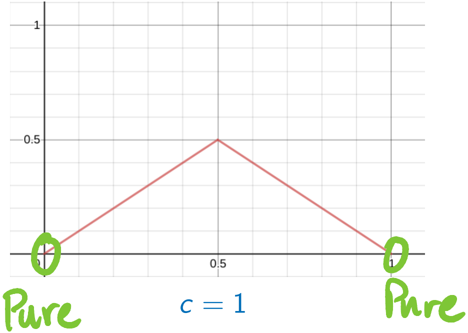




A better impurity function

- Misclassification rate is linear

Ratio of minority



$c = 1$

c = Yes

A better impurity function

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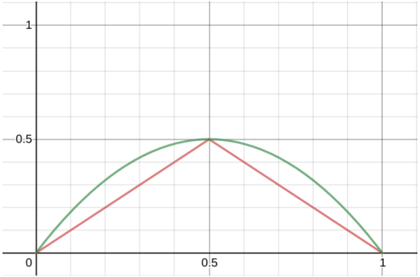
- Impurity measure that increases more sharply performs better, empirically



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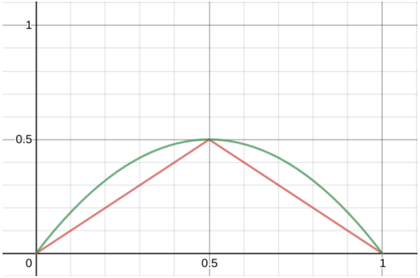
- Entropy — [Quinlan]



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A better impurity function

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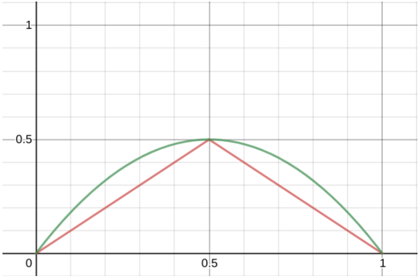
- Entropy — [Quinlan]
- Gini index — [Breiman]



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  - n_0 with $c = 0$, $p_0 = n_0/n$
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  $E = -(p_0 \log_2 p_0 + p_1 \log_2 p_1)$

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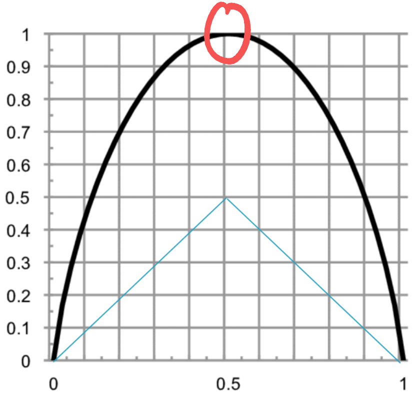
- Entropy
  $\frac{1}{2} \times -1 \quad + \frac{1}{2} \times -1$
  $E = -(p_0 \log_2 p_0 + p_1 \log_2 p_1)$
- Minimum when $p_0 = 1, p_1 = 0$ or vice versa — note, declare $0 \log_2 0$ to be 0
- Maximum when $p_0 = p_1 = 0.5$

$0 \log 0$
$+ 1 \log 1$
0

$2^0 = 1$



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Gini Index

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

0 1

1 0

$\frac{1}{4} + \frac{1}{4}$

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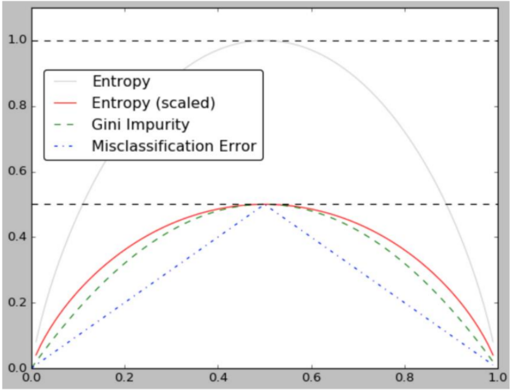
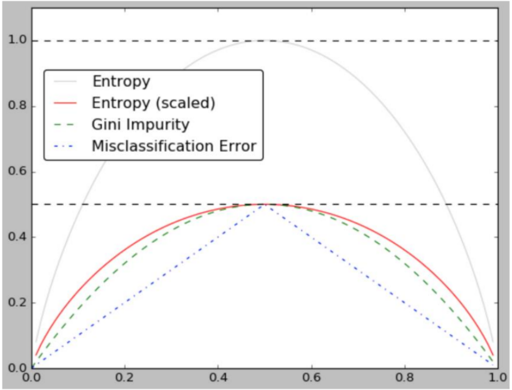
  - n_1 with $c = 1$, $p_1 = n_1/n$
- Gini Index $G = 1 - (p_0^2 + p_1^2)$
- $G = 0$ when $p_0 = 0$, $p_1 = 0$ or v.v.
  $G = 0.5$ when $p_0 = p_1 = 0.5$



$c = 1$

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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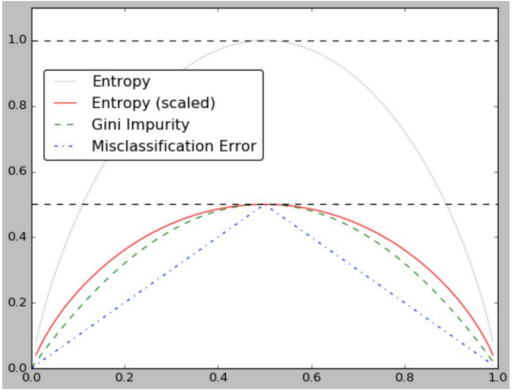
- Gini Index $G = 1 - (p_0^2 + p_1^2)$
- $G = 0$ when $p_0 = 0$, $p_1 = 0$ or v.v.
  $G = 0.5$ when $p_0 = p_1 = 0.5$
- Entropy curve is slightly steeper, but Gini index is easier to compute
- Decision tree libraries usually use Gini index



$c = 1$